BIRKHÄUSER

Progress in Mathematical Physics

54

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Birkhäuser
Basel · Boston · Berlin

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2000 Mathematics Subject Classification: 00-01, 81Q10 , 47A05 , 47A07, 47B25, 42B10

Library of Congress Control Number: 2008935753

Bibliographic information published by Die Deutsche Bibliothek.
Die Deutsche Bibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data is available in the Internet at http://dnb.ddb.de

ISBN 978-3-7643-8794-5 Birkhäuser Verlag AG, Basel · Boston · Berlin

Basel · Boston · Berlin
P.O. Box 133, CH-4010 Basel, Switzerland
Part of Springer Science+Business Media
Printed on acid-free paper produced from chlorine-free pulp. TCF ∞
Printed in Germany

ISBN 978-3-7643-8794-5
e-ISBN 978-3-7643-8795-2
9 8 7 6 5 4 3 2 1
www.birkhauser.ch

Dedicated to

my parents (Marly, João)

and

my parents-in-law (Elza, Geraldo)

Contents

Preface

The spectral theory of linear operators in Hilbert spaces is the most important tool in the mathematical formulation of quantum mechanics; in fact, linear operators and quantum mechanics have had a symbiotic relationship. However, typical physics textbooks on quantum mechanics give just a rough sketch of operator theory, occasionally treating linear operators as matrices in finite-dimensional spaces; the implicit justification is that the details of the theory of unbounded operators are involved and those texts are most interested in applications. Further, it is also assumed that mathematical intricacies do not show up in the models to be discussed or are skipped by "heuristic arguments." In many occasions some questions, such as the very definition of the hamiltonian domain, are not touched, leaving an open door for controversies, ambiguities and choices guided by personal tastes and ad hoc prescriptions. All in all, sometimes a blank is left in the mathematical background of people interested in nonrelativistic quantum mechanics.

Quantum mechanics was the most profound revolution in physics; it is not natural to our common sense (check, for instance, the wave-particle duality) and the mathematics may become crucial when intuition fails. Even some very simple systems present nontrivial questions whose answers need a mathematical approach. For example, the Hamiltonian of a quantum particle confined to a box involves a choice of boundary conditions at the box ends; since different choices imply different physical models, students should be aware of the basic difficulties intrinsic to this (in principle) very simple model, as well as in more sophisticated situations. The theory of linear operators and their spectra constitute a wide field and it is expected that the selection of topics in this book will help to fill this theoretical gap. Of course this selection is greatly biased toward the preferences of the author.

Besides the customary role of working as a computational instrument, a mathematically rigorous approach could lead to a more profound insight into the nature of quantum mechanics, and provide students and researchers with appropriate tools for a better understanding of their own research work. So the first aim of this book is to present the basic mathematics of nonrelativistic quantum mechanics of one particle, that is, developing the spectral theory of self-adjoint operators in infinite-dimensional Hilbert spaces from the beginning. The reader is assumed to have had some contact with functional analysis and, in applications to differential operators, with rudiments of distribution theory. Traditional results of the theory of linear operators in Banach spaces are addressed in Chapter 1, whereas necessary results of Sobolev spaces are described in Chapter 3. The definition and basic properties of (unbounded) self-adjoint operators appear in Chapter 2.

The second aim of this book is to give an overview of many of the basic functional analysis aspects of quantum theory, from its physical principles to the mathematical methods. This end is illustrated by:

1. The use of von Neumann theory of self-adjoint extensions (2), Fourier transform (3), sesquilinear forms (4), Kato-Rellich and KLMN theorems (6) and boundary triples (7) as tools to properly define Schrödinger (self-adjoint) operators in quantum mechanics. These matters are developed in the chapters indicated above in parentheses.
2. The spectral theorem and first applications in Chapters 8 and 9.
3. Convergence of (unbounded) self-adjoint operators in Chapter 10.
4. Spectral decomposition (essential, discrete, continuous and point) in Chapters 11 and 12.

In case of time evolution, which is ruled by the quantum energy operator, item 1 above is closely related to the question in classical mechanics whether the motion is unambiguously determined by the force.

Another aim of this book is to strive to present many examples illustrating concepts and build up confidence with methods. Some examples are simple and are meant to reduce the effort of beginning graduate students to learn the subject of spectral theory and its relation to quantum mechanics.

The last aim of the book is to discuss the relation between spectral type of the hamiltonian (energy) operator and asymptotic quantum dynamics, i.e., the quantum behavior as time goes to infinity. In Chapter 5, the existence of quantum dynamics is shown to be equivalent to the self-adjointness of the Hamiltonian, but the discussion is not restricted to time evolution and the general theory of unitary evolution groups is addressed in detail. Various aspects of the role played by the spectral type in quantum dynamics are given in Chapter 13. Some results seem not to have appeared in book form yet, such as the discussions on precompact orbits and almost periodic trajectories. Chapters 11, 12 and 13 make heavy use of spectral measures and are more advanced than previous chapters.

Selected quantum relations are discussed in Chapter 14. The idea is to complement a text that emphasizes mathematics with additional rigorous approaches to some standard quantum concepts; e.g., why the quantum observables are represented by self-adjoint operators instead of just hermitian ones. But no exhaustive presentation of quantum relations should be expected and parallel reading of traditional books on quantum mechanics is highly recommended.

The book does not offer a quantum mechanics course, but the necessary quantum concepts are introduced when needed (usually with Planck's constant

$\hbar = 1$ and mass particle $m = 1/2$). Hence, it can also be useful to readers who are only interested in an introduction to spectral theory, since its focus is mathematics and proofs of theorems. The level is suitable for graduate students (or advanced undergraduates) who already have some familiarity with linear functional analysis. Thus, more advanced methods in spectral theory, mainly those related to singular continuous and dense point spectra, are not discussed (see [DeKr05] for a collection of advanced methods and the four volumes by Reed and Simon in the references); this is the reason for the term "Intermediate" in the title of the book. However, a certain level of mathematical literacy is desired from the reader.

Different readers may have different backgrounds, and each one will easily find which sections to skip and a suitable pathway to the particular topics of interest. But most of them will usually start on the introduction of a spectrum in Section 1.5 or Chapter 2. After working through this book, a student should be able to follow more specialized texts and research articles, and should find it easier to select a topic for future research.

Exercises present different levels of difficulties; many of them are related to missing details in proofs and examples. Due to the nature of the book, the set of references includes literature on both physics and mathematics.

Parts of the book have been used in courses addressed to graduate students interested in spectral theory at the Department of Mathematics of the Federal University of São Carlos, in 2004 and 2006; in fact, the book grew out of such lectures. The author thanks students and colleagues who have attended those courses and made helpful comments. Partial financial support by a Brazilian federal agency, CNPq, is very much acknowledged.

I want to thank the patience and support of my wife, Ana Teresa, and our children, Daniel and Natália, that gave me stability during the revisions of the text.

Hopefully, you, mathematician or physicist, will enjoy reading the book and will profit from it. The following page on the internet

`http://www.dm.ufscar.br/~oliveira/ISTbook.html`

is related to this book and it may include a possible errata page. Any remark, suggestion and correction (including those that have arisen from "copy-paste" manipulations) from readers will be welcome!

May 2008 São Carlos,

César R. de Oliveira

Selected Notation

- The set of natural numbers: $\mathbb{N} = \{1, 2, 3, \dots\}$.
- The term "enumerable" refers to the cardinality of $\mathbb{N}$, whereas "countable" refers to enumerable or finitely many (including zero).
- "a.e." abbreviates *almost everywhere* with respect to some measure.
- $\mathcal{N}, \mathcal{B}, \mathcal{H}$ denote normed, Banach and Hilbert spaces, respectively.
- $Y \sqsubseteq X$ means that Y is a dense subset of X.
- The identity operator is denoted by $\mathbf{1}$.
- The range, domain and kernel (i.e., null set) of a transformation T will be denoted by $\operatorname{rng} T, \operatorname{dom} T$ and $\mathrm{N}(T)$, respectively.
- An action "T in X" means that $\operatorname{dom} T \subset X$, whereas "$T$ on X" means that $\operatorname{dom} T = X$. They are abbreviations of "T acting in X" and "T acting on X," respectively.
- An element x of $\mathbb{R}^n$ is simply denoted by $x = (x_1, \dots, x_n)$ and $dx = dx_1 dx_2 \cdots dx_n$. Also, the inner product, $xy = x_1 y_1 + \cdots + x_n y_n$.
- A linear operator T in $\mathcal{H}$ is *symmetric* if $\langle T\xi, \eta \rangle = \langle \xi, T\eta \rangle$, $\forall \xi, \eta \in \operatorname{dom} T$. A *hermitian* operator is a symmetric one whose domain is dense in $\mathcal{H}$.
- "dominated convergence" always refers to Lebesgue's dominated convergence theorem.
- "Schrödinger operator", "hamiltonian operator" and "energy operator" are synonymous. The "standard Schrödinger operator" is the formal action $H = -\Delta + V$ acting in $\mathrm{L}^2(\Omega)$, $\Omega \subset \mathbb{R}^n$.
- r.h.s. (l.h.s.) means "right- (left-) hand side."
- The end of a proof is signalled by the symbol $\square$.

A Glance at Quantum Mechanics

Since this book is closely connected to quantum mechanics, these introductory words will briefly and informally recall some postulates of this theory. Interested readers are urged to consult traditional books on quantum mechanics to complement the discussion ahead and for descriptions of experimental evidence that give rise to the postulates. In physics there are several "equivalent formulations" of quantum mechanics, and a catalogue of the most important appears in [Sty02]. The discussion here is restricted to the nonrelativistic case.

Quantum mechanics is the physical theory of microscopic phenomena, and it was found that nature has peculiarities that were essentially revealed only at distances of the order of an atomic radius ($\approx 10^{-10}$meters); of course there are interesting pure quantum effects in some macroscopic phenomena as well. Due to the work of many talented people, a beautiful and, more important, greatly useful theory has emerged. In the common formulation of a quantum mechanical system (as proposed by the members – in a broad sense – of the so-called Copenhagen school), the dynamics is linear with "pure" physical states represented by normalized vectors ξ in a complex separable Hilbert space $\mathcal{H}$ (with inner product $\langle \cdot, \cdot \rangle$ and $\|\xi\| = 1$), and physical observables (such as position, energy, etc.) by self-adjoint operators acting in such spaces. Usually these operators are not continuous and are defined only on a dense subset of $\mathcal{H}$ (see Hellinger-Toeplitz Theorem 2.1.27), which cause subtle and intricate technical difficulties (and, it should be said, richness of possibilities). Two normalized states ξ, η are equivalent if there is $\theta \in \mathbb{R}$ so that $\xi = e^{i\theta}\eta$. Of course the precise forms of the Hilbert space and operators to be selected depend on details of the system under study.

Let $\xi, \eta \in \mathcal{H}$ be possible states of a quantum system. The linear structure implies that states are additive, which in physics is called the *superposition principle*; that is, after normalization, any nonzero linear combination $a\xi + b\eta$, $a, b \in \mathbb{C}$, is another possible state. If two states ξ, η are normalized, the transition probability from ξ to η is $|\langle \xi, \eta \rangle|^2$. More precisely, if the system is in the state ξ, then it can be observed in any state η with nonzero projection $|\langle \xi, \eta \rangle|^2 \neq 0$, and this quantity is exactly the probability that such quantum transition will occur. It should then be clear that one state can interfere with another one and so the "quantum interpretations are nonlinear!"

If a system is in the (normalized) state ξ, then a measurement of an observable, represented by the self-adjoint operator T, is not guaranteed to give a unique answer, due to possible quantum transitions; thus, usually an observable has no definite value. However, the average value of T over many measurements over copies of the system in the same state ξ will result in the average value given by

$$\mathcal{E}_\xi^T = \langle \xi, T\xi \rangle,$$

which is called the expectation value of T in the state ξ. Further, $\mathcal{E}_\xi^T$ is strictly related to the spectrum of T and all measurements will result in a definite value λ iff $T\xi = \lambda\xi$, that is, iff ξ is an eigenvector of T with corresponding eigenvalue λ (and in this case $\mathcal{E}_\xi^T = \lambda$). Thus, it becomes clear that there is a close relation between spectral theory of self-adjoint operators and measurements of physical observables. More explicitly, the probability that the value of a measurement of the observable T will result in a value in the set $\Lambda \subset \mathbb{R}$ is $\mu_\xi^T(\Lambda)$, with μ_ξ^T denoting the spectral measure of T at the quantum state ξ.

The time evolution of a quantum system is given by a family of unitary operators $U(t)$ so that $U(t+s) = U(t)U(s)$, with $t, s \in \mathbb{R}$ playing the role of time. It turns out that $U(t)$ is generated by the total energy observable H of the system, a prominent self-adjoint operator which is also called a hamiltonian or Schrödinger operator. The equation governing this time evolution is the famous Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\xi(t) = H\xi(t), \qquad \xi(0) = \xi,$$

whose solution is $\xi(t) = U(t)\xi$, and one naturally writes $U(t) = e^{-itH/\hbar}$. $\hbar$ denotes Planck's constant

The process of associating a quantum system to a classical one is called quantization. It is not always a well-defined process, since a rule and physical arguments are necessary to associate self-adjoint operators to observables. Consider a standard quantum system, that is, the Hilbert space is $\mathrm{L}^2(\mathbb{R}^n)$ (or $\mathrm{L}^2(\Lambda)$, $\Lambda \subset \mathbb{R}^n$) with coordinates $x = (x_1, \ldots, x_n)$, for which the jth coordinate of the position operator is just the multiplication by x_j, while for the conjugate momentum component p_j the operator is $P_j = -i\hbar\partial/\partial x_j$. The quantum version of a function $f(x_j, p_k)$ should be the operator $f(x_j, -i\partial/\partial x_k)$. Therefore, in case of a particle of mass m under a potential energy $V(x)$, the total (classical) mechanical energy is $p^2/(2m) + V(x)$ and the quantum hamiltonian operator will take the form

$$H = -\frac{\hbar^2}{2m}\Delta + V(x),$$

with Δ denoting the Laplacian in $\mathbb{R}^n$. In this setting the states are normalized vectors $\psi \in \mathrm{L}^2(\mathbb{R}^n)$, usually called *wave functions*, and, according to a proposal of Max Born, the probability of finding the particle in $\Lambda \subset \mathbb{R}^n$ at time t is

$$\text{Prob}_{\psi(t)}(\Lambda) = \int_\Lambda \left|(e^{-itH}\psi)(x)\right|^2 \, dx.$$

Thus $|\psi(x)|^2$ is interpreted as the probability density of the particle position at time $t = 0$.

Note that no domain has been assigned to the operators mentioned above, and it is not at all clear that bona fide domains do exist so that those operators become self-adjoint. Occasionally there are infinitely many self-adjoint extensions and finding and interpreting them are of considerable interest. These are some of the main questions to be considered when a mathematical theory of quantum mechanics is addressed, and they turn out to be directly connected to a properly defined unitary time evolution.

Besides the development of the theory of unbounded self-adjoint operators in Hilbert spaces, including spectral theory, many other related issues are treated in this book. Some specific quantities (e.g., quantum return probability, expectation values, test operators) are introduced and motivated on the basis of quantum interpretations and aim at a better understanding of possible quantum behaviors, how they depend on the self-adjoint extensions and spectral type, particularly the asymptotic behavior as time increases.

The above discussion summarizes some important postulates of (nonrelativistic) quantum mechanics and the motivation for writing this book. The physical discussion is restricted to one-particle systems without spin, so that fermionic (including Pauli exclusion principle) and bosonic statistics are disregarded in the text.

There is a huge literature on attempts at an axiomatization of quantum mechanics aiming at the justification of its postulates. Usually one tries to isolated a suitable set of ad hoc elements. The book [vonN67], originally published in 1932, can be considered the first one to attempt a mathematical justification of quantum postulates; the book [Mac04] (originally published in 1963) is also a classic whose ideas established the so-called *quantum logic*. Pleasant pedagogical descriptions of some modern experiments and interpretations of quantum mechanics can be found in [GreZ97]; however, experience indicates that one needs some acquaintance with quantum mechanics to fully understand its interpretations.

It should be mentioned that there have been attempts to formulate quantum mechanics in terms of real Hilbert spaces [Stue60] and by using Hilbert spaces over the field of quaternions rather than the field of complex numbers [FJSS62]. These references were cited because they are seminal works.

In spite of such motivations, in this book the theory of linear operators in Hilbert spaces is presented at an abstract level, so that the reader can have an introduction to the subject and take advantage of the book even if quantum mechanics is not his/her primary interest.

Chapter 1

Linear Operators and Spectra

This chapter recalls some basic concepts of the theory of linear operators in normed spaces, with emphasis on Hilbert spaces. It also fixes some notation and introduces the concept of a spectrum along with various proofs. Compact operators are discussed. The readers are supposed to have had a first contact with functional analysis.

1.1 Bounded Operators

Let $\mathbb{F}$ denote either the field of real numbers $\mathbb{R}$ or complex numbers $\mathbb{C}$. For $z \in \mathbb{C}$, let $\overline{z}$ denote its complex conjugate. As usual in mathematics, *iff* will be an abbreviation for "if and only if."

Definition 1.1.1. A *linear operator* between the vector spaces X and Y is a transformation $T : \mathrm{dom}\, T \subset X \to Y$, for which its domain $\mathrm{dom}\, T$ is a vector subspace and $T(\xi + \alpha\eta) = T(\xi) + \alpha T(\eta)$, for all $\xi, \eta \in \mathrm{dom}\, T$ and all scalar $\alpha \in \mathbb{F}$.

Note that $T(0) = 0$ for any linear operator T, and that the set of linear operators with the same domain and codomain is a vector space with pointwise operations; frequently $T(\xi)$ will also be denoted by $T\xi$. Simple examples of linear operators are the *identity operator* $\mathbf{1} : X \to X$, with $\mathbf{1}(\xi) = \xi$, and the *null* (or *zero*) *operator* $T\xi = 0$, $\forall \xi$.

In many cases it is imperative to consider domains dense in another set; so throughout this text the notation $A \sqsubseteq B$ will indicate that A is a dense subset of B, with respect to the appropriate topology. The natural numbers $\{1, 2, 3, \dots\}$ will be denoted by $\mathbb{N}$ and the term *enumerable* indicates the cardinality $\aleph_0$ of the set of natural numbers, while *countable* refers to finite numbers (including zero); so, *uncountable* indicates that something is infinite and with cardinality different from $\aleph_0$.

$\mathcal{N}, \mathcal{B}, \mathcal{H}$ always denote a normed space, a Banach space and a Hilbert space, respectively. In any metric space, the sphere, open and closed balls centered at ξ and of radius $r > 0$ will be denoted by $S(\xi; r)$, $B(\xi; r)$ and $\overline{B}(\xi; r)$, respectively. If A is a subset of a vector space, then $\mathrm{Lin}(A)$ denotes the linear subspace spanned by A.

Example 1.1.2. Let $\phi \in \mathrm{L}^\infty_\mu(\Omega)$, with μ being σ-finite. Then the multiplication operator by ϕ, defined by $\mathcal{M}_\phi : \mathrm{L}^p_\mu(\Omega) \to \mathrm{L}^p_\mu(\Omega)$,

$$(\mathcal{M}_\phi \psi)(t) := \phi(t)\psi(t), \quad \psi \in \mathrm{L}^p_\mu(\Omega),$$

is a linear operator $\forall\, 1 \le p \le \infty$. Note that $(\mathcal{M}_\phi \psi) \in \mathrm{L}^p_\mu$ for $\psi \in \mathrm{L}^p_\mu$.

Remark 1.1.3. The notation of the Banach spaces $\mathrm{L}^p_\mu(\Omega)$, $1 \le p \le \infty$, is standard. In case $\Omega \subset \mathbb{R}^n$ and the measure is Lebesgue measure, the simplified notation $\mathrm{L}^p(\Omega)$ will be employed.

Example 1.1.4. Let X and Y be compact metric spaces and $u : Y \to X$ continuous. Then $T_u : C(X) \to C(Y)$, $(T_u\psi)(y) = \psi(u(y))$, is a linear operator.

Exercise 1.1.5. Let $T : \mathrm{dom}\, T \subset X \to Y$ be a linear operator. Verify the following items:

a) The range of T, $\mathrm{rng}\, T := T(\mathrm{dom}\, T) \subset Y$, and the *kernel* (or *null space*) of T, $\mathrm{N}(T) := \{\xi \in \mathrm{dom}\, T : T\xi = 0\}$, are vector spaces.
b) If the dimension $\dim(\mathrm{dom}\, T) = n < \infty$, then $\dim(\mathrm{rng}\, T) \le n$.
c) The inverse operator of T, $T^{-1} : \mathrm{rng}\, T \to \mathrm{dom}\, T$, exists if, and only if, $T\xi = 0 \Rightarrow \xi = 0$ and, in case it exists, it is also a linear operator.
d) If T, S are invertible linear operators, then $(TS)^{-1} = S^{-1}T^{-1}$ (by supposing, of course, that the operations are well posed).

A rich theory is obtained through the fusion of linear operators with the natural topology generated by norms. The next result is an example of such fusion; it shows that if a linear operator is continuous at some point of its domain, then it is uniformly continuous on its whole domain.

Theorem 1.1.6. *Let $T : \mathcal{N}_1 \to \mathcal{N}_2$ be a linear operator. Then the following assertions are equivalent:*

i) $\sup_{\|\xi\| \le 1} \|T\xi\| < \infty$.
ii) $\exists C > 0$ *such that* $\|T\xi\| \le C\|\xi\|$, $\forall \xi \in \mathcal{N}_1$.
iii) T *is uniformly continuous.*
iv) T *is continuous.*
v) T *is continuous at zero* (*i.e., the null vector*).

Proof. i) $\Longrightarrow$ ii) Let $C = \sup_{\|\xi\| \le 1} \|T\xi\|$. If $0 \ne \xi \in \mathcal{N}_1$, then $\|T(\xi/\|\xi\|)\| \le C$, i.e., $\|T\xi\| \le C\|\xi\|$, $\forall \xi \in \mathcal{N}_1$.

ii) $\Longrightarrow$ iii) If $\xi, \eta \in \mathcal{N}_1$, then $\|T\xi - T\eta\| = \|T(\xi - \eta)\| \le C\|\xi - \eta\|$.

iii) $\Longrightarrow$ iv) and iv) $\Longrightarrow$ v) are obvious.

v) $\Longrightarrow$ i) Since T is continuous at zero, there exists $\delta > 0$ with $\|T\xi\| \le 1$ if $\|\xi\| \le \delta$. Thus, if $\|\xi\| \le 1$, it follows that $\|\delta\xi\| \le \delta$ and $\|T(\delta\xi)\| \le 1$; therefore, $\|T\xi\| \le 1/\delta$, and i) holds. □

Definition 1.1.7. A continuous linear operator is also called *bounded*, and the set of bounded linear operators from $\mathcal{N}_1$ to $\mathcal{N}_2$ will be denoted by $\mathrm{B}(\mathcal{N}_1, \mathcal{N}_2)$. The notation $\mathrm{B}(\mathcal{N})$ will also be used as an abbreviation of $\mathrm{B}(\mathcal{N}, \mathcal{N})$.

Note the distinct use of the term *bounded linear operator* compared to the use in *bounded application* in general, i.e., one with bounded range; in the latter sense every linear (nonzero) operator is not bounded; verify this.

Example 1.1.8. The operator T_u in Example 1.1.4 is continuous, since for all $\psi \in C(X)$ one has $\|T_u\psi\|_\infty = \sup_{t\in Y} |\psi(u(t))| \le \sup_{t\in X} |\psi(t)| = \|\psi\|_\infty$, and T_u is bounded by Theorem 1.1.6(ii).

Exercise 1.1.9. Let X and Y be finite-dimensional vector spaces and $T : X \to Y$ a linear operator. Choose bases in X and Y and show that T can be represented by a matrix, and discuss how the matrix that represents T changes if other bases are considered.

Proposition 1.1.10. *If* $T : \mathcal{N}_1 \to \mathcal{N}_2$ *be linear and* $\dim \mathcal{N}_1 < \infty$, *then* T *is bounded.*

Proof. Consider in $\mathcal{N}_1$ the norm $|||\xi||| = \|\xi\| + \|T\xi\|$; then there exists $C > 0$ such that $|||\xi||| \le C\|\xi\|$, because all norms on finite-dimensional vector spaces are equivalent. Hence, $\|T\xi\| \le |||\xi||| \le C\|\xi\|$ and T is bounded. □

Example 1.1.11. For $1 \le p < \infty$, $l^p(\mathbb{N})$ denotes the Banach space of sequences $\xi = (\xi_j)_{j\in\mathbb{N}}$ so that $\|\xi\|_p = \left(\sum_j |\xi_j|^p\right)^{1/p} < \infty$. For $p = \infty$ the space $l^\infty(\mathbb{N})$ carries the norm $\|\xi\|_\infty = \sup_j |\xi_j|$. Similarly one defines $l^p(\mathbb{Z})$, $1 \le p \le \infty$.

Let $T : \left\{(\xi_n) \in l^p(\mathbb{N}) : \sum_n |n^2\xi_n|^p < \infty\right\} \to l^p(\mathbb{N})$, with $1 \le p < \infty$, $T(\xi_n) = (n^2\xi_n)$; this operator is linear, but is not continuous, since if $\{e_n\}_{n=1}^\infty$ denotes the canonical basis of $l^p(\mathbb{N})$, i.e., $e_n = (\delta_{j,n})_j$, then $e_n/n \to 0$, while Te_n does not converge to zero. Another argument: T is not bounded since $\|e_n\|_p = 1$ and $\|Te_n\|_p = n^2, \forall n$.

Example 1.1.12 (Shifts). The *right* (*left*) *shift* operator in $l^p(\mathbb{Z})$, $1 \le p \le \infty$, is defined by $S_r : l^p(\mathbb{Z}) \to l^p(\mathbb{Z})$ (resp. S_l), $\eta = S_r\xi$ (resp. $\eta = S_l\xi$), with $\eta_j = \xi_{j-1}$ (resp. $\eta_j = \xi_{j+1}$), $j \in \mathbb{Z}$. Note that the shift operator in $l^p(\mathbb{Z})$ is a bijective isometry (i.e., an isometric mapping), so bounded. They are also defined on $l^p(\mathbb{N})$ in an analogous way, but if $\eta = S_r\xi$ then it is defined $\eta_1 = 0$; these operators are also bounded, but S_r in $l^p(\mathbb{N})$ is not onto, although it is isometric.

Note that $\mathrm{B}(\mathcal{N}_1, \mathcal{N}_2)$ is a vector space with pointwise operations, and it turns out that

$$\|T\| := \sup_{\substack{\xi\in\mathcal{N}_1 \\ \|\xi\|\le 1}} \|T\xi\|$$

is a norm on $\mathrm{B}(\mathcal{N}_1, \mathcal{N}_2)$. In fact, if $T \in \mathrm{B}(\mathcal{N}_1, \mathcal{N}_2)$, $\|T\| = 0 \Longleftrightarrow T\xi = 0$, $\forall \xi \in \mathcal{N}_1$, that is, $T = 0$; $\|\alpha T\| = |\alpha|\|T\|$ is immediate; if $S \in \mathrm{B}(\mathcal{N}_1, \mathcal{N}_2)$, then

$$\|T + S\| = \sup_{\|\xi\| \le 1} \|T\xi + S\xi\| \le \sup_{\|\xi\| \le 1} (\|T\xi\| + \|S\xi\|) \le \|T\| + \|S\|.$$

If a topology is not explicitly given in $\mathrm{B}(\mathcal{N}_1, \mathcal{N}_2)$, it is supposed that the topology is the one induced by this norm.

Exercise 1.1.13. a) If $T \in \mathrm{B}(\mathcal{N}_1, \mathcal{N}_2)$, check that

$$\|T\| = \inf_{C>0} \{\|T\xi\| \le C\|\xi\|, \ \forall \xi \in \mathcal{N}_1\} = \sup_{\|\xi\|=1} \|T\xi\| = \sup_{\xi \ne 0} \frac{\|T\xi\|}{\|\xi\|}.$$

b) If T, S are bounded linear operators and TS (the composition, but usually called product of operators) is defined, show that TS is bounded and $\|TS\| \le \|T\|\|S\|$. Therefore, if T^n (nth iterate of T) is defined, then $\|T^n\| \le \|T\|^n$.

Example 1.1.14. The zero operator is the unique operator whose norm is zero, and for the identity operator $\|\mathbf{1}\| = 1$ (with $\mathcal{N} \ne \{0\}$).

Example 1.1.15. Let X be the vector space of polynomials in $C[0,1]$ and $D : X \hookleftarrow$ the differential operator $(Dp)(t) = p'(t)$, $p \in X$. This operator is linear and does not belong to $\mathrm{B}(X)$, since if $p_n(t) = t^n$, then for all $n \ge 1$ one has $(Dp_n)(t) = nt^{n-1}$, $\|p_n\|_\infty = 1$, while $\|Dp_n\|_\infty = n$.

Example 1.1.16. The operator $\mathcal{M}_\phi$, with $\phi \in \mathrm{L}^\infty_\mu(\Omega)$ (see Example 1.1.2) is bounded in $\mathrm{L}^p_\mu(\Omega), 1 \le p \le \infty$, and $\|\mathcal{M}_\phi\| = \|\phi\|_\infty$ $(= \sup\operatorname{ess} |\phi|)$.

Proof. It will be supposed that $\|\phi\|_\infty \ne 0$ and demonstrated for $1 \le p < \infty$. The cases $p = \infty$ and $\|\phi\|_\infty = 0$ are left as exercises. If $\|\psi\|_p = 1$, then by

$$\|\mathcal{M}_\phi \psi\|_p^p = \int_\Omega |\phi(t)|^p |\psi(t)|^p d\mu(t) \le \|\phi\|_\infty^p \|\psi\|_p^p,$$

one gets that $\mathcal{M}_\phi$ is bounded and $\|\mathcal{M}_\phi\| \le \|\phi\|_\infty$.

Let $0 < \theta < \|\phi\|_\infty$; then there exists a measurable set A, with $0 < \mu(A) < \infty$ (recall that μ is σ-finite) obeying $\|\phi\|_\infty \ge |\phi(t)| > \theta$, $\forall t \in A$. Thus, χ_A, the characteristic function of A (i.e., $\chi_A(t) = 1$ if $t \in A$ and $\chi_A(t) = 0$ if $t \notin A$), belongs to $\mathrm{L}^p_\mu(\Omega)$ and

$$\|\mathcal{M}_\phi \chi_A\|_p^p = \int_A |\phi(t)|^p |\chi_A(t)|^p d\mu(t) \ge \theta^p \|\chi_A\|_p^p;$$

so $\|\mathcal{M}_\phi\| \ge \theta$ and, therefore, $\|\mathcal{M}_\phi\| = \|\phi\|_\infty$. □

Example 1.1.17. Let $K : (\Omega, \mathcal{A}, \mu) \times (\Omega, \mathcal{A}, \mu) \to \mathbb{F}$ measurable (σ-finite space) and suppose that there exists $C > 0$ with

$$\int_\Omega |K(x,y)| d\mu(x) \le C, \quad \text{for } y \ \ \mu - \text{a.e.}$$

Then, $T_K : \mathrm{L}^1_\mu(\Omega) \hookleftarrow$ given by

$$(T_K\psi)(x) = \int_\Omega K(x,y)\psi(y)d\mu(y), \quad \psi \in \mathrm{L}^1_\mu(\Omega),$$

is bounded and $\|T_K\| \le C$.

Proof. If $\psi \in \mathrm{L}^1_\mu(\Omega)$ then

$$|(T_K\psi)(x)| \le \int_\Omega |K(x,y)\psi(y)|d\mu(y);$$

thus, $\|T_K\psi\|_1 = \int_\Omega |(T_K\psi)(x))|d\mu(x) \le \iint |K(x,y)|\,|\psi(y)|d\mu(y)d\mu(x)$. By the Fubini Theorem it is found that

$$\|T_K\psi\|_1 \le \iint_{\Omega\times\Omega} |K(x,y)|d\mu(x)\,|\psi(y)|d\mu(y) \le C\|\psi\|_1.$$

Therefore $\|T_K\| \le C$. □

Exercise 1.1.18. Let $(e_n)_{n=1}^\infty$ be the usual basis of $l^2(\mathbb{N})$ and $(\alpha_n)_{n=1}^\infty$ a sequence in $\mathbb{F}$. Show that the operator $T : l^2(\mathbb{N}) \hookleftarrow$ with $Te_n = \alpha_n e_n$ is bounded if, and only if, $(\alpha_n)_{n=1}^\infty$ is a bounded sequence. Verify that, in this case, $\|T\| = \sup_n |\alpha_n|$.

Exercise 1.1.19. Let $C^1(0,1)$ be the set of continuously differentiable real functions on $(0,1)$, as a subspace of $\mathrm{L}^2(0,1)$ (i.e., use the norm of L^2). Apply the differential operator $(D\psi)(t) = \psi'(t)$, $D : C^1(0,1) \to \mathrm{L}^2(0,1)$, to functions $\psi_n(t) = \sin(n\pi t)$ and conclude that D is not bounded.

Exercise 1.1.20. Show that the differential operator $D : C^\infty[a,b] \hookleftarrow$ is not bounded for any norm on $C^\infty[a,b]$.

The next result gives a simple answer to an important question. Under which conditions $\mathrm{B}(\mathcal{N}_1,\mathcal{N}_2)$ is a Banach space?

Theorem 1.1.21. *If $\mathcal{N}$ is a normed space and $\mathcal{B}$ a Banach space, then* $\mathrm{B}(\mathcal{N},\mathcal{B})$ *is Banach.*

Proof. Let $(T_n)_{n=1}^\infty$ be a Cauchy sequence in $\mathrm{B}(\mathcal{N},\mathcal{B})$. Since for each $\xi \in \mathcal{N}$ one has $\|T_n\xi - T_k\xi\| \le \|T_n - T_k\|\|\xi\|$, then $(T_n\xi)$ is Cauchy in $\mathcal{B}$ and converges to $\eta \in \mathcal{B}$. Define $T : \mathcal{N} \to \mathcal{B}$ by $T\xi = \eta$, which is clearly linear. It will be shown that this operator is bounded and $T_n \to T$ in $\mathrm{B}(\mathcal{N},\mathcal{B})$.

Given $\varepsilon > 0$ there exists $N(\varepsilon)$ such that, if $n,k \ge N(\varepsilon)$, then $\|T_n - T_k\| < \varepsilon$. By the continuity of the norm it follows that

$$\|T_n\xi - T\xi\| = \lim_{k\to\infty} \|T_n\xi - T_k\xi\| \le \varepsilon\|\xi\|, \qquad n \ge N(\varepsilon),$$

and $(T_n - T) \in \mathrm{B}(\mathcal{N},\mathcal{B})$ with $\|T_n - T\| \le \varepsilon$. Since $\mathrm{B}(\mathcal{N},\mathcal{B})$ is a vector space, and $T = T_n + (T - T_n)$, then $T \in \mathrm{B}(\mathcal{N},\mathcal{B})$. The inequality $\|T_n - T\| \le \varepsilon$, valid for all $n \ge N(\varepsilon)$, shows that $T_n \to T$ and $\mathrm{B}(\mathcal{N},\mathcal{B})$ is complete. □

Exercise 1.1.22. Suppose that $T_n \to T$ in $\mathrm{B}(\mathcal{N})$ and $\xi_n \to \xi$ in $\mathcal{N}$. Show that $T_n\xi_n \to T\xi$.

Exercise 1.1.23. Let $T \in \mathrm{B}(\mathcal{B})$. Show that, for all $t \in \mathbb{F}$, the operator e^{tT} defined by the series

$$e^{tT} := \sum_{j=0}^{\infty} \frac{(tT)^j}{j!}$$

belongs to $\mathrm{B}(\mathcal{B})$ and $\|e^{tT}\| \le e^{|t|\|T\|}$.

Exercise 1.1.24. Let $T \in \mathrm{B}(\mathcal{B})$, with $\|T\| < 1$. Show that the operator defined by the series $S = \sum_{j=0}^{\infty} T^j$ belongs to $\mathrm{B}(\mathcal{B})$ and $S = (\mathbf{1} - T)^{-1}$.

Uniformly continuous functions on metric spaces have uniformly continuous extensions to the closure of their domains; in the case of linear operators there is an analogous result, which is a consequence of the uniform continuity of bounded operators (Theorem 1.1.6).

Definition 1.1.25. If $\mathcal{N}$ is a normed space, then the Banach space $\mathrm{B}(\mathcal{N}, \mathbb{F})$ will be denoted by $\mathcal{N}^*$ and termed *dual space* of $\mathcal{N}$. Each element of $\mathcal{N}^*$ is called a continuous *linear functional* on $\mathcal{N}$ (Why is $\mathcal{N}^*$ complete?).

Remark 1.1.26. a) Recall that by the Hahn-Banach theorem $\mathcal{N}^*$ separates points of $\mathcal{N}$, that is, if $\eta \neq \xi \in \mathcal{N}$, then there exists $f \in \mathcal{N}^*$ with $f(\xi) \neq f(\eta)$. In particular, if $f(\xi) = 0$ for all $f \in \mathcal{N}^*$, then $\xi = 0$.

b) The Hahn-Banach theorem can also be used to prove the converse of Theorem 1.1.21, so that $\mathrm{B}(\mathcal{N}_1, \mathcal{N}_2)$ is complete iff $\mathcal{N}_2$ is a Banach space.

Example 1.1.27. The integral on $C[a, b]$ is an element of the dual of $C[a, b]$, since $\psi \mapsto \int_a^b \psi(t)\, dt$ is linear and continuous. In fact, every finite Borel (complex) measure μ over $[a, b]$ defines an element of the dual of $C[a, b]$ through the integral $\psi \mapsto \int_a^b \psi(t)\, d\mu(t)$, because

$$\left| \int_a^b \psi(t)\, d\mu(t) \right| \le \|\psi\|_\infty\, |\mu|([a, b]).$$

Example 1.1.28 (Unbounded functional). Consider the linear functional

$$f : C[-1, 1] \subset \mathrm{L}^1[-1, 1] \to \mathbb{F}, \quad f(\psi) = \psi(0).$$

Pick a function $\psi \in C[-1, 1]$ with $\psi(-1) = \psi(1) = 0$ and $\psi(0) \neq 0$. For each $n \ge 2$, set $\psi_n(t) = \psi(nt)$ if $|t| \le 1/n$, and equal to zero otherwise. Note that $\|\psi_n\|_1 = \int_{-1}^1 |\psi_n(t)|\, dt = \|\psi\|_1/n$, which converges to zero for $n \to \infty$. However, $f(\psi_n) = \psi(0) \neq 0$ for all n, and f is not continuous.

Example 1.1.29. Let $1 < p < \infty$ and $1/p + 1/q = 1$. Each $\phi \in \mathrm{L}^q_\mu(\Omega)$ defines an element of the dual of $\mathrm{L}^p_\mu(\Omega)$, since by Hölder inequality the product $\phi\psi \in \mathrm{L}^1_\mu(\Omega)$, for all $\psi \in \mathrm{L}^p_\mu(\Omega)$, and

$$\psi \mapsto \int_\Omega \phi\psi d\mu$$

is linear and bounded with norm $\le \|\phi\|_q$ (again by Hölder). Hence, $\mathrm{L}^q_\mu(\Omega) \subset \mathrm{L}^p_\mu(\Omega)^*$. The proof is found in books on Integration Theory that $\mathrm{L}^p_\mu(\Omega)^* = \mathrm{L}^q_\mu(\Omega)$, for $1 < p < \infty$ and, if the measure μ is σ-finite, one also has $\mathrm{L}^1_\mu(\Omega)^* = \mathrm{L}^\infty_\mu(\Omega)$.

Exercise 1.1.30. Show that the dual of l^p is l^q, with $1 < p < \infty$ and $1/p + 1/q = 1$.

Theorem 1.1.31 (Uniform Boundedness Principle). *Any family of operators* $\{T_\alpha\}_{\alpha \in J}$ *in* $\mathrm{B}(\mathcal{B}, \mathcal{N})$ *so that, for each* $\xi \in \mathcal{B}$,

$$\sup_{\alpha \in J} \|T_\alpha \xi\| < \infty,$$

satisfies $\sup_{\alpha \in J} \|T_\alpha\| < \infty$.

Proof. Put $E_k = \{\xi \in \mathcal{B} : \|T_\alpha \xi\| \le k, \forall \alpha \in J\}$, which is a closed set; indeed, since T_α is continuous, it is the intersection of the closed sets $T_\alpha^{-1}\overline{B}(0;k)$ for all $\alpha \in J$. Since $\mathcal{B} = \bigcup_{k=1}^\infty E_k$, by the Baire theorem there exists E_m with nonempty interior. Let $B_{\mathcal{B}}(\xi_0; r)$ $(r > 0)$ be an open ball contained in E_m; then, for any $\alpha \in J$ one has $\|T_\alpha \xi\| \le m$ for all $\xi \in B_{\mathcal{B}}(\xi_0; r)$.

If $\xi \in \mathcal{B}$, $\|\xi\| = 1$, it is found that $\eta = \xi_0 + r\xi/2$ belongs to $B_{\mathcal{B}}(\xi_0; r)$ and

$$\|T_\alpha \xi\| = \frac{2}{r} \|T_\alpha \eta - T_\alpha \xi_0\| \le \frac{2}{r} (\|T_\alpha \eta\| + \|T_\alpha \xi_0\|) \le \frac{4m}{r};$$

thus $\|T_\alpha \xi\| \le 4m/r$ for all $\alpha \in J$ and $\|\xi\| = 1$; it then follows that $\sup_\alpha \|T_\alpha\| \le 4m/r < \infty$. □

Corollary 1.1.32. *A subset* $H \subset \mathcal{B}^* = \mathrm{B}(\mathcal{B}, \mathbb{F})$ *is bounded if, and only if, for all* $\xi \in \mathcal{B}$, $\sup_{f \in H} |f(\xi)| < \infty$.

Proof. If H is bounded, then $M = \sup_{f \in H} \|f\| < \infty$ and for all $\xi \in \mathcal{B}$ one has $\sup_{f \in H} |f(\xi)| \le M\|\xi\| < \infty$. To show the other statement, by using the notation presented in the uniform boundedness principle, it is enough to consider H as the family T_α in the Banach space $\mathcal{B}^*$. □

Corollary 1.1.33 (Banach-Steinhaus Theorem). *Let* $(T_n)_{n=1}^\infty$ *be a sequence in* $\mathrm{B}(\mathcal{B}, \mathcal{N})$ *so that for each* $\xi \in \mathcal{B}$ *there exists the limit*

$$T\xi := \lim_{n \to \infty} T_n \xi.$$

Then $\sup_n \|T_n\| < \infty$ *and* T *is a bounded operator in* $\mathrm{B}(\mathcal{B}, \mathcal{N})$.

Proof. Clearly T is linear. Since for all $\xi \in \mathcal{B}$ there exists $\lim_{n \to \infty} T_n \xi$, then $\sup_n \|T_n \xi\| < \infty$, and by the uniform boundedness principle one has $\sup_n \|T_n\| < \infty$. By the definition of T it follows that

$$\|T\xi\| \le (\sup_n \|T_n\|) \|\xi\|, \qquad \forall \xi \in \mathcal{B}$$

and, therefore, T is bounded. □

Example 1.1.34. Let $\mathcal{N}$ be the normed space of the elements $\xi = (\xi_j) \in l^\infty(\mathbb{N})$ that have just a finite number of nonzero entries ξ_j. Define $T_n : \mathcal{N} \to l^\infty$ by $T_n\xi = (n\xi_n)_{j\in\mathbb{N}}$. Then $T_n \in \mathrm{B}(\mathcal{N}, l^\infty)$ for all n, and for each $\xi \in \mathcal{N}$ there exists the limit $\lim_{n\to\infty} T_n\xi = 0$, but $\lim_{n\to\infty} \|T_n\| = \infty$. This shows that the conclusions of the Banach-Steinhaus theorem (and of the uniform boundedness principle) may fail if the domain of the operators is not complete.

Exercise 1.1.35. Let $S_l : l^2(\mathbb{N}) \hookleftarrow$ be the shift

$$S_l(\xi_1, \xi_2, \xi_3, \dots) = (\xi_2, \xi_3, \xi_4, \dots)$$

and $T_n = S_l^n$. Find $\|T_n\xi\|$, and the limit operator described in the Banach-Steinhaus theorem.

Proposition 1.1.36. *Let* $\{T_\alpha\}_{\alpha\in J}$ *be a family in* $\mathrm{B}(\mathcal{B}, \mathcal{N})$ *with*

$$\sup_{\alpha\in J} \|T_\alpha\| = \infty.$$

Then the set $\mathcal{I} = \{\xi \in \mathcal{B} : \sup_\alpha \|T_\alpha\xi\| < \infty\}$ *is meager in* $\mathcal{B}$ (*that is, it is a subset of a countable union of closed subsets of* $\mathcal{B}$ *with empty interior*).

Proof. By using the notation of the proof of the uniform boundedness principle, one has $\mathcal{I} = \cup_{k=1}^\infty E_k$, and by that proof it follows that the interior of every E_k is empty, since if not one would get $\sup_{\alpha\in J} \|T_\alpha\| < \infty$. Since E_k is closed, then $\mathcal{I}$ is meager. □

Denote $C_p[0, 2\pi] = \{\psi \in C[0, 2\pi] : \psi(0) = \psi(2\pi)\}$, which is a closed subspace of $C[0, 2\pi]$, so it is Banach, and

$$(\mathrm{F}\psi)_n = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} e^{-int}\psi(t)\, dt, \qquad \psi \in C_p[0, 2\pi].$$

Corollary 1.1.37. *The set of elements* $\psi \in C_p[0, 2\pi]$ *whose Fourier series* $\sum_{n\in\mathbb{Z}} (\mathrm{F}\psi)_n\, e^{int}$ *converges for* $t = 0$ *is meager.*

Proof. By working with trigonometric relations it is found that, for each N, the partial sum $(S_N\psi)(t) = \sum_{|n|\le N} (\mathrm{F}\psi)_n\, e^{int}$ can be written in the form

$$(S_N\psi)(t) = \frac{1}{2\pi} \int_0^{2\pi} \frac{\sin[(2N+1)(t-s)/2]}{\sin[(t-s)/2]} \psi(s)\, ds.$$

Note that $f_N : C_p[0, 2\pi] \to \mathbb{C}$, $f_N(\psi) = (S_N\psi)(0)$, is an element of the dual of $C_p[0, 2\pi]$; thus, in order to conclude this proof it is enough to show that $\sup_N \|f_N\| = \infty$ and use Proposition 1.1.36 with f_N represented by T_α.

Consider $\phi_N(t) = \sin[(2N+1)t/2]$, an element of $C_p[0, 2\pi]$ with norm equal to 1; thus

$$\begin{aligned} f_N(\phi_N) &= \frac{1}{2\pi}\int_0^{2\pi} \frac{\sin^2[(2N+1)s/2]}{\sin(s/2)}\,ds \\ &\geq \frac{1}{\pi}\int_0^{2\pi} \frac{\sin^2[(2N+1)s/2]}{s}\,ds \\ &= \frac{1}{\pi}\int_0^{(2N+1)\pi} \frac{\sin^2 u}{u} du \\ &\geq \frac{1}{\pi}\sum_{n=1}^{2N+1}\int_{(n-1)\pi}^{n\pi} \frac{\sin^2 u}{n\pi} du = \frac{1}{2\pi}\sum_{n=1}^{2N+1}\frac{1}{n}. \end{aligned}$$

Since the harmonic series is divergent, one concludes that $\lim_{N\to\infty} \|f_N\| = \infty$, and the proof is complete. □

Exercise 1.1.38. Verify that $C_p[0, 2\pi]$ is a Banach space, and also the validity of the expression for a partial sum for the Fourier series used in the proof of Corollary 1.1.37.

Now the famous Riesz representation theorem of Hilbert spaces $\mathcal{H}$, which shows that every Hilbert space is naturally identified to its dual, is recalled and demonstrated. In order to fix notation, remember that an inner product in a vector space X is a map $(\xi, \eta) \mapsto \langle\xi, \eta\rangle$, $X \times X \to \mathbb{F}$, so that for any $\xi, \eta, \zeta \in X$ and $\alpha \in \mathbb{F}$ it satisfies:

i) $\langle\alpha\xi + \eta, \zeta\rangle = \bar{\alpha}\langle\xi, \zeta\rangle + \langle\eta, \zeta\rangle$,
ii) $\langle\xi, \eta\rangle = \overline{\langle\eta, \xi\rangle}$,
iii) $\langle\xi, \xi\rangle \geq 0$, and $\langle\xi, \xi\rangle = 0$ iff $\xi = 0$.

In an inner product space one has the induced norm $\|\xi\| := \sqrt{\langle\xi, \xi\rangle}$, so that the Cauchy-Schwarz $|\langle\xi, \eta\rangle| \leq \|\xi\|\|\eta\|$ and triangular $\|\xi + \eta\| \leq \|\xi\| + \|\eta\|$ inequalities always hold.

Exercise 1.1.39. Show that equality in Cauchy-Schwarz occurs iff $\{\xi, \eta\}$ is linearly dependent, while equality in the triangular occurs iff either $\xi = 0$ or $\eta = t\xi$ for some $t \geq 0$.

Let $\{\xi_\alpha\}_{\alpha\in J}$ be an orthonormal set in $\mathcal{H}$. One of the advantages of the presence of an inner product in a Hilbert space $\mathcal{H}$ is the existence of orthonormal basis of $\mathcal{H}$, that is, if $\overline{\mathrm{Lin}(\{\xi_\alpha\}_{\alpha\in J})} = \mathcal{H}$. The following facts illustrate such advantages quite well. For each $\xi \in \mathcal{H}$, the Bessel inequality

$$\|\xi\|^2 \geq \sum_{\alpha\in J} |\langle\xi_\alpha, \xi\rangle|^2$$

holds; in particular, $\langle\xi_\alpha, \xi\rangle \neq 0$ only for a countable number of indices $\alpha \in J$. Furthermore, the following assertions are equivalent:

i) $\{\xi_\alpha\}_{\alpha\in J}$ is an orthonormal basis of $\mathcal{H}$.
ii) If $\xi \in \mathcal{H}$, then the Fourier series of ξ, with respect to $\{\xi_\alpha\}_{\alpha\in J}$, converges in $\mathcal{H}$ for ξ (and independent of the sum order), that is,

$$\xi = \sum_{\alpha\in J} \langle \xi_\alpha, \xi\rangle\, \xi_\alpha, \qquad \forall \xi \in \mathcal{H}.$$

iii) [Parseval Identity] For all $\xi \in \mathcal{H}$,

$$\|\xi\|^2 = \sum_{\alpha\in J} |\langle \xi_\alpha, \xi\rangle|^2.$$

Furthermore, if $\{\xi_\alpha\}_{\alpha\in J}$ is an orthonormal basis and $\eta = \sum_{\alpha\in J}\langle \xi_\alpha, \eta\rangle \xi_\alpha$, then

$$\langle \xi, \eta\rangle = \sum_\alpha \langle \xi, \xi_\alpha\rangle\, \langle \xi_\alpha, \eta\rangle.$$

Theorem 1.1.40 (Riesz Representation). *Let $\mathcal{H}$ be a Hilbert space and $\mathcal{H}^*$ its dual. The map $\gamma : \mathcal{H} \to \mathcal{H}^*$, $\gamma(\xi) = f_\xi$, for $\xi \in \mathcal{H}$, given by*

$$\gamma(\xi)(\eta) = f_\xi(\eta) = \langle \xi, \eta\rangle, \qquad \forall \eta \in \mathcal{H},$$

is an antilinear (i.e., $\alpha\xi \mapsto \overline{\alpha}\xi$, $\forall \alpha \in \mathbb{F}$) and onto isometry on $\mathcal{H}^*$.

Remark 1.1.41. This theorem implies that each element of $\mathcal{H}^*$ is identified to a unique $\xi \in \mathcal{H}$, via f_ξ, and $\|f_\xi\| = \|\xi\|$; one then says such ξ represents f_ξ. Note that two distinct notations for this map were introduced: $\gamma(\xi)$ and f_ξ; this is convenient in certain situations.

Proof. If $\xi = 0$, clearly $f_\xi = 0$. If $\xi \in \mathcal{H}$, then f_ξ is a linear functional and $|f_\xi(\eta)| = |\langle \xi, \eta\rangle| \le \|\xi\|\|\eta\|$, so that $f_\xi \in \mathcal{H}^*$ with $\|f_\xi\| \le \|\xi\|$. In view of $\|\xi\|^2 = f_\xi(\xi) \le \|f_\xi\|\|\xi\|$ one has $\|f_\xi\| \ge \|\xi\|$. Hence $\|f_\xi\| = \|\xi\|$, and the map γ is an isometry, obviously antilinear (linear in the real case). Then we only need to show that every $f \in \mathcal{H}^*$ is of the form f_ξ for some $\xi \in \mathcal{H}$. If $f = 0$, then $f = f_\xi$ for $\xi = 0$. If $f \ne 0$, since the kernel $\mathrm{N}(f)$ is a proper closed vector subspace (since f is continuous) of $\mathcal{H}$, it is found that

$$\mathcal{H} = \mathrm{N}(f) \oplus \mathrm{N}(f)^\perp,$$

and there exists $\zeta \in \mathrm{N}(f)^\perp$ with $\|\zeta\| = 1$. Now, by noticing that the vector $(f(\eta)\zeta - f(\zeta)\eta) \in \mathrm{N}(f)$, for all $\eta \in \mathcal{H}$ (this remark is simple but essential in this proof), one concludes that

$$\langle \zeta, f(\eta)\zeta - f(\zeta)\eta\rangle = 0, \qquad \forall \eta \in \mathcal{H},$$

that is, $f(\eta) = \langle \overline{f(\zeta)}\zeta, \eta\rangle$. Therefore, $f = \gamma(\overline{f(\zeta)}\zeta)$. □

Exercise 1.1.42. If $f \in \mathcal{H}^*$, what is the dimension of $\mathrm{N}(f)^\perp$?

Example 1.1.43. The hypothesis that the inner product space is complete can not be dispensed with in Theorem 1.1.40. Consider the subspace $\mathcal{N}$ of $l^2(\mathbb{N})$ whose elements have just a finite number of nonzero entries; then $f : \mathcal{N} \to \mathbb{F}$, $f(\eta) = \sum_{j=1}^{\infty} \eta_j/j$, belongs to $\mathcal{N}^*$, but there is no $\xi \in \mathcal{N}$ with $f = f_\xi$, since the vector $(1, 1/2, 1/3, \dots) \notin \mathcal{N}$.

Now a simple and useful technical result, although it is restricted to complex inner product spaces, as illustrated by Example 1.1.45.

Lemma 1.1.44. *Let $(X, \langle\cdot,\cdot\rangle)$ be a complex inner product space. If $T : X \hookleftarrow$ is a linear operator and $\langle T\xi, \xi\rangle = 0$ for all $\xi \in X$, then $T = 0$. Hence, if T, S are linear operators and $\langle T\xi, \xi\rangle = \langle S\xi, \xi\rangle$ for all $\xi \in X$, then $T = S$.*

Proof. For all $\alpha \in \mathbb{C}$ and any $\xi, \eta \in X$ one has

$$0 = \langle T(\alpha\xi + \eta), \alpha\xi + \eta\rangle = \bar{\alpha}\langle T\xi, \eta\rangle + \alpha\langle T\eta, \xi\rangle.$$

By picking, successively, $\alpha = 1$ and $\alpha = -i$ one obtains

$$\langle T\xi, \eta\rangle + \langle T\eta, \xi\rangle = 0 \ \text{ and } \ \langle T\xi, \eta\rangle - \langle T\eta, \xi\rangle = 0,$$

whose unique solution is $\langle T\xi, \eta\rangle = 0$, for all $\xi, \eta \in X$, that is, T is the zero operator. □

Example 1.1.45. Consider the rotation R by the right angle on $\mathbb{R}^2$, so that $R \neq 0$ while $\langle R\xi, \xi\rangle = 0$, $\forall \xi \in \mathbb{R}^2$.

Before closing this section, recall the parallelogram law

$$\|\xi + \eta\|^2 + \|\xi - \eta\|^2 = 2\|\xi\|^2 + 2\|\eta\|^2, \qquad \forall \xi, \eta \in X$$

as well as the polarization identity

$$\langle \xi, \eta\rangle = \frac{1}{4}\left(\|\xi + \eta\|^2 - \|\xi - \eta\|^2 + i\|\xi + i\eta\|^2 - i\|\xi - i\eta\|^2\right),$$

which hold in any (complex) inner product space.

1.2 Closed Operators

Before discussing closed operators it can be useful to recall the so-called open mapping theorem. A map between topological spaces is open if the image of every open subset is also open. There are invertible continuous maps that are not open, as shown by the following examples.

Example 1.2.1. The identity map between $\mathbb{R}^n$ with the discrete topology and $\mathbb{R}^n$ with the usual topology is continuous and invertible, but its inverse map is not continuous, that is, this bijective continuous map is not open.

Example 1.2.2. Let $X = [-1,0] \cup (1,2]$ in $\mathbb{R}$ and $\psi : X \to [0,4]$, $\psi(t) = t^2$. ψ is a continuous bijection, but its inverse $\psi^{-1} : [0,4] \to X$, given by

$$\psi^{-1}(t) = \begin{cases} -\sqrt{t} & \text{if } 0 \le t \le 1 \\ \sqrt{t} & \text{if } 1 < t \le 4 \end{cases},$$

is not continuous.

Exercise 1.2.3. Show that $T : l^1(\mathbb{N}) \hookleftarrow$ given by $T(\xi_1, \xi_2, \xi_3, \dots) = (\xi_1/1, \xi_2/2, \xi_3/3, \dots)$ is linear, continuous and invertible, but its inverse T^{-1}, defined on the range of T, is not a continuous operator.

Theorem 1.2.4 (Open Mapping). *If $T \in \mathrm{B}(\mathcal{B}_1, \mathcal{B}_2)$ with* rng $T = \mathcal{B}_2$*, then T is an open map.*

Proof. The following properties will be used, and only the last one is not immediate:

- **a)** for all $r, s > 0$ one has $TB(0;r) = \frac{r}{s} TB(0;s)$.
- **b)** for all $\xi \in \mathcal{B}_1$ and $r > 0$, one has $TB(\xi;r) = T\xi + TB(0;r)$ (sum of sets).
- **c)** if $B(0;\varepsilon) \subset \overline{TB(0;r)}$, then $B(0;\alpha\varepsilon) \subset \overline{TB(0;\alpha r)}$, for all $\alpha > 0$. Then if there is $r > 0$ so that $\overline{TB(0;r)}$ contains a neighborhood of the origin, then $\overline{TB(0;s)}$ contains a neighborhood of the origin for all $s > 0$ (note that such implications also hold without closures of the sets).
- **d)** if $B(\eta_0;\varepsilon) \subset \overline{TB(0;r)}$, then there exists $\delta > 0$ so that $B(0;\delta) \subset \overline{TB(0;r)}$ (note that it also holds without closure of the sets).

To prove the last property, pick $\xi_1 \in B(0;r)$ so that $\|\eta_1 - \eta_0\| < \varepsilon/2$, with $\eta_1 = T\xi_1$. Thus,

$$B(\eta_1;\varepsilon/2) \subset B(\eta_0;\varepsilon) \subset \overline{TB(0;r)},$$

and so

$$\begin{aligned} B(0;\varepsilon/2) &= B(\eta_1;\varepsilon/2) - \eta_1 \subset \{B(\eta_0;\varepsilon) - T\xi_1\} \\ &\subset \left\{\overline{TB(0;r)} - T\xi_1\right\} \subset \overline{T[B(0;r) - \xi_1]} \subset \overline{TB(0;2r)}\,. \end{aligned}$$

Then it follows that $B(0;\varepsilon/2) \subset \overline{TB(0;2r)}$ and, therefore, $B(0;\delta) \subset \overline{TB(0;r)}$ with $\delta = \varepsilon/4$, proving **d)**.

Lemma 1.2.5. *If $T \in \mathrm{B}(\mathcal{N}_1, \mathcal{N}_2)$ and there exists $r > 0$ so that the interior of $\overline{TB(0;r)}$ is nonempty, then T is an open map.*

Proof. Since the interior of $\overline{TB(0;r)} \neq \emptyset$, from the above properties it follows that for all $s > 0$, $\overline{TB(0;s)}$ contains an open ball centered at the origin. To show that T is an open map it is enough to show that for all $\xi \in \mathcal{N}_1$ and all $s > 0$, $TB(\xi;s)$ contains a neighborhood of $T\xi$. In view of $TB(\xi;s) = T\xi + TB(0;s)$, one may consider $\xi = 0$ and verify that for all $s > 0$ the set $TB(0;s)$ contains a neighborhood of the origin, but this is exactly what was observed at the beginning of this proof. □

By this lemma, to prove the open mapping theorem it is enough to verify that there exists some $r > 0$ so that $TB(0;r)$ contains an open ball centered at the origin. Note that only from this point will the completeness of $\mathcal{B}_1, \mathcal{B}_2$ and that T is onto be used; the Baire theorem will be crucial.

Since T is onto $\mathcal{B}_2 = \bigcup_{n=1}^{\infty} \overline{TB(0;n)}$, and by the Baire theorem there is some m so that the interior of $\overline{TB(0;m)}$ is nonempty. By property **c)** it is possible to take $m = 1$.

By property **d)** one may suppose that there is $\delta > 0$ so that $B(0;\delta) \subset \overline{TB(0;1)}$. The goal now is to show that the relation $\overline{TB(0;1)} \subset TB(0;2)$ holds, which, by Lemma 1.2.5, proves the theorem.

Let $\eta \in \overline{TB(0;1)}$. Pick $\xi_1 \in B(0;1)$ with

$$(\eta - T\xi_1) \in B(0;\delta/2) \subset \overline{TB(0;1/2)}.$$

In the last step property **c)** was invoked. Pick now ξ_2 in $B(0;1/2)$ so that (again by **c)**)

$$(\eta - T\xi_1 - T\xi_2) \in B(0;\delta/2^2) \subset \overline{TB(0;1/2^2)}.$$

By induction, pick $\xi_n \in B(0;1/2^{n-1})$ satisfying

$$\left(\eta - \sum_{j=1}^{n} T\xi_j\right) \in B(0;\delta/2^n) \subset \overline{TB(0;1/2^n)}.$$

$(\sum_{j=1}^{n} \xi_j)_n$ is a Cauchy sequence and, since $\mathcal{B}_1$ is complete, there exists $\xi = \sum_{j=1}^{\infty} \xi_j$ and, by the continuity of the map T it follows that $\eta = T\xi$. Since $\|\xi\| < 2$, one gets $\overline{TB(0;1)} \subset TB(0;2)$. □

By the open mapping theorem the next result is evident; it is sometimes called the *inverse mapping theorem*.

Corollary 1.2.6. *If* $T \in \mathrm{B}(\mathcal{B}_1, \mathcal{B}_2)$ *is a bijection between* $\mathcal{B}_1$ *and* $\mathcal{B}_2$*, then* T^{-1} *is also a linear continuous map.*

Recall that the cartesian product $\mathcal{N}_1 \times \mathcal{N}_2$ of two normed spaces has a natural structure of vector space given by $\alpha(\xi,\eta) = (\alpha\xi, \alpha\eta)$, $\alpha \in \mathbb{F}$, and $(\xi_1,\eta_1)+(\xi_2,\eta_2) = (\xi_1+\xi_2, \eta_1+\eta_2)$; furthermore, this cartesian product becomes a normed space with the norm $\|(\xi,\eta)\| = (\|\xi\|^2_{\mathcal{N}_1} + \|\eta\|^2_{\mathcal{N}_2})^{\frac{1}{2}}$; such a norm is equivalent to $\|\xi\|_{\mathcal{N}_1} + \|\eta\|_{\mathcal{N}_2}$ and both may be employed.

Definition 1.2.7. The *graph* of a linear operator $T : \mathrm{dom}\, T \subset \mathcal{N}_1 \to \mathcal{N}_2$ is the vector subspace $\mathcal{G}(T) = \{(\xi, T\xi) : \xi \in \mathrm{dom}\, T\}$ of $\mathcal{N}_1 \times \mathcal{N}_2$. The *graph norm* of T on dom T is $\|\xi\|_T := \left(\|T\xi\|^2 + \|\xi\|^2\right)^{1/2}$.

Definition 1.2.8. A linear operator $T : \mathrm{dom}\, T \subset \mathcal{N}_1 \to \mathcal{N}_2$ is *closed* if for all convergent sequences $(\xi_n) \subset \mathrm{dom}\, T$, $\xi_n \to \xi \in \mathcal{N}_1$, with $(T\xi_n) \subset \mathcal{N}_2$ also convergent, $T\xi_n \to \eta$, then $\xi \in \mathrm{dom}\, T$ and $\eta = T\xi$. In other words, T is closed iff $\mathcal{G}(T)$ is a closed subspace of $\mathcal{N}_1 \times \mathcal{N}_2$.

Exercise 1.2.9. a) Show that $\mathcal{B}_1 \times \mathcal{B}_2$ with the norm $\|(\xi, \eta)\|$ defined above is a Banach space. b) Show that T is a closed operator iff dom T with the graph norm is a Banach space.

Exercise 1.2.10. Verify that $\mathcal{G}(T)$ is a vector subspace of $\mathcal{N}_1 \times \mathcal{N}_2$ and the equivalence quoted in the above definition of closed operator.

Remark 1.2.11. Pay attention to the difference between a continuous and a closed operator: a linear operator T is continuous if for $\xi_n \to \xi$ in dom T, then necessarily $T\xi_n \to T\xi$, while for a closed operator it is asked that if both $(\xi_n) \subset$ dom T and $(T\xi_n)$ are convergent, then necessarily $\xi = \lim_n \xi_n$ belongs to dom T and $T\xi_n \to T\xi$.

Exercise 1.2.12. Consider the linear operator $T : \text{dom } T \subset \mathcal{N}_1 \to \mathcal{N}_2$, and let $\pi_1 : \mathcal{G}(T) \to \text{dom } T$ and $\pi_2 : \mathcal{G}(T) \to \text{rng } T$ be the natural projections $\pi_1(\xi, T\xi) = \xi$ and $\pi_2(\xi, T\xi) = T\xi$, for $\xi \in \text{dom } T$. Show that such projections are continuous linear operators.

It is important to give conditions to guarantee that closed operators are continuous, since the requirement for being closed is in general easier to verify; the closed graph theorem, presented below, says that such concepts are equivalent for linear operators between Banach spaces.

A first result in this direction appears in:

Proposition 1.2.13. *Any operator* $T \in \mathrm{B}(\mathcal{B}_1, \mathcal{B}_2)$ *is closed.*

Proof. Let $\xi_n \to \xi$ with $T\xi_n \to \eta$. Since $\xi \in \text{dom } T$ and T is continuous, then $T\xi_n \to T\xi = \eta$; thus T is closed. □

Exercise 1.2.14. If $\dim \mathcal{N}_1 < \infty$, show that every linear operator $T : \text{dom } T \subset \mathcal{N}_1 \to \mathcal{N}_2$ is closed.

Example 1.2.15 (Bounded and nonclosed). Let $\mathbf{1} : \text{dom } \mathbf{1} \to \mathcal{B}$, with dom $\mathbf{1}$ a proper dense subspace of $\mathcal{B}$, the identity operator $\mathbf{1}(\xi) = \xi$ for $\xi \in \text{dom } \mathbf{1}$; such operator is bounded. Let $(\xi_n) \subset \text{dom } \mathbf{1}$ with $\xi_n \to \xi \in \mathcal{B} \backslash \text{dom } \mathbf{1}$. Since $\xi_n \to \xi$ and $\mathbf{1}(\xi_n) \to \xi$, but $\xi \notin \text{dom } \mathbf{1}$, this operator is not closed. It is a rather artificial example, but it illustrates the difference between bounded and closed linear operators.

Exercise 1.2.16. If $\mathcal{N} \subset \mathcal{B}$, show that $T \in \mathrm{B}(\mathcal{N}, \mathcal{B})$ is closed if, and only if, $\mathcal{N}$ is a Banach space.

Remark 1.2.17. If $T \in \mathrm{B}(\mathcal{N}_1, \mathcal{B}_2)$ with $\mathcal{N}_1 \subset \mathcal{B}_1$, then its unique continuous linear extension $\overline{T} : \overline{\mathcal{N}_1} \to \mathcal{B}_2$ is a closed operator (Proposition 1.2.13). Then, every continuous linear operator is "basically" closed, and the artificiality in Example 1.2.15 is unavoidable.

Example 1.2.18 (Unbounded and closed). Let $C^1[0, \pi] \subset C[0, \pi]$ (both with the uniform convergence topology) be the subspace of continuously differentiable functions on $[0, \pi]$ and $D : C^1[0, \pi] \to C[0, \pi]$, $(D\psi)(t) = \psi'(t)$. D is not continuous, since the sequence $\psi_n(t) = \sin(nt)/n \to 0$, while $(D\psi_n)(t) = \cos(nt)$ does not converge uniformly to zero. However, this operator is closed. In fact, if $\psi_n \to \psi$ and $D\psi_n = \psi_n' \to \varphi$, then, as these limits are uniform,

$$\int_0^t \varphi(s)\,ds = \int_0^t \lim_{n\to\infty} \psi_n'(s)\,ds = \lim_{n\to\infty} \int_0^t \psi_n'(s)\,ds = \psi(t) - \psi(0).$$

Thus, $\psi \in \operatorname{dom} D = C^1[0,\pi]$ and $(D\psi)(t) = \varphi(t)$, $\forall t$, and D is closed.

Exercise 1.2.19. From Example 1.2.18, show that if $(\psi_j)_{j=1}^\infty \subset C^1[0,\pi]$ is such that the series $\psi(t) = \sum_{j=1}^\infty \psi_j(t)$ and $\varphi(t) = \sum_{j=1}^\infty \psi_j'(t)$ converge uniformly, then ψ is continuously differentiable and $\varphi = \psi'$.

Example 1.2.20 (Unbounded and nonclosed). Let dom T be the set of continuous functions in $\mathrm{L}^1[-1,1]$ and $(T\psi)(t) = \psi(0)$, $\forall t$, as element of $\mathrm{L}^1[-1,1]$. This operator is neither continuous nor closed, since $\psi_n(t) = e^{-|t|n} \to 0$ in $\mathrm{L}^1[-1,1]$, while $(T\psi_n)(t) = 1$, $\forall t$, for all n. Note that it has no closed extensions.

Theorem 1.2.21 (Closed Graph). *If $T : \mathcal{B}_1 \to \mathcal{B}_2$ is a linear operator, then T is continuous if, and only if, T is closed.*

Proof. One of the assertions of the closed graph theorem was already discussed; it is only needed to show that, under such conditions, if the linear operator T is closed, then it is bounded; the open mapping theorem will be used.

By hypotheses $\mathcal{G}(T)$ is closed in $\mathcal{B}_1 \times \mathcal{B}_2$, then $\mathcal{G}(T)$ is also a Banach space. The projection operators π_1 and π_2 (see Exercise 1.2.12) are both linear and continuous. Moreover, π_1 is a bijection between the Banach spaces $\mathcal{G}(T)$ and $\mathcal{B}_1$; thus, by the open mapping theorem, its inverse $\pi_1^{-1} : \mathcal{B}_1 \to \mathcal{G}(T)$ is continuous. Since T is the composition

$$T = \pi_2 \circ \pi_1^{-1},$$

it follows that it is a bounded operator. □

Example 1.2.22 (Unbounded and closed). It is essential that the operator range is a complete space. The operator $T^{-1} : \operatorname{rng} T \to l^1(\mathbb{N})$ in Exercise 1.2.3 has closed graph but is not continuous.

Remark 1.2.23. One could imagine that a linear operator is not closed because its domain was chosen too small, and by considering the closure $\overline{\mathcal{G}(T)}$ in $\mathcal{N}_1 \times \mathcal{N}_2$ a closed operator would result. This may not work, since $\overline{\mathcal{G}(T)}$ is not necessarily the graph of an operator; see Example 1.2.20 where the point $(0,1)$ belongs to $\overline{\mathcal{G}(T)}$, however it is not of the form $(0, S0)$ for any linear operator S.

Exercise 1.2.24. Let E be a subspace of $\mathcal{N}_1 \times \mathcal{N}_2$. Show that E is the graph of a linear operator if, and only if, E does not contain any element of the form $(0,\eta)$, with $\eta \neq 0$.

Definition 1.2.25.

(a) The linear operators T, for which $\overline{\mathcal{G}(T)}$ is the graph of a linear extension $\overline{T}$ of T, are called *closable operators* and $\overline{T}$ is the *closure* of T (see Proposition 1.2.27).

(b) If the operator $T : \text{dom}\, T \sqsubseteq \mathcal{N}_1 :\to \mathcal{N}_2$ is closed, a subspace $\mathcal{D} \subset \text{dom}\, T$ is called a *core* of T if $\overline{T|_{\mathcal{D}}} = T$, that is, if the closure of the restriction $T|_{\mathcal{D}}$ is T.

Exercise 1.2.26. Show that X is a core of the closed operator T iff $\{(\xi, T\xi) : \xi \in X\}$ is dense in $\mathcal{G}(T)$.

If the linear operator $T : \text{dom}\, T \subset \mathcal{N}_1 \to \mathcal{N}_2$ is closable, then

$$\mathcal{D} = \{\xi \in \mathcal{N}_1 : \exists (\xi_n) \subset \text{dom}\, T, \xi_n \to \xi \text{ and exists } \eta \in \mathcal{N}_2 \text{ with } T\xi_n \to \eta\}$$

is a subset of all closed extensions of T. Define $\text{dom}\, \tilde{T} = \mathcal{D}$ and, for $\xi \in \mathcal{D}$, $\tilde{T}\xi := \eta$, and note that, by construction, $\mathcal{G}(\tilde{T})$ is closed in $\mathcal{N}_1 \times \mathcal{N}_2$, and so $\tilde{T}$ is closed. Note also that $\mathcal{G}(\tilde{T}) = \overline{\mathcal{G}(T)}$. Therefore $\tilde{T}$ is the closure of T, that is, $\tilde{T} = \overline{T}$. In summary:

Proposition 1.2.27. *If $T : \text{dom}\, T \subset \mathcal{N}_1 \to \mathcal{N}_2$ is closable, then $\overline{\mathcal{G}(T)}$ is the graph of its closure $\overline{T}$, which is the smallest closed extension of T.*

Exercise 1.2.28. Show that T is a closed operator acting in $\mathcal{H}$ iff $\text{dom}\, T$ with the *graph inner product of* T, given by $\langle \eta, \xi \rangle_T := \langle T\eta, T\xi \rangle + \langle \eta, \xi \rangle$, is a Hilbert space. This inner product generates a graph norm (Definition 1.2.7) and the corresponding orthogonality will be denoted by $\perp_T$.

1.3 Compact Operators

The compact operators have some similarities with operators on finite-dimensional spaces and so the theory presents several technical simplifications. These operators are important in many applications, sometimes as integral operators, a historically important example of compact operator.

It is convenient to recall some definitions and properties – in the form of exercises – of metric spaces theory. A set A in the metric space (X, d) is *relatively compact*, or *precompact*, if its closure $\overline{A}$ is compact. A is *totally bounded* if, for all $\varepsilon > 0$, A is in the finite union of open balls in X with radii ε; so, any totally bounded set is also bounded.

Exercise 1.3.1. Show that if $A \subset (X, d)$ is precompact, then A is totally bounded and, so, bounded.

Exercise 1.3.2. If $A \subset (X, d)$ is totally bounded, show that, for all $\varepsilon > 0$, A is in the union of a finite number of open balls of radii ε centered at points of A. Conclude then that a totally bounded set is separable with the induced topology, that is, it contains a countable dense subset.

Lemma 1.3.3. *Any totally bounded subset of a complete metric space is precompact.*

Proof. Let A be a totally bounded set; then its closure is also totally bounded (from a cover of balls, the family of balls with the same centers but with double radii covers the closure of the set). Since this set is in a complete metric space, to show that its closure is compact it is enough to check that every sequence $(\xi_n) \subset \overline{A}$ has a Cauchy subsequence. Such a set being totally bounded, there is a subsequence $(\xi_{1,n})$ of (ξ_n) contained in an open ball of radius 1. In the same way, there exists a subsequence $(\xi_{2,n})$ of $(\xi_{1,n})$ contained in an open ball of radius $1/2$; it is possible to construct subsequences $(\xi_{k,n})_{n\geq 1}$ of $(\xi_{k-1,n})_{n\geq 1}$ contained in some open ball of radius $1/k$, for all $k \in \mathbb{N}$. To finish the proof note that $(\xi_{k,k})_{k\geq 1}$ is a Cauchy subsequence of the original sequence. □

Definition 1.3.4. A linear operator $T : \mathcal{N}_1 \to \mathcal{N}_2$ is *compact*, also called *completely continuous*, if the range $T(A)$, of any bounded set $A \subset \mathcal{N}_1$ is precompact in $\mathcal{N}_2$. The set of such compact operators will be denoted by $\mathrm{B}_0(\mathcal{N}_1, \mathcal{N}_2)$ (or $\mathrm{B}_0(\mathcal{N})$ in case $\mathcal{N}_1 = \mathcal{N}_2 = \mathcal{N}$).

Remark 1.3.5. Equivalently, $T : \mathcal{N}_1 \to \mathcal{N}_2$ linear is compact if $(T\xi_n)$ has a convergent subsequence in $\mathcal{N}_2$ for every bounded sequence $(\xi_n) \subset \mathcal{N}_1$. Verify this!

Exercise 1.3.6. If $\dim \mathcal{N} = \infty$, show that the identity operator $\mathbf{1} : \mathcal{N} \hookleftarrow$ is not compact (use, for instance, Riesz's Lemma 1.6.2).

Proposition 1.3.7. *Let $\mathcal{N}_1, \mathcal{N}_2$ be normed spaces and $T, S : \mathcal{N}_1 \to \mathcal{N}_2$ linear operators. Then:*

i) $\mathrm{B}_0(\mathcal{N}_1, \mathcal{N}_2)$ *is a vector subspace of* $\mathrm{B}(\mathcal{N}_1, \mathcal{N}_2)$.

ii) *If T is compact and S bounded, then TS and ST are compact operators* (*suppose all operations are well posed*).

Proof. i) Let $T \in \mathrm{B}_0(\mathcal{N}_1, \mathcal{N}_2)$; since $T(S(0; 1))$ is precompact, it is bounded. Thus, $T \in \mathrm{B}(\mathcal{N}_1, \mathcal{N}_2)$. The proof that $\mathrm{B}_0(\mathcal{N}_1, \mathcal{N}_2)$ is a vector subspace is left to the readers.

ii) If A is a bounded set, then $S(A)$ is also bounded and, so, $T(S(A))$ is precompact. Therefore, TS is compact.

Given a bounded set A, the range by T of any sequence $(\xi_n) \subset A$ has a convergent subsequence $(T\xi_{n_j})$, since T is compact. S being continuous, $(ST\xi_{n_j})$ is also convergent. Therefore, $ST(A)$ is precompact and ST is a compact operator. □

Remark 1.3.8. A map between metric spaces is *compact* if the range of bounded sets is precompact; the Dirichlet function $h : \mathbb{R} \to \mathbb{R}$, $h(t) = 1$ if $t \in \mathbb{Q}$ and $h(t) = 0$ otherwise, is compact, but not continuous in any point of its domain (cf. Proposition 1.3.7).

Important examples of compact operators are the finite-rank operators.

Definition 1.3.9. $T \in \mathrm{B}(\mathcal{N}_1, \mathcal{N}_2)$ is of *finite rank* if $\dim \operatorname{rng} T < \infty$. The vector space of finite rank operators between these spaces will be denoted by $\mathrm{B}_\mathrm{f}(\mathcal{N}_1, \mathcal{N}_2)$ (it will also be used the obvious notation $\mathrm{B}_\mathrm{f}(\mathcal{N})$).

Proposition 1.3.10. *All finite rank operators are compact. In particular $\mathcal{N}^* = \mathrm{B}_0(\mathcal{N}, \mathbb{F})$.*

Proof. Let $T \in \mathrm{B_f}(\mathcal{N}_1, \mathcal{N}_2)$ and $A \subset \mathcal{N}_1$ a bounded set. Since T is a bounded operator, $T(A)$ is bounded and its closure $\overline{T(A)}$ is a closed and bounded set and, in view of $\dim \operatorname{rng} T < \infty$, it follows that $\overline{T(A)}$ is a compact set. □

Lemma 1.3.11. *If* $T \in \mathrm{B_0}(\mathcal{N}_1, \mathcal{N}_2)$*, then* $T(\mathcal{N}_1)$ *is separable.*

Proof. Since $\mathcal{N}_1 = \bigcup_{j=1}^{\infty} B(0;j)$, then for $T : \mathcal{N}_1 \to \mathcal{N}_2$, $\operatorname{rng} T = \bigcup_{j=1}^{\infty} T(B(0;j))$. In order to conclude the lemma, it is sufficient to show that for each $j \in \mathbb{N}$ the set $TB(0;j)$ has a countable dense subset. If T is compact, $TB(0;j)$ is totally bounded; thus, for each $m \in \mathbb{N}$ it can be covered by a finite number of open balls of radii $1/m$, centered at points of $TB(0;j)$. The union of the centers of such open balls for all $m \in \mathbb{N}$ is a dense countable set of $TB(0;j)$. □

Exercise 1.3.12. Let $T : \mathcal{N}_1 \to \mathcal{N}_2$ linear. Show that it is compact if, and only if, $TB(0;1)$ is precompact in $\mathcal{N}_2$.

Theorem 1.3.13. $\mathrm{B_0}(\mathcal{N}, \mathcal{B})$ *is a closed subspace of* $\mathrm{B}(\mathcal{N}, \mathcal{B})$*; therefore,* $\mathrm{B_0}(\mathcal{N}, \mathcal{B})$ *is a Banach space.*

Proof. Let $(T_n) \subset \mathrm{B_0}(\mathcal{N}, \mathcal{B})$, with $T_n \to T$ in $\mathrm{B}(\mathcal{N}, \mathcal{B})$. It will be shown that for all $r > 0$ the set $TB(0;r)$ is totally bounded and, therefore, precompact by Lemma 1.3.3. From this it follows that T is also a compact operator.

Given $\varepsilon > 0$, there is n such that $\|T_n - T\| < \varepsilon/r$. Since T_n is compact, the set $T_nB(0;r)$ is totally bounded and, so, it is in the union of certain balls $B(T_n\xi_1;\varepsilon), B(T_n\xi_2;\varepsilon), \ldots, B(T_n\xi_m;\varepsilon)$, with $\xi_j \in B(0;r)$, for all $1 \le j \le m$. Hence, if $\xi \in B(0;r)$ there is one of these ξ_j such that $T_n\xi \in B(T_n\xi_j;\varepsilon)$. From this

$$\begin{aligned}\|T\xi - T\xi_j\| &\le \|T\xi - T_n\xi\| + \|T_n\xi - T_n\xi_j\| + \|T_n\xi_j - T\xi_j\| \\ &< \|T - T_n\|\|\xi\| + \varepsilon + \|T_n - T\|\|\xi_j\| \\ &< \frac{\varepsilon}{r}r + \varepsilon + \frac{\varepsilon}{r}r = 3\varepsilon,\end{aligned}$$

showing that $TB(0;r) \subset \bigcup_{j=1}^{m} B(T_n\xi_j;3\varepsilon)$. Therefore $TB(0;r)$ is totally bounded for all $r > 0$. □

Corollary 1.3.14. *If* $(T_n) \subset \mathrm{B_f}(\mathcal{N}, \mathcal{B})$ *and* $T_n \to T$ *in* $\mathrm{B}(\mathcal{N}, \mathcal{B})$*, then the operator* T *is compact.*

Proof. Combine Proposition 1.3.10 and Theorem 1.3.13. □

Recall that a sequence $(\xi_n) \subset \mathcal{N}$ *converges weakly* to $\xi \in \mathcal{N}$ if $\lim_{n\to\infty} f(\xi_n) = f(\xi)$ for all $f \in \mathcal{N}^*$, and that all weakly convergent sequences are bounded. $\xi_n \xrightarrow{\mathrm{w}} \xi$ and $\mathrm{w} - \lim \xi_n = \xi$ will be used to indicate that (ξ_n) converges weakly to ξ. The convergence of (ξ_n) to ξ in the norm of $\mathcal{N}$ will be called *strong convergence* and indicated by $\xi_n \to \xi$, $\xi_n \xrightarrow{\mathrm{s}} \xi$ and $\mathrm{s} - \lim \xi_n = \xi$.

There are also corresponding notions of convergence of a sequence (T_n) of bounded operators in $\mathrm{B}(\mathcal{N})$.

Definition 1.3.15. Let (T_n) be a sequence of operators in $B(\mathcal{N}_1, \mathcal{N}_2)$ and $T : \mathcal{N}_1 \to \mathcal{N}_2$ linear. One says that

a) T_n *converges uniformly*, or *in norm*, to T if

$$\|T_n - T\| \to 0.$$

The uniform convergence is denoted by $T_n \to T$ or $\lim_{n\to\infty} T_n = T$.

b) T_n *converges strongly* to T if

$$\|T_n\xi - T\xi\|_{\mathcal{N}_2} \to 0, \qquad \forall \xi \in \mathcal{N}_1.$$

The strong convergence of linear operators will be denoted by $T_n \xrightarrow{\text{s}} T$ or $\text{s} - \lim_{n\to\infty} T_n = T$.

c) T_n *converges weakly* to T if

$$|f(T_n\xi) - f(T\xi)| \to 0, \qquad \forall \xi \in \mathcal{N}_1,\ f \in \mathcal{N}_2^*.$$

The weak convergence of linear operators will be denoted by $T_n \xrightarrow{\text{w}} T$ or $\text{w} - \lim_{n\to\infty} T_n = T$.

Exercise 1.3.16. Show that in $B(\mathcal{N}_1, \mathcal{N}_2)$ the three kinds of limits defined above are well defined and unique (if they exist, of course). Moreover, verify that the uniform convergence $\Longrightarrow$ strong convergence $\Longrightarrow$ weak convergence, and with the same limits.

Example 1.3.17. Let $P_N : l^1(\mathbb{N}) \hookleftarrow$, $P_N\xi = (\xi_1, \xi_2, \dots, \xi_N, 0, 0, \dots)$, with $\xi = (\xi_1, \xi_2, \xi_3, \dots)$. Since $\|P_N\xi - \xi\| = \sum_{j=N+1}^{\infty} |\xi_j|$ it is found that $P_N \xrightarrow{\text{s}} \mathbf{1}$. On the other hand, $\|P_N\xi - \xi\| \le \|\xi\|$ and $\|P_N e_{(N+1)} - e_{(N+1)}\| = \|e_{(N+1)}\| = 1$, $\forall N$, and then (P_N) is not uniformly convergent ((e_j) is the canonical basis of $l^1(\mathbb{N})$). Adapt it to l^p, $1 < p < \infty$.

Exercise 1.3.18. Show that the sequence of operators $T_n : l^2(\mathbb{N}) \hookleftarrow$

$$T_n\xi = (\underbrace{0, 0, \dots, 0}_{n \text{ entries}}, \xi_{n+1}, \xi_{n+2}, \xi_{n+3}, \dots)$$

converges strongly to zero, but does not converge uniformly.

Exercise 1.3.19. Show that the sequence of operators $T_n : l^2(\mathbb{N}) \hookleftarrow$

$$T_n\xi = (\underbrace{0, 0, \dots, 0}_{n \text{ entries}}, \xi_1, \xi_2, \xi_3, \dots)$$

converges weakly to zero, but does not converge strongly.

As a reformulation of the Banach-Steinhaus theorem, one has (by using an obvious generalization of convergence of operators):

Proposition 1.3.20. *If (T_n) in $B(\mathcal{B}, \mathcal{N})$ converges strongly to the operator $T : \mathcal{B} \to \mathcal{N}$, then $T \in B(\mathcal{B}, \mathcal{N})$.*

Note that due to the Riesz representation Theorem 1.1.40, a sequence $(\xi_n) \subset \mathcal{H}$ converges weakly to ξ if, and only if,

$$\lim_{n\to\infty} \langle \eta, \xi_n \rangle = \langle \eta, \xi \rangle, \qquad \forall \eta \in \mathcal{H}.$$

Exercise 1.3.21. Show that every orthonormal sequence in a Hilbert space converges weakly to zero and has no strongly convergent subsequence.

Recall the Hilbert adjoint T^* of a bounded operator $T \in \mathrm{B}(\mathcal{H}_1, \mathcal{H}_2)$. It is the unique linear operator so that

$$\langle \xi, T\eta \rangle = \langle T^*\xi, \eta \rangle, \qquad \forall \xi \in \mathcal{H}_2, \eta \in \mathcal{H}_1.$$

Further, $T^* \in \mathrm{B}(\mathcal{H}_2, \mathcal{H}_1)$ and $\|T^*\| = \|T\|$. The bounded linear operator T is self-adjoint if $T^* = T$. See a generalization of the concept of adjoint to certain unbounded operators in Definition 2.1.2. Finally, recall that an operator $P \in \mathrm{B}(\mathcal{H})$ is an *orthogonal projection* if it is self-adjoint and $P^2 = P$, and it projects onto the closed subspace rng P.

Proposition 1.3.22. *Let $T \in \mathrm{B}_0(\mathcal{H}_1, \mathcal{H}_2)$. If $\xi_n \xrightarrow{w} \xi$ in $\mathcal{H}_1$, then $T\xi_n \to T\xi$, i.e., a compact operator takes weakly convergent sequences to strongly convergent ones (this result also holds in normed spaces).*

Proof. Suppose $\xi_n \xrightarrow{w} \xi$ in $\mathcal{H}_1$. If $\eta \in \mathcal{H}_2$,

$$\langle \eta, T\xi_n \rangle = \langle T^*\eta, \xi_n \rangle \to \langle T^*\eta, \xi \rangle = \langle \eta, T\xi \rangle,$$

showing that $T\xi_n \xrightarrow{w} T\xi$. If $T\xi_n$ does not converge strongly to $T\xi$, there exists $\varepsilon > 0$ and a subsequence $(T\xi_{n_j})$ with $\|T\xi_{n_j} - T\xi\| \geq \varepsilon$. Since T is a compact operator, $T\xi_{n_j}$ has the strongly convergent subsequence and, necessarily, it converges to $T\xi$. The contradiction with the above inequality proves the proposition. □

In a Hilbert space the closure (with the usual norm of $\mathrm{B}(\mathcal{H})$) of the vector space of finite-rank operators coincides with the set of compact operators; to show this the following technical result will be useful. Remember that a Hilbert space is separable iff it has a countable orthonormal basis.

Lemma 1.3.23. *If $T \in \mathrm{B}_0(\mathcal{H}_1, \mathcal{H}_2)$, then* rng T *and* $\mathrm{N}(T)^\perp$ *are separable vector spaces.*

Proof. rng T is separable by Lemma 1.3.11. Let $\{e_\alpha\}_{\alpha\in J}$ be an orthonormal basis of $\mathrm{N}(T)^\perp$. If J is finite the result is clear.

Suppose that J is not finite; the goal is to show that J is enumerable. Every sequence $(e_{\alpha_j})_{j=1}^\infty$ of pairwise distinct elements of $\{e_\alpha\}_{\alpha\in J}$ weakly converges to zero (Exercise 1.3.21) and, by Proposition 1.3.22, $Te_{\alpha_j} \to 0$, for $j \to \infty$. Thus, for each $n \in \mathbb{N}$ there exists only a finite number of $\alpha \in J$ with $\|Te_\alpha\| \geq 1/n$. Hence, J is enumerable, for

$$J = \bigcup_{n=1}^\infty \{\alpha : \|Te_\alpha\| \geq 1/n\}.$$

Recall that $Te_\alpha \neq 0$, $\forall \alpha \in J$, since $e_\alpha \in \mathrm{N}(T)^\perp$. □

Remark 1.3.24. If $T : \mathcal{H}_1 \to \mathcal{H}_2$ is a finite rank operator of rank $N < \infty$, then there exist vectors $\xi_1, \eta_1, \dots, \xi_N, \eta_N$ so that

$$T\xi = \sum_{j=1}^{N} \langle \eta_j, \xi \rangle \, \xi_j,$$

the so-called *canonical form* of T. Indeed, if $\{\xi_1, \dots, \xi_N\}$ is an orthonormal basis of rng T, then

$$T\xi = \sum_{j=1}^{N} \langle \xi_j, T\xi \rangle \, \xi_j = \sum_{j=1}^{N} \langle T^*\xi_j, \xi \rangle \, \xi_j;$$

now put $\eta_j = T^*\xi_j$.

Theorem 1.3.25. *An operator $T \in \mathrm{B}(\mathcal{H}_1, \mathcal{H}_2)$ is compact if, and only if, there is a sequence of finite rank operators $(T_n) \subset \mathrm{B_f}(\mathcal{H}_1, \mathcal{H}_2)$, which converges to T in $\mathrm{B}(\mathcal{H}_1, \mathcal{H}_2)$.*

Proof. If T is the limit of finite-rank operators, then T is compact by Corollary 1.3.14. Let $T \in \mathrm{B}_0(\mathcal{H}_1, \mathcal{H}_2)$ and P the orthogonal projection on $\mathrm{N}(T)^\perp$, so that $T = TP$. If $\dim \mathrm{N}(T)^\perp < \infty$ the result is clear; suppose then that $\dim \mathrm{N}(T)^\perp = \infty$ and pick an orthonormal basis $(e_j)_{j=1}^\infty$ of $\mathrm{N}(T)^\perp$, which is enumerable by Lemma 1.3.23. Denote by P_n the orthogonal projection on $\mathrm{Lin}(\{e_1, \dots, e_n\})$. Thus, the operator $T_n = TP_n$ has finite rank. It will be shown that $T_n \to T$.

For each n there exists $\xi_n \in \mathcal{H}_1$, $\|\xi_n\| = 1$, with

$$\frac{1}{2}\|T - T_n\| \leq \|(T - T_n)\xi_n\| = \|T(P - P_n)\xi_n\|.$$

Since $(P_n - P) \xrightarrow{\mathrm{s}} 0$ and for all $\eta \in \mathcal{H}_1$,

$$|\langle \eta, (P - P_n)\xi_n \rangle| = |\langle (P - P_n)\eta, \xi_n \rangle| \leq \|(P - P_n)\eta\|,$$

then $(P - P_n)\xi_n \xrightarrow{\mathrm{w}} 0$. Since T is a compact operator, by Proposition 1.3.22 it follows that $T(P - P_n)\xi_n \to 0$ and, by the inequality above, it is found that $\|T - T_n\| \to 0$. □

Exercise 1.3.26. Let $T \in \mathrm{B}(\mathcal{H})$, with $\mathcal{H}$ separable. Show that there is a sequence (T_n) of finite rank operators which converges strongly to T, that is, $T_n \xrightarrow{\mathrm{s}} T$.

Corollary 1.3.27. *Let $T \in \mathrm{B}(\mathcal{H}_1, \mathcal{H}_2)$. Then T is compact if, and only if, its Hilbert adjoint T^* is compact.*

Proof. T is compact if, and only if, there exists a sequence $(T_n) \subset \mathrm{B_f}(\mathcal{H}_1, \mathcal{H}_2)$ so that $T_n \to T$. Since T_n^* has also finite rank and $\|T^* - T_n^*\| = \|(T - T_n)^*\| = \|T - T_n\|$, one concludes that T is compact if, and only if, T^* is compact. □

Proposition 1.3.28. *Let T be an operator in* $\mathrm{B}(\mathcal{H})$*. Then T is compact if, and only if, $(T\xi_n)$ is convergent in $\mathcal{H}$ for all weakly convergent sequences (ξ_n).*

Proof. If $\dim\mathcal{H} < \infty$ the proof is quite simple. Suppose that $\dim\mathcal{H} = \infty$. Taking into account the hypotheses and Proposition 1.3.22, it is enough to show that for each bounded sequence (ξ_n) in $\mathcal{H}$ the sequence $(T\xi_n)$ has a convergent subsequence. Since in a Hilbert space any bounded set has a weakly convergent sequence, (ξ_n) has a weakly convergent subsequence (ξ_{n_j}); by hypothesis, $(T\xi_{n_j})$ is convergent. Thus, the image of every bounded sequence admits a convergent subsequence, and so, T is a compact operator. □

Proposition 1.3.29. *Let $S_n, S \in \mathrm{B}(\mathcal{H})$ with $S_n \xrightarrow{\mathrm{s}} S$. If T is a compact operator, then $TS_n \to TS$ and $S_nT \to ST$ in the norm of* $\mathrm{B}(\mathcal{H})$*.*

Proof. By considering $S_n - S$ it is possible to suppose that $S = 0$. Since $\|T^*S_n^*\| = \|S_nT\|$, by Corollary 1.3.27, it is enough to prove that $S_nT \to 0$ uniformly. For each $\varepsilon > 0$ there is an operator $F_\varepsilon \in \mathrm{B_f}(\mathcal{H})$ so that $T = T_\varepsilon + F_\varepsilon$, and $\|T_\varepsilon\| < \varepsilon$. The last preparatory remark is that there exists $M > 0$ so that $\sup_n \|S_n\| \le M$, a consequence of the Banach-Steinhaus theorem.

In view of

$$\begin{aligned}\|S_nT\| &\le \|S_n(F_\varepsilon + T_\varepsilon)\|\\ &\le \|S_nF_\varepsilon\| + \|T_\varepsilon\|\,\|S_n\|\\ &\le \|S_nF_\varepsilon\| + \varepsilon\, M,\end{aligned}$$

it is sufficient to prove that $\|S_nF_\varepsilon\| \le \varepsilon$ if n is large enough.

Write $F_\varepsilon(\cdot) = \sum_{j=1}^k \langle \eta_j, \cdot\rangle \xi_j$, $\eta_j \ne 0$. If $\xi \in \mathcal{H}$ with $\|\xi\| = 1$ one has

$$\|S_nF_\varepsilon\xi\| \le \sum_{j=1}^k |\langle \eta_j, \xi\rangle|\,\|S_n\xi_j\| \le \sum_{j=1}^k \|\eta_j\|\,\|S_n\xi_j\|$$

and since $S_n \xrightarrow{\mathrm{s}} 0$ if n is large $\|S_n\xi_j\| < \varepsilon/(\|\eta_j\|k)$, $1 \le j \le k$. Thus, as required, $\|S_nF_\varepsilon\| \le \varepsilon$ for n large enough. Thereby the proof of the proposition is complete. □

Example 1.3.30. Let $K : Q \to \mathbb{F}$ be continuous, with $Q = [a,b] \times [a,b]$. Then the integral operator $T_K : \mathrm{L}^2[a,b] \hookleftarrow$ given by

$$(T_K\psi)(t) = \int_a^b K(t,s)\psi(s)\, ds, \qquad \psi \in \mathrm{L}^2[a,b],$$

is compact.

Proof. For each $t \in [a,b]$ the function $s \mapsto K(t,s)$ is an element of $\mathrm{L}^2[a,b]$. Let $\psi \in B(0;R) \subset \mathrm{L}^2[a,b]$ and $M = \max_{(t,s)\in Q} |K(t,s)|$. For all $t \in [a,b]$ one has

$$\begin{aligned}|(T_K\psi)(t)| &\leq \int_a^b |K(t,s)||\psi(s)|\,ds \\ &\leq \left(\int_a^b |K(t,s)|^2\,ds\right)^{\frac{1}{2}} \|\psi\|_2 \leq M\sqrt{b-a}R,\end{aligned}$$

and $T_K B(0;R)$ is a bounded set. This set is also equicontinuous, since for $\psi \in B(0;R)$,

$$|(T_K\psi)(t) - (T_K\psi)(r)| \leq \|K(t,\cdot) - K(r,\cdot)\|_2\|\psi\|_2 \leq \varepsilon\sqrt{b-a}R,$$

if $|t-r| < \delta$. Hence, by the Ascoli theorem, $T_K B(0;R)$ is precompact in $(C[a,b], \|\cdot\|_\infty)$. Since $\|\phi\|_2 \leq \sqrt{b-a}\|\phi\|_\infty$, for all continuous ϕ (especially for $\phi = T_K\psi$), then $T_K B(0;R)$ is precompact in $\mathrm{L}^2[a,b]$. □

Exercise 1.3.31. Show that a precompact set (compact) in $(C[a,b], \|\cdot\|_\infty)$ is precompact (compact) in $\mathrm{L}^2[a,b]$. This occurs because the identity map $\mathbf{1} : (C[a,b], \|\cdot\|_\infty) \to \mathrm{L}^2[a,b]$ is continuous.

Example 1.3.32. Let $K \in \mathrm{L}^2(Q)$, with $Q = [a,b]\times[a,b]$. Then the integral operator $T_K : \mathrm{L}^2[a,b] \hookleftarrow$ given by $(T_K\psi)(t) = \int_a^b K(t,s)\psi(s)ds$, for $\psi \in \mathrm{L}^2[a,b]$, is compact.

Proof. Since the set of continuous functions on Q is dense in $\mathrm{L}^2(Q)$, there exists a sequence $K_n : Q \to \mathbb{F}$ of continuous functions so that $\|K - K_n\|_{\mathrm{L}^2(Q)} \to 0$. Thus, by defining $T_n : \mathrm{L}^2[a,b] \hookleftarrow$,

$$(T_n\psi)(t) = \int_a^b K_n(t,s)\psi(s)\,ds, \qquad \psi \in \mathrm{L}^2[a,b],$$

and using estimates similarly to those in preceding examples, one obtains $\|T_n\psi - T_K\psi\|_2 \leq \|K_n - K\|_{\mathrm{L}^2(Q)}\|\psi\|_2$, and $\|T_n - T_K\| \leq \|K_n - K\|_{\mathrm{L}^2(Q)}$, which vanishes as $n \to \infty$. By Example 1.3.30 each T_n is a compact operator, and so T_K is compact (Theorem 1.3.13). □

1.4 Hilbert-Schmidt Operators

One of the most important classes of compact operators on Hilbert spaces is constituted by the Hilbert-Schmidt operators, discussed in this section. Sometimes the shortest way to show that an operator on a Hilbert space is compact is to verify that it is Hilbert-Schmidt.

Definition 1.4.1. An operator $T \in \mathrm{B}(\mathcal{H}_1, \mathcal{H}_2)$ is *Hilbert-Schmidt* if there is an orthonormal basis $\{e_j\}_{j\in J}$ of $\mathcal{H}_1$ with

$$\|T\|_{\mathrm{HS}} := \left(\sum_{j\in J} \|Te_j\|^2\right)^{\frac{1}{2}} < \infty.$$

The set of Hilbert-Schmidt operators between such Hilbert spaces will be denoted by $\mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$ or, briefly, by $\mathrm{HS}(\mathcal{H})$ if $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}$.

Proposition 1.4.2. *Let $T \in \mathrm{B}(\mathcal{H}_1, \mathcal{H}_2)$. Then*

i) $\|T\|_{\mathrm{HS}}$ *does not depend on the orthonormal basis considered.*
ii) $T \in \mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$ *if, and only if, its adjoint $T^* \in \mathrm{HS}(\mathcal{H}_2, \mathcal{H}_1)$. Furthermore,* $\|T\|_{\mathrm{HS}} = \|T^*\|_{\mathrm{HS}}$.

Proof. If $\{e_j\}_{j\in J}$ and $\{f_k\}_{k\in K}$ are orthonormal bases of $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, then, by Parseval,

$$\sum_{j\in J} \|Te_j\|^2 = \sum_{\substack{j\in J\\ k\in K}} |\langle Te_j, f_k\rangle|^2 = \sum_{\substack{j\in J\\ k\in K}} |\langle e_j, T^* f_k\rangle|^2 = \sum_{k\in K} \|T^* f_k\|^2.$$

Since such orthonormal bases are arbitrary $\|T\|_{\mathrm{HS}} = \|T^*\|_{\mathrm{HS}}$, and such values do not depend on the orthonormal bases considered. □

Corollary 1.4.3. *Let S, T be bounded operators between two Hilbert spaces. If one of them is Hilbert-Schmidt, then the product TS is also Hilbert-Schmidt (assuming the product is defined).*

Proof. If S is Hilbert-Schmidt, then for any orthonormal basis $\{e_j\}_{j\in J}$ of its domain

$$\|TS\|_{\mathrm{HS}}^2 = \sum_{j\in J} \|TSe_j\|^2 \le \|T\|^2 \sum_{j\in J} \|Se_j\|^2 = \|T\|^2 \|S\|_{\mathrm{HS}}^2,$$

and TS is Hilbert-Schmidt.

If the operator T is Hilbert-Schmidt, then by Proposition 1.4.2, one has that S^*T^* is Hilbert-Schmidt. Since $TS = (S^*T^*)^*$, then TS is Hilbert-Schmidt. □

Theorem 1.4.4. $\mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$ *is a vector subspace of* $\mathrm{B}(\mathcal{H}_1, \mathcal{H}_2)$*, it is a Hilbert space with the norm $\|\cdot\|_{\mathrm{HS}}$, which is called Hilbert-Schmidt norm, and it is induced by the (Hilbert-Schmidt) inner product*

$$\langle T, S\rangle_{\mathrm{HS}} := \sum_{j\in J} \langle Te_j, Se_j\rangle, \qquad T, S \in \mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2),$$

with $\{e_j\}_{j\in J}$ being any orthonormal basis of $\mathcal{H}_1$. Furthermore, the inequality $\|T\| \le \|T\|_{\mathrm{HS}}$ holds.

Proof. If $T, S \in \mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$, then for any orthonormal basis $\{e_j\}_{j\in J}$ of $\mathcal{H}_1$ and all $\alpha \in \mathbb{F}$ one has (by Cauchy-Schwarz applied to the inner product $\sum_{j\in J} \|Te_j\|\|Se_j\|$ in l^2)

$$\begin{aligned}\|T + \alpha S\|_{\mathrm{HS}}^2 &\le \sum_{j\in J} \|Te_j\|^2 + |\alpha|^2 \sum_{j\in J} \|Se_j\|^2 + 2|\alpha| \sum_{j\in J} \|Te_j\|\|Se_j\| \\ &\le (\|T\|_{\mathrm{HS}} + |\alpha|\,\|S\|_{\mathrm{HS}})^2 ,\end{aligned}$$

and so $\mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$ is a vector space. From the same inequality it follows that $\|\cdot\|_{\mathrm{HS}}$ is a norm.

Now it will be verified that $\langle T, S\rangle_{\mathrm{HS}}$ is well posed and is independent of the orthonormal basis considered. By Cauchy-Schwarz

$$\begin{aligned}\sum_{j\in J} |\langle Te_j, Se_j\rangle| &\le \sum_{j\in J} \|Te_j\|\|Se_j\| \\ &\le \left(\sum_{j\in J} \|Te_j\|^2\right)^{\frac{1}{2}} \left(\sum_{j\in J} \|Se_j\|^2\right)^{\frac{1}{2}} \\ &= \|T\|_{\mathrm{HS}}\,\|S\|_{\mathrm{HS}},\end{aligned}$$

(note that this corresponds to $|\langle T, S\rangle_{\mathrm{HS}}| \le \|T\|_{\mathrm{HS}}\|S\|_{\mathrm{HS}}$) and the series defining $\langle T, S\rangle_{\mathrm{HS}}$ converges absolutely. By the polarization identity (or similarly to the proof of Proposition 1.4.2) it is found that

$$\sum_j \langle Te_j, Se_j\rangle = \sum_k \langle S^* f_k, T^* f_k\rangle,$$

for any orthonormal basis $\{f_k\}$ of $\mathcal{H}_2$; so $\langle T, S\rangle_{\mathrm{HS}}$ is independent of the orthonormal basis and, therefore, well posed. The properties of inner product are simple and left to the reader.

If $\xi \in \mathcal{H}_1$, $\|\xi\| = 1$, pick an orthonormal basis of $\mathcal{H}_1$ of the following form $\{\xi, \eta_l\}_l$. Thus, $\|T\xi\|^2 \le \sum_l \|T\eta_l\|^2 + \|T\xi\|^2 = \|T\|_{\mathrm{HS}}^2$, and so $\|T\| \le \|T\|_{\mathrm{HS}}$.

We only need to show that $\mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$ is complete; for this, consider a Cauchy sequence $(T_n) \subset \mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$. From the inequality $\|\cdot\|_{\mathrm{B}(\mathcal{H}_1,\mathcal{H}_2)} \le \|\cdot\|_{\mathrm{HS}}$ it is found that (T_n) is Cauchy in $\mathrm{B}(\mathcal{H}_1, \mathcal{H}_2)$ and, therefore, it converges to some $T \in \mathrm{B}(\mathcal{H}_1, \mathcal{H}_2)$. It will be shown that $T \in \mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$ and that $T_n \to T$ in this space.

For $\varepsilon > 0$, there exists $N(\varepsilon)$ with $\|T_n - T_m\|_{\mathrm{HS}}^2 < \varepsilon$ if $n, m \ge N(\varepsilon)$. Consider an orthonormal basis $\{e_j\}_{j\in J}$ of $\mathcal{H}_1$. If $F \subset J$ is finite,

$$\sum_{j\in F} \|T_n e_j - T_m e_j\|^2 \le \|T_n - T_m\|_{\mathrm{HS}}^2 < \varepsilon.$$

Taking $m \to \infty$ one obtains $\sum_{j\in F} \|(T_n - T)e_j\|^2 \le \varepsilon$, for all finite subsets F. Therefore, $\|T_n - T\|_{\mathrm{HS}}^2 = \sum_{j\in J} \|(T_n - T)e_j\|^2 \le \varepsilon$, so that $(T - T_n) \in \mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$

and $(T_n - T) \to 0$ in this space. Since $\mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$ is a vector space, then $T = (T - T_n) + T_n$ belongs to $\mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$, and this space is Hilbert. $\square$

Exercise 1.4.5. Show that $\|\cdot\|_{\mathrm{HS}}$ is a norm and that $\|TS\|_{\mathrm{HS}} \le \|T\|_{\mathrm{HS}}\|S\|_{\mathrm{HS}}$.

At this point all the tools necessary to verify that Hilbert-Schmidt operators are compact are available.

Theorem 1.4.6. $\mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2) \subset \mathrm{B}_0(\mathcal{H}_1, \mathcal{H}_2)$.

Proof. Let $T \in \mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$ and $(\xi_n) \subset \mathcal{H}_1$, with $\xi_n \xrightarrow{\mathrm{w}} \xi$. By Proposition 1.3.28, in order to show that T is compact it is sufficient to verify that $T\xi_n \to T\xi$. Note that, by linearity, it is sufficient to consider the case $\xi_n \xrightarrow{\mathrm{w}} 0$.

Let $\{e_j\}_{j\in J}$ be an orthonormal basis of $\mathcal{H}_2$. For each n it is known that the set $\{j \in J : \langle e_j, T\xi_n\rangle \ne 0\}$ is countable (if it is finite for all n the argument ahead is easily adapted) and, for notational simplicity, it will be denoted by the natural numbers. Thus,

$$\|T\xi_n\|^2 = \sum_{j=1}^{\infty} |\langle e_j, T\xi_n\rangle|^2 \le \sum_{j=1}^{N} |\langle T^* e_j, \xi_n\rangle|^2 + M \sum_{j=N+1}^{\infty} \|T^* e_j\|^2,$$

with $M = \sup_{n\in\mathbb{N}} \|\xi_n\|^2$ (M is finite since every weakly convergent sequence is bounded).

For $\varepsilon > 0$, pick N with $\sum_{j=N+1}^{\infty} \|T^* e_j\|^2 < \varepsilon/M$, which exists since $T^* \in \mathrm{HS}(\mathcal{H}_2, \mathcal{H}_1)$. Now, in view of $\xi_n \xrightarrow{\mathrm{w}} 0$, there exists K so that $\sum_{j=1}^{N} |\langle T^* e_j, \xi_n\rangle|^2 < \varepsilon$ if $n \ge K$. Thus, if $n \ge K$ one has $\|T\xi_n\|^2 < 2\varepsilon$, and one concludes that $T\xi_n \to 0$. $\square$

Exercise 1.4.7. Let $T : l^2(\mathbb{N}) \hookleftarrow$ given by $(T\xi)_n = \sum_{j=1}^{\infty} a_{nj}\xi_j$, $n \in \mathbb{N}$, with $(a_{nj})_{n,j\in\mathbb{N}}$ an infinite matrix with $\sum_{n,j\in\mathbb{N}} |a_{nj}|^2 < \infty$. Show that T is a Hilbert-Schmidt operator and find its Hilbert-Schmidt norm.

The next lemma will be used in the important example ahead.

Lemma 1.4.8. *Let $\mathcal{H}_1 = \mathrm{L}^2_\mu(\Omega)$ and $\mathcal{H}_2 = \mathrm{L}^2_\nu(\Lambda)$ be separable spaces, with μ, ν σ-finite measures, and $\mathcal{H}_3 = \mathrm{L}^2_{\mu\times\nu}(\Omega \times \Lambda)$. Then, if (ψ_n) and (ϕ_j) are (countable) orthonormal bases of $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, then $(\overline{\psi_n}\phi_j)$ is an orthonormal basis of $\mathcal{H}_3$, which is also separable.*

Proof. By Fubini $(\overline{\psi_n}\phi_j)$ is an orthonormal set of $\mathcal{H}_3$. In order to prove this lemma it is enough to show that if $f \in \mathcal{H}_3$ satisfies $\langle f, \overline{\psi_n}\phi_j\rangle_{\mathcal{H}_3} = 0$, $\forall n, j$, then $f = 0$. For each $s \in \Lambda$, denote the function sector $f^s : \Omega \to \mathbb{F}$ by $f^s(t) = f(t, s)$, which belongs to $\mathcal{H}_1$ for s in a set of total measure ν, and for each n the function $F_n(s) = \langle \overline{f^s}, \psi_n\rangle_{\mathcal{H}_1}$ (it is measurable since ν is $\sigma-$finite), then $\langle f, \overline{\psi_n}\phi_j\rangle_{\mathcal{H}_3} = \langle F_n, \phi_j\rangle_{\mathcal{H}_2}$. Note that by Cauchy-Schwarz $\nu-$a.e. one has $|F_n(s)| \le \|f^s\|_{\mathcal{H}_1}$, so that $F_n \in \mathcal{H}_2$ for all n, in view of $\|F_n\|^2_{\mathcal{H}_2} \le \int_\Lambda \|f^s\|^2_{\mathcal{H}_1}\, d\nu(s) = \|f\|^2_{\mathcal{H}_3}$.

Thus, one obtains the condition $\langle F_n, \phi_j\rangle_{\mathcal{H}_2} = 0$, $\forall n, j$; since (ϕ_j) is a basis of $\mathcal{H}_2$, for all n one has $F_n(s) = 0$ ν-a.e. and, therefore, since (ψ_n) is a basis of $\mathcal{H}_1$, one finds that $f^s = 0$ (in $\mathcal{H}_1$) ν-a.e. Then the result $\|f\|_{\mathcal{H}_3} = 0$ follows. □

Example 1.4.9. Let $\mathcal{H}_1$, $\mathcal{H}_2$ and $\mathcal{H}_3$ be as in Lemma 1.4.8. Then, the operator $T \in \mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$ if, and only if, there exits $K \in \mathcal{H}_3$ so that

$$(T\psi)(t) = (T_K\psi)(t) := \int_\Omega K(t,s)\psi(s)d\mu(s), \qquad \psi \in \mathcal{H}_1.$$

Furthermore, $\|T\|_{\mathrm{HS}} = \|K\|_{\mathcal{H}_3}$.

Proof. If (ψ_n) and (ϕ_j) are orthonormal bases of $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, then, by Lemma 1.4.8, $(\overline{\psi_n}\phi_j)$ is an orthonormal basis of $\mathcal{H}_3$. Suppose that $T = T_K$; then

$$\sum_n \|T_K\psi_n\|^2_{\mathcal{H}_2} = \sum_{n,j} |\langle T_K\psi_n, \phi_j\rangle_{\mathcal{H}_2}|^2 = \sum_{n,j} |\langle K, \overline{\psi_n}\phi_j\rangle_{\mathcal{H}_3}|^2 = \|K\|^2_{\mathcal{H}_3},$$

and so $T_K \in \mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$ and $\|T_K\|_{\mathrm{HS}} = \|K\|_{\mathcal{H}_3}$.

Pick $T \in \mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$. By using the above notation, one has

$$\sum_{n,j} |\langle \phi_j, T\psi_n\rangle_{\mathcal{H}_2}|^2 = \sum_n \|T\psi_n\|^2 = \|T\|^2_{\mathrm{HS}} < \infty,$$

consequently the function $K_0(t,s) = \sum_{n,j}\langle \phi_j, T\psi_n\rangle_{\mathcal{H}_2}\overline{\psi_n(s)}\phi_j(t)$ is well defined in the space $\mathcal{H}_3$; note that $\|K_0\|_{\mathcal{H}_3} = \|T\|_{\mathrm{HS}}$. It will be shown that $T = T_{K_0}$.

If $\psi \in \mathcal{H}_1$ and $\phi \in \mathcal{H}_2$, since T is bounded and the inner product is continuous,

$$\begin{aligned}
\langle \phi, T_{K_0}\psi\rangle_{\mathcal{H}_2} &= \int_\Lambda d\nu(t)\left(\overline{\phi(t)}\int_\Omega K_0(t,s)\psi(s)d\mu(s)\right)\\
&= \langle \phi\overline{\psi}, K_0\rangle_{\mathcal{H}_3} = \sum_{n,j}\langle \phi_j, T\psi_n\rangle_{\mathcal{H}_2}\langle \phi\overline{\psi}, \phi_j\overline{\psi_n}\rangle_{\mathcal{H}_3}\\
&= \sum_{n,j}\langle \phi_j, T\psi_n\rangle_{\mathcal{H}_2}\langle \phi, \phi_j\rangle_{\mathcal{H}_2}\langle \psi_n, \psi\rangle_{\mathcal{H}_1}\\
&= \left\langle \sum_j \langle \phi_j, \phi\rangle_{\mathcal{H}_2}\phi_j, \sum_n \langle \psi_n, \psi\rangle_{\mathcal{H}_1} T\psi_n\right\rangle_{\mathcal{H}_2}\\
&= \left\langle \phi, \sum_n \langle \psi_n, \psi\rangle_{\mathcal{H}_1} T\psi_n\right\rangle_{\mathcal{H}_2} = \left\langle \phi, T\sum_n \langle \psi_n, \psi\rangle_{\mathcal{H}_1}\psi_n\right\rangle_{\mathcal{H}_2}\\
&= \langle \phi, T\psi\rangle_{\mathcal{H}_2}.
\end{aligned}$$

Therefore, $T = T_{K_0}$. □

Remark 1.4.10. There is a family of compact operators in $\mathrm{B}(\mathcal{H})$ for each $1 \le p < \infty$, with certain norm $\|T\|_p < \infty$ (this norm is based on that of l^p); the Hilbert-Schmidt operators are obtained through $p = 2$. The case $p = 1$, discussed in Subsection 9.4.1, is important in mathematical physics, particularly in statistical mechanics and scattering theory, and such operators are called *trace class* ($\|T\|_1$ is a generalization of the trace of the absolute values of the entries of a matrix).

Exercise 1.4.11. Show that $\mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$ is the closure of the set of finite rank operators with the norm $\|\cdot\|_{\mathrm{HS}}$.

Exercise 1.4.12. Fix $\eta \in \mathcal{H}$ with $\|\eta\| = 1$. Let $T_\eta : \mathcal{H} \to \mathcal{H}$ be defined by $T_\eta \xi = \langle \eta, \xi \rangle\, \eta$, $\xi \in \mathcal{H}$. Show that T_η is a linear Hilbert-Schmidt operator and find its norm $\|T\|_{\mathrm{HS}}$.

Exercise 1.4.13. Let $\mathcal{H}$ be separable and $T \in \mathrm{B}(\mathcal{H})$ an operator whose eigenvectors form an orthonormal basis (ξ_j) of $\mathcal{H}$, that is, for all j, $T\xi_j = \lambda_j \xi_j$, $\lambda_j \in \mathbb{F}$. Present conditions for $T \in \mathrm{HS}(\mathcal{H})$. Verify that on infinite-dimensional Hilbert spaces there always are compact operators that are not Hilbert-Schmidt.

Exercise 1.4.14. Are there sequences $(T_n) \subset \mathrm{HS}(\mathcal{H})$ that converge in $\mathrm{B}(\mathcal{H})$ but do not converge in $\mathrm{HS}(\mathcal{H})$?

1.5 The spectrum

Intuitively, the spectrum of a linear operator comprises of "the values in $\mathbb{C}$ this operator assumes;" the very definition of spectrum justifies this interpretation. The spectrum is a generalization of the set of eigenvalues of linear operators. The point is that, for a linear operator acting on a finite-dimensional space, the property of being injective is equivalent to being surjective; however, in infinite dimensions such properties are not equivalent and the definition of spectrum must be properly generalized. From now on, vector spaces are assumed complex.

The spectral question is directly related to the solvability and uniqueness of solutions of linear equations in Banach spaces, boundary problems, approximations of nonlinear problems by linear versions, stability and, in an essential way, to the mathematical apparatus of quantum mechanics.

Definition 1.5.1. Let $T : \mathrm{dom}\, T \subset \mathcal{B} \to \mathcal{B}$ be linear in the complex Banach space $\mathcal{B} \neq \{0\}$. The *resolvent set* of T, denoted by $\rho(T)$, is the set of $\lambda \in \mathbb{C}$ for which the *resolvent operator* of T at λ,

$$R_\lambda(T) : \mathcal{B} \to \mathrm{dom}\, T, \qquad R_\lambda(T) := (T - \lambda \mathbf{1})^{-1},$$

exists and is bounded, i.e., $R_\lambda(T)$ belongs to $\mathrm{B}(\mathcal{B})$.

Definition 1.5.2. The *spectrum* of T is the set $\sigma(T) = \mathbb{C} \backslash \rho(T)$.

Remark 1.5.3. a) If $T \in \mathrm{B}(\mathcal{B})$ and $(T - \lambda \mathbf{1})$ is one-to-one with range $\mathcal{B}$, then, by the Open Mapping Theorem 1.2.6, $R_\lambda(T) \in \mathrm{B}(\mathcal{B})$ and $\lambda \in \rho(T)$.

b) Every eigenvalue λ of T (i.e., there is an eigenvector $\xi \neq 0$ with $T\xi = \lambda\xi$) belongs to the spectrum of T, for $(T - \lambda\mathbf{1})$ is not invertible in this case.
c) Notation: if it is clear which operator T is involved, $R_\lambda = R_\lambda(T)$.

The definition of spectrum is not restricted to the real numbers in order to be nonempty for continuous operators (see Corollary 1.5.17). For example, if $\dim \mathcal{B} < \infty$, the spectrum is the set of its eigenvalues, but the rotation by a right angle operator on $\mathbb{R}^2$ has no real eigenvalue (check this!).

Exercise 1.5.4. Let $T : \mathcal{B} \hookleftarrow$ be linear with $\dim \mathcal{B} < \infty$. Show that $\sigma(T)$ is the set of eigenvalues of T and, by the fundamental theorem of algebra, conclude that $\sigma(T) \neq \emptyset$ in this case.

Exercise 1.5.5. Let $T : \mathrm{dom}\, T \subset \mathcal{B} \to \mathcal{B}$ be linear. Show that the eigenvectors $\{\xi_j\}_{j\in J}$ of T, corresponding to pairwise distinct eigenvalues $\{\lambda_j\}_{j\in J}$, form a linearly independent set of $\mathrm{dom}\, T$.

Proposition 1.5.6. *If $\sigma(T) \neq \mathbb{C}$, then T is a closed operator.*

Proof. Pick $\lambda_0 \in \rho(T)$; so $R_{\lambda_0}(T) \in \mathrm{B}(\mathcal{B})$. If $(\xi_n) \subset \mathrm{dom}\, T$ with $\xi_n \to \xi$ and $T\xi_n \to \eta$, then

$$R_{\lambda_0}(T)(\eta - \lambda_0\xi) = \lim_{n\to\infty} R_{\lambda_0}(T)(T\xi_n - \lambda_0\xi_n) = \lim_{n\to\infty} \xi_n = \xi;$$

hence $\xi \in \mathrm{dom}\, T$ and

$$\eta - \lambda_0\xi = (T - \lambda_0\mathbf{1})R_{\lambda_0}(T)(\eta - \lambda_0\xi) = (T - \lambda_0\mathbf{1})\xi.$$

Therefore $T\xi = \eta$ and T is closed. □

The converse of Proposition 1.5.6 may not hold:

Example 1.5.7. Let $D : \mathrm{dom}\, D = C^1[0,1] \subset C[0,1] \to C[0,1]$ and $(D\psi)(t) = \psi'(t)$, which is a closed and unbounded operator. If $\lambda \in \mathbb{C}$, the function $\psi_\lambda(t) = e^{\lambda t} \in \mathrm{dom}\, D$ and $D\psi_\lambda = \lambda\psi_\lambda$, showing that $\sigma(D) = \mathbb{C}$ and it is constituted exclusively of eigenvalues. Therefore $\rho(D) = \emptyset$.

Given an operator action, the spectrum may drastically depend on the domain assigned to it. This is illustrated by Examples 1.5.7 and 1.5.8.

Example 1.5.8. Let $\mathrm{dom}\, d = \{\psi \in (C^1[0,1], \|\cdot\|_\infty) : \psi(0) = 0\}$, $d : \mathrm{dom}\, d \to C[0,1]$, $(d\psi)(t) = \psi'(t)$, which is a closed and unbounded operator. If $\lambda \in \mathbb{C}$, the operator $W_\lambda : C[0,1] \to \mathrm{dom}\, d$, $(W_\lambda\phi)(t) = e^{\lambda t}\int_0^t e^{-\lambda s}\phi(s)\, ds$, $\phi \in C[0,1]$, is bounded and satisfies $(d - \lambda\mathbf{1})W_\lambda = \mathbf{1}$ (identity on $C[0,1]$) and $W_\lambda(d - \lambda\mathbf{1}) = \mathbf{1}$ (identity in $\mathrm{dom}\, d$). Therefore W_λ is the resolvent operator for d at λ and $\rho(d) = \mathbb{C}$, showing that $\sigma(d) = \emptyset$ (the resolvent W_λ was obtained by considering the solution of the differential equation $\psi' - \lambda\psi = \phi$ with $\psi(0) = 0$).

Below there are three useful identities involving resolvent operators; except the third one, the nomenclature is standard. The first identity relates the resolvent of a fixed operator at two points in its resolvent set; the second resolvent identity relates the resolvent of two different operators at a point in both resolvent sets; the third identity relates the difference of resolvents of two operators at a point in both resolvent sets with the difference at another point.

Proposition 1.5.9. *Let* $T : \mathrm{dom}\, T \subset \mathcal{B} \to \mathcal{B}$. *Then for any* $z, s \in \rho(T)$ *one has the first resolvent identity* (*also known as first resolvent equation*)

$$R_z(T) - R_s(T) = (z - s)R_z(T)R_s(T).$$

Furthermore, $R_z(T)$ *commutes with* $R_s(T)$.

Proof. Write

$$\begin{aligned} R_z - R_s &= R_z(T - s\mathbf{1})R_s - R_z(T - z\mathbf{1})R_s \\ &= R_z\left((T - s\mathbf{1}) - (T - z\mathbf{1})\right)R_s = (z - s)R_zR_s, \end{aligned}$$

which shows the first resolvent identity. The commutation claim is immediate from this relation. □

Exercise 1.5.10. For linear operators T, S acting in $\mathcal{B}$, with $\mathrm{dom}\, S \subset \mathrm{dom}\, T$, and $\lambda \in \rho(T) \cap \rho(S)$, verify the *second resolvent identity*

$$R_\lambda(T) - R_\lambda(S) = R_\lambda(T)(S - T)R_\lambda(S).$$

If $\mathrm{dom}\, T = \mathrm{dom}\, S$, such identity also equals $R_\lambda(S)(S - T)R_\lambda(T)$.

Proposition 1.5.11. *Let* S *and* T *be linear operators acting in* $\mathcal{B}$. *Then, for* $z, z_0 \in \rho(T) \cap \rho(S)$ *one has the third resolvent identity*

$$\begin{aligned} &R_z(T) - R_z(S) \\ &\quad = \left(\mathbf{1} + (z - z_0)R_z(T)\right)\left[R_{z_0}(T) - R_{z_0}(S)\right]\left(\mathbf{1} + (z - z_0)R_z(S)\right). \end{aligned}$$

Proof. By the first resolvent identity $R_z(T) = (\mathbf{1} + (z - z_0)R_z(T))R_{z_0}(T)$ and $R_z(S) = R_{z_0}(S)(\mathbf{1} + (z - z_0)R_z(S))$. By using such relations on the r.h.s. above one gets $R_z(T) - R_z(S)$. □

Theorem 1.5.12. *Let* $T : \mathrm{dom}\, T \subset \mathcal{B} \to \mathcal{B}$ *and* $\lambda_0 \in \rho(T)$. *Then for all* λ *in the disk* $|\lambda - \lambda_0| < 1/\|R_{\lambda_0}(T)\|$ *of the complex plane,* $R_\lambda(T) \in \mathrm{B}(\mathcal{B})$ *and*

$$R_\lambda(T) = \sum_{j=0}^{\infty} (\lambda - \lambda_0)^j R_{\lambda_0}(T)^{j+1},$$

with an absolutely convergent series.

Proof. Note initially that $R_{\lambda_0}(T) \neq 0$, since it is the inverse of an operator. By the relation

$$\begin{aligned} T - \lambda\mathbf{1} &= T - (\lambda_0 + (\lambda - \lambda_0))\mathbf{1} \\ &= (T - \lambda_0\mathbf{1})\left[\mathbf{1} + (\lambda_0 - \lambda)R_{\lambda_0}\right], \end{aligned}$$

just formally it would follow that

$$R_\lambda = \left(\sum_{j=0}^{\infty}(\lambda-\lambda_0)^j R_{\lambda_0}^j\right) R_{\lambda_0}.$$

It is left to justify this expression and show that it defines $(T-\lambda\mathbf{1})^{-1}$ in $\mathrm{B}(\mathcal{B})$. For $|\lambda-\lambda_0| < 1/\|R_{\lambda_0}(T)\|$ the series is absolutely convergent in $\mathrm{B}(\mathcal{B})$ and defines an operator satisfying

$$\begin{aligned}\left(\sum_{j=0}^{N}(\lambda-\lambda_0)^j R_{\lambda_0}^{j+1}\right)(T-\lambda\mathbf{1}) &= \sum_{j=0}^{N}(\lambda-\lambda_0)^j R_{\lambda_0}^{j+1}\left(T-(\lambda_0+(\lambda-\lambda_0))\mathbf{1}\right)\\ &= \sum_{j=0}^{N}(\lambda-\lambda_0)^j R_{\lambda_0}^j - \sum_{j=0}^{N}(\lambda-\lambda_0)^{j+1} R_{\lambda_0}^{j+1}\\ &= \mathbf{1} - \left[(\lambda-\lambda_0)R_{\lambda_0}\right]^{N+1}.\end{aligned}$$

Now $\lim_{N\to\infty}\left[(\lambda-\lambda_0)R_{\lambda_0}\right]^N = 0$ in $\mathrm{B}(\mathcal{B})$, since $|\lambda-\lambda_0| < 1/\|R_{\lambda_0}(T)\|$; then $\left(\sum_{j=0}^{\infty}(\lambda-\lambda_0)^j R_{\lambda_0}^{j+1}\right)(T-\lambda\mathbf{1}) = \mathbf{1}$. Similarly it is shown that

$$(T-\lambda\mathbf{1})\left(\sum_{j=0}^{\infty}(\lambda-\lambda_0)^j R_{\lambda_0}^{j+1}\right) = \mathbf{1}.$$ □

Corollary 1.5.13. *$\rho(T)$ is an open set and $\sigma(T)$ is a closed set of $\mathbb{C}$.*

Proof. One sees that $\rho(T)$ is open directly from Theorem 1.5.12, hence $\sigma(T)$ is closed. □

Corollary 1.5.14. *The map $\rho(T) \to \mathrm{B}(\mathcal{B})$ given by $\lambda \mapsto R_\lambda(T)$ is continuous and uniformly holomorphic, i.e., it has a derivative in $\mathrm{B}(\mathcal{B})$ defined by the limit*

$$\frac{dR_\lambda(T)}{d\lambda} := \lim_{h\to 0}\frac{R_{\lambda+h}(T)-R_\lambda(T)}{h} = R_\lambda(T)^2,$$

for all λ in a neighborhood of each point $\lambda_0 \in \rho(T)$.

Proof. By Theorem 1.5.12, if $\lambda_0 \in \rho(T)$ and $|\lambda-\lambda_0| < 1/\|R_{\lambda_0}(T)\|$,

$$\begin{aligned}\|R_\lambda(T)-R_{\lambda_0}(T)\| &\le \sum_{j=1}^{\infty}|\lambda-\lambda_0|^j\,\|R_{\lambda_0}(T)\|^{j+1}\\ &= |\lambda-\lambda_0|\,\|R_{\lambda_0}(T)\|^2\sum_{j=0}^{\infty}|\lambda-\lambda_0|^j\,\|R_{\lambda_0}(T)\|^j\\ &= \frac{|\lambda-\lambda_0|\,\|R_{\lambda_0}(T)\|^2}{1-|\lambda-\lambda_0|\,\|R_{\lambda_0}(T)\|} \longrightarrow 0 \ \text{ as } \ \lambda\to\lambda_0,\end{aligned}$$

showing that the map $\lambda \mapsto R_\lambda(T)$ in $\rho(T)$ is continuous.

By the first resolvent identity $(R_{\lambda+h} - R_\lambda)/h = R_{\lambda+h}R_\lambda$; taking $h \to 0$ and using the continuity shown above, it follows that the derivative exists and $dR_\lambda(T)/d\lambda = R_\lambda(T)^2$ holds. □

Corollary 1.5.15. *If both $\sigma(T)$ and $\rho(T)$ are nonempty, then*

$$\|R_\lambda(T)\| \geq 1/d(\lambda, \sigma(T))$$

for all $\lambda \in \rho(T)$ (with $d(\lambda, \sigma(T)) := \inf_{\mu\in\sigma(T)} |\mu - \lambda|$).

Proof. By Theorem 1.5.12, if $\lambda_0 \in \rho(T)$ and $\|R_{\lambda_0}(T)\| \, |\lambda - \lambda_0| < 1$, then $\lambda \in \rho(T)$. Thus, if $\lambda \in \sigma(T)$, necessarily $\|R_{\lambda_0}(T)\| \, |\lambda - \lambda_0| \geq 1$, that is,

$$\|R_{\lambda_0}(T)\| \geq \frac{1}{|\lambda - \lambda_0|}, \qquad \forall \lambda \in \sigma(T),$$

and (since $\sigma(T) \neq \emptyset$) the result follows. □

Now certain specific results on the spectrum of bounded operators will be discussed.

Corollary 1.5.16. *Let $T \in \mathrm{B}(\mathcal{B})$. If $|\lambda| > \|T\|$, then $\lambda \in \rho(T)$ and $\|R_\lambda(T)\| \to 0$ for $|\lambda| \to \infty$.*

Proof. Following the proof of the above theorem (write $T - \lambda\mathbf{1} = -\lambda(\mathbf{1} - T/\lambda)$), one concludes that the representation of $R_\lambda(T)$ by the series, called *Neumann's series* of T,

$$R_\lambda(T) = -\frac{1}{\lambda}\sum_{j=0}^{\infty}\left(\frac{T}{\lambda}\right)^j$$

is absolutely convergent if $|\lambda| > \|T\|$ and, in this case, that

$$\|R_\lambda(T)\| \leq 1/|\lambda| \sum_{j\geq 0} (\|T\|/\lambda)^j = 1/(|\lambda| - \|T\|).$$

It then follows that the spectrum $\sigma(T) \subset \{\lambda \in \mathbb{C} : |\lambda| \leq \|T\|\}$ and

$$\lim_{|\lambda|\to\infty} \|R_\lambda(T)\| = 0. \qquad □$$

Corollary 1.5.17. *If $T \in \mathrm{B}(\mathcal{B})$, then $\sigma(T) \neq \emptyset$.*

Proof. If $f \in \mathrm{B}(\mathcal{B})^*$ (the dual of $\mathrm{B}(\mathcal{B})$) define $F : \rho(T) \to \mathbb{C}$ by $F(\lambda) = f(R_\lambda(T))$. Thus, by Corollary 1.5.14 it is found that

$$\frac{dF(\lambda)}{d\lambda} = \lim_{h\to 0} \frac{F(\lambda + h) - F(\lambda)}{h} = f\left(R_\lambda(T)^2\right),$$

which is continuous; hence, F is holomorphic in $\rho(T)$. By using the inequality $|F(\lambda)| \leq \|f\|\|R_\lambda(T)\|$ and Corollary 1.5.16, $\lim_{|\lambda|\to\infty} F(\lambda) = 0$.

If $\sigma(T) = \emptyset$, i.e., $\rho(T) = \mathbb{C}$, by continuity F is bounded in any ball in $\mathbb{C}$, and since it converges to zero for $|\lambda| \to \infty$, it is found that $F : \mathbb{C} \to \mathbb{C}$ is an entire and bounded function, hence constant by Liouville's Theorem. In view of $\lim_{|\lambda|\to\infty} F(\lambda) = 0$, one has $F(\lambda) = f(R_\lambda(T)) = 0$ for all $\lambda \in \mathbb{C}$, $f \in \mathrm{B}(\mathcal{B})^*$. By the Hahn-Banach Theorem one gets $R_\lambda(T) = 0$, $\forall \lambda \in \mathbb{C}$, but this can not occur, since $R_\lambda(T)$ is the inverse of some operator. This contradiction shows that $\sigma(T)$ is nonempty. □

Definition 1.5.18. The *spectral radius* of a bounded linear operator $T \in \mathrm{B}(\mathcal{B})$ is $r_\sigma(T) := \sup_{\lambda\in\sigma(T)} |\lambda|$.

The next result is the so-called *spectral radius formula* and is due to I. Gelfand, who has shown it in the context of Banach algebras, around 1940. This formula is a relation between a limit strongly related to the metric, and the spectral radius defined via the supremum of a set.

Theorem 1.5.19. *If $T \in \mathrm{B}(\mathcal{B})$, then $r_\sigma(T) = \lim_{n\to\infty} \|T^n\|^{1/n} \le \|T\|$.*

Proof. Note, initially, that due to Corollary 1.5.16, $r_\sigma(T) \le \|T\|$. To demonstrate Theorem 1.5.19 we will use results from the Holomorphic Functions Theory combined with "any weakly convergent sequence is bounded," and the following simple observation: if $\lambda \in \mathbb{C}$ and $\lambda_1, \lambda_2, \ldots, \lambda_n$ are its nth roots in $\mathbb{C}$, then

$$T^n - \lambda\mathbf{1} = (T - \lambda_1\mathbf{1})(T - \lambda_2\mathbf{1}) \cdots (T - \lambda_n\mathbf{1}).$$

This implies that $\lambda \in \sigma(T^n)$ if, and only if, $\lambda_j \in \sigma(T)$ for some $1 \le j \le n$. Hence, $\sigma(T^n) = \sigma(T)^n := \{\lambda^n : \lambda \in \sigma(T)\}$. From this relation one concludes that for all $n \in \mathbb{N}$ one has $r_\sigma(T) = r_\sigma(T^n)^{1/n} \le \|T^n\|^{1/n}$.

For each f in the dual of $\mathrm{B}(\mathcal{B})$, define $F : \rho(T) \to \mathbb{C}$ by $F(\lambda) = f(R_\lambda(T))$, which is a holomorphic function (see the proof of Corollary 1.5.17). If $|\lambda| > \|T\|$, by using the Neumann series

$$F(\lambda) = -\frac{1}{\lambda} \sum_{n=0}^{\infty} \frac{1}{\lambda^n} f(T^n),$$

and by the uniqueness of Laurent expansion the above series converge for all $\lambda \in \mathbb{C}$ in the region $|\lambda| > r_\sigma(T)$ (or Taylor expansion if the variable $s = 1/\lambda$, with $F(0) = 0$, is considered).

Given $\varepsilon > 0$, for $r_\sigma(T) < \alpha < r_\sigma(T) + \varepsilon$ and all $f \in \mathrm{B}(\mathcal{B})^*$, the series $\sum_{n=0}^{\infty} f(T^n/\alpha^n)$ converge. Thus, the sequence T^n/α^n converges weakly to zero in $\mathrm{B}(\mathcal{B})$; hence it is bounded and there exists $C = C(\alpha) > 0$ with

$$\|T^n/\alpha^n\| \le C \Longrightarrow \|T^n\|^{1/n} \le \alpha C^{1/n}, \qquad \forall n \in \mathbb{N}.$$

Since $\lim_{n\to\infty} C^{1/n} = 1$, there is $N(\varepsilon) > 0$ such that

$$\|T^n\|^{\frac{1}{n}} < r_\sigma(T) + \varepsilon, \qquad \forall n \ge N(\varepsilon).$$

This relation, along with $r_\sigma(T) \le \|T^n\|^{1/n}$ verified above, show that $\lim_{n\to\infty} \|T\|^{1/n}$ exists and equals $r_\sigma(T)$. □

Exercise 1.5.20. If all pairs of the operators $\{T_1, \ldots, T_n\} \subset \mathrm{B}(\mathcal{B})$ are *commuting*, i.e., $T_jT_k = T_kT_j$, $\forall j, k$, show that the *product* $T_1T_2\cdots T_n$ is invertible with bounded inverse if, and only if, each T_j is invertible in $\mathrm{B}(\mathcal{B})$.

Corollary 1.5.21. *If* $T \in \mathrm{B}(\mathcal{B})$, *then* $\sigma(T^n) = \sigma(T)^n$ *and* $r_\sigma(T^n) = r_\sigma(T)^n$.

Exercise 1.5.22. Present a proof of Corollary 1.5.21.

Example 1.5.23. Let $S_e : l^\infty(\mathbb{N}) \hookleftarrow$ be the shift operator

$$S_e(\xi_1, \xi_2, \xi_3, \ldots) = (\xi_2, \xi_3, \xi_4, \ldots).$$

Since $\|S_e\| = 1$, then $\sigma(S_e) \subset \overline{B}(0;1)$. Every $|\lambda| \le 1$ is an eigenvalue of S_e, for the equation $S_e\xi^\lambda = \lambda\xi^\lambda$ has the solution $\xi^\lambda = (1, \lambda, \lambda^2, \lambda^3, \ldots)$ in $l^\infty(\mathbb{N})$. Therefore $\sigma(S_e) = \overline{B}(0;1)$, $r_\sigma(S_e) = 1$, and every point of its spectrum is an eigenvalue.

Example 1.5.24. The Volterra operator $T : C[0,1] \hookleftarrow$, given by $(T\psi)(t) = \int_0^t \psi(s)\, ds$ has no eigenvalues. In fact, by the eigenvalue equation

$$(T\psi)(t) = \lambda\psi(t) = \int_0^t \psi(s)\, ds$$

one finds $\lambda\psi'(t) = \psi(t)$ (ψ is differentiable since it is the integral of a continuous function). If $\lambda = 0$ then $\psi = 0$ and zero is not an eigenvalue; if $\lambda \ne 0$, the solutions of this differential equation are $\psi(t) = C\exp(t/\lambda)$, and since $\psi(0) = 0$ it follows that the constant $C = 0$, and so $\psi = 0$ and no $\lambda \in \mathbb{C}$ is an eigenvalue of T.

From the inequality $|(T\psi)(t)| \le t\|\psi\|_\infty$ it is found, by induction, that

$$|(T^2\psi)(t)| \le \int_0^t s\|\psi\|_\infty\, ds = \frac{t^2}{2}\|\psi\|_\infty, \qquad |(T^n\psi)(t)| \le \frac{t^n}{n!}\|\psi\|_\infty.$$

Thus, $\|T^n\| \le 1/n!$ and $r_\sigma(T) \le \lim_{n\to\infty}(1/n!)^{1/n} = 0$. Therefore $r_\sigma(T) < \|T\|$, $\sigma(T) = \{0\}$ (since $\ne \emptyset$) and T has no eigenvalues.

Example 1.5.25. Let $\mathcal{M}_h$ on $\mathrm{L}^2[0,1]$, with $h(t) = t$. Then $\mathcal{M}_h$ has no eigenvalues, since from $\mathcal{M}_h\psi = \lambda\psi$ it follows that $(t - \lambda)\psi(t) = 0$, or $\psi(t) = 0$ for a.e. $t \ne \lambda$, i.e., $\psi = 0$ in $\mathrm{L}^2[0,1]$.

Exercise 1.5.26. Show that in Example 1.5.25 one has $\sigma(\mathcal{M}_h) = [0,1]$.

Exercise 1.5.27. If $T \in \mathrm{B}(\mathcal{B})$, show that $\lim_{|\lambda|\to\infty} \lambda R_\lambda(T) = -\mathbf{1}$.

Exercise 1.5.28. For $T \in \mathrm{B}(\mathcal{B})$, define $V(t) := e^{tT}$, $t \in \mathbb{R}$, as in Exercise 1.1.23. Show that: a) The map $t \mapsto V(t) \in \mathrm{B}(\mathcal{B})$ is continuous with $V(0) = \mathbf{1}$ and $V(t+s) = V(t)V(s)$. b) If $S \in \mathrm{B}(\mathcal{B})$ commutes with T, then it also commutes with $V(t), \forall t$. c) This map is uniformly holomorphic and $dV(t)/dt = TV(t)$. See related results in Section 5.2.

1.6 Spectra of Compact Operators

As expected, the spectral theory of compact linear operators has many similarities with the spectral theory on finite-dimensional spaces; for example, with the possible exception of zero, each eigenvalue of a compact operator has finite multiplicity. However, there are compact operators with no eigenvalues.

Example 1.6.1. Consider the operator $T : l^2(\mathbb{N}) \hookleftarrow$,

$$T(\xi_1, \xi_2, \xi_3, \dots) = (0, \xi_1/1, \xi_2/2, \xi_3/3, \dots).$$

T is compact and $0 \in \sigma(T)$ since T^{-1} is not bounded. However this operator has no eigenvalues (check this!).

The next lemma is a key tool to construct bounded sequences with no convergent subsequence in infinite-dimensional $\mathcal{N}$. Although there is no explicit notion of orthogonality, a geometric interpretation is important for turning its proof natural.

Lemma 1.6.2 (Riesz Lemma). *Let X be a proper closed vector subspace of a normed space $(\mathcal{N}, \|\cdot\|)$. Then, for each $0 < \alpha < 1$ there exists $\xi \in \mathcal{N} \setminus X$ with $\|\xi\| = 1$ and $\inf_{\eta \in X} \|\xi - \eta\| \geq \alpha$.*

Proof. Let $\zeta \in \mathcal{N} \setminus X$ and $c = \inf_{\eta \in X} \|\eta - \zeta\|$. Since X is closed, $c > 0$. Thus, for all $d > c$ there exists $\omega \in X$ with $c \leq \|\zeta - \omega\| \leq d$. The vector $\xi = (\zeta - \omega)/\|\zeta - \omega\|$ belongs to $\mathcal{N} \setminus X$ and $\|\xi\| = 1$. Moreover, for all $\eta \in X$ one has

$$\|\xi - \eta\| = \frac{1}{\|\zeta - \omega\|} \Big\| \zeta - (\omega + \|\zeta - \omega\| \eta) \Big\| \geq \frac{c}{\|\zeta - \omega\|} \geq \frac{c}{d}.$$

For $0 < \alpha < 1$ choose $d = c/\alpha$ and the result follows. □

Theorem 1.6.3. *The closed ball $\overline{B}(0; 1)$ in a normed vector space $\mathcal{N}$ is compact if, and only if, $\dim \mathcal{N} < \infty$.*

Proof. If $\dim \mathcal{N} < \infty$, it is known that $\overline{B}(0; 1)$ is compact. If $\dim \mathcal{N}$ is not finite, then Riesz's lemma will be used to construct a sequence in $\overline{B}(0; 1)$ with no convergent subsequence.

Let $\xi_1 \in \mathcal{N}$, $\|\xi_1\| = 1$. By Riesz's lemma there exists $\xi_2 \in \mathcal{N}$, with $\|\xi_2\| = 1$, and $\|\xi_1 - \xi_2\| \geq 1/2$ (by choosing $\alpha = 1/2$ in Riesz's lemma). The vector space $\mathrm{Lin}(\{\xi_1, \xi_2\})$ is closed, since its dimension is finite. Again by Riesz's lemma, there exists $\xi_3 \in \mathcal{N}$, with $\|\xi_3\| = 1$, $\|\xi_3 - \xi_1\| \geq 1/2$ and $\|\xi_3 - \xi_2\| \geq 1/2$. In this way, a sequence $(\xi_n)_{n=1}^\infty$, $\|\xi_n\| = 1$, $\forall n$, and $\|\xi_j - \xi_k\| \geq 1/2$ for all $j \neq k$ is constructed. Since such sequence has no convergent subsequence , the closed ball $\overline{B}(0; 1)$ is not compact. □

Proposition 1.6.4. *If $T \in \mathrm{B}_0(\mathcal{B})$, then every nonzero eigenvalue of T is of finite multiplicity, that is, $\dim \mathrm{N}(T - \lambda \mathbf{1}) < \infty$.*

Proof. Let B_1 be the closed ball centered at zero and radius 1 in the vector space $\mathrm{N}(T - \lambda\mathbf{1})$. It will be shown that B_1 is compact and, hence, $\dim \mathrm{N}(T - \lambda\mathbf{1}) < \infty$ by Theorem 1.6.3. Since T is compact, for a sequence $(\xi_n) \subset B_1$ $(T\xi_n = \lambda\xi_n)$, there is a convergent subsequence $(T\xi_{n_j})$ and, so, $(\xi_{n_j} = T\xi_{n_j}/\lambda)$ also converges to an element of B_1; hence that ball is compact. □

Exercise 1.6.5. Use the next argument as a variant of the proof of Proposition 1.6.4: suppose that B_1 is not compact; thus there exists a sequence $(\xi_n) \subset B_1$ with no convergent subsequence; use the compactness of T to reach a contradiction.

Proposition 1.6.6. *If $T \in \mathrm{B}_0(\mathcal{B})$, then for all $\varepsilon > 0$ the number of eigenvalues λ of T with $|\lambda| \geq \varepsilon$ is finite.*

Proof. Suppose that it is possible to choose $\varepsilon > 0$ so that there are infinitely many eigenvalues $\{\lambda_j\}_{j\in\mathbb{N}}$ of T with absolute values greater than or equal to ε. By Proposition 1.6.4 one may assume that such eigenvalues are pairwise distinct; denote by $\{\xi_j\}$ the respective eigenvectors. Recall that this set is linearly independent (Exercise 1.5.5).

Let $E_0 = \{0\}$ and $E_n = \mathrm{Lin}(\{\xi_1, \ldots, \xi_n\})$; note that such subspaces are closed for all n. By Riesz's Lemma 1.6.2 there exists a sequence $\{\eta_n\}$, $\eta_n \in E_n$, $\|\eta_n\| = 1$ and $\|\eta_n - \xi\| \geq 1/2$, $\forall \xi \in E_{n-1}$. The aim is to show that $\|T\eta_n - T\eta_m\| \geq \varepsilon/2$ for all distinct n, m, which then has no convergent subsequence, a contradiction with the compactness of T.

If $m < n$, then $T\eta_n - T\eta_m = \lambda_n\eta_n + [(T - \lambda_n\mathbf{1})\eta_n - T\eta_m]$. Clearly $T\eta_m \in E_m$ and, writing $\eta_n = \sum_{j=1}^n \alpha_j\xi_j$, one has

$$(T - \lambda_n\mathbf{1})\eta_n = \left[\sum_{j=1}^{n-1} \alpha_j(\lambda_j - \lambda_n)\xi_j\right] \in E_{n-1},$$

so that $\zeta_m := -[(T - \lambda_n\mathbf{1})\eta_n - T\eta_m]/\lambda_n$ belongs to the subspace E_{n-1}. Therefore, $\|T\eta_n - T\eta_m\| = |\lambda_n|\|\eta_n - \zeta_m\| \geq \frac{|\lambda_n|}{2} \geq \varepsilon/2$, and $\{T\eta_n\}$ has no convergent subsequence. □

From such propositions (and some simple extra argument) follows the important

Corollary 1.6.7. *Let $T \in \mathrm{B}_0(\mathcal{B})$ and Λ the set of eigenvalues of T. Then:*

i) *The unique possible accumulation point of Λ is zero.*
ii) *Λ is countable and, if $\lambda \neq 0$, then $\dim \mathrm{N}(T - \lambda\mathbf{1}) < \infty$.*
iii) *If Λ is an infinite set, then the eigenvalues of T can be ordered in a sequence converging to zero.*
iv) *If $\dim \mathcal{B} = \infty$, then zero belongs to the spectrum of T.*

Exercise 1.6.8. Present the details of the proof of Corollary 1.6.7.

Example 1.6.9. Any finite rank operator is compact and has finite spectrum.

Example 1.6.10. Consider the operator $T : l^2(\mathbb{N}) \hookleftarrow$,

$$T(\xi_1, \xi_2, \xi_3, \dots) = (\xi_1/1, \xi_2/2, \xi_3/3, \dots).$$

T is compact and zero is not an eigenvalue of T, however it belongs to its spectrum, since $\{1, 1/2, 1/3, \dots\}$ is a subset of $\sigma(T)$ (they are eigenvalues) and the spectrum is closed. It is also possible to infer directly that the resolvent operator $R_0(T)$ exists, with dense domain, but it is not bounded.

Chapter 2

Adjoint Operator

The basics of (linear) unbounded self-adjoint operators is discussed in this chapter. Cayley transform, von Neumann criterion on self-adjoint extensions, Weyl spectral criterion and many examples are presented. These are the first steps to the mathematical formulation of quantum mechanics. From now on the Hilbert spaces are supposed to be separable and, unless it is explicitly remarked, also complex.

2.1 Adjoint Operator

The concept of Hilbert adjoint will be extended to some unbounded operators. T always denotes a linear operator.

Definition 2.1.1. A linear operator $T : \text{dom}\ T \subset \mathcal{H} \to \mathcal{H}$ is *symmetric if*

$$\langle T\xi, \eta\rangle = \langle \xi, T\eta\rangle, \qquad \forall \xi, \eta \in \text{dom}\ T.$$

T is hermitian if it is symmetric and dom T *is dense in* $\mathcal{H}$.

Let $T : \text{dom}\ T \sqsubseteq \mathcal{H}_1 \to \mathcal{H}_2$ and define dom T^* as the vector space of elements $\eta \in \mathcal{H}_2$ such that the linear functional

$$\xi \mapsto \langle \eta, T\xi\rangle, \qquad \xi \in \text{dom}\ T,$$

can be represented by $\zeta \in \mathcal{H}_1$, that is,

$$\langle \eta, T\xi\rangle = \langle \zeta, \xi\rangle, \qquad \forall \xi \in \text{dom}\ T.$$

Definition 2.1.2. The (Hilbert) *adjoint* of T is the operator T^* with domain dom T^* defined above and, for $\eta \in \text{dom}\ T^*$, $T^*\eta = \zeta$. Hence

$$\langle \eta, T\xi\rangle = \langle T^*\eta, \xi\rangle, \qquad \forall \xi \in \text{dom}\ T, \forall \eta \in \text{dom}\ T^*.$$

Observe that it is essential that dom T is dense in $\mathcal{H}$ for T^* to be uniquely defined. If S is also a linear operator and $z \in \mathbb{C}$, then T^* is linear and $(S + zT)^* = S^* + \overline{z}T^*$.

Exercise 2.1.3. Show that $T : \mathrm{dom}\, T \sqsubseteq \mathcal{H} \to \mathcal{H}$ is hermitian iff $T \subset T^*$ (recall that, given two operators R, S, then $S \subset R$ indicates that R is an extension of S).

Remark 2.1.4. Note that $\eta \in \mathrm{dom}\, T^*$ iff the map $\mathrm{dom}\, T \ni \xi \mapsto \langle \eta, T\xi \rangle$ is uniformly continuous. In fact, since dom T is dense in $\mathcal{H}$, this linear map has a unique continuous extension to $\mathcal{H}$ and so, by Riesz's Theorem 1.1.40, it can be represented by a unique $\zeta \in \mathcal{H}$ as above. Then the definition $T^*\eta = \zeta$.

Example 2.1.5. The domain of the adjoint can be quite small. Let $\mathcal{H} = \mathrm{L}^2[-1, 1]$, $\mathrm{dom}\, T = C[-1, 1] \sqsubseteq \mathcal{H}$ and $(T\psi)(x) = \psi(0)$. Since dom T is dense in $\mathcal{H}$, its adjoint is well defined. $g \in \mathrm{dom}\, T^*$ iff the map $\mathrm{dom}\, T \ni \psi \mapsto \langle g, T\psi \rangle = \int_{-1}^{1} \overline{g(x)}\, (T\psi)(x)\, dx = \int_{-1}^{1} \overline{g(x)}\, \psi(0)\, dx$ is continuous, i.e.,

$$\sup_{\psi \in \mathrm{dom}\ T,\, \|\psi\|=1} \left| \psi(0) \int_{-1}^{1} \overline{g(x)}\, dx \right| < \infty.$$

Since $|\psi(0)|$ can be arbitrarily large, then $\int_{-1}^{1} \overline{g(x)}\, dx = 0$ and dom T^* is the subspace orthogonal to the constant functions in $\mathcal{H}$. Moreover, for $g \in \mathrm{dom}\, T^*$ one has $0 = \langle g, \psi(0) \rangle = \langle g, T\psi \rangle = \langle T^*g, \psi \rangle$, $\forall \psi \in C[-1, 1]$, so that $T^*g = 0$.

Proposition 2.1.6 shows that the above definition of adjoint actually generalizes the one recalled on page 24 for the specific case of bounded operators.

Proposition 2.1.6. *If* $T \in \mathrm{B}(\mathcal{H}_1, \mathcal{H}_2)$*, then* $T^* \in \mathrm{B}(\mathcal{H}_2, \mathcal{H}_1)$*,* $T^{**} = T$ *and* $\|T^*\| = \|T\|$*. Hence*

$$\langle \eta, T\xi \rangle = \langle T^*\eta, \xi \rangle, \qquad \forall \xi \in \mathcal{H}_1, \forall \eta \in \mathcal{H}_2.$$

Proof. Clearly, for bounded T one has $\mathrm{dom}\, T^* = \mathcal{H}_2$. By Riesz's Theorem 1.1.40, for each $\xi_2 \in \mathcal{H}_2$ one has $f_{T^*\xi_2} \in \mathcal{H}_1^*$ and

$$\begin{aligned} \|T^*\xi_2\| = \|f_{T^*\xi_2}\| &= \sup_{\|\xi_1\|=1} |f_{T^*\xi_2}(\xi_1)| = \sup_{\|\xi_1\|=1} |\langle T^*\xi_2, \xi_1 \rangle| \\ &= \sup_{\|\xi_1\|=1} |\langle \xi_2, T\xi_1 \rangle| \le \|T\|\|\xi_2\|, \end{aligned}$$

so $T^* \in \mathrm{B}(\mathcal{H}_2, \mathcal{H}_1)$ and $\|T^*\| \le \|T\|$.

Directly from the definition of adjoint

$$\langle T^*\xi_2, \xi_1 \rangle = \langle \xi_2, T\xi_1 \rangle, \quad \forall \xi_1 \in \mathcal{H}_1, \forall \xi_2 \in \mathcal{H}_2,$$

and so $T^{**} = T$. Now $\|T\| = \|T^{**}\| \le \|T^*\|$; hence $\|T^*\| = \|T\|$. □

Definition 2.1.7.

a) A linear operator $T : \operatorname{dom} T \sqsubseteq \mathcal{H} \to \mathcal{H}$ is *self-adjoint* if $T = T^*$ (including equality of domains, of course).

b) A bounded linear $T : \mathcal{H}_1 \to \mathcal{H}_2$ is *unitary* if $\operatorname{rng} T = \mathcal{H}_2$, it is one-to-one and $T^* = T^{-1}$.

c) A bounded linear operator $T : \mathcal{H} \hookleftarrow$ is *normal* if $T^*T = TT^*$.

Remark 2.1.8. a) Note that $T : \mathcal{H}_1 \to \mathcal{H}_2$ is unitary iff $\langle T\xi, T\eta\rangle = \langle \xi, T^*T\eta\rangle = \langle \xi, \eta\rangle$, $\forall \xi, \eta \in \mathcal{H}_1$ and $\operatorname{rng} T = \mathcal{H}_2$; in particular unitary operators are isometries (and so $\|T\| = 1$) and T^{-1} is also unitary. The unitary operators are the isomorphisms on Hilbert spaces.

b) T^{**} will denote $(T^*)^*$ and so on. It is possible to define unbounded normal operators; see Definition 8.2.9.

c) If T is self-adjoint (or just symmetric), then $\langle T\xi, \xi\rangle \in \mathbb{R}$ for all $\xi \in \operatorname{dom} T$. Further, a self-adjoint operator is symmetric and the addition of elements to its domain will necessarily deform this property (see Theorem 2.1.24).

d) It is usually not difficult to check if an operator is symmetric, however self-adjointness is a much more subtle property to verify. It turns out that for bounded operators with domain all $\mathcal{H}$, the concepts of hermitian and self-adjoint coincide.

Example 2.1.9. Let $z \in \mathbb{C}$ and $\mathbf{1}$ be the identity operator on $\mathcal{H}$. The operator $z\mathbf{1}$ is: 1) normal for all $z \in \mathbb{C}$; 2) self-adjoint iff $z \in \mathbb{R}$; 3) unitary iff $|z| = 1$.

Example 2.1.10. For each fixed $0 \neq s \in \mathbb{R}$ the operator $T_s \in \mathrm{B}(\mathrm{L}^2(\mathbb{R}))$, $(T_s\psi)(t) := \frac{1}{2s}[\psi(t+s) + \psi(t-s)]$, $\psi \in \mathrm{L}^2(\mathbb{R})$, is self-adjoint.

Example 2.1.11. The operator $S_r : l^2(\mathbb{N}) \hookleftarrow$ given by

$$S_r(\xi_1, \xi_2, \xi_3, \dots) = (0, \xi_1, \xi_2, \dots)$$

is a linear isometry (i.e., an isometric mapping) between Hilbert spaces, but it is not unitary, because it is not onto.

Proposition 2.1.12.

a) *If* $T \in \mathrm{B}(\mathcal{H})$ *then* $\|TT^*\| = \|T^*T\| = \|T\|^2$. *Therefore,*

 i) $T^*T = 0$ *if, and only if,* $T = 0$.

 ii) *If* T *is normal, then* $\|T^2\| = \|T\|^2$.

b) *If* $T \in \mathrm{B}(\mathcal{H})$ *is normal* (*especially it holds for bounded self-adjoint operators*), *then its spectral radius* $r_\sigma(T) = \|T\|$ (*see Definition 1.5.18*).

Proof. a) If $T \in \mathrm{B}(\mathcal{H})$,

$$\begin{aligned}\|T\|^2 &= \sup_{\|\xi\|=1} \|T\xi\|^2 = \sup_{\|\xi\|=1} \langle T\xi, T\xi\rangle = \sup_{\|\xi\|=1} \langle T^*T\xi, \xi\rangle \le \sup_{\|\xi\|=1} \|T^*T\|\,\|\xi\|^2 \\ &= \|T^*T\| \le \|T^*\|\,\|T\| = \|T\|^2,\end{aligned}$$

and $\|T^*T\| = \|T\|^2$. By adapting the roles of T and T^* in this relation one obtains $\|TT^*\| = \|T\|^2$. Then i) is immediate from such a relation.

Now, if T commutes with its adjoint, then for all $\xi \in \mathcal{H}$ one has $\|T^*T\xi\|^2 = \langle T^*T\xi, T^*T\xi\rangle = \langle T^2\xi, T^2\xi\rangle = \|T^2\xi\|^2$, consequently $\|T^2\| = \|T^*T\| = \|T\|^2$, which is ii).

b) If T is normal then, by ii) above, $\|T^{2^n}\| = \|T\|^{2^n}$ for all $n \in \mathbb{N}$; thus

$$r_\sigma(T) = \lim_{n\to\infty} \|T^{2^n}\|^{1/2^n} = \|T\|.$$

Recall that, if a limit does exist, then one may use any subsequence to evaluate it. □

Proposition 2.1.13. *If $T \in \mathrm{B}(\mathcal{H})$ is self-adjoint, then*

$$\|T\| = \sup_{\|\xi\|=1} \langle T\xi, \xi\rangle.$$

Proof. Let κ denote the above right-hand side. Thus, $|\langle T\xi,\xi\rangle| \le \|T\|\,\|\xi\|^2$ and so $\kappa \le \|T\|$. Since $\langle T\xi,\xi\rangle \in \mathbb{R}$ for all $\xi \in \mathcal{H}$, by polarization and then using the parallelogram law,

$$\begin{aligned} 4\,|\mathrm{Re}\,\langle T\xi,\eta\rangle| &= |\langle T(\xi+\eta),\xi+\eta\rangle - \langle T(\xi-\eta),\xi-\eta\rangle| \\ &= \left|\left\langle T\frac{\xi+\eta}{\|\xi+\eta\|}, \frac{\xi+\eta}{\|\xi+\eta\|}\right\rangle \|\xi+\eta\|^2 - \left\langle T\frac{\xi-\eta}{\|\xi-\eta\|}, \frac{\xi-\eta}{\|\xi-\eta\|}\right\rangle \|\xi-\eta\|^2\right| \\ &\le \kappa\left(\|\xi+\eta\|^2 + \|\xi-\eta\|^2\right) = 2\kappa\left(\|\xi\|^2+\|\eta\|^2\right). \end{aligned}$$

Hence, if $\|\xi\| = \|\eta\| = 1$ one has $|\mathrm{Re}\,\langle T\xi,\eta\rangle| \le \kappa$. By choosing $\eta = T\xi/\|T\xi\|$ it follows that $\|T\xi\| \le \kappa$ for all $\|\xi\| = 1$. Therefore, $\|T\| \le \kappa$ and so $\|T\| = \kappa$. □

Remark 2.1.14. a) The distinction between hermitian and self-adjoint operators is a famous subtlety in mathematics with outstanding physical and mathematical implications. See, for instance, Theorem 2.2.17 and Section 14.1.

b) For some applications (especially to quantum mechanics), it may be important that the operator in question is self-adjoint. However, often what is initially supplied is just an operator action (a differential one, for instance) which is hermitian on certain domain, and one is left with the hard task of finding suitable self-adjoint extensions.

Lemma 2.1.15. $\mathcal{G}(T^*) = (J\mathcal{G}(T))^\perp$ *in $\mathcal{H}\times\mathcal{H}$, with $J(\xi,\eta) = (-\eta,\xi)$ a unitary operator.*

Proof. By the equivalent relations

$$\begin{aligned} (\eta,\phi) \in \mathcal{G}(T^*) &\Leftrightarrow \langle T\xi,\eta\rangle = \langle \xi,\phi\rangle,\ \forall\xi \in \mathrm{dom}\,T \\ &\Leftrightarrow \langle(-T\xi,\xi),(\eta,\phi)\rangle_{\mathcal{H}\times\mathcal{H}} = 0,\ \forall\xi\in\mathrm{dom}\,T \\ &\Leftrightarrow \langle J(\xi,T\xi),(\eta,\phi)\rangle_{\mathcal{H}\times\mathcal{H}} = 0,\ \forall\xi\in\mathrm{dom}\,T \\ &\Leftrightarrow (\eta,\phi) \in (J\mathcal{G}(T))^\perp \end{aligned}$$

the assertion follows. □

Corollary 2.1.16.

a) *Let T be a linear operator in $\mathcal{H}$. T^* is a closed operator, specifically every self-adjoint operator is closed.*

b) *Any hermitian operator is closable and its closure is hermitian.*

Proof. a) By Lemma 2.1.15 $\mathcal{G}(T^*)$ is a closed subspace.

b) Since T is hermitian then $T \subset T^*$ and, by item a), T is closable. To show that $\overline{T}$ is hermitian, let $\xi, \zeta \in \mathrm{dom}\ \overline{T}$, and pick $(\xi_n), (\zeta_n) \subset \mathrm{dom}\ T$ with $\xi_n \to \xi$, $\zeta_n \to \zeta$ and $T\xi_n \to \overline{T}\xi$, $T\zeta_n \to \overline{T}\zeta$; in view of

$$\langle \overline{T}\zeta, \xi \rangle = \lim_{n\to\infty} \langle T\zeta_n, \xi_n \rangle = \lim_{n\to\infty} \langle \zeta_n, T\xi_n \rangle = \langle \zeta, \overline{T}\xi \rangle,$$

it follows that $\overline{T}$ is hermitian. □

Corollary 2.1.17.

a) *Let T be a densely defined linear operator. Then T is closable iff* dom T^* *is dense in $\mathcal{H}$. In this case*

$$\mathcal{H} \times \mathcal{H} = \overline{J\mathcal{G}(T)} \oplus \mathcal{G}(T^*) = \overline{\mathcal{G}(T)} \oplus J\mathcal{G}(T^*), \quad \textit{and} \quad T^{**} = \overline{T}.$$

b) *If T is closable, then $(\overline{T})^* = T^*$.*

Proof. a) Since J is unitary and $J^2 = -\mathbf{1}$, if T is closable, then $\overline{\mathcal{G}(T)}$ and $J\overline{\mathcal{G}(T)}$ are closed subspaces and

$$\mathcal{H} \times \mathcal{H} = J\overline{\mathcal{G}(T)} \oplus \left(J\overline{\mathcal{G}(T)}\right)^{\perp} = \overline{J\mathcal{G}(T)} \oplus \mathcal{G}(T^*) = \overline{\mathcal{G}(T)} \oplus J\mathcal{G}(T^*).$$

Let $\zeta \in (\mathrm{dom}\ T^*)^{\perp}$. Thus, $\langle \xi, \zeta \rangle = 0 = \langle T^*\xi, 0 \rangle$, $\forall \xi \in \mathrm{dom}\ T^*$, that is,

$$\langle (0, \zeta), (-T^*\xi, \xi) \rangle_{\mathcal{H}\times\mathcal{H}} = 0 \Rightarrow (0, \zeta) \in (J\mathcal{G}(T^*))^{\perp} = \overline{\mathcal{G}(T)},$$

so $\overline{T}(0) = \zeta = 0$ and dom T^* is dense in $\mathcal{H}$. Note that these arguments also show that if dom T^* is dense in $\mathcal{H}$, then, for no $\zeta \neq 0$, $(0, \zeta) \in \overline{\mathcal{G}(T)}$ so that $\overline{\mathcal{G}(T)}$ is the graph of an operator and T is closable.

Now (apply Lemma 2.1.15), for T closable T^{**} is well defined and $\mathcal{H} \times \mathcal{H} = J\mathcal{G}(T^*) \oplus \mathcal{G}(T^{**})$; since $\mathcal{G}(T^{**}) = (J\mathcal{G}(T^*))^{\perp} = \overline{\mathcal{G}(T)}$, it is found that $T^{**} = \overline{T}$.

b) By applying Corollary 2.1.16a) once and then item a) twice: $T^* = \overline{T^*} = T^{***} = \overline{T}^*$. □

Remark 2.1.18. Due to Corollaries 2.1.16b) and 2.1.17b), in many theoretical discussions one assumes that hermitian operators are closed.

Exercise 2.1.19. a) Show that a self-adjoint operator has no proper hermitian extensions. b) Show that each eigenvalue of a symmetric operator is a real number. c) Check that if $S \subset T$, then $T^* \subset S^*$.

Exercise 2.1.20. If T and S are linear operators in $\mathcal{H}$, define dom $(S+T) :=$ dom $S \cap$ dom T, and dom $(ST) := \{\xi \in \text{dom } T : T\xi \in \text{dom } S\}$,

$$(T+S)\xi := T\xi + S\xi \qquad \text{and} \qquad (ST)\xi := S(T\xi),$$

which are called *operator sum* and *operator product*, respectively (of course such operations are well defined in normed spaces). If these operators are densely defined, show that $T^*S^* \subset (ST)^*$, and if $S \in \mathrm{B}(\mathcal{H})$ then $T^*S^* = (ST)^*$.

Exercise 2.1.21. Let T be a densely defined closed linear operator. Use Corollary 2.1.17 to show that for any pair $\xi', \eta' \in \mathcal{H}$ there is a unique pair $\xi \in$ dom T and $\eta \in$ dom T^* obeying

$$\xi' = \eta - T\xi, \qquad \eta' = \xi + T^*\eta.$$

Moreover, $\|\xi'\|^2 + \|\eta'\|^2 = \|\xi\|^2 + \|T\xi\|^2 + \|\eta\|^2 + \|T^*\eta\|^2$.

Definition 2.1.22. A hermitian operator T is *essentially self-adjoint* if $\overline{T}$ is self-adjoint.

Remark 2.1.23. If T is self-adjoint, then a subspace $\mathcal{D} \subset$ dom T is a *core* of T (see Definition 1.2.25) iff the restriction $T|_{\mathcal{D}}$ is essentially self-adjoint.

Let T, S be linear operators. If $S \subset T$ one has $T^* \subset S^*$, then if T is hermitian (i.e., $T \subset T^*$) it follows that $\overline{T} = T^{**} \subset T^*$.

If A is a self-adjoint extension of the hermitian operator T, i.e., $T \subset A$, then $A = A^* \subset T^*$, consequently T^* is an extension of all self-adjoint extensions of T. Now if T is also essentially self-adjoint with $T \subset A$, one has

$$A \subset T^* \Rightarrow \overline{T} = T^{**} \subset A \Rightarrow A \subset \overline{T}^* = \overline{T},$$

so that $\overline{T} = A$.

Theorem 2.1.24. *Let T be a hermitian operator. Then:*

a) *T^* is an extension of all self-adjoint* (*or hermitian*) *extensions of T.*
b) *If T is essentially self-adjoint, then it has just one self-adjoint extension* (*see also Corollary* 2.2.14).
c) *T is essentially self-adjoint iff T^* is hermitian, and in this case $\overline{T} = T^{**} = T^*$* (*so T^* is, in fact, self-adjoint*).

Proof. Items a) and b) were discussed above.

c) If T is essentially self-adjoint, then $T^* = \overline{T}^* = \overline{T} = T^{**}$ and T^* is self-adjoint, so $\overline{T} = T^{**} = T^*$. Now assume that T^* is hermitian; one has $T^* = \overline{T}^*$ and, since $\overline{T}$ is also hermitian, $\overline{T} \subset \overline{T}^* = T^* \subset T^{**} = \overline{T}$, and so $\overline{T} = \overline{T}^*$ and T is essentially self-adjoint. □

Thus a hermitian operator has at least two natural closed extensions: a "minimal" one given by its closure, and a "maximal" one given by its adjoint. Hence, its fortuitous self-adjoint extensions are half-way between such minimal and maximal closed extensions.

Definition 2.1.25. If there is a unitary operator $U : \mathcal{H}_1 \to \mathcal{H}_2$, then these spaces are said to be *unitarily equivalent*. In this case, two linear operators $T_j : \mathrm{dom}\ T_j \subset \mathcal{H}_j \to \mathcal{H}_j$, $j = 1, 2$, are *unitarily equivalent* if $\mathrm{dom}\ T_2 := U\mathrm{dom}\ T_1$ and $T_2 = UT_1U^*$.

Exercise 2.1.26. Let $U \in \mathrm{B}(\mathcal{H}_1, \mathcal{H}_2)$ be a unitary operator and T_1, T_2 unitarily equivalent linear operators. Show that: a) T_2 is closed iff T_1 is closed. b) T_2 is hermitian, essentially self-adjoint, self-adjoint iff the corresponding statement holds for T_1. c) T_1 and T_2 have the same eigenvalues. d) $z \in \rho(T_2)$ iff $z \in \rho(T_1)$ and $\|R_z(T_2)\| = \|R_z(T_1)\|$; conclude that $\sigma(T_2) = \sigma(T_1)$.

Now it is interesting to present the Hellinger-Toeplitz argument. It shows that in the study of the adjoint of an unbounded operator subtle domain questions will actually appear, since such operators can not be defined on all elements of the Hilbert space.

Proposition 2.1.27 (Hellinger-Toeplitz). *Let $T : \mathcal{H} \hookleftarrow$ be a linear operator with*

$$\langle T\eta, \xi\rangle = \langle \eta, T\xi\rangle, \qquad \forall \eta, \xi \in \mathcal{H}.$$

Then $T \in \mathrm{B}(\mathcal{H})$ and it is self-adjoint.

Proof. From the definitions it follows that T is self-adjoint, so closed. Since its domain is $\mathcal{H}$, then T is bounded by the Closed Graph Theorem 1.2.21. □

Exercise 2.1.28. If $T : \mathcal{H}_1 \to \mathcal{H}_2$ is linear and there exists $S : \mathcal{H}_2 \to \mathcal{H}_1$, not necessarily linear, with $\langle T\xi, \eta\rangle = \langle \xi, S(\eta)\rangle$ for all $\xi \in \mathcal{H}_1$ and $\eta \in \mathcal{H}_2$, conclude that S is linear, T and S are bounded and, finally, that $T^* = S$.

Remark 2.1.29. There are some ongoing attempts to construct an adjoint for operators on separable Banach spaces that parallels the construction in Hilbert spaces, also aiming at introducing the notion of self-adjoint operators in Banach spaces; however, usually some expected properties fail. See [GiBZS04].

2.2 Cayley Transform I

The basic and motivating observation for the developments ahead is that for a hermitian operator $T : \mathrm{dom}\ T \sqsubseteq \mathcal{H} \to \mathcal{H}$ one has

$$\|(T \pm i\mathbf{1})\xi\|^2 = \|T\xi\|^2 + \|\xi\|^2 = \|\xi\|_T^2, \qquad \forall \xi \in \mathrm{dom}\ T.$$

Hence, the operator

$$U(T) := (T - i\mathbf{1})(T + i\mathbf{1})^{-1} : \mathrm{rng}\ (T + i\mathbf{1}) \to \mathrm{rng}\ (T - i\mathbf{1})$$

is one-to-one, linear and isometric.

Definition 2.2.1. $U(T)$ as above is called the *Cayley transform* of the hermitian operator T.

Exercise 2.2.2. Show that for a densely defined operator $T : \mathrm{dom}\, T \sqsubseteq \mathcal{H} \to \mathcal{H}$ one has $\mathrm{N}(T^*) = (\mathrm{rng}\ (T))^\perp$.

Definition 2.2.3. Let T be a hermitian operator. The closed linear subspaces $\mathrm{K}_\pm(T) := \mathrm{N}(T^* \pm i\mathbf{1}) = (\mathrm{rng}\ (T \mp i\mathbf{1}))^\perp$ are the *deficiency subspaces* of T and the integer numbers, given by the respective dimensions,

$$n_+(T) := \dim \mathrm{N}(T^* + i\mathbf{1}) = \dim(\mathrm{rng}\ (T - i\mathbf{1}))^\perp,$$
$$n_-(T) := \dim \mathrm{N}(T^* - i\mathbf{1}) = \dim(\mathrm{rng}\ (T + i\mathbf{1}))^\perp,$$

are its *deficiency indices*.

Proposition 2.2.4. *Let T be a hermitian operator. Then:*

i) *T is closed iff* $\mathrm{rng}\ (T - i\mathbf{1})$ *is closed iff* $\mathrm{rng}\ (T + i\mathbf{1})$ *is closed.*

ii) *T is self-adjoint iff* $\mathrm{rng}\ (T + i\mathbf{1}) = \mathrm{rng}\ (T - i\mathbf{1}) = \mathcal{H}$ *iff its Cayley transform is a unitary operator $U(T) : \mathcal{H} \to \mathcal{H}$.*

iii) *If there is $\lambda \in \mathbb{R}$ so that* $\mathrm{rng}\ (\overline{T} - \lambda\mathbf{1}) = \mathcal{H}$*, then T is essentially self-adjoint (recall that $\overline{T}$ is the closure of T).*

iv) *If there is $\lambda \in \mathbb{R} \cap \rho(T)$, then T is self-adjoint.*

Proof. i) It is enough to observe that the maps

$$\mathrm{rng}\ (T \pm i\mathbf{1}) \ni (T \pm i\mathbf{1})\xi \mapsto (\xi, T\xi) \in \mathcal{G}(T), \qquad \xi \in \mathrm{dom}\ T,$$

are isometric (so one-to-one) and onto.

ii) The two last assertions are clearly equivalent.

Let $T = T^*$; then T is closed and, by Exercise 2.2.2 if $\xi \in (\mathrm{rng}\ (T + i\mathbf{1}))^\perp = \mathrm{N}(T^* - i\mathbf{1})$ one has $T\xi = i\xi$, and $\xi = 0$ since its eigenvalues are real. So $\mathrm{rng}\ (T + i\mathbf{1})$ is dense in $\mathcal{H}$; by i) it is also closed, so $\mathrm{rng}\ (T + i\mathbf{1}) = \mathcal{H}$. Similarly one gets $\mathrm{rng}\ (T - i\mathbf{1}) = \mathcal{H}$.

For the converse, recall that $T \subset T^*$. If $\eta \in \mathrm{dom}\ T^*$, then for all $\phi \in \mathrm{dom}\ T$, $\langle \eta, (T + i\mathbf{1})\phi \rangle = \langle (T^* - i\mathbf{1})\eta, \phi \rangle$. Pick $\xi \in \mathrm{dom}\ T$ with $(T - i\mathbf{1})\xi = (T^* - i\mathbf{1})\eta$. Hence

$$\langle \eta, (T + i\mathbf{1})\phi \rangle = \langle (T - i\mathbf{1})\xi, \phi \rangle = \langle \xi, (T + i\mathbf{1})\phi \rangle, \qquad \forall \phi \in \mathrm{dom}\ T.$$

Since $\mathrm{rng}\ (T + i\mathbf{1}) = \mathcal{H}$, then $\xi = \eta$ and $\mathrm{dom}\ T^* = \mathrm{dom}\ T$.

iii) If $\eta \in \mathrm{dom}\ (\overline{T})^*$, then for all $\phi \in \mathrm{dom}\ \overline{T}$, $\langle \eta, (\overline{T} - \lambda\mathbf{1})\phi \rangle = \langle (T^* - \lambda\mathbf{1})\eta, \phi \rangle$. Pick $\xi \in \mathrm{dom}\ \overline{T}$ with $(T - \lambda\mathbf{1})\xi = (T^* - \lambda\mathbf{1})\eta$. Hence

$$\langle \eta, (\overline{T} - \lambda\mathbf{1})\phi \rangle = \langle (\overline{T} - \lambda\mathbf{1})\xi, \phi \rangle = \langle \xi, (\overline{T} - \lambda\mathbf{1})\phi \rangle, \qquad \forall \phi \in \mathrm{dom}\ \overline{T}.$$

Since $\mathrm{rng}\ (\overline{T} - \lambda\mathbf{1}) = \mathcal{H}$, it follows that $\xi = \eta$ and $\mathrm{dom}\ T^* = \mathrm{dom}\ \overline{T}$; hence $\overline{T}$ is self-adjoint.

iv) Since $\lambda \in \rho(T)$ one has $\mathrm{rng}\ (T - \lambda\mathbf{1}) = \mathcal{H}$. The proof then follows the same lines of iii) above. □

Remark 2.2.5. Due to Proposition 2.2.4ii), $n_+, n_-, \mathrm{K}_+, \mathrm{K}_-$ quantify the "lack of self-adjointness" of a hermitian operator; so the terminology. See also Theorem 2.2.11.

Exercise 2.2.6. Show that a hermitian operator T is closed iff $U(T)$ is closed.

Exercise 2.2.7. If T is hermitian, show that T is self-adjoint iff there exists $z \in \mathbb{C}\backslash\mathbb{R}$ so that $\mathrm{rng}\ (T + z\mathbf{1}) = \mathrm{rng}\ (T + \overline{z}\mathbf{1}) = \mathcal{H}$.

Exercise 2.2.8. Let T be a hermitian operator. Show that $\mathrm{rng}\ (\overline{T} \pm i\mathbf{1}) = \overline{\mathrm{rng}\ (T \pm i\mathbf{1})}$ (the bar denotes closure).

Remark 2.2.9. From the proof of Proposition 2.2.4, one concludes that, if T is hermitian but not self-adjoint, then either $+i$ or $-i$ (or both) belongs to $\sigma(T)$, although neither of them is an eigenvalue of T. This verification is a nice exercise left to you.

Theorem 2.2.10. *If $\mathcal{H}$ has an orthonormal basis of eigenvectors of the symmetric operator $T : \mathrm{dom}\ T \subset \mathcal{H} \to \mathcal{H}$, then T is essentially self-adjoint and $\sigma(\overline{T})$ is the closure of the set of eigenvalues of T.*

Proof. Note that in this case $\mathrm{dom}\ T \sqsubseteq \mathcal{H}$, so T is in fact hermitian and $\overline{T}$ exists and is hermitian. Since its eigenvalues are real numbers, it follows that $\mathrm{rng}\ (\overline{T} \pm i\mathbf{1}) \supset \mathrm{rng}\ (T \pm i\mathbf{1})$ contains the subspace spanned by each of such eigenvectors and so it is dense in $\mathcal{H}$; by Proposition 2.2.4i) $\mathrm{rng}\ (\overline{T} \pm i\mathbf{1}) = \mathcal{H}$, since those sets are closed. Hence, by Proposition 2.2.4ii), $\overline{T}$ is self-adjoint and T is essentially self-adjoint.

Denote by (λ_j) and (ξ_j) the set of eigenvalues and eigenvectors of T, respectively. If Σ is the closure of the set of such eigenvalues in $\mathbb{C}$, then $\Sigma \subset \sigma(\overline{T})$ as the spectrum is a closed set and eigenvalues of T are also eigenvalues of $\overline{T}$. Note that every vector of $\mathcal{H}$ can be written in the form $\sum_j a_j \xi_j$. If $z \notin \Sigma$, then the operator S defined on $\mathcal{H}$ given by

$$S\left(\sum_j a_j \xi_j\right) = \sum_j \frac{a_j}{(\lambda_j - z)} \xi_j$$

is one-to-one and bounded. Since $\overline{T}$ is a closed operator, by considering partial sums of $\sum_j a_j \xi_j$ a direct verification shows that $S = R_z(\overline{T})$, so that $z \notin \sigma(\overline{T})$. Therefore, $\sigma(\overline{T}) = \Sigma$. □

Now an important result will be stated and its proof postponed to Section 2.5; this is expected to speed up the presentation. In any case one could try to get some intuition behind proofs as follows. If T is closed and hermitian, then

$$\mathcal{H} = \mathrm{rng}\ (T \pm i\mathbf{1}) \oplus (\mathrm{rng}\ (T \pm i\mathbf{1}))^\perp = \mathrm{rng}\ (T \pm i\mathbf{1}) \oplus \mathrm{K}_\mp(T),$$

and the Cayley transform $U(T)$ is an isometry between $\mathrm{rng}\ (T + i\mathbf{1})$ and $\mathrm{rng}\ (T - i\mathbf{1})$. By Proposition 2.2.4ii), in order to get a self-adjoint extension $\tilde{T}$ of T one needs to extend its domain so that $\mathrm{rng}\ (\tilde{T} \pm i\mathbf{1}) = \mathcal{H}$, that is, $U(\tilde{T})$ should be a unitary map in $\mathcal{H}$. This extension requires $n_+(T) = n_-(T)$. Here is the precise formulation:

Theorem 2.2.11 (von Neumann). *Let T be a hermitian operator with* dom $T \sqsubseteq \mathcal{H}$ *and $\overline{T}$ its closure. Then:*

a) *With respect to the graph inner product of T^* one has*

$$\text{dom } T^* = \text{dom } \overline{T} \oplus_{T^*} \text{K}_+(T) \oplus_{T^*} \text{K}_-(T).$$

So, in case T is also closed: dom $T^* = \text{dom } T \oplus_{T^*} \text{K}_+(T) \oplus_{T^*} \text{K}_-(T)$.

b) *T is essentially self-adjoint iff $n_+ = n_- = 0$.*

c) *T has self-adjoint extensions iff $n_+ = n_-$, and there exists a one-to-one correspondence between self-adjoint extensions of T and unitary operators between* K_- *and* K_+ (*and so infinitely many self-adjoint extensions if $n_+ = n_- \geq 1$*).

Remark 2.2.12. Theorem 2.2.11 was published in 1929 by von Neumann, as a generalization of a result of Weyl of 1910 for second-order differential operators. Maybe it should be called the "von Neumann-Weyl theorem."

Remark 2.2.13. A slightly different proof that "if $\mathcal{H}$ has an orthonormal basis (ξ_j) of eigenvectors of the symmetric operator $T : \text{dom } T \subset \mathcal{H} \to \mathcal{H}$, with respectively (real) eigenvalues (λ_j), then T is essentially self-adjoint" is the following: if $(T^* \pm i\mathbf{1})\eta = 0$, then for all j one has

$$0 = \langle (T^* \pm i\mathbf{1})\eta, \xi_n\rangle = \langle \eta, (T \mp i\mathbf{1})\xi_n\rangle = (\lambda_j \mp i)\langle \eta, \xi_j\rangle,$$

and so $\eta \perp \xi_j$ for all j; hence $\eta = 0$ and $n_\pm(T) = 0$.

Corollary 2.2.14. *The hermitian operator T is essentially self-adjoint iff T has exactly one self-adjoint extension.*

Proof. Half of the statement is Theorem 2.1.24b). Suppose, now, that $\overline{T}$ is not self-adjoint. By Theorem 2.2.11 either $n_- \neq n_+$ or $n_- = n_+ \geq 1$. The former possibility implies that T has no self-adjoint extensions at all. The latter possibility implies the existence of infinitely many self-adjoint extensions of T. □

Definition 2.2.15. An antilinear map $\mathcal{C} : \mathcal{H} \to \mathcal{H}$ is a *conjugation* if it is an isometry and $\mathcal{C}^2 = \mathbf{1}$.

Proposition 2.2.16 (von Neumann). *If T is hermitian and there exists a conjugation $\mathcal{C}$ such that $\mathcal{C}(\text{dom } T) \subset \text{dom } T$ and $\mathcal{C}$ commutes with T (that is, $T\mathcal{C}\xi = \mathcal{C}T\xi$, $\forall \xi \in \text{dom } T$), then T has a self-adjoint extension.*

Proof. In view of $\mathcal{C}(\text{dom } T) \subset \text{dom } T$ one has $\text{dom } T = \mathcal{C}^2(\text{dom } T) \subset \mathcal{C}\text{dom } T$, and so $\mathcal{C}(\text{dom } T) = \text{dom } T$. If $\xi \in \text{rng } (T - i\mathbf{1})^\perp$, then for any $\eta \in \text{dom } T$ (by using the polarization identity)

$$0 = \langle \xi, (T - i\mathbf{1})\eta\rangle = \langle \mathcal{C}\xi, \mathcal{C}(T - i\mathbf{1})\eta\rangle = \langle \mathcal{C}\xi, (T + i\mathbf{1})\mathcal{C}\eta\rangle,$$

and so $\mathcal{C}\xi \in \text{rng }(T + i\mathbf{1})^{\perp}$. Hence, $\mathcal{C}$ maps $\text{rng }(T - i\mathbf{1})^{\perp}$ into $\text{rng }(T + i\mathbf{1})^{\perp}$; a similar argument concludes that $\mathcal{C}$ maps $\text{rng }(T + i\mathbf{1})^{\perp}$ into $\text{rng }(T - i\mathbf{1})^{\perp}$. Since $\mathcal{C}$ is an isometry it follows that $n_+ = n_-$. By Theorem 2.2.11, T has self-adjoint extensions. □

Before presenting some applications, certain basic spectral properties of self-adjoint and unitary operators will be addressed. Since a unitary operator is bounded, its spectrum is nonempty (Corollary 1.5.17); for the corresponding result in case of unbounded self-adjoint operators see Theorem 2.4.4.

Theorem 2.2.17. *Let T be a closed hermitian operator. Then T is self-adjoint iff $\sigma(T) \subset \mathbb{R}$. In this case, for $z \in \mathbb{C} \setminus \mathbb{R}$, one has*

$$\|R_z(T)\| \le \frac{1}{|\text{Im } z|} \qquad \text{and} \qquad R_z(T)^* = R_{\overline{z}}(T).$$

Furthermore, if $0 \neq y \in \mathbb{R}$, then $\|TR_{iy}(T)\| \le 1$.

Proof. If $\sigma(T) \subset \mathbb{R}$, then $\pm i \in \rho(T)$ and $\text{rng }(T \pm i\mathbf{1}) = \mathcal{H}$; so T is self-adjoint by Proposition 2.2.4.

Now, assume that T is self-adjoint. Take a complex number $z = x + iy$, $y \neq 0$; then

$$T - z\mathbf{1} = y(S - i\mathbf{1}),$$

where $S = (T - x\mathbf{1})/y$ is self-adjoint with the same domain as T. From the relation

$$\|(S \pm i\mathbf{1})\xi\|^2 = \|S\xi\|^2 + \|\xi\|^2 \ge \|\xi\|^2$$

and $\text{rng }(S \pm i\mathbf{1}) = \mathcal{H}$ (Proposition 2.2.4), it is found that $R_{\pm i}(S) \in \mathrm{B}(\mathcal{H})$ and $\|R_{\pm i}(S)\| \le 1$. By noting that $S - i\mathbf{1} = (T - z\mathbf{1})/y$, one finds $1 \ge \|R_i(S)\| = \|R_z(T)\|\,|y|$, and so

$$\|R_z(T)\| \le \frac{1}{|\text{Im } z|}.$$

Therefore $z \in \rho(T)$ and $\sigma(T) \subset \mathbb{R}$.

For self-adjoint T and $z \in \rho(T)$ one has

$$\langle \xi, (T - z\mathbf{1})\eta \rangle = \langle (T - \overline{z}\mathbf{1})\xi, \eta \rangle, \qquad \forall \xi, \eta \in \text{dom } T.$$

Since $\text{rng }(T - z\mathbf{1}) = \text{rng }(T - \overline{z}\mathbf{1}) = \mathcal{H}$, and taking $\xi_1 = (T - \overline{z}\mathbf{1})\xi$, $\eta_1 = (T - z\mathbf{1})\eta$ one concludes that

$$\langle R_{\overline{z}}(T)\xi_1, \eta_1 \rangle = \langle \xi_1, R_z(T)\eta_1 \rangle, \qquad \forall \xi_1, \eta_1 \in \mathcal{H},$$

i.e., $R_z(T)^* = R_{\overline{z}}(T)$.

Finally the last assertion of the theorem; for $y \neq 0$ and $\xi \in \text{dom } T$ one has

$$\|(T - iy\mathbf{1})\xi\|^2 = \|T\xi\|^2 + y^2\|\xi\|^2 \ge \|T\xi\|^2.$$

Write $\xi = R_{iy}(T)\eta$; then the above inequality leads to $\|\eta\| \ge \|TR_{iy}(T)\eta\|$, $\forall \eta \in \mathcal{H}$, and so $\|TR_{iy}(T)\| \le 1$. □

Exercise 2.2.18. Show that if T is hermitian but not self-adjoint, then $\mathbb{R} \subset \sigma(T)$ and $\sigma(T) \setminus \mathbb{R} \neq \emptyset$.

Corollary 2.2.19. *Let T be self-adjoint. Then* $\mathrm{s} - \lim_{y\to\pm\infty} TR_{iy}(T) = 0$*, that is, for all $\xi \in \mathcal{H}$ one has* $\lim_{y\to\pm\infty} TR_{iy}(T)\xi = 0$.

Proof. Since dom T is dense in $\mathcal{H}$, given $\varepsilon > 0$ write $\xi = \eta + \zeta$, with $\eta \in \operatorname{dom} T$ and $\|\zeta\| < \varepsilon$. Thus, according to Theorem 2.2.17,

$$\begin{aligned}\|TR_{iy}(T)\xi\| &\leq \|TR_{iy}(T)\eta\| + \|TR_{iy}(T)\zeta\| \\ &\leq \|R_{iy}(T)T\eta\| + \|\zeta\| < \frac{\|T\eta\|}{|y|} + \varepsilon.\end{aligned}$$

For $|y| \to \infty$ one gets $\|TR_{iy}(T)\xi\| \leq \varepsilon$, and the result follows. □

Exercise 2.2.20. If T is linear and $z \in \rho(T)$, verify that $TR_z(T)$ is bounded by showing that $\|TR_z(T)\| \leq 1 + |z|\|R_z(T)\|$.

It is not difficult to check that any eigenvalue of a unitary operator has unity absolute value. This extends to all points of its spectrum:

Proposition 2.2.21. *If $U : \mathcal{H} \to \mathcal{H}$ is a unitary operator, then $\sigma(U)$ is a subset of* $\{\lambda \in \mathbb{C} : |\lambda| = 1\}$.

Proof. Since $\|U\| = 1$, Corollary 1.5.16 implies that $|\lambda| > 1$ belongs to the resolvent set of U. Since $U^{-1} = R_0(U)$ is unitary and $UU^{-1} = \mathbf{1} = U^{-1}U$, then $0 \in \rho(U)$ and if $|\lambda| = |\lambda - 0| < 1/\|U^{-1}\| = 1$ it is found, by using Theorem 1.5.12, that λ also belongs to the resolvent set of U. Therefore, if $\lambda \in \sigma(U)$, then $|\lambda| = 1$. □

2.3 Examples

In this section a series of applications of previously discussed results will be presented. For didactic reasons, sometimes different aspects of an operator will be separated into more than one example; see also Section 2.6. The Schwartz space of smooth fast decaying functions (see Section 3.1) on $\mathbb{R}^n$ will be denoted by $\mathcal{S} = \mathcal{S}(\mathbb{R}^n)$, and $C_0^\infty(\Omega)$ will indicate the set of functions with compact support and continuous derivatives of any order in $\Omega \subset \mathbb{R}^n$. Keep in mind that physical observables in quantum mechanics are represented by self-adjoint operators; see page 1 and Section 14.1.

2.3.1 Momentum and Energy

Example 2.3.1. [Standard Schrödinger (energy) operator] Let $V : \mathbb{R}^n \to \mathbb{R}$ be a real function in $\mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ and Δ denote the usual Laplacian. The operator domain is dom $H = C_0^\infty(\mathbb{R}^n) \sqsubseteq \mathrm{L}^2(\mathbb{R}^n)$ (the common practice of writing just V instead of $\mathcal{M}_V$ will be followed; see Subsection 2.3.2 for a discussion about unbounded multiplication operators),

$$(H\psi)(x) = -(\Delta\psi)(x) + V(x)\psi(x), \qquad \psi \in \text{dom } H,$$

i.e., $H = -\Delta + V$ is hermitian (use integration by parts) and has at least one self-adjoint extension. In fact, dom H is dense in $L^2(\mathbb{R}^n)$, and it is enough to apply Proposition 2.2.16 with $\mathcal{C}$ being the complex conjugation. V is called the *potential* and $-\Delta$ represents the quantum kinetic energy. These self-adjoint extensions are candidates for the quantum energy operator. Note that $V \in L^2_{\text{loc}}(\mathbb{R}^n)$ is the minimum requirement for $V\psi$ to be an element of $L^2(\mathbb{R}^n)$ with $\psi \in C_0^\infty(\mathbb{R}^n)$.

Example 2.3.2. [Polynomial potential] Example 2.3.1 applies, in particular, to potentials $V(x)$ given by real polynomials $p(x)$, $x \in \mathbb{R}^n$. As an alternative, in this case one can also take dom $H = \mathcal{S} \subset L^2(\mathbb{R}^n)$.

Example 2.3.3. [Energy operator of the harmonic oscillator] The Hilbert space is $L^2(\mathbb{R})$ and the operator is $H = -\Delta + x^2$, dom $H = \mathcal{S}$; more precisely, for $\psi \in \mathcal{S}$, $(H\psi)(x) = -\psi''(x) + x^2\psi(x)$. By Example 2.3.2 this hermitian operator has self-adjoint extensions. However, more can be said. The eigenvalue equation for this operator $H\psi = \lambda\psi$ has the well-known Hermite functions (see [Zei95], [Will03])

$$\psi_j(x) = N_j\, e^{x^2/2} \frac{d^j e^{-x^2}}{dx^j}, \qquad j = 0, 1, 2, \ldots,$$

as solutions (N_j is a normalization constant). The subsequent eigenvalues are $\lambda_j = 2(j + 1/2)$. Since $\{\psi_j\}$ form a complete orthonormal set in $L^2(\mathbb{R})$, by Theorem 2.2.10, this operator is essentially self-adjoint, its closure $\overline{H}$ is the energy operator of the quantum one-dimensional harmonic oscillator and $\sigma(\overline{H}) = \{\lambda_j\}$. Note that the minimum of the energy spectrum is greater than zero, in contrast to the classical case whose minimum of the harmonic oscillator energy is zero; this is a purely quantum fact, as well as the discrete possible values of energy.

After including all physical constants (particle mass m, oscillator frequency ω and Planck constant $\hbar$), the formal energy operator for the quantum harmonic oscillator energy looks like

$$H = -\frac{\hbar^2}{2m}\Delta + \frac{1}{2}m\omega^2 x^2,$$

and its eigenvalues are $\lambda_j = \omega\hbar(j + 1/2)$, so that the minimum energy is $\omega\hbar/2$. All eigenvalues are simple, that is, they have multiplicity 1.

Remark 2.3.4. If in Example 2.3.1 $V(x) \in L^2_{\text{loc}}(\mathbb{R}^n)$ and $V(x) \geq \beta$, for some $\beta \in \mathbb{R}$, then it is shown in Corollary 6.3.5 that the corresponding Schrödinger operator $H = -\Delta\psi + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$. This unique self-adjoint extension plays the unequivocal role of the quantum energy operator in this case.

Example 2.3.5. [Free particle energy in the "box" $[0, 1]$ with Dirichlet boundary conditions] Here $\mathcal{H} = L^2[0, 1]$. Set dom $T_D = \{\psi \in C^2[0, 1] : \psi(0) = \psi(1) = 0\}$

and $(T_D\psi)(x) = -\Delta\psi = -\psi''(x)$. It is a hermitian operator. The set $\psi_j^D(x) = \sqrt{2}\sin(j\pi x)$, $j \geq 1$, is an orthonormal basis of $L^2[0,1]$ and since $T_D\psi_j^D = j^2\pi^2\psi_j^D$, by Theorem 2.2.10, it follows that T_D is essentially self-adjoint and the spectrum of its unique self-adjoint extension $\overline{T}_D$ is $\{j^2\pi^2 : j \geq 1\}$; all eigenvalues are simple. See Example 4.4.3.

Example 2.3.6. [Free particle energy in the "box" $[0,1]$ with Neumann boundary conditions] Here $\mathcal{H} = L^2[0,1]$. Set dom $T_N = \{\psi \in C^2[0,1] : \psi'(0) = \psi'(1) = 0\}$ and $(T_N\psi)(x) = -\psi''(x)$. It is a hermitian operator. The set $\psi_0^N(x) = 1$, $\psi_j^N(x) = \sqrt{2}\cos(j\pi x)$, $j \geq 1$, is an orthonormal basis of $L^2[0,1]$ and since $T_N\psi_j^N = j^2\pi^2\psi_j^N$, $\forall j$, it follows that T_N is essentially self-adjoint and the spectrum of its unique self-adjoint extension $\overline{T}_N$ is $\{j^2\pi^2 : j \geq 0\}$. All eigenvalues are simple.

Example 2.3.7. [Free particle energy in the "box" $[0,1]$ with periodic boundary conditions] Here $\mathcal{H} = L^2[0,1]$. Set dom $T_P = \{\psi \in C^2[0,1] : \psi(0) = \psi(1), \psi'(0) = \psi'(1)\}$ and $(T_P\psi)(x) = -\psi''(x)$. It is a hermitian operator. The set $\psi_j^P(x) = \exp(j2\pi ix)$, $j \in \mathbb{Z}$, is an orthonormal basis of $L^2[0,1]$ and since $T_P\psi_j^P = 4j^2\pi^2\psi_j^N$, it follows that T_P is essentially self-adjoint, the spectrum of its unique self-adjoint extension $\overline{T}_P$ is $\{4j^2\pi^2 : j \geq 0\}$ and, except the zero, each eigenvalue has multiplicity 2. This multiplicity can be understood physically: the case of periodic boundary conditions means the particle is in fact on a circumference, so that given a nonzero energy value it can be reached by either clockwise or counterclockwise rotations, so the multiplicity 2. For a description of $\overline{T}_P$ see Exercise 4.4.4.

Example 2.3.8. The operator T : dom $T_D \cap$dom $T_N \to L^2[0,1]$ (see Examples 2.3.5 and 2.3.6), $(T\psi)(x) = -\psi''(x)$, is hermitian (its domain is dense in the Hilbert space since it contains $C_0^\infty(0,1)$) and has at least three different self-adjoint extensions: $\overline{T}_D$, $\overline{T}_N$ and $\overline{T}_P$.

Let $I \subset \mathbb{R}$ be an interval and $\psi^{(k)}$ the kth derivative of the function $\psi : I \to \mathbb{C}$; the space of absolutely continuous functions on every closed bounded subinterval of I is denoted by AC(I). Recall that ψ belongs to AC(I) iff it can be written in the form

$$\psi(x) = \psi(c) + \int_c^x \phi(s)\,ds, \qquad c \in I,\ \phi \in L^1_{\text{loc}}(I),$$

and a.e. $\psi'(x) = \phi(x)$, i.e., the fundamental theorem of calculus holds. Such functions map sets of zero Lebesgue measure into sets of zero Lebesgue measure. In case of a bounded closed interval $I = [a,b]$ one has $\psi' \in L^1[a,b]$ and $\psi \in C[a,b]$.

For $m \in \mathbb{N}$, recall the Sobolev spaces $\mathcal{H}^m(I)$ (more details appear in Section 3.2; in this sense the discussion here could be considered premature, but important for applications), which consists of all $\psi \in L^2(I)$ obeying $\psi^{(k)} \in \text{AC}(I) \cap L^2(I)$ for $k = 0, 1, \ldots, m-1$ and $\psi^{(m)} \in L^2(I)$. The spaces $\mathcal{H}^m(I)$ are Hilbert spaces with the norm

$$|||\psi|||_m := \left(\sum_{k=0}^m \|\psi^{(k)}\|^2 \right)^{\frac{1}{2}}$$

and $\psi \in C(\overline{I})$, so that ψ is bounded and, when applicable, $\lim_{x\to\pm\infty} \psi(x) = 0$. Furthermore, for $\psi \in \mathcal{H}^m(I)$ the above derivatives $\psi^{(k)}$ coincide with the corresponding distributional (also called weak) derivatives.

An important property of absolutely continuous functions ψ, φ is the integration by parts formula

$$\int_a^b \psi(s)\varphi'(s)\,ds = \psi(b)\varphi(b) - \psi(a)\varphi(a) - \int_a^b \psi'(s)\varphi(s)\,ds.$$

The failure of the integration by parts formula is related to the existence of strictly monotone continuous functions for which the derivatives vanish almost everywhere; consequently, for $\mathcal{H}^m$ it is not enough to ask for functions in L^2 with derivatives in L^2, and distributional derivatives must be invoked.

As a rule, the rudiments of distributions are assumed to be known. In any event, it is worth presenting the following fundamental uniqueness result.

Lemma 2.3.9. *Let $I = (a, b) \subset \mathbb{R}$ be an open interval* ($-\infty \le a < b \le \infty$) *and u a distribution acting on $C_0^\infty(I)$ with derivative $u' = 0$. Then u is constant.*

Proof. Note first that if $\phi \in C_0^\infty(I)$, then its primitive $\Phi(x) = \int_a^x \phi(t)dt$ also belongs to $C_0^\infty(I)$ iff $\int_I \phi(t)\,dt = 0$. Recall that (see Section 3.2) $u' = 0$ means $u'(\phi) := -u(\phi') = 0$ for all $\phi \in C_0^\infty(I)$.

Pick $\phi_0 \in C_0^\infty(I)$ with $\int_I \phi_0(t)\,dt = 1$, and for each $\phi \in C_0^\infty(I)$ consider

$$\psi = \phi - \left(\int_I \phi(t)\,dt\right)\phi_0.$$

Since $\psi \in C_0^\infty(I)$ and $\int_I \psi(t)\,dt = 0$ it follows that this function is the derivative of an element of $C_0^\infty(I)$ and so

$$0 = u(\psi) = u(\phi) - \left(\int_I \phi(t)\,dt\right)u(\phi_0).$$

Therefore, for any $\phi \in C_0^\infty(I)$, $u(\phi) = \int_I u(\phi_0)\phi(t)\,dt$ and u is represented by the constant function $u(\phi_0)$. □

Remark 2.3.10. a) From the above proof and discussion it should be clear that, in open intervals in $\mathbb{R}$, the derivative of a distribution u is a locally integrable function iff u is represented by an absolutely continuous function.

b) Lemma 2.3.9 has a natural generalization for connected open subsets Ω of $\mathbb{R}^n$: if a distribution u has partial distributional derivatives at all points of Ω, that is, $\frac{\partial u}{\partial x_j} = 0$, $1 \le j \le n$, then u is constant.

Example 2.3.11. [Momentum operator on $\mathbb{R}$] Let $\mathrm{dom}\, P_0 = C_0^\infty(\mathbb{R}) \sqsubseteq \mathcal{H} = \mathrm{L}^2(\mathbb{R})$, $(P_0\psi)(x) = -i\psi'(x)$, $\psi \in \mathrm{dom}\, P_0$. An integration by parts shows that P_0 is hermitian. Accept, for a moment, that $\mathrm{dom}\, P_0^* = \mathcal{H}^1(\mathbb{R})$ and $P_0^* u = -iu'$, $u \in \mathcal{H}^1(\mathbb{R})$.

Another integration by parts shows that P_0^* is hermitian. Then (see Theorem 2.1.24c)) $P_0 \subset P_0^* \subset P_0^{**} = \overline{P_0}$; denote $P = \overline{P_0}$. From the first inclusion $P_0^{**} = P \subset P_0^*$ and so $P = P_0^{**} = P_0^*$, concluding that P is self-adjoint and so P_0 is essentially self-adjoint. The operator P is the quantum momentum operator for a particle in the line $\mathbb{R}$.

Now we will check the claims about the adjoint P_0^*. If $u \in \mathcal{H}^1(\mathbb{R})$, a direct verification implies that $u \in \operatorname{dom} P_0^*$ and $P_0^* u = -iu'$; indeed, if $\psi \in \operatorname{dom} P_0$ its support is contained in an interval (a, b), consequently

$$\begin{aligned}\langle u, P_0\psi\rangle &= \int_a^b \overline{u(x)}(-i\psi'(x))\,dx \\ &= -i\left[\overline{u(b)}\psi(b) - \overline{u(a)}\psi(z) - \int_a^b \overline{u'(x)}\psi(x)\right] \\ &= \int_a^b \overline{-iu'(x)}\psi(x).\end{aligned}$$

Now let $u \in \operatorname{dom} P_0^*$; set $w = P_0^* u$ and $W(x) = \int_0^x w(t)\,dt$, which is absolutely continuous in any bounded interval $(-m, m) \subset \mathbb{R}$. If $\psi \in C_0^\infty(-m, m)$, then an integration by parts gives us

$$\begin{aligned}\langle u, P_0\psi\rangle &= \langle P_0^* u, \psi\rangle = \langle w, \psi\rangle \\ &= \int_{-m}^m \overline{u(x)}(-i\psi'(x))\,dx = \int_{-m}^m \overline{w(x)}\psi(x)\,dx \\ &= \overline{W(m)}\psi(m) - \overline{W(-m)}\psi(-m) - \int_{-m}^m \overline{W(x)}\psi'(x)\,dx \\ &= -\int_{-m}^m \overline{W(x)}\psi'(x)\,dx.\end{aligned}$$

Hence, $\int_{-m}^m (\overline{W(x) + iu(x)})\psi'(x)\,dx = 0$ for all $\psi \in C_0^\infty(-m, m)$ and, by Lemma 2.3.9, $y(x) = W(x)+iu(x)$ is a constant function in $(-m, m)$; m being arbitrary, $y(x)$ is constant in all $\mathbb{R}$. Therefore, u is absolutely continuous in any bounded interval and $0 = y' = W' + iu' = P_0^* u + iu$, so that $P_0^* u = -iu$.

Exercise 2.3.12. By using P_0^* as in Example 2.3.11, compute the deficiency subspaces K_- and K_+ and show explicitly that $n_+ = n_- = 0$. Conclude again that P_0 is essentially self-adjoint.

Exercise 2.3.13. Verify that the operator $\operatorname{dom} P_0 = \mathcal{S}(\mathbb{R}) \sqsubseteq \mathrm{L}^2(\mathbb{R})$, with the action $(P_0\psi)(x) = -i\psi'(x)$, $\psi \in \operatorname{dom} P_0$, is essentially self-adjoint and its unique self-adjoint extension is the same operator P obtained in Example 2.3.11.

Example 2.3.14. [Momentum operator on $[0, 1]$] Let $\operatorname{dom} P = C_0^\infty(0, 1) \sqsubseteq \mathcal{H} = \mathrm{L}^2[0, 1]$, and $(P\psi)(x) = -i\psi'(x), \psi \in \operatorname{dom} P$. An integration by parts shows that P is hermitian. By following the lines of the argument used in Example 2.3.11 it can be shown that dom $P^* = \mathcal{H}^1[0,1]$ and $(P^*\psi)(x) = -i\psi'(x), \psi \in \text{dom } P^*$. The next step is to calculate its deficiency indices $n_\pm$.

n_+: if $u \in \mathrm{N}(P^* + i\mathbf{1})$, then $-iu' = -iu$ and, since u is a continuous function this equation implies that it is also continuously differentiable, so $u(x) = ce^x$, for some constant c; thus $n_+ = 1$.

n_-: if $u \in N(P^* - i\mathbf{1})$, then $-iu' = iu$ and, since u is a continuous function, $u(x) = ce^{-x}$, and $n_- = 1$.

Therefore $n_- = n_+ = 1$ and P has infinitely many self-adjoint extensions.

Exercise 2.3.15. Verify that the closure of P in Example 2.3.14 has the same action but with domain $\{\psi \in \mathcal{H}^2[0,1] : \psi(0) = \psi(1) = 0\}$.

Example 2.3.16. This is P in Example 2.3.14 revisited. Now the deficiency indices will be obtained by computing $(\text{rng } (P \pm i\mathbf{1}))^\perp$, that is, with no explicit need of the adjoint operator. The idea can be adapted to other situations. Let

$$\text{dom } P = C_0^\infty(0,1) \sqsubseteq \mathcal{H} = \mathrm{L}^2[0,1],$$

$(P\psi)(x) = -i\psi'(x), \psi \in \text{dom } P$. An integration by parts shows that P is hermitian.

If $\phi \in \text{rng } (P + i\mathbf{1})$, then there is $\psi \in \text{dom } P$ so that

$$-i\frac{d\psi}{dx} + i\psi = \phi.$$

Clearly $\phi \in C_0^\infty(0,1)$. After multiplying by the integrating factor e^{-x}, one gets

$$\frac{d(e^{-x}\psi)}{dx}(x) = ie^{-x}\phi(x),$$

and since ψ has compact support $\int_0^1 e^{-x}\phi(x)\,dx = 0$. Conversely, if $\phi \in C_0^\infty(0,1)$ satisfies this latter condition, then $\psi(x) = i\int_0^x e^{(x-t)}\phi(t)dt$ belongs to dom P and $(P + i\mathbf{1})\psi = \phi$. Therefore, $(\text{rng } (P + i\mathbf{1}))^\perp$ is the vector space spanned by e^{-x} and $n_- = 1$. Similarly one gets $n_+ = 1$. Therefore $n_- = n_+ = 1$ and P has infinitely many self-adjoint extensions.

Example 2.3.17. [Momentum operator on $[0,\infty)$?] Let

$$\text{dom } P = C_0^\infty(0,\infty) \sqsubseteq \mathcal{H} = \mathrm{L}^2[0,\infty),$$

$(P\psi)(x) = -i\psi'(x), \psi \in \text{dom } P$. An integration by parts shows that P is hermitian. As in Example 2.3.11, it can be shown that dom $P^* = \mathcal{H}^1[0,\infty)$ and $(P^*\psi)(x) = -i\psi'(x), \psi \in \text{dom } P^*$.

The next step is to calculate its deficiency indices.

n_+: if $u \in \mathrm{N}(P^* + i\mathbf{1})$, then $-iu' = -iu$ and, as in Example 2.3.14 one gets $u(x) = ce^x$. Since $u \notin \mathcal{H}$ for $c \neq 0$, $n_+ = 0$.

n_-: if $u \in \mathrm{N}(P^* - i\mathbf{1})$, then $-iu' = iu$ and $u(x) = ce^{-x}$; so $n_- = 1$.

Therefore $n_- \neq n_+$ and P has no self-adjoint extensions!

Example 2.3.18. [Free particle energy operator on $\mathbb{R}$] Let dom $H = C_0^\infty(\mathbb{R}) \sqsubseteq \mathrm{L}^2(\mathbb{R})$, $(H\psi)(x) = -\psi''(x)$, $\psi \in$ dom H, which is clearly hermitian. Accept, for a moment, that dom $H^* = \mathcal{H}^2(\mathbb{R})$ and $H^*\psi = -\psi''$ for $\psi \in$ dom H^*; then H^* is hermitian (check it!) so that, by Theorem 2.1.24c), $\overline{H} = H^{**} = H^*$ is the unique self-adjoint extension of H. $\overline{H}$ is the free particle energy operator on $\mathbb{R}$.

Now we will check the claims about the adjoint H^*; the arguments resemble those in Example 2.3.11. If $u \in \mathcal{H}^2(\mathbb{R})$ then a direct verification shows that $u \in$ dom H^* and $H^*u = -u''$.

Now let $u \in$ dom H^*, set $v = H^*u$, $V(x) = \int_0^x v(t)\,dt$, and $W(x) = \int_0^x V(t)\,dt = \int_0^x \int_0^t v(s)\,ds\,dt$. V and W are absolutely continuous in any bounded interval $[-m,m] \subset \mathbb{R}$. If $\psi \in C_0^\infty(-m,m)$, then integrations by parts imply

$$\begin{aligned}\langle u, H\psi\rangle = \langle u, -\psi''\rangle &= \int_{-m}^{m} \overline{u(x)}(-\psi''(x))\,dx = \langle v, \psi\rangle \\ &= \int_{-m}^{m} \overline{v(x)}\psi(x)\,dx = -\int_{-m}^{m} \overline{V(x)}\psi'(x)\,dx \\ &= \int_{-m}^{m} \overline{W(x)}\psi''(x)\,dx\end{aligned}$$

so that

$$\int_{-m}^{m} (\overline{u(x) + W(x)})\psi''(x)\,dx = 0$$

and the distributional derivative $(u(x) + W(x))'' = 0$. Hence there exists a constant c_1 so that $(u(x) + W(x))' = c_1$ in $(-m,m)$, so $(u(x) + W(x) - c_1 x)' = 0$ and there is another constant c_2 for which $u(x) = -W(x) + c_1 x + c_2$. Since W and $W' = V$ are absolutely continuous functions and $W'' = v \in \mathrm{L}^2(\mathbb{R})$, it follows that $u \in \mathcal{H}^2(\mathbb{R})$ and $H^*u = v = -u''$.

Example 2.3.19. [Free particle energy operator on $[0,\infty)$] Let

$$\text{dom } H = C_0^\infty(0,\infty) \sqsubseteq \mathrm{L}^2[0,\infty),$$

$(H\psi)(x) = -\psi''(x), \psi \in$ dom H. Integrations by parts show that H is hermitian. By following the lines of Example 2.3.18, it is found that dom $H^* = \mathcal{H}^2[0,\infty)$ and $(H^*\psi)(x) = -\psi''(x), \psi \in$ dom H^*. The next step is to calculate its deficiency indices.

n_-: if $u \in \mathrm{N}(H^* - i\mathbf{1})$, then $-u'' = iu$ and, since u is a continuously differentiable function, there are exactly two linearly independent solutions, say $e^{(1-i)x/\sqrt{2}}$ and $e^{-(1-i)x/\sqrt{2}}$; since only the latter belongs to dom H^* one gets $n_- = 1$.

n_+: similarly one gets $n_+ = 1$.

Therefore, H has infinitely many self-adjoint extensions; they are candidates for representing the free energy operator for a particle in the half-line $[0,\infty)$. See Exercise 4.4.15. All self-adjoint extensions of H are described in Example 7.3.1.

Proposition 2.3.20. *Let* $V : (a,b) \to \mathbb{R}$ *be a real function (potential energy) in* $\mathrm{L}^2_{\mathrm{loc}}(a,b)$ $(-\infty \le a < b \le +\infty)$*. Then the minimal operator* $\mathrm{dom}\ H = C_0^\infty(a,b) \subset \mathcal{H} = \mathrm{L}^2(a,b)$ *(see Example* 2.3.1 *and Remark* 2.3.4*),*

$$(H\psi)(x) = -\psi''(x) + V(x)\psi(x), \qquad \psi \in \mathrm{dom}\ H,$$

is hermitian,

$$\mathrm{dom}\ H^* = \left\{\psi \in \mathrm{L}^2(a,b) : \psi, \psi' \in \mathrm{AC}(a,b), (-\psi'' + V\psi) \in \mathrm{L}^2(a,b)\right\}$$

and

$$(H^*\psi)(x) = -\psi''(x) + V(x)\psi(x), \qquad \psi \in \mathrm{dom}\ H^*.$$

Proof. Integrations by parts show that the above set is in $\mathrm{dom}\ H^*$ and that $H^*\psi$ is as above for such vectors. Now let $u \in \mathrm{dom}\ H^*$; then

$$\langle H\phi, u\rangle = \langle -\phi'' + V\phi, u\rangle = \langle \phi, H^*u\rangle, \qquad \forall \phi \in C_0^\infty(a,b).$$

Note that $u, H^*u \in \mathrm{L}^2[a,b] \subset \mathrm{L}^1_{\mathrm{loc}}(a,b)$ and since $V \in \mathrm{L}^2_{\mathrm{loc}}(a,b)$ it follows that $Vu \in \mathrm{L}^1_{\mathrm{loc}}(a,b)$ (check this!); so, for a fixed $c \in (a,b)$, the function

$$W(x) := \int_c^x ds \int_c^s dt\ (V(t)u(t) - (H^*u)(t))$$

and its derivative $W'(x)$ are absolutely continuous in the open interval (a,b), and Lebesgue a.e. $W''(x) = V(x)u(x) - (H^*u)(x)$. One can thus integrate by parts to get

$$\begin{aligned}\int_a^b dx\, \overline{\phi''(x)} u(x) = \langle \phi'', u\rangle &= \langle V\phi - H\phi, u\rangle \\ &= \int_a^b dx\, \overline{\phi(x)}\left((H^*u)(x) - V(x)u(x)\right) \\ &= \int_a^b dx\, \overline{\phi(x)} W''(x) = \int_a^b dx\, \overline{\phi''(x)} W(x).\end{aligned}$$

Hence, $0 = \int_a^b dx\, \phi''\, (\overline{u - W})$ for all $\phi \in C_0^\infty(a,b)$, so that the distributional second derivative $(u - W)'' = 0$ and, by Lemma 2.3.9, $u(x) = W(x) + c_1 x + c_2$ for suitable constants c_1, c_2. Since W and W' are absolutely continuous functions, then u, u' are also absolutely continuous in (a,b), and since $W'' = Vu - H^*u$, it follows that $-u'' + Vu = H^*u \in \mathrm{L}^2(a,b)$. The result is proved. Another proof appears in Example 3.2.16. □

Remark 2.3.21. Note the general strategy: except if there are strong reasons for the choice of specific boundary conditions, the domain of the original hermitian operator does not "touch" the boundary of the region (e.g., for a particle in $[0,\infty)$ one considers $C_0^\infty(0,\infty)$), so that what happens at the boundary is left for the self-adjoint extensions, each one corresponding to a different physical situation. In fact, more can be said: the self-adjoint extensions that are found are mathematical indications of the physical possibilities (which are embodied in the choice of the original domain of the hermitian operator).

Example 2.3.22. In the case of a sum of operators $T_1\xi + T_2\xi$ it is possible that neither $T_1\xi$ nor $T_2\xi$ is in the Hilbert space, but their sum is, due to suitable cancellations! For instance, if dom $T = C_0^\infty(0,1) \subset \mathrm{L}^2[0,1]$,

$$T\phi = -\phi'' - \frac{1}{4x^2}\phi, \qquad \phi \in \text{dom } T,$$

it follows that $\psi(x) = \sqrt{x} \in \text{dom } T^*$ (see Proposition 2.3.20); although neither ψ'' nor $\psi/(4x^2)$ belong to the Hilbert space, one has $T^*\psi = -\psi'' - \frac{1}{4x^2}\psi = 0 \in \mathrm{L}^2[0,1]$, i.e., ψ is an eigenvector of T^*. The self-adjoint extensions of this operator are discussed in Example 7.4.1.

Exercise 2.3.23. Show that the operator $P_-\psi = -i\psi'$, with domain

$$\text{dom } P_- = C_0^\infty(-\infty, 0) \subset \mathrm{L}^2(-\infty, 0],$$

is hermitian and has deficiency indices $n_- = 0$ and $n_+ = 1$. Given nonnegative integers m_-, m_+, use direct sums of this operator P_- and P of Example 2.3.17 to construct hermitian operators with deficiency indices $n_- = m_-$ and $n_+ = m_+$.

2.3.2 Multiplication Operator

Let μ be a positive Borel measure over a metric space X obeying $\mu(E) < \infty$ for all bounded Borel sets $E \subset X$. Fix a Borel set E and let $\varphi : E \to \mathbb{C}$ be a measurable function; define the *multiplication operator* by φ as the linear operator (cf. the bounded case in Example 1.1.2)

$$\text{dom } \mathcal{M}_\varphi := \left\{\psi \in \mathrm{L}^2_\mu(E) : (\varphi\psi) \in \mathrm{L}^2_\mu(E)\right\},$$
$$(\mathcal{M}_\varphi\psi)(x) := \varphi(x)\psi(x), \qquad \psi \in \text{dom } \mathcal{M}_\varphi.$$

A very important example of a multiplication operator is the potential energy $\mathcal{M}_V$, with $V : E \to \mathbb{R}$, $E \subset \mathbb{R}^n$, which will usually be denoted simply by V. The total mechanical energy is $H = H_0 + V$, with $H_0 = -\Delta$ denoting the quantum kinetic energy, after a suitable domain is provided. This H is commonly referred to as the standard Schrödinger operator.

Proposition 2.3.24. dom $\mathcal{M}_\varphi$ *is dense in* $\mathrm{L}^2_\mu(E)$ *and* ${\mathcal{M}_\varphi}^* = \mathcal{M}_{\overline{\varphi}}$.

Proof. Let $\phi \in (\text{dom } \mathcal{M}_\varphi)^\perp$ and $E_n := |\varphi|^{-1}([0,n))$, which is measurable. If $\phi_n = \chi_{E_n}\phi$, then $\phi_n \in \text{dom } \mathcal{M}_\varphi$ and

$$0 = \langle \phi, \phi_n \rangle = \int_{E_n} |\phi|^2 \, d\mu,$$

so that μ-a.e. $\phi_n = 0$. By dominated convergence

$$\int_E |\phi|^2 \, d\mu = \lim_{n\to\infty} \int_{E_n} |\phi|^2 \, d\mu = 0$$

and so $\phi = 0$; it follows that dom $\mathcal{M}_\varphi$ is dense in $\mathrm{L}^2_\mu(E)$.

Thus, the adjoint operator ${\mathcal{M}_\varphi}^*$ is well defined and if $f \in \mathrm{dom}\ {\mathcal{M}_\varphi}^*$, there is $g \in \mathrm{L}^2_\mu(E)$ with

$$\int_E \overline{\overline{\varphi} f}\, \psi \, d\mu = \int_E \overline{f}\, \varphi\psi \, d\mu = \langle f, \mathcal{M}_\varphi \psi\rangle = \langle g, \psi\rangle, \qquad \forall \psi \in \mathrm{dom}\ \mathcal{M}_\varphi.$$

The goal is to verify that $\mathcal{M}_{\overline{\varphi}} f \in \mathrm{L}^2_\mu(E)$. Define $f_n = \chi_{E_n} f \in \mathrm{dom}\ \mathcal{M}_{\overline{\varphi}} = \mathrm{dom}\ \mathcal{M}_\varphi$, and so $\int_E (\overline{\varphi} f_n - {\mathcal{M}_\varphi}^* f_n)\psi \, d\mu = 0$, and by taking ψ properly one gets $\int_{E_n} |\overline{\varphi} f - {\mathcal{M}_\varphi}^* f|\, \psi \, d\mu = 0$, so that μ-a.e. in E_n one has $\int_E (\overline{\varphi} f_n - {\mathcal{M}_\varphi}^* f_n)\psi \, d\mu = 0$ and $({\mathcal{M}_\varphi}^* f)(x) = \overline{\varphi(x)} f(x)$. Therefore

$$f \in \mathrm{dom}\ \mathcal{M}_{\overline{\varphi}}, \qquad \mathcal{M}_{\overline{\varphi}} f = g = {\mathcal{M}_\varphi}^* f,$$

and $\mathcal{M}_{\overline{\varphi}} = {\mathcal{M}_\varphi}^*$. □

Corollary 2.3.25. *$\mathcal{M}_\varphi$ is self-adjoint iff φ is a real function.*

Proof. It follows directly by Proposition 2.3.24. It is instructive to mention an alternative argument. Note that $\mathcal{M}_\varphi$ is hermitian iff φ is real and in this case $\mathcal{M}_{(\varphi \pm i\mathbf{1})^{-1}}$ is the bounded resolvent operator $R_{\pm i}(\mathcal{M}_\varphi)$, so that rng $(\mathcal{M}_\varphi \pm i\mathbf{1}) = \mathrm{L}^2_\mu(E)$ and $\mathcal{M}_\varphi$ is self-adjoint by Proposition 2.2.4. □

Definition 2.3.26. The (μ-) *essential image* of $\varphi : E \to \mathbb{C}$ is the set of all $y \in \mathbb{C}$ so that $\mu\left(\{x \in E : |\varphi(x) - y| < \varepsilon\}\right) > 0$, $\forall \varepsilon > 0$.

Proposition 2.3.27.

a) *The spectrum $\sigma(\mathcal{M}_\varphi)$ is the essential image of φ.*

b) *λ is an eigenvalue of $\mathcal{M}_\varphi$ iff $\mu(\{\varphi^{-1}(\lambda)\}) > 0$.*

Proof. a) If $\lambda \notin \sigma(\mathcal{M}_\varphi)$, then $0 \notin \sigma(\mathcal{M}_{\varphi-\lambda})$ and there is $S \in \mathrm{B}(\mathrm{L}^2_\mu(E))$ with $(S\mathcal{M}_{\varphi-\lambda}\psi)(x) = \psi(x)$, $\forall \psi \in \mathrm{dom}\ \mathcal{M}_\varphi$; for such vectors $\|\psi\|^2 \le \|S\|^2\, \|\mathcal{M}_{\varphi-\lambda}\psi\|^2$. Thus

$$\int_E \left(\frac{1}{\|S\|^2} - |\varphi(x) - \lambda|^2 \right) |\psi(x)|^2 \, d\mu(x) \le 0,$$

and so μ-a.e. $|\varphi(x) - \lambda| \ge \frac{1}{\|S\|}$ (e.g., consider $\psi = \chi_{E_n}$ with $E_n = \varphi^{-1}(-n, n)$), which shows that λ does not belong to the essential image of φ.

On the other hand, if $\exists \varepsilon_0 > 0$ with μ-a.e. $|\varphi(x) - \lambda| \ge \varepsilon_0$, then $\mathcal{M}_{\frac{1}{\varphi-\lambda}}$ is a bounded inverse of $\mathcal{M}_{\varphi-\lambda}$, since $\|\mathcal{M}_{\frac{1}{\varphi-\lambda}}\psi\| \le \frac{1}{\varepsilon_0}\|\psi\|$, $\forall \psi \in \mathrm{L}^2_\mu(E)$; therefore $\lambda \notin \sigma(\mathcal{M}_\varphi)$.

b) λ is an eigenvalue of $\mathcal{M}_\varphi$ iff there exists an element $0 \ne \psi \in \mathrm{L}^2_\mu(E)$ with $(\varphi(x) - \lambda)\psi(x) = 0$ a.e. iff $\mu(\varphi^{-1}(\lambda)) > 0$ since one has $\mu(\{x \in E : \psi(x) \ne 0\}) > 0$. □

Exercise 2.3.28. Let E be a Borel subset of $\mathbb{R}^n$. Show that the subspace of compactly supported functions $\psi \in \mathrm{L}^2_\mu(E)$ is a core of $\mathcal{M}_\varphi$ acting in $\mathrm{L}^2_\mu(E)$.

Exercise 2.3.29. Let E be an open subset of $\mathbb{R}^n$ and $\varphi : E \to \mathbb{C}$ continuous. For $\mathcal{M}_\varphi$ acting in $\mathrm{L}^2(\mathbb{R}^n)$, show that $\sigma(\mathcal{M}_\varphi) = \overline{\mathrm{rng}\ \varphi}$ (the bar indicates closure).

Exercise 2.3.30. Let ℓ denote Lebesgue measure over $\mathbb{R}$ and set

$$\mu = \ell + \delta_4 + \delta_{-4}$$

over $\mathbb{R}$ (δ_y denotes the Dirac measure at y, that is, for each $\Lambda \subset \mathbb{R}$, $\delta_y(\Lambda) = 1$ if $y \in \Lambda$ and 0 otherwise) and

$$\varphi(x) = \begin{cases} x^2 & x \geq 0 \\ 3 & x < 0 \end{cases}.$$

Find the spectrum and eigenvalues of $\mathcal{M}_\varphi$ acting in $\mathrm{L}^2_\mu(\mathbb{R})$.

Exercise 2.3.31. [Position operator on $\mathbb{R}$] Let $q : \mathbb{R} \to \mathbb{R}$, $q(x) = x$ and $\mathcal{M}_q$ acting in $\mathrm{L}^2(\mathbb{R})$. Then $\mathcal{M}_q$ is self-adjoint and represents the quantum position operator. Show that $\mathcal{M}_q$ has no eigenvalues and that its spectrum is $\mathbb{R}$.

2.4 Weyl Sequences

It is possible to characterize the spectrum of some linear operators, including self-adjoint and unitary, by means of Weyl sequences, which are especial sequences in the operator domain that give a flavor of "generalized eigenvalue" for each spectral point. Before defining them, it will be shown that any self-adjoint operator has nonempty spectrum.

Lemma 2.4.1. *Let T be densely defined in $\mathcal{H}$.*

a) *If* $\mathrm{rng}\ T$ *is dense in $\mathcal{H}$ and T is one-to-one, then T^* is one-to-one and $(T^*)^{-1} = (T^{-1})^*$. In particular, if T is self-adjoint and T^{-1} exists, then T^{-1} is also self-adjoint (recall* $\overline{\mathrm{rng}\ T} = \mathcal{H}$, *since* $\mathcal{H} = \mathrm{N}(T) \oplus \overline{\mathrm{rng}\ T}$ *and if T^{-1} exists* $\mathrm{N}(T) = \{0\}$).
b) *If $z \in \rho(T)$, then $R_z(T)^* = R_{\overline{z}}(T^*)$.*
c) *If T is closed, then $\sigma(T^*) = \overline{\sigma(T)}$ (here the bar indicates complex conjugation).*

Proof. a) From $\mathrm{N}(T^*) = (\mathrm{rng}\ T)^\perp$ one gets $\mathrm{N}(T^*) = \{0\}$ and so T^* is injective. Since $\mathcal{G}(T^*) = (J\mathcal{G}(T))^\perp$ and $\mathcal{G}(T^{-1}) = W\mathcal{G}(T)$, with $W(\xi, \eta) = (\eta, \xi)$, which is unitary and $W^{-1} = W$, one has

$$\begin{aligned}\mathcal{G}((T^{-1})^*) &= (J\mathcal{G}(T^{-1})^\perp = (JW\mathcal{G}(T))^\perp \\ &= W(J\mathcal{G}(T))^\perp = W\mathcal{G}(T^*) = \mathcal{G}((T^*)^{-1}),\end{aligned}$$

so that $(T^*)^{-1} = (T^{-1})^*$.

b) If $z \in \rho(T)$, then $T - z\mathbf{1}$ is one-to-one with rng $(T - z\mathbf{1}) = \mathcal{H}$. Thus, by a), $(T - z\mathbf{1})^*$ is one-to-one and

$$\left((T - z\mathbf{1})^{-1}\right)^* = ((T - z\mathbf{1})^*)^{-1} = (T^* - \overline{z}\mathbf{1})^{-1},$$

that is, $R_z(T)^* = R_{\overline{z}}(T^*)$.

c) Recall that here the bar indicates complex conjugation. By b) one has $\overline{\rho(T)} \subset \rho(T^*)$; since T is closed, $T = T^{**}$, and consequently

$$\overline{\rho(T)} \subset \rho(T^*) \subset \overline{\rho(T^{**})} = \overline{\rho(T)}.$$

This finishes the proof. □

Lemma 2.4.2. *Let T be a linear operator in $\mathcal{H}$.*

a) *If for $z_0 \in \mathbb{C}$ the operator $T - z_0\mathbf{1}$ is one-to-one, then*

$$\sigma((T - z_0)^{-1}) \setminus \{0\} = \left\{(z - z_0)^{-1} : z_0 \neq z \in \sigma(T)\right\}.$$

b) *If $z_0 \in \rho(T)$ then the spectral radius*

$$r_\sigma(R_{z_0}(T)) = \frac{1}{d(z_0, \sigma(T))}.$$

Proof. a) It is enough to consider $z_0 = 0$. As motivation note that, for nonzero $x, z \in \mathbb{C}$, $(x^{-1} - z^{-1})^{-1} = -zx(x - z)^{-1}$.

If $z \in \rho(T)$, $z \neq 0$, then $\forall \xi \in \mathcal{H}$,

$$(T^{-1} - z^{-1}\mathbf{1})zTR_z(T)\xi = -(T - z\mathbf{1})R_z(T)\xi = -\xi,$$

and for $T\xi = \eta \in \text{dom}\, T^{-1} = \text{rng}\, T$ one has

$$zTR_z(T)(T^{-1} - z^{-1}\mathbf{1})\eta = TR_z(T)(z\mathbf{1} - T)\xi = -T\xi = -\eta.$$

Hence $R_{1/z}(T^{-1}) = -zTR_z(T) = -z^2R_z(T) - z\mathbf{1}$, which is an operator in $\mathrm{B}(\mathcal{H})$. Therefore $z^{-1} \in \rho(T^{-1})$. Similarly one gets the other inclusion; the statement on the spectra follows.

b) The result follows at once from a) after recalling that: $r_\sigma(R_{z_0}(T)) = \sup\{|z| : z \in \sigma(R_{z_0}(T))\}$ and $d(z_0, \sigma(T)) = \inf\{|z - z_0| : z \in \sigma(T)\}$. □

Exercise 2.4.3. If $0 \neq z$ is an eigenvalue of T, show that z^{-1} is an eigenvalue of T^{-1}.

Theorem 2.4.4. *Every self-adjoint operator has nonempty spectrum* (*see also Theorem* 8.2.14).

Proof. Let T be self-adjoint. $\sigma(T) \subset \mathbb{R}$ by Theorem 2.2.17. If $0 \in \sigma(T)$, then there is nothing to prove. If $0 \notin \sigma(T)$, then T is one-to-one, onto $\mathcal{H}$ and $0 \neq T^{-1} = R_0(T) \in \mathrm{B}(\mathcal{H})$. So $\sigma(T^{-1}) \neq \emptyset$ and there is $0 \neq \lambda \in \sigma(T^{-1})$ ($\lambda \in \mathbb{R}$, since T^{-1} is also self-adjoint). By Lemma 2.4.2, $\lambda^{-1} \in \sigma(T)$ and so the spectrum $\sigma(T)$ is nonempty. □

Corollary 2.4.5. *If T is self-adjoint and $z \in \rho(T)$, then*

$$\|R_z(T)\| = \frac{1}{d(z, \sigma(T))}.$$

Proof. Since $R_z(T)^* = R_{\overline{z}}(T)$, it follows from the first resolvent identity, Proposition 1.5.9, that $R_z(T)$ is a normal operator. Then, by Proposition 2.1.12, $\|R_z(T)\| = r_\sigma(R_z(T))$. Apply Lemma 2.4.2b) to conclude the equality in the corollary. In Chapter 9 this result will also be derived as a consequence of the spectral theorem. □

Exercise 2.4.6. If T is not hermitian the inequality $\|R_\lambda(T)\| \le 1/d(\lambda, \sigma(T))$ may fail already in the Hilbert space $\mathbb{R}^2$. Conclude this by considering the operator represented by the matrix

$$T_a = \begin{bmatrix} 0 & a \\ 0 & 0 \end{bmatrix},$$

whose spectrum is $\sigma(T_a) = \{0\}$, $\forall a \in \mathbb{R}$, and, for fixed $0 \neq \lambda \in \mathbb{R}$, show that $\|R_\lambda(T_a)\| \to \infty$ as $a \to \infty$.

Definition 2.4.7. Let T be a linear operator in $\mathcal{H}$. A sequence $(\xi_n) \subset \operatorname{dom} T$ is a Weyl sequence for T at $z \in \mathbb{C}$ if

$$\|\xi_n\| = 1, \forall n, \qquad \text{and} \qquad \lim_{n\to\infty} (T - z\mathbf{1})\xi_n = 0.$$

A direct verification shows that if T is closed and the Weyl sequence (ξ_n) at z converges to ξ, then $\|\xi\| = 1$ and $T\xi = z\xi$, so that z is an eigenvalue of T. Thus, if there is a Weyl sequence for T at z one interprets z as a generalized eigenvalue; this is supported by Theorem 2.4.8 and Corollary 2.4.9.

Theorem 2.4.8. *Let T be a linear operator in $\mathcal{H}$ so that both sets $\rho(T)$ and $\sigma(T)$ are nonempty. Then:*

a) *If there exists a Weyl sequence for T at $z \in \mathbb{C}$, then $z \in \sigma(T)$.*
b) *If z belongs to the boundary of $\sigma(T)$ in $\mathbb{C}$, then there exists a Weyl sequence for T at z (since the spectrum is closed, $z \in \sigma(T)$).*

Proof. a) Let (ξ_n) be a Weyl sequence for T at z. If $z \in \rho(T)$ then

$$1 = \|\xi_n\| = \|R_z(T)(T - z\mathbf{1})\xi_n\| \le \|R_z(T)\| \|(T - z\mathbf{1})\xi_n\|;$$

since the right-hand side vanishes for $n \to \infty$, $z \notin \rho(T)$.

b) Let $(z_n) \subset \rho(T)$ with $z_n \to z \in \sigma(T)$. By Corollary 1.5.15, $\|R_{z_n}(T)\| \to \infty$; so there exists a sequence $(\eta_n) \subset \mathcal{H}$ with $\|\eta_n\| = 1$, $\forall n$, and $\|R_{z_n}(T)\eta_n\| \to \infty$. Define $\zeta_n = \eta_n / \|R_{z_n}(T)\eta_n\|$ and $\xi_n = R_{z_n}(T)\zeta_n$; so $\zeta_n \to 0$ as $n \to \infty$, $\xi_n \in \operatorname{dom} T$ and $\|\xi_n\| = 1$, $\forall n$. Now, since for $n \to \infty$ one has

$$(T - z\mathbf{1})\xi_n = (T - z_n\mathbf{1})\xi_n + (z_n - z)\xi_n = \zeta_n + (z_n - z)\xi_n \to 0,$$

it follows that (ξ_n) is a Weyl sequence for T at z. □

Corollary 2.4.9. *λ belongs to the spectrum of a self-adjoint or unitary operator iff there exists a Weyl sequence for this operator at λ.*

Proof. If the operator is self-adjoint its spectrum is real (Theorem 2.2.17); if it is unitary its spectrum belongs to the unit circumference in $\mathbb{C}$ (Proposition 2.2.21). In both cases all points in the spectrum are also boundary points. Apply Theorem 2.4.8. □

Example 2.4.10. Let P, dom $P = \mathcal{H}^1(\mathbb{R})$, be the momentum operator on $\mathbb{R}$ discussed in Example 2.3.11. This operator has no eigenvalues; indeed, if $\lambda \in \mathbb{R}$ (recall that its spectrum is real) satisfies

$$(P\psi)(x) = -i\frac{d\psi}{dx}(x) = \lambda\psi(x), \qquad \psi \in \mathcal{H}^1(\mathbb{R}),$$

then $\psi(x) = ce^{i\lambda x}$, which belongs to $\mathrm{L}^2(\mathbb{R})$ iff $c = 0$; however, by "cutting off" such ψ, it will be possible to determine the spectrum of P. It should be noted that the "cutting off" that follows is a usual procedure.

Now fix $\lambda \in \mathbb{R}$ and let $\phi(x) = (2/\pi)^{1/4}e^{-x^2}$; then $1 = \|\phi\|^2 = \int_{\mathbb{R}} |\phi(x)|^2\, dx$. For each n set

$$\xi_n(x) = \frac{1}{\sqrt{n}}\phi\left(\frac{x}{n}\right) e^{i\lambda x},$$

which belongs to dom P and $\|\xi_n\| = 1$. Since

$$\|P\xi_n - \lambda\xi_n\|^2 = \frac{1}{n^2}\int_{\mathbb{R}} |\phi'(t)|^2\, dt$$

which vanishes as $n \to \infty$. Then (ξ_n) is a Weyl sequence for P at λ, and $\lambda \in \sigma(P)$. Therefore, $\sigma(P) = \mathbb{R}$ and it has no eigenvalues.

Example 2.4.11. Let $q : \mathbb{R} \to \mathbb{R}$, $q(x) = x$ be the position operator on $\mathbb{R}$ (see Exercise 2.3.31; here an alternative solution to that exercise is discussed). If $\lambda \in \mathbb{R}$, for each n set

$$\xi_n(x) = \frac{\sqrt{n}}{\pi^{1/4}}e^{-n^2(x-\lambda)^2},$$

which belongs to dom $\mathcal{M}_q$, $\|\xi_n\|^2 = 1$ and

$$\|q\xi_n - \lambda\xi_n\|^2 = \frac{1}{\sqrt{\pi}\, n^2}\int_{\mathbb{R}} x^2\, e^{-x^2}\, dx,$$

vanishes as $n \to \infty$, then (ξ_n) is a Weyl sequence for q at λ. Therefore, $\sigma(\mathcal{M}_q) = \mathbb{R}$ and it is easy to check that it has no eigenvalues.

Example 2.4.12. If T is a bounded self-adjoint operator so that $T^{2k} = \mathbf{1}$, for some $k \in \mathbb{N}$, then $\sigma(T) \subset \{z \in \mathbb{C} : z^{2k} = 1\}$. In fact, if $k = 1$ and (ξ_n) is a Weyl sequence for T at z, then

$$(\mathbf{1} - z^2\mathbf{1})\xi_n = (T^2 - z^2\mathbf{1})\xi_n = (T + z\mathbf{1})(T - z\mathbf{1})\xi_n$$

that vanishes as $n \to \infty$ iff $z^2 = 1$, since $\|\xi_n\| = 1$. For $k = 2$ write $(\mathbf{1} - z^4\mathbf{1}) = (T^2 + z^2\mathbf{1})(T^2 - z^2\mathbf{1}) = (T^2 + z^2\mathbf{1})(T + z\mathbf{1})(T - z\mathbf{1})$ and invoke the same argument. Use induction for the general case.

Recall that the Fourier transform $\mathcal{F} : \mathrm{L}^2(\mathbb{R}^n) \hookleftarrow$ (see Section 3.1) is a unitary operator and $\mathcal{F}^4 = \mathbf{1}$, so $\sigma(\mathcal{F}) \subset \{i, -i, 1, -1\}$ (in fact the spectrum of $\mathcal{F}$ is exactly this set, since it is possible to exhibit eigenvectors of $\mathcal{F}$ for each complex quartic root of 1; try the eigenvectors of the harmonic oscillator).

Exercise 2.4.13. Show that if T is self-adjoint, then λ is an eigenvalue of T iff the closure $\overline{\mathrm{rng}\ (T - \lambda\mathbf{1})} \neq \mathcal{H}$.

Exercise 2.4.14. Let T be self-adjoint. Show that the following assertions are equivalent:

a) $z \in \rho(T)$.
b) $\mathrm{rng}\ (T - z\mathbf{1}) = \mathcal{H}$.
c) $\exists c > 0$ so that $\|(T - z\mathbf{1})\xi\| \geq c\|\xi\|$, $\forall \xi \in \mathrm{dom}\ T$.

Exercise 2.4.15. Let T be self-adjoint. Use Exercise 2.4.14 to give an alternative proof that $\lambda \in \sigma(T)$ iff there is a Weyl sequence for T at λ.

Definition 2.4.16. A hermitian operator T is *lower bounded*, also called *bounded from below*, if there is $\beta \in \mathbb{R}$ so that $\langle \xi, T\xi \rangle \geq \beta\|\xi\|^2$, $\forall \xi \in \mathrm{dom}\ T$; this will be denoted by $T \geq \beta\mathbf{1}$ and such β is called a *lower limit* or *lower bound* of T. In case $\beta = 0$ the operator T is also called a *positive operator*.

Exercise 2.4.17. Let T be self-adjoint with $T \geq \beta\mathbf{1}$. Use Weyl sequences, or Exercise 2.4.14, to show that $\sigma(T) \subset [\beta, \infty)$.

Exercise 2.4.18. If T is self-adjoint or unitary, show that

$$\sigma(T) \subset \overline{\{\langle \xi, T\xi \rangle : \xi \in \mathrm{dom}\ T, \|\xi\| = 1\}}.$$

2.5 Cayley Transform II

The main goal of this section is to prove Theorem 2.2.11. To reach this, a more detailed study of the Cayley transform will be performed.

Lemma 2.5.1. *Let T be hermitian and the isometry $U(T)$ its Cayley transform (Definition 2.2.1).*

a) *$U(T)$ is unitary (with $\mathrm{dom}\ U(T) = \mathrm{rng}\ U(T) = \mathcal{H}$) iff T is self-adjoint.*
b) *If $\mathrm{rng}\ (\mathbf{1} - U(T))$ is dense in $\mathcal{H}$, then $(\mathbf{1} - U(T))$ is one-to-one (so 1 is not an eigenvalue of $U(T)$). Note that this holds for any linear isometry.*
c) *$U(T)$ is closed iff T is closed.*
d) *S is a hermitian extension of T, i.e., $T \subset S$ iff $U(T) \subset U(S)$.*

Proof. Write $U = U(T)$.

a) Straight from Proposition 2.2.4.

b) Suppose $\xi - U\xi = 0$. Then, for any $\eta \in \text{dom }(\mathbf{1} - U)$

$$\begin{aligned} 0 &= \langle U\xi - \xi, \eta \rangle = \langle U\xi, \eta \rangle - \langle \xi, \eta \rangle \\ &= \langle U\xi, \eta \rangle - \langle U\xi, U\eta \rangle = \langle U\xi, (\mathbf{1} - U)\eta \rangle, \end{aligned}$$

so $U\xi = 0$ in case rng $(\mathbf{1} - U)$ is dense in $\mathcal{H}$; since $\|U\xi\| = \|\xi\|$ it follows that $\xi = 0$ and $\mathbf{1} - U$ is one-to-one.

c) Since U is an isometry, then it is a closed operator iff its domain and range (i.e., rng $(T \pm i\mathbf{1})$) are closed subspaces iff $\mathcal{G}(T)$ is closed (recall that $\|(T \pm i\mathbf{1})\xi\| = \|\xi\|_T$).

d) Denote by $\Xi : \mathcal{H} \times \mathcal{H} \hookleftarrow$ the one-to-one map $\Xi(\eta, \xi) = (\xi + i\eta, \xi - i\eta)$. Thus, for any hermitian operator S one has

$$\begin{aligned} \mathcal{G}(U(S)) &= \{((S + i\mathbf{1})\eta, (S - i\mathbf{1})\eta) : \eta \in \text{dom } S\} \\ &= \{(\xi + i\eta, \xi - i\eta) : (\eta, \xi) \in \mathcal{G}(S)\} = \Xi\mathcal{G}(S). \end{aligned}$$

Hence, for hermitian operators T, S one has $\mathcal{G}(T) \subset \mathcal{G}(S)$ iff $\mathcal{G}(U(T)) \subset \mathcal{G}(U(S))$. □

Proposition 2.5.2. *If T is hermitian in $\mathcal{H}$, then* rng $(\mathbf{1} - U(T)) =$ dom T, $(\mathbf{1} - U(T))$ *is injective and*

$$T = i(\mathbf{1} + U(T))(\mathbf{1} - U(T))^{-1}.$$

Hence rng $T =$ rng $(\mathbf{1} + U(T))$.

Proof. Write $U = U(T)$. One has

$$\begin{aligned} \text{rng }(\mathbf{1} - U) &= \{\xi - U\xi : \xi \in \text{dom } U = \text{rng }(T + i\mathbf{1})\} \\ &= \{(T + i\mathbf{1})\eta - (T - i\mathbf{1})\eta = 2i\eta : \eta \in \text{dom } T\} = \text{dom } T. \end{aligned}$$

Since dom T is dense, Lemma 2.5.1b) implies that $(\mathbf{1} - U)$ is one-to-one.

Now for $\xi \in \text{dom } T$, if $\eta = (T + i\mathbf{1})\xi$, then $U\eta = (T - i\mathbf{1})\xi$,

$$(\mathbf{1} - U)\eta = 2i\xi \qquad \text{and} \qquad (\mathbf{1} + U)\eta = 2T\xi.$$

Hence

$$2T\xi = (\mathbf{1} + U)\eta = 2i(\mathbf{1} + U)(\mathbf{1} - U)^{-1}\xi, \qquad \forall \xi \in \text{dom } T,$$

and $T\xi = i(\mathbf{1} + U)(\mathbf{1} - U)^{-1}\xi$. This concludes the verification. □

Corollary 2.5.3. *If S and T are hermitian operators in $\mathcal{H}$, then $S = T$ iff $U(S) = U(T)$.*

Exercise 2.5.4. Prove Corollary 2.5.3.

Proposition 2.5.5. *Let Y be a linear isometry between* dom $Y \subset \mathcal{H}$ *and its range in $\mathcal{H}$. If* rng $(\mathbf{1} - Y)$ *is dense in $\mathcal{H}$, then Y is the Cayley transform $Y = U(T)$ of a hermitian operator $T :$* rng $(\mathbf{1} - Y) \to$ rng $(\mathbf{1} + Y)$.

Proof. Since rng $(\mathbf{1}-Y)$ is dense in $\mathcal{H}$, by Lemma 2.5.1 $(\mathbf{1}-Y)$ is one-to-one and the operator

$$T := i(\mathbf{1}+Y)(\mathbf{1}-Y)^{-1} : \text{rng } (\mathbf{1}-Y) \to \text{rng } (\mathbf{1}+Y)$$

is well posed and with dense domain. It will be checked that T is hermitian and Y is its Cayley transform.

For $\xi, \eta \in \text{dom } T$, there exist $\eta_1, \xi_1 \in \text{dom } Y$ obeying $\eta = (\mathbf{1}-Y)\eta_1$ and $\xi = (\mathbf{1}-Y)\xi_1$. Then,

$$\begin{aligned}\langle T\eta, \xi\rangle &= \langle i(\mathbf{1}+Y)\eta_1, (\mathbf{1}-Y)\xi_1\rangle \\ &= -i\left(\langle \eta_1, \xi_1\rangle + \langle Y\eta_1, \xi_1\rangle - \langle \eta_1, Y\xi_1\rangle - \langle Y\eta_1, Y\xi_1\rangle\right) \\ &= i\left(\langle \eta_1, Y\xi_1\rangle - \langle Y\eta_1, \xi_1\rangle\right) \\ &= i\left(\langle \eta_1, Y\xi_1\rangle - \langle Y\eta_1, \xi_1\rangle + \langle \eta_1, \xi_1\rangle - \langle Y\eta_1, Y\xi_1\rangle\right) \\ &= \langle (\mathbf{1}-Y)\eta_1, i(\mathbf{1}+Y)\xi_1\rangle = \langle \eta, T\xi\rangle,\end{aligned}$$

and T is hermitian.

By definition, for $\xi = (\mathbf{1}-Y)\xi_1$, $\xi \in \text{dom } T$, one has $T\xi = i(\mathbf{1}+Y)\xi_1$. A direct computation leads to

$$\begin{aligned}Y(T+i\mathbf{1})\xi &= Y(i(\xi_1 + Y\xi_1) + i\xi_1 - iY\xi_1)) = 2iY\xi_1 \\ &= iY\xi_1 + iY\xi_1 = i(Y\xi_1 + \xi_1) + i(Y\xi_1 - \xi_1) \\ &= T\xi - i\xi,\end{aligned}$$

so that $Y((T+i\mathbf{1})\xi) = (T-i\mathbf{1})\xi$, $\forall \xi \in \text{dom } T$, and $Y = U(T)$. □

Corollary 2.5.6. *Let T be a hermitian operator.*

a) *There is a one-to-one correspondence between hermitian extensions of T and isometric extensions of its Cayley transform $U(T)$.*
b) *There is a one-to-one correspondence between self-adjoint extensions of T and unitary extensions of its Cayley transform $U(T)$.*

Proof. a) Let S be a hermitian operator. By Lemma 2.5.1 one has $T \subset S$ iff $U(T) \subset U(S)$. If Y is an isometry with $U(T) \subset Y$, then rng Y is dense in the Hilbert space and, by Proposition 2.5.5, $Y = U(R)$ for some hermitian operator R. By the proof of Lemma 2.5.1d) one has $T \subset R$.

b) It follows directly by a) and Proposition 2.2.4. □

The time is ripe for concluding Theorem 2.2.11.

Proof. [**Theorem 2.2.11**] a) The inner product in question is

$$\langle \xi, \eta\rangle_{T^*} = \langle \xi, \eta\rangle + \langle T^*\xi, T^*\eta\rangle, \quad \xi, \eta \in \text{dom } T^*;$$

see Exercise 1.2.28. Clearly one has $\{\text{dom } T, \mathrm{K}_-, \mathrm{K}_-\} \subset \text{dom } T^*$.

- If $\xi_+ \in \mathrm{K}_+ = \mathrm{K}_+(T)$ and $\xi_- \in \mathrm{K}_- = \mathrm{K}_-(T)$, then

$$\begin{aligned}\langle \xi_+, \xi_- \rangle_{T^*} &= \langle \xi_+, \xi_- \rangle + \langle T^*\xi_+, T^*\xi_- \rangle \\ &= \langle \xi_+, \xi_- \rangle + \langle -i\xi_+, i\xi_- \rangle = 0,\end{aligned}$$

so, with respect to this inner product, $\mathrm{K}_+ \perp_{T^*} \mathrm{K}_-$.

- If $\xi \in \mathrm{dom}\ T$ and $\xi_+ \in \mathrm{K}_+$ (similarly for $\xi_- \in \mathrm{K}_-$), then

$$\begin{aligned}\langle \xi, \xi_+ \rangle_{T^*} &= \langle \xi, \xi_+ \rangle + \langle T^*\xi, T^*\xi_+ \rangle = \langle \xi, \xi_+ \rangle + \langle T\xi, -i\xi_+ \rangle \\ &= \langle \xi, \xi_+ \rangle + \langle \xi, -iT^*\xi_+ \rangle = \langle \xi, \xi_+ \rangle + \langle \xi, -\xi_+ \rangle = 0.\end{aligned}$$

Hence, $\mathrm{K}_\pm \perp_{T^*} \mathrm{dom}\ T$.

- Let $\xi \in (\mathrm{dom}\ T)^{\perp_{T^*}}$. Then, for all $\eta \in \mathrm{dom}\ T$ one has $0 = \langle \xi, \eta \rangle_{T^*} = \langle \xi, \eta \rangle + \langle T^*\xi, T^*\eta \rangle$, so that $\langle T^*\xi, T^*\eta \rangle = \langle -\xi, \eta \rangle$. Hence, $T^*\xi \in \mathrm{dom}\ T^*$ and $T^*(T^*\xi) = -\xi$, which is equivalent to

$$(T^* + i\mathbf{1})(T^* - i\mathbf{1})\xi = 0 = (T^* - i\mathbf{1})(T^* + i\mathbf{1})\xi.$$

Therefore, $(T^* - i\mathbf{1})\xi \in \mathrm{K}_+$ and $(T^* + i\mathbf{1})\xi \in \mathrm{K}_-$. Since

$$\xi = \frac{1}{2i}\left[(T^* + i\mathbf{1})\xi - (T^* - i\mathbf{1})\xi\right],$$

one has $(\mathrm{dom}\ T)^{\perp_{T^*}} \subset \mathrm{K}_+ \oplus_{T^*} \mathrm{K}_-$ and, due to T^* being closed,

$$(\mathrm{dom}\ T)^{\perp_{T^*}\perp_{T^*}} = \overline{\mathrm{dom}\ T} = \mathrm{dom}\ \overline{T} \subset \mathrm{dom}\ T^*$$

(the closure $\overline{\mathrm{dom}\ T}$ with respect to the graph norm of T^*) and item a) follows.

b) and c) The Cayley transform $U(T)$ is an isometry and it has unitary extensions from $\mathcal{H}$ onto $\mathcal{H}$ iff $\dim \mathrm{rng}\ (T + i\mathbf{1})^\perp = \dim \mathrm{rng}\ (T - i\mathbf{1})^\perp$, i.e., iff $n_- = n_+$. There is exactly one extension iff $n_- = n_+ = 0$, i.e., the case U(T) is densely defined and with dense range, so a single unitary extension exists; otherwise there are infinitely many of them. The other assertion follows directly by Corollary 2.5.6. □

Exercise 2.5.7. Let T be a hermitian operator. Show that the closure of dom T with respect to the graph norm of T^* is $\mathrm{dom}\ \overline{T}$.

Proposition 2.5.8. *Let T be hermitian and $\mathrm{K}_\pm$ its deficiency subspaces. If $\mathcal{U}$: $\mathrm{dom}\ \mathcal{U} \subset \mathrm{K}_- \to \mathrm{rng}\ \mathcal{U} \subset \mathrm{K}_+$ is a linear isometry, then the corresponding hermitian extension $T_\mathcal{U}$ of T, associated with $Y = U(T) \oplus \mathcal{U}$ (see Proposition 2.5.5), is given by*

$$\begin{aligned}\mathrm{dom}\ T_\mathcal{U} &= \{\xi + \xi_- - \mathcal{U}\xi_- : \xi \in \mathrm{dom}\ T,\ \xi_- \in \mathrm{dom}\ \mathcal{U}\}, \\ T_\mathcal{U}(\xi + \xi_- - \mathcal{U}\xi_-) &= T^*(\xi + \xi_- - \mathcal{U}\xi_-) = T\xi + i\xi_- + i\mathcal{U}\xi_-.\end{aligned}$$

Proof. The map

$$Y : \text{rng } (T + i\mathbf{1}) \oplus \text{dom } \mathcal{U} \to \text{rng } (T - i\mathbf{1}) \oplus \text{rng } \mathcal{U},$$

$$Y := U(T) \oplus \mathcal{U},$$

is the Cayley transform of a hermitian operator $T_{\mathcal{U}}$, that is, $Y = U(T_{\mathcal{U}})$. Since $T \subset T_{\mathcal{U}}$, by Theorem 2.1.24a), one has $T_{\mathcal{U}} \subset T^*$. Thus

$$\begin{aligned}\text{dom } T_{\mathcal{U}} &= \text{rng } (\mathbf{1} - Y) = \text{rng } \left(\mathbf{1} - (U(T) \oplus_{T^*} \mathcal{U})\right)\\ &= \{(\mathbf{1} - (U(T) \oplus_{T^*} \mathcal{U}))((T\xi + i\xi) \oplus_{T^*} \xi_-) : \xi \in \text{dom } T, \xi_- \in \text{dom } \mathcal{U}\}\\ &= \{(T\xi + i\xi) \oplus_{T^*} \xi_- - ((T\xi - i\xi) \oplus_{T^*} \mathcal{U}\xi_-)\\ &\quad : \xi \in \text{dom } T, \xi_- \in \text{dom } \mathcal{U}\}\\ &= \{2i\xi + \xi_- - \mathcal{U}\xi_- : \xi \in \text{dom } T, \xi_- \in \text{dom } \mathcal{U}\}\end{aligned}$$

which is the set in the statement of the proposition (and dense in $\mathcal{H}$). Thus, for vectors in this domain, since $T_{\mathcal{U}} \subset T^*$,

$$\begin{aligned}T_{\mathcal{U}}(\xi + \xi_- - \mathcal{U}\xi_-) &= T^*(\xi + \xi_- - \mathcal{U}\xi_-)\\ &= T\xi + T^*\xi_- - T^*\mathcal{U}\xi_-\\ &= T\xi + i\xi_- + i\mathcal{U}\xi_-,\end{aligned}$$

as claimed. □

If T is hermitian and $\mathcal{U} : \mathrm{K}_- \to \mathrm{K}_+$ is unitary onto K_+, then the subsequent self-adjoint extension $T_{\mathcal{U}}$ has domain

$$\left\{\xi + \xi_- - \mathcal{U}\xi_- : \xi \in \text{dom } \overline{T},\ \xi_- \in \mathrm{K}_-\right\}.$$

Certainly, in applications it may be interesting to have the closure $\overline{T}$ at hand.

Exercise 2.5.9. By following the notation in Proposition 2.5.8, show that if $\dim \text{dom } \mathcal{U} < \infty$, then

$$n_\pm(T_{\mathcal{U}}) = n_\pm(T) - \dim \text{dom } \mathcal{U}.$$

Exercise 2.5.10. Let T be self-adjoint in $\mathcal{H}$. Use that in the graph norm of T the operators $T \pm i\mathbf{1}$ are unitary, to show that a subspace $\mathcal{D} \subset \text{dom } T$ is a core of T iff $\mathcal{D}$ is dense in dom T with respect to the graph norm of T.

Exercise 2.5.11. If T is hermitian and closed with $n_+ \neq 0$ and $n_- = 0$ (or vice versa), show that T has no proper hermitian extensions.

Exercise 2.5.12. Let T be a hermitian operator. Show that λ is an eigenvalue of T iff $(\lambda - i)/(\lambda + i)$ is an eigenvalue of $U(T)$.

Exercise 2.5.13. Let T be hermitian and $T \geq \beta\mathbf{1}$. Show that if the vector space rng $(T - \lambda\mathbf{1})$ is dense in $\mathcal{H}$ for some $\lambda < \beta$, then T is essentially self-adjoint.

Exercise 2.5.14. Show that the mapping

$$x \mapsto z = \frac{x-i}{x+i},$$

is a one-to-one relation between $\mathbb{R}$ and $\{1 \neq z \in \mathbb{C} : |z| = 1\}$ whose inverse is

$$z \mapsto x = -i\,\frac{z+1}{z-1}.$$

Take this as another motivation for the definition of Cayley transform, giving rise to a one-to-one relation between self-adjoint and unitary operators for which 1 is not an eigenvalue.

2.6 Examples

Example 2.6.1. Let $\Lambda \subset \mathbb{R}^n$ be an open set and $\varphi : \Lambda \to \mathbb{R}$ a Borel function. Consider the multiplication operator $\mathcal{M}_\varphi$ (see Subsection 2.3.2); its Cayley transform is $U(\mathcal{M}_\varphi) = \mathcal{M}_\tau$, with function $\tau : \Lambda \to \{z \in \mathbb{C} : |z| = 1\}$ and action

$$\tau(x) = \frac{\varphi(x) - i}{\varphi(x) + i}.$$

Since $|\tau(x)| = 1, \forall x$, $\mathcal{M}_\tau$ is a unitary operator and thus $\mathcal{M}_\varphi$ is self-adjoint. Check the details.

Example 2.6.2. Let $\mathcal{H} = l^2(\mathbb{N})$ and $S_r : \mathcal{H} \hookleftarrow$ the right shift

$$S_r(\xi_1, \xi_2, \xi_3, \dots) = (0, \xi_1, \xi_2, \xi_3, \dots).$$

Since S_r is an isometry and rng $(\mathbf{1} - S_r) = \mathcal{H}$, by Proposition 2.5.5 there is a hermitian operator T_r so that $S_r = U(T_r)$. In view of dom $U(T_r) = \mathcal{H}$ and $\dim(\text{rng } U(T_r))^\perp = 1$, it follows that $n_+(T_r) = 1$ and $n_-(T_r) = 0$. Therefore, T_r has no self-adjoint extensions.

Example 2.6.3. This is a standard example for which the role of boundary conditions is apparent. Let $\mathcal{H} = \mathcal{H}^1[0,1]$, dom $P_1 = \mathcal{H}^1[0,1]$, dom $P_2 = \{\psi \in \mathcal{H}^1[0,1] : \psi(0) = \psi(1)\}$, dom $P_3 = \{\psi \in \mathcal{H}^1[0,1] : \psi(0) = \psi(1) = 0\}$, and

$$(P_j\psi)(x) = -i\frac{d\psi}{dx}(x), \qquad \psi \in \text{dom } P_j,\ j = 1, 2, 3.$$

Exercise 2.6.4. Show that P_1, P_2 and P_3 are closed.

If $g \in \text{dom}\ P_j^* \subset \mathcal{H}^1[0,1]$, then for all $\psi \in \text{dom}\ P_j$, on integrating by parts one gets the relation

$$\begin{aligned}\langle g, P_j\psi\rangle &= \int_0^1 \overline{g(x)}\,(-i\psi'(x))\,dx \\ &= -i\left(\overline{g(1)}\psi(1) - \overline{g(0)}\psi(0)\right) + \int_0^1 \overline{-ig'(x)}\,\psi(x)\,dx \\ &= -i\left(\overline{g(1)}\psi(1) - \overline{g(0)}\psi(0)\right) + \langle -ig', \psi\rangle.\end{aligned}$$

For self-adjointness the boundary terms must vanish, i.e., the following key relation must hold true

$$\overline{g(1)}\psi(1) = \overline{g(0)}\psi(0).$$

For $j = 1$ such a relation must hold for all $\psi \in \mathcal{H}^1[0,1]$, so $g(0) = g(1) = 0$, i.e., $P_1^* = P_3$. Conversely, for $j = 3$ this relation must hold for all $\psi(0) = \psi(1) = 0$, so no boundary condition is imposed on g and $P_3^* = P_1$. For $j = 2$ it is found that g must satisfy the same boundary condition as ψ, that is, $g(0) = g(1)$, so that P_2 is self-adjoint; it has "well-balanced" boundary conditions. Note that P_2 is a self-adjoint extension of P_3 and that P_1 is not hermitian, since P_1 is a proper extension of its adjoint P_3.

Example 2.6.5. This is Example 2.3.14 continued, i.e., momentum on an interval. It has become a standard and remarkable illustration of self-adjoint extensions in quantum mechanics. It is, however, convenient to work with its closure (Exercise 2.3.15) dom $P = \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = \psi(1) = 0\}$ and

$$(P\psi)(x) = -i\frac{d\psi}{dx}(x), \qquad \psi \in \text{dom}\ P.$$

Note that the same notation was kept for the operator closure. Its adjoint is dom $P^* = \mathcal{H}^1[0,1]$, $P^*g = -ig'$. The point here is to classify all self-adjoint extensions of P.

First natural conditions for self-adjointness can be reached by inspection of the relation $\overline{g(1)}\psi(1) = \overline{g(0)}\psi(0)$, as in Example 2.6.3. For a self-adjoint extension the same conditions must be imposed on both, ψ and g; rewrite such key relation so that it becomes evident that there is a complex number α obeying

$$\frac{\overline{g(1)}}{\overline{g(0)}} = \frac{\psi(0)}{\psi(1)} = \alpha,$$

that is $\psi(0) = \alpha\psi(1)$ and $\overline{g(1)} = \alpha\overline{g(0)}$. The latter relation is $g(0) = g(1)/\overline{\alpha}$, and the same condition on ψ and g is obtained if $\alpha = 1/\overline{\alpha}$, or $|\alpha|^2 = 1$, that is, if $\alpha = e^{i\theta}$ for some $0 \le \theta < 2\pi$. As expected, one readily checks that the operators

$$\text{dom}\ P^\theta = \left\{\psi \in \mathcal{H}^1[0,1] : \psi(0) = e^{i\theta}\psi(1)\right\}, \qquad P^\theta\psi = -i\psi',$$

are actually self-adjoint. Note that the self-adjoint operator P_2 in Example 2.6.3 corresponds to $\theta = 0$.

Arguments using the extensions of the Cayley transform are as follows. The vector spaces $\mathrm{K}_+(P)$ and $\mathrm{K}_-(P)$ are spanned by the normalized vectors

$$u_+(x) = \sqrt{\frac{2}{e^2-1}}\, e^x, \qquad u_-(x) = \sqrt{\frac{2}{1-e^{-2}}}\, e^{-x},$$

respectively, so that $n_+ = n_- = 1$ (see Example 2.3.14). All unitary maps $\mathcal{U}$ of K_- onto K_+ have the form $u_- \mapsto e^{i\omega}u_+$, $0 \le \omega < 2\pi$, i.e., $\mathcal{U}u_- = e^{i\omega}u_+$, so that for each ω a self-adjoint extension P_ω is associated, and by Proposition 2.5.8,

$$\mathrm{dom}\ P_\omega = \{\psi + c(u_- - e^{i\omega}u_+) : \psi \in \mathrm{dom}\ P,\ c \in \mathbb{C}\},$$

and for $g = \psi + c(u_- - e^{i\omega}u_+) \in \mathrm{dom}\ P_\omega$, one gets the expected expression

$$\begin{aligned}(P_\omega g) &= -i\psi' + cP^*u_- - ce^{i\omega}P^*u_+\\ &= -i\psi' + icu_- + ice^{i\omega}u_+\\ &= -i(\psi + c(u_- - e^{i\omega}u_+))' = -ig'.\end{aligned}$$

Now note that there is a unique $0 \le \theta < 2\pi$ so that for all $g = \psi + c(u_- - e^{i\omega}u_+) \in \mathrm{dom}\ P_\omega$,

$$\kappa := \frac{g(1)}{g(0)} = \frac{1-e^{i\omega}e}{e-e^{i\omega}} = e^{i\theta},$$

because $|\kappa| = 1$. Therefore the relation between P_ω and P^θ has been uncovered. Such operators P^θ (alternatively P_ω) constitute all self-adjoint extensions of P. This finishes the example.

Exercise 2.6.6. Show that all points of the complex plane are eigenvalues of the adjoint operator P^* in Example 2.6.5; conclude then that it is not hermitian and so P is not essentially self-adjoint.

Example 2.6.7. Consider again the free particle energy operator from Example 2.3.18: $\overline{H} = -d^2/dx^2$ on $\mathbb{R}$, $\mathrm{dom}\ \overline{H} = \mathcal{H}^2(\mathbb{R})$. Introduce the function $\phi(x) = (2/\pi)^{1/4}e^{-x^2}$. Given $\lambda > 0$, for each n set

$$\xi_n(x) = \frac{1}{\sqrt{n}}\phi\left(\frac{x}{n}\right)e^{ix\sqrt{\lambda}},$$

so that $\|\xi_n\| = 1$, $\xi_n \in \mathrm{dom}\ \overline{H}$, and, after some manipulations,

$$\|-\xi'' - \lambda\xi_n\| \le \frac{2\sqrt{\lambda}}{\sqrt{n}}\|\phi'\| + \frac{1}{n^{3/2}}\|\phi''\|,$$

which vanishes as $n \to \infty$; thus (ξ_n) is a Weyl sequence and $\lambda \in \sigma(\overline{H})$ by Corollary 2.4.9. Since the spectrum is a closed set, $[0,\infty) \subset \sigma(\overline{H})$. To deal with $\lambda < 0$, note first that $\langle\overline{H}\psi,\psi\rangle = \langle\psi',\psi'\rangle \ge 0$, $\forall\psi \in \mathrm{dom}\ \overline{H}$; so,

$$0 \le \big\langle(\overline{H} - \lambda\mathbf{1} + \lambda\mathbf{1})\psi,\psi\big\rangle \implies -\lambda\|\psi\|^2 \le \big\langle(\overline{H} - \lambda\mathbf{1})\psi,\psi\big\rangle$$

and, by Exercise 2.4.14, it follows that $\lambda \in \rho(\overline{H})$ if $\lambda < 0$. Therefore, $\sigma(\overline{H}) = [0, \infty)$.

Example 2.6.8. [Free particle energy operator on $[0,1]$] Let

$$\text{dom } H = C_0^\infty(0,1) \sqsubseteq \mathrm{L}^2[0,1],$$

$(H\psi)(x) = -\psi''(x), \psi \in \text{dom } H$. Integrations by parts show that H is hermitian. By following the lines of Example 2.3.18, it is found that $\text{dom } H^* = \mathcal{H}^2[0,1]$ and $(H^*\psi)(x) = -\psi''(x)$, $\psi \in \text{dom } H^*$. For its deficiency indices one has:

n_-: if $u \in \mathrm{N}(H^* - i\mathbf{1})$, then $-u'' = iu$ and, since u is a continuously differentiable function, there are just two linearly independent solutions, e.g., $u_-^1(x) = e^{(1-i)x/\sqrt{2}}$ and $u_-^2(x) = e^{-(1-i)x/\sqrt{2}}$; since both belong to $\mathcal{H}$ one gets $n_- = 2$.

n_+: similarly one gets $u_+^1(x) = e^{(i+1)x/\sqrt{2}}$, $u_+^2(x) = e^{-(i+1)x/\sqrt{2}}$, and since both belong to $\mathcal{H}$ one gets $n_+ = 2$.

Therefore, H has infinitely many self-adjoint extensions; they are candidates for representing the free energy operator for a particle on the half-line $[0,1]$. All such extensions are described in Example 7.3.4; for particular instances see Examples 2.3.5, 2.3.6 and 2.3.7.

Example 2.6.9. Let $v : \mathbb{R} \hookleftarrow$ be a continuous function, $\text{dom } T = C_0^1(\mathbb{R}) \sqsubseteq \mathrm{L}^2(\mathbb{R})$ and

$$(T\psi)(x) = -i\frac{d\psi}{dx}(x) + v(x)\psi(x), \qquad \psi \in \text{dom } T.$$

An integration by parts shows that T is hermitian. Arguing as in previous examples leads to $\text{dom } T^* = \{\psi \in \mathcal{H}^1(\mathbb{R}) : (-i\psi' + v\psi) \in \mathrm{L}^2(\mathbb{R})\}$ and

$$(T^*\psi)(x) = -i\frac{d\psi}{dx}(x) + v(x)\psi(x), \qquad \psi \in \text{dom } T^*.$$

Now one can either compute the operator deficiency indices $n_- = n_+ = 0$ or note that T^* is hermitian, in order to conclude that T is essentially self-adjoint and $\overline{T} = T^*$ is its unique self-adjoint extension.

Next let $V(x) = \int_0^x v(t)\,dt$ and $U = e^{-iV(x)}$, i.e., $U = \mathcal{M}_{e^{-iV(x)}}$, a unitary operator, for which $U^* = e^{iV(x)}$. If $P = -id/dx$, $\text{dom } P = \mathcal{H}^1(\mathbb{R})$, is the momentum operator on $\mathbb{R}$ (Example 2.3.11) one readily checks that $U^*\text{dom } \overline{T} = \text{dom } P$ and

$$U^*\overline{T}U\psi = P\psi, \qquad \psi \in \text{dom } \overline{T}.$$

Therefore, by Exercise 2.1.26, one finds $\sigma(\overline{T}) = \sigma(P) = \mathbb{R}$. The latter equality follows from Example 2.4.10.

Exercise 2.6.10. Check that T in Example 2.6.9 is essentially self-adjoint.

Example 2.6.11. Let $\mathcal{H} = \mathrm{L}^2(\mathbb{R}^3)$. The initial quantum energy (Schrödinger) operator for the hydrogen atom is

$$H = -\Delta - \frac{\gamma}{\|x\|}, \qquad \text{dom } H = C_0^\infty(\mathbb{R}^3) \sqsubseteq \mathcal{H}.$$

By Proposition 2.2.16 H has self-adjoint extensions. In the 1950's Kato proved that this prominent operator is essentially self-adjoint; its unique self-adjoint extension has the same action with domain $\mathcal{H}^2(\mathbb{R}^3)$. Details are described in Example 6.2.3.

Exercise 2.6.12 (Free Dirac energy operator). Let I be an interval in $\mathbb{R}$, dom $D_0 := C_0^\infty(I;\mathbb{C}^2) \sqsubseteq \mathrm{L}^2(I;\mathbb{C}^2)$ and

$$\left(D_0\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}\right)(x) = \begin{pmatrix} mc^2 & -ic\frac{d}{dx}\\ -ic\frac{d}{dx} & -mc^2\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}(x),$$

with m representing the mass of the particle and c the speed of light. The adjoint operator D_0^* has the same action as D_0 but with dom $D_0^* = \mathcal{H}^1(I;\mathbb{C}^2)$ (see [BulT90]). Show that D_0 is hermitian and find $\mathrm{K}_\pm(D_0)$ to conclude that $n_+ = n_- = 0$ if $I = \mathbb{R}$, $n_+ = n_- = 1$ if $I = [0,\infty)$ and $n_+ = n_- = 2$ if I is a bounded closed interval.

Chapter 3

Fourier Transform and Free Hamiltonian

The standard free energy and momentum operators are also properly defined in $\mathbb{R}^n$ through Fourier transform. It is also an opportunity to briefly discuss some aspects of Sobolev spaces and related differential operators. The definitions of distributions $C_0^\infty(\Omega)'$ and tempered distributions $\mathcal{S}'(\Omega)$, as well as their derivatives, are also recalled.

3.1 Fourier Transform

Fourier transform is a very useful tool in dealing with differential operators in $\mathrm{L}^p(\mathbb{R}^n)$, with especial interest in $p = 2$. So some of its main properties will be reviewed and summarized in the first sections, including its relation to Sobolev spaces. Few simple proofs will be presented. Applications to the quantum free particle appear in other sections. Details can be found in the references [Ad75] and [ReeS75]; a nice introduction to distributions and Fourier transform is [Str94]. Readers familiar with the subject are referred to Sections 3.3 and 3.4, which discuss some (quantum) physical quantities.

Recall that the Fourier transform $\mathcal{F} = \hat{\ } : \mathrm{L}^2(\mathbb{R}^n) \to \mathrm{L}^2(\mathbb{R}^n)$ is a unitary operator onto $\mathrm{L}^2(\mathbb{R}^n)$. This is known as the *Plancherel Theorem*, and it implies the *Parseval identity*

$$\|\mathcal{F}\psi\|_2 = \|\psi\|_2, \qquad \forall \psi \in \mathrm{L}^2(\mathbb{R}^n).$$

Note the two notations for the Fourier transform $\mathcal{F}\psi = \hat{\psi}$. For functions $\psi \in \mathrm{L}^1(\mathbb{R}^n)$ there is an explicit expression for this transform, that is,

$$(\mathcal{F}\psi)(p) = \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} e^{-i\,xp}\, \psi(x)\, dx,$$

with $p = (p_1, \ldots, p_n), x = (x_1, \ldots, x_n) \in \mathbb{R}^n$ and $px = \sum_{j=1}^n p_j x_j$, i.e., the usual inner product in $\mathbb{R}^n$. Denote the norm $|x| = (\sum_{j=1}^n x_j^2)^{1/2}$ and $x^2 = \sum_{j=1}^n x_j^2$. Similarly for the variable p.

Besides the use of variables x and p, sometimes it is convenient to distinguish $\mathrm{L}^2(\mathbb{R}^n)$ from $\mathcal{F}\mathrm{L}^2(\mathbb{R}^n)$ by denoting the latter by $\mathrm{L}^2(\hat{\mathbb{R}}^n)$; functions ψ and operators T acting in $\mathrm{L}^2(\mathbb{R}^n)$ are said to be in the *position representation*, while the corresponding $\hat{\psi}$ and $\hat{T} := \mathcal{F}T\mathcal{F}^{-1}$ acting in $\mathrm{L}^2(\hat{\mathbb{R}}^n)$ are said to be in the *momentum representation*; see Section 3.4 for illustrations that justify the nomenclature.

The inverse Fourier transform $\mathcal{F}^{-1}\mathrm{L}^2(\hat{\mathbb{R}}^n) = \mathrm{L}^2(\mathbb{R}^n)$ has the expression, for $\phi \in \mathrm{L}^1(\hat{\mathbb{R}}^n)$,

$$(\mathcal{F}^{-1}\phi)(x) = \check{\phi}(x) = \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} e^{i\,xp}\, \phi(p)\, dp,$$

again with two different notations. These expressions hold, especially, for functions in the Schwartz space

$$\mathcal{S} = \mathcal{S}(\mathbb{R}^n) = \{\psi \in C^\infty(\mathbb{R}^n) : \lim_{|x|\to\infty} \left| x^m \psi^{(k)}(x) \right| = 0, \forall k, m\},$$

where $m = (m_1, \ldots, m_n)$, $k = (k_1, \ldots, k_n)$ are multiindices,

$$x^m = x_1^{m_1} \cdots x_n^{m_n}, \qquad \psi^{(k)}(x) = \frac{\partial^{k_1} \cdots \partial^{k_n} \psi}{\partial x_1^{k_1} \cdots \partial x_n^{k_n}}(x).$$

Also, $|m| = m_1 + \cdots + m_n$, $|k| = k_1 + \cdots + k_n$ (which should not be confused with the norm $|x|, |p|$ above) and $\partial_j^{k_j} \psi$ may also indicate

$$\partial_j^{k_j} \psi = \frac{\partial^{k_j} \psi}{\partial x_j^{k_j}}.$$

It is possible to show that $\mathcal{F}\mathcal{S} = \mathcal{S}$ (one-to-one). Since $\mathcal{S}$ is a dense subspace of all $\mathrm{L}^p(\mathbb{R}^n)$, $1 \le p < \infty$, any bounded linear operator defined on this space can be uniquely extended to $\mathrm{L}^p(\mathbb{R}^n)$. This holds in particular for the Fourier transform, and it is the usual road for its definition on such spaces. If $p = 2$ one has the Plancherel Theorem, and so many authors consider that this is the natural space of Fourier transforms. Instead of $\mathcal{S}$ it is possible to work with $C_0^\infty(\mathbb{R}^n)$ because this space is also dense in $\mathrm{L}^2(\mathbb{R}^n)$ and also $\mathcal{F}C_0^\infty(\mathbb{R}^n)$ is dense in $\mathrm{L}^2(\hat{\mathbb{R}}^n)$.

Recall the famous integral $\int_{\mathbb{R}} \exp(-t^2)\, dt = \sqrt{\pi}$. A sample of Fourier transform evaluations, which will be used repeated times (e.g., in the proof of Theorem 5.5.1), is

$$\mathcal{F}(e^{-wx - zx^2/2})(p) = \frac{1}{\sqrt{z}}\, e^{w^2/(2z)}\, e^{iwp/z - p^2/(2z)},$$

where $w \in \mathbb{C}$ and the branch of the complex number z with $\operatorname{Re} z > 0$ has been chosen so that $\operatorname{Re} \sqrt{z} > 0$. It is worth remarking that the linear subspace spanned by all such functions

$$\{e^{-wx-zx^2/2} : w, z \in \mathbb{C}, \operatorname{Re} z > 0\}$$

is dense in L^2, and so it is a way to extend (and define) the Fourier transform to every element of L^2. Note that $e^{-x^2/2}$ is an eigenvector of $\mathcal{F}$ with eigenvalue 1 (pick $w = 0$ and $z = 1$). More generally, one has that $(\mathcal{F}^2\psi)(x) = \psi(-x)$, $\forall \psi \in \mathrm{L}^2(\mathbb{R}^n)$, so that every even function is an eigenvector corresponding to this eigenvalue.

For computations it is also useful to invoke the limit in $\mathrm{L}^2(\mathbb{R}^n)$

$$(\mathcal{F}\psi)(p) = \lim_{R\to\infty} \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{|x|\le R} e^{-i\,xp}\,\psi(x)\,dx, \qquad \forall \psi \in \mathrm{L}^2(\mathbb{R}^n),$$

which is usually denoted in the literature by

$$(\mathcal{F}\psi)(p) = \text{l.i.m.}\ \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} e^{-i\,xp}\,\psi(x)\,dx.$$

l.i.m. means "limit in the mean."

Exercise 3.1.1. Let $\psi \in \mathrm{L}^2(\mathbb{R}^n)$ and $B_R = \{x \in \mathbb{R}^n : |x| \le R\}$ a closed ball. Show that the function $\psi_R = \psi\chi_{B_R}$ is integrable and so the above explicit expression for the Fourier transform $\hat{\psi}_R$ is valid. This justifies the use of l.i.m. above.

Exercise 3.1.2. Find eigenfunctions of the Fourier transform corresponding to the eigenvalues -1 and $\pm i$.

Many utilities of the Fourier transform come from its property of exchanging multiplication and differentiation, as in the next propositions, whose simple proofs are quite instructive. The roots of those properties are the relations

$$\frac{\partial}{\partial x_j} e^{-i\,xp} = -ip_j\,e^{-i\,xp}, \qquad \frac{\partial}{\partial p_j} e^{-i\,xp} = -ix_j\,e^{-i\,xp}.$$

Proposition 3.1.3. *Let $\psi \in \mathcal{S}$. Then,*

a) $(\mathcal{F}\psi^{(k)})(p) = (-i)^{|k|} p^k \hat{\psi}(p)$.
b) $(\mathcal{F}^{-1}\psi)^{(k)}(x) = i^{|k|}\mathcal{F}^{-1}(p^k\hat{\psi}(p))(x)$.

Proposition 3.1.4. *Let $\psi \in \mathrm{L}^2(\mathbb{R}^n)$. Then, for fixed $y \in \mathbb{R}^n$,*

a) $(\mathcal{F}\psi(x-y))(p) = e^{-iyp}\hat{\psi}(p)$.
b) $\mathcal{F}(e^{ixy}\psi(x))(p) = \hat{\psi}(p-y)$.

Similar properties hold for the inverse Fourier transform.

Proposition 3.1.5. *Let $\psi, \phi \in \mathcal{S}$. Then, for the convolution*

$$(\psi * \phi)(x) := \int_{\mathbb{R}^n} \psi(x-y)\,\phi(y)\,dy = \int_{\mathbb{R}^n} \psi(y)\,\phi(x-y)\,dy$$

one has $\mathcal{F}(\psi * \phi)(p) = (2\pi)^{n/2}\,\hat{\psi}(p)\,\hat{\phi}(p)$.

Exercise 3.1.6. Since $\mathcal{S} \subset \mathrm{L}^1(\mathbb{R}^n)$, by using the above explicit integral representation of the Fourier transform, provide proofs of Propositions 3.1.3, 3.1.4 and 3.1.5.

Exercise 3.1.7. Compute the Fourier transform of the following functions in $\mathrm{L}^1(\mathbb{R})$:

a) $\psi(x) = \chi_{[a,b]}(x)$.
b) For $a > 0$, $\psi(x) = e^{-ax}$ if $x \geq 0$ and $\psi(x) = 0$ if $x < 0$.

Exercise 3.1.8. Parseval identity can be used to compute certain integrals. For $a > 0$, consider the characteristic function $\chi_{[-a,a]}(x)$; compute its Fourier transform $\hat{\chi}_{[-a,a]}$ and use Parseval to show that

$$\int_{\mathbb{R}} \left(\frac{\sin ax}{x} \right)^2 dx = \pi a.$$

It is possible to extend the convolution to spaces $\mathrm{L}^p(\mathbb{R}^n)$ by using Young's inequality, which is now recalled.

Proposition 3.1.9 (Young's Inequality). *Let* $1 \leq p, q, r \leq \infty$ *with* $1/p + 1/q = 1 + 1/r$. *If* $\psi \in \mathrm{L}^p(\mathbb{R}^n)$ *and* $\phi \in \mathrm{L}^q(\mathbb{R}^n)$, *then the convolution* $\psi * \phi \in \mathrm{L}^r(\mathbb{R}^n)$ *and*

$$\|\psi * \phi\|_r \leq \|\psi\|_p \, \|\phi\|_q.$$

The expression for $\psi * \phi$ *is the same as that in Proposition* 3.1.5.

3.2 Sobolev Spaces

In Chapter 2 the particular classes of Sobolev spaces $\mathcal{H}^m(\mathbb{R})$ were recalled via distributional (i.e., weak) derivatives and absolutely continuous functions. A main point is that the existence of sufficiently many weak derivatives in $\mathrm{L}^2(\mathbb{R})$ implies some derivatives in the classical sense. In this section additional properties of suitable Sobolev spaces are collected, and the discussion extended to higher dimensions.

Before going on, for reader's convenience, the definition of distribution and its derivatives are suitably recalled. Let Ω be an open subset of $\mathbb{R}^n$; a sequence $(\phi_j)_j \subset C_0^\infty(\Omega)$ is said to converge to $\phi \in C_0^\infty(\Omega)$ if there is a compact set $K \subset \Omega$ so that the support of ϕ_j is contained in K, $\forall j$, and for each multiindex k the sequence of derivatives $\phi^{(k)} \to \phi^{(k)}$ uniformly. $C_0^\infty(\Omega)$ is called the space of *test functions*.

A distribution u on Ω, is a linear functional on $C_0^\infty(\Omega)$ that are continuous under the above sequential convergence, that is, $u(\phi_j) \to u(\phi)$ whenever $\phi_j \to \phi$ in $C_0^\infty(\Omega)$. Its derivative is the distribution $u^{(k)}$ defined by

$$u^{(k)}(\phi) := (-1)^{|k|} u(\phi^{(k)}), \qquad \forall \phi \in C_0^\infty(\Omega).$$

The space of distributions on Ω is denoted by $C_0^\infty(\Omega)'$.

A distribution u is represented by a function $\psi \in \mathrm{L}^1_{\mathrm{loc}}(\Omega)$ if

$$u(\phi) = \int_\Omega \psi(x)\,\phi(x)\,dx, \qquad \forall \phi \in C_0^\infty(\Omega),$$

and in this case one usually says that $u = \psi$ in the sense of distributions. Note that $\mathrm{L}^1_{\mathrm{loc}}(\Omega)$ is naturally included in the space of distributions, and this fact suggests the extra terminology *generalized function* for distributions. The fundamental fact here is that if $u \in \mathrm{L}^1_{\mathrm{loc}}(\Omega)$ and

$$\int_\Omega u(x)\,\phi(x)\,dx = 0, \qquad \forall \phi \in C_0^\infty(\Omega),$$

then $u = 0$ a.e. in Ω. This justifies $u = 0$ in the sense of distributions as well as $u = \psi$ above. The Dirac δ is a well-known example of a distribution that is not represented by any function in $\mathrm{L}^1_{\mathrm{loc}}$.

The statement $u \in \mathrm{L}^1_{\mathrm{loc}}(\Omega)$ has distributional derivative $u^{(k)} = v \in \mathrm{L}^1_{\mathrm{loc}}(\Omega)$ means

$$u^{(k)}(\phi) := (-1)^{|k|} \int_\Omega u(x)\,\phi^{(k)}(x)\,dx = \int_\Omega v(x)\,\phi(x)\,dx,$$

for all $\phi \in C_0^\infty(\Omega)$. An important result is discussed in Lemma 2.3.9 and Remark 2.3.10, that is, if Ω is an open connected set and u is a distribution with null derivative, then u is constant.

A sequence of distributions $(u_j)_j$ in $C_0^\infty(\Omega)'$ converges to the distribution u, in the same space, if for every $\phi \in C_0^\infty(\Omega)$ the sequence $(u_j(\phi))_j$ converges in $\mathbb{C}$ to $u(\phi)$.

Example 3.2.1. To illustrate how weak is the notion of convergence of distributions, consider the sequence $u_j(x) = e^{ijx}$ in $\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R})$, which has a bad behavior in terms of convergence as a sequence of functions (e.g., it has constant absolute values and it does not converge pointwise to any function). However, for each $\phi \in C_0^\infty(\mathbb{R})$, on integrating by parts

$$\begin{aligned} |u_j(\phi)| &= \left| \int_{\mathbb{R}} e^{ijx}\,\phi(x)\,dx \right| = \left| \frac{1}{j} \int_{\mathbb{R}} e^{ijx}\,\phi'(x)\,dx \right| \\ &\le \frac{C_\phi}{j} \|\phi'\|_\infty \longrightarrow 0 \end{aligned}$$

as $j \to \infty$, where C_ϕ is the Lebesgue measure of the support of ϕ. Hence $u_j \to 0$ in the sense of distributions. The mechanism is the fast oscillations as $j \to \infty$ implying cancellations in the integral.

Example 3.2.2. If $0 \le \psi \in \mathrm{L}^1(\mathbb{R}^n)$ and $\int \psi(x)\,dx = 1$, then $\psi_j(x) := j^n \psi(jx)$ converges to Dirac δ at the origin as $j \to \infty$. Indeed, for $\phi \in C_0^\infty(\mathbb{R}^n)$,

$$\begin{aligned} \psi_j(\phi) &= \int_{\mathbb{R}^n} \psi_j(x)\,(\phi(x) - \phi(0))\,dx + \int_{\mathbb{R}^n} \psi_j(x)\,\phi(0)\,dx \\ &= \int_{\mathbb{R}^n} \psi_j(x)\,(\phi(x) - \phi(0))\,dx + \phi(0), \end{aligned}$$

since $\int \psi_j(x)\,dx = 1$. Now a change of variable gives

$$\int_{\mathbb{R}^n} \psi_j(x)\,(\phi(x)-\phi(0))\,dx = \int_{\mathbb{R}^n} \psi(x)\,(\phi(x/j)-\phi(0))\,dx$$

which vanishes as $j \to \infty$ by dominated convergence. Hence $\psi_j(\phi) \to \phi(0)$ for all $\phi \in C_0^\infty(\mathbb{R}^n)$, that is, $\psi_j \to \delta$ in the sense of distributions.

A sequence $(\psi_j)_j \subset \mathcal{S}(\mathbb{R}^n)$ is said to converge to $\psi \in \mathcal{S}(\mathbb{R}^n)$ if for every polynomial $p : \mathbb{R}^n \to \mathbb{C}$ and all multiindex k, $p\psi_j^{(k)} \to p\psi^{(k)}$ uniformly. A *tempered distribution* u on $\mathbb{R}^n$, is a continuous linear functional on $\mathcal{S}(\mathbb{R}^n)$, that is, $u(\psi_j) \to u(\psi)$ whenever $\psi_j \to \psi$ in $\mathcal{S}(\mathbb{R}^n)$. The space of tempered distributions is denoted by $\mathcal{S}'(\mathbb{R}^n)$. Note that $\mathcal{S}'(\mathbb{R}^n) \subset C_0^\infty(\mathbb{R}^n)'$, so that tempered distributions are indeed distributions.

The exponential function e^x is an example of $\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R})$ function that defines a distribution but not a tempered distribution.

At last the definition of (some) Sobolev spaces! For positive integers m, one defines $\mathcal{H}^m(\Omega)$, for an open $\Omega \subset \mathbb{R}^n$, as the Hilbert spaces of $\psi \in \mathrm{L}^2(\Omega)$ so that the weak derivatives $\psi^{(k)}$ exist and $\psi^{(k)} \in \mathrm{L}^2(\Omega)$ for all $|k| \le m$, and it is considered the norm

$$|||\psi|||_m := \left(\sum_{|k|\le m} \left\| \psi^{(k)} \right\|_2^2 \right)^{\frac{1}{2}}.$$

In case $\Omega = \mathbb{R}^n$ the Fourier transform provides another approach to $\mathcal{H}^m(\mathbb{R}^n)$. Proofs of some of the next results will be provided as examples of typical arguments.

Proposition 3.2.3. *Let $\psi \in \mathcal{H}^m(\mathbb{R}^n)$. Then, for $|k| \le m$ one has*

$$\mathcal{F}(\psi^{(k)})(p) = (-i)^{|k|} p^k \hat{\psi}(p),$$

with $\psi^{(k)}$ denoting distributional derivatives.

Proof. It is enough to consider that only one $k_j \ne 0$; the general case follows by induction. Since the weak derivatives belong to $\mathrm{L}^2(\mathbb{R}^n)$, one can use Plancherel's theorem. Let $\phi \in C_0^\infty(\mathbb{R}^n)$. Then, by Proposition 3.1.3,

$$\begin{aligned} \left\langle \mathcal{F}\psi^{(k_j)}), \hat{\phi} \right\rangle &= \left\langle \psi^{(k_j)}, \phi \right\rangle = (-1)^{k_j} \left\langle \psi, \phi^{(k_j)} \right\rangle \\ &= (-1)^{k_j} \left\langle \hat{\psi}, \mathcal{F}\phi^{(k_j)} \right\rangle = (-1)^{k_j} \left\langle \hat{\psi}, (-i)^{k_j} p_j^{k_j} \hat{\phi} \right\rangle \\ &= \left\langle (-i)^{k_j} p_j^{k_j} \hat{\psi}, \hat{\phi} \right\rangle, \end{aligned}$$

and the result follows since $\mathcal{F}C_0^\infty(\mathbb{R}^n)$ is dense in $\mathrm{L}^2(\hat{\mathbb{R}}^n)$. □

Corollary 3.2.4. *If $\psi \in \mathcal{H}^m(\mathbb{R}^n)$, then*

$$p^k \hat{\psi}(p) \in \mathrm{L}^2(\hat{\mathbb{R}}^n) \quad and \quad \psi^{(k)} = \mathcal{F}^{-1}(-i)^{|k|} p^k \mathcal{F}\psi, \ \forall |k| \leq m.$$

Corollary 3.2.4 has a converse statement, but for its proof it is necessary to recall that, for a tempered distributions $u \in \mathcal{S}'(\mathbb{R}^n)$, the Fourier transform $\hat{u}$ is defined by

$$\hat{u}(\phi) = u(\hat{\phi}), \qquad \forall \phi \in \mathcal{S}(\mathbb{R}^n),$$

and due to Proposition 3.1.3 the relation

$$\mathcal{F}(u^{(k)})(p) = (-i)^{|k|} p^k \hat{u}(p)$$

follows. The space $\mathrm{L}^p(\mathbb{R}^n)$ can be identified with a subset of $\mathcal{S}'(\mathbb{R}^n)$ (the inclusion $\mathrm{L}^p(\mathbb{R}^n) \mapsto \mathcal{S}'(\mathbb{R}^n)$ is a continuous injection). With this, a very important characterization will be presented.

Proposition 3.2.5. *The above norm $|||\cdot|||_m$ in $\mathcal{H}^m(\mathbb{R}^n)$ is equivalent to*

$$|||\psi|||'_m := \left(\int_{\mathbb{R}^n} \left(1 + |p|^2\right)^m |\hat{\psi}(p)|^2 \, dp \right)^{\frac{1}{2}}.$$

Proof. Let $\psi \in \mathcal{S}(\mathbb{R}^n)$; since $|p|^k \leq (1+|p|^2)^{|k|/2}$, then if $p^k\hat{\psi} \in \mathrm{L}^2(\hat{\mathbb{R}}^n)$ for $|k| \leq m$,

$$\begin{aligned}\int_{\mathbb{R}^n} \left|\psi^{(k)}(x)\right|^2 dx &= \int_{\mathbb{R}^n} \left|p^k \hat{\psi}(p)\right|^2 dp \leq \int_{\mathbb{R}^n} (1 + |p|^2)^{|k|} \left|\hat{\psi}(p)\right|^2 dp \\ &\leq \int_{\mathbb{R}^n} (1 + |p|^2)^m \left|\hat{\psi}(p)\right|^2 dp,\end{aligned}$$

and there is a constant $a > 0$ obeying $|||\psi|||_m \leq a|||\psi|||'_m$, since $\mathcal{S}(\mathbb{R}^n) \sqsubseteq \mathcal{H}^m(\mathbb{R}^n)$ and the norms are continuous, the latter inequality extends to $\psi \in \mathcal{H}^m(\mathbb{R}^n)$. Conversely, if $\psi \in \mathcal{H}^2(\mathbb{R}^m)$, it follows by the binomial relation that there are positive constants b_j so that

$$(1 + |p|^2)^m \left|\hat{\psi}(p)\right|^2 = \sum_{j=0}^{m} b_j |p|^{2j} \left|\hat{\psi}(p)\right|^2$$

and so

$$|||\psi|||'^2_m = \sum_{j=0}^{m} b_j \int_{\mathbb{R}^n} |p|^{2j} \left|\hat{\psi}(p)\right|^2 dp,$$

and because the right-hand side is a linear combination of terms of the form $\|p^k\hat{\psi}(p)\|_2^2$, then, by Proposition 3.2.3, there is $b > 0$ with $|||\psi|||'_m \leq b|||\psi|||_m$. The proposition is proved. □

Remark 3.2.6. By using the norm $|||\cdot|||'$, it is possible to define $\mathcal{H}^s(\mathbb{R}^n)$ for any $s \in \mathbb{R}$.

Theorem 3.2.7. *Let u be a tempered distribution in $\mathcal{S}'(\mathbb{R}^n)$. Then the following statements are equivalent:*

1. *u belongs to $\mathcal{H}^m(\mathbb{R}^n)$.*
2. *$u^{(m)} \in \mathrm{L}^2(\mathbb{R}^n)$ (weak derivative).*
3. *$p^k \hat{u}(p) \in \mathrm{L}^2(\hat{\mathbb{R}}^n)$, $\forall |k| \leq m$.*
4. *$p^m \hat{u}(p) \in \mathrm{L}^2(\hat{\mathbb{R}}^n)$.*

Moreover, if such statements hold, then $\mathcal{F}(u^{(k)})(p) = (-i)^{|k|} p^k \hat{u}(p)$.

Proof. (*Sketch*) The equivalences $1 \Leftrightarrow 2$ and $3 \Leftrightarrow 4$ will not be discussed here. $1 \Rightarrow 3$ is Corollary 3.2.4. Finally, $3 \Rightarrow 1$ follows by Proposition 3.2.5. □

Some of the above results show that, for $\psi \in \mathrm{L}^2(\mathbb{R}^n)$, the existence of weak derivatives implies integrability properties of $\hat{\psi}$. The next discussion is about differentiability properties.

Lemma 3.2.8. *If $\psi \in \mathrm{L}^1(\mathbb{R}^n)$, then $p \mapsto \hat{\psi}(p)$ is a continuous function and*

$$\|\hat{\psi}\|_\infty = \sup_{p \in \mathbb{R}^n} |\hat{\psi}(p)| \leq \frac{1}{(2\pi)^{\frac{n}{2}}} \|\psi\|_1 = \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} |\psi(x)|\, dx.$$

Similarly, if $\phi \in \mathrm{L}^1(\hat{\mathbb{R}}^n)$, then $\check{\phi}(x)$ is a continuous function and

$$\|\check{\phi}\|_\infty \leq \frac{1}{(2\pi)^{\frac{n}{2}}} \|\phi\|_1.$$

Proof. Write

$$|\hat{\psi}(p+h) - \hat{\psi}(p)| \leq \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} \left| e^{-i(p+h)x} - e^{-i(p)x} \right| |\psi(x)|\, dx$$

and note that, since ψ is integrable, the right-hand side vanishes by dominated convergence as $h \to 0$; hence $\hat{\psi}(p)$ is continuous. The inequality in the statement of the proposition is immediate. □

Exercise 3.2.9. Verify the inequalities in Lemma 3.2.8.

Proposition 3.2.10. *Let $\psi \in \mathrm{L}^1(\mathbb{R}^n)$. If $x^k \psi(x)$ is integrable for all $|k| \leq m$, then $\hat{\psi}^{(k)}$ is a continuous and bounded function, and*

$$(\mathcal{F}\psi)^{(k)} = (-i)^{|k|}\, \mathcal{F}(x^k \psi(x)), \qquad \forall |k| \leq m.$$

Proof. It is enough to consider $k_j = 1$ for some j and $k_l = 0$ if $l \neq j$; the general case follows by induction. One has

$$\hat{\psi}(p) = \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} e^{-i\,xp}\, \psi(x)\, dx.$$

Consider also the differentiation of this integrand with respect to p_j, that is,

$$\phi(p) = \phi(p_j) = \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} (-ix_j) e^{-i\,xp}\, \psi(x)\, dx;$$

this integral is $\phi(p) = -i\mathcal{F}(x_j\psi)(p)$, which is a continuous function of p_j since, by hypothesis, $x_j\psi(x)$ is integrable (see Lemma 3.2.8). For $p_j \in \mathbb{R}$, denote $\hat{\psi}(p_j)$ the function obtained by keeping fixed p_k for $k \neq j$. By using Fubini's theorem it is found that, for $h \neq 0$,

$$\begin{aligned} \left| \frac{1}{h}[\hat{\psi}(p_j + h) - \hat{\psi}(p_j)] - \phi(p_j) \right| &= \left| \frac{1}{h} \int_0^h [\phi(p_j + r) - \phi(p_j)]\, dr \right| \\ &\leq \sup_{|r| \leq |h|} |\phi(p_j + r) - \phi(p_j)|, \end{aligned}$$

and since $\phi(s)$ is uniformly continuous in any closed interval, the above expression vanishes as $h \to 0$. Therefore, $\partial_{p_j}\hat{\psi}(p) = \phi(p)$. □

Corollary 3.2.11. *If $\psi \in \mathrm{L}^2(\mathbb{R}^n)$ and $p^k\hat{\psi}(p)$ is integrable for all $|k| \leq m$, then $\psi^{(k)}$ is a continuous and bounded function, and*

$$\psi^{(k)} = i^{|k|}\, \mathcal{F}^{-1}(p^k \hat{\psi}(p)), \qquad \forall |k| \leq m.$$

Proof. This is essentially Proposition 3.2.10 adapted to the inverse Fourier transform. □

The functions $\psi \in \mathcal{H}^m(\mathbb{R}^n)$ are characterized as those that have weak derivatives $\psi^{(k)} \in \mathrm{L}^2(\hat{\mathbb{R}}^n)$ for any $|k| \leq m$ and, by a set of results called Sobolev embedding theorems (also called Sobolev lemmas), they become more regular with increasing m. One of such (nontrivial) results is the following one:

Theorem 3.2.12 (Sobolev Embedding). *Let Ω be an open subset of $\mathbb{R}^n$. If $\psi \in \mathcal{H}^m(\Omega)$ and $m > r + \frac{n}{2}$, then $\psi^{(k)}$ is a continuous and bounded function for all $|k| \leq r$. Furthermore, in case $\Omega = \mathbb{R}^n$ the inclusion map $\mathcal{H}^m(\mathbb{R}^n) \mapsto C^r(\mathbb{R}^n)$ is bounded.*

By way of illustration, take $n = 1$; it follows that if $\psi \in \mathcal{H}^m(\mathbb{R})$ then $\psi^{(k)}$ are bounded continuous functions for $0 \leq k < m$. For $n = 3$ and $\psi \in \mathcal{H}^2(\mathbb{R}^3)$, then $\psi^{(k)}$ is surely continuous only for $k = 0$. In case of bounded open intervals (a, b) one has $C(a, b) \subset \mathcal{H}^1(a, b) \subset C[a, b]$; so, roughly speaking, for $n = 1$ the elements of $\mathcal{H}^1$ are continuous functions that are primitives of functions in L^2.

For the curious readers, Exercise 3.2.13 gives a flavor of how such results can be obtained; of course it does not replace a specific text about Sobolev spaces.

Exercise 3.2.13. The case $m > r + n$ and $\Omega = \mathbb{R}^n$ in Theorem 3.2.12 has a simpler proof. The interested reader may follow the steps ahead to prove this restricted version of the first part of Sobolev's embedding theorem, that is, if $\psi \in \mathcal{H}^m(\mathbb{R}^n)$ and $m > r + n$, then $\psi^{(k)}$ is a continuous and bounded function for all $|k| \leq r$.

1. If $\psi \in \mathcal{H}^m(\mathbb{R}^n)$ then, by Corollary 3.2.11, conclude that it is enough to show that $p^k\hat{\psi} \in \mathrm{L}^1(\hat{\mathbb{R}}^n)$, for all $|k| \le r$.
2. Write $p^k\hat{\psi} = \phi_1\phi_2$, with

$$\phi_1(p) = \left(\Pi_{j=1}^k \left(1+|p_j|^{1+k_j}\right)\right)\hat{\psi}(p), \qquad \phi_2(p) = \frac{p^k}{\Pi_{j=1}^k \left(1+|p_j|^{1+k_j}\right)},$$

and show that if $|k| \le r$ both ϕ_1 and ϕ_2 belong to $\mathrm{L}^2(\hat{\mathbb{R}}^n)$, so that $\phi_1\phi_2$ is integrable. For ϕ_1, dominate it by a finite sum of integrable functions of the form $|p_j|^{r_j}|\hat{\psi}(p)|$, with $0 \le r_j \le |k|$. For ϕ_2 use Fubini's theorem and note that

$$\frac{|p|^n}{1+|p|^{1+n}} \le \frac{1}{|p|}$$

for $|p|$ large enough.

Exercise 3.2.14. If $\Omega \subset \mathbb{R}^n$ is a bounded set, show that $\psi(t) = |t|^\alpha$ belongs to $\mathcal{H}^m(\Omega)$ iff $(\alpha - m) > -n/2$.

It is also worth mentioning (see [Ad75]):

Lemma 3.2.15. *Let Ω be an open set in $\mathbb{R}^n$ with a regular bounded boundary. Then the norm $|||\psi|||_m$ in $\mathcal{H}^m(\Omega)$ is equivalent to the norm*

$$[\psi]_m := \left(\|\psi\|_2^2 + \sum_{|k|=m}\left\|\psi^{(k)}\right\|_2^2\right)^{\frac{1}{2}}.$$

Example 3.2.16. As an application of Sobolev's embedding theorem, another proof of Proposition 2.3.20 will be provided. Recall that $\mathrm{dom}\, H = C_0^\infty(a,b) \subset \mathcal{H} = \mathrm{L}^2(a,b)$, $V \in \mathrm{L}^2_{\mathrm{loc}}(a,b)$, $-\infty \le a < b \le \infty$, and

$$(H\psi)(x) = -\psi''(x) + V(x)\psi(x), \qquad \psi \in \mathrm{dom}\, H.$$

The question is to find H^*. If $\psi \in \mathrm{dom}\, H^*$, then $H^*\psi \in \mathrm{L}^2(a,b)$ and for all $\phi \in C_0^\infty(a,b)$,

$$\int_a^b \left(-\phi''(x) + V(x)\phi(x)\right)\psi(x)\,dx = \langle\overline{\phi}, H^*\psi\rangle,$$

that is

$$\int_a^b \phi''(x)\psi(x)\,dx = \int_a^b \phi(x)\,\left(V(x)\psi(x) - H^*\psi\right)\,dx,$$

so that the second distributional derivative of ψ belongs to $\mathrm{L}^2_{\mathrm{loc}}(a,b)$; by Sobolev embedding ψ, ψ' are absolutely continuous functions and

$$\psi'' = V\psi - H^*\psi,$$

that is,

$$\text{dom } H^* = \left\{\psi \in \mathrm{L}^2(a,b) : \psi, \psi' \in \mathrm{AC}(a,b), (-\psi'' + V\psi) \in \mathrm{L}^2(a,b)\right\},$$
$$(H^*\psi)(x) = -\psi''(x) + V(x)\psi(x), \qquad \psi \in \text{dom } H^*.$$

Thereby the proof is complete. □

3.3 Momentum Operator

This section begins with a summary of a very important statement. For $\psi \in \mathcal{H}^m(\mathbb{R}^n)$ there are two equivalent ways of differentiating it: if $|k| \le m$, under Fourier transform the derivative in the sense of distributions $\psi \mapsto \psi^{(k_j)}$ corresponds to the multiplication operator $\hat{\psi} \mapsto (-i)^{k_j} p_j^{k_j} \hat{\psi}$ in $\mathrm{L}^2(\hat{\mathbb{R}}^n)$. It is also worth recalling some integration by parts formulae: if $\psi, \phi \in \mathcal{H}^1(\mathbb{R}^n)$, then

$$\int_{\mathbb{R}^n} \psi(x)\partial_j\phi(x)\,dx = -\int_{\mathbb{R}^n} \partial_j(\psi(x))\,\phi(x)\,dx,$$

and for $\psi, \phi \in \mathcal{H}^2(\mathbb{R}^n)$ then

$$\int_{\mathbb{R}^n} \psi(x)\Delta\phi(x)\,dx = -\int_{\mathbb{R}^n} \nabla\psi(x)\cdot\nabla\psi(x)\,dx.$$

Two particular cases will be discussed in detail: related to the first derivative $P_j\psi = -i\partial_j\psi$, corresponding to the jth component of the quantum momentum operator and, related to the laplacian $H_0\psi = -\Delta\psi = -\sum_{j=1}^n \partial_j^2\psi$, corresponding to the quantum kinetic energy in $\mathrm{L}^2(\mathbb{R}^n)$, discussed in Section 3.4.

In $\mathrm{L}^2(\mathbb{R})$ the quantum momentum operator was previously introduced, in Chapter 2), as $\text{dom } P = \mathcal{H}^1(\mathbb{R})$,

$$(P\psi)(x) = -i\psi'(x), \qquad \psi \in \text{dom } P.$$

See Examples 2.3.11 and 2.4.10. By Fourier transform one gets

$$(\mathcal{F}P\psi)(p) = p\hat{\psi}(p) = \mathcal{M}_{\varphi(p)}\hat{\psi}(p), \qquad \varphi(p) = p.$$

Note also that $\mathcal{H}^1(\hat{\mathbb{R}}) = \left\{\hat{\psi} \in \mathrm{L}^2(\hat{\mathbb{R}}) : |||\psi|||_1' < \infty\right\}$, that is,

$$|||\psi|||_1' = \left(\int_{\mathbb{R}} \left(1 + |p|^2\right)|\hat{\psi}(p)|^2\,dp\right)^{\frac{1}{2}} < \infty,$$

which is the graph norm of $\mathcal{M}_{\varphi(p)}$ in $\mathrm{L}^2(\hat{\mathbb{R}})$, and $\text{dom } P = \mathcal{F}^{-1}\mathcal{H}^1(\hat{\mathbb{R}})$. Then,

$$(\mathcal{F}P\mathcal{F}^{-1})\hat{\psi}(p) = p\hat{\psi}(p), \qquad (P\psi)(x) = (\mathcal{F}^{-1}p\mathcal{F})\psi(x),$$

and it follows that the momentum operator is unitarily equivalent (via Fourier transform) to this multiplication operator $\mathcal{M}_p$ by a continuous real function. Therefore, see Subsection 2.3.2, it provides another proof that this operator is self-adjoint with no eigenvalues, and that its spectrum is $\mathbb{R}$, since such properties hold for $\mathcal{M}_p$ (see Exercise 2.1.26).

This construction is readily generalized to the jth component of the momentum operator P_j in $\mathrm{L}^2(\mathbb{R}^n)$, given by

$$\mathcal{F}(P_j\psi)(p) = p_j\hat{\psi}(p) = \mathcal{M}_{p_j}\hat{\psi}(p), \qquad 1 \le j \le n,$$

which is also self-adjoint, with no eigenvalues and its spectrum is $\mathbb{R}$. The (total) momentum operator is defined through the gradient

$$P = -i\nabla = -i\,(\partial_1, \ldots, \partial_n),$$

i.e., $P = \mathcal{F}^{-1}(p_1, \ldots, p_n)\mathcal{F} = (\mathcal{F}^{-1}p_1\mathcal{F}, \ldots, \mathcal{F}^{-1}p_n\mathcal{F})$.

3.4 Kinetic Energy and Free Particle

The nonrelativistic quantum *kinetic energy* operator in $\mathrm{L}^2(\mathbb{R}^n)$ (or $\mathrm{L}^2(\Omega)$, Ω an open subset of $\mathbb{R}^n$) is denoted by H_0 and (up to a sign) it is the self-adjoint realization of the laplacian (distributional derivatives), that is, $H_0 = -\Delta$ with domain $\mathcal{H}^2(\mathbb{R}^n)$.

For the one-dimensional case $\mathrm{L}^2(\mathbb{R})$ the kinetic energy corresponds to $\mathrm{dom}\, H_0 = \mathcal{H}^2(\mathbb{R})$ and $H_0\psi = -\psi''$. By using Fourier transform, this operator is unitarily equivalent to the multiplication operator

$$\mathcal{F}H_0\psi = \mathcal{F}H_0\mathcal{F}^{-1}\mathcal{F}\psi = \mathcal{M}_{p^2}\hat{\psi}.$$

In higher dimensions $\mathrm{L}^2(\mathbb{R}^n)$, $n \ge 2$, an alternative way of defining the kinetic energy operator is $\mathrm{dom}\, H_0 = \mathcal{H}^2(\mathbb{R}^n)$ and

$$(H_0\psi)(x) = -\Delta\psi(x) = \mathcal{F}^{-1}[p^2\hat{\psi}(p)](x), \qquad \psi \in \mathrm{dom}\, H_0.$$

That is, it is unitarily equivalent to the multiplication operator $\mathcal{F}H_0\psi = \mathcal{M}_{p^2}\hat{\psi}$ in $\mathrm{L}^2(\hat{\mathbb{R}}^n)$,

$$H_0 = \mathcal{F}^{-1}p^2\mathcal{F}.$$

Since $p \mapsto p^2$ is a positive continuous function, it follows that its spectrum is $\sigma(H_0) = \mathrm{rng}\, p^2 = [0, \infty)$; see Exercise 2.3.29. Further, H_0 has no eigenvalues.

Note that the unitarity of the Fourier transform allows one to conclude that if $\psi \in \mathrm{L}^2(\mathbb{R}^n)$ with $\Delta\psi \in \mathrm{L}^2(\mathbb{R}^n)$, then $\psi \in \mathcal{H}^2(\mathbb{R}^n)$; see other comments on page 197.

Since only kinetic energy is present (there is no interaction among particles), the operator H_0 is also called the *Schrödinger operator for the free particle*.

Another terminology is *free hamiltonian* or *free Schrödinger operator*. Perturbations of H_0 by a potential energy $V(x)$, resulting in the total energy operator, are considered in other chapters.

Proposition 3.4.1. *The operators T_C, T_S with domains $C_0^\infty(\mathbb{R}^n)$ and $\mathcal{S}(\mathbb{R}^n)$, respectively, both with action $\psi \mapsto -\Delta\psi$, are essentially self-adjoint and*

$$\overline{T_C} = H_0 = \overline{T_S}.$$

In other words, $C_0^\infty(\mathbb{R}^n)$ and $\mathcal{S}(\mathbb{R}^n)$ are cores of H_0.

Proof. If $g \in \operatorname{dom} T_C^* \subset \mathrm{L}^2(\mathbb{R}^n)$, then

$$\langle g, -\Delta\psi\rangle = \langle T_C^* g, \psi\rangle, \qquad \forall\psi \in C_0^\infty(\mathbb{R}^n);$$

thus the distributional derivative $-\Delta g = T_C^* g \in \mathrm{L}^2(\mathbb{R}^n)$ and so $g \in \mathcal{H}^2(\mathbb{R}^n)$ and $T_C^* g = -\Delta g = H_0 g$, so that $T_C^* \subset H_0$. Conversely, if $\phi \in \mathcal{H}^2(\mathbb{R}^n)$ then $-\Delta\phi \in \mathrm{L}^2(\mathbb{R}^n)$ and, via integration by parts,

$$\langle \phi, T_C\psi\rangle = \langle \phi, -\Delta\psi\rangle = \langle -\Delta\phi, \psi\rangle, \qquad \forall\psi \in C_0^\infty(\mathbb{R}^n);$$

by definition, $\phi \in \operatorname{dom} T_C^*$ and $T_C^*\phi = -\Delta\phi = H_0\phi$, so that $H_0 \subset T_C^*$. Hence $T_C^* = H_0$. Since H_0 is self-adjoint, one has $\overline{T_C} = T_C^{**} = H_0$, and it is found that T_C is essentially self-adjoint.

For T_S, note that $T_C \subset T_S \subset H_0$. Thus, since T_C is essentially self-adjoint, $T_C^* = \overline{T_C} = H_0$, and so $H_0 \subset T_S^* \subset T_C^* = H_0$. Therefore, $T_S^* = H_0$ and T_S is essentially self-adjoint (also $\overline{T_S} = T_S^{**} = H_0$). □

Exercise 3.4.2. Show that $(\mathbf{1} + H_0)\mathcal{S} = \mathcal{S}$.

In view of $H_0 = \mathcal{F}^{-1} p^2 \mathcal{F}$, one has

$$R_z(H_0) = \mathcal{F}^{-1} \frac{1}{p^2 - z} \mathcal{F},$$

for the resolvent of H_0 at $z \notin [0, \infty)$ (check this!). The operator of multiplication by the functions

$$\frac{1}{p^2 - z} \qquad \text{and} \qquad e^{-itp^2}$$

correspond to important quantum operators in the momentum representation $\mathrm{L}^2(\hat{\mathbb{R}}^n)$; their actions in the position representation $\mathrm{L}^2(\mathbb{R}^n)$ will be discussed in Subsection 3.4.1 and Section 5.5, respectively.

Exercise 3.4.3. Use Fourier transform to show that for all complex numbers $z \notin [0, \infty)$ the operator $P_j R_z(H_0)$ is bounded for any momentum component P_j.

For a measurable function $f : \mathbb{R} \to \mathbb{C}$ one defines the operator

$$\operatorname{dom} f(H_0) = \mathcal{F}^{-1} \operatorname{dom} f(p^2), \qquad f(H_0) := \mathcal{F}^{-1} f(p^2) \mathcal{F};$$

since dom $f(p^2)$ is a dense set and $\mathcal{F}$ is unitary, then dom $f(H_0)$ is dense and if $f(p^2)$ is real valued the operator $f(H_0)$ is also self-adjoint – see Subsection 2.3.2. If f is a (essentially) bounded function, then $f(H_0) \in \mathrm{B}(\mathcal{H})$. According to the nomenclature on page 80, $f(p^2)$ is the operator $f(H_0)$ in momentum representation.

In a similar way one defines the function of momentum operators $f(P_j)$ and $f(P)$, the latter with $f : \mathbb{R}^n \to \mathbb{C}$. Note, as before, the abuse of notation by indicating the multiplication operator $\mathcal{M}_{f(p)}$ by just $f(p)$.

Exercise 3.4.4. Verify that if $f(p) = p^k$, $k \in \mathbb{N}$, then the corresponding operator $f(H_0)$ in $\mathrm{L}^2(\mathbb{R})$ is

$$\operatorname{dom} f(H_0) = \mathcal{H}^{2k}(\mathbb{R}), \qquad f(H_0)\psi = (-1)^k \psi^{(2k)}.$$

Challenge: What about $\sqrt{H_0}$?

3.4.1 Free Resolvent

In this subsection the resolvent of the free hamiltonian $R_z(H_0)$ in $\mathbb{R}^3$, in position representation, will be computed from its momentum representation $(p^2 - z)^{-1}$. First, a result also of general interest.

Lemma 3.4.5. *If $f \in \mathrm{L}^2(\mathbb{R}^n)$, then the operator $f(P)$ in position representation is an integral operator whose kernel is $1/(2\pi)^{\frac{n}{2}} \check{f}(y-x)$, that is, for all $\psi \in \mathrm{L}^2(\mathbb{R}^n)$,*

$$(f(P)\psi)(x) := \mathcal{F}^{-1}\left[f(p)\hat{\psi}(p)\right](x) = \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} \check{f}(y-x)\psi(y)\, dy.$$

Proof. Since $f\hat{\psi} \in \mathrm{L}^1(\hat{\mathbb{R}}^n)$ there is an explicit expression for its inverse Fourier transform. Fix $x \in \mathbb{R}^n$. Then, since $\mathcal{F}^{-1}$ is unitary and by a simple variation of Proposition 3.1.4,

$$\begin{aligned}(2\pi)^{\frac{n}{2}} \mathcal{F}^{-1}\left[f(p)\hat{\psi}(p)\right](x) &= \int_{\mathbb{R}^n} e^{i\,xp} f(p)\hat{\psi}(p)\, dp \\ &= \left\langle e^{-i\,xp}\overline{f(p)}, \hat{\psi}(p)\right\rangle = \left\langle \mathcal{F}^{-1}(e^{-i\,xp}\overline{f(p)})(y), \psi(y)\right\rangle \\ &= \left\langle \overline{\check{f}(y-x)}, \psi(y)\right\rangle = \int_{\mathbb{R}^n} \check{f}(y-x)\psi(y)\, dy.\end{aligned}$$

This is the desired expression. □

Theorem 3.4.6. *Fix a complex number $z \notin [0,\infty)$. Then the resolvent of the free hamiltonian H_0 in $\mathrm{L}^2(\mathbb{R}^3)$ at z, in position representation, is given by*

$$(R_z(H_0)\psi)(x) = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{e^{i\sqrt{z}|x-y|}}{|x-y|}\, \psi(y)\, dy, \qquad \forall \psi \in \mathrm{L}^2(\mathbb{R}^3),$$

with the branch of the square root given by $\operatorname{Im} \sqrt{z} > 0$.

Proof. The resolvent is $(R_z(H_0)\psi)(x) = \mathcal{F}^{-1}[f(p)\hat{\psi}(p)](x)$ with $f(p) = (p^2 - z)^{-1}$ which belongs to $L^2(\mathbb{R}^3)$ (and is also bounded). By Lemma 3.4.5, the resolvent is an integral operator with kernel

$$G_0(x-y;z) := 1/(2\pi)^{\frac{3}{2}}\, \check{f}(x-y).$$

The task now is to compute

$$X = (2\pi)^{3/2}\check{f}(x) = \text{l.i.m.} \int_{\mathbb{R}^3} \frac{e^{i\,xp}}{p^2 - z}\, dp = \lim_{R\to\infty} \int_{|p|\le R} \frac{e^{i\,xp}}{p^2 - z}\, dp.$$

Introduce spherical coordinates $xp = |x||p|\cos\theta$, $r = |p|$, $0 \le \theta \le \pi$, $-\pi \le \vartheta < \pi$ and also $a = \cos\theta$. Then

$$\begin{aligned} X &= \lim_{R\to\infty} \int_0^R \int_{-1}^1 \int_{-\pi}^{\pi} \frac{e^{i\,r|x|a}}{r^2 - z}\, r^2\, d\vartheta da\, dr \\ &= \frac{2\pi}{i\,|x|} \lim_{R\to\infty} \int_{-R}^{R} \frac{re^{i\,r|x|}}{r^2 - z} dr = \frac{2\pi}{i\,|x|} \lim_{R\to\infty} \int_{C_R} \frac{we^{i\,w|x|}}{(w-\sqrt{z})(w+\sqrt{z})} dw, \end{aligned}$$

where $\text{Im}\,\sqrt{z} > 0$, C_R is the rectangle in the upper half complex plane, delimited by the vertices $(-R,0), (R,0), (R,\sqrt{R}), (-R,\sqrt{R})$, and w the complex integration variable. Then, by residues, one gets

$$X = 2\pi^2\, \frac{e^{i\,\sqrt{z}|x|}}{|x|}, \qquad \text{Im}\,\sqrt{z} > 0,$$

so that

$$G_0(x-y;z) = \frac{1}{4\pi} \frac{e^{i\,\sqrt{z}\,|x-y|}}{|x-y|}, \qquad \text{Im}\,\sqrt{z} > 0,$$

and the proof is complete. □

Definition 3.4.7. The function $G_0(x-y;z)$, introduced in the proof of Theorem 3.4.6, is called the three-dimensional *free Green function*. It is the kernel of the free resolvent operator in $L^2(\mathbb{R}^3)$.

Exercise 3.4.8. Given a potential $V : \mathbb{R}^3 \to \mathbb{R}$, assume that $\psi \in L^2(\mathbb{R}^3)$ is an eigenfunction of $H_0 + V$ with eigenvalue $\lambda < 0$, that is, $(H_0 + V)\psi = \lambda\psi$ and, also, $V\psi \in L^2(\mathbb{R}^3)$. Show that

$$\psi(x) = -\frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{e^{-\sqrt{-\lambda}|x-y|}}{|x-y|}\, V(y)\psi(y)\, dy.$$

This is an integral equation for ψ closely related to the *Lippmann-Schwinger equation* in scattering theory.

Exercise 3.4.9. Check that the kernel of the free resolvent operator in $L^2(\mathbb{R})$, i.e., the one-dimensional free Green function, at $z \notin [0,\infty)$ is

$$G_0(x-y;z) = \frac{i}{2\sqrt{z}}\, e^{i\sqrt{z}\,|x-y|}, \qquad \text{with Im}\,\sqrt{z} > 0.$$

Remark 3.4.10. For dimensions different from one and three, the computation of the free Green function is more difficult to handle; it can be performed in terms of modified Bessel functions of the second kind. The situation is simpler for odd dimensions, since spherical Bessel functions can be employed. Nonetheless, they are not too illuminating. See the full expression in [HiS96] page 164 and details in [CouH53], and for Bessel functions [Wa62].

Exercise 3.4.11. Check that for $\mathrm{L}^2(\mathbb{R}^n)$, $n = 1, 3$, there exists (a.e.) the limit of the free Green function for $z = \lambda + i\varepsilon$, $\lambda > 0$,

$$G_0(x - y; \lambda \pm 0) := \lim_{\varepsilon \to 0^\pm} G_0(x - y; \lambda + i\varepsilon).$$

So the operators $R_{\lambda\pm0}(H_0)$ are also defined as integral operators with kernels $G_0(x-y; \lambda\pm0)$. Verify that $R_{\lambda+0}(H_0) \neq R_{\lambda-0}(H_0)$. Are these operators bounded?

Exercise 3.4.12. Write out the one-dimensional harmonic oscillator energy operator (Example 2.3.3) $(H\psi)(x) = -\psi''(x) + x^2\psi(x)$ in the position and momentum representations.

Remark 3.4.13. The kinetic energy, the j-component of the momentum and the total momentum operators in $\mathrm{L}^2(\mathbb{R}^n)$, with all physical constants included, have the expressions

$$H_0 = -\frac{\hbar^2}{2m}\Delta, \qquad P_j = -i\hbar\partial_j, \qquad P = -i\hbar\nabla,$$

respectively. For the Green function in $\mathrm{L}^2(\mathbb{R}^3)$,

$$G_0(x - y; z) = \frac{m}{\hbar^2 2\pi} \, \frac{1}{|x - y|} \exp\left(i \, \frac{\sqrt{2mz}}{\hbar} \, |x - y| \right),$$

while in $\mathrm{L}^2(\mathbb{R})$

$$G_0(x - y; z) = \frac{i}{\hbar} \sqrt{\frac{m}{2z}} \exp\left(i \, \frac{\sqrt{2mz}}{\hbar} \, |x - y| \right).$$

Finally, the expression of Fourier transform in $\mathrm{L}^2(\mathbb{R}^n)$ usually employed in quantum mechanics takes the form

$$\hat{\psi}(p) = \frac{1}{(2\pi\hbar)^{\frac{n}{2}}} \int_{\mathbb{R}^n} e^{-i\frac{xp}{\hbar}} \, \psi(x) \, dx.$$

Remark 3.4.14. In the context of quantum mechanics, usually the term "Green function" refers to a representation (e.g., in position or momentum representation) of the resolvent of a self-adjoint operator. The Green function for the hydrogen atom Schrödinger operator was studied in [Ho64] and [Schw64] (see Example 6.2.3).

Chapter 4

Operators via Sesquilinear Forms

The basics of self-adjoint extensions via sesquilinear forms are discussed. The main points are form representations, Friedrichs extensions and examples. Additional information appears in Sections 6.1, 9.3 and 10.4. Some sesquilinear forms can be sources of self-adjoint operators related to "singular interactions" and/or ill-posed operator sums.

4.1 Sesquilinear Forms

Let dom b be a dense subspace of the Hilbert space $\mathcal{H}$. A *sesquilinear form* in $\mathcal{H}$,

$$b : \text{dom } b \times \text{dom } b \to \mathbb{C}$$

is a map linear in the second variable and antilinear in the first one. b is hermitian if $b(\xi, \eta) = \overline{b(\eta, \xi)}$. The map $\xi \mapsto b(\xi, \xi)$, $\xi \in \text{dom } b$, is called the *quadratic form* associated with b. Usually dom b is referred to as the domain of b, instead of dom $b \times$ dom b, and only the term *form* is used as a shorthand for sesquilinear form. Sometimes the notation $b(\xi) = b(\xi, \xi)$ for the quadratic form is used. Here all forms are assumed to be densely defined.

Exercise 4.1.1. Verify the polarization identity for sesquilinear forms

$$4b(\xi, \eta) = b(\xi + \eta) - b(\xi - \eta) - ib(\xi + i\eta) + ib(\xi - i\eta),$$

for all $\xi, \eta \in \text{dom } b$. Use polarization to show that b is hermitian iff the associated quadratic form is real valued.

Definition 4.1.2. A sesquilinear form b is *bounded* if its *form norm*

$$\|b\| := \sup_{\substack{0\neq\xi_1\in\mathrm{dom}\ b\\ 0\neq\xi_2\in\mathrm{dom}\ b}} \frac{|b(\xi_1,\xi_2)|}{\|\xi_1\|\,\|\xi_2\|}$$

is finite, i.e., $\|b\| < \infty$.

The standard example of bounded sesquilinear form is the inner product on a Hilbert space, whose norm is 1. The next result is the structure of bounded sesquilinear forms; the corresponding results when boundedness is not required appear in Theorems 4.2.6 and 4.2.9.

Proposition 4.1.3. *If $b : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ is a bounded sesquilinear form, then there exists a unique operator $T_b \in \mathrm{B}(\mathcal{H})$ obeying*

$$b(\xi_1, \xi_2) = \langle T_b\xi_1, \xi_2\rangle, \qquad \forall\xi_1, \xi_2 \in \mathcal{H}.$$

Furthermore, $\|T_b\| = \|b\|$ and if b is hermitian then T_b is self-adjoint.

Proof. For each $\xi_1 \in \mathcal{H}$ the functional $L_{\xi_1} : \mathcal{H} \to \mathbb{C}$, $L_{\xi_1}(\xi_2) = b(\xi_1, \xi_2)$ is linear, and since

$$|L_{\xi_1}(\xi_2)| = |b(\xi_1, \xi_2)| \leq \|b\|\|\xi_1\|\,\|\xi_2\|,$$

then $\|L_{\xi_1}\| \leq \|b\|\,\|\xi_1\|$ and $L_{\xi_1} \in \mathcal{H}^*$ (the dual space of $\mathcal{H}$).

By Riesz's Representation Theorem 1.1.40 there exists a unique $\eta_2 \in \mathcal{H}$ with $L_{\xi_1}(\xi_2) = \langle\eta_2, \xi_2\rangle$, for all $\xi_2 \in \mathcal{H}$. Define $T_b : \mathcal{H} \to \mathcal{H}$ by $T_b\xi_1 = \eta_2$, for which $b(\xi_1, \xi_2) = \langle T_b\xi_1, \xi_2\rangle$, $\forall\xi_1 \in \mathcal{H}, \xi_2 \in \mathcal{H}$, and it is linear. Note that $T_b = 0$ if, and only if, b is null (the definition is clear!).

Thus, if $b \neq 0$,

$$\begin{aligned}
\|T_b\| &= \sup_{\substack{0\neq\xi_1\\ T_b\xi_1\neq 0}} \frac{\|T_b\xi_1\|}{\|\xi_1\|} = \sup_{\substack{0\neq\xi_1\\ T_b\xi_1\neq 0}} \frac{|\langle T_b\xi_1, T_b\xi_1\rangle|}{\|\xi_1\|\,\|T_b\xi_1\|} \leq \|b\| \\
&= \sup_{\substack{0\neq\xi_1\\ 0\neq\xi_2}} \frac{|\langle T_b\xi_1, \xi_2\rangle|}{\|\xi_1\|\,\|\xi_2\|} \leq \sup_{\substack{0\neq\xi_1\\ 0\neq\xi_2}} \frac{\|T_b\xi_1\|\,\|\xi_2\|}{\|\xi_1\|\,\|\xi_2\|} = \|T_b\|,
\end{aligned}$$

showing that $T_b \in \mathrm{B}(\mathcal{H})$ and $\|T_b\| = \|b\|$. The uniqueness of the operator follows from the relation $\langle T_b\xi_1, \xi_2\rangle = \langle S\xi_1, \xi_2\rangle$, for any ξ_1, ξ_2, consequently the operators S and T_b coincide.

Now if such b is hermitian then $\langle T_b\xi, \eta\rangle = b(\xi, \eta) = \overline{b(\eta, \xi)} = \langle\xi, T_b\eta\rangle$, and T_b is self-adjoint. □

Hence, there is a one-to-one correspondence between such bounded (and hermitian) sesquilinear forms on $\mathcal{H} \times \mathcal{H}$ and bounded (and self-adjoint) linear operators on $\mathcal{H}$. Observe that if the sesquilinear form is given by the inner product on $\mathcal{H}$, then Proposition 4.1.3 gives rise to the identity operator $T_b = \mathbf{1}$.

One then wonders whether it is possible to adapt the above construction to get unbounded self-adjoint operators from more general forms. In fact, part of this construction can be carried out for suitable forms, as discussed below; a chief result will be that there is a one-to-one correspondence between “closed lower bounded sesquilinear forms” and lower bounded self-adjoint operators. Other motivations appear in Remark 4.1.14. Now some definitions.

Definition 4.1.4. Let b be a hermitian sesquilinear form. Then b is:

a) *positive* if the quadratic form $b(\xi,\xi) \geq 0, \forall \xi \in \text{dom } b$.

b) *lower bounded* if there is $\beta \in \mathbb{R}$ with $b(\xi,\xi) \geq \beta\|\xi\|^2$, $\forall \xi \in \text{dom } b$, and this situation will be briefly denoted by $b \geq \beta$; such β is called a *lower limit* or *lower bound* of b. Notice that $b - \beta$ defines a positive sesquilinear form by $(b-\beta)(\xi,\eta) := b(\xi,\eta) - \beta\langle\xi,\eta\rangle$.

Exercise 4.1.5. Verify that Cauchy-Schwarz and triangular inequalities

$$|b(\xi,\eta)| \leq b(\xi)^{\frac{1}{2}}\, b(\eta)^{\frac{1}{2}}, \qquad b(\xi+\eta)^{\frac{1}{2}} \leq b(\xi)^{\frac{1}{2}} + b(\eta)^{\frac{1}{2}},$$

respectively, hold for positive sesquilinear forms ($\forall \xi,\eta \in \text{dom } b$).

Let b be a hermitian form and $(\xi_n) \subset \text{dom } b$. Even though b is not necessarily positive, this sequence is called a *Cauchy sequence* with respect to b (or in $(\text{dom } b, b)$) if $b(\xi_n - \xi_m) \to 0$ as $n,m \to \infty$. It is said that (ξ_n) *converges* to ξ with respect to b (or in $(\text{dom } b, b)$) if $\xi \in \text{dom } b$ and $b(\xi_n - \xi) \to 0$ as $n \to \infty$.

Definition 4.1.6. A sesquilinear form b is *closed* if for each Cauchy sequence (ξ_n) in $(\text{dom } b, b)$ with $\xi_n \to \xi$ in $\mathcal{H}$, one has $\xi \in \text{dom } b$ and $\xi_n \to \xi$ in $(\text{dom } b, b)$. b is *closable* if it has a closed extension in $\mathcal{H}$.

If β is a lower bound of the sesquilinear form b, one introduces the inner product $\langle\cdot,\cdot\rangle_+$ on $\text{dom } b \subset \mathcal{H}$ by the expression

$$\langle\xi,\eta\rangle_+ := b(\xi,\eta) + (1-\beta)\langle\xi,\eta\rangle,$$

and one has $\langle\xi,\xi\rangle_+ = b(\xi,\xi) - \beta\|\xi\|^2 + \|\xi\|^2 \geq \|\xi\|^2$, so that the norm $\|\xi\|_+ := \sqrt{\langle\xi,\xi\rangle_+} \geq \|\xi\|$.

Definition 4.1.7.

a) If $b \geq \beta$, the abstract completion of the inner product space $(\text{dom } b, \langle\cdot,\cdot\rangle_+)$ will be denoted by $(\mathcal{H}_+, b_+)$.

b) Let b denote a closed and lower bounded form $b \geq \beta$. A *form core* of b is a subset $\mathcal{D} \subset \text{dom } b$ which is dense in $\text{dom } b$ equipped with the inner product $\langle\cdot,\cdot\rangle_+ = b_+(\cdot)$.

Remark 4.1.8. If $b \geq \beta \geq 0$ is closed and also an inner product, then $\mathcal{D}$ is a form core of b is equivalent to $\mathcal{D}$ being dense in $(\text{dom } b, b)$, i.e., it is not necessary to take $\langle\cdot,\cdot\rangle_+$. This applies, in particular, when a form core of $\langle\cdot,\cdot\rangle_+$ is considered.

Lemma 4.1.9. *Suppose that the hermitian sesquilinear form $b \geq \beta$, for some $\beta \in \mathbb{R}$. Then the following assertions are equivalent:*

i) $(\text{dom } b, \langle\cdot,\cdot\rangle_+)$ *is a Hilbert space* (*and so it coincides with* $(\mathcal{H}_+, b_+)$).
ii) b *is closed.*

Proof. First note that every Cauchy sequence in $\mathcal{K} := (\text{dom } b, \langle\cdot,\cdot\rangle_+)$ is also a Cauchy sequence in the other three spaces: $\mathcal{H}$, $(\text{dom } b, b-\beta)$ and also in $(\text{dom } b, b)$.

Suppose that i) holds. If (ξ_n) is Cauchy in $\mathcal{K}$ then there is $\xi \in \text{dom } b$ so that $\xi_n \to \xi$ in $\mathcal{K}$; also $\|\xi_n - \xi\| \to 0$ and so $\xi_n \to \xi$ in $\mathcal{H}$. That is, ii) holds.

Conversely, suppose that ii) holds. If (ξ_n) is Cauchy in $\mathcal{K}$, then it is also Cauchy with respect to b and in $\mathcal{H}$, and so there is ξ with $\xi_n \to \xi$ in $\mathcal{H}$. By ii), $\xi \in \text{dom } b$ and $\xi_n \to \xi$ in $\mathcal{K}$. So $\mathcal{K}$ is complete, that is, i) holds. □

The above lemma shows that any lower bound β can be used to construct $\mathcal{H}_+$; in particular if $b \geq \beta > 0$, a preferred choice is the zero lower bound. Note that $b_+(\cdot,\cdot)$ is the inner product on the Hilbert space $\mathcal{H}_+$ and if $\xi, \eta \in \text{dom } b$, then $b_+(\xi,\eta) = \langle\xi,\eta\rangle_+$; moreover, b_+ is a closed sesquilinear form on $\mathcal{H}_+$.

Example 4.1.10. To a densely defined operator T one introduces two positive hermitian sesquilinear forms $b, \tilde{b}$, with $\text{dom } b = \text{dom } \tilde{b} = \text{dom } T$, via $b(\xi,\eta) = \langle T\xi, T\eta\rangle$ and $\tilde{b}(\xi,\eta) = \langle T\xi, T\eta\rangle + \langle\xi,\eta\rangle$. Since $\tilde{b}(\xi,\xi) = \|\xi\|_T^2$, i.e., the square of the graph norm of T, it is closed iff T is closed; one has $\tilde{b} \geq 1$. See also Example 4.1.11.

Note that $\tilde{b}(\xi,\eta) = b(\xi,\eta) + \langle\xi,\eta\rangle$; this was a motivation for the introduction of the inner product $\langle\xi,\eta\rangle_+$ and the definition of closed form above.

Example 4.1.11. A hermitian operator $T : \text{dom } T \sqsubseteq \mathcal{H} \to \mathcal{H}$ defines a hermitian sesquilinear form b^T as

$$b^T(\xi,\eta) := \langle\xi, T\eta\rangle, \qquad \text{dom } b^T = \text{dom } T.$$

b^T is lower bounded iff T is (see Definition 2.4.16). Since this b^T is easily extended to any $\xi \in \mathcal{H}$ and $\eta \in \text{dom } T$, it has a potential advantage over the forms in Example 4.1.10 while searching extensions of T. See Theorem 4.3.1.

Definition 4.1.12. If $T : \text{dom } T \sqsubseteq \mathcal{H} \to \mathcal{H}$ is a hermitian operator, the form b^T introduced in Example 4.1.11 is called the sesquilinear form *generated by* T.

Remark 4.1.13. In the specific case of positive self-adjoint operators $T \geq 0$, the form b^T generated by T will be naturally extended in Section 9.3, and keeping the same notation b^T and nomenclature, to the form $\text{dom } b^T = \text{dom } T^{\frac{1}{2}}$, $b^T(\xi,\eta) = \langle T^{\frac{1}{2}}\xi, T^{\frac{1}{2}}\eta\rangle$, $\forall \xi,\eta \in \text{dom } T^{\frac{1}{2}}$. Refer to Section 9.3 for explanation of these symbols.

Remark 4.1.14. There are many appealing reasons for considering sesquilinear forms as sources of operators.

- In physics it is a common procedure to deal with “matrix elements” of an operator, i.e., $b^T(\xi,\eta) = \langle\xi, T\eta\rangle$. Also $\langle\xi, T\xi\rangle$ is the expectation value of the observable T (see discussion on page 132) if the system is in the normalized state ξ, and one asks how to construct the (self-adjoint) operator T from its matrix elements. Some authors argue that physically the expectation values are more fundamental than the square $\|T\xi\|^2 = \langle T\xi, T\xi\rangle$.

- Usually the conditions on the form domain are less restrictive than the ones on the operator domain. For instance, for the second derivative operator $\psi \mapsto -\psi''$, in suitable subspaces of $\mathrm{L}^2(\mathbb{R})$, on integrating by parts one can write $\langle \psi, -\phi''\rangle = \langle \psi', \phi'\rangle$, and the right-hand side inner product imposes conditions only on the first derivative of the functions.
- Given hermitian operators T_1, T_2 and a form b, due to less stringent domain conditions (e.g., dom $T_1 \cap$ dom T_2 can be rather small), sesquilinear forms open the possibility of defining an operator T via the sum of forms by imposing $b^T(\xi,\eta) = b^{T_1}(\xi,\eta) + b^{T_2}(\xi,\eta)$ (see Example 4.2.15, Corollary 9.3.12 and Subsection 9.3.1), and also through $b^T(\xi,\eta) = b^{T_1}(\xi,\eta) + b(\xi,\eta)$ even in some cases b is not directly related to an operator; see Examples 4.1.15, 4.4.9, 6.2.16 and 6.2.19.

The primary point relates to the representation theorems in Section 4.2, which associate self-adjoint operators to forms. Eventually, other reasons supporting the use of sesquilinear forms will appear spread over the book.

Example 4.1.15. Let dom $b_\delta = \mathcal{H}^1(\mathbb{R}) \subset \mathcal{H} = \mathrm{L}^2(\mathbb{R})$, and the action

$$b_\delta(\psi,\phi) = \overline{\psi(0)}\,\phi(0), \qquad \psi,\phi \in \text{dom } b_\delta.$$

This form is hermitian and positive, but not closable. In fact, the sequence $\psi_n(x) = e^{-nx^2}$ is contained in dom b_δ, $b_\delta(\psi_n - \psi_m) \to 0$ (so a Cauchy sequence with respect to b_δ) and converges to zero in $\mathcal{H}$, but $b_\delta(\psi_n) \to 1$ while $b_\delta(0,0) = 0$ (apply Lemma 4.1.9). Thus, in contrast to hermitian operators, a (lower bounded) hermitian form need not be closable.

Nevertheless, by naively pushing on the comparison with b^T, one would get

$$\overline{\psi(0)}\phi(0) = \langle \psi, T\phi\rangle = \int_{\mathbb{R}} \overline{\psi(x)}T\phi(x)\,dx,$$

and this form should represent an operator T "generated by the Dirac delta $\delta(x)$ at the origin;" such informal association can be useful in some contexts, as in Examples 4.4.9 and 6.2.16 in attempts to make sense of a Schrödinger operator with a delta potential. Clearly $\mathcal{H}^1(\mathbb{R})$ can be replaced by other domains, e.g., $C_0^\infty(\mathbb{R})$.

Remark 4.1.16. Sometimes it is convenient to put $b(\xi,\xi) = \infty$ if $\xi \in \mathcal{H} \setminus$ dom b. See Theorem 9.3.11 and Subsection 10.4.1.

4.2 Operators Associated with Forms

Definition 4.2.1. Consider the lower bounded sesquilinear form $b \geq \beta$. b_+ as above is *compatible with* $\mathcal{H}$ if $\mathcal{H}_+$ can be identified with a vector subspace of $\mathcal{H}$ and the (linear) inclusion $j : \mathcal{H}_+ \to \mathcal{H}$ is continuous.

Lemma 4.2.2. *If b_+ is compatible with $\mathcal{H}$, then the inclusion $j : \mathcal{H}_+ \to \mathcal{H}$ can be taken as the natural inclusion $j(\xi) = \xi$, $\forall \xi \in \mathcal{H}_+$, with $\|j\| \leq 1$.*

Proof. The natural inclusion $\hat{j} : (\text{dom } b, \langle \cdot, \cdot \rangle_+) \to \mathcal{H}$, $\hat{j}(\xi) = \xi$, is linear and satisfies

$$\|\xi\|^2 = \|\hat{j}(\xi)\|^2 \leq \langle \xi, \xi \rangle_+ = b_+(\xi, \xi),$$

and so it is continuous with $\|\hat{j}\| \leq 1$. Since b_+ is compatible with $\mathcal{H}$, $\hat{j}$ has a unique linear extension $j : \mathcal{H}_+ \to \mathcal{H}$, with $\|j\| \leq 1$.

If $\xi \in \mathcal{H}_+$, there is a sequence $(\xi_k) \subset \text{dom } b$ with $\xi_k \to \xi$ in $\mathcal{H}_+$; the above inequality implies $\xi_k \to \xi$ in $\mathcal{H}$. Thus,

$$\begin{aligned} 0 &= \lim_{k \to \infty} j(\xi_k - \xi) = \lim_{k \to \infty} j(\xi_k) - j(\xi) \\ &= \lim_{k \to \infty} \xi_k - j(\xi) = \xi - j(\xi). \end{aligned}$$

Therefore $j(\xi) = \xi$ and j is clearly injective. □

Exercise 4.2.3. Let $(\mathcal{H}_+^{b_\delta}, b_{\delta +})$ be the abstract completion of $(\text{dom } b_\delta, b_\delta + 1)$, b_δ the form in Example 4.1.15. Show that the extension j of the natural inclusion $\hat{j} : (\text{dom } b_\delta, \langle \cdot, \cdot \rangle_+) \to \mathcal{H}$, $\hat{j}(\xi) = \xi$, $\forall \xi \in \text{dom } b_\delta$, is not injective. Conclude that $b_{\delta +}$ is not compatible with $\mathcal{H}$.

Example 4.2.4. Let $T : \text{dom } T \sqsubseteq \mathcal{H} \to \mathcal{H}$ be a hermitian and lower bounded operator with lower bound $\beta \in \mathbb{R}$, that is, $T \geq \beta \mathbf{1}$. Consider the form b^T generated by T, the inner product

$$\begin{aligned} \langle \xi, \eta \rangle_+ &= b^T(\xi, \eta) + (1 - \beta)\langle \xi, \eta \rangle \\ &= \langle \xi, (T - \beta \mathbf{1})\eta \rangle + \langle \xi, \eta \rangle, \qquad \xi, \eta \in \text{dom } T, \end{aligned}$$

and its completion $(\mathcal{H}_+^T, b_+^T)$. The subject now is to show that b_+^T is compatible with $\mathcal{H}$; consequently b^T is closable.

The linear natural inclusion $\hat{j} : (\text{dom } T, \langle \cdot, \cdot \rangle_+) \to \mathcal{H}$, $\hat{j}(\xi) = \xi$, satisfies

$$\|\hat{j}(\xi)\|^2 = \|\xi\|^2 \leq \|\xi\|^2 + \langle \xi, (T - \beta \mathbf{1})\xi \rangle = \langle \xi, \xi \rangle_+,$$

and so it is continuous with $\|\hat{j}\| \leq 1$. Thus $\hat{j}$ has a unique linear extension $j : \mathcal{H}_+^T \to \mathcal{H}$ and with $\|j\| \leq 1$. If $j(\xi) = 0$, then there exists a sequence $(\xi_k) \subset (\text{dom } T, \langle \cdot, \cdot \rangle_+)$ with $\xi_k \to \xi$ in $\mathcal{H}_+^T$ and $\xi_k = j(\xi_k) \to 0$ in $\mathcal{H}$. Thus, for any $\eta \in \text{dom } T$,

$$\begin{aligned} b_+^T(\eta, \xi) &= \lim_{k \to \infty} b_+^T(\eta, j(\xi_k)) = \lim_{k \to \infty} b_+^T(\eta, \xi_k) \\ &= \lim_{k \to \infty} \langle \eta, \xi_k \rangle_+ = \lim_{k \to \infty} \left(\langle \eta, (T - \beta \mathbf{1})\xi_k \rangle + \langle \eta, \xi_k \rangle \right) \\ &= \lim_{k \to \infty} \langle [T + (1 - \beta)\mathbf{1}]\eta, \xi_k \rangle = 0. \end{aligned}$$

Since dom $T \sqsubseteq \mathcal{H}_+^T$, it follows that $\xi = 0$. Therefore, besides $\|j\| \le 1$, it was found that j is injective and so it is possible to regard $\mathcal{H}_+^T$ as a vector subspace of $\mathcal{H}$, that is, b_+^T is compatible with $\mathcal{H}$. Finally, by Lemma 4.2.2, $j(\xi) = \xi$ for all $\xi \in \mathcal{H}_+^T$.

Given a densely defined operator T, the sesquilinear form $\tilde{b}$ with dom $\tilde{b}$ = dom T, $\tilde{b}(\xi,\eta) := \langle \eta, \xi\rangle_T = \langle T\eta, T\xi\rangle + \langle \eta, \xi\rangle$, satisfies $\tilde{b}(\xi,\xi) \ge \|\xi\|^2$, $\forall \xi \in \text{dom } \tilde{b}$, and it is closed iff T is closed. Now if $\eta \in \text{dom } (T^*T)$, then

$$\tilde{b}(\xi,\eta) = \langle \xi, (T^*T + \mathbf{1})\eta\rangle, \qquad \forall \xi \in \text{dom } \tilde{b},$$

and, on the basis of Example 4.1.11 and Proposition 4.1.3, one is tempted to link the operator $T^*T+\mathbf{1}$ to $\tilde{b}$. With this motivation in mind, one has the main theorem of this section, ensuring that closed lower bounded forms are actually the forms of lower bounded self-adjoint operators.

Definition 4.2.5. Given a hermitian sesquilinear form b, the *operator* T_b *associated with* b is defined as

$$\text{dom } T_b := \{\xi \in \text{dom } b : \exists \zeta \in \mathcal{H} \text{ with } b(\eta,\xi) = \langle \eta, \zeta\rangle,\ \forall \eta \in \text{dom } b\},$$
$$T_b\xi := \zeta, \qquad \xi \in \text{dom } T_b,$$

that is, $b(\eta,\xi) = \langle \eta, T_b\xi\rangle$, $\forall \eta \in \text{dom } b$, $\forall \xi \in \text{dom } T_b$. Such operator T_b is well defined since dom b is dense in $\mathcal{H}$.

Note that T_b is automatically symmetric; for $\xi, \eta \in \text{dom } T_b$,

$$\langle \eta, T_b\xi\rangle = b(\eta,\xi) = \overline{b(\xi,\eta)} = \overline{\langle \xi, T_b\eta\rangle} = \langle T_b\eta, \xi\rangle.$$

Furthermore, in case of a bounded hermitian sesquilinear form b, the operator T_b in Definition 4.2.5 coincides with the one in Proposition 4.1.3.

The next two theorems are known as representations of sesquilinear forms.

Theorem 4.2.6. *Let* dom $b \sqsubseteq \mathcal{H}$ *and* $b : \text{dom } b \times \text{dom } b \to \mathbb{C}$ *be a closed sesquilinear form with lower bound* $\beta \in \mathbb{R}$ *(so hermitian).*

Then the operator T_b *associated with* b *is the unique self-adjoint operator with* dom $T_b \sqsubseteq$ dom $b \mapsto \mathcal{H}$ *so that*

$$b(\eta,\xi) = \langle \eta, T_b\xi\rangle, \qquad \forall \eta \in \text{dom } b,\ \forall \xi \in \text{dom } T_b.$$

Further, $T_b \ge \beta\mathbf{1}$ *and* dom T_b *is a form core of* b*. The subspace* dom b *is called the form domain of* T_b*.*

Proof. Set $\mathcal{H}_b := (\text{dom } b, \langle\cdot,\cdot\rangle_+)$, which is a Hilbert space by hypothesis. As remarked above, T_b is symmetric. For $\xi \in \text{dom } T_b \subset \text{dom } b$ one has

$$\langle \xi, T_b\xi\rangle = b(\xi,\xi) \ge \beta\|\xi\|^2,$$

so that $T_b \ge \beta\mathbf{1}$.

For all $\eta \in \mathcal{H}_b$ one has $\|\eta\|_+^2 = \langle \eta, \eta \rangle_+ = (b(\eta) - \beta\|\eta\|^2) + \|\eta\|^2\| \geq \|\eta\|^2$; thus, for each $\phi \in \mathcal{H}$,

$$|\langle \phi, \eta \rangle| \leq \|\phi\| \, \|\eta\| \leq \|\phi\| \, \|\eta\|_+, \qquad \forall \eta \in \mathcal{H}_b,$$

so that the linear functional $f_\phi : \mathcal{H}_b \to \mathbb{C}$, $f_\phi(\eta) = \langle \phi, \eta \rangle$ is continuous; since $\mathcal{H}_b$ is a Hilbert space, by Riesz's Theorem 1.1.40 there is a unique $\phi_b \in \mathcal{H}_b$ with

$$\langle \phi, \eta \rangle = \langle \phi_b, \eta \rangle_+, \qquad \forall \eta \in \mathcal{H}_b.$$

The last relation will be crucial in what follows.

We then define a linear map $M : \mathcal{H} \to \mathcal{H}_b$, $M\phi := \phi_b$; since dom b is dense in $\mathcal{H}$, note that if $\phi_b = 0$, then $\langle \phi, \eta \rangle = 0, \forall \eta \in \mathcal{H}_b$, and so $\phi = 0$. Hence M is invertible, and for M^{-1} : dom M^{-1} = rng $M \to \mathcal{H}$ write $M^{-1}\phi_b = \phi$, and note that rng $M^{-1} = \mathcal{H}$. Further, since $\|f_\phi\| \leq \|\phi\|$ and, by Riesz $\|f_\phi\| = \|\phi_b\|_+$, it is found that $\|M\phi\|_+ = \|\phi_b\|_+ \leq \|\phi\|$. Thus, M is bounded (with domain $\mathcal{H}$) with norm ≤ 1.

Now it will be shown that rng M is dense in $\mathcal{H}$. Since rng $M \subset$ dom b and $\|\cdot\| \leq \|\cdot\|_1$, it is enough to show that rng $M \sqsubseteq \mathcal{H}_b$. If $\eta \in \mathcal{H}_b$ and $\langle M\xi, \eta \rangle_+ = 0$, $\forall \xi \in \mathcal{H}$, then, by the above crucial relation,

$$0 = \langle M\xi, \eta \rangle_+ = \langle \xi_b, \eta \rangle_+ = \langle \xi, \eta \rangle,$$

and so $\eta = 0$, which proves that density.

The operator M^{-1} is directly related to T_b. Indeed, if $\xi_b \in$ dom M^{-1}, then for all $\eta \in$ dom b,

$$\langle \eta, M^{-1}\xi_b \rangle = \langle \eta, \xi \rangle = \langle \eta, \xi_b \rangle_+ = b(\eta, \xi_b) + (1 - \beta)\langle \eta, \xi_b \rangle,$$

or

$$b(\eta, \xi_b) = \langle \eta, M^{-1}\xi_b \rangle - (1 - \beta)\langle \eta, \xi_b \rangle = \langle \eta, Q\xi_b \rangle,$$

where $Q := M^{-1} - (1 - \beta)\mathbf{1}$, with dom Q = dom M^{-1}. Hence, $\xi_b \in$ dom T_b and $T_b\xi_b = Q\xi_b$; in other words, $Q \subset T_b$. From this relation one infers that T_b is densely defined (because dom Q is dense in $\mathcal{H}$), so hermitian, and the operator Q is also hermitian (because it has a hermitian extension T_b).

Observe that $M^{-1} = Q + (1 - \beta)\mathbf{1}$ is also hermitian, and a simple exercise shows that M is also hermitian; since M is bounded ($M \in \mathrm{B}(\mathcal{H})$), it is in fact self-adjoint. By Lemma 2.4.1 one infers that M^{-1} is self-adjoint, so Q is also self-adjoint (very general arguments appear in Theorem 6.1.8 and Exercise 6.1.11). Finally, the relation $Q \subset T_b$ implies $Q = T_b$, since a self-adjoint operator has no proper hermitian extension. The self-adjointness of T_b is hereby verified.

Recall that it was shown above that dom T_b = dom Q = rng M is dense in $\mathcal{H}_b$, that is, dom T_b is a form core of b.

For the uniqueness, suppose that S is self-adjoint with dom $S \subset$ dom b and

$$b(\eta, \xi) = \langle \eta, S\xi \rangle, \qquad \forall \eta \in \text{dom } b, \, \xi \in \text{dom } S.$$

By construction (Definition 4.2.5), $\xi \in \mathrm{dom}\, T_b$ and $T_b\xi = S\xi$; thus $S \subset T_b$. Since S is self-adjoint it has no proper hermitian extension; it then follows that $S = T_b$. □

Exercise 4.2.7. Show that if a linear invertible operator is hermitian, then its inverse is also hermitian.

Exercise 4.2.8. Adapt the statement and proof of Theorem 4.2.6 to the case $b \geq \beta > 0$ and $(\mathrm{dom}\, b, b)$ is complete; in this case write $\mathcal{H}_b$ for $(\mathrm{dom}\, b, b)$ and note that with such approach the inner product $\langle \cdot, \cdot \rangle_+$ does not play any role. Show, in particular, that $\mathrm{dom}\, T_b$ (T_b is the resulting self-adjoint operator, of course) is a form core of b.

Now the hypothesis of $(\mathrm{dom}\, b, b(\cdot, \cdot))$ being closed in Theorem 4.2.6 will be replaced by the assumption that its completion b_+ is compatible with the original Hilbert space $\mathcal{H}$.

Theorem 4.2.9. *Let b be a hermitian sesquilinear form with $b \geq \beta$ for some $\beta \in \mathbb{R}$, its completion $(\mathcal{H}_+, b_+)$ as above and T_{b_+} the self-adjoint operator associated with b_+.*

If b_+ is compatible with $\mathcal{H}$, then there exists a unique self-adjoint operator $\tilde{T}_b : \mathrm{dom}\, \tilde{T}_b \sqsubseteq \mathcal{H}_+ \to \mathcal{H}$, with

$$b(\eta, \xi) = \langle \eta, \tilde{T}_b \xi \rangle, \qquad \forall \eta \in \mathrm{dom}\, b,\ \forall \xi \in \mathrm{dom}\, \tilde{T}_b \cap \mathrm{dom}\, b.$$

Further, $\tilde{T}_b \geq \beta \mathbf{1}$, $\mathrm{dom}\, \tilde{T}_b = \mathrm{dom}\, T_{b_+}$, $\tilde{T}_b = T_{b_+} - (1-\beta)\mathbf{1}$ and $\mathrm{dom}\, \tilde{T}_b$ is a form core of b_+. $\mathcal{H}_+$ is called the form domain of $\tilde{T}_b$.

Proof. Recall that

$$\langle \eta, \xi \rangle_+ = b(\eta, \xi) + (1-\beta)\langle \eta, \xi \rangle, \qquad \forall \eta, \xi \in \mathrm{dom}\, b.$$

So $\langle \eta, \eta \rangle_+ \geq \|\eta\|^2$, $\forall \eta \in \mathrm{dom}\, b$, and since b_+ is compatible with $\mathcal{H}$ it follows that, by Lemma 4.2.2,

$$b_+(\eta, \eta) \geq \|\eta\|^2, \qquad \forall \eta \in \mathrm{dom}\, b_+ = \mathcal{H}_+,$$

that is, $b_+ \geq 1$. Since b_+ is closed, by Theorem 4.2.6, there is a unique self-adjoint operator T_{b_+} with domain dense in $\mathcal{H}_+$ and

$$b_+(\eta, \xi) = \langle \eta, T_{b_+} \xi \rangle, \qquad \forall \eta \in \mathcal{H}_+,\ \xi \in \mathrm{dom}\, T_{b_+}.$$

It also follows that $T_{b_+} \geq \mathbf{1}$.

Now define $\tilde{T}_b := T_{b_+} - (1-\beta)\mathbf{1}$, $\mathrm{dom}\, \tilde{T}_b = \mathrm{dom}\, T_{b_+}$, which is also self-adjoint and $\tilde{T}_b \geq \beta \mathbf{1}$. In case $\eta \in \mathrm{dom}\, b$ and $\xi \in \mathrm{dom}\, b \cap \mathrm{dom}\, T_{b_+}$, one has

$$\langle \eta, T_{b_+} \xi \rangle = b_+(\eta, \xi) = \langle \eta, \xi \rangle_+ = b(\eta, \xi) + (1-\beta)\langle \eta, \xi \rangle,$$

and so

$$b(\eta, \xi) = \langle \eta, (T_{b_+} - (1-\beta)\mathbf{1})\xi \rangle = \langle \eta, \tilde{T}_b \xi \rangle;$$

thus $b(\eta, \xi) = \langle \eta, \tilde{T}_b \xi \rangle$, $\forall \eta \in \mathrm{dom}\, b$, $\forall \xi \in \mathrm{dom}\, \tilde{T}_b \cap \mathrm{dom}\, b$.

Next the uniqueness. Suppose that $\tilde{S} : \mathrm{dom}\ \tilde{S} \sqsubseteq \mathcal{H}_+ \to \mathcal{H}$ is a self-adjoint operator with

$$b(\eta,\xi) = \langle \eta, \tilde{S}\xi\rangle, \qquad \forall \eta \in \mathrm{dom}\ b,\ \forall \xi \in \mathrm{dom}\ \tilde{S} \cap \mathrm{dom}\ b.$$

Define $S := \tilde{S} + (1-\beta)\mathbf{1}$; note that $\tilde{S} \neq \tilde{T}_b$ iff $S \neq T_{b_+}$. The above condition on $\tilde{S}$ can be rewritten as

$$b_+(\eta,\xi) = \langle \eta, \tilde{S}\xi\rangle + (1-\beta)\langle \eta, \xi\rangle = \langle \eta, S\xi\rangle,$$

$\forall \eta \in \mathrm{dom}\ b$, $\forall \xi \in \mathrm{dom}\ S \cap \mathrm{dom}\ b$. Since $(\mathcal{H}_+, b_+)$ is complete and S is closed, together with the continuity of the inner product, one gets

$$b_+(\eta,\xi) = \langle \eta, S\xi\rangle, \qquad \forall \eta \in \mathcal{H}_+,\ \forall \xi \in \mathrm{dom}\ S;$$

but, by construction, this means that $\xi \in \mathrm{dom}\ T_{b_+}$ and $T_{b_+}\xi = S\xi$, that is, $S \subset T_{b_+}$. Since both are self-adjoint $S = T_{b_+}$, so $\tilde{S} = \tilde{T}_b$ and such an operator is unique. Since $\mathrm{dom}\ \tilde{T}_b = \mathrm{dom}\ T_{b_+}$, Theorem 4.2.6 immediately implies that $\mathrm{dom}\ \tilde{T}_b$ is a form core of b_+. □

Remark 4.2.10. Note that Definition 4.2.5 and the relation

$$b(\eta,\xi) = \langle \eta, \tilde{T}_b\xi\rangle, \qquad \forall \eta \in \mathrm{dom}\ b,\ \forall \xi \in \mathrm{dom}\ \tilde{T}_b \cap \mathrm{dom}\ b,$$

in the statement of Theorem 4.2.6 imply that $\mathrm{dom}\ \tilde{T}_b$ is given by

$$\{\xi \in \mathcal{H}_+ : \exists \zeta \in \mathcal{H} \text{ with } b_+(\eta,\xi) - (1-\beta)\xi = \langle \eta, \zeta\rangle,\ \forall \eta \in \mathrm{dom}\ b\},$$

and $\tilde{T}_b\xi = \zeta$.

Recall that the quantum kinetic energy operator in $\mathrm{L}^2(\mathbb{R}^n)$ is the operator $H_0 = -\Delta$ with $\mathrm{dom}\ H_0 = \mathcal{H}^2(\mathbb{R}^n)$ and both $C_0^\infty(\mathbb{R}^n), \mathcal{S}(\mathbb{R}^n)$ are cores of H_0; the laplacian Δ is obtained through distributional derivatives and $\mathcal{H}^2$ is a Sobolev space. Below ∇ indicates the distributional gradient operator.

Example 4.2.11. Let $\mathrm{dom}\ b = \mathcal{H}^1(\mathbb{R}^n) \sqsubseteq \mathrm{L}^2(\mathbb{R}^n)$,

$$b(\phi,\psi) := \langle \nabla\phi, \nabla\psi\rangle, \qquad \phi,\psi \in \mathrm{dom}\ b.$$

Since $b(\phi) = \|\nabla\phi\|^2$, the hermitian sesquilinear form b is positive. Let $(\phi_j) \subset \mathrm{dom}\ b$ be a sequence obeying $b(\phi_j - \phi_k) \to 0$ and $\phi_j \to \phi$ in $\mathrm{L}^2(\mathbb{R}^n)$ as $j,k \to \infty$. Note that this is equivalent to $\phi_j \to \phi$ in $\mathcal{H}^1(\mathbb{R}^n)$, which is a Hilbert space and so $\phi \in \mathrm{dom}\ b$; hence the form b is also closed and $(\mathrm{dom}\ b, \langle\cdot,\cdot\rangle_+)$, with $\langle \phi,\psi\rangle_+ = b(\phi,\psi) + \langle\phi,\psi\rangle$, is a Hilbert space ($\mathcal{H}^1(\mathbb{R}^n)$ in fact!).

It is easily checked that the subsequent self-adjoint operator T_b in Theorem 4.2.6 is H_0; indeed, H_0 is positive and self-adjoint, $\mathrm{dom}\ H_0 = \mathcal{H}^2(\mathbb{R}^n) \sqsubseteq \mathrm{dom}\ b$ and on integrating by parts

$$b(\phi,\psi) = \langle \phi, -\Delta\psi\rangle, \qquad \forall \phi \in \mathrm{dom}\ b, \psi \in \mathrm{dom}\ H_0.$$

Hence, $\mathcal{H}^1(\mathbb{R}^n)$ is the form domain of H_0 and both $C_0^\infty(\mathbb{R}^n), \mathcal{S}(\mathbb{R}^n)$ are form cores of b (since these sets are dense in $\mathcal{H}^1(\mathbb{R}^n)$). In summary, $T_b = H_0$. Usually such form b is denoted by b^{H_0}.

Example 4.2.12. Consider the Hilbert space $\mathcal{H} = \mathrm{L}^2[0,1]$. Let $\alpha = (\alpha_0, \alpha_1)$, $\alpha_0 > 0, \alpha_1 > 0$ (for simplicity), dom $b_\alpha = \mathcal{H}^1[0,1]$ and, for $\phi, \psi \in$ dom b_α,

$$b_\alpha(\phi,\psi) := \langle \phi', \psi' \rangle + \alpha_0\, \overline{\phi(0)}\psi(0) + \alpha_1\, \overline{\phi(1)}\psi(1),$$

which is a densely defined sesquilinear form. For (say!) $a > 1$, integrations by parts show the validity of the integral representations

$$\psi(1) = \int_0^1 t^a \psi'(t)\, dt + \int_0^1 a t^{a-1}\psi(t)\, dt,$$
$$\psi(0) = \int_0^1 -(1-t)^a \psi'(t)\, dt + \int_0^1 a(1-t)^{a-1}\psi(t)\, dt,$$

and by Cauchy-Schwarz,

$$\begin{aligned} b_\alpha(\psi) &\geq \|\psi'\|^2 - \alpha_0\, |\psi(0)|^2 - \alpha_1\, |\psi(1)|^2 \\ &\geq \left(1 - \frac{\alpha_0 + \alpha_1}{2a+1}\right) \|\psi'\|^2 - (\alpha_0 + \alpha_1)\frac{a^2}{2a-1}\|\psi\|^2, \end{aligned}$$

and for a large enough the coefficient of $\|\psi'\|^2$ becomes positive so that $b_\alpha(\psi) \geq \beta\|\psi\|^2$, with $\beta = -(\alpha_0+\alpha_1)a^2/(2a-1)$. In other words, b_α is lower bounded.

Now it will be argued that b_α is closed, so that it defines a self-adjoint operator T_{b_α} as in Theorem 4.2.6. Let (ψ_n) be a sequence in dom b_α with $b_\alpha(\psi_n - \psi_m) \to 0$ and $\psi_n \to \psi$ in $\mathcal{H}$ as $n, m \to \infty$. Write out such conditions to get that (ψ_n') is also a Cauchy sequence in $\mathcal{H}$ and so $\psi_n' \to \phi \in \mathcal{H}$ (note that $(\psi_n(0))$ and $(\psi_n(1))$ are Cauchy in $\mathbb{C}$). The relation (recall that on bounded intervals convergence in L^2 implies convergence in L^1)

$$\int_0^t \phi(s)\, ds = \lim_{n\to\infty} \int_0^t \psi_n'(s)\, ds = \psi(t) - \psi(0)$$

implies that $\psi \in$ dom b_α and $\psi' = \phi$. By continuity of the elements of $\mathcal{H}^1[0,1]$ and the above integral representations for $\psi_n(0), \psi_n(1)$, one has $\psi_n(0) \to \psi(0)$ and $\psi_n(1) \to \psi(1)$. A direct verification that $b_\alpha(\psi_n - \psi) \to 0$ concludes that b_α is closed.

The next step is to find T_{b_α} via $b_\alpha(\phi,\psi) = \langle \phi, T_{b_\alpha}\psi\rangle$. After a formal integration by parts in the expression of $b_\alpha(\phi,\psi)$ one gets

$$\begin{aligned} \langle \phi, T_{b_\alpha}\psi\rangle &= b_\alpha(\phi,\psi) \\ &= \langle \phi, -\psi'' \rangle + \overline{\phi(0)}\,(\alpha_0\psi(0) + \psi'(0)) - \overline{\phi(1)}(\alpha_1\psi(1) - \psi'(1)), \end{aligned}$$

which suggests to try $\text{dom}\, T_{b_\alpha} = \{\psi \in \mathcal{H}^2[0,1] : \psi'(0) = -\alpha_0\psi(0), \psi'(1) = \alpha_1\psi(1)\}$, $T_{b_\alpha}\psi = -\psi''$. One can check that this operator T_{b_α} is actually self-adjoint; since $\text{dom}\, T_{b_\alpha} \sqsubseteq \text{dom}\, b_\alpha$ and

$$b_\alpha(\phi,\psi) = \langle \phi, T_{b_\alpha}\psi\rangle, \qquad \forall \phi \in \text{dom}\, b_\alpha, \psi \in \text{dom}\, T_{b_\alpha},$$

one has that T_α is the operator associated with the form b_α in Theorem 4.2.6, and $\mathcal{H}^1[0,1]$ is the form domain of T_α.

Exercise 4.2.13. Verify that T_{b_α} in Example 4.2.12 is self-adjoint (a possible solution can be obtained from a characterization in Example 7.3.4).

Exercise 4.2.14. Consider the Hilbert space $\mathcal{H} = \mathrm{L}^2[0,1]$, $\text{dom}\, \tilde{b} = \{\psi \in \mathcal{H}^1[0,1] : \psi(0) = 0 = \psi(1)\}$ and, for $\phi, \psi \in \text{dom}\, \tilde{b}$,

$$\tilde{b}(\phi,\psi) = \langle \phi', \psi'\rangle.$$

Based on Example 4.2.12, show that $\tilde{b}$ is a positive closed form whose corresponding associated operator is $\text{dom}\, T_{\tilde{b}} = \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = 0 = \psi(1)\}$, $T_{\tilde{b}}\psi = -\psi''$, $\psi \in \text{dom}\, T_{\tilde{b}}$.

Let b_1, b_2 be two closed and lower bounded forms and T_{b_1}, T_{b_2} the subsequent self-adjoint operators associated with b_1 and b_2, respectively. It can happen that the sesquilinear form sum $b = b_1 + b_2$, with $\text{dom}\,(b_1 + b_2) = \text{dom}\, b_1 \cap \text{dom}\, b_2$, is either closed and lower bounded or its completion b_+ is compatible with the original Hilbert space; in either way the operator T_b associated with b is self-adjoint and called the *form sum* of T_{b_1} and T_{b_2}, and denoted by

$$T_b = T_{b_1} \dot{+} T_{b_2}.$$

This concept is illustrated in the following example; see also Subsection 6.1.1 and Remark 9.3.13.

Example 4.2.15. Let T_α, $\alpha = (\alpha_0, \alpha_1)$, be the operator obtained in Example 4.2.12, and consider also T_τ, $\tau = (\tau_0, \tau_1)$, obtained in the same way. The aim here is to describe the operator $T_\alpha/2 \dot{+} T_\tau/2$. First note that $T_\alpha/2$ is the operator associated with the form $b_\alpha/2$.

Let $b = b_\alpha/2 + b_\tau/2$, i.e., $\text{dom}\, b = \mathcal{H}^1[0,1]$,

$$b(\phi,\psi) = \langle \phi', \psi'\rangle + \frac{\alpha_0 + \tau_0}{2}\overline{\phi(0)}\,\psi(0) + \frac{\alpha_1 + \tau_1}{2}\,\overline{\phi(1)}\psi(1),$$

consequently

$$\frac{T_\alpha}{2} \dot{+} \frac{T_\tau}{2} = T_\omega, \qquad \omega = \left(\frac{\alpha_0 + \tau_0}{2}, \frac{\alpha_1 + \tau_1}{2}\right).$$

See also Example 4.4.8.

4.3 Friedrichs Extension

Given T hermitian, consider the form generated by T, that is, $b^T(\xi,\eta) = \langle \xi, T\eta\rangle$, $\xi,\eta \in \mathrm{dom}\ T$; if $T \geq \beta\mathbf{1}$, one has $b^T(\xi,\xi) \geq \beta\|\xi\|^2$, and it is possible to apply Theorem 4.2.9 in order to get the so-called Friedrichs extension of T (a fundamental result by Friedrichs of 1934).

Theorem 4.3.1 (Friedrichs Extension). *Let T be a lower bounded hermitian operator with $T \geq \beta\mathbf{1}$, $\beta \in \mathbb{R}$, b^T the form generated by T, i.e.,*

$$b^T(\xi,\eta) = \langle \xi, T\eta\rangle, \qquad \xi,\eta \in \mathrm{dom}\ b^T = \mathrm{dom}\ T,$$

and $(\mathcal{H}_+^T, b_+^T)$ as in Example 4.2.4. Then the operator T has a unique self-adjoint extension $T_F : \mathrm{dom}\ T_F \to \mathcal{H}$ with $\mathrm{dom}\ T_F \sqsubseteq \mathcal{H}_+^T$. Further, $T_F \geq \beta\mathbf{1}$ and $\mathrm{dom}\ T_F$ is a form core of b_+^T. $\mathcal{H}_+^T$ is the form domain of T_F.

Proof. Recall that $\langle \xi,\eta\rangle_+ = b^T(\xi,\eta) + (1-\beta)\langle \xi,\eta\rangle$, $\xi,\eta \in \mathrm{dom}\ T$, and its completion is $(\mathcal{H}_+^T, b_+^T)$. On account of Example 4.2.4, b_+^T is compatible with $\mathcal{H}$ and $b_+^T(\xi,\xi) \geq \|\xi\|^2$, $\forall\xi \in \mathcal{H}_+^T$. By Theorem 4.2.9 there is a unique self-adjoint operator

$$T_F = \tilde{T}_{b^T} := T_{b_+^T} - (1-\beta)\mathbf{1}, \qquad \mathrm{dom}\ T_F = \mathrm{dom}\ T_{b_+^T} \sqsubseteq \mathcal{H}_+^T,$$

so that

$$b^T(\eta,\xi) = \langle \eta, T_F\xi\rangle, \qquad \forall\eta \in \mathrm{dom}\ T,\ \xi \in \mathrm{dom}\ T \cap \mathrm{dom}\ T_F.$$

Since $T_{b_+^T} \geq \mathbf{1}$ one finds that $T_F \geq \beta\mathbf{1}$. In order to show that $T \subset T_F$, take note initially that for $\xi,\eta \in \mathrm{dom}\ T$,

$$b_+^T(\eta,\xi) = \langle \eta,\xi\rangle_+ = \langle \eta, [T + (1-\beta)\mathbf{1}]\xi\rangle\,.$$

By continuity of the inner product, density of $\mathrm{dom}\ T$ in $\mathcal{H}_+^T$ and the continuity of the inclusion $j : \mathcal{H}_+^T \to \mathcal{H}$, it follows that, for each $\xi \in \mathrm{dom}\ T$,

$$b_+^T(\eta,\xi) = \langle \eta, [T + (1-\beta)\mathbf{1}]\xi\rangle$$

holds true for any $\eta \in \mathcal{H}_+^T$. Hence, by the construction in Definition 4.2.5, $\xi \in \mathrm{dom}\ T_{b_+^T}$ and $T_{b_+^T}\xi = T\xi + (1-\beta)\xi$, showing that

$$T\xi = T_{b_+^T}\xi - (1-\beta)\xi = T_F\xi, \qquad \forall\xi \in \mathrm{dom}\ T.$$

Hence $T \subset T_F$.

Now the uniqueness of T_F. If S is a self-adjoint operator so that $T \subset S$ and $\mathrm{dom}\ S \subset \mathcal{H}_+^T$, the above proof that $T \subset T_F$ applies, and so one concludes that $S \subset T_F$; since both operators are self-adjoint, $S = T_F$. As in Theorem 4.2.6, one concludes that $\mathrm{dom}\ T_F$ is a form core of b_+^T. □

Exercise 4.3.2. Conclude that (see Remark 4.2.10) dom T_F is given by

$$\left\{\xi \in \mathcal{H}_+^T : \exists \zeta \in \mathcal{H} \text{ with } b_+^T(\xi,\eta) - (1-\beta)\langle \xi,\eta\rangle = \langle \zeta,\eta\rangle,\ \forall \eta \in \text{dom } T\right\},$$

and $T_F\xi = \zeta$. Given $\xi \in \text{dom } T_F$, by taking $(\xi_n) \subset \text{dom } T$ with $\xi_n \to \xi$ in $\mathcal{H}_+^T$, show that

$$\begin{aligned} b_+^T(\xi,\eta) - (1-\beta)\langle \xi,\eta\rangle &= \lim_{n\to\infty} [b_+^T(\xi_n,\eta) - (1-\beta)\langle \xi_n,\eta\rangle] \\ &= \langle \xi, T\eta\rangle, \qquad \forall \eta \in \text{dom } T, \end{aligned}$$

and conclude that dom $T_F = \text{dom } T^* \cap \mathcal{H}_+^T$.

Definition 4.3.3. The self-adjoint operator T_F introduced in Theorem 4.3.1 is called the Friedrichs extension of the hermitian and lower bounded T.

Proposition 4.3.4. *Let $T \geq \beta\mathbf{1}$ and T_0 a lower bounded self-adjoint extension of T. Then $\mathcal{H}_+^{T_F} \subset \mathcal{H}_+^{T_0}$, that is, the Friedrichs extension has the smallest form domain among the form domains of lower bounded self-adjoint extensions of T.*

Proof. Assume that β is the largest lower bound of T and let $\alpha \in \mathbb{R}$ be strictly less than a lower bound of T_0; so $\alpha < \beta$.

It is known that the form domain $\mathcal{H}_+^{T_F}$ of T_F is the completion of dom T in the norm $\langle \xi,\xi\rangle_+ = \langle \xi, [T + (1-\beta)\mathbf{1}]\xi\rangle$, which is the same space obtained after completion of dom T in the norm

$$\langle \xi, [T + (1-\alpha)\mathbf{1}]\xi\rangle = \langle \xi, [T_0 + (1-\alpha)\mathbf{1}]\xi\rangle.$$

Since dom $T \subset$ dom T_0 and the form domain $\mathcal{H}_+^{T_0}$ of T_0 is the completion of dom T_0 in the above norm $\langle \xi, [T_0 + (1-\alpha)\mathbf{1}]\xi\rangle$, it follows that $\mathcal{H}_+^{T_F} \subset \mathcal{H}_+^{T_0}$. □

It is interesting to point out that T_F is the only self-adjoint extension of T whose domain is dense in $\mathcal{H}_+^T$; particularly, the only self-adjoint extension whose form domain is $\mathcal{H}_+^T$. Thus, in this sense and in view of Proposition 4.3.4, T_F is canonically constructed.

Corollary 4.3.5. *If T is hermitian and lower bounded, then its deficiency indices are equal.*

Proof. T_F is a self-adjoint extension of the operator T. Now apply Theorem 2.2.11. □

Exercise 2.4.17 implies an important lower bound of the spectrum of the Friedrichs extension:

Corollary 4.3.6. *Let $T \geq \beta$ be as in Theorem* 4.3.1 *and T_F the consequent Friedrichs extension. Then $\sigma(T_F) \subset [\beta,\infty)$.*

However, Example 4.4.13 presents another self-adjoint extension of a lower bounded hermitian operator T with the same spectrum of T_F.

In case the Hilbert space is $\mathrm{L}^2(\mathbb{R}^n)$, one can anticipate an important result if Corollary 6.3.5 is invoked:

Corollary 4.3.7. *If there is $\beta \in \mathbb{R}$ so that $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ satisfies $V(x) \geq \beta$, $\forall x \in \mathbb{R}^n$, then the Friedrichs extension of the standard Schrödinger operator*

$$\mathrm{dom}\ H = C_0^\infty(\mathbb{R}^n), \qquad H\psi = -\Delta\psi + V\psi, \quad \psi \in \mathrm{dom}\ H,$$

is the unique self-adjoint extension of H.

If $T \in \mathrm{B}(\mathcal{H})$, then T^*T is self-adjoint and positive. Form extensions will be used to adapt this result to a more general case. Recall that $\mathrm{dom}\ (T^*T) := \{\xi \in \mathrm{dom}\ T : (T\xi) \in \mathrm{dom}\ T^*\}$ and $(T^*T)\xi = T^*(T\xi)$. However, it can happen that $\mathrm{dom}\ (T^*T)$ is not dense in $\mathcal{H}$. See Example 2.1.5; another classical example is the following.

Example 4.3.8 ($\mathrm{dom}\ T^*$ is not dense in $\mathcal{H}$). Let $\mathcal{H} = \mathrm{L}^2(\mathbb{R})$, $0 \neq \psi_0 \in \mathcal{H}$, $\phi(x) = 1, \forall x \in \mathbb{R}$ and $\mathrm{dom}\ T := \{\psi \in \mathcal{H} : \int_{\mathbb{R}} |\psi| dx < \infty\}$. Write $\langle \phi, \psi \rangle = \int_{\mathbb{R}} \psi dx$, and define

$$(T\psi)(x) := \langle \phi, \psi \rangle \psi_0(x), \qquad \psi \in \mathrm{dom}\ T.$$

Thus, if $u \in \mathrm{dom}\ T^*$, then for every $\psi \in \mathrm{dom}\ T$ one has

$$\begin{aligned}\langle T^*u, \psi \rangle &= \langle u, T\psi \rangle = \langle u, \langle \phi, \psi \rangle \psi_0 \rangle \\ &= \langle \phi, \psi \rangle \langle u, \psi_0 \rangle = \langle \langle \psi_0, u \rangle \phi, \psi \rangle .\end{aligned}$$

Hence, $(T^*u)(x) = \langle \psi_0, u \rangle \phi(x)$, and it belongs to $\mathcal{H}$ iff $\langle \psi_0, u \rangle = 0$. Thus, $\mathrm{dom}\ T^* \subset \{\psi_0\}^\perp$ and it is not dense in $\mathcal{H}$. Furthermore, for $u \in \mathrm{dom}\ T^*$ one has $T^*u = 0$.

However, if T is closed a remarkable result of von Neumann is found.

Proposition 4.3.9. *Let T be a closed operator with* $\mathrm{dom}\ T \sqsubseteq \mathcal{H}$*. Then* $\mathrm{dom}\ (T^*T) \sqsubseteq \mathcal{H}$, *$T^*T$ is a positive self-adjoint operator and* $\mathrm{dom}\ T$ *is the form domain of T^*T.*

Proof. Since T is closed, by taking the form

$$b(\xi, \eta) := \langle \xi, \eta \rangle_T = \langle T\xi, T\eta \rangle + \langle \xi, \eta \rangle$$

as the inner graph product, it follows that $(\mathcal{H}_+, b_+) = (\mathrm{dom}\ T, b)$ is a Hilbert space and $b(\xi) = \|\xi\|_T \geq \|\xi\|$, $\forall \xi \in \mathrm{dom}\ T$. Thus, by Theorem 4.2.6 the operator T_b associated with b is self-adjoint, $T_b \geq \mathbf{1}$,

$$\mathrm{dom}\ T_b = \{\xi \in \mathrm{dom}\ T : \exists \phi \in \mathcal{H} \text{ with } b(\eta, \xi) = \langle \eta, \phi \rangle, \forall \eta \in \mathrm{dom}\ T\}$$

and $T_b\xi = \phi$. Explicitly, $\xi \in \mathrm{dom}\ T_b$ iff for all $\eta \in \mathrm{dom}\ T$,

$$\langle T\eta, T\xi \rangle + \langle \eta, \xi \rangle = b(\eta, \xi) = \langle \eta, T_b\xi \rangle,$$

so that

$$\langle T\eta, T\xi \rangle = \langle \eta, (T_b - \mathbf{1})\xi \rangle, \qquad \forall \eta \in \mathrm{dom}\ T.$$

Therefore, $\xi \in \mathrm{dom}\ T_b$ iff $T\xi \in \mathrm{dom}\ T^*$ and $T^*(T\xi) = (T_b - \mathbf{1})\xi$, that is, $T^*T = T_b - \mathbf{1}$ is self-adjoint and positive. By Theorem 4.2.6, $\mathrm{dom}\ T_b$ is dense in $(\mathrm{dom}\ T, b)$, and it follows that $\mathrm{dom}\ (T^*T)$ is dense in $(\mathrm{dom}\ T, b)$. By construction, the form domain of T^*T is $\mathrm{dom}\ T$. □

Although the next result could be obtained directly from general theorems, it is worth presenting a specific short proof.

Corollary 4.3.10. *If T is self-adjoint, then for all $n \in \mathbb{N}$ the operator T^{2^n} is positive and self-adjoint. In particular T^2 is self-adjoint.*

Proof. If T^j is self-adjoint, Proposition 4.3.9 implies that T^{2j} is self-adjoint; use recursion in j starting from $j = 1$. □

Proposition 4.3.11. *Let T be closed and densely defined.*

i) *Then* dom (T^*T) *is a core of T.*
ii) *If T is self-adjoint, then T^2 is self-adjoint and* dom T^2 *is a core of T.*

Proof. i) In the graph inner product of T, let

$$(\eta, T\eta) \in \{(\xi, T\xi) : \xi \in \text{dom } (T^*T)\}^{\perp}.$$

Thus $0 = \langle \xi, \eta \rangle + \langle T\xi, T\eta \rangle = \langle (\mathbf{1} + T^*T)\xi, \eta \rangle$. Since T^*T is a positive self-adjoint operator, $-1 \in \rho(T^*T)$ and so rng $(T^*T + \mathbf{1}) = \mathcal{H}$. Hence $\eta = 0$ and, by Exercise 1.2.26 (or Exercise 2.5.10), dom (T^*T) is a core of T.

ii) Combine Corollary 4.3.10 with i). □

Remark 4.3.12. The following property is attractive. If T is self-adjoint and dom $T^2 =$ dom T, then T is bounded.

Proof. Clearly dom $T^2 \subset$ dom T and we introduce the notation $\mathbf{h} = (\text{dom } T, \| \cdot \|_T)$, which is a Hilbert space since T is closed. Pay attention to the following facts:

1. $T - i\mathbf{1} : \mathbf{h} \to (\mathcal{H}, \| \cdot \|)$ is bounded. Indeed, for $\xi \in$ dom T, $\|(T - i\mathbf{1})\xi\|^2 = \|\xi\|^2 + \|T\xi\|^2 = \|\xi\|_T^2$.
2. Since dom $T^2 =$ dom T one has Tdom $T \subset$ dom T and so the linear mapping

$$R_i(T) : (\text{dom } T, \| \cdot \|) \to \mathbf{h}$$

is bounded. Indeed, for $\xi \in$ dom T use triangular inequality to get

$$\begin{aligned}\|R_i(T)\xi\|_T^2 &= \|R_i(T)\xi\|^2 + \|TR_i(T)\xi\|^2 \\ &\le \|\xi\|^2 + \|(T - i\mathbf{1})R_i(T)\xi + iR_i(T)\xi\|^2 \le 5\|\xi\|^2.\end{aligned}$$

3. Since dom $T^2 =$ dom T, define

$$\tilde{T} : \mathbf{h} \to \mathbf{h}, \qquad \tilde{T}\xi := T\xi,$$

which is a closed operator; indeed, if $\xi_n \xrightarrow{\mathbf{h}} \xi$ and $T\xi_n \xrightarrow{\mathbf{h}} \eta$, then $\xi \in$ dom T, $T\xi_n \xrightarrow{\mathcal{H}} T\xi$, $T\xi_n \xrightarrow{\mathcal{H}} \eta$, so that $\eta = T\xi$. Hence, $\tilde{T}$ is bounded by the closed graph theorem.

Now observe that $T : (\mathrm{dom}\ T, \|\cdot\|) \to (\mathcal{H}, \|\cdot\|)$ can be written in the form

$$T = (T - i\mathbf{1})\,\tilde{T}\,R_i(T),$$

which shows that T is bounded. □

Exercise 4.3.13. Let T be a closed hermitian operator with dom T^2 dense in $\mathcal{H}$. Show that T^*T is the Friedrichs extension of T^2.

Exercise 4.3.14. Let dom $a = \{\psi \in \mathrm{L}^2(\mathbb{R}) : \psi \in \mathrm{AC}(\mathbb{R}), \psi' + x\psi \in \mathrm{L}^2(\mathbb{R})\}$, $a\psi = \psi' + x\psi$, $\psi \in \mathrm{dom}\ a$. Show that a is a closed operator and that its adjoint is dom $a^* = \{\psi \in \mathrm{L}^2(\mathbb{R}) : \psi \in \mathrm{AC}(\mathbb{R}), -\psi' + x\psi \in \mathrm{L}^2(\mathbb{R})\}$, $a^*\psi = -\psi' + x\psi$, $\psi \in \mathrm{dom}\ a^*$. Find the operator a^*a and relate it to the harmonic oscillator. a^*, a are called *creation* and *annihilation* operators, respectively.

Exercise 4.3.15. If T is self-adjoint and E is a dense subspace of $\mathcal{H}$, show that $R_i(T)E$ is also dense in $\mathcal{H}$. Observe that dom $T^{n+1} = R_i(T)$dom T^n for all $n \in \mathbb{N}$, and conclude that dom T^n is dense in $\mathcal{H}$.

Exercise 4.3.16. Let T be a closed operator with dom $T \sqsubseteq \mathcal{H}$. Choose $\xi' = 0$ in Exercise 2.1.21 and work to show that $(\mathbf{1} + T^*T)^{-1}$ is a bounded self-adjoint operator. Conclude that T^*T is self-adjoint. This is a sketch of a proof of the first part of Proposition 4.3.9 without using forms.

4.4 Examples

Example 4.4.1. Let $\varphi : \mathbb{R} \to [0, \infty)$ be a Borel function and $T = \mathcal{M}_\varphi \geq 0$ the subsequent self-adjoint multiplication operator in $\mathrm{L}^2(\mathbb{R})$, as in Subsection 2.3.2. The sesquilinear form generated by T is dom $b^T = \mathrm{dom}\ \mathcal{M}_\varphi$,

$$b^T(\psi, \phi) = \langle \psi, \mathcal{M}_\varphi \phi\rangle = \int_{\mathbb{R}} \overline{\psi(x)}\, \varphi(x)\phi(x)\, dx.$$

By writing

$$b^T(\psi, \phi) = \int_{\mathbb{R}} \overline{\varphi(x)^{\frac{1}{2}}\psi(x)}\ \varphi(x)^{\frac{1}{2}}\phi(x)\, dx$$

one has

$$\langle \psi, \phi\rangle_+ = \langle \mathcal{M}_{\sqrt{\varphi}}\psi, \mathcal{M}_{\sqrt{\varphi}}\phi\rangle + \langle \psi, \phi\rangle, \qquad \psi, \phi \in \mathrm{dom}\ T,$$

which is the graph inner product of $\mathcal{M}_{\sqrt{\varphi}}$ restricted to dom T. Now, it is possible to show (Lemma 4.4.2) that dom $\mathcal{M}_\varphi$ is dense in dom $\mathcal{M}_{\sqrt{\varphi}}$ and since the operator $\mathcal{M}_{\sqrt{\varphi}}$ is closed, it follows that $b^T_+ = \langle\cdot,\cdot\rangle_+$ and $\mathcal{H}^T_+$ is the domain of $\mathcal{M}_{\sqrt{\varphi}}$. In summary, the form domain of the positive self-adjoint operator $\mathcal{M}_\varphi$ (so equal to its Friedrichs extension) is dom $\mathcal{M}_{\sqrt{\varphi}}$. Note that, for general function φ, dom $T =$ dom $\mathcal{M}_\varphi$ is a proper subset of $\mathcal{H}^T_+ = \mathrm{dom}\ \mathcal{M}_{\sqrt{\varphi}}$. Later on this will be generalized (see Section 9.3).

Lemma 4.4.2. *Consider all symbols as in Example* 4.4.1*. In both spaces,* $\mathcal{H}$ *and* $\mathcal{H}_+ = (\mathrm{dom}\ \mathcal{M}_{\sqrt{\varphi}}, \langle\cdot,\cdot\rangle_{\mathcal{M}_{\sqrt{\varphi}}})$*, one has* $\mathrm{dom}\ \mathcal{M}_\varphi \sqsubseteq \mathrm{dom}\ \mathcal{M}_{\sqrt{\varphi}}$ *(see also general arguments in Proposition* 4.3.11*).*

Proof. If $\psi \in \mathrm{dom}\ \mathcal{M}_\varphi$ then, by Cauchy-Schwarz,

$$\|\sqrt{\varphi}\psi\|^2 = \int_E \overline{\psi(x)}\,\varphi(x)\,\psi(x)\,d\mu(x) \le \|\psi\|\|\varphi\psi\| < \infty,$$

and $\mathrm{dom}\ \mathcal{M}_\varphi \subset \mathrm{dom}\ \mathcal{M}_{\sqrt{\varphi}}$.

Given $\psi \in \mathrm{dom}\ \mathcal{M}_{\sqrt{\varphi}}$, for each positive integer n set $E_n = \{x \in E : 0 \le \varphi(x) \le n\}$ and $\psi_n(x) = \chi_{E_n}(x)\psi(x)$. Then $\psi_n \in \mathrm{dom}\ \mathcal{M}_\varphi$ and

$$\|\sqrt{\varphi}\,(\psi_n - \psi)\|^2 = \int_E \varphi(x)\,|1 - \chi_{E_n}(x)|^2\ |\psi(x)|^2\,d\mu(x)$$

which vanishes as $n \to \infty$, by the dominated convergence theorem. In a similar way one checks that $\psi_n \to \psi$ in $\mathcal{H}$, that is, in this space $\mathrm{dom}\ \mathcal{M}_\varphi$ is dense in $\mathrm{dom}\ \mathcal{M}_{\sqrt{\varphi}}$.

Taking these two convergences together, it follows that

$$\|\psi_n - \psi\|_+^2 = \|\sqrt{\varphi}\,(\psi_n - \psi)\|^2 + \|\psi_n - \psi\|^2 \stackrel{n\to\infty}{\longrightarrow} 0,$$

which shows that $\mathrm{dom}\ \mathcal{M}_\varphi$ is dense in $\mathrm{dom}\ \mathcal{M}_{\sqrt{\varphi}}$ in $\mathcal{H}_+$. □

The next examples indicate that occasionally the Friedrichs extension naturally allocates boundary conditions.

Example 4.4.3. Let $\mathrm{dom}\ P = \{\psi \in \mathcal{H}^1[0,1] : \psi(0) = 0 = \psi(1)\}$, $P\psi = -i\psi'$, and $H = P^2$, with

$$\begin{aligned}\mathrm{dom}\ H &= \{\psi \in \mathrm{dom}\ P : P\psi \in \mathrm{dom}\ P\}\\ &= \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = \psi(1) = 0 = \psi'(0) = \psi'(1)\},\end{aligned}$$

and $H\psi = -\psi''$. P is a closed hermitian operator and its adjoint has the same action but with domain $\mathrm{dom}\ P^* = \mathcal{H}^1[0,1]$. Therefore, by Proposition 4.3.9, P^*P is self-adjoint,

$$\begin{aligned}\mathrm{dom}\ P^*P &= \{\psi \in \mathcal{H}^1[0,1] : \psi(0) = 0 = \psi(1),\ \psi' \in \mathcal{H}^1[0,1]\}\\ &= \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = 0 = \psi(1)\}.\end{aligned}$$

By results of Section 4.3, P^*P is the Friedrichs extension of H, i.e., $P^*P = H_F$. This is the unique self-adjoint extension of the free particle energy operator T_D in $[0,1]$, Example 2.3.5, with Dirichlet boundary conditions. This is a general feature of the Friedrichs extension of differential operators, that is, it corresponds to the Dirichlet boundary conditions; see other examples below.

Exercise 4.4.4. Show that the unique self-adjoint extension of the free particle energy operator T_P in $[0,1]$, with periodic boundary conditions of Example 2.3.7, is the Friedrichs extension of P^2, where dom $P = \{\psi \in \mathcal{H}^1[0,1] : \psi(0) = \psi(1)\}$, $P\psi = -i\psi'$. Find the domain of this extension.

Example 4.4.5. [Energy operator on $[0,1]$] Set $\mathcal{H} = \mathrm{L}^2[0,1]$, dom $H = C_0^\infty(0,1)$,

$$(H\psi)(x) := -\psi''(x) + V(x)\psi(x),$$

with $V : [0,1] \to [0,\infty)$ continuous. Consider the form generated by this operator, that is, b^H : dom $H \times$ dom $H \to \mathbb{C}$, $b^H(\psi,\phi) := \langle \psi, H\phi\rangle$. Thus

$$\begin{aligned} b^H(\psi,\psi) &= \int_0^1 \overline{\psi(x)}\,(-\psi''(x) + V(x)\psi(x))\;dx \\ &= \int_0^1 \left(|\psi'(x)|^2 + V(x)|\psi(x)|^2\right)\,dx \ge \beta\|\psi\|^2, \end{aligned}$$

with $0 \le \beta = \min_{x\in[0,1]} V(x)$. Thus $H \ge \beta\mathbf{1}$.

Let H_F be the Friedrichs extension of H; so dom $H_F \subset \mathcal{H}_+^H$. For $\psi \in$ dom H, by Cauchy-Schwarz one has

$$\begin{aligned} |\psi(x) - \psi(0)| &= \left|\int_0^x \psi'(t)dt\right| \le |x|^{\frac12}\left(\int_0^x |\psi'(t)|^2\,dt\right)^{\frac12} \\ &\le |x|^{\frac12}\; b^H(\psi,\psi)^{\frac12}. \end{aligned}$$

Since $\psi(0) = 0$ one has

$$\|\psi\|_\infty = \sup_{x\in[0,1]} |\psi(x)| \le b^H(\psi,\psi)^{\frac12} \le \langle\psi,\psi\rangle_+^{\frac12};$$

thus each Cauchy sequence according to either $b^H(\cdot,\cdot)$ or $\langle\cdot,\cdot\rangle_+$ norm converges uniformly, and so its limit is also continuous and vanishing at the boundary. Then this holds for every element of the complete space $\mathcal{H}_+^H$, in particular for the elements of dom H_F. Therefore, null Dirichlet boundary conditions $\psi(0) = 0 = \psi(1)$ hold in dom H_F. Note that the result is in fact valid for more general positive potentials $V(x)$.

Exercise 4.4.6. Let $\mathcal{H} = \mathrm{L}^2[0,1]$, $V : [0,1] \to [0,\infty)$ continuous, dom $\underline{b} = \{\psi \in \mathcal{H}^1[0,1] : \psi(0) = 0 = \psi(1)\}$ and, for $\phi,\psi \in$ dom $\underline{b}$,

$$\underline{b}(\phi,\psi) = \langle\phi',\psi'\rangle + \langle\phi, V\psi\rangle$$

Based on Example 4.2.12, show that $\underline{b}$ is a positive closed form whose respective associated operator is dom $T_{\underline{b}} = \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = 0 = \psi(1)\}$, $T_{\underline{b}}\psi = -\psi'' + V\psi$, $\psi \in$ dom $T_{\underline{b}}$. Show that $\underline{b}$ here is the closure of the form b in Example 4.4.5, and conclude that $T_{\underline{b}}$ is the Friedrichs extension H_F of the operator H in that example.

Example 4.4.7. Let $\mathcal{H} = \mathrm{L}^2[0,1]$, $p, V : [0,1] \to \mathbb{R}$ continuous functions, with $p(x) \geq 0$, $\forall x \in [0,1]$, and continuous derivative p'. Given $a \geq 0$, consider the operator

$$\begin{aligned} \mathrm{dom}\; T &= \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = 0,\ \psi'(1) = -a\psi(1)\}, \\ (T\psi)(x) &= -[p\psi']'(x) + V(x)\psi(x), \qquad \psi \in \mathrm{dom}\; T. \end{aligned}$$

Integrations by parts show that T is hermitian, and since

$$\begin{aligned} \langle \psi, T\psi \rangle &= a\, p(1)|\psi(1)|^2 + \int_0^1 p(x)|\psi'(x)|^2\, dx + \int_0^1 V(x)|\psi(x)|^2\, dx \\ &\geq \int_0^1 V(x)|\psi(x)|^2\, dx \geq \beta \|\psi\|^2, \qquad \beta = \inf\{V(x) : x \in [0,1]\}, \end{aligned}$$

it follows that $T \geq \beta\mathbf{1}$. Therefore, this operator has a self-adjoint extension T_F, its Friedrichs extension, and $T_F \geq \beta\mathbf{1}$. In particular $\sigma(T_F) \subset [\beta, \infty)$.

Example 4.4.8. Let T_α, T_τ be operators as introduced in Example 4.2.15 and assume that $\alpha_0 \neq \tau_0$, $\alpha_1 \neq \tau_1$ (recall that they are not zero). Consider the operator sum $(T_\alpha + T_\tau)/2$, whose domain is

$$\begin{aligned} \mathrm{dom}\; (T_\alpha/2) \cap \mathrm{dom}\; (T_\tau/2) &= \Big\{\psi \in \mathcal{H}^2[0,1] : \\ &\qquad \psi'(0) = \frac{\alpha_0}{2}\psi(0) = \frac{\tau_0}{2}\psi(0), \psi'(1) = -\frac{\alpha_1}{2}\psi(1) = -\frac{\tau_1}{2}\psi(1)\Big\} \\ &= \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = 0 = \psi(1), \psi'(0) = 0 = \psi'(1)\}. \end{aligned}$$

Since the situation is very similar to Exercise 4.2.14 and Example 4.4.3, one concludes that $(T_\alpha + T_\tau)/2 \geq 0$ and the domain of its Friedrichs extension $((T_\alpha + T_\tau)/2)_F$ carries Dirichlet boundary conditions, i.e., $\psi(0) = 0 = \psi(1)$. Therefore

$$\frac{T_\alpha}{2} \dot{+} \frac{T_\tau}{2} \neq \left(\frac{T_\alpha}{2} + \frac{T_\tau}{2}\right)_F;$$

see Example 4.2.15.

Example 4.4.9. [Schrödinger operator with delta-function potential] Let $c > 0$ and $\delta(x)$ be the Dirac delta at the origin (see also Example 6.2.16 and Subsection 7.4.2). A way to interpret the formal energy operator (in $\mathrm{L}^2(\mathbb{R})$)

$$T^c = -\frac{d^2}{dx^2} + c\,\delta(x),$$

under this δ potential with positive intensity c, is to consider a suitable domain for T^c, which contains all information on $\delta(x)$, and then construct a self-adjoint extension via sesquilinear forms (see Example 4.1.15). Physically, $\delta(x)$ models a very strong (positive) interaction concentrated at the origin.

As a guide for defining such domain, for $\varepsilon > 0$ integrate $T^c\psi$ formally

$$\int_{-\varepsilon}^{\varepsilon} (T^c\psi)(x)\,dx = \int_{-\varepsilon}^{\varepsilon} -\psi''(x)\,dx + \int_{-\varepsilon}^{\varepsilon} c\,\delta(x)\psi(x)\,dx$$
$$= \psi'(-\varepsilon) - \psi'(\varepsilon) + c\,\psi(0).$$

The term $c\psi(0)$ induces 1. below. If the function $(T^c\psi)$ is bounded (so 3. below), then as $\varepsilon \to 0^+$ one gets

$$0 = \psi'(0^-) - \psi'(0^+) + c\,\psi(0),$$

and so 2. below. Based on this motivating digression, define dom T^c as the set of $\psi \in \mathcal{H}^2(\mathbb{R} \setminus \{0\})$ obeying

1. ψ is continuously extended at zero, that is, $\psi(0^+) = \psi(0^-) := \psi(0)$;
2. $\psi'(0^+) - \psi'(0^-) = c\psi(0)$;
3. $\psi''(0^+) - \psi''(0^-)$ is finite.

This set dom T^c contains $C_0^\infty(\mathbb{R} \setminus \{0\})$ and so is dense in $\mathrm{L}^2(\mathbb{R})$. Finally define

$$T^c\psi := -\psi'', \qquad \psi \in \mathrm{dom}\; T^c.$$

For $\psi, \phi \in \mathrm{dom}\; T^c$ one has, after integration by parts,

$$b^{T^c}(\psi,\phi) = \langle \psi, T^c\phi\rangle = -\int_{-\infty}^{0^-} \overline{\psi(x)}\,\phi''(x)\,dx - \int_{0^+}^{\infty} \overline{\psi(x)}\,\phi''(x)\,dx$$
$$= \overline{\psi(0^+)}\,\phi'(0^+) - \overline{\psi(0^-)}\,\phi'(0^-) + \int_{\mathbb{R}} \overline{\psi'(x)}\,\phi'(x)\,dx$$
$$= c\,\overline{\psi(0)}\,\phi(0) + \langle \psi', \phi'\rangle = \langle \psi', \phi'\rangle + c\,b_\delta(\psi,\phi),$$

where b_δ is the form in Example 4.1.15. Two important conclusions follow. First, the form $b^{T^c}(\psi,\phi)$ is the sum

$$b^{T^c}(\psi,\phi) = \langle \psi', \phi'\rangle + c\,b_\delta(\psi,\phi),$$

supporting the interpretation of the presence of a δ potential with intensity $c > 0$. Second, another integration by parts shows that T^c is hermitian, and for $\psi = \phi$ one has

$$\langle \psi, T^c\psi\rangle = c\,|\psi(0)|^2 + \|\psi'\|^2,$$

so that T^c is a positive operator. Therefore, it has a (Friedrichs) self-adjoint extension T_F^c, a candidate for the energy operator in this situation.

Note that if ψ is in the domain of this Friedrichs extension and it is meaningful to write $u = -\psi'' + c\delta\psi = -\psi'' + c\psi(0)$, then such functions ψ have a slope discontinuity at the origin equal to $c\psi(0)$, so that $u \in \mathrm{L}^2(\mathbb{R})$ even if ψ'' and the constant function $c\psi(0)$ do not.

Exercise 4.4.10. Consider again the formal operator

$$T^c = -\frac{d^2}{dx^2} + c\,\delta(x),$$

as in Example 4.4.9. A possible way to address the problem of getting a well-defined self-adjoint operator is to note that formally on the set

$$E = \{\psi \in \mathcal{H}^2(\mathbb{R}) : \psi(0) = 0\},$$

T^c coincides with $T_0 = -d^2/dx^2$. Show that T_0 with dom $T_0 = E$ is hermitian, that its adjoint has the same action but with dom ${T_0}^* = \{\psi \in \mathcal{H}^2(\mathbb{R} \setminus \{0\}) : \psi(0^-) = \psi(0^+)\}$. Check that its deficiency indices are both equal to 1; the corresponding self-adjoint extensions should contain the rigorous definition of T^c for any $c \in \mathbb{R}$.

Example 4.4.11. The derivative of the Dirac delta $\delta'(x)$ acts formally as

$$\int \delta'(x)\psi(x)dx = -\psi'(x).$$

Here a construction will be discussed so that it becomes meaningful to talk about the energy operator, in $\mathrm{L}^2(\mathbb{R})$,

$$S^c = -\frac{d^2}{dx^2} + c\,\delta'(x), \qquad c < 0.$$

Physically $\delta'(x)$ would model a very strong interaction concentrated at the origin but of positive intensity on the left and of negative intensity on the right, something like a dipole concentrated at the origin (think of the derivative of a function that approximates $\delta(x)$, which has a positive peak on the left and a negative one on the right).

Introduce dom S^c as the set of elements $\psi \in \mathcal{H}^2(\mathbb{R} \setminus \{0\})$ obeying $\psi'(0^+) = \psi'(0^-)$ (both lateral limits do exist), so it becomes meaningful to talk about $\psi'(0) := \psi'(0^+)$ and (a formal integration imposes) $\psi(0^+) - \psi(0^-) = -c\psi'(0)$. This subspace is dense in $\mathrm{L}^2(\mathbb{R})$ since it contains $C_0^\infty(\mathbb{R} \setminus \{0\})$. On dom S^c define the sesquilinear form

$$b_{\delta'}(\psi, \phi) := -\psi'(0)\phi'(0),$$

heuristically corresponding to a δ' potential. Finally, define on dom S^c the operator and subsequent sesquilinear form

$$S^c\psi := -\psi'', \qquad b^{S^c}(\psi, \phi) := \langle \psi, S^c\phi \rangle.$$

On integrating by parts it is found that S^c is hermitian and

$$b^{S^c}(\psi, \phi) = \langle \psi', \phi' \rangle + c\, b_{\delta'}(\psi, \phi),$$

so that

$$b^{S^c}(\psi, \psi) = -c|\psi'(0)|^2 + \|\psi'\|^2$$

and S^c is positive for $c < 0$. Its Friedrichs extension S_F^c is a candidate for the energy operator in this situation. Additional information about δ' potential can be obtained from [Še86] and [ExNZ01].

Exercise 4.4.12. Show that S^c in Example 4.4.11 is hermitian and positive.

Example 4.4.13. Let $\mathcal{H} = \mathrm{L}^2[0,1]$,

$$\begin{aligned} \mathrm{dom}\ T_0 &= \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = \psi(1) = 0 = \psi'(0) = \psi'(1)\}, \\ \mathrm{dom}\ T_1 &= \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = 0 = \psi(1)\}, \\ T_j\psi &= -\psi'', \qquad \psi \in \mathrm{dom}\ T_j,\ j = 0, 1. \end{aligned}$$

Then $\mathrm{dom}\ T_0^* = \mathcal{H}^2[0,1]$, T_0 is hermitian, lower bounded, with deficiency indices $n_- = n_+ = 2$ (see Example 2.6.8), and the Friedrichs extension of T_0 is $T_F = T_1$. In fact, observe that $T_0 = P^2$, with P as in Example 4.4.3 and $T_1 = P^*P$.

The eigenvectors of T_F form an orthogonal basis of $\mathcal{H}$ and its spectrum is $\{(n\pi)^2 : n = 1, 2, 3, \dots\}$ (see Example 2.3.5). Then $T_F \geq \pi^2\mathbf{1}$, and the constant π^2 cannot be increased. Check this, for instance, by considering an eigenfunction (of T_F) expansions.

Note, however, that the operator

$$\mathrm{dom}\ T_2 = \left\{\psi \in \mathcal{H}^2[0,1] : \psi(0) = -\psi(1),\ \psi'(0) = -\psi'(1)\right\},$$

$T_2\psi = -\psi''$, is another self-adjoint extension of T_0, with the same spectrum as T_F, and so with the same lower bound π^2. Therefore, the sole lower bound is not enough to characterize the Friedrichs extension of lower bounded hermitian operators.

Exercise 4.4.14. Fill in the missing details in Example 4.4.13.

Exercise 4.4.15. This is closely related to Example 2.3.19. The Hilbert space is $\mathcal{H} = \mathrm{L}^2[0,\infty)$,

$$\mathrm{dom}\ T = \left\{\psi \in \mathcal{H}^2[0,\infty) : \psi(0) = 0,\ \psi'(0) = 0\right\},$$

and $T\psi = -\psi''$.

1. Check that this operator is hermitian and positive.
2. Show that its deficiency indices are $n_- = n_+ = 1$ and that its self-adjoint extensions T_c have the same operator action as T but with domain labeled by $c \in \mathbb{R} \cup \{\infty\}$ with

   $$\mathrm{dom}\ T_c = \left\{\psi \in \mathcal{H}^2[0,\infty) : \psi(0) = c\psi'(0)\right\}, \qquad c \in \mathbb{R},$$

   and $\psi'(0) = 0$ for $c = \infty$.
3. Find the Friedrichs extension T_F of T and conclude that it corresponds to $c = 0$, i.e., the Dirichlet boundary condition is selected.

4.4.1 Hardy's Inequality

An important inequality will be used in the next example. It has versions for $\mathbb{R}^n$, $n > 3$, but with constants different from 1/4 in Lemma 4.4.16; see Exercise 4.4.21 for $n = 1$.

Lemma 4.4.16 (Hardy's Inequality). *For $\psi \in \mathcal{H}^1(\mathbb{R}^3)$ (in particular for $\psi \in C_0^\infty(\mathbb{R}^3)$)*

$$\int_{\mathbb{R}^3} |\nabla\psi(x)|^2 \, dx \geq \frac{1}{4} \int_{\mathbb{R}^3} \frac{|\psi(x)|^2}{|x|^2} \, dx.$$

Proof. By considering the real and imaginary parts of functions, it is possible to restrict the argument to real-valued ψ. Consider first $\psi \in C_0^\infty(\mathbb{R}^3)$.

For $x = (x_1, x_2, x_3) \in \mathbb{R}^3$ denote $r = |x|$ (standard norm in $\mathbb{R}^3$), and recall that in spherical coordinates (r, θ, φ) one has $dx = r^2 \sin\theta \, dr d\theta d\varphi$. For real-valued $\psi \in C_0^\infty(\mathbb{R}^3)$ set $\phi = r^{\frac{1}{2}}\psi$, so that

$$\begin{aligned}|(\nabla\psi)(x)|^2 &= (\partial_1\psi)^2 + (\partial_2\psi)^2 + (\partial_3\psi)^2 \\ &= \frac{1}{r}|\nabla\phi|^2 - \frac{1}{r^2}\frac{\partial(\phi^2)}{\partial r} + \frac{1}{4r^3}(\phi^2).\end{aligned}$$

Since $\phi(0) = 0$ and there exists $R > 0$ so that $\phi(x) = 0$ if $r \geq R$, then

$$\begin{aligned}\int_{\mathbb{R}^3} \frac{1}{r^2}\frac{\partial(\phi^2)}{\partial r} dx &= \int_0^{2\pi}\int_0^{\pi} \sin\theta \, d\theta d\varphi \int_0^R \frac{\partial(\phi^2)}{\partial r} dr \\ &= \pi \left(\phi(R)^2 - \phi(0)^2\right) = 0.\end{aligned}$$

Therefore

$$\int_{\mathbb{R}^3} |\nabla\psi|^2 \, dx \geq \frac{1}{4}\int_{\mathbb{R}^3} \frac{1}{r^3}\phi^2 \, dx = \frac{1}{4}\int_{\mathbb{R}^3} \frac{1}{r^2}\psi^2 \, dx,$$

which implies the desired inequality in case $\psi \in C_0^\infty(\mathbb{R}^3)$.

For $\psi \in \mathcal{H}^1(\mathbb{R}^3)$, take a sequence $(\psi_j)_j \subset C_0^\infty(\mathbb{R}^3)$ with $\psi_j \to \psi$ in $\mathcal{H}^1(\mathbb{R}^3)$; thus both $\psi_j \to \psi$ and (the components of) $\nabla\psi_j \to \nabla\psi$ in $\mathrm{L}^2(\mathbb{R}^3)$, and the inequality follows for all $\psi \in \mathcal{H}^1(\mathbb{R}^3)$. □

Exercise 4.4.17. Inspect the proof of Hardy's inequality to show that equality holds for $\psi \in C_0^\infty(\mathbb{R}^3)$ iff $\psi = 0$.

Remark 4.4.18. There is a version of Hardy's inequality in $\mathbb{R}^n$, $n \geq 3$, that holds for all $\psi \in \mathcal{H}^1(\mathbb{R}^n)$ and takes the form

$$\int_{\mathbb{R}^n} |\nabla\psi(x)|^2 \, dx \geq \frac{(n-2)^2}{4} \int_{\mathbb{R}^n} \frac{|\psi(x)|^2}{|x|^2} \, dx,$$

and the constant $(n-2)^2/4$ is the best possible for all $\psi \in C_0^\infty(\mathbb{R}^n)$ [Sh31], [KaSW75].

Example 4.4.19. [The Friedrichs Extension for the 3D hydrogen atom] Let $\mathcal{H} = \mathrm{L}^2(\mathbb{R}^3)$ and consider dom $H = C_0^\infty(\mathbb{R}^3)$ and

$$(H\psi)(x) = -\frac{\hbar^2}{2m}(\Delta\psi)(x) - \alpha\frac{e^2}{|x|}\psi(x), \qquad \psi \in \mathrm{dom}\ H,$$

with $\alpha > 0$. This is related to the quantum three-dimensional (briefly 3D) hydrogen atom energy operator (with some physical constants included: Planck constant $\hbar$, electron mass m and charge $-e$). Integration by parts shows that H is hermitian and, together with Lemma 4.4.16 that, for real-valued $\psi \in \mathrm{dom}\ H$,

$$\begin{aligned}\langle\psi, H\psi\rangle &= \int_{\mathbb{R}^3}\left(\frac{\hbar^2}{2m}|\nabla\psi(x)|^2 - \alpha\frac{e^2}{|x|}\psi(x)^2\right)dx \\ &\geq \int_{\mathbb{R}^3}\left(\frac{\hbar^2}{8m}\frac{1}{|x|^2} - \alpha\frac{e^2}{|x|}\right)\psi(x)^2\,dx.\end{aligned}$$

Now pick $a > 0$ so that

$$\frac{\alpha e^2}{|x|} \leq \frac{\hbar^2}{8m|x|^2} + a, \qquad \forall x \neq 0.$$

Thus

$$\langle\psi, H\psi\rangle \geq -a\int_{\mathbb{R}^3}\psi(x)^2\,dx = -a\|\psi\|^2.$$

For $\psi = \psi_1 + i\psi_2 \in \mathrm{dom}\ H$, with ψ_1, ψ_2 real-valued, one gets

$$\begin{aligned}\langle\psi, H\psi\rangle &= \langle\psi_1, H\psi_1\rangle + i\langle\psi_1, H\psi_2\rangle - i\langle\psi_2, H\psi_1\rangle + \langle\psi_2, H\psi_2\rangle \\ &= \langle\psi_1, H\psi_1\rangle + \langle\psi_2, H\psi_2\rangle \\ &\geq -a\|\psi_1\|^2 - a\|\psi_2\|^2 = -a\|\psi\|^2,\end{aligned}$$

and the same relation holds for all elements of dom H. Therefore, it follows that $H \geq -a\mathbf{1}$ and H has the self-adjoint Friedrichs extension H_F. Further, $H_F \geq -a\mathbf{1}$ and its spectrum $\sigma(T_F)$ is lower bounded.

Remark 4.4.20. By using results of Rellich, in the 1950s Tosio Kato showed that H in Example 4.4.19 with domain $C_0^\infty(\mathbb{R}^3)$ is essentially self-adjoint; this is discussed in Example 6.2.3.

Exercise 4.4.21. Let ψ be a real-valued element of $C_0^\infty(\mathbb{R}\setminus\{0\})$ or $C_0^\infty(0,\infty)$. On integrating by parts

$$\int \psi(x)^2\frac{1}{x^2}\,dx,$$

and then applying Cauchy-Schwarz, conclude the Hardy's inequality

$$\frac{1}{4}\int\left(\frac{\psi(x)}{x}\right)^2 dx \leq \int \psi'(x)^2\,dx.$$

The integrations are over $\mathbb{R}$ or $[0,\infty)$, respectively.

Chapter 5

Unitary Evolution Groups

Unitary evolution groups are in one-to-one correspondence with self-adjoint operators. They are also responsible for the time evolution of quantum states, that is, the solutions of Schrödinger equations. In this chapter such relations are described in detail, including standard examples of unitary evolution groups and infinitesimal generators. Different continuity assumptions on the unitary groups are discussed.

5.1 Unitary Evolution Groups

A major interest here is in solutions of the initial value problem

$$i\frac{d\xi}{dt}(t) = T\xi(t), \qquad \xi(0) = \xi \in \operatorname{dom} T,$$

for $T : \operatorname{dom} T \sqsubseteq \mathcal{H} \to \mathcal{H}$ a linear self-adjoint operator, with t playing the role of time. In quantum mechanics this equation is known as the Schrödinger equation and it rules the dynamics in quantum mechanics; in this setting T corresponds to the total system energy. The imaginary factor i imposes that the solutions of this problem are via unitary operators, as discussed below. A mathematical and physical pertinent question is about the behavior of $\xi(t)$ for large values of t; this will be one of the main concerns of this text, but first the existence of solutions must be addressed.

Sometimes integrals of vector and operator-valued functions will be used; they can be defined via limits of Riemann sums in a similar way to the usual Riemann integral. Since their definitions and properties are quite similar to the ordinary case, no attempt will be made to present details of this theory.

Definition 5.1.1. A map $G : \mathbb{R} \to \mathrm{B}(\mathcal{H})$ is a *one-parameter unitary evolution group*, or simply a *unitary evolution group*, on $\mathcal{H}$ if $G(t)$ is a unitary operator onto $\mathcal{H}$ and $G(t+s) = G(t)G(s)$, $\forall t, s \in \mathbb{R}$.

Note that $G(0)G(t) = G(t)$, so $G(0) = \mathbf{1}$, $G(-t) = G(t)^{-1} = G(t)^*$, $\forall t \in \mathbb{R}$, and the map $t \mapsto G(t)$ is a representation of the abelian group $\mathbb{R}$ in $\mathrm{B}(\mathcal{H})$.

Definition 5.1.2. If $G(t)$ is a unitary evolution group, the operator T defined by

$$\text{dom } T := \left\{ \xi \in \mathcal{H} : \exists \lim_{h\to 0} \frac{1}{h} \left(G(h) - \mathbf{1} \right) \xi \right\},$$

that is, $\xi \in \text{dom } T$ iff $t \mapsto G(t)\xi$ is *differentiable* at $t = 0$,

$$T\xi := i \lim_{h\to 0} \frac{1}{h} \left(G(h) - \mathbf{1} \right) \xi, \qquad \xi \in \text{dom } T,$$

is called the *infinitesimal generator* of $G(t)$ (note that dom T is actually a vector subspace of $\mathcal{H}$ and T is uniquely defined).

Since for each $t \in \mathbb{R}$ the operator $G(t)$ is unitary, so continuous, for $\xi \in \text{dom } T$ take $h \to 0$ in

$$\frac{1}{h} \left[G(h) - \mathbf{1} \right] G(t)\xi = \frac{1}{h} \left[G(t+h)\xi - G(t)\xi \right] = G(t) \frac{1}{h} (G(h) - \mathbf{1})\xi,$$

to conclude that $G(t)(\text{dom } T) \subset \text{dom } T$, $\forall t \in \mathbb{R}$; apply $G(-t)$ to this inclusion and conclude that $G(t)(\text{dom } T) = \text{dom } T$. Explicitly, for $h \to 0$ one gets

$$G(t)T\xi = TG(t)\xi, \qquad \forall t \in \mathbb{R},\ \xi \in \text{dom } T.$$

The parameter t is not necessarily time; some examples in this chapter will point out the richness of other possibilities. The case of t actually representing time is very important in quantum mechanics and, as already mentioned, in this case the infinitesimal generator is the operator corresponding to the total quantum energy; see Example 5.4.1. So the terminology "evolution groups."

Proposition 5.1.3. *Let $t \mapsto G(t)$ be a unitary evolution group. Then its infinitesimal generator T is symmetric and for $\xi \in \text{dom } T$ the curve $\xi(t) := G(t)\xi$ in $\mathcal{H}$ is the unique solution of*

$$i\frac{d\xi}{dt}(t) = T\xi(t), \qquad \xi(0) = \xi.$$

Proof. Since by definition

$$\frac{d\xi}{dt}(t) := \lim_{h\to 0} \frac{1}{h} \left[G(t+h)\xi - G(t)\xi \right],$$

the preceding discussion has already shown that $\xi(t)$ is a solution of this initial value problem. For $\xi, \eta \in \text{dom } T$ one has

$$\begin{aligned}
\langle T\xi, \eta \rangle &= \lim_{h\to 0} \left\langle i \frac{G(h) - \mathbf{1}}{h} \xi, \eta \right\rangle = -i \lim_{h\to 0} \frac{1}{h} \left\langle \left(G(h) - \mathbf{1} \right) \xi, \eta \right\rangle \\
&= -i \lim_{h\to 0} \frac{1}{h} \left\langle \xi, \left(G(-h) - \mathbf{1} \right) \eta \right\rangle \\
&= \lim_{h\to 0} \left\langle \xi,\, i\, \frac{G(-h) - \mathbf{1}}{-h} \eta \right\rangle = \langle \xi, T\eta \rangle,
\end{aligned}$$

and so T is a symmetric operator. For the uniqueness of the solution of the initial value problem, let $\eta(t)$ be another solution to the problem; then, for all t,

$$\begin{aligned}\frac{d}{dt}\|\xi(t)-\eta(t)\|^2 &= 2\mathrm{Re}\ \left\langle [\xi(t)-\eta(t)], \frac{d}{dt}[\xi(t)-\eta(t)]\right\rangle \\ &= 2\mathrm{Re}\ \langle [\xi(t)-\eta(t)], -iT[\xi(t)-\eta(t)]\rangle = 0\end{aligned}$$

since T is symmetric (thus, $\langle \phi, T\phi\rangle \in \mathbb{R}$, $\forall \phi \in \mathrm{dom}\ T$). So $\|\xi(t)-\eta(t)\|$ is constant, and owing to $\xi(0)-\eta(0)=0$, it is found that $\xi(t)=\eta(t)$ for all $t\in\mathbb{R}$. □

It is interesting to observe that, according to Proposition 5.1.3, the infinitesimal generator of a unitary evolution group $G(t)$ is symmetric with no explicit continuity assumption on $G(t)$. Now suitable continuity properties will be required and some of their consequences explored.

Definition 5.1.4. Let $G(t)$ be a unitary evolution group acting on $\mathcal{H}$. Then the map $t\mapsto G(t)$ is

a) *norm (or uniformly) continuous* if in $\mathrm{B}(\mathcal{H})$ one has $\lim_{t\to t_0}\|G(t)-G(t_0)\| = 0$, $\forall t_0\in\mathbb{R}$.
b) *strongly continuous* if $\lim_{t\to t_0} G(t)\xi = G(t_0)\xi$, $\forall t_0\in\mathbb{R}$, $\forall \xi\in\mathcal{H}$.
c) *weakly continuous* if $\lim_{t\to t_0}\langle G(t)\xi,\eta\rangle = \langle G(t_0)\xi,\eta\rangle$, $\forall t_0\in\mathbb{R}$, $\forall \xi,\eta\in\mathcal{H}$.
d) *measurable* if the map $\mathbb{R}\ni t\mapsto \langle G(t)\xi,\eta\rangle$ is (Lebesgue) measurable $\forall\xi,\eta\in\mathcal{H}$.

Exercise 5.1.5. By using basic properties of $G(t)$ discussed at the beginning of this section, show that it is enough to consider only $t_0=0$ in items a), b) and c) of Definition 5.1.4.

Example 5.1.6. Let $\varphi: E\to\mathbb{R}$ be a measurable function and bounded on each bounded subset of the open set $E\subset\mathbb{R}^n$; by Corollary 2.3.25, $\mathcal{M}_\varphi$ is self-adjoint. Consider $U(t)=e^{-it\varphi(x)} := \mathcal{M}_{e^{-it\varphi}}$, $t\in\mathbb{R}$, acting on $\mathrm{L}^2_\mu(E)$, which is a unitary evolution group (check this!).

For $\psi\in\mathrm{L}^2_\mu(E)$, it follows by the dominated convergence theorem that

$$\lim_{h\to 0}\|U(h)\psi-\psi\|^2 = \lim_{h\to 0}\int_E \left|e^{-ih\varphi(x)}-1\right|^2 |\psi(x)|^2\,d\mu(x) = 0.$$

Hence $U(t)$ is strongly continuous.

Now let T be the infinitesimal generator of $U(t)$, which is symmetric by Proposition 5.1.3. If $\psi\in\mathrm{dom}\ \mathcal{M}_\varphi$, then

$$\left\|\frac{i}{h}(U(h)\psi-\psi)-\mathcal{M}_\varphi\psi\right\|^2 = \int_E \left|\frac{i}{h}(e^{-ih\varphi(x)}-1)-\varphi(x)\right|^2 |\psi(x)|^2\,d\mu(x).$$

Since $|e^{iy}-1|\le |y|$ for $y\in\mathbb{R}$,

$$\left|\frac{i}{h}(e^{-ih\varphi(x)}-1)-\varphi(x)\right| \le \left|\frac{1}{h}(e^{-ih\varphi(x)}-1)\right| + |\varphi(x)| \le 2\,|\varphi(x)|\,,$$

and by dominated convergence one finds that

$$\lim_{h\to 0}\left\|\frac{i}{h}(U(h)\psi-\psi)-\mathcal{M}_\varphi\psi\right\|=0$$

and so $\psi\in\text{dom}\,T$ and $T\psi=\mathcal{M}_\varphi\psi$, that is, $\mathcal{M}_\varphi\subset T$. Since T is symmetric and $\mathcal{M}_\varphi$ self-adjoint, one has $\mathcal{M}_\varphi=T$ (see Exercise 2.1.19). By Proposition 5.1.3, $U(t)\psi=e^{-it\varphi(x)}\psi$ is a solution of

$$i\frac{d\psi}{dt}(t)=\mathcal{M}_\varphi\psi(t),\qquad \psi(0)=\psi\in\text{dom}\,\mathcal{M}_\varphi,$$

and the unique one.

Proposition 5.1.7. *If $G(t)$ is a unitary evolution group on the Hilbert space $\mathcal{H}$, then* b), c) *and* d) *in Definition* 5.1.4 *are equivalent.*

Proof. Recall that due to the group property it is enough to take $t_0=0$ in b), c); also, $\mathcal{H}$ is separable (it is known that d) $\Rightarrow$ c) may not hold if $\mathcal{H}$ is not separable).

• b) $\Rightarrow$ c) $\Rightarrow$ d) They are clear from the definitions.

• c) $\Rightarrow$ b) One has

$$\begin{aligned}\|G(t)\xi-\xi\|^2&=\|G(t)\xi\|^2+\|\xi\|^2-\langle G(t)\xi,\xi\rangle-\langle\xi,G(t)\xi\rangle\\&=2\|\xi\|^2-\langle G(t)\xi,\xi\rangle-\langle\xi,G(t)\xi\rangle,\end{aligned}$$

and if c) holds then $\langle\xi,G(t)\xi\rangle\to\|\xi\|^2$ as $t\to 0$ and so $\|G(t)\xi-\xi\|\to 0$, that is, b) holds.

• d) $\Rightarrow$ c) This is a rather surprising result of von Neumann. Pick $\xi\in\mathcal{H}$. Since $t\mapsto\langle G(t)\xi,\eta\rangle$ is measurable and $|\langle G(t)\xi,\eta\rangle|\le\|\xi\|\,\|\eta\|$, given $s>0$ it is possible to use integration to define the linear functional $f:\mathcal{H}\to\mathbb{C}$ by

$$f(\eta)=\int_0^s\langle G(t)\xi,\eta\rangle\,dt,\qquad\forall\eta\in\mathcal{H},$$

which is continuous since $|f(\eta)|\le s\|\xi\|\,\|\eta\|$; thus, by Riesz's Representation 1.1.40, there is $\xi_s\in\mathcal{H}$ so that

$$\langle\xi_s,\eta\rangle=\int_0^s\langle G(t)\xi,\eta\rangle\,dt,\qquad\forall\eta\in\mathcal{H}.$$

Note that $\|\xi_s\|=\|f\|\le s\|\xi\|$. A similar construction defines ξ_s for $s\le 0$.

Denote by S the subspace

$$S=\text{Lin}\left(\{\xi_s\in\mathcal{H}:\xi\in\mathcal{H},s\in\mathbb{R}\}\right).$$

The next step is to show that S is dense in $\mathcal{H}$. Let $\{\xi^j\}_j$ be a countable orthonormal basis of $\mathcal{H}$ and take $\zeta\in S^\perp$. Thus, for all $s\in\mathbb{R}$,

$$0=\langle\xi^j_s,\zeta\rangle=\int_0^s\langle G(t)\xi^j,\zeta\rangle\,dt$$

and so $\langle G(t)\xi^j, \zeta\rangle = 0$ Lebesgue a.e. in $\mathbb{R}$, say for $t \in A_j$ and A_j with total measure. Thus the set $A = \cap_j A_j \subset \mathbb{R}$ also has total Lebesgue measure and

$$\langle G(t)\xi^j, \zeta\rangle = \langle \xi^j, G(-t)\zeta\rangle = 0, \qquad \forall j, \forall t \in A.$$

Therefore, $G(-t)\zeta = 0$ if $t \in A$, and since $\|\zeta\| = \|G(-t)\zeta\| = 0$, it follows that $\zeta = 0$ and S is dense in $\mathcal{H}$.

Now, for $\xi, \eta \in \mathcal{H}$ (for convenience the argument is restricted to $s > 0$),

$$\begin{aligned}\langle G(r)\xi_s, \eta\rangle = \langle \xi_s, G(-r)\eta\rangle &= \int_0^s \langle G(t)\xi, G(-r)\eta\rangle\, dt \\ &= \int_0^s \langle G(t+r)\xi, \eta\rangle\, dt = \int_r^{s+r} \langle G(t)\xi, \eta\rangle\, dt,\end{aligned}$$

and one gets, for $0 \le r < s$,

$$\begin{aligned}|\langle G(r)\xi_s, \eta\rangle - \langle \xi_s, \eta\rangle| &= \left| \int_r^{s+r} \langle G(t)\xi, \eta\rangle\, dt - \int_0^s \langle G(t)\xi, \eta\rangle\, dt \right| \\ &= \left| \left(\int_r^{s+r} - \int_r^s - \int_0^r \right) \langle G(t)\xi, \eta\rangle\, dt \right| \\ &\le \left(\int_s^{s+r} + \int_0^r \right) |\langle G(t)\xi, \eta\rangle|\; dt \le 2\, r \|\xi\|\, \|\eta\|\end{aligned}$$

which vanishes as $r \to 0$. Similarly for $r < 0$. Therefore, for all $\eta \in \mathcal{H}$ and all $\phi \in S$, the maps $t \mapsto \langle G(t)\phi, \eta\rangle$ are continuous.

Let $\xi \in \mathcal{H}$; given $\varepsilon > 0$ pick $\phi \in S$ with $\|\phi - \xi\| < \varepsilon$. Since $t \mapsto G(t)$ is uniformly bounded, for each $\eta \in \mathcal{H}$,

$$\begin{aligned}|\langle G(h)\xi, \eta\rangle - \langle \xi, \eta\rangle| &\le |\langle G(h)\xi, \eta\rangle - \langle G(h)\phi, \eta\rangle| \\ &\quad + |\langle G(h)\phi, \eta\rangle - \langle \phi, \eta\rangle| + |\langle \phi, \eta\rangle - \langle \xi, \eta\rangle| \\ &< \|G(h)\xi - G(h)\phi\|\, \|\eta\| \\ &\quad + |\langle G(h)\phi, \eta\rangle - \langle \phi, \eta\rangle| + \|\xi - \phi\|\, \|\eta\| \\ &\le 2\varepsilon + |\langle G(h)\phi, \eta\rangle - \langle \phi, \eta\rangle|\,.\end{aligned}$$

Since $\phi \in S$, by continuity there exists $h_0 > 0$ so that, if $|h| < h_0$ one has $|\langle G(h)\phi, \eta\rangle - \langle \phi, \eta\rangle| \le \varepsilon$, consequently

$$|\langle G(h)\xi, \eta\rangle - \langle \xi, \eta\rangle| \le 3\varepsilon, \qquad |h| < h_0.$$

Therefore, $\lim_{h\to 0}\langle G(h)\xi, \eta\rangle = \langle \xi, \eta\rangle$, $\forall \xi, \eta \in \mathcal{H}$, and $G(t)$ is weakly continuous at zero. This finishes the proof of the proposition. □

5.2 Bounded Infinitesimal Generators

If $T \in \mathrm{B}(\mathcal{H})$ and $z \in \mathbb{C}$, the exponential operator e^{zT} can be defined by the series

$$e^{zT} = \sum_{j=0}^{\infty} \frac{z^j T^j}{j!},$$

which is norm convergent in $\mathrm{B}(\mathcal{H})$. Since T is bounded, the manipulations with such series are very similar to the ones with the corresponding numerical series, and so one can conclude, for instance, that

1. $Te^{zT} = e^{zT}T, \qquad \forall z \in \mathbb{C}.$
2. $e^{(z+y)T} = e^{zT}\, e^{yT} = e^{yT}\, e^{zT}, \qquad \forall z, y \in \mathbb{C}.$
3. For $t = 0$ one has $e^{0T} = \mathbf{1}$, and $e^{-zT} = (e^{zT})^{-1}$.
4. For the adjoint operator
$$(e^{zT})^* = \sum_{j=0}^{\infty} \frac{(\overline{z}T^*)^j}{j!} = e^{\overline{z}T^*}.$$
5. The map $\mathbb{R} \ni t \mapsto e^{tT}$ is norm differentiable in $\mathrm{B}(\mathcal{H})$ (so continuous) with
$$\frac{d}{dt} e^{tT} := \lim_{h\to 0} \frac{1}{h}(e^{(t+h)T} - e^{tT}) = Te^{tT}, \qquad \forall t \in \mathbb{R}.$$

As an illustration of the arguments, consider 2 above. Since the involved series are norm convergent, one has

$$\begin{aligned} e^{zT} e^{yT} &= \sum_{m,j=0}^{\infty} \frac{z^j T^j}{j!} \frac{y^m T^m}{m!} = \sum_{k=0}^{\infty} \sum_{j+m=k} \frac{(zT)^j (yT)^m}{j!\, m!} \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{j+m=k} \frac{k!}{j!\, m!} (zT)^j (yT)^m \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{m=0}^{k} \frac{k!}{m!\, (k-m)!} (zT)^{k-m} (yT)^m \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \, ((z+y)T)^k = e^{(z+y)T} \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \, ((y+z)T)^k = e^{(y+z)T}. \end{aligned}$$

Exercise 5.2.1. Verify the validity of the other properties of e^{zT} presented above. Note that 5. also holds with $t \in \mathbb{C}$.

In the specific case T is a bounded self-adjoint operator, the map $t \mapsto e^{-itT}$ is a unitary evolution group, T is its infinitesimal generator and the differentiation can be taken even in the norm of $\mathrm{B}(\mathcal{H})$, instead of strongly as in Definition 5.1.2. This situation is the general one, as discussed in Theorem 5.2.3.

Exercise 5.2.2. For a bounded self-adjoint T, verify that $t \mapsto e^{-itT}$ is a unitary evolution group and also that T is its infinitesimal generator.

Theorem 5.2.3. *If $G(t)$ is a unitary evolution group on $\mathcal{H}$, then the following assertions are equivalent:*

i) *$t \mapsto G(t)$ is norm continuous.*

ii) *$t \mapsto G(t)$ is norm differentiable and there exists $T \in \mathrm{B}(\mathcal{H})$ with*

$$\lim_{h\to 0} \left\| \frac{i}{h}\left[G(t+h) - G(t)\right] - T \right\| = \lim_{h\to 0} \left\| \frac{i}{h}[G(h) - \mathbf{1}] - T \right\| = 0.$$

So $T \in \mathrm{B}(\mathcal{H})$ is the infinitesimal generator of $G(t)$.

iii) *There exists $T \in \mathrm{B}(\mathcal{H})$ so that*

$$G(t) = e^{-itT} = \sum_{j=0}^{\infty} \frac{1}{j!}\,(-itT)^j, \qquad \forall t \in \mathbb{R}.$$

Furthermore, T in ii) *and* iii) *is the same operator and self-adjoint.*

Proof. By repeating an argument in Proposition 5.1.3, one gets that if ii) holds, then T is symmetric with $\operatorname{dom} T = \mathcal{H}$, so T in ii) is self-adjoint. The implications iii) $\Rightarrow$ ii) $\Rightarrow$ i) and iii) $\Rightarrow$ i) basically follow by the discussion above. Since iii) $\Rightarrow$ ii), then e^{-itT} in iii) is a unitary evolution group and T its self-adjoint infinitesimal generator. It is then needed only to show that

i) $\Rightarrow$ iii) As a motivation for what follows, note that for $x \in \mathbb{R}$, $x \int_0^t e^{-isx}\, ds = i(e^{-itx} - 1)$ and so iii) allows one to guess

$$i(G(t) - \mathbf{1}) \approx T \int_0^t G(s)\, ds.$$

Suppose i) holds. Compute the relation

$$\begin{aligned}(G(t) - \mathbf{1}) \times \int_0^h G(s)\, ds &= \int_t^{t+h} G(s)\, ds - \int_0^h G(s)\, ds \\ &= \int_t^h G(s)\, ds + \int_h^{t+h} G(s)\, ds - \int_0^t G(s)\, ds - \int_t^h G(s)\, ds \\ &= \int_h^{t+h} G(s)\, ds - \int_0^t G(s)\, ds \\ &= (G(h) - \mathbf{1}) \times \int_0^t G(s)\, ds.\end{aligned}$$

Set

$$X = X(h) = \int_0^h G(s)\, ds.$$

Fix $0 \neq |h|$ small enough so that, by norm continuity of $G(t)$,

$$\begin{aligned}\left\| \frac{1}{h} X - \mathbf{1} \right\| &= \left\| \frac{1}{h} \int_0^h G(s)\, ds - \frac{1}{h} \int_0^h \mathbf{1}\, ds \right\| \\ &= \left\| \frac{1}{h} \int_0^h (G(s) - \mathbf{1})\, ds \right\| \leq \sup_{|s| \leq |h|} \|G(s) - \mathbf{1}\| < 1.\end{aligned}$$

Hence for such h it follows that X^{-1} is well defined and belongs to $\mathrm{B}(\mathcal{H})$ (see Exercise 1.1.24).

So, after composition with X^{-1} in the above relation, one gets (since all operators in question commute)

$$i(G(t) - \mathbf{1}) = Y \int_0^t G(s)\, ds,$$

where $Y := i(G(h) - \mathbf{1})X^{-1} \in \mathrm{B}(\mathcal{H})$. Therefore $G(t)$ is norm differentiable and

$$i \frac{d}{dt} G(t) = Y G(t), \qquad G(0) = \mathbf{1},$$

whose unique solution is $G(t) = e^{-itY}$. In fact, one explicitly finds

$$\frac{d}{dt} \left(G(t) e^{itY} \right) = 0, \qquad \forall t \in \mathbb{R},$$

so that $G(t)e^{itY} = \text{cte}$ and, together with $G(0) = \mathbf{1}$, it necessarily follows that $G(t) = e^{-itY}$. Note that both ii) and iii) were obtained and Y is the infinitesimal generator of $G(t)$. Since ii) follows by iii), Y equals the operator T in ii) and the last assertion of the theorem is also valid. □

Therefore, if the infinitesimal generator of the unitary evolution group $G(t)$ is unbounded, then at most strong continuity is possible for $t \mapsto G(t)$. Such possibility will be discussed in the next section. This complements the results in Proposition 5.1.7.

Exercise 5.2.4. Provide the details of the proofs that iii) ⇒ ii) ⇒ i) and iii) ⇒ i) in Theorem 5.2.3.

Exercise 5.2.5. From $G(t) - \mathbf{1} = -iY \int_0^t G(s)\, ds$, $T \in \mathrm{B}(\mathcal{H})$, in the proof of Theorem 5.2.3, use iteration under the integral sign to check that $G(t) = e^{-itY}$.

Exercise 5.2.6. Let T, S be bounded operators and Q a bounded operator so that $QT = SQ$. Show that $Q = e^{zS} Q e^{-zT}$ for all $z \in \mathbb{C}$.

5.3 Stone Theorem

Often a self-adjoint operator $T : \operatorname{dom} T \sqsubseteq \mathcal{H} \to \mathcal{H}$ is given and one tries to construct a unitary evolution group for which T is its infinitesimal generator. This is a common situation in quantum mechanics.

Theorem 5.3.1. *If T is self-adjoint, there exists a strongly continuous unitary evolution group $U(t)$ for which T is its infinitesimal generator. In this case one writes $U(t) = e^{-itT}$, $t \in \mathbb{R}$.*

Remark 5.3.2. The proof of Theorem 5.3.1 will be postponed until after the discussion of the spectral theorem (see Section 9.2). An alternative proof which does not use the spectral theorem can be found in [Am81]. Based on Theorem 5.2.3 and Example 5.1.6, given a self-adjoint operator T one could try to construct a unitary evolution group through the series

$$e^{-itT} = \sum_{j=0}^{\infty} \frac{1}{j!} (-itT)^j.$$

However, unlike the case of bounded T, it would make sense only for vectors in $\cap_n \operatorname{dom} T^n$, a not simple set to control; see, however, Section 9.9. So, for unitary evolution groups, the difference between norm continuity and strong continuity has very important consequences.

The converse of Theorem 5.3.1 is the well-known Stone theorem.

Theorem 5.3.3 (Stone). *If $U(t)$ is a measurable unitary evolution group on $\mathcal{H}$, then its infinitesimal generator T is self-adjoint, that is, $U(t) = e^{-itT}$ (and hence $\operatorname{dom} T \sqsubseteq \mathcal{H}$).*

Proof. By Proposition 5.1.7, $t \mapsto U(t)$ is strongly continuous. The domain $\operatorname{dom} T$ of its infinitesimal generator T is nonempty since the null vector belongs to it. The proof will be split into three parts, as follows:

1. $\operatorname{dom} T$ is dense in $\mathcal{H}$.
2. T is essentially self-adjoint.
3. $T = \overline{T}$ and so self-adjoint.

• For each $\eta \in \mathcal{H}$ and $f \in C_0^\infty(\mathbb{R})$ the map $\mathbb{R} \ni t \mapsto f(t)U(t)\eta$ is measurable and integrable. If $\eta_f := \int_{\mathbb{R}} f(t)U(t)\eta \, dt$, then

$$\begin{aligned}\frac{1}{h}(U(h) - \mathbf{1})\eta_f &= \frac{1}{h} \int_{\mathbb{R}} [f(t)U(t+h) - f(t)U(t)]\, \eta \, dt \\ &= \int_{\mathbb{R}} \frac{f(t-h) - f(t)}{h} U(t)\eta \, dt \stackrel{h\to 0}{\longrightarrow} -\int_{\mathbb{R}} f'(t)U(t)\eta \, dt.\end{aligned}$$

In the last passage the dominated convergence theorem was invoked. This shows that $\eta_f \in \operatorname{dom} T$ for all $f \in C_0^\infty(\mathbb{R})$, $\eta \in \mathcal{H}$.

Since $U(t)$ is strongly continuous, given $\varepsilon > 0$ there exists $\delta > 0$ with $\sup_{t\in[-\delta,\delta]} \|\eta - U(t)\eta\| < \varepsilon$, and for a positive $g \in C_0^\infty(\mathbb{R})$ with support in $[-\delta, \delta]$ and $\int_{\mathbb{R}} g(t)\,dt = 1$, one has

$$\begin{aligned}\|\eta - \eta_g\| &= \left\| \int_{[-\delta,\delta]} g(t)[\eta - U(t)\eta]\,dt \right\| \\ &\le \sup_{t\in[-\delta,\delta]} \|\eta - U(t)\eta\| < \varepsilon.\end{aligned}$$

Hence, dom T is dense in $\mathcal{H}$.

• By Proposition 5.1.3, T is known to be symmetric and, since its domain is dense in $\mathcal{H}$, T is hermitian. It will be checked that $n_-(T) = n_+(T) = 0$, so that T is essentially self-adjoint.

Let $\eta \in \mathrm{K}_+(T) = \mathrm{N}(T^* + i\mathbf{1})$. Then, $\eta \in \operatorname{dom} T^*$ and, for all $\xi \in \operatorname{dom} T$,

$$\frac{d}{dt}\langle U(t)\xi, \eta\rangle = \langle -iTU(t)\xi, \eta\rangle = i\langle U(t)\xi, T^*\eta\rangle = \langle U(t)\xi, \eta\rangle.$$

The unique solution of this differential equation with initial condition $\langle \xi, \eta\rangle$ at $t = 0$ is

$$\langle U(t)\xi, \eta\rangle = e^t\langle \xi, \eta\rangle, \qquad t \in \mathbb{R},$$

and since the left-hand side is bounded we find that $\langle \xi, \eta\rangle = 0$, $\forall \xi \in \operatorname{dom} T$. Due to the density of dom T in $\mathcal{H}$, it follows that $\eta = 0$ and so $n_+ = 0$. Similarly one gets $n_- = 0$.

• Let $\overline{T}$ be the closure of T, which coincides with its unique self-adjoint extension. By Theorem 5.3.1, $\overline{T}$ is the (unique) infinitesimal generator of a strongly continuous unitary evolution group $G(t) := e^{-it\overline{T}}$. It will be shown that $U(t) = G(t)$, $\forall t$, so that necessarily $T = \overline{T}$.

Since $U(t)$ and $G(t)$ are unitary operators, we only need to show that $U(t)\xi = G(t)\xi$ for all ξ in the dense set dom $T \subset$ dom $\overline{T}$. For such vectors both $U(t)\xi$ and $G(t)\xi$ are strongly differentiable and if one denotes

$$\phi(t) = U(t)\xi - G(t)\xi,$$

then, in view of $U(t)\operatorname{dom} T = \operatorname{dom} T$, one has $d\phi/dt = -i\overline{T}\phi(t)$, and $\overline{T}$ being self-adjoint,

$$\frac{d}{dt}\|\phi(t)\|^2 = 2\mathrm{Re}\,\langle -i\overline{T}\phi(t), \phi(t)\rangle = 0, \qquad \forall t.$$

Thus, $\|\phi(t)\|$ is a constant function and equal to $\|\phi(0)\| = 0$. Therefore, $U(t) = G(t)$, $\forall t$. Thereby the proof is complete. □

Corollary 5.3.4. *Let T be self-adjoint and the infinitesimal generator of the unitary evolution group $U(t)$. If $\mathcal{D} \sqsubseteq$ dom T with $U(t)\mathcal{D} \subset \mathcal{D}$, $\forall t \in \mathbb{R}$, then $\mathcal{D}$ is a core of T.*

Exercise 5.3.5. Prove Corollary 5.3.4. Note that it is a consequence of the proof of Theorem 5.3.3.

Exercise 5.3.6. If $G(t)$ and $F(t)$ are strongly continuous unitary evolution groups on $\mathcal{H}$ and there exists $\varepsilon > 0$ so that $G(t) = F(t)$ for $-\varepsilon < t < \varepsilon$, show that $G(t) = F(t)$, $\forall t$.

Exercise 5.3.7. The map $\mathbb{R} \ni t \mapsto G(t)$ is a *contraction evolution group* on $\mathcal{H}$ if $G(t)G(s) = G(t+s)$, $\forall s, t \in \mathbb{R}$, $G(0) = \mathbf{1}$ and $\|G(t)\| \le 1$, $\forall t$. Show that if $G(t)$ is a contraction evolution group, then it is in fact a unitary evolution group.

Remark 5.3.8. It follows, by the results of this section, that in a Hilbert space there is a one-to-one correspondence between the set of measurable (so strongly continuous) unitary evolution groups and self-adjoint operators. This is another motivation for the abstract study of self-adjoint operators.

Proposition 5.3.9. *Let T be self-adjoint, $U(t) = e^{-itT}$, E a closed vector subspace of $\mathcal{H}$ and P_E the subsequent orthogonal projection. If $U(t)E \subset E$, $\forall t$, then*

a) $U(t)E = E,\ U(t)E^\perp = E^\perp, \qquad \forall t.$
b) $P_E U(t) = U(t) P_E$, *$\forall t$, and $P_E T \subset T P_E$. (If the latter holds one says that E reduces T or that E is a reducing subspace for T; see Section* 9.8.)

Proof. Apply $U(-t)$ to $U(t)E \subset E$, $\forall t$, to show that $U(t)E = E$, $\forall t$. If $\eta \in E^\perp$, then for all $\xi \in E$,

$$\langle U(t)\eta, \xi\rangle = \langle \eta, U(-t)\xi\rangle = 0,$$

and so $U(t)E^\perp \subset E^\perp \Rightarrow U(t)E^\perp = E^\perp$, and a) is verified. Note that such relations also show that $P_E U(t) = U(t) P_E$, $\forall t$.

Now, for $\xi \in \operatorname{dom} T$,

$$P_E T\xi = P_E \lim_{h\to 0} \frac{i}{h}(U(h)\xi - \xi) = \lim_{h\to 0} \frac{i}{h}(U(h)P_E\xi - P_E\xi),$$

which shows that $P_E\xi \in \operatorname{dom} T$ and $P_E T\xi = T P_E \xi$; in other symbols, $P_E T \subset T P_E$. The proof of b) is complete. □

Exercise 5.3.10. Let $G(t)$ be a strongly continuous unitary evolution group on $\mathcal{H}$. For $\xi \in \mathcal{H}$ show that the function

$$\mathbb{R} \ni t \longmapsto f(t) = \langle \xi, G(t)\xi\rangle \in \mathbb{C},$$

is *positive definite*, i.e., $f(t)$ is continuous, $f(-t) = \overline{f(t)}$ and for all $\{t_1, \ldots, t_n\} \subset \mathbb{R}$ and $\{c_1, \ldots, c_n\} \subset \mathbb{C}$,

$$\sum_{k,j=1}^{n} f(t_j - t_k)\, c_j \overline{c_k} \ge 0.$$

5.4 Examples

Example 5.4.1. [Schrödinger equation] This equation gives the quantum dynamics of a system in a Hilbert space $\mathcal{H}$. If the energy observable is represented by the (usually unbounded) self-adjoint operator H, the so-called Schrödinger operator (or hamiltonian operator), then the corresponding Schrödinger equation is the following first-order (with respect to time t) linear differential equation

$$i\frac{d}{dt}\xi(t) = H\xi(t), \qquad \xi(0) = \xi \in \operatorname{dom} H.$$

Previous results show that for $\xi \in \operatorname{dom} H$, the unique solution of this equation is $U(t)\xi = e^{-itH}\xi$, i.e., it is ruled by a strongly continuous unitary evolution group whose infinitesimal generator is H.

Note that since $e^{-itH}\operatorname{dom} H = \operatorname{dom} H$, $\forall t$, this solution is global, in the sense that it is defined for all $t \in \mathbb{R}$. So, in contrast to classical mechanics, the quantum time evolution is globally defined as soon as it exists, which corresponds to the self-adjointness of the associated energy operator H. Since e^{-itH} is unitary, even for $\eta \notin \operatorname{dom} H$ the time evolution $\eta(t) = e^{-itH}\eta$ is still defined, although not differentiable; in this case it is said that $\eta(t)$ is a *weak solution* of the Schrödinger equation.

Remark 5.4.2. If H is self-adjoint and represents the energy of a quantum system, i.e., a Schrödinger operator, then the time evolution is ruled by $U(t) = e^{-itH}$. If $\xi \in \operatorname{dom} H$, then the relation

$$\langle U(t)\xi, HU(t)\xi\rangle = \langle U(t)\xi, U(t)H\xi\rangle = \langle \xi, H\xi\rangle, \qquad \forall t \in \mathbb{R},$$

is interpreted as the conservation of energy in quantum mechanics. More precisely, such relation shows that the *expectation value* $\mathcal{E}^{\xi}_{H}(t) := \langle \xi(t), H\xi(t)\rangle$ of H in the state $\xi(t) = e^{-itH}\xi$ is a constant function of time.

Exercise 5.4.3. Let H be the quantum energy operator in $\mathcal{H}$ and $A \in \mathrm{B}(\mathcal{H})$ self-adjoint representing a physical observable. If

$$e^{-itH}A = Ae^{-itH}, \qquad \forall t \in \mathbb{R},$$

check that the expectation value

$$\mathcal{E}^{\xi}_{A}(t) = \left\langle e^{-itH}\xi, Ae^{-itH}\xi\right\rangle$$

is conserved, i.e., it does not depend on time t so that $\mathcal{E}^{\xi}_{A}(t) = \mathcal{E}^{\xi}_{A}(0)$. How can we adapt such a "conservation law" to observables represented by unbounded self-adjoint operators?

An additional word on physical interpretations: the expectation value $\mathcal{E}^{\xi}_{A}(t)$, introduced in Exercise 5.4.3, is the result obtained by averaging out over a large number of measurements of the observable A at time t in identical systems, each one prepared in the initial *quantum state* $\xi \in \mathcal{H}$ at $t = 0$. Quantum states are assumed normalized, i.e., $\|\xi\| = 1$. Finally, the Schrödinger equation with explicit Planck constant $\hbar$ reads

$$i\hbar \frac{d}{dt}\xi(t) = H\xi(t),$$

so that the unitary evolution group is $e^{-itH/\hbar}$.

In many situations a one-parameter unitary group is naturally associated with space transformations, as translations in $\mathbb{R}$. The next examples illustrate this.

Example 5.4.4 (Spatial translations). Let $\mathcal{H} = \mathrm{L}^2(\mathbb{R})$ and, for $s \in \mathbb{R}$,

$$(G(s)\psi)(x) := \psi(x - s), \qquad \psi \in \mathcal{H}.$$

Then $G(s)$ is a strongly continuous unitary evolution group whose infinitesimal generator is the momentum operator

$$P : \mathrm{dom}\, P = \mathcal{H}^1(\mathbb{R}) \to \mathcal{H}, \qquad P\psi = -i\psi',$$

discussed in Section 3.3 (see also Examples 2.3.11 and 2.4.10).

Proof. First note that $G(s)$ is clearly a unitary evolution group (Lebesgue measure is invariant under translations). If $\psi, \phi \in C_0^\infty(\mathbb{R})$ one has, by dominated convergence,

$$\langle G(h)\psi, \phi\rangle = \int_{\mathbb{R}} \overline{\psi(x - h)}\, \phi(x)\, dx \stackrel{h\to 0}{\longrightarrow} \langle \psi, \phi\rangle.$$

Since $C_0^\infty(\mathbb{R}) \sqsubseteq \mathcal{H}$, it follows that

$$\mathrm{w} - \lim_{h\to 0} G(h) = \mathbf{1}.$$

By Proposition 5.1.7, $G(s)$ is strongly continuous (another argument can be found in the proof of Lemma 13.3.2).

Let T be the (self-adjoint) infinitesimal generator of $G(s)$. Thus, for $\psi \in C_0^\infty(\mathbb{R})$,

$$\frac{i}{h}(G(h) - \mathbf{1})\psi(x) = \frac{i}{h}(\psi(x-h) - \psi(x)) = -\frac{i}{h}\int_{x-h}^{x} \psi'(s)\, ds,$$

and if $h > 0$ (similarly for $h < 0$),

$$\left| i\frac{G(h) - \mathbf{1}}{h}\psi(x) + i\psi'(x)\right| \le \frac{1}{h}\int_{x-h}^{x} |\psi'(x) - \psi'(s)|\, ds$$

and since ψ' is continuous with compact support, it is uniformly continuous and so

$$\frac{1}{h}\int_{x-h}^{x} |\psi'(x) - \psi'(s)|\, ds \le \sup_{s\in[x-h,x]} |\psi'(x) - \psi'(s)| \stackrel{h\to 0}{\longrightarrow} 0.$$

Thus,

$$T|_{C_0^\infty} = P|_{C_0^\infty} ,$$

and since $C_0^\infty(\mathbb{R})$ is a core of P, it follows that $T = P$. □

Remark 5.4.5. The following formal derivation is instructive. By Taylor series around $s = 0$,

$$\begin{aligned}\psi(x-s) &= \psi(x) - s\psi'(x) + \frac{s^2}{2}\psi''(x) - \frac{s^3}{3!}\psi'''(x) + \cdots \\ &= \left(\mathbf{1} + s\left(-\frac{d}{dx}\right) + \frac{s^2}{2}\left(-\frac{d}{dx}\right)^2 + \frac{s^3}{3!}\left(-\frac{d}{dx}\right)^3 + \cdots\right)\psi(x) \\ &= \exp\left(-s\frac{d}{dx}\right)\psi(x) = \exp\left(-isP\right)\psi(x),\end{aligned}$$

and the momentum operator has appeared.

Exercise 5.4.6. Let P be the momentum operator in $\mathrm{L}^2(\mathbb{R})$. For $\phi \in C_0^\infty(\mathbb{R})$, verify that the Schrödinger equation with momentum P playing the role of "energy operator", that is, if $G(t) = e^{-itP}$,

$$i\frac{d}{dt}(G(t)\psi)(x) = P(G(t)\psi)(x),$$

is just a manifestation of the chain rule:

$$i\frac{d}{dt}\psi(x-t) = P\psi(x-t) = -i\frac{d}{dx}\psi(x-t).$$

Remark 5.4.7. Due to Example 5.4.4, it is often said that "the momentum operator generates translations in $\mathbb{R}$." With natural adaptations to different directions in $\mathbb{R}^n$. See also Exercise 5.5.9.

With such interpretation one can intuitively understand the self-adjoint extensions of the momentum operator P in different types of intervals, that is, the whole line $\mathbb{R}$, finite interval (say, $[0,1]$) and half-line (say, $[0,\infty)$). Such extensions are discussed in Chapter 2.

Since it is possible to translate wave functions ψ to both sides in $\mathbb{R}$, the generator of translations is well posed and so P is essentially self-adjoint. In case of the bounded interval, one can translate wave functions up to to an end when they "enter" at the other end with a possible fixed different phase $\psi(0) = e^{i\theta}\psi(1)$; each phase $e^{i\theta}$ corresponds to a distinct type of translation and so to a different self-adjoint extension of P, and there are infinitely many of them. For the half-line, it is possible to freely translate wave functions to the right, however what reaches the origin is not able to enter at the other end, since it is infinity; thus, the translations are ill posed in this case and consequently the momentum can not be realized as a self-adjoint operator.

Example 5.4.8 (Dilations). Let $\mathcal{H} = \mathrm{L}^2(\mathbb{R})$. The dilation on $\mathbb{R}$ is the map $x \mapsto e^{-s}x$, $s \in \mathbb{R}$, which induces the operator $U_d(s) : \mathcal{H} \to \mathcal{H}$,

$$(U_d(s)\psi)(x) := e^{-s/2}\psi(e^{-s}x), \qquad \psi \in \mathcal{H}.$$

$U_d(s)$ is a change of scale since x is multiplied by e^{-s}; the factor $e^{-s/2}$ is just to preserve the norm. $U_d(s)$ is a strongly continuous unitary evolution group, $C_0^\infty(\mathbb{R})$ is a core of its infinitesimal generator T_d and, for $\phi \in C_0^\infty(\mathbb{R})$,

$$(T_d\phi)(x) = \frac{1}{2}(xp + px)\phi(x) = \left(xp - \frac{i}{2}\right)\phi(x), \qquad p = -i\frac{d}{dx}.$$

The same conclusions hold if $C_0^\infty(\mathbb{R})$ is replaced by $\mathcal{S}(\mathbb{R})$. The version of the group of dilations in $\mathbb{R}^n$ is given by $(U_d(s)\psi)(x) := e^{-ns/2}\psi(e^{-s}x)$, $s \in \mathbb{R}$ and $\psi \in \mathrm{L}^2(\mathbb{R}^n)$.

Proof. Again it is a simple exercise to check that $U_d(s)$ is a unitary evolution group. If $\phi \in C_0^\infty(\mathbb{R})$ one has

$$\langle \phi, U_d(h)\phi\rangle = \int_{\mathbb{R}} \overline{\phi(x)}\, e^{-h/2}\phi(e^{-h}x)\, dx.$$

If $|h| \le 2$, then $|\overline{\phi(x)}\, e^{-h/2}\phi(e^{-h}x)| \le e\,\|\phi\|_\infty\, |\phi(x)| \in \mathrm{L}^1(\mathbb{R})$ and, by dominated convergence,

$$\langle \phi, U_d(h)\phi\rangle \stackrel{h\to 0}{\longrightarrow} \langle \phi, \phi\rangle.$$

Being that $C_0^\infty(\mathbb{R})$ is dense in $\mathcal{H}$, such convergence is valid for every element of $\mathcal{H}$. By polarization,

$$\langle \psi, U_d(h)\phi\rangle \stackrel{h\to 0}{\longrightarrow} \langle \psi, \phi\rangle, \qquad \forall \psi, \phi \in \mathcal{H},$$

and $U_d(s)$ is weakly continuous. If T_d is its (self-adjoint) infinitesimal generator, then for $\phi \in C_0^\infty(\mathbb{R})$ one has the pointwise convergence

$$\begin{aligned}
\frac{i}{s}(U_d(s) - \mathbf{1})\phi(x) &= i\left(\frac{e^{-s/2}\phi(e^{-s}x) - \phi(x)}{s}\right) \\
&\stackrel{s\to 0}{\longrightarrow} i\frac{d}{ds}(e^{-s/2}\phi(e^{-s}x))\Big|_{s=0}. \\
&= i\left(-\frac{1}{2}e^{-s/2}\phi(e^{-s}x) - e^{-s/2}e^{-s}x\,\phi'(e^{-s}x)\right)\Big|_{s=0}. \\
&= \left(\frac{-i}{2}\phi(x) + xp\phi(x)\right) = \left(xp - \frac{i}{2}\right)\phi(x),
\end{aligned}$$

with $p\phi = -i\phi'$. Again by dominated convergence, the above pointwise limit can be translated into $\mathrm{L}^2(\mathbb{R})$; then $C_0^\infty(\mathbb{R}) \subset \mathrm{dom}\, T_d$ and since for $\phi \in C_0^\infty(\mathbb{R})$ one has $xp\phi(x) - px\phi(x) = i\phi(x)$, it is found that

$$(T_d\phi)(x) = \frac{1}{2}(xp + px)\phi(x).$$

Finally, since $U_d(s)C_0^\infty(\mathbb{R}) \subset C_0^\infty(\mathbb{R})$, $\forall s \in \mathbb{R}$, by Corollary 5.3.4 it follows that $C_0^\infty(\mathbb{R})$ is a core of T_d. □

Exercise 5.4.9 (Rotation). If $(x, y) \in \mathbb{R}^2$, the rotation $(x, y) \mapsto (x_\theta, y_\theta)$, $x_\theta = x\cos\theta - y\sin\theta$, $y_\theta = x\sin\theta + y\cos\theta$, induces the operator

$$U_R(\theta) : \mathrm{L}^2(\mathbb{R}^2) \hookleftarrow, \qquad (U_R(\theta)\psi)(x, y) := \psi(x_\theta, y_\theta).$$

Show that $U_R(\theta)$, $\theta \in \mathbb{R}$, is a strongly continuous unitary evolution group, $C_0^\infty(\mathbb{R}^2)$ is a core of its infinitesimal generator T_R and for $\phi \in C_0^\infty(\mathbb{R})$ one has

$$(T_R\phi)(x, y) = (xp_y - yp_x)\phi(x, y), \qquad p_x = -i\frac{d}{dx},\ p_y = -i\frac{d}{dy}.$$

T_R is identified with the z-component of the angular momentum, and so it is often said that "the angular momentum generates rotations."

Example 5.4.10. Let T be a self-adjoint operator with an orthonormal basis $(\xi_j)_{j\geq 1}$ of $\mathcal{H}$ constituted of eigenvectors $T\xi_j = \lambda_j\xi_j$. Every vector of $\mathcal{H}$ can be written in the form $\xi = \sum_{j\geq 1} a_j\xi_j$, with $\sum_j |a_j|^2 = \|\xi\|^2 < \infty$. The vector $\xi \in \operatorname{dom} T$ iff $\sum_j \lambda_j^2 |a_j|^2 < \infty$ and in this case $T\xi = \sum_{j\geq 1} \lambda_j a_j\xi_j$. The claim is that the unitary evolution group $U(t) = e^{-itT}$ is given by

$$e^{-itT}\xi = \sum_{j\geq 1} e^{-it\lambda_j} a_j\xi_j, \qquad \forall \xi \in \mathcal{H}.$$

Actually, define $G(t)\xi := \sum_{j\geq 1} e^{-it\lambda_j} a_j\xi_j$, which is a strongly continuous unitary evolution group; in fact, $\langle \xi, G(t)\xi\rangle = \lim_{N\to\infty} \sum_{j=1}^N e^{-it\lambda_j} |a_j|^2$ is measurable, since it is the limit of a sequence of continuous functions; by polarization it follows that $t \mapsto G(t)$ is measurable. Let S be its self-adjoint infinitesimal generator and $X = \mathrm{Lin}(\{\xi_j\}_j)$, which is dense in $\mathcal{H}$. For each j one has $G(t)\xi_j = e^{-it\lambda_j}\xi_j$, which is differentiable and

$$S\xi_j = i\frac{d}{dt}G(t)\xi_j\bigg|_{t=0} = \lambda_j\xi_j = T\xi_j,$$

so that $S\xi_j = T\xi_j$, $\forall j$. So, for $X \ni \xi = \sum_{j=1}^N a_j\xi_j$, one has $S\xi = T\xi$. Since $G(t)X \subset X$, it follows that X is a core of S, and, by self-adjointness, $T = S$. Therefore, both unitary evolution groups have the same infinitesimal generator and so coincide, that is, $G(t) = U(t)$, for all $t \in \mathbb{R}$.

Example 5.4.11 (Projection as infinitesimal generator). Let E be a closed subspace of $\mathcal{H}$ and P_E the orthogonal projection onto E. Then

$$G(t) := P_{E^\perp} + e^{-it}P_E$$

is a unitary evolution group, whose infinitesimal generator is P_E. In fact, since P_E is self-adjoint it is the infinitesimal generator of the strongly continuous unitary evolution group e^{-itP_E}. Taking into account that $P_E^2 = P_E$ and P_E is bounded, Theorem 5.2.3 implies that

$$e^{-itP_E} = \sum_{j=0}^{\infty} \frac{(-itP_E)^j}{j!} = \mathbf{1} + \left(\sum_{j=1}^{\infty} \frac{(-it)^j}{j!} \right) P_E$$
$$= \mathbf{1} + \left(-1 + e^{-it}\right) P_E = G(t), \qquad \forall t \in \mathbb{R}.$$

Note that the trajectory $t \mapsto G(t)\xi$ is periodic for all $\xi \in \mathcal{H}$.

Exercise 5.4.12. Use the action of $G(t)$ in Example 5.4.11 to check that it is a norm continuous unitary evolution group and P_E is its infinitesimal generator.

Exercise 5.4.13. Let $G(t) : l^2(\mathbb{N}) \to l^2(\mathbb{N})$, defined by

$$G(t)\left(\xi_1, \xi_2, \xi_3, \dots\right) := \left(e^{-it}\xi_1, e^{-i2t}\xi_2, e^{-i3t}\xi_3, \dots\right).$$

Verify that $G(t)$ is a strongly continuous unitary evolution group, but it is not norm continuous. Find its infinitesimal generator.

Exercise 5.4.14. Let $\mathcal{H} = \mathrm{L}^2[0,1]$ and for $s \in \mathbb{R}$ define $G(s) : \mathcal{H} \hookleftarrow$ given by $G(s)\psi(x) = \psi(x-s)$, with $(x-s)$ understood mod 1. Show that $G(s)$ is a strongly continuous unitary group and find its infinitesimal generator.

Exercise 5.4.15. Let $G(t)$ be a measurable unitary evolution group on $\mathcal{H}$ and T its infinitesimal generator. If W is a unitary operator on $\mathcal{H}$ with $G(t)W = WG(t)$, $\forall t \in \mathbb{R}$, show that $W\mathrm{dom}\; T \subset \mathrm{dom}\; T$ and

$$WT\xi = TW\xi, \qquad \forall \xi \in \mathrm{dom}\; T.$$

What can we conclude in case $W = G(s)$?

Exercise 5.4.16. Let $G(t)$ and $U(t)$ be two measurable unitary evolution groups on $\mathcal{H}$, and T, A their infinitesimal generators, respectively. Based on Exercises 5.4.15 and 5.4.3, if

$$U(t)G(s) = G(s)U(t), \qquad \forall s, t \in \mathbb{R},$$

discuss possible relations between T and A.

5.5 Free Quantum Dynamics

By Example 5.1.6, the map $t \mapsto e^{-itp^2}$ is a strong continuous unitary evolution group on $\mathrm{L}^2(\hat{\mathbb{R}}^n)$, i.e., in momentum representation, whose infinitesimal generator is the multiplication operator by p^2. Since $H_0 = \mathcal{F}^{-1}p^2\mathcal{F}$ (see Section 3.4), one has

$$e^{-itH_0} = \mathcal{F}^{-1}e^{-itp^2}\mathcal{F},$$

which is a unitary evolution group on $\mathrm{L}^2(\mathbb{R}^n)$, called a *free evolution group*, whose infinitesimal generator is the free hamiltonian H_0.

In this subsection the free unitary evolution group e^{-itH_0} will be computed in position representation $\mathrm{L}^2(\mathbb{R}^n)$. Then some consequences on quantum free dynamics are derived.

Theorem 5.5.1. *If* $\psi \in \mathrm{L}^1(\mathbb{R}^n) \cap \mathrm{L}^2(\mathbb{R}^n)$, *then*

$$\left(e^{-itH_0}\psi\right)(x) = \frac{1}{(4\pi it)^{\frac{n}{2}}} \int_{\mathbb{R}^n} e^{i\frac{(x-y)^2}{4t}}\, \psi(y)\, dy, \qquad t \neq 0.$$

The branch of the square root $(4\pi it)^{\frac{1}{2}}$ *is chosen so that its real part is positive.*

Proof. The proof will be done for $n = 1$; the general case is similar. Since $e^{-itH_0} = \mathcal{F}^{-1}e^{-itp^2}\mathcal{F}$, if $\hat{\psi} \in \mathrm{L}^1(\hat{\mathbb{R}})$ one has

$$\left(e^{-itH_0}\psi\right)(x) = \frac{1}{(2\pi)^{\frac{1}{2}}} \int_{\mathbb{R}} e^{i\,xp}e^{-ip^2t}\, \hat{\psi}(p)\, dp.$$

However, if $\psi \in \mathrm{L}^2(\mathbb{R})$, then for any $\varepsilon > 0$ the function $p \mapsto e^{-\varepsilon p^2}\hat{\psi}(p)$ belongs to $\mathrm{L}^1(\hat{\mathbb{R}})$, and since $e^{-i(t-i\varepsilon)H_0} = \mathcal{F}^{-1}e^{-i(t-i\varepsilon)p^2}\mathcal{F}$ one has, for any $\psi \in \mathrm{L}^2(\mathbb{R})$,

$$\left(e^{-i(t-i\varepsilon)H_0}\psi\right)(x) = \frac{1}{(2\pi)^{\frac{1}{2}}} \int_{\mathbb{R}} e^{i\,xp}e^{-ip^2t}e^{-\varepsilon p^2}\, \hat{\psi}(p)\, dp.$$

In case $\psi \in \mathrm{L}^2(\mathbb{R}) \cap \mathrm{L}^1(\mathbb{R})$, write out the expression of the Fourier transform $\hat{\psi}(p)$ and apply Fubini to get

$$\begin{aligned}
\left(e^{-i(t-i\varepsilon)H_0}\psi\right)(x) &= \frac{1}{2\pi} \int_{\mathbb{R}} \int_{\mathbb{R}} e^{-ip(y-x)}e^{-p^2(it+\varepsilon)}\psi(y)\, dp\, dy \\
&= \frac{1}{(2\pi)^{\frac{1}{2}}} \int_{\mathbb{R}} \mathcal{F}\left(e^{-p^2(it+\varepsilon)}\right)(y-x)\, \psi(y)\, dy \\
&= \frac{1}{(2\pi)^{\frac{1}{2}}} \frac{1}{(2(it+\varepsilon))^{\frac{1}{2}}} \int_{\mathbb{R}} \exp\left(-\frac{(x-y)^2}{4(it+\varepsilon)}\right)\, \psi(y)\, dy.
\end{aligned}$$

The idea now is to take $\varepsilon \to 0^+$. Note first that for any $\psi \in \mathrm{L}^2(\mathbb{R})$ one has the convergence in $\mathrm{L}^2(\mathbb{R})$

$$\begin{aligned}
\left\| e^{-(it+\varepsilon)H_0}\psi - e^{-itH_0}\psi \right\|_2^2 &= \left\| \mathcal{F}\left(e^{-(it+\varepsilon)H_0}\psi - e^{-itH_0}\psi\right)\right\|_2^2 \\
&= \int_{\mathbb{R}} \left|e^{-\varepsilon p^2} - 1\right|^2 \left|\hat{\psi}(p)\right|^2\, dp \longrightarrow 0
\end{aligned}$$

as $\varepsilon \to 0^+$ by dominated convergence. Then there is a subsequence $\varepsilon_j \to 0^+$ so that the convergence is Lebesgue a.e.; note that this convergence is uniform in t.

For $\psi \in \mathrm{L}^2(\mathbb{R}) \cap \mathrm{L}^1(\mathbb{R})$, use the above expression and dominated convergence again, to get

$$\left(e^{-itH_0}\psi\right)(x) = \lim_{\varepsilon_j \to 0^+} \left(e^{-i(t-i\varepsilon_j)H_0}\psi\right)(x) = \frac{1}{(4\pi i t)^{\frac{1}{2}}} \int_{\mathbb{R}} \exp\left(i\frac{(x-y)^2}{4t}\right) \psi(y)\, dy,$$

and the theorem is proven. □

Corollary 5.5.2. *If* $\psi \in \mathrm{L}^2(\mathbb{R}^n)$, *then*

$$\left(e^{-itH_0}\psi\right)(x) = \text{l.i.m.}\, \frac{1}{(4\pi i t)^{\frac{n}{2}}} \int_{\mathbb{R}^n} e^{i\frac{(x-y)^2}{4t}}\, \psi(y)\, dy, \qquad t \neq 0.$$

Exercise 5.5.3. With respect to the expression for the free unitary evolution group in position representation, verify that $(4\pi i t)^{\frac{n}{2}} = ((4\pi i t)^{\frac{1}{2}})^n$ equals

$$|4\pi i t|^{\frac{n}{2}}\, e^{in\pi/4}, \qquad |4\pi i t|^{\frac{n}{2}}\, e^{-in\pi/4},$$

if $t > 0$ and $t < 0$, respectively.

Definition 5.5.4. The function

$$x \mapsto K_t(x) := \frac{1}{(4\pi i t)^{\frac{n}{2}}}\, e^{i\frac{x^2}{4t}}$$

is called the *free propagator kernel* in $\mathrm{L}^2(\mathbb{R}^n)$.

Note that the free unitary evolution group can be written as

$$\left(e^{-itH_0}\psi\right)(x) = (K_t * \psi)(x) = \text{l.i.m.} \int_{\mathbb{R}^n} K_t(x-y)\, \psi(y)\, dy,$$

that is, it is an integral operator whose kernel is the free propagator.

The following result is also a direct consequence of Theorem 5.5.1.

Corollary 5.5.5. *Let* $\psi \in \mathrm{L}^1(\mathbb{R}^n) \cap \mathrm{L}^2(\mathbb{R}^n)$. *Then, for each* $0 \neq t \in \mathbb{R}$, *one has*

$$\left|\left(e^{-itH_0}\psi\right)(x)\right| \leq \frac{1}{|4\pi t|^{\frac{n}{2}}}\, \|\psi\|_1, \qquad \text{a.e. } x \in \mathbb{R}^n.$$

For $\psi \in \mathrm{L}^1(\mathbb{R}^n) \cap \mathrm{L}^2(\mathbb{R}^n)$ this corollary implies that, in a set of points $x \in \mathbb{R}^n$ of full Lebesgue measure, $\left|(e^{-itH_0}\psi)(x)\right|$ vanishes uniformly as $t \to \pm\infty$.

According to quantum mechanics (as proposed by Max Born), if H is the hamiltonian operator of a particle acting in $\mathrm{L}^2(\mathbb{R}^n)$, given a bounded measurable set $\Lambda \subset \mathbb{R}^n$, if the initial state of the system is ψ, then the probability of finding the particle in Λ at time t is

$$\mathrm{Prob}_{\psi(t)}(\Lambda) = \int_{\Lambda} \left|(e^{-itH}\psi)(x)\right|^2\, dx.$$

If $\ell(\Lambda) < \infty$ is the Lebesgue measure of Λ, then by Corollary 5.5.5, for the free particle one has

$$\mathrm{Prob}_{\psi(t)}(\Lambda) \leq \frac{\ell(\Lambda)}{|4\pi t|^n}\, \|\psi\|_1^2,$$

which decays with rate t^{-n} for $t \to \infty$. The interpretation is that for large times the particle escapes from every bounded region of $\mathbb{R}^n$ and so it goes to infinity, as expected for a free particle. Later on (see Chapters 12 and 13) it will be seen that the root of such behavior is the spectral type of the free Schrödinger operator H_0. For historical details of the transition from classical to quantum mechanics one is invited to consult [Ste94] and for some pedagogical descriptions of modern experiments on the quantum foundations [GreZ97].

Exercise 5.5.6. Let H be the hamiltonian operator of a system for which an orthonormal basis $(\psi_j)_{j\geq 1}$ of $\mathrm{L}^2(\mathbb{R}^n)$ is comprised of its eigenvectors $H\psi_j = \lambda_j \psi_j$; see Example 5.4.10. Verify that for each eigenvector ψ_j the probability of finding the free particle in a measurable set $\Lambda \subset \mathbb{R}^n$ at time t,

$$\mathrm{Prob}_{\psi_j(t)}(\Lambda) = \int_\Lambda \left|(e^{-itH}\psi_j)(x)\right|^2 \, dx,$$

is constant. This is interpreted as the lack of fast mobility of the particles in this case, that is, under time evolution they become localized in space. Compare with the free particle time evolution discussed above.

Exercise 5.5.7. Verify that the solution for $t > 0$ of the Schrödinger equation

$$i\frac{d}{dt}\psi(t) = H_0\psi(t), \qquad \psi(0) = \phi_u,$$

where $\phi_u(x) = e^{-(x-u)^2}$, with fixed parameter $u \in \mathbb{R}$, is

$$\psi(t) = \left(e^{-itH_0}\phi_u\right)(x) = \frac{1}{(1+4it)^{\frac{1}{2}}}\, e^{-\frac{(x-u)^2}{1+4it}}.$$

What is the behavior of these $\psi(t)$ for large t? Compare with the result of Corollary 5.5.5.

Exercise 5.5.8. For $\psi \in C_0^\infty(\mathbb{R}^n)$, use the change of integration variable $y = x + 2|t|^{1/2}s$ in the expression for the free propagator (Theorem 5.5.1) to show that

$$\lim_{t\to 0} e^{-itH_0}\psi = \psi.$$

How general can ψ be in this (strong) limit?

Exercise 5.5.9. Show that the position operator $\mathcal{M}_x$ "generates translations in $\hat{\mathbb{R}}$," that is, $(\hat{G}(t)\hat{\psi})(p) := \hat{\psi}(p+t)$, $\hat{\psi} \in \mathrm{L}^2(\hat{\mathbb{R}})$, is a unitary evolution group whose infinitesimal generator is $\mathcal{M}_x$ (cf. Example 5.4.4).

Remark 5.5.10. Taking into account all physical constants, the kinetic energy and the free unitary evolution group in $\mathrm{L}^2(\mathbb{R}^n)$ have the expressions

$$H_0 = -\frac{\hbar^2}{2m}\Delta,$$

and

$$\left(e^{-itH_0/\hbar}\psi\right)(x) = \left(\frac{m}{2\pi\hbar it}\right)^{\frac{n}{2}} \int_{\mathbb{R}^n} \exp\left(\frac{im(x-y)^2}{2\hbar t}\right)\psi(y)\,dy,$$

respectively.

Remark 5.5.11. The inequality in Corollary 5.5.5 is known as a *dispersive bound*; see [Gol06] for a proof of similar estimates, with the same decay rate $|t|^{-3/2}$, for $H = H_0 + V$ with potentials $V \in \mathrm{L}^p(\mathbb{R}^3) \cap \mathrm{L}^q(\mathbb{R}^3)$, $p < 3/2 < q$, and additional hypotheses on V.

5.5.1 Heat Equation

In a situation analogous to the above discussion, the solution of the heat equation for $t > 0$ and initial conditions

$$\frac{\partial}{\partial t}\psi(t,x) = -(H_0\psi)(t,x), \qquad \psi(0,x) = \psi(x) \in \mathcal{H}^2(\mathbb{R}^n),$$

is given by

$$\left(e^{-H_0 t}\psi\right)(x) := \left(K_t * \psi\right)(x) = \int_{\mathbb{R}^n} K_t(x-y)\psi(y)\,dy,$$

with

$$K_t(x) := \frac{1}{(4\pi t)^{n/2}} \exp\left(-\frac{x^2}{4t}\right).$$

$\psi(x,t)$ means the temperature distribution at time t, given the temperature distribution $\psi(x)$ at the initial time 0. K_t is called the heat kernel. This is the most traditional model for heat propagation.

Remark 5.5.12. Note that the above expression for $(e^{-H_0 t}\psi)(x)$ is well posed for any initial condition in $\psi \in \mathrm{L}^2(\mathbb{R}^n)$. With respect to notation, it is also common to write $e^{-H_0 t} = e^{\Delta t}$.

Exercise 5.5.13. Verify that

$$\mathcal{F}\left(e^{\Delta t}\psi\right)(p) = \frac{1}{(2\pi)^{n/2}} \exp\left(-p^2 t\right)\hat{\psi}(p),$$

for all $\psi \in \mathrm{L}^2(\mathbb{R}^n)$.

Exercise 5.5.14. Show that e^{-tH_0} is *positive preserving*, that is, if $0 \neq \psi \in \mathrm{L}^2(\mathbb{R}^n)$ is a nonnegative function, then $e^{-tH_0}\psi$ is also nonzero and nonnegative for all $t > 0$.

Exercise 5.5.15. Show that if $\psi \in \mathcal{H}^2(\mathbb{R}^n)$, then

$$\lim_{h \downarrow 0} \frac{1}{h}\left(\|\psi\|_2^2 - \langle \psi, e^{-H_0 h}\psi\rangle\right) = \|\nabla\psi\|_2^2.$$

5.6 Trotter Product Formula

Let T, S be self-adjoint operators acting in $\mathcal{H}$ so that $T+S$, with $\mathrm{dom}\,(T+S) = \mathrm{dom}\,T \cap \mathrm{dom}\,S$, is also self-adjoint; see Chapter 6 for some sufficient conditions. How do we write $e^{-it(T+S)}$ in terms of the individual unitary evolution groups e^{-itT} and e^{-itS}? This is a nontrivial question since in general T and S do not commute and one expects that $e^{-it(T+S)} \neq e^{-itT}e^{-itS}$ (see Example 5.6.1). For operators in infinite-dimensional spaces, the first results in this direction were published in [Tr58] and [Tr59], which have a flavor of perturbation results. The folklore rule that "infinitesimal transformations" do commute even though the macroscopic transformations do not, plays an intuitive role in Trotter's formula ahead.

Example 5.6.1 (Weyl form of commutation relation). Let x and P be the position and momentum operators in $\mathrm{L}^2(\mathbb{R})$, and the corresponding evolution groups e^{-itP} and e^{-isx}, $t, s \in \mathbb{R}$. By Example 5.4.4, for all $\psi \in \mathrm{L}^2(\mathbb{R})$, one has

$$
\begin{aligned}
e^{-isx}e^{-itP}\psi(x) &= e^{-isx}\psi(x-t),\\
e^{-itP}e^{-isx}\psi(x) &= e^{-is(x-t)}\psi(x-t) = e^{ist}e^{-isx}e^{-itP}\psi(x),
\end{aligned}
$$

that is, $e^{-itP}e^{-isx} = e^{ist}e^{-isx}e^{-itP}$. This is called the *Weyl form of the canonical commutation relation* of position and momentum, and it is basic to the Stone-von Neumann representation theorem of canonical commutation relations; see [Su01], a mathematical justification of the action $P = -id/dx$. Thus $e^{-itP}e^{-itx} \neq e^{-itx}e^{-itP}$, $t \neq 0$

Theorem 5.6.2 (Trotter Product Formula). *Suppose that T, S are self-adjoint operators acting in $\mathcal{H}$ so that $T+S$, with* $\mathrm{dom}\,(T+S) = \mathcal{D} := \mathrm{dom}\,T \cap \mathrm{dom}\,S$, *is also self-adjoint. Then, for each $t \in \mathbb{R}$,*

$$
e^{-it(T+S)} = \mathrm{s-}\lim_{n\to\infty} \left(e^{-i\frac{t}{n}T} e^{-i\frac{t}{n}S} \right)^n .
$$

Proof. There are two initial key points in the proof of the theorem:

1. For $0 \neq h \in \mathbb{R}$ and $\xi \in \mathcal{D}$, denote

$$
u_h(\xi) := \frac{1}{h}\left(e^{-ihT}e^{-ihS}\xi - e^{-ih(T+S)}\xi \right).
$$

   The domain $\mathcal{D}$ is left invariant by e^{-isT}, e^{-isS} and $e^{-is(T+S)}$, $\forall s \in \mathbb{R}$, and for $\xi \in \mathcal{D}$ the identity

$$
u_h(\xi) = \frac{(e^{-ihT} - \mathbf{1})}{h}\xi + e^{-ihT}\frac{(e^{-ihS} - \mathbf{1})}{h}\xi - \frac{(e^{-ih(T+S)} - \mathbf{1})}{h}\xi
$$

   implies $\lim_{h\to 0} u_h(\xi) = 0$. Then define $u_0(\xi) := 0$, $\xi \in \mathcal{D}$.

2. For bounded operators A, B and all $n \in \mathbb{N}$, one has (expand the r.h.s.)

$$\begin{aligned}\left(e^{-itT/n}e^{-itS/n}\right)^n - \left(e^{-it(T+S)/n}\right)^n &= \left(e^{-itT/n}e^{-itS/n}\right)^n - e^{-it(T+S)} \\ &= \sum_{j=0}^{n-1} \left(e^{-itT/n}e^{-itS/n}\right)^j \\ &\times \left[e^{-itT/n}e^{-itS/n} - e^{-it(T+S)/n}\right] \left(e^{-it(T+S)/n}\right)^{n-1-j}.\end{aligned}$$

By 1 above, for each $h \in \mathbb{R}$ the map $u_h : \mathcal{D} \to \mathcal{H}$ is linear and bounded. For fixed $\xi \in \mathcal{D}$, it is continuous as a function of $h \in \mathbb{R}$ and one also has the pointwise convergence $u_h(\xi) \to 0$ as $h \to \infty$; thus there exists $c(\xi) > 0$ for which $\|u_h(\xi)\| \le c(\xi)$, $\forall h \in \mathbb{R}$.

Since the operator $T + S$ is closed, its domain $\mathcal{D}$ is a Banach space in the graph norm $\|\cdot\|_{T+S}$, and so, by the Uniform Boundedness Principle 1.1.31 applied to the family $u_h : (\mathcal{D}, \|\cdot\|_{T+S}) \to \mathcal{H}$, there is $C > 0$ so that

$$\|u_h(\xi)\| \le C\|\xi\|_{T+S}, \qquad \forall h \in \mathbb{R}, \xi \in \mathcal{D}.$$

For each fixed $\xi \in \mathcal{D}$, introduce the map

$$\mathbb{R} \ni t \mapsto \xi_t := e^{-it(T+S)}\xi \in (\mathcal{D}, \|\cdot\|_{T+S});$$

by properties of unitary evolution groups,

$$\begin{aligned}\|\xi_t - \xi_s\|_{T+S}^2 &= \|\xi_t - \xi_s\|^2 + \|(T+S)\xi_t - (T+S)\xi_s\|^2 \\ &= \|\xi - e^{-i(s-t)(T+S)}\xi\|^2 + \|(T+S)\xi - e^{-i(s-t)(T+S)}(T+S)\xi\|^2\end{aligned}$$

which vanishes as $s \to t$, that is, the map $t \mapsto \xi_t$ into $(\mathcal{D}, \|\cdot\|_{T+S})$ is continuous. Thus, for fixed $t \in \mathbb{R}$, the compactness of the interval $[-|t|, |t|]$ imply that

$$J_{\xi,t} = \{\xi_s : |s| \le |t|\}$$

is a compact set in $(\mathcal{D}, \|\cdot\|_{T+S})$. Hence $J_{\xi,t}$ is totally bounded in $(\mathcal{D}, \|\cdot\|_{T+S})$, and the triangular inequality together with the above uniform boundedness conclude that the restriction to the continuous family of linear operators $u_h : J_{\xi,t} \to \mathcal{H}$ vanishes uniformly as $h \to 0$; in other symbols $\max_{|s|\le|t|} \|u_h(\xi_s)\| \to 0$ as $h \to 0$.

Write $h = t/n$ and note that $(n-1-j)/n \le 1$. Thus, by 2 above,

$$\begin{aligned}&\left\|\left(e^{-itT/n}e^{-itS/n}\right)^n \xi - e^{-it(T+S)}\xi\right\| \\ &\le \max_{|s|\le|t|} \left\|n\left[e^{-itT/n}e^{-itS/n} - e^{-it(T+S)/n}\right] e^{-is(T+S)}\xi\right\| \\ &\le |t| \max_{|s|\le|t|} \left\|\frac{1}{h}\left[e^{-ihT}e^{-ihS} - e^{-ih(T+S)}\right] e^{-is(T+S)}\xi\right\| \\ &= |t| \max_{|s|\le|t|} \|u_h(\xi_s)\|\end{aligned}$$

which vanishes as $h \to 0$, that is, as $n \to \infty$; therefore

$$\left(e^{-itT/n}e^{-itS/n}\right)^n \xi \to e^{-it(T+S)}\xi, \qquad \forall \xi \in \mathcal{D}.$$

Since the involved operators are unitary, this convergence extends to the closure of $\mathcal{D}$, that is, it holds on $\mathcal{H}$. □

Exercise 5.6.3. Present details that, in the above proof of the Trotter product formula, $u_h : J_{\xi,t} \to \mathcal{H}$, $h \in \mathbb{R}$, satisfies $u_h(\xi_s) \to 0$ uniformly as $h \to 0$.

The following is a consequence of the proof of the Trotter formula.

Corollary 5.6.4. *Let T and S be as in Theorem* 5.6.2*. For a fixed $\xi \in \mathcal{D}$, the convergence $\left(e^{-itT/n}e^{-itS/n}\right)^n \xi \to e^{-it(T+S)}\xi$ is uniform for t in compact intervals $[a, b]$.*

A first version of the Trotter formula for matrices was demonstrated by Sophus Lie, so sometimes it is also called the *Lie-Trotter product formula*. It can be used in numerical implementations of the time evolution $e^{-it(T+S)}\xi$ in case e^{-itT} and e^{-itS} are easier to handle. In Theorem 5.6.2 it is possible to assume that $T + S$ is just essentially self-adjoint [Ch68]. The above proof of Theorem 5.6.2 is based on Appendix B of [Nel64]; for recent results and references related to the Trotter formula see [IchT04]. The version that appears in Exercise 9.9.3 is used in statistical mechanics to relate quantum and classical spin systems.

Exercise 5.6.5. Let E, F be two closed subspaces of $\mathcal{H}$ with $E \cap F = \{0\}$, and P_E, P_F the respective orthogonal projections. Show that

$$\lim_{n\to\infty} (P_E P_F)^n = P_{E\cap F}$$

and

$$\text{s} - \lim_{n\to\infty} \left(e^{-i\frac{t}{n}P_E} e^{-i\frac{t}{n}P_F}\right)^n = e^{-itP_M}, \qquad \forall t \in \mathbb{R},$$

where $M = E \oplus F$.

Chapter 6

Kato-Rellich Theorem

In this and the next chapters, the preservation of self-adjointness under hermitian perturbations are considered. The classical application of Rellich's theorem by Kato to a hydrogen atom hamiltonian is discussed in detail. Examples, the virial and KLMN theorems and an outstanding Kato distributional inequality are also presented in this chapter.

6.1 Relatively Bounded Perturbations

Self-adjointness is a delicate property. It may not be preserved by a sum of operators. For instance, if T, S are self-adjoint operators in $\mathcal{H}$, then dom $T \cap$ dom S is the subspace on which $T + S$ is a priori defined. However, this intersection may be too small for $T + B$ be self-adjoint (e.g., both $C_0^\infty(\mathbb{R})$ and the set of simple functions are both dense in $\mathrm{L}^2(\mathbb{R})$, but their intersection contains only the null vector; see a specific instance in Exercise 6.2.25). It may also happen that such an intersection is dense but $T + S$ is not self-adjoint.

If T is self-adjoint and B is hermitian, under which conditions is $T + B$ self-adjoint? This is the general question to be addressed now. Although the main interest is in perturbations of the free Schrödinger operators H_0 acting in $\mathrm{L}^2(\Lambda), \Lambda \subset \mathbb{R}^n$, by potentials V, it is useful to deal with abstract hermitian perturbations B of a general self-adjoint operator T.

The motivation for the next results is the following. Let T be hermitian; then T is self-adjoint iff λT is self-adjoint for some (and so any) $0 \neq \lambda \in \mathbb{R}$. It is known (Proposition 2.2.4) that a hermitian T is self-adjoint iff rng $(T \pm i\mathbf{1}) = \mathcal{H}$. One has

$$\begin{aligned} T + B \pm i\lambda\mathbf{1} &= (BR_{\pm i\lambda}(T) + \mathbf{1})(T \pm i\lambda\mathbf{1}) \\ &= \lambda(BR_{\pm i\lambda}(T) + \mathbf{1}) \left(\frac{1}{\lambda}T \pm i\mathbf{1}\right), \end{aligned}$$

so that if for some real λ one has $\|BR_{\pm i\lambda}(T)\| < 1$, then $(BR_{\pm i\lambda}(T) + \mathbf{1})$ has also a bounded inverse in $\mathrm{B}(\mathcal{H})$ and so $\operatorname{rng}\,(BR_{\pm i\lambda}(T) + \mathbf{1}) = \mathcal{H}$. If T is self-adjoint $\operatorname{rng}\,(T \pm i\lambda\mathbf{1}) = \lambda \operatorname{rng}\,(T/\lambda \pm i\mathbf{1}) = \mathcal{H}$, and the above relation implies

$$\operatorname{rng}\,(T + B \pm i\lambda\mathbf{1}) = \mathcal{H},$$

so that $(T + B)$ would also be self-adjoint. We now explore some details of these ideas.

Definition 6.1.1. Let $T : \operatorname{dom} T \sqsubseteq \mathcal{H} \to \mathcal{H}$ and $B : \operatorname{dom} B \sqsubseteq \mathcal{H} \to \mathcal{H}$ be linear operators. Then B is *T-bounded* (or *relatively bounded with respect to T*) if $\operatorname{dom} B \supset \operatorname{dom} T$ and there exist $a, b \geq 0$ so that

$$\|B\xi\| \leq a\|T\xi\| + b\|\xi\|, \qquad \forall \xi \in \operatorname{dom} T.$$

The *T-bound* of B is the infimum $N_T(B)$ of the admissible a's in this inequality.

Remark 6.1.2. An equivalent definition is $\operatorname{dom} B \supset \operatorname{dom} T$ and there exist $c, d \geq 0$ so that

$$\|B\xi\|^2 \leq c^2\|T\xi\|^2 + d^2\|\xi\|^2, \qquad \forall \xi \in \operatorname{dom} T.$$

Further, $N_T(B)$ coincides with the infimum of the admissible c's. Therefore, both formulations will be freely used.

Proof. If the latter relation holds, then

$$\begin{aligned}\|B\xi\|^2 &\leq c^2\|T\xi\|^2 + d^2\|\xi\|^2 + 2cd\,\|T\xi\|\,\|\xi\| \\ &\leq (c\|T\xi\| + d\|x\|)^2,\end{aligned}$$

and one can take $a = c$ and $b = d$. For the other inequality, consider the following

Lemma 6.1.3. *Let $\xi, \eta \in \mathcal{H}$ and $s, t > 0$. Then, for all $r > 0$ one has*

$$2st\|\eta\|\,\|\xi\| \leq r^2 s^2\,\|\eta\|^2 + \frac{t^2}{r^2}\|\xi\|^2.$$

Proof. It is enough to expand $0 \leq \left(rs\|\eta\| - \frac{t}{r}\|\xi\|\right)^2$. □

Suppose then that $\|B\xi\| \leq a\|T\xi\| + b\|\xi\|$. By Lemma 6.1.3 it follows that

$$\|B\xi\|^2 \leq (a\|T\xi\| + b\|\xi\|)^2 \leq a^2\left(1 + r^2\right)\|T\xi\|^2 + b^2\left(1 + \frac{1}{r^2}\right)\|\xi\|^2$$

and the second relation holds with $c^2 = a^2(1 + r^2)$ and $d^2 = b^2(1 + 1/r^2)$. By taking $r \to 0$ it is found that the same value of $N_T(B)$ is obtained from both relations. □

Lemma 6.1.4. *Let T be a linear operator in $\mathcal{H}$ with $\rho(T) \neq \emptyset$ and B a closed operator with* $\operatorname{dom} T \subset \operatorname{dom} B$. *Then B is T-bounded and $N_T(B) \leq \|BR_z(T)\|$, $\forall z \in \rho(T)$.*

Proof. If $z \in \rho(T)$, then $BR_z(T) : \mathcal{H} \hookleftarrow$ is a closed operator (check this!) and, by the closed graph theorem, it is bounded. Thus, for $\xi \in \operatorname{dom} T$ and $z \in \rho(T)$ one has

$$\|B\xi\| = \|BR_z(T)(T - z\mathbf{1})\xi\| \le \|BR_z(T)\| \left(\|T\xi\| + |z|\|\xi\|\right),$$

and B is T-bounded. □

Proposition 6.1.5. *If T is self-adjoint and* $\operatorname{dom} T \subset \operatorname{dom} B$*, then B is T-bounded iff $BR_z(T) \in \mathrm{B}(\mathcal{H})$ for some $z \in \rho(T)$; in this case $BR_z(T) \in \mathrm{B}(\mathcal{H})$, $\forall z \in \rho(T)$, and* $N_T(B) = \lim_{|\lambda|\to\infty} \|BR_{i\lambda}(T)\|$ *($\lambda \in \mathbb{R}$).*

Proof. If $BR_z(T)$ is a bounded operator for some $z \in \rho(T)$, then by the proof of Lemma 6.1.4 it follows that B is T-bounded and $N_T(B) \le \|BR_z(T)\|$; moreover, by the first resolvent identity,

$$BR_y(T) = BR_z(T) + (y - z)BR_z(T)R_y(T),$$

so that $BR_y(T)$ is bounded for all $y \in \rho(T)$. Hence, since T is self-adjoint one can consider $z = \pm i\lambda$, with $0 \ne \lambda \in \mathbb{R}$, which belongs to $\rho(T)$.

Suppose now that B is T-bounded, so that there are $a, b \ge 0$ obeying, for all $\xi \in \mathcal{H}$,

$$\|BR_{i\lambda}(T)\xi\| \le a\|TR_{i\lambda}(T)\xi\| + b\|R_{i\lambda}(T)\xi\|,$$

and since $\|T\eta - i\lambda\eta\|^2 = \|T\eta\|^2 + \lambda^2\|\eta\|^2 \ge \|T\eta\|^2$, one has, with $\eta = R_{i\lambda}(T)\xi$,

$$\begin{aligned}\|BR_{i\lambda}(T)\xi\| &\le a\|(T - i\lambda\mathbf{1})R_{i\lambda}(T)\xi\| + b\|R_{i\lambda}(T)\|\,\|\xi\| \\ &\le \left(a + \frac{b}{|\lambda|}\right)\|\xi\|,\end{aligned}$$

and $BR_{i\lambda}(T)$ is bounded (Theorem 2.2.17 was employed). Together with the inequality at the beginning of this proof,

$$N_T(B) \le \|BR_{i\lambda}(T)\| \le a + \frac{b}{|\lambda|}.$$

From the definition of $N_T(B)$ it then follows that

$$N_T(B) = \lim_{|\lambda|\to\infty} \|BR_{i\lambda}(T)\|.$$

Thereby the proof is complete. □

Exercise 6.1.6. If T is a self-adjoint operator, show that $\|TR_{i\lambda}(T)\| \le 1$, $\forall 0 \ne \lambda \in \mathbb{R}$.

Exercise 6.1.7. Let $T \ge \beta\mathbf{1}$ be self-adjoint, $\beta \in \mathbb{R}$. Inspect the proof of Proposition 6.1.5 and check that for $\lambda < 0$, $|\lambda|$ large enough, $\|TR_\lambda(T)\| < 1$, and that $N_T(B) = \lim_{\lambda\to-\infty} \|BR_\lambda(T)\|$.

Theorem 6.1.8 (Rellich or Kato-Rellich). *Let T be self-adjoint and B hermitian. If B is T-bounded with $N_T(B) < 1$, then the operator*

$$\text{dom}\,(T+B) = \text{dom}\,T, \qquad (T+B)\xi := T\xi + B\xi, \qquad \forall \xi \in \text{dom}\,T,$$

is self-adjoint.

Proof. Clearly $(T+B)$ is hermitian. Since $N_T(B) < 1$, by Proposition 6.1.5 there exists $\lambda_0 > 0$ so that $\|BR_{i\lambda_0}(T)\| < 1$. Thus, $(\mathbf{1} + BR_{\pm i\lambda_0}(T))$ is invertible in $\mathrm{B}(\mathcal{H})$ and onto. Hence,

$$\begin{aligned}(T+B) \pm i\lambda_0\mathbf{1} &= B + (T \pm i\lambda_0\mathbf{1}) \\ &= (BR_{\pm i\lambda_0}(T) + \mathbf{1})\,(T \pm i\lambda_0\mathbf{1})\end{aligned}$$

and so $\text{rng}\,(T+B\pm i\lambda_0) = \mathcal{H}$. By Proposition 2.2.4 (see also the discussion at the beginning of this section), (T+B) is self-adjoint. □

Corollary 6.1.9. *Let T and B be as in Theorem* 6.1.8*. If $\mathcal{D} \subset \text{dom}\,T$ is a core of T, then $\mathcal{D}$ is a core of $(T+B)$.*

Proof. Take λ_0 as in the proof of Thm. 6.1.8. Then the operator $(\mathbf{1}+BR_{\pm i\lambda_0}(T))$ is a homeomorphism onto $\mathcal{H}$. Thus, if $(T\pm i\lambda_0\mathbf{1})\mathcal{D}$ is dense in $\mathcal{H}$, then $(T+B\pm i\lambda_0\mathbf{1})\mathcal{D}$ is also dense in $\mathcal{H}$. Therefore the deficiency indices of $(T+B)|_{\mathcal{D}}$ are both zero (see Theorem 2.2.11), consequently $\mathcal{D}$ is a core of $(T+B)$. □

Example 6.1.10. In $\mathrm{L}^2(\mathbb{R}^n)$ the momentum operators $P_j = -i\partial_j$, $1 \le j \le n$, are H_0-bounded with $N_{H_0}(P_j) = 0$; thus the operator

$$H\psi = H_0\psi - i\lambda \sum_j \partial_j\psi$$

is self-adjoint in the domain $\mathcal{H}^2(\mathbb{R}^n)$, $\forall \lambda \in \mathbb{R}$. In fact, for $\psi \in \mathcal{H}^2(\mathbb{R}^n) \subset \text{dom}\,P_j$, $\|P_j\psi\|_2 = \|p_j\hat{\psi}(p)\|_2$, and given $a > 0$ there is $b \ge 0$ so that $|p_j| \le (ap^2 + b)$, and so (assume that $\lambda \ne 0$)

$$\|\lambda P_j\psi\|_2 \le a\,|\lambda|\,\|p^2\hat{\psi}(p)\|_2 + b\,|\lambda|\,\|\hat{\psi}(p)\|_2 = a\,|\lambda|\,\|H_0\psi\|_2 + b\,|\lambda|\,\|\psi\|_2.$$

Since $a > 0$ was arbitrary, the result follows by Theorem 6.1.8.

Exercise 6.1.11. Let T and B be self-adjoint operators in $\mathcal{H}$. If $B \in \mathrm{B}(\mathcal{H})$, verify that

a) $N_T(B) = 0$.
b) $T + B$ is self-adjoint with $\text{dom}\,(T+B) = \text{dom}\,T$.
c) Every core of T is also a core of $T+B$.

Exercise 6.1.12.

a) If B is T-bounded with $N_T(B) < 1$, show that B is also $(T+B)$-bounded.
b) If T is self-adjoint and B hermitian and T-bounded with $N_T(B) < 1/2$, show that $(T+2B)$ is also self-adjoint.

Exercise 6.1.13. Let T be closed and B a T-bounded operator with T-bound $N_T(B) < 1$. Show that $T + B$ with domain dom T is closed. If $N_T(B) = 1$ take $B = -T$ and conclude that $T + B$ can be nonclosed.

6.1.1 KLMN Theorem

This theorem is a partial counterpart for sesquilinear forms of the Kato-Rellich theorem, and it was dubbed KLMN by J.T. Cannon in 1968 from the initials of Kato, Lions, Lax, Milgram and Nelson. In this subsection b_1 and b_2 denote two (densely defined) hermitian sesquilinear forms in $\mathcal{H}$, with b_1 lower bounded $b_1 \geq \beta$. The domain of $b_1 + b_2$ is dom $b_1 \cap$ dom b_2.

Definition 6.1.14. b_2 is b_1-bounded if dom $b_1 \subset$ dom b_2 and there are $a \geq 0, c \geq 0$ so that

$$|b_2(\xi)| \leq a\,|b_1(\xi)| + c\|\xi\|^2, \qquad \forall \xi \in \text{dom } b_1.$$

The infimum of the admissible $a's$ in this inequality is called the b_1-*bound* of b_2.

Exercise 6.1.15. Show that the b_1-bound of b_2 coincides with the $(b_1 + \alpha)$-bound of b_2 for any $\alpha \in \mathbb{R}$.

By Exercise 6.1.15 there is no loss if it is assumed that $b_1 \geq 0$, i.e., that b_1 is positive.

Lemma 6.1.16. *Suppose that $b_1 \geq 0$ and b_2 is b_1-bounded with b_1-bound < 1, that is, the inequality in Definition* 6.1.14 *holds for some $0 \leq a < 1$ and $0 \leq c \in \mathbb{R}$. Then:*

i) *$b_1 + b_2 \geq -c$, that is, $b_1 + b_2$ is also lower bounded.*
ii) *$b_1 + b_2$ is closed iff b_1 is closed.*

Proof. For all $\xi \in$ dom $b_1 =$ dom $(b_1 + b_2)$,

$$\begin{aligned} -c\|\xi\|^2 &\leq -c\|\xi\|^2 + (1-a)b_1(\xi) = -\left(c\|\xi\|^2 + a\,b_1(\xi)\right) + b_1(\xi) \\ &\leq b_2(\xi) + b_1(\xi) = (b_1 + b_2)(\xi) \leq a\,b_1(\xi) + c\|\xi\|^2 + b_1(\xi) \\ &= (1+a)\,b_1(\xi) + c\|\xi\|^2. \end{aligned}$$

Then i) follows at once. By adding $(1 + c)\|\xi\|^2$ to the terms in the above chain of inequalities, one gets

$$\begin{aligned} (1-a)(b_1(\xi) + \|\xi\|^2) &\leq (1-a)b_1(\xi) + \|\xi\|^2 \\ &\leq (b_1 + b_2)(\xi) + (1+c)\|\xi\|^2 \\ &\leq (1+a)b_1(\xi) + (1+2c)\|\xi\|^2 \\ &\leq A\left(b_1(\xi) + \|\xi\|^2\right), \qquad A = \max\{1+a, 1+2c\}; \end{aligned}$$

thus the norms $\xi \mapsto \sqrt{b_1(\xi) + \|\xi\|^2}$ and $\xi \mapsto \sqrt{(b_1 + b_2)(\xi) + (1+c)\|\xi\|^2}$ are equivalent on dom b_1 and ii) follows (see Lemma 4.1.9). ☐

Theorem 6.1.17 (KLMN). *Suppose that $b_1 \geq 0$ and b_2 is b_1-bounded with b_1-bound < 1. Then there exists a unique self-adjoint operator T with* dom $T \sqsubseteq$ dom b_1, *whose form domain is* dom b_1, *and*

$$\langle \xi, T\eta \rangle = b_1(\xi, \eta) + b_2(\xi, \eta), \qquad \forall \xi \in \text{dom } b_1, \eta \in \text{dom } T.$$

Further, T is lower bounded and dom T *is a core of* $b_1 + b_2$.

Proof. By Lemma 6.1.16, $b_1 + b_2$ is closed and lower bounded. The operator T is the one associated with $b_1 + b_2$ as in Definition 4.2.5. The other statements follow by Theorem 4.2.6. □

Although the hypotheses of KLMN are weaker than those of Kato-Rellich, in the latter the domain of the operator sum is explicitly found. Be aware that in concrete situations it can be a nontrivial task to decide if such theorems are applicable.

Typical applications of Theorem 6.1.17 involve the definition of the sum of two hermitian operators $T_1 \geq \beta \mathbf{1}$ and T_2 via $b^{T_1} + b^{T_2}$ (see Example 4.1.11), in particular when Kato-Rellich does not apply, as in Example 6.2.15, and cases of forms not directly related to a potential, as in Examples 6.2.16 and 6.2.19.

One can roughly think of the KLMN theorem as a definition of an adequate quantum observable from the addition of expectation values.

6.2 Applications

6.2.1 H-Atom and Virial Theorem

Now the Kato-Rellich Theorem is applied to perturbations of the free particle hamiltonian

$$\text{dom } H_0 = \mathcal{H}^2(\mathbb{R}^n), \qquad H_0\psi = -\Delta\psi,$$

discussed in Section 3.4. Recall that, by Proposition 3.4.1, $C_0^\infty(\mathbb{R}^n)$ is a core of H_0. Besides the Sobolev embedding theorem, the next result gives valuable information on elements of the Sobolev space $\mathcal{H}^2(\mathbb{R}^n)$, $n \leq 3$.

Lemma 6.2.1. *If $n \leq 3$, then $\mathcal{H}^2(\mathbb{R}^n) \subset C(\mathbb{R}^n) \cap \mathrm{L}^\infty(\mathbb{R}^n)$ and for each $a > 0$ there exists $b > 0$ so that*

$$\|\psi\|_\infty \leq a\|H_0\psi\| + b\|\psi\|, \qquad \forall \psi \in \mathcal{H}^2(\mathbb{R}^n).$$

Proof. Technically, the point of the argument is that for $n \leq 3$ the function $p \mapsto (1+p^2)^{-1} \in \mathrm{L}^2(\mathbb{R}^n)$, and also $(1+p^2)\hat{\psi}(p) = \mathcal{F}(\psi + H_0\psi)$.

If $\psi \in$ dom H_0, by Cauchy-Schwarz,

$$\left(\int_{\mathbb{R}^n} |\hat{\psi}(p)|\, dp\right)^2 \leq \int_{\mathbb{R}^n} (1+p^2)^2 |\hat{\psi}(p)|^2\, dp \int_{\mathbb{R}^n} \frac{dp}{(1+p^2)^2} < \infty,$$

and so $\hat{\psi} \in \mathrm{L}^1(\mathbb{R}^n)$. By Lemma 3.2.8 it follows that $\psi \in C(\mathbb{R}^n) \cap \mathrm{L}^\infty(\mathbb{R}^n)$. Note that since $\psi \in \mathrm{L}^2(\mathbb{R}^n)$ and is continuous, then $\lim_{|x|\to\infty} \psi(x) = 0$.

Let $\lambda > 1$ and $\kappa = \|(1+p^2)^{-1}\|_2/(2\pi)^{\frac{n}{2}}$. Then, for $\psi \in \mathrm{dom}\, H_0$, again by Cauchy-Schwarz,

$$\begin{aligned}|\psi(x)| &= \frac{1}{(2\pi)^{n/2}} \left| \int_{\mathbb{R}^n} (\lambda^2 + p^2) e^{ipx}\, \hat{\psi}(p)\, \frac{dp}{(\lambda^2 + p^2)} \right| \\ &\le \frac{1}{(2\pi)^{n/2}} \left\| (\lambda^2 + p^2)\, \hat{\psi}(p) \right\|_2 \left\| \frac{1}{(\lambda^2 + p^2)} \right\|_2 \\ &\le \frac{\kappa}{\lambda^{2-\frac{n}{2}}} \left(\lambda^2 \left\| \hat{\psi}(p) \right\|_2 + \left\| p^2 \hat{\psi}(p) \right\|_2 \right) \\ &= \frac{\kappa}{\lambda^{2-\frac{n}{2}}} \|H_0 \psi\|_2 + \kappa \lambda^{\frac{n}{2}} \|\psi\|_2,\end{aligned}$$

since the Fourier transform is a unitary operator. Now take λ large enough. □

For the potential $V : \mathbb{R}^n \to \mathbb{R}$ in $\mathrm{L}^\infty(\mathbb{R}^n)$, one associates a bounded self-adjoint multiplication operator $V = \mathcal{M}_V$, and so

$$H := H_0 + V, \qquad \mathrm{dom}\, H := \mathrm{dom}\, H_0,$$

is self-adjoint (see Exercise 6.1.11). This situation can be generalized to some unbounded potentials V.

The notation $V \in \mathrm{L}^r_\mu + \mathrm{L}^s_\mu$ means that the function $V = V_r + V_s$ with $V_r \in \mathrm{L}^r_\mu$ and $V_s \in \mathrm{L}^s_\mu$, and it has already been incorporated into the main stream of Schrödinger operator theory.

Theorem 6.2.2 (Kato). *If $n \le 3$ and $V \in \mathrm{L}^2(\mathbb{R}^n) + \mathrm{L}^\infty(\mathbb{R}^n)$ is a real-valued function, then V is H_0-bounded with $N_{H_0}(V) = 0$, the operator*

$$H := H_0 + V, \qquad \mathrm{dom}\, H = \mathrm{dom}\, H_0,$$

is self-adjoint and $C_0^\infty(\mathbb{R}^n)$ is a core of H.

Proof. By hypothesis $V = V_2 + V_\infty$ with $V_2 \in \mathrm{L}^2(\mathbb{R}^n)$ and $V_\infty \in \mathrm{L}^\infty(\mathbb{R}^n)$. Thus, by Lemma 6.2.1, for all $a > 0$ there is $b \ge 0$ so that, for all $\psi \in \mathrm{dom}\, H_0$,

$$\begin{aligned}\|V\psi\|_2 &\le \|V_2\psi\|_2 + \|V_\infty\psi\|_2 \le \|V_2\|_2\, \|\psi\|_\infty + \|V_\infty\|_\infty\, \|\psi\|_2 \\ &\le \|V_2\|_2\, (a\|H_0\psi\|_2 + b\|\psi\|_2) + \|V_\infty\|_\infty\, \|\psi\|_2 \\ &= (a\|V_2\|_2)\, \|H_0\psi\|_2 + (b\|V_2\|_2 + \|V_\infty\|_\infty)\, \|\psi\|_2.\end{aligned}$$

Since $a > 0$ is arbitrary, it follows that $N_{H_0}(V) = 0$. To finish the proof apply Theorem 6.1.8 and Corollary 6.1.9. □

Example 6.2.3. Consider the class of negative power potentials in $\mathbb{R}^3$,

$$V(x) = -\frac{\kappa}{|x|^\alpha}, \qquad \kappa \in \mathbb{R},\ 0 < \alpha < 3/2.$$

Fix $R > 0$; then $V = V_2 + V_\infty$, with

$$V_2(x) = V(x)\chi_{[0,R)}(|x|), \qquad V_\infty(x) = V(x)\chi_{[R,\infty)}(|x|),$$

where χ_A denotes the characteristic function of the set A. Since $V_2 \in \mathrm{L}^2(\mathbb{R}^3)$ and $V_\infty \in \mathrm{L}^\infty(\mathbb{R}^3)$, it follows that the Schrödinger operator

$$H = H_0 - \frac{\kappa}{|x|^\alpha}, \qquad \mathrm{dom}\ H = \mathcal{H}^2(\mathbb{R}^3),$$

is self-adjoint and $C_0^\infty(\mathbb{R}^3)$ is a core of H (recall $0 < \alpha < 3/2$).

The very important Coulomb potential $\alpha = 1$ gives rise to 3D hydrogenic atoms; if also $\kappa > 0$, it is briefly referred to as an *H-atom* Schrödinger operator H_H (see Remark 6.2.6); as discussed on page 295, this operator is lower bounded (see also Remark 11.4.9). The unidimensional version of the H-atom presents additional technical issues and is addressed in Subsection 7.4.1.

Example 6.2.4. The same conclusions of Example 6.2.3 hold for the "generalized Yukawa-like potential" in $\mathbb{R}^3$,

$$V_Y(x) = -\frac{\kappa}{|x|^\alpha} e^{-a|x|}, \qquad \kappa \in \mathbb{R},\ 0 < \alpha < 3/2,\ a > 0,$$

since $V_Y \in \mathrm{L}^2(\mathbb{R}^3)$. Hence the Schrödinger operator $H = H_0 + V_Y$ with dom $H = \mathcal{H}^2(\mathbb{R}^3)$ is self-adjoint. The genuine *Yukawa potential* is obtained for $\kappa > 0$ and $\alpha = 1$.

Exercise 6.2.5. Apply the Kato-Rellich theorem to the Schrödinger operators of Example 6.2.3, but in dimensions 1 and 2, i.e., for the cases of Hilbert spaces $\mathrm{L}^2(\mathbb{R})$ and $\mathrm{L}^2(\mathbb{R}^2)$, respectively. For which values of $\alpha > 0$ are self-adjoint operators H obtained?

Remark 6.2.6. The expression for the Coulomb potential above describes the electrostatic interaction between two charged particles, and one of them is supposed to be at rest at the origin, so heavy with respect to the other that this approximation is taken. For a hydrogenic atom, that is, with just one electron of mass m and charge $-e$ ($e > 0$), and nuclear mass M and charge Ze, with $M \gg m$ and Z a positive integer indicating the total number of protons in the nucleus, the corresponding Schrödinger operator with all physical constants made explicit is

$$H_H = -\frac{\hbar^2}{2\mu}\Delta - \frac{KZe^2}{|x|},$$

with K indicating the electrostatic constant, $\mu = mM/(m + M)$ the so-called reduced mass, and x corresponding to the relative position between the electron and the nucleus. Note that in the limit of a fixed nucleus, represented here by the condition $M \to \infty$, one has $\mu \to m$. Throughout this discussion the center of mass has been "removed" [Will03], so that only the relative motion remains.

Remark 6.2.7. For $\mathbb{R}^n$, $n \geq 4$, the Kato Theorem 6.2.2 holds for $V \in \mathrm{L}^p(\mathbb{R}^n) + \mathrm{L}^\infty(\mathbb{R}^n)$, with $p > 2$ if $n = 4$ and $p \geq n/2$ if $n \geq 5$.

By using the Virial Theorem 6.2.8, with relatively little effort it is possible to say something about the spectrum of the H-atom Schrödinger operator. Let $U_d(s)$ be the strongly continuous dilation unitary evolution group discussed in Example 5.4.8, adapted to $\mathbb{R}^n$,

$$(U_d(s)\psi)(x) = e^{-ns/2}\psi(e^{-s}x), \qquad s \in \mathbb{R}, \psi \in \mathrm{L}^2(\mathbb{R}^n).$$

Assume that V is an H_0-bounded potential with $N_{H_0}(V) < 1$, so that $H := H_0+V$ with dom $H = \mathcal{H}^2(\mathbb{R}^n)$ is self-adjoint.

Theorem 6.2.8 (Virial). *Let V be an H_0-bounded potential with $N_{H_0}(V) < 1$. Suppose there exists $0 \neq \alpha \in \mathbb{R}$ so that*

$$U_d(-s)VU_d(s) = e^{-\alpha s}V.$$

If λ is an eigenvalue of H and ψ_λ the subsequent normalized eigenvector, i.e., $H\psi_\lambda = \lambda\psi_\lambda$, $\|\psi_\lambda\| = 1$, then

$$\langle\psi_\lambda, H_0\psi_\lambda\rangle = -\frac{\alpha}{2}\langle\psi_\lambda, V\psi_\lambda\rangle$$

and

$$\lambda = \left(1 - \frac{2}{\alpha}\right)\langle\psi_\lambda, H_0\psi_\lambda\rangle = \left(1 - \frac{\alpha}{2}\right)\langle\psi_\lambda, V\psi_\lambda\rangle.$$

Proof. Note that $U_d(-s)H_0U_d(s) = e^{-2s}H_0$. Since $\psi_\lambda \in$ dom $H_0 =$ dom H and $U_d(s)$dom $H_0 =$ dom H_0, $\forall s \in \mathbb{R}$, one has

$$\begin{aligned}
0 &= \langle U_d(-s)\psi_\lambda, \lambda\psi_\lambda\rangle - \langle U_d(-s)\lambda\psi_\lambda, \psi_\lambda\rangle \\
&= \langle U_d(-s)\psi_\lambda, H\psi_\lambda\rangle - \langle U_d(-s)H\psi_\lambda, \psi_\lambda\rangle \\
&= \langle U_d(-s)\psi_\lambda, H\psi_\lambda\rangle - \langle H\psi_\lambda, U_d(s)\psi_\lambda\rangle \\
&= \langle U_d(-s)\psi_\lambda, H\psi_\lambda\rangle - \langle U_d(-s)\psi_\lambda, U_d(-s)HU_d(s)\psi_\lambda\rangle \\
&= \langle U_d(-s)\psi_\lambda, [H - U_d(-s)HU_d(s)]\,\psi_\lambda\rangle, \qquad \forall s \in \mathbb{R}.
\end{aligned}$$

Write out $H = H_0 + V$ in the above expression and use the hypothesis on V to get

$$\begin{aligned}
0 &= \lim_{s\to 0}\left\langle U_d(-s)\psi_\lambda, \frac{1}{s}\,[H - U_d(-s)HU_d(s)]\,\psi_\lambda\right\rangle \\
&= \langle\psi_\lambda 2H_0\psi_\lambda + \alpha V\psi_\lambda\rangle\,,
\end{aligned}$$

so that

$$\langle\psi_\lambda, H_0\psi_\lambda\rangle = -\frac{\alpha}{2}\langle\psi_\lambda, V\psi_\lambda\rangle,$$

which is the first equality in the theorem. Since

$$\lambda = \langle\psi_\lambda, (H_0 + V)\psi_\lambda\rangle = \langle\psi_\lambda, H_0\psi_\lambda\rangle + \langle\psi_\lambda, V\psi_\lambda\rangle,$$

the other equality follows. □

Corollary 6.2.9. *Let V and α be as in the virial theorem.*

a) *If $\alpha < 2$, then all eigenvalues of H are negative and, if also $V \geq 0$, then H has no eigenvalues.*
b) *The Schrödinger operator $H_0 + V$ with the negative power potential (Example 6.2.3)*

$$V(x) = -\frac{\kappa}{|x|^\alpha}, \qquad 0 < \alpha < 3/2,$$

in $L^2(\mathbb{R}^3)$ has no eigenvalues if $\kappa < 0$ and all its eigenvalues are negative if $\kappa > 0$ (note that the H-atom is a particular case).

Proof. It is enough to recall that H_0 is a positive operator, to note that

$$U_d(-s)VU_d(s) = e^{-\alpha s}V$$

and apply the conclusions of Theorem 6.2.8. For instance, if $\alpha < 2$ and λ is an eigenvalue of H, then the relation

$$\lambda = \left(1 - \frac{2}{\alpha}\right) \langle \psi_\lambda, H_0 \psi_\lambda \rangle$$

implies $\lambda < 0$. □

Exercise 6.2.10. Look for an eigenfunction of the hydrogen atom hamiltonian in the form $\psi(x) = e^{-a|x|}$, for some $a > 0$. Find the corresponding eigenvalue, which is the lowest possible energy value ("ground level" in the physicists' nomenclature) of the electron (see, for instance, [Will03]).

Exercise 6.2.11. Verify the relation $U_d(-s)H_0U_d(s) = e^{-2s}H_0$, and that

$$U_d(s)\text{dom } H_0 = \text{dom } H_0, \quad \forall\, s \in \mathbb{R}.$$

Exercise 6.2.12. Consider the energy expectation value (see the discussion in Section 14.1)

$$\mathcal{E}^\psi = \langle \psi, H_0\psi \rangle + \langle \psi, V\psi \rangle, \qquad \psi \in C_0^\infty(\mathbb{R}^n),$$

and let $\psi(s) = U_d(s)\psi$. By taking appropriate values of s, show that

$$\inf_{\|\psi\|=1} \mathcal{E}^\psi = -\infty$$

in case $V(x) = -1/|x|^\alpha$ and $\alpha > 2$. Comment on the physical meaning of this result – see Remark 11.4.9.

Example 6.2.13. The condition $U_d(-s)VU_d(s) = e^{-\alpha s}V$ in the virial theorem is not strictly necessary. Consider the bounded potential

$$V_a(x) = -\frac{\kappa}{|x| + a}, \qquad a > 0,$$

acting on $L^2(\mathbb{R})$. Then $U_d(-s)V_aU_d(s) = e^{-s}V_{e^{-s}a}$; if $H\psi_\lambda = \lambda\psi_\lambda$, by following the proof of Theorem 6.2.8 one gets

$$0 \le \langle \psi_\lambda, H_0\psi_\lambda\rangle = \frac{1}{2\kappa}\langle \psi_\lambda, |x|V_a^2\psi_\lambda\rangle,$$

and if $\kappa < 0$ the operator $H = H_0 + V_a$ has no eigenvalues.

Exercise 6.2.14. Present the missing details in Example 6.2.13.

The virial theorem is closely related to its version in classical mechanics. Both relate averages of the potential energy and kinetic energy, and was originally considered by Clausius in the investigation of problems in molecular physics (recall that average kinetic energy is directly related to temperature in equilibrium statistical mechanics). Restricting to dimension 1, Clausius considered the classical quantity $G = xp$, the so-called *virial*; note that in the quantum version this quantity corresponds to the infinitesimal generator of $U_d(s)$ – see Example 5.4.8. Some domain issues are avoided by working directly with the unitary group $U_d(s)$ (as in the virial theorem above) instead of its infinitesimal generator. It has applications to thermodynamics and astrophysics, among others. For several aspects of the quantum virial theorem the reader is referred to [GeoG99].

6.2.2 KLMN: Applications

Let b^{H_0} be the (closed and positive) form generated by the free hamiltonian $H_0 = -\Delta$ in $L^2(\mathbb{R}^n)$, so that

$$b^{H_0}(\psi,\phi) = \langle \psi, -\Delta\phi\rangle, \qquad \forall\psi \in \text{dom } b^{H_0}, \forall\phi \in \text{dom } H_0.$$

According to Examples 4.2.11 and 9.3.9, dom $b^{H_0} = \mathcal{H}^1(\mathbb{R}^n)$ and

$$b^{H_0}(\psi,\phi) = \langle \nabla\psi, \nabla\phi\rangle, \qquad \forall\psi,\phi \in \text{dom } b^{H_0}.$$

The following three examples consider form perturbations of b^{H_0}.

Example 6.2.15. In $L^2(\mathbb{R}^3)$ the Kato-Rellich theorem allows the definition of a self-adjoint realization of $H_0 + V$ for

$$V(x) = -\frac{\kappa}{|x|^\alpha}, \qquad 0 < \alpha < 3/2,$$

since such potential belongs to $L^2 + L^\infty$. The KLMN theorem can be used to give meaning also for $3/2 \le \alpha < 2$.

Let b_α be the form generated by $|x|^{-\alpha}$. Fix $0 < \alpha < 2$ and note that dom $b_\alpha \supset$ dom b^{H_0} in this case; given $a > 0$, choose $\varepsilon > 0$ so that $|x|^{-\alpha} \le a|x|^{-2}/4$ for all

$|x| \le \varepsilon$. By Hardy's Inequality 4.4.16, for all $\psi \in \operatorname{dom} b^{H_0} = \mathcal{H}^1(\mathbb{R}^3)$,

$$\begin{aligned} b_\alpha(\psi) &= \int_{\mathbb{R}^3} \frac{|\psi(x)|^2}{|x|^\alpha}\,dx = \int_{|x|\le\varepsilon} \frac{|\psi(x)|^2}{|x|^\alpha}\,dx + \int_{|x|>\varepsilon} \frac{|\psi(x)|^2}{|x|^\alpha}\,dx \\ &\le a\int_{|x|\le\varepsilon} \frac{|\psi(x)|^2}{4|x|^2}\,dx + \frac{1}{\varepsilon^\alpha}\int_{|x|>\varepsilon} |\psi(x)|^2\,dx \\ &\le a\int_{\mathbb{R}^3} \frac{|\psi(x)|^2}{4|x|^2}\,dx + \frac{1}{\varepsilon^\alpha}\int_{\mathbb{R}^3} |\psi(x)|^2\,dx \\ &\le a\int_{\mathbb{R}^3} |\nabla\psi(x)|^2\,dx + \frac{1}{\varepsilon^\alpha}\int_{\mathbb{R}^3} |\psi(x)|^2\,dx \\ &= a\,b^{H_0}(\psi) + \frac{1}{\varepsilon^\alpha}\|\psi\|^2. \end{aligned}$$

Since $a > 0$ was arbitrary in the above inequality, the b^{H_0}-bound of b_α is zero. Hence the KLMN Theorem 6.1.17 defines a self-adjoint realization of $H_0 - \kappa/|x|^\alpha$ in $\mathrm{L}^2(\mathbb{R}^3)$, $0 < \alpha < 2$, given by the operator associated with $b^{H_0} + b_\alpha$.

Example 6.2.16 (Delta-function potential in $\mathbb{R}$). In $\mathrm{L}^2(\mathbb{R})$, perturb the free form $b^{H_0}(\psi,\phi) = \langle\psi',\phi'\rangle$ by the nonclosable form $b_\delta(\psi,\phi) = \overline{\psi(0)}\,\phi(0)$ of Example 4.1.15, which simulates a Dirac delta interaction at the origin. Here $\operatorname{dom} b_\delta = \operatorname{dom} b^{H_0} = \mathcal{H}^1(\mathbb{R})$. The KLMN theorem permits the association of a self-adjoint operator with the form

$$b^{H_0} + \alpha b_\delta, \qquad \alpha \in \mathbb{R},$$

with domain $\mathcal{H}^1(\mathbb{R})$; see also Example 4.4.9.

In fact, if $\psi \in \mathcal{H}^1(\mathbb{R})$ one has $\psi(x) \to 0$ as $|x| \to \infty$, and by using Lemma 6.1.3 with $s = t = 1, \varepsilon = r^2$, for all $M > 0$,

$$\begin{aligned} |b_\delta(\psi)| &= |\psi(0)|^2 \le \big||\psi(0)|^2 - |\psi(M)|^2\big| + |\psi(M)|^2 \\ &= \left|\int_0^M \frac{d}{dx}|\psi(x)|^2\,dx\right| + |\psi(M)|^2 \\ &= \left|\int_0^M \left(\overline{\psi'(x)}\,\psi(x) + \overline{\psi(x)}\,\psi'(x)\right) dx\right| + |\psi(M)|^2 \\ &\le |\psi(M)|^2 + 2\|\psi'\|\,\|\psi\| \le |\psi(M)|^2 + \varepsilon\,\|\psi'\|^2 + \frac{1}{\varepsilon}\,\|\psi\|^2 \\ &\xrightarrow{M\to\infty} \varepsilon\,\|\psi'\|^2 + \frac{1}{\varepsilon}\,\|\psi\|^2 = \varepsilon\,b^{H_0}(\psi) + \frac{1}{\varepsilon}\,\|\psi\|^2. \end{aligned}$$

Since $\varepsilon > 0$ is arbitrary, it follows that the b^{H_0}-bound of αb_δ is zero for all $\alpha \in \mathbb{R}$. By KLMN theorem, there is a unique self-adjoint operator T_α with $\operatorname{dom} T_\alpha \sqsubseteq \mathcal{H}^1(\mathbb{R})$, whose form domain is $\mathcal{H}^1(\mathbb{R})$, and

$$\langle\psi, T_\alpha\phi\rangle = \langle\psi',\phi'\rangle + \alpha\overline{\psi(0)}\phi(0), \qquad \forall\psi \in \mathcal{H}^1(\mathbb{R}), \phi \in \operatorname{dom} T_\alpha.$$

Further, T_α is lower bounded.

Exercise 6.2.17. If $\alpha < 0$, verify that $e^{\alpha|x|/2}$ is an eigenvector of T_α in Example 6.2.16, whose corresponding eigenvalue is $-\alpha^2/4$.

Remark 6.2.18. In the KLMN theorem it is strictly necessary that $a < 1$. In fact, one has $|-b^{H_0}| \le b^{H_0} + b_\delta$ (so $a = 1$) but the "perturbed" form $(b^{H_0} + b_\delta) - b^{H_0} = b_\delta$ is not closable.

Example 6.2.19. Let ν be a positive Radon measure in $\mathbb{R}^n$, that is, a Borel, finite on compact sets and regular measure. Under suitable conditions, the KLMN theorem will be used to give meaning to the operator

$$H = H_0 + \alpha\nu,$$

that is, the interaction potential is ruled by the measure ν with intensity $\alpha \in \mathbb{R}$, as proposed in [BraEK94]. The "interaction" form $b^{\alpha,\nu}$ associated with this "potential" is introduced by the expression

$$b^{\alpha,\nu}(\psi, \phi) = \alpha \int_{\mathbb{R}^n} \overline{\psi(x)}\phi(x)\, d\nu(x).$$

Singular (with respect to Lebesgue measure) ν are the most interesting cases, but in view of the KLMN theorem one faces the difficulty of getting $\operatorname{dom} b^{\alpha,\nu} \supset \operatorname{dom} b^{H_0} = \mathcal{H}^1(\mathbb{R}^n)$, since the elements of $\mathcal{H}^1(\mathbb{R}^n)$ are not necessarily continuous and the restriction to the support of ν can be meaningless. The idea is to define $b^{\alpha,\nu}$ as above initially on $C_0^\infty(\mathbb{R}^n)$, and assume that ν is such that there are $0 \le a < 1$ and $c \ge 0$ so that (see Remark 6.2.20)

$$(1 + |\alpha|) \int_{\mathbb{R}^n} |\psi(x)|^2\, d\nu(x) \le a \int_{\mathbb{R}^n} |\nabla\psi(x)|^2\, dx + c \int_{\mathbb{R}^n} |\psi(x)|^2\, dx$$

for all $\psi \in C_0^\infty(\mathbb{R}^n)$. Since $C_0^\infty(\mathbb{R}^n)$ is dense in $\mathcal{H}^1(\mathbb{R}^n)$, the map $J : C_0^\infty(\mathbb{R}^n) \to \mathrm{L}^2_\nu(\mathbb{R}^n)$, $J\psi = \psi$, has a unique extension to a continuous linear map (also denoted by J; note that ψ is being used to denote elements in both equivalence classes $\mathrm{L}^2(\mathbb{R}^n)$ and $\mathrm{L}^2_\nu(\mathbb{R}^n)$)

$$J : \mathcal{H}^1(\mathbb{R}^n) \to \mathrm{L}^2_\nu(\mathbb{R}^n),$$

and, by continuity, the above inequality holds for all $\psi \in \mathcal{H}^1(\mathbb{R}^n)$, that is,

$$(1 + |\alpha|) \int_{\mathbb{R}^n} |J\psi(x)|^2\, d\nu(x) \le a \int_{\mathbb{R}^n} |\nabla\psi(x)|^2\, dx + c \int_{\mathbb{R}^n} |\psi(x)|^2\, dx.$$

Finally, the precise definition of the interaction form $b^{\alpha,\nu}$ is presented: $\operatorname{dom} b^{\alpha,\nu} = \mathcal{H}^1(\mathbb{R}^n)$ and for $\psi, \phi \in \operatorname{dom} b^{\alpha,\nu}$,

$$b^{\alpha,\nu}(\psi, \phi) := \alpha \int_{\mathbb{R}^n} \overline{J\psi(x)}\, J\phi(x)\, d\nu(x).$$

For $\psi \in \mathcal{H}^1(\mathbb{R}^n)$, one then has

$$\begin{aligned}|b^{\alpha,\nu}(\psi)| &= |\alpha| \int_{\mathbb{R}^n} |J\psi(x)|^2 \, d\nu(x) \\ &\leq \frac{a|\alpha|}{1+|\alpha|} \int_{\mathbb{R}^n} |\nabla\psi(x)|^2 \, dx + \frac{c|\alpha|}{1+|\alpha|} \int_{\mathbb{R}^n} |\psi(x)|^2 \, dx \\ &= \frac{a|\alpha|}{1+|\alpha|} b^{H_0}(\psi) + \frac{c|\alpha|}{1+|\alpha|} \|\psi\|^2.\end{aligned}$$

Since $a|\alpha|/(1+|\alpha|) < 1$, for such measures ν the KLMN Theorem 6.1.17 provides a self-adjoint realization of $H_0 + \alpha\nu$ rigorously defined by the operator associated with $b^{H_0} + b^{\alpha,\nu}$.

Remark 6.2.20. Sufficient conditions for the above inequality to be valid for positive Radon measures ν in $\mathbb{R}^n$ appear in [StoV96]: e.g., all finite measures over $\mathbb{R}$,

$$\lim_{\varepsilon\downarrow 0} \sup_{x\in\mathbb{R}^2} \int_{B(x;\varepsilon)} |\ln|x-y|| \, d\nu(y) = 0, \qquad n = 2,$$

and

$$\lim_{\varepsilon\downarrow 0} \sup_{x\in\mathbb{R}^n} \int_{B(x;\varepsilon)} \frac{1}{|x-y|^{n-2}} \, d\nu(y) = 0, \qquad n \geq 3.$$

Particular interesting cases are $\nu = \mu^{\mathcal{C}}$, that is, a measure concentrated on the ternary Cantor set in $\mathbb{R}$ (see Example 12.2.13), and when ν is supported by smooth curves and other manifolds in $\mathbb{R}^n$, which is part of the set of so-called *leaky quantum graphs*.

6.2.3 Some $\mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ Potentials

Theorem 6.2.21. *Let $V : \mathbb{R}^n \to \mathbb{R}$ be a measurable potential and $\overline{B}_x = \overline{B}(x;1)$ denote the closed ball of center $x \in \mathbb{R}^n$ and radius 1.*

a) *If* dom $H_0 \subset$ dom V*, then*

$$d(V) := \sup_{x\in\mathbb{R}^n} \int_{\overline{B}_x} |V(y)|^2 \, dy < \infty,$$

in particular $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$.

b) *If* dom $H_0 \subset$ dom V *and* $\limsup_{|x|\to\infty} |V(x)| = s < \infty$*, then $V \in \mathrm{L}^2(\mathbb{R}^n) + \mathrm{L}^\infty(\mathbb{R}^n)$.*

Proof. a) Since V is a closed operator and $\rho(H_0) \neq \emptyset$, by Lemma 6.1.4 there is $c > 0$ so that

$$\|V\psi\|^2 \leq c\left(\|H_0\psi\|^2 + \|\psi\|^2\right), \qquad \forall\psi \in \operatorname{dom} H_0.$$

If $x \in \mathbb{R}^n$, pick $\phi \in C_0^\infty(\mathbb{R}^n)$ so that $\phi(y) = 1$ for $y \in \overline{B}_0$, and set $\phi_x(y) = \phi(y-x)$. Thus,

$$\begin{aligned}\int_{\overline{B}_x} |V(y)|^2\, dy \le \|V\phi_x\|^2 \le c\left(\|H_0\phi_x\|^2 + \|\phi_x\|^2\right) \\ = c\left(\|H_0\phi\|^2 + \|\phi\|^2\right) < \infty,\end{aligned}$$

and note that this upper bound does not depend on x. Hence $d(V) < \infty$.

b) Let $E_s = \{x \in \mathbb{R}^n : |V(x)| \le 2s\}$, $V_\infty = V\chi_{E_s}$ and $V_2 = V\chi_{E_s^c}$, with $E_s^c = \mathbb{R}^n \setminus E_s$. Then $V = V_2 + V_\infty$, $V_\infty \in \mathrm{L}^\infty(\mathbb{R}^n)$ and, by the definition of s, there exists $R > 0$ so that $V_2(x) = 0$ if $x \notin \overline{B}(0; R)$. Pick $\phi \in C_0^\infty(\mathbb{R}^n)$ so that $\phi(x) = 1$ for $x \in \overline{B}(0; R)$; then $\phi \in \mathrm{dom}\ H_0 \subset \mathrm{dom}\ \mathcal{M}_V$ and

$$\|V_2\|^2 = \int_{\mathbb{R}^n} |V_2(x)|^2\, |\phi(x)|^2\, dx = \|V_2\phi\|^2 \le \|V\phi\|^2 < \infty,$$

so that $V_2 \in \mathrm{L}^2(\mathbb{R}^n)$. □

Exercise 6.2.22. Show that if $\limsup_{|x|\to\infty} |V(x)| = 0$ in Theorem 6.2.21, then the $\mathrm{L}^\infty(\mathbb{R}^n)$ part of V can be chosen with arbitrarily small L^∞ norm.

Theorem 6.2.23. *Let V and $d(V)$ be as in Theorem* 6.2.21*. Then for $n = 1$, i.e., in* $\mathrm{L}^2(\mathbb{R})$*, the following assertions are equivalent:*

a) $\mathrm{dom}\ H_0 \subset \mathrm{dom}\ V$.
b) $d(V) < \infty$.
c) *V is H_0-bounded.*
d) *V is H_0-bounded with $N_{H_0}(V) = 0$.*

Proof. The implications a) ⇒ c) ⇒ b) were already discussed in the proof of Theorem 6.2.21. d) ⇒ a) is clear. It is only needed to show that b) ⇒ d).

Assume that b) holds. If $\psi \in \mathrm{dom}\ H_0 = \mathcal{H}^2(\mathbb{R})$, then ψ is continuous and continuously differentiable. Assume first that ψ is real valued. By using an idea in Lemma 6.1.3, given $\varepsilon > 0$ for $z, y \in \overline{B}_x$, one has

$$\begin{aligned}\psi(y)^2 - \psi(z)^2 &= \int_z^y \left(\psi(t)^2\right)'\, dt = 2\int_z^y \psi(t)\,\psi'(t)\, dt \\ &\le \frac{1}{\varepsilon}\int_{\overline{B}_x} \psi(t)^2\, dt + \varepsilon\int_{\overline{B}_x} \psi'(t)^2\, dt.\end{aligned}$$

By the mean value theorem, choose $z \in \overline{B}_x$ so that $\psi(z)^2 = \int_{\overline{B}_x} \psi(t)^2\, dt$, thus

$$\psi(y)^2 \le \left(1 + \frac{1}{\varepsilon}\right)\int_{\overline{B}_x} \psi(t)^2\, dt + \varepsilon\int_{\overline{B}_x} \psi'(t)^2\, dt.$$

For complex $\psi \in \mathcal{H}^2(\mathbb{R})$ one gets, for all $\varepsilon > 0$ and all $x \in \mathbb{R}$,

$$|\psi(y)|^2 \le \left(1 + \frac{1}{\varepsilon}\right)\int_{\overline{B}_x} |\psi(t)|^2\, dt + \varepsilon\int_{\overline{B}_x} |\psi'(t)|^2\, dt.$$

Hence,

$$\int_{\overline{B}_x} |V(y)\psi(y)|^2\,dy \le d(V)\left(1+\frac{1}{\varepsilon}\right)\int_{\overline{B}_x} |\psi(t)|^2\,dt + d(V)\varepsilon\int_{\overline{B}_x} |\psi'(t)|^2\,dt,$$

and so (denote the set of even integers by $2\mathbb{Z}$)

$$\begin{aligned}\|V\psi\|^2 = \int_{\mathbb{R}} |V(y)\psi(y)|^2\,dy &= \sum_{x\in 2\mathbb{Z}} \int_{\overline{B}_x} |V(y)\psi(y)|^2\,dy \\ &\le d(V)\left(1+\frac{1}{\varepsilon}\right)\int_{\mathbb{R}} |\psi(t)|^2\,dt + d(V)\varepsilon\int_{\mathbb{R}} |\psi'(t)|^2\,dt, \\ &\le d(V)\left(1+\frac{1}{\varepsilon}\right)\|\psi\|^2\,dt + d(V)\varepsilon\|\psi'\|^2.\end{aligned}$$

Since $0 \le (p^2-1)^2$ it follows that $p^2 \le (p^4+1)/2 < (p^4+1)$, and then

$$\begin{aligned}\|\psi'\|^2 = \|p\hat\psi(p)\|^2 &= \int_{\mathbb{R}} p^2|\hat\psi(p)|^2\,dp \\ &\le \|p^2\hat\psi(p)\|^2 + \|\hat\psi\|^2 = \|H_0\psi\|^2 + \|\psi\|^2,\end{aligned}$$

and one obtains

$$\|V\psi\|^2 \le \varepsilon\, d(V)\,\|H_0\psi\|^2 + \left(\varepsilon + 1 + \frac{1}{\varepsilon}\right) d(V)\,\|\psi\|^2.$$

Since this holds for all $\varepsilon > 0$, d) follows. □

Hence, in order to apply the Kato-Rellich theorem to conclude that $H := H_0 + V$, with $\mathrm{dom}\, H = \mathrm{dom}\, H_0$, is self-adjoint and $C_0^\infty(\mathbb{R}^n)$ is a core of H, it is necessary that $d(V) < \infty$, and for $n = 1$ this condition is also sufficient.

Example 6.2.24. Let $V_e(x) = e^{|x|}$ and $V_\alpha(x) = |x|^\alpha$, $0 < \alpha < 1/2$, $x \in \mathbb{R}$; then $d(V_e) = \infty$ while $d(V_\alpha) < \infty$. Thus, by Theorem 6.2.23, the operator $H_\alpha := H_0 + V_\alpha$ with domain $\mathcal{H}^2(\mathbb{R})$ is self-adjoint and $C_0^\infty(\mathbb{R})$ is a core of it; however, $H_e := H_0 + V_e$ can not be defined on $\mathcal{H}^2(\mathbb{R})$, although $C_0^\infty(\mathbb{R})$ is a core of H_e by Corollary 6.3.5.

Exercise 6.2.25. For $x \in \mathbb{R}$, let

$$\phi(x) = \begin{cases} 1/\sqrt{|x|}, & \text{if } |x| \le 1 \\ 0, & \text{if } |x| > 1 \end{cases}.$$

Consider the enumeration of rational numbers $\mathbb{Q} = (r_j)_{j=1}^\infty$ and the potential $V(x) := \sum_{j=1}^\infty \phi(x - r_j)/2^j$. Show that:

a) $V \in \mathrm{L}^1(\mathbb{R})$ and V is not L^2 over any open interval in $\mathbb{R}$.
b) If $\psi \in (\mathrm{dom}\, V \cap C(\mathbb{R}))$, show that $\psi \equiv 0$.

Conclude then that $\mathrm{dom}\, H_0 \cap \mathrm{dom}\, V = \{0\}$.

Exercise 6.2.26. Discuss for which dimensions n (i.e., spaces $\mathrm{L}^2(\mathbb{R}^n)$) each of the potentials $V_m(x) = |x|$, $V_l(x) = \ln|x|$ and $V_c(x) = -|x|^{-1}$ have $d(V) < \infty$.

Remark 6.2.27. Note that $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ is the minimum requirement for $V\psi$ to be an element of $\mathrm{L}^2(\mathbb{R}^n)$ with $\psi \in C_0^\infty(\mathbb{R}^n)$. It is shown in Section 6.3 that if $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ and is bounded from below $V(x) \geq \beta$, then the operator $H = H_0 + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

6.3 Kato's Inequality and Pointwise Positivity

An outstanding distributional inequality due to Kato will be discussed (the original reference is [Kat72]; see also [Sim79]). It involves functions and here applications are restricted to standard hamiltonians in the Hilbert space $\mathrm{L}^2(\mathbb{R}^n)$. It will be used to show that lower bounded $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ leads to essentially self-adjoint hamiltonians $-\Delta + V$ with domain $C_0^\infty(\mathbb{R}^n)$. See Subsection 9.3.1 for other applications. In this section a.e. refers to Lebesgue measure.

Definition 6.3.1. A distribution u in $\mathbb{R}^n$ is *positive* if $u(\phi) \geq 0$ for all test functions $\phi \in C_0^\infty(\mathbb{R}^n)$ with $\phi(x) \geq 0$, $\forall x \in \mathbb{R}^n$. This fact will be denoted by $u \geq 0$ and $u \geq v$ will indicate $(u - v) \geq 0$.

Example 6.3.2.

a) If $F : \mathbb{R}^n \to [0, \infty)$ is continuous, then the distribution $u_F(\phi) = \int F(x)\phi(x)dx$, $\phi \in C_0^\infty(\mathbb{R}^n)$, is positive.

b) If $u_n \geq 0$, $\forall n$, and $u_n \to u$ in the distributional sense (i.e., $u_n(\phi) \to u(\phi)$, $\forall \phi \in C_0^\infty$), then $u \geq 0$.

If $\psi \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$, define the function $(\operatorname{sgn}\psi)(x) := 0$ if $\psi(x) = 0$, otherwise set

$$(\operatorname{sgn}\psi)(x) := \frac{\overline{\psi(x)}}{|\psi(x)|},$$

which belongs to $\mathrm{L}^\infty(\mathbb{R}^n)$ and $|\psi(x)| = \psi(x)(\operatorname{sgn}\psi)(x)$ (this is the motivation for introducing the function sgn). Given $\varepsilon > 0$, denote $\psi_\varepsilon(x) := \left(|\psi(x)|^2 + \varepsilon^2\right)^{1/2}$, which converges $\psi_\varepsilon(x) \to |\psi(x)|$ pointwise as $\varepsilon \to 0$. Denote also $\operatorname{sgn}_\varepsilon\psi(x) := \overline{\psi(x)}/\psi_\varepsilon(x)$. In the following, the derivatives of $\mathrm{L}^1_{\mathrm{loc}}$ functions mean distributional derivatives.

Theorem 6.3.3 (Kato's Inequality). *If both* $u, \Delta u$ *are elements of* $\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$*, then* $(\operatorname{sgn} u)\Delta u \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$*, so it defines a distribution, and*

$$\Delta((\operatorname{sgn} u)u) = \Delta|u| \geq \operatorname{Re}\,((\operatorname{sgn} u)\Delta u),$$

that is to say,

$$\int_{\mathbb{R}^n} |u(x)|\Delta\phi(x)\,dx \geq \int_{\mathbb{R}^n} ((\operatorname{sgn} u)\Delta u(x))\,\phi(x)\,dx$$

for all $0 \leq \phi \in C_0^\infty(\mathbb{R}^n)$.

Example 6.3.4. It is instructive to play with some standard functions $u : \mathbb{R} \to \mathbb{C}$ in this inequality. For instance:

1. If $u(x) = e^{ax+ibx}$, $a, b \in \mathbb{R}$, then a straight computation shows that Kato's inequality reads $a^2 e^{ax} \geq (a^2 - b^2)e^{ax}$.
2. If $u(x) = x$, then Kato's inequality expresses that the Dirac delta distribution is positive, i.e., $\delta(x) \geq 0$.
3. If $u(x) = x^3$, then it turns into an equality $6|x| = 6|x|$.

We leave it as an exercise to check details in the above statements.

A very important consequence of this inequality implies that some standard Schrödinger operators in $\mathrm{L}^2(\mathbb{R}^n)$ are well posed; recall $H_0 = -\Delta$.

Corollary 6.3.5. *If there is $\beta \in \mathbb{R}$ so that $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ satisfies $V(x) \geq \beta$, $\forall x \in \mathbb{R}^n$, then the operator*

$$H\psi := H_0\psi + V\psi, \qquad \psi \in \mathrm{dom}\ H = C_0^\infty(\mathbb{R}^n),$$

is essentially self-adjoint.

Remark 6.3.6. The domain and action of the unique self-adjoint extension of H in Corollary 6.3.5 are described in Corollary 9.3.17, and its domain can be strictly smaller than dom $H_0 = \mathcal{H}^2(\mathbb{R}^n)$, even for $n = 1$; see Example 6.2.24.

Example 6.3.7. a) The operator $H_0 + \kappa/|x|$, $\kappa > 0$, with domain $C_0^\infty(\mathbb{R}^3)$ is essentially self-adjoint. Compare with Example 6.2.3 where negative κ is allowed.

b) The operator $H_0 + \kappa/|x|^j$, $j, \kappa > 0$, with domain $C_0^\infty(\mathbb{R}^n)$ is essentially self-adjoint if $n \geq 2j + 1$.

Remark 6.3.8. Note the great generality of Corollary 6.3.5, since the operator sum $H = -\Delta + V$ is defined on $C_0^\infty(\mathbb{R}^n)$ iff $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$; hence, if V is bounded from below, then H is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$ iff it is defined (as a sum of operators)!

Before proceeding to proofs, a rough idea and figurative arguments of how Theorem 6.3.3 can be used to get Corollary 6.3.5 are presented. Let $\lambda \in \mathbb{R}$ obeying $\lambda + \beta > 0$; so $V + \lambda > 0$. By Proposition 2.2.4iii), to show that the deficiency index $n_\pm(H) = 0$, it will suffice to show that the solution of

$$(H_0 + V + \lambda\mathbf{1})^*\, u = 0, \qquad u \in \mathrm{L}^2(\mathbb{R}^n) \subset \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n),$$

is solely $u = 0$ (recall that $(\mathrm{rng}\ T)^\perp = \mathrm{N}(T^*)$). Since H_0 is a positive operator, one could guess that $H_0|u| \geq 0$; the positivity of $V + \lambda$ and Kato's inequality will imply $H_0|u| \leq 0$, so that $H_0|u| = 0$ and, since $u \in \mathrm{L}^2$, $u = 0$. Now the proofs.

An important step in the proof of Kato's inequality is first to prove it when u is smooth, and then use the so-called mollifiers to create sequences of smooth functions, via convolutions, approximating certain distributions and nonsmooth functions.

Let $m \in C_0^\infty(\mathbb{R}^n)$, $m(x) \geq 0, \forall x$, with $\int_{\mathbb{R}^n} m(x)\, dx = 1$ (i.e., m is normalized). Given $r \neq 0$ (usually $r > 0$) set

$$m_r(x) := \frac{1}{r^n} m\left(\frac{x}{r}\right), \qquad u^{(r)} := u * m_r,$$

where $*$ denotes the convolution, which was recalled in Section 3.1. The family $r \mapsto m_r$ is called a *mollifier* and m a *mollifier generator*. The standard example of mollifier a generator is

$$m(x) = C \exp\left(-\frac{1}{1-x^2}\right), \qquad |x| < 1,$$

and $m(x) = 0$ for $|x| \geq 1$; C is just a normalization constant. Thus, $\int m_r(x) dx = 1$, $u^{(r)} \in C^\infty(\mathbb{R}^n)$ for all $u \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$, $r \neq 0$, and, by Lemma 6.3.9,

$$\Delta(u^{(r)})_\varepsilon \; \geq \; \mathrm{Re} \; \left(\mathrm{sgn}_\varepsilon(u^{(r)})\, \Delta u^{(r)}\right).$$

Lemma 6.3.9. *For any $v \in C^\infty(\mathbb{R}^n)$ one has, pointwise and in the distributional sense,*

$$\Delta v_\varepsilon \; \geq \; \mathrm{Re} \; (\mathrm{sgn}_\varepsilon(v)\, \Delta v)\,.$$

Proof. Clearly $|v_\varepsilon| \geq |v|$. On differentiating $v_\varepsilon^2 = |v|^2 + \varepsilon^2$ one gets $2v_\varepsilon \nabla v_\varepsilon = \overline{v} \nabla v + v \nabla \overline{v} = 2\mathrm{Re}\,(\overline{v}\, \nabla v)$. This expression will derive two relations. The first one is obtained by taking the divergence of it:

$$|\nabla v_\varepsilon|^2 + v_\varepsilon\, \Delta v_\varepsilon = \mathrm{Re}\,(\overline{v}\, \Delta v) + |\nabla v|^2.$$

The second one is

$$|\nabla v_\varepsilon| = \frac{|\mathrm{Re}\,(\overline{v}\, \nabla v)|}{|v_\varepsilon|} \leq \frac{|\overline{v}\, \nabla v|}{|v|} \leq |\nabla v|.$$

Combine these two relations to get

$$v_\varepsilon\, \Delta v_\varepsilon \geq \mathrm{Re}\,(\overline{v}\, \Delta v) \Longrightarrow \Delta v_\varepsilon \geq \mathrm{Re}\; ((\mathrm{sgn}_\varepsilon v) \Delta v)$$

pointwise; thus, for every $0 \leq \phi \in C_0^\infty(\mathbb{R}^n)$,

$$\int_{\mathbb{R}^n} v_\varepsilon \Delta\phi\, dx = \int_{\mathbb{R}^n} \Delta v_\varepsilon\, \phi\, dx \geq \mathrm{Re} \int_{\mathbb{R}^n} (\mathrm{sgn}_\varepsilon(v)\, \Delta v)\, \phi\, dx,$$

and the inequality also holds in the distributional sense. □

Exercise 6.3.10. If $\phi \in C_0^\infty(\mathbb{R}^n)$, write

$$\phi(x) - \phi^{(r)}(x) = \int_{\mathbb{R}^n} (\phi(x) - \phi(x-y))\; m_r(y)\, dy,$$

for a fixed mollifier generator m, and use the uniform continuity of ϕ to show that $\lim_{r \downarrow 0} \|\phi^{(r)} - \phi\|_\infty = 0$.

Lemma 6.3.11.

a) *For any* $r > 0$ *the linear map* $\mathrm{L}^p(\mathbb{R}^n) \mapsto \mathrm{L}^p(\mathbb{R}^n)$, $u \mapsto u^{(r)}$, *is bounded and with norm* ≤ 1, *for all* $1 \leq p < \infty$.

b) *If* $u \in \mathrm{L}^p(\mathbb{R}^n)$, $1 \leq p < \infty$, *then* $\lim_{r\downarrow 0} \|u^{(r)} - u\|_p = 0$.

c) *If* $u \in \mathrm{L}^p(\mathbb{R}^n)$, $1 \leq p < \infty$, *then* $\Delta u^{(r)} \in \mathrm{L}^p(\mathbb{R}^n)$, $\forall r > 0$ (*the laplacian can be replaced by any derivative*).

d) *If* $u \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$, *then* $u^{(r)} \to u$ *in the distributional sense as* $r \downarrow 0$.

Proof. a) Since $m_r \in \mathrm{L}^1(\mathbb{R}^n)$, for $u \in \mathrm{L}^p(\mathbb{R}^n)$ it follows by Young's inequality (Proposition 3.1.9) that (take "$r = p$" in Young's inequality)

$$\|u^{(r)}\|_p = \|u * m_r\|_p \leq \|u\|_p \|m_r\|_1 = \|u\|_p.$$

b) If $\phi \in C_0^\infty(\mathbb{R}^n)$ and Ω_ϕ is the support of ϕ, one has

$$\|\phi^{(r)} - \phi\|_p \leq \|\phi^{(r)} - \phi\|_\infty \, \ell(\Omega_\phi)^{\frac{1}{p}},$$

where $\ell(\cdot)$ denotes Lebesgue measure over $\mathbb{R}^n$. Hence $\|\phi^{(r)} - \phi\|_p \to 0$ as $r \to 0$ (see Exercise 6.3.10). Now take $u \in \mathrm{L}^p(\mathbb{R}^n)$. Given $\varepsilon > 0$, choose $\phi \in C_0^\infty(\mathbb{R}^n)$ so that $\|u - \phi\|_p < \varepsilon$. By triangle inequality and a), for r small enough,

$$\begin{aligned} \|u^{(r)} - u\|_p &\leq \|u^{(r)} - \phi^{(r)}\|_p + \|\phi^{(r)} - \phi\|_p + \|\phi - u\|_p \\ &< \|u - \phi\|_p + \varepsilon + \varepsilon < 3\varepsilon. \end{aligned}$$

Item b) follows.

c) It is a consequence of

$$\frac{\partial}{\partial x_j} u^{(r)} = \frac{\partial}{\partial x_j}(u * m_r) = u * \frac{\partial}{\partial x_j} m_r$$

and Young's inequality, i.e.,

$$\left\| \frac{\partial}{\partial x_j} u^{(r)} \right\|_p \leq \|u\|_p \left\| \frac{\partial}{\partial x_j} m_r \right\|_1 .$$

d) Since $u^{(r)} \in C^\infty(\mathbb{R}^n)$ it also defines a distribution. If $\phi \in C_0^\infty(\mathbb{R}^n)$ and Ω_ϕ is the support of ϕ, a change of variable and Fubini's theorem lead to

$$u^{(r)}(\phi) = \int_{\mathbb{R}^n} u^{(r)}(x)\, \phi(x)\, dx = \int_{\mathbb{R}^n} (-1)^n u(x) \phi^{(-r)}(x)\, dx = (-1)^n u(\phi^{(-r)}),$$

and so

$$\left| u(\phi) - u^{(r)}(\phi) \right| = \left| u\left(\phi - (-1)^n \phi^{(-r)}\right) \right| \leq \left\| \phi - (-1)^n \phi^{(-r)} \right\|_\infty \int_{\Omega_\phi} |u(x)|\, dx.$$

Note that $(-1)^n \phi^{(-r)} = \phi * \tilde{m}_r$, where $\tilde{m}(x) := m(-x)$ also satisfies the assumptions required for $\tilde{m}_r$ to be a mollifier; so $\|\phi - (-1)^n \phi^{(-r)}\|_\infty$ vanishes as $r \to 0$ by Exercise 6.3.10. Therefore, $u^{(r)} \to u$ in the distributional sense. □

Other properties needed to complete the proof of Corollary 6.3.5 will be collected in the following proposition.

Proposition 6.3.12. *Let $u \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$ and $r \downarrow 0$. Then:*

i) *There exists a subsequence $u^{(r)}(x)$ obeying $u^{(r)}(x) \to u(x)$ a.e., and so also $(\operatorname{sgn}_\varepsilon u^{(r)})(x) \to \operatorname{sgn}_\varepsilon u(x)$ a.e.*

ii) *$\Delta u^{(r)} = (\Delta u)^{(r)}$ and, if also $\Delta u \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$, one has $\Delta u^{(r)} \to \Delta u$ in $\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$ (that is, $\int_K |u^{(r)} - u|\, dx \to 0$ for every compact $K \subset \mathbb{R}^n$) and a.e. as well.*

Proof. i) Let m be a mollifier generator with support Ω_m. Let K be a compact subset of $\mathbb{R}^n$ and χ_K its characteristic function. By the definition of convolution and Fubini,

$$\left\| (u^{(r)} - u)\chi_K \right\|_1 \le \int_{\Omega_m} m(y) \, \|(u(x) - u(x - ry))\chi_K\|_1 \, dy.$$

It turns out that $\|(u(x) - u(x - ry))\chi_K\|_1$ vanishes as $r \to 0$ (see the proof of Lemma 13.3.2), and so $\left\|(u^{(r)} - u)\chi_K\right\|_1 \to 0$. Thus, $u^{(r)} \to u$ in $\mathrm{L}^1(K)$, for any compact K. Hence there is a subsequence with a.e. convergence.

ii) After an interchange of integration and differentiation (by dominated convergence), it is simple to verify that $\Delta u^{(r)} = (\Delta u)^{(r)}$. By hypothesis $\Delta u \in \mathrm{L}^1_{\mathrm{loc}}$; so the convergences stated in ii) follow by i). □

Proof. [**Corollary 6.3.5**] Pick λ so that $\lambda + \beta > 0$ and $u \in \operatorname{dom} H^* \subset \mathrm{L}^2(\mathbb{R}^n)$ a solution of $(H + \lambda \mathbf{1})^* u = 0$, which amounts to

$$0 = \langle (H + \lambda\mathbf{1})^* u, \phi \rangle = \langle u, (H + \lambda\mathbf{1})\phi \rangle, \qquad \forall \phi \in C_0^\infty(\mathbb{R}^n),$$

and since $H + \lambda\mathbf{1} = -\Delta + V + \lambda\mathbf{1}$ one finds that, in the distributional sense,

$$0 = -\Delta u + (V + \lambda\mathbf{1})u.$$

Since $u, Vu \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$, it follows that $\Delta u = (V + \lambda\mathbf{1})u \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$ and Theorem 6.3.3 implies

$$\Delta|u| \ge \operatorname{Re}\left((\operatorname{sgn} u)\, \Delta u\right) = \operatorname{Re}\left((\operatorname{sgn} u)\,(V + \lambda\mathbf{1})u\right) = (V + \lambda\mathbf{1})|u| \ge 0.$$

However, $|u|$ is not ensured to belong to dom Δ, and a "regularization process" is necessary. Thus, for any $r > 0$, $\Delta|u|^{(r)} = \Delta|u| * m_r \ge 0$ pointwise and in the distributional sense; also, by Lemma 6.3.11c), $\Delta|u|^{(r)} \in \mathrm{L}^2(\mathbb{R}^n)$ and so

$$\left\langle |u|^{(r)}, \Delta|u|^{(r)} \right\rangle = \int_{\mathbb{R}^n} |u|^{(r)} \Delta|u|^{(r)} \, dx \ge 0.$$

On the other hand, again by Lemma 6.3.11c), $\partial|u|^{(r)}/\partial x_j, \Delta|u|^{(r)} \in \mathrm{L}^2(\mathbb{R}^n)$, consequently $|u|^{(r)} \in \mathcal{H}^2(\mathbb{R}^n) = \operatorname{dom} H_0$ (see Section 3.2); hence (recall $H_0 \ge 0$)

$$\left\langle |u|^{(r)}, \Delta|u|^{(r)} \right\rangle \le 0.$$

Combining with the other inequality one finds $\langle |u|^{(r)}, \Delta|u|^{(r)}\rangle = 0$, and thus $|u|^{(r)} = 0$. Since $u \in \mathrm{L}^2(\mathbb{R}^n)$, by Lemma 6.3.11b) one can consider a subsequence and assume that $|u|^{(r)} \to |u|$ a.e. as $r \downarrow 0$, so that $u = 0$. By Proposition 2.2.4, the deficiency indices of H are null. The corollary is proved. □

Exercise 6.3.13. Use results of Section 3.4 to show that if $\psi \in \operatorname{dom} H_0 = \mathcal{H}^2(\mathbb{R}^n)$ and $\langle \psi, H_0\psi\rangle = 0$, then $\psi = 0$. This was used in the proof of Corollary 6.3.5.

Proof. [**Theorem 6.3.3**] Let $u, \Delta u \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$. Thus, $u^{(r)} \in C^\infty(\mathbb{R}^n)$ and, by Lemma 6.3.9,

$$\Delta(u^{(r)})_\varepsilon \geq \operatorname{Re}\left(\operatorname{sgn}_\varepsilon(u^{(r)})\,\Delta u^{(r)}\right), \qquad \forall \varepsilon, r > 0,$$

that is, for every $0 \leq \phi \in C_0^\infty(\mathbb{R}^n)$,

$$\int_{\mathbb{R}^n} u_\varepsilon^{(r)}\,\Delta\phi\,dx \geq \operatorname{Re}\int_{\mathbb{R}^n} (\operatorname{sgn}_\varepsilon u^{(r)})\,\Delta u^{(r)}\phi\,dx.$$

The point now is to take the limit $r \downarrow 0$ in both terms of this inequality. Since $u, \Delta u \in \mathrm{L}^1_{\mathrm{loc}}$, by Lemma 6.3.11c), d) and Proposition 6.3.12ii), $u^{(r)} \to u$ and $\Delta u^{(r)} = (\Delta u)^{(r)} \to \Delta u$ in $\mathrm{L}^1_{\mathrm{loc}}$ and in the distributional sense. By passing to a subsequence one can suppose that $u^{(r)} \to u$ and $\Delta u^{(r)} = (\Delta u)^{(r)} \to \Delta u$ a.e. Together with the inequality

$$\begin{aligned}
|u_\varepsilon^{(r)} - u_\varepsilon| &= \left|\left(|u^{(r)}|^2 + \varepsilon^2\right)^{1/2} - \left(|u|^2 + \varepsilon^2\right)^{1/2}\right| \\
&= \frac{\left||u^{(r)}|^2 - |u|^2\right|}{\left(|u^{(r)}|^2 + \varepsilon^2\right)^{1/2} + \left(|u|^2 + \varepsilon^2\right)^{1/2}} \\
&\leq \left||u^{(r)}| - |u|\right| \leq \left|u^{(r)} - u\right|
\end{aligned}$$

the convergence $u^{(r)} \to u$ implies that $u_\varepsilon^{(r)} \to u_\varepsilon$ in $\mathrm{L}^1_{\mathrm{loc}}$ and a.e. as $r \downarrow 0$ (for a subsequence), and so

$$\int_{\mathbb{R}^n} u_\varepsilon^{(r)}\,\Delta\phi\,dx \to \int_{\mathbb{R}^n} u_\varepsilon\,\Delta\phi\,dx.$$

Taking into account the uniform boundedness of $\operatorname{sgn}_\varepsilon u^{(r)}$ (that is, $|\operatorname{sgn}_\varepsilon u^{(r)}| \leq 1$) and $\Delta u^{(r)} \to \Delta u$, in a similar way it is found that (for a subsequence)

$$\operatorname{sgn}_\varepsilon(u^{(r)})\left(\Delta u^{(r)} - \Delta u\right) \to 0,$$

in the distributional sense as $r \downarrow 0$. By dominated convergence

$$\int_{\mathbb{R}^n} \operatorname{sgn}_\varepsilon(u^{(r)})\Delta u\,\phi\,dx \to \int_{\mathbb{R}^n} \operatorname{sgn}_\varepsilon(u)\Delta u\,\phi\,dx, \qquad r \to 0.$$

By collecting these convergences and taking the appropriate subsequence $r \downarrow 0$, for $0 \le \phi \in C_0^\infty(\mathbb{R}^n)$,

$$\begin{aligned}\mathrm{Re} \int_{\mathbb{R}^n} (\mathrm{sgn}_\varepsilon u^{(r)})\, \Delta u^{(r)} \phi \, dx &= \mathrm{Re} \int_{\mathbb{R}^n} (\mathrm{sgn}_\varepsilon u^{(r)}) \left(\Delta u^{(r)} - \Delta u\right) \phi \, dx \\ &\quad + \mathrm{Re} \int_{\mathbb{R}^n} (\mathrm{sgn}_\varepsilon u^{(r)})\, \Delta u \phi \, dx \\ &\to \int_{\mathbb{R}^n} \mathrm{sgn}_\varepsilon (u) \Delta u \, \phi \, dx\end{aligned}$$

as $r \downarrow 0$, that is,

$$\int_{\mathbb{R}^n} u_\varepsilon \, \Delta \phi \, dx \ge \mathrm{Re} \int_{\mathbb{R}^n} ((\mathrm{sgn}_\varepsilon u)\, \Delta u) \phi \, dx,$$

which is equivalent to the distributional inequality

$$\Delta u_\varepsilon \ge \mathrm{Re}\, ((\mathrm{sgn}_\varepsilon u)\, \Delta u).$$

Since $u_\varepsilon \to |u|$ uniformly as $\varepsilon \to 0$, the left-hand side in the above integral inequality converges to $\int |u|\, \Delta\phi \, dx$. Now $\mathrm{sgn}_\varepsilon u \to \mathrm{sgn}\, u$ as $\varepsilon \to 0$ and since $|\mathrm{sgn}_\varepsilon \Delta u| \le |\Delta u|$ and $\Delta u \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$, one can apply dominated convergence on the right-hand side of the above integral inequality to get

$$\mathrm{Re} \int_{\mathbb{R}^n} ((\mathrm{sgn}_\varepsilon u)\, \Delta u) \phi \, dx \to \mathrm{Re} \int_{\mathbb{R}^n} ((\mathrm{sgn}\, u)\, \Delta u) \phi \, dx$$

as $\varepsilon \to 0$. Therefore, the final result, i.e., Kato's inequality, follows by taking the limit $\varepsilon \to 0$ in the latter distributional inequality. □

Remark 6.3.14. In [LeiS81] there is a generalization of Corollary 6.3.5 that includes magnetic fields; for an introduction to Schrödinger operators with magnetic fields see Sections 10.5 and 12.4. The Leinfelder-Simader proof also makes use of Kato's inequality and their theorem reads as follows: Let $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ be bounded from below, the components of the magnetic vector potential $A_j \in \mathrm{L}^4_{\mathrm{loc}}(\mathbb{R}^n)$, $j = 1, \ldots, n$, and the distributional divergent $(\sum_j \partial_j A_j) \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$; then the Schrödinger operator with magnetic field

$$H = \sum_{j=1}^n \left(-i \frac{\partial}{\partial x_j} - \frac{e}{c} A_j \right)^2 + V, \qquad \mathrm{dom}\, H = C_0^\infty(\mathbb{R}^n),$$

is essentially self-adjoint.

Chapter 7

Boundary Triples and Self-Adjointness

A simple variation of the not so popular approach to self-adjoint extensions via boundary triples is discussed. The idea is exemplified through a series of examples, including the one-dimensional hydrogen atom, free hamiltonian in an interval and spherically symmetric potentials. At the end, important self-adjoint extensions of a quantum particle hamiltonian in a multiply connected domain are found.

7.1 Boundary Forms

If $T \subset S$ are hermitian operators one has $T \subset S \subset S^* \subset T^*$, that is, any hermitian extension of T is a hermitian restriction of T^*. The larger the domain of a hermitian operator the smaller the domain of its adjoint. The choice of the domain of S has to be properly adjusted in order to get a self-adjoint extension of T; recall also that a self-adjoint operator is maximal, in the sense that it has no proper hermitian extensions.

Definition 7.1.1. Let T be a hermitian operator. The *boundary form* of T is the sesquilinear map $\Gamma = \Gamma_{T^*} : \mathrm{dom}\, T^* \times \mathrm{dom}\, T^* \to \mathbb{C}$ given by

$$\Gamma(\xi, \eta) := \langle T^*\xi, \eta\rangle - \langle \xi, T^*\eta\rangle\,, \qquad \xi, \eta \in \mathrm{dom}\, T^*.$$

$\Gamma(\xi)$ will also denote $\Gamma(\xi, \xi)$.

In case T^* is known, Γ can be used to find the closure of T, that is, $\overline{T}$. Since $\overline{T} = T^{**} \subset T^*$, by the definition of the adjoint operator T^{**} one has that $\xi \in \mathrm{dom}\, \overline{T}$ iff there is $\eta \in \mathcal{H}$ with

$$\langle \xi, T^*\zeta\rangle = \langle \eta, \zeta\rangle\,, \qquad \forall \zeta \in \mathrm{dom}\, T^*,$$

and $\eta = \overline{T}\xi$. Since $\overline{T} \subset T^*$ one has $\eta = T^*\xi$ and so the above relation is equivalent to

$$0 = \Gamma(\xi, \zeta) = \langle T^*\xi, \zeta\rangle - \langle \xi, T^*\zeta\rangle, \qquad \forall \zeta \in \mathrm{dom}\, T^*,$$

which is a (anti)linear equation for $\xi \in \mathrm{dom}\, \overline{T}$.

Exercise 7.1.2. Use the above characterization of $\overline{T}$ to show that the closure of a hermitian operator is also hermitian.

Proposition 7.1.3. *$\Gamma(\xi, \eta) = 0$, $\forall \xi, \eta \in \mathrm{dom}\, T^*$, iff T^* is self-adjoint, that is, iff T is essentially self-adjoint.*

Exercise 7.1.4. Present a proof of Proposition 7.1.3. Hence, the boundary form Γ quantifies the "lack of self-adjointness" of T^*.

Proposition 7.1.5. *If T is hermitian then*

$$\mathrm{dom}\, \overline{T} = \{\xi \in \mathrm{dom}\, T^* : \Gamma(\xi, \eta_\pm) = 0, \forall \eta_\pm \in \mathrm{K}_\pm(T)\}.$$

Proof. Recall that if $\zeta \in \mathrm{dom}\, T^*$, then $\zeta = \eta + \eta_+ + \eta_-$, with $\eta \in \mathrm{dom}\, \overline{T}$, and $\eta_\pm \in \mathrm{K}_\pm(T)$ (the deficiency subspaces). Since $\Gamma(\xi, \eta) = 0$ for all $\xi \in \mathrm{dom}\, T^*, \eta \in \mathrm{dom}\, \overline{T}$, it follows that $\xi \in \mathrm{dom}\, \overline{T}$ iff for all $\zeta \in \mathrm{dom}\, T^*$

$$0 = \Gamma(\xi, \zeta) = \Gamma(\xi, \eta + \eta_+ + \eta_-) = \Gamma(\xi, \eta_+ + \eta_-).$$

The result follows. □

Exercise 7.1.6. Show that an operator S so that $T \subset S \subset T^*$ is hermitian iff $\Gamma(\xi, \eta) = 0$ for all $\xi, \eta \in \mathrm{dom}\, S$.

Let $\zeta^1 = \eta^1 + \eta^1_+ + \eta^1_-$ and $\zeta^2 = \eta^2 + \eta^2_+ + \eta^2_-$, with $\eta^1, \eta^2 \in \mathrm{dom}\, \overline{T}$, $\eta^1_+, \eta^2_+ \in \mathrm{K}_+(T)$, $\eta^1_-, \eta^2_- \in \mathrm{K}_-(T)$, be general elements of $\mathrm{dom}\, T^*$; since $T^*\eta_\pm = \mp i\eta_\pm$, it follows by Theorem 2.2.11 that

$$\Gamma(\zeta^1, \zeta^2) = \Gamma(\eta^1_+ + \eta^1_-, \eta^2_+ + \eta^2_-) = 2i\left(\langle \eta^1_+, \eta^2_+\rangle - \langle \eta^1_-, \eta^2_-\rangle\right).$$

It is then clear that the nonvanishing of Γ is related to the deficiency subspaces. Boundary forms can be used to determine self-adjoint extensions of T by noting that such extensions are restrictions of T^* on suitable domains $\mathcal{D}$ so that $\Gamma(\xi, \eta) = 0, \forall \xi, \eta \in \mathcal{D}$ (Lemma 7.1.7). Recall that each self-adjoint extension of T is related to a unitary operator $\mathcal{U} : \mathrm{K}_-(T) \to \mathrm{K}_+(T)$ onto $\mathrm{K}_+(T)$; denote by $T_\mathcal{U}$ the corresponding self-adjoint extension, whose domain is $\mathrm{dom}\, T_\mathcal{U} = \{\eta = \zeta + \eta_- - \mathcal{U}\eta_- : \zeta \in \mathrm{dom}\, \overline{T}, \eta_- \in \mathrm{K}_-(T)\}$. Then, explicitly one has

Lemma 7.1.7. *The boundary form Γ_{T^*} restricted to* $\mathrm{dom}\, T_\mathcal{U}$ *vanishes identically.*

Proof. For any two elements $\eta = \zeta_1 + \eta_- - \mathcal{U}\eta_-$ and $\xi = \zeta_2 + \xi_- - \mathcal{U}\xi_-$ in $\mathrm{dom}\, T_\mathcal{U}$ ($\zeta_1, \zeta_2 \in \mathrm{dom}\, \overline{T}$) one has

$$\Gamma(\xi, \eta) = 2i\left(\langle \mathcal{U}\xi_-, \mathcal{U}\eta_-\rangle - \langle \xi_-, \eta_-\rangle\right) = 0,$$

which vanishes since $\mathcal{U}$ is unitary. □

Proposition 7.1.8. *Assume that T has self-adjoint extensions. Then each self-adjoint extension of T is of the form*

$$\mathrm{dom}\ T_{\mathcal{U}} = \{\xi \in \mathrm{dom}\ T^* : \Gamma(\xi, \eta_- - \mathcal{U}\eta_-) = 0, \forall \eta_- \in \mathrm{K}_-(T)\},$$

$T_{\mathcal{U}}\xi = T^*\xi$, $\xi \in \mathrm{dom}\ T_{\mathcal{U}}$ *($\mathcal{U}$ as above).*

Proof. If $T_{\mathcal{U}}$ is a self-adjoint extension of T, then $\mathrm{dom}\ T_{\mathcal{U}} = \{\eta = \zeta + \eta_- - \mathcal{U}\eta_- : \zeta \in \mathrm{dom}\ \overline{T}, \eta_- \in \mathrm{K}_-(T)\}$; since Γ restricted to $\mathrm{dom}\ T_{\mathcal{U}}$ vanishes, by Proposition 7.1.5 one has, for $\xi \in \mathrm{dom}\ T_{\mathcal{U}}$,

$$0 = \Gamma(\xi, \zeta + \eta_- - \mathcal{U}\eta_-) = \Gamma(\xi, \eta_- - \mathcal{U}\eta_-), \qquad \forall \eta_- \in \mathrm{K}_-.$$

Hence, $\mathrm{dom}\ T_{\mathcal{U}} \subset A := \{\xi \in \mathrm{dom}\ T^* : \Gamma(\xi, \eta_- - \mathcal{U}\eta_-) = 0, \forall \eta_- \in \mathrm{K}_-(T)\}$.

Now, given $\mathcal{U}$, consider the linear equation for $\zeta + \xi_- + \xi_+ = \xi \in \mathrm{dom}\ T^*$ (of course $\xi_\pm \in \mathrm{K}_\pm(T)$)

$$0 = \Gamma(\xi, \eta_- - \mathcal{U}\eta_-), \qquad \forall \eta_- \in \mathrm{K}_-(T).$$

By Lemma 7.1.7, any $\xi \in \mathrm{dom}\ T_{\mathcal{U}}$ is a solution of this equation. Let $\xi \in \mathrm{dom}\ T^*$ be a solution and write

$$\xi = \zeta + \xi_- - \mathcal{U}\xi_- + \xi_+ + \mathcal{U}\xi_-;$$

thus

$$\begin{aligned} 0 &= \Gamma(\xi, \eta_- - \mathcal{U}\eta_-) = \Gamma(\xi_- - \mathcal{U}\xi_- + \xi_+ + \mathcal{U}\xi_-, \eta_- - \mathcal{U}\eta_-) \\ &= 2i\,(\langle (\xi_+ + \mathcal{U}\xi_-) - \mathcal{U}\xi_-, \mathcal{U}\eta_-\rangle - \langle \xi_-, \eta_-\rangle) \\ &= 2i\,(\langle \xi_+ + \mathcal{U}\xi_-, -\mathcal{U}\eta_-\rangle + \langle \mathcal{U}\xi_-, \mathcal{U}\eta_-\rangle - \langle \xi_-, \eta_-\rangle) \\ &= 2i\,\langle \xi_+ + \mathcal{U}\xi_-, -\mathcal{U}\eta_-\rangle, \qquad \forall \eta_- \in K(T). \end{aligned}$$

Since $\mathrm{rng}\,\mathcal{U} = \mathrm{K}_+$, it follows that $\xi_+ + \mathcal{U}\xi_- = 0$, or $\xi_+ = -\mathcal{U}\xi_-$; thus $\xi = \zeta + \xi_- - \mathcal{U}\xi_- \in \mathrm{dom}\ T_{\mathcal{U}}$ so that $A \subset \mathrm{dom}\ T_{\mathcal{U}}$. Therefore $\mathrm{dom}\ T_{\mathcal{U}} = A$, and the proposition is proved. □

Remark 7.1.9. Note that the specification of the self-adjoint extensions $T_{\mathcal{U}}$ in Proposition 7.1.8 does not require the explicit knowledge of $\overline{T}$; sometimes this can be handy and an advantage over the specification presented in Section 2.5.

Example 7.1.10. As an illustration of the above ideas, the simple case of the momentum differential operator on a bounded interval (a, b) of Example 2.3.14 will be discussed. Let

$$\mathrm{dom}\ P = C_0^\infty(0,1) \sqsubseteq \mathcal{H} = \mathrm{L}^2[0,1],$$

$(P\psi)(x) = -i\psi'(x), \psi \in \mathrm{dom}\ P$. On integrating by parts it is found that P is hermitian. One has $\mathrm{dom}\ P^* = \mathcal{H}^1[0,1]$ and $(P^*\psi)(x) = -i\psi'(x), \psi \in \mathrm{dom}\ P^*$. In this case the boundary form is

$$\Gamma(\psi, \phi) = i\left(\overline{\psi(1)}\phi(1) - \overline{\psi(0)}\phi(0)\right), \qquad \psi, \phi \in \mathrm{dom}\ P^*.$$

By choosing $\psi = \phi \in \mathcal{H}^1[0,1]$ with $\phi(0) = 0$ and $\phi(1) \neq 0$ one has $\Gamma(\phi) \neq 0$, and so P^* is not self-adjoint; consequently P is not essentially self-adjoint. Now ψ is in the domain of the closure $\overline{P}$ iff

$$0 = \Gamma(\psi, \phi) = i\left(\overline{\psi(1)}\phi(1) - \overline{\psi(0)}\phi(0)\right), \qquad \forall \phi \in \mathcal{H}^1[0,1];$$

taking ϕ vanishing at only one end, it follows that $\psi(0) = 0 = \psi(1)$, that is, $\operatorname{dom} \overline{P} = \{\psi \in \mathcal{H}^1[0,1] : \psi(0) = 0 = \psi(1)\}$. For the self-adjoint extensions Proposition 7.1.8 leads exactly to the characterization presented in Example 2.6.5, although now the specification of $\operatorname{dom} \overline{P}$ is not necessary.

7.1.1 Boundary Triples

A boundary triple is an abstraction of the notion of boundary values in function spaces; this idea goes back to Calkin in 1939 [Ca39] and Vishik in 1952 [Vi63].

Definition 7.1.11. Let T be a hermitian operator in $\mathcal{H}$ with $n_-(T) = n_+(T)$. A *boundary triple* $(\mathbf{h}, \rho_1, \rho_2)$ for T is composed of a Hilbert space $\mathbf{h}$ and two linear maps $\rho_1, \rho_2 : \operatorname{dom} T^* \to \mathbf{h}$ with dense ranges and so that

$$a\,\Gamma_{T^*}(\xi, \eta) = \langle \rho_1(\xi), \rho_1(\eta)\rangle - \langle \rho_2(\xi), \rho_2(\eta)\rangle, \ \forall \xi, \eta \in \operatorname{dom} T^*,$$

for some constant $0 \neq a \in \mathbb{C}$. Note that $\langle \cdot, \cdot \rangle$ is also denoting the inner product in $\mathbf{h}$.

In general, given a hermitian operator T with equal deficiency indices, different boundary triples can be associated with it; since for $\zeta^1, \zeta^2 \in \operatorname{dom} T^*$ (by using the above notation)

$$\Gamma(\zeta^1, \zeta^2) = 2i\left(\langle \eta_+^1, \eta_+^2\rangle - \langle \eta_-^1, \eta_-^2\rangle\right),$$

only the deficiency subspaces effectively appear in the boundary form, consequently one may take either $\mathbf{h} = \mathrm{K}_-(T)$ or $\mathbf{h} = \mathrm{K}_+(T)$ (with ρ properly chosen); in this case, say $\mathbf{h} = \mathrm{K}_-(T)$, by von Neumann theory it is known that self-adjoint extensions are in one-to-one relation with unitary operators $\mathcal{U} : \mathrm{K}_-(T) \to \mathrm{K}_+(T)$. However, it is convenient to allow a general $\mathbf{h}$ with $\dim \mathbf{h} = n_+(T)$ (recall that two Hilbert spaces are unitarily equivalent iff they have the same dimension), and Theorem 7.1.13 will adapt von Neumann theory to this situation.

Again, self-adjoint extensions of T are restrictions of T^* on suitable domains $\mathcal{D}$ so that $\Gamma(\xi, \eta) = 0, \forall \xi, \eta \in \mathcal{D}$, and given a boundary triple for T, such $\mathcal{D}$ are related to isometric maps $\hat{\mathcal{U}} : \mathbf{h} \to \mathbf{h}$ (which can be taken to be onto; extend it by continuity, if necessary) so that $\hat{\mathcal{U}}\rho_1(\xi) = \rho_2(\xi)$ and

$$\langle \rho_1(\xi), \rho_1(\eta)\rangle = \langle \rho_2(\xi), \rho_2(\eta)\rangle = \left\langle \hat{\mathcal{U}}\rho_1(\xi), \hat{\mathcal{U}}\rho_1(\eta)\right\rangle,$$

$\forall \xi, \eta \in \mathcal{D}$. Next the linearity of $\hat{\mathcal{U}}$ will be established.

Lemma 7.1.12. *Each $\hat{\mathcal{U}}$ above is a linear and unitary map.*

Proof. Note that rng $\hat{\mathcal{U}} = \mathbf{h}$ and it will suffice to show that this operator is invertible and linear. To simplify the notation, ρ_1 and ρ_2 will not appear in what follows.

If $\hat{\mathcal{U}}(\xi) = \hat{\mathcal{U}}(\eta)$, then

$$\begin{aligned}0 &= \left\langle \hat{\mathcal{U}}(\xi) - \hat{\mathcal{U}}(\eta), \hat{\mathcal{U}}(\xi) - \hat{\mathcal{U}}(\eta) \right\rangle \\ &= \left\langle \hat{\mathcal{U}}(\xi), \hat{\mathcal{U}}(\xi) \right\rangle - \left\langle \hat{\mathcal{U}}(\xi), \hat{\mathcal{U}}(\eta) \right\rangle - \left\langle \hat{\mathcal{U}}(\eta), \hat{\mathcal{U}}(\xi) \right\rangle + \left\langle \hat{\mathcal{U}}(\eta), \hat{\mathcal{U}}(\eta) \right\rangle \\ &= \langle \xi, \xi\rangle - \langle \xi, \eta\rangle - \langle \eta, \xi\rangle + \langle \eta, \eta\rangle = \|\xi - \eta\|^2;\end{aligned}$$

therefore $\xi = \eta$ and so $\hat{\mathcal{U}}$ is injective and $\hat{\mathcal{U}}^{-1} : \mathbf{h} \to \mathbf{h}$ exists.

If $\hat{\mathcal{U}}^{-1}(\xi_1) = \xi$ and $\hat{\mathcal{U}}^{-1}(\eta_1) = \eta$, since by hypothesis $\left\langle \hat{\mathcal{U}}(\xi), \hat{\mathcal{U}}(\eta) \right\rangle = \langle \xi, \eta\rangle$, $\forall \xi, \eta$, then $\langle \xi_1, \eta_1\rangle = \left\langle \hat{\mathcal{U}}^{-1}(\xi_1), \hat{\mathcal{U}}^{-1}(\eta_1) \right\rangle$; since $\hat{\mathcal{U}}$ is bijective such a relation holds for every vector in the space. In this relation, if $\xi_1 = \hat{\mathcal{U}}(\xi_2)$, then $\left\langle \hat{\mathcal{U}}(\xi_2), \eta_1 \right\rangle = \left\langle \xi_2, \hat{\mathcal{U}}^{-1}(\eta_1) \right\rangle$, again for all vectors of $\mathbf{h}$.

Now, for all $\eta, \xi, \zeta \in \mathbf{h}$ and $a, b \in \mathbb{C}$, one has

$$\begin{aligned}\left\langle \hat{\mathcal{U}}(a\xi + b\eta), \zeta \right\rangle &= \left\langle a\xi + b\eta, \hat{\mathcal{U}}^{-1}(\zeta) \right\rangle \\ &= \bar{a} \left\langle \xi, \hat{\mathcal{U}}^{-1}(\zeta) \right\rangle + \bar{b} \left\langle \eta, \hat{\mathcal{U}}^{-1}(\zeta) \right\rangle \\ &= \bar{a} \left\langle \hat{\mathcal{U}}(\xi), \zeta \right\rangle + \bar{b} \left\langle \hat{\mathcal{U}}(\eta), \zeta \right\rangle = \left\langle a\hat{\mathcal{U}}(\xi) + b\hat{\mathcal{U}}(\eta), \zeta \right\rangle,\end{aligned}$$

showing that $\hat{\mathcal{U}}(a\xi + b\eta) = a\hat{\mathcal{U}}(\xi) + b\hat{\mathcal{U}}(\eta)$, that is, $\hat{\mathcal{U}}$ is linear. □

Theorem 7.1.13. *Let T be a hermitian operator with equal deficiency indices. If $(\mathbf{h}, \rho_1, \rho_2)$ is a boundary triple for T, then the self-adjoint extensions $T_{\hat{\mathcal{U}}}$ of T are precisely*

$$\operatorname{dom} T_{\hat{\mathcal{U}}} = \left\{ \xi \in \operatorname{dom} T^* : \rho_2(\xi) = \hat{\mathcal{U}} \rho_1(\xi) \right\}, \qquad T_{\hat{\mathcal{U}}}\xi = T^*\xi,$$

for every unitary map $\hat{\mathcal{U}} : \mathbf{h} \to \mathbf{h}$.

Proof. A necessary condition for the restriction of T^* to a domain $\mathcal{D}$ be self-adjoint is that the corresponding boundary form vanishes identically on $\mathcal{D}$. Given the boundary triple, taking into account Lemma 7.1.12 and the discussion that precedes it, Lemma 7.1.7 and Proposition 7.1.8, such $\mathcal{D}$'s are necessarily obtained through unitary maps $\hat{\mathcal{U}} : \mathbf{h} \to \mathbf{h}$ and it is enough to check that actually each $T_{\hat{\mathcal{U}}}$ is self-adjoint.

Clearly $T_{\hat{\mathcal{U}}}$ is a hermitian extension of T. If $\eta \in \mathrm{dom}\, T_{\hat{\mathcal{U}}}^*$ one has

$$\langle T_{\hat{\mathcal{U}}}^* \eta, \xi\rangle = \langle \eta, T_{\hat{\mathcal{U}}} \xi\rangle = \langle \eta, T_{\hat{\mathcal{U}}}^* \xi\rangle, \qquad \forall \xi \in \mathrm{dom}\, T_{\hat{\mathcal{U}}}.$$

Then,

$$\begin{aligned} 0 = \Gamma_{T_{\hat{\mathcal{U}}}^*}(\eta, \xi) &= \langle T_{\hat{\mathcal{U}}}^* \eta, \xi\rangle - \langle \eta, T_{\hat{\mathcal{U}}}^* \xi\rangle \\ &= \langle \rho_1(\eta), \rho_1(\xi)\rangle - \langle \rho_2(\eta), \rho_2(\xi)\rangle \\ &= \langle \rho_1(\eta), \rho_1(\xi)\rangle - \langle \rho_2(\eta), \hat{\mathcal{U}} \rho_1(\xi)\rangle \\ &= \langle \rho_1(\eta), \rho_1(\xi)\rangle - \langle \hat{\mathcal{U}}^* \rho_2(\eta), \rho_1(\xi)\rangle \\ &= \langle \rho_1(\eta) - \hat{\mathcal{U}}^* \rho_2(\eta), \rho_1(\xi)\rangle, \qquad \forall \xi \in \mathrm{dom}\, T_{\hat{\mathcal{U}}}. \end{aligned}$$

Since ρ_1 has dense range in $\mathbf{h}$, it follows that $\rho_1(\eta) - \hat{\mathcal{U}}^* \rho_2(\eta) = 0$, that is, $\rho_2(\eta) = \hat{\mathcal{U}} \rho_1(\eta)$ and $\eta \in \mathrm{dom}\, T_{\hat{\mathcal{U}}}$. Therefore, $T_{\hat{\mathcal{U}}}$ is self-adjoint. □

Often a boundary triple for differential operators gives self-adjoint extensions in terms of boundary conditions, and different choices of the triple correspond to different parametrizations of such extensions. In applications sometimes it is convenient to distinguish the spaces $\rho_1(\mathbf{h})$ from $\rho_2(\mathbf{h})$ by different symbols.

Remark 7.1.14. The definition of boundary triple presented here is slightly different from the current definition in the literature; maybe the term *modified boundary triple* should be used. For the usual approach and related results and references in case of differential operators see [GorG91] and [BrGP08].

7.2 Schrödinger Operators on Intervals

Important Schrödinger operators are self-adjoint extensions of the minimal operator

$$H = -\frac{d^2}{dx^2} + V(x), \qquad \mathrm{dom}\, H = C_0^\infty(a,b) \sqsubseteq \mathrm{L}^2(a,b),$$

with $-\infty \le a < b \le +\infty$; the weakest request on the (real-valued) potential is $V \in \mathrm{L}^2_{\mathrm{loc}}(a,b)$, and this will be henceforth supposed in this chapter.

Note that $\mathrm{L}^2(a,b) = \mathrm{L}^2[a,b]$ since the set of end points $\{a,b\}$ has zero Lebesgue measure. However, in case of bounded intervals one has $C_0^\infty(a,b) \neq C_0^\infty[a,b]$ and for absolutely continuous functions $\mathrm{AC}(a,b) \neq \mathrm{AC}[a,b]$ (recall that $\mathrm{AC}(a,b)$ denotes the set of absolutely continuous functions in every bounded and closed interval $[c,d] \subset (a,b)$). By Proposition 2.2.16, H has equal deficiency indices and so self-adjoint extensions do exist. In this and the next sections some results related to this matter will be addressed, as well as some ways of getting self-adjoint extensions of H, mainly illustrated by means of boundary forms. In this section H always refers to this minimal differential operator.

Again note the open interval (a,b) and in general $V \in \mathrm{L}^2_{\mathrm{loc}}$ is allowed to "drastically diverge" at the end points. For $V \in \mathrm{L}^2_{\mathrm{loc}}(a,b)$, Proposition 2.3.20 ensures that dom H^* equals

$$\left\{\psi \in \mathrm{L}^2(a,b) : \psi, \psi' \in \mathrm{AC}(a,b), (-\psi'' + V\psi) \in \mathrm{L}^2(a,b)\right\},$$

so that if $\psi \in \mathrm{dom}\, H^*$ then ψ, ψ' are absolutely continuous functions in (a,b), and in case the potential V has a discontinuity at a point $c \in (a,b)$, then ψ and ψ' must be continuous at c for any ψ in the domain of a self-adjoint extension of H. Such continuity conditions at c are habitually imposed on wave functions (i.e., ψ) in quantum mechanics textbooks, and here the justification is seen to be related to regularity properties of elements of dom H^*.

Lemma 7.2.1. *The boundary form of the above minimal operator H is*

$$\Gamma(\psi,\varphi) = W_b[\psi,\varphi] - W_a[\psi,\varphi], \qquad \psi,\varphi \in \mathrm{dom}\, H^*,$$

where $W_x[\psi,\varphi] = \overline{\psi(x)}\varphi'(x) - \overline{\psi'(x)}\varphi(x)$ is the wronskian of ψ,φ at $x \in (a,b)$, and $W_a[\psi,\varphi] := \lim_{x\to a^+} W_x[\psi,\varphi]$, $W_b[\psi,\varphi] := \lim_{x\to b^-} W_x[\psi,\varphi]$.

Proof. Let $[c,d] \subset (a,b)$ and $\psi,\varphi \in \mathrm{dom}\, H^*$. In view of $V \in \mathrm{L}^2_{\mathrm{loc}}(a,b)$, on integrating by parts one gets that $\Gamma(\psi,\phi)$ is reduced to

$$\int_c^d \left(\overline{(H^*\psi)(x)}\varphi(x) - \overline{\psi(x)}(H^*\varphi)(x)\right) dx = W_d[\psi,\varphi] - W_c[\psi,\varphi];$$

since the integral over the whole interval $[a,b]$ is finite, the limits defining $W_a[\psi,\varphi]$ and $W_b[\psi,\varphi]$ exist (modify the functions so that they vanish in a neighborhood of a; then $W_b[\psi,\varphi]$ exists; similarly for the other end) and $\Gamma(\psi,\varphi) = W_b[\psi,\varphi] - W_a[\psi,\varphi]$. □

Exercise 7.2.2. Let H be the above minimal operator and $u \in \mathrm{L}^1_{\mathrm{loc}}(a,b)$. If ψ,φ are solutions of $H^*\psi = u$, show that the wronskian $W_x[\overline{\psi},\varphi] = \gamma$ is constant. Furthermore, if $\{\overline{\psi},\varphi\}$ is a linearly independent set, show that such a constant $\gamma \neq 0$, and given $c \in (a,b)$,

$$\phi(x) := \frac{1}{\gamma}\int_c^x [\psi(x)\varphi(t) - \varphi(x)\psi(t)]\, u(t)\, dt$$

is the unique solution of $H^*\psi = u$ with initial conditions $\phi(c) = 0$ and $\phi'(c) = 0$.

7.2.1 Regular and Singular End Points

Definition 7.2.3. The end point a is *regular* for the differential operator $H = -d^2/dx^2 + V$ if $-\infty < a$ and for some $c \in (a,b)$ (and so for all such c) one has $\int_a^c |V(x)|\, dx := \lim_{d\to a^+} \int_d^c |V(x)|\, dx < \infty$; b is regular for H if $b < \infty$ and $\int_c^b |V(x)|\, dx := \lim_{d\to b^-} \int_c^d |V(x)|\, dx < \infty$. If an end point is not regular it is called *singular*.

From the theory of differential equations [Na69] it is known that the space of solutions of the $K_{\mp}$-*equation*

$$H^*\psi = -\psi'' + V\psi = \pm i\psi, \qquad \psi \in \text{dom } H^*,$$

is two-dimensional and if a is a regular point for H then any solution ψ has finite limits $\psi(a) := \psi(a^+) = \lim_{x\to a^+}\psi(x)$ and $\psi'(a) := \psi'(a^+) = \lim_{x\to a^+}\psi'(x)$; if a is singular then such limits can be divergent.

Recall also that if V is a continuous function (even complex-valued) on (a,b), then any solution of

$$-\psi'' + (V - z)\psi = 0, \qquad z \in \mathbb{C},$$

is a twice continuously differentiable function in (a,b), and in case $V \in C^\infty(a,b)$ then $\psi \in C^\infty(a,b)$.

Proposition 7.2.4. *Let H be the above minimal differential operator.*

i) *The closure of H is given by*

$$\begin{aligned} \text{dom } \overline{H} &= \{\psi \in \text{dom } H^* : W_b[\psi,\varphi] = 0, W_a[\psi,\varphi] = 0, \forall\varphi \in \text{dom } H^*\}, \\ \overline{H}\psi &= H^*\psi, \qquad \forall\psi \in \text{dom } \overline{H}. \end{aligned}$$

ii) *Let $\psi \in$ dom H^*. In case a is a regular end point, then the condition $W_a[\psi,\varphi] = 0$, $\forall\varphi \in$ dom H^*, means $\psi(a) = 0 = \psi'(a)$ (similarly for b).*

Proof. i) Combine Proposition 7.1.5 and Lemma 7.2.1 to get

$$\text{dom } \overline{H} = \{\psi \in \text{dom } H^* : W_b[\psi,\varphi] - W_a[\psi,\varphi] = 0, \forall\varphi \in \text{dom } H^*\}.$$

Since the behavior of functions in dom H^* near a is independent of their values near b, it follows that the statement $W_b[\psi,\varphi] - W_a[\psi,\varphi] = 0, \forall\varphi \in$ dom H^*, is equivalent to $W_b[\psi,\varphi] = 0 = W_a[\psi,\varphi], \forall\varphi \in$ dom H^* (e.g., given φ, pick $u \in$ dom H^* that coincides with φ in a neighborhood of a and is zero in a neighborhood of b; then $W_a[\psi,\varphi] = W_a[\psi,u] = W_b[\psi,u] = 0$).

ii) If a is a regular point, then $\varphi(a), \varphi'(a)$ are well defined (i.e., they have finite limits) for all $\varphi \in$ dom H^*; hence $0 = W_a[\psi,\varphi] = \overline{\psi(a)}\varphi'(a) - \overline{\psi'(a)}\varphi(a)$, $\forall\varphi \in$ dom H^*, implies $\psi(a) = 0 = \psi'(a)$, since $\varphi(a), \varphi'(a)$ can take arbitrary values. □

Corollary 7.2.5. *If both end points a, b are regular, then*

$$\text{dom } \overline{H} = \{\psi \in \text{dom } H^* : \psi(b) = \psi'(b) = 0 = \psi(a) = \psi'(a)\}.$$

Corollary 7.2.6. *If H has a regular end point, then its closure $\overline{H}$ has no eigenvalues.*

Proof. Say a is a regular end point. Then the solution of $\overline{H}\psi = \lambda\psi$, $\psi \in$ dom $\overline{H}$, $\lambda \in \mathbb{C}$, must satisfy $\psi(a) = 0 = \psi'(a)$, and so, by uniqueness, ψ is the null solution. □

Definition 7.2.7. A measurable function $u : (a,b) \to \mathbb{C}$ is in L^2 *near the end point* a if there exists $c \in (a,b)$ so that $u \in \mathrm{L}^2(a,c)$ (in fact the restriction $u|_{(a,c)} \in \mathrm{L}^2(a,c)$); similarly for u that is L^2 near b.

Remark 7.2.8. Note that if ψ is a solution of the K_--equation for H, then $\overline{\psi}$ is a solution of the corresponding K_+-equation. So for each solution L^2 near a of the K_--equation corresponds a solution L^2 near a of the K_+-equation and vice versa. Similarly for the end point b.

Theorem 7.2.9. *Let H be the minimal operator introduced on page* 174.

i) *The deficiency indices of the above minimal operator H are finite and bounded by $0 \le n_-(H) = n_+(H) \le 2$.*
ii) *If both end points a, b are regular, then $n_-(H) = n_+(H) = 2$.*

Proof. i) By Proposition 2.2.16, $n_-(H) = n_+(H)$. From the above discussion on solutions of linear differential equations of second order one has, say, $0 \le n_-(H) \le 2$.

ii) If u is a solution of

$$H^*\psi = -\psi'' + V\psi = -i\psi, \qquad \psi \in \mathrm{dom}\ H^*,$$

then u, u' are absolutely continuous in (a,b) and so for any $[c,d] \subset (a,b)$ one has $\int_c^d |u(x)|^2\, dx < \infty$. Since the limits $u(a^+), u(b^-)$ exist and a, b are finite, one gets $\int_a^b |u(x)|^2\, dx < \infty$, consequently all elements of $\mathrm{K}_+(H)$ are in $\mathrm{L}^2[a,b]$. Hence $n_+(H) = 2$. By item i), $n_-(H) = 2$. □

Lemma 7.2.10. *Let H be the minimal operator introduced on page* 174. *For each end point, at least one* (*nonzero*) *solution of*

$$H^*\psi = -\psi'' + V\psi = \pm i\psi, \qquad \psi \in \mathrm{dom}\ H^*,$$

is L^2 *near it.*

Proof. Let a, b be the end points and $a < a' < b' < b$; it is enough to consider $-i$ on the right-hand side of the above equation, since the arguments are the same for the other possibility.

For the hermitian operator $\mathrm{dom}\ S = \{\psi, \psi' \in \mathrm{AC}[a',b'] \subset \mathrm{L}^2[a',b'] : \psi(a') = \psi'(a') = 0 = \psi(b') = \psi'(b')\}$,

$$S\psi = -\psi'' + V\psi,$$

a', b' are regular end points and, by Theorem 7.2.9, $n_-(S) = 2 = n_+(S)$. Thus, $\overline{\mathrm{rng}\ (S + i\mathbf{1})} = \mathrm{K}_-(S)^\perp \ne \{0\}$, and since $C_0^\infty(a',b') \sqsubseteq \mathrm{L}^2[a',b']$, there exists $\phi \in C_0^\infty(a',b')$ with $\phi \notin \mathrm{rng}\ (S + i\mathbf{1})$. Let $\hat{H}$ be a self-adjoint extension of H and $\psi \in \mathrm{dom}\ \hat{H} \subset \mathrm{dom}\ H^*$ with $(\hat{H} + i\mathbf{1})\psi = \phi$ (recall that $\mathrm{rng}\ (\hat{H} + i\mathbf{1}) = \mathcal{H}$ by Proposition 2.2.4); note that the support of ψ does not lie in (a',b'), for otherwise ψ would belong to $\mathrm{dom}\ S$ and $(S + i\mathbf{1})\psi = \phi$, so that a contradiction would arise.

Now suppose that ψ does not vanish identically on (a, a') (similarly if it does not vanish identically on (b', b)). Then the restriction $u := \psi|_{(a,a')}$ is a solution of the above equation in the statement of the lemma (recall that $\hat{H} \subset H^*$) and it is L^2 near a. The construction of the solution L^2 near b is as follows.

Consider the operator dom $Q = \{\varphi \in \mathrm{dom}\ \hat{H} : \varphi(x) = 0, \forall x \in [b', b)\}$ (under restriction, this set is dense in $\mathrm{L}^2(a, a')$), $Q := \hat{H}|_{\mathrm{dom}\ Q}$; in view of $u \in \mathrm{dom}\ Q$ and

$$Qu = -u'' + Vu = -iu,$$

it is found that $\bar{u} \in \mathrm{dom}\ Q^*$ (the complex conjugate of u above) and

$$(Q^* - i\mathbf{1})\bar{u} = 0;$$

it then follows that rng $(Q + i\mathbf{1})$ is not dense and, as above, there exists $\phi \in C_0^\infty(a, a')$ with $\phi \notin \mathrm{rng}\ (Q + i\mathbf{1})$. The self-adjointness of $\hat{H}$ implies that rng $(\hat{H} + i\mathbf{1}) = \mathrm{L}^2(a, b)$, and so there is $v \in \mathrm{dom}\ \hat{H}$ with $(\hat{H} + i\mathbf{1})v = \phi$. Finally, v does not vanish identically on $[b', b)$ since $\phi \notin \mathrm{rng}\ (Q + i\mathbf{1})$, and so a (nonzero) L^2 near b solution of the equation in the statement of the lemma was found. This completes the proof. □

Corollary 7.2.11. *If $n_-(H) = n_+(H) = 0$, that is, H is essentially self-adjoint, then both ends a, b are singular.*

Proof. If one end is regular then all solutions of the corresponding $\mathrm{K}_\mp$-equation are L^2 near it and, by Lemma 7.2.10, there is at least one solution of the above equation that is L^2 near the other end point, so at least one solution belongs to $\mathrm{L}^2(a, b)$ and $n_+(H) \geq 1$. Both ends being singular is the only remaining possibility if $n_- = n_+ = 0$. □

7.2.2 Limit Point, Limit Circle

Corollary 7.2.11 shows that a necessary condition for H to be essentially self-adjoint is that both ends a, b are singular. This is related to interesting results by Weyl (around 1910) and further developed by Levinson, Friedrichs and many others. For details justifying the terms in the next definition – although not immediate, they are quite interesting – consult [CoL55] or [Pea88].

Definition 7.2.12. The minimal differential operator H is in the *limit point* (resp. *limit circle*) at one end point if the vector space of solutions of the $\mathrm{K}_\pm$-equation that are L^2 near this end point is unidimensional (resp. two-dimensional).

Theorem 7.2.13 (Weyl). *The operator H is essentially self-adjoint iff it is in the limit point at both ends a and b.*

Proof. By Corollary 7.2.11 and the proof of Lemma 7.2.10, if H is essentially self-adjoint, then both ends are limit point and the unique nonzero solution φ of the K_+-equation that is L^2 near a and the unique nonzero solution ψ that is L^2 near b compose a linearly independent set, so that no solution belongs to $\mathrm{L}^2(a, b)$.

The task now is to show that if H is limit point at both end points, then $n_- = n_+ = 0$, which is equivalent to H^* being self-adjoint.

By Lemma 7.2.1,

$$\Gamma_{H^*}(\psi, \varphi) = W_b[\psi, \varphi] - W_a[\psi, \varphi], \qquad \forall \psi, \varphi \in \text{dom } H^*;$$

also H^* is self-adjoint iff the boundary form Γ_{H^*} vanishes identically. Let $c \in (a, b)$ and A, B be operators with the same action as H but domains dom $B = C_0^\infty(a, c)$ and dom $A = \{\varphi \in C^\infty(a, c) : \varphi(c) = 0, \exists \varepsilon > 0, \varphi(x) = 0, \forall x \in (a, a + \varepsilon)\}$. Since $B \subset A$ one has $\overline{B} \subset \overline{A}$.

Claim. $\overline{A}$ is self-adjoint.

In fact, by hypothesis the solutions of $-\varphi'' + V\varphi = \pm i\varphi$ that are L^2 near a constitute a one-dimensional subspace, and since c is a regular end point, all solutions are L^2 near c; hence $n_-(B) = 1 = n_+(B)$. By noting that $\overline{A}$ is a proper hermitian extension of $\overline{B}$ (there are functions φ in dom $\overline{A}$ with $\varphi'(c) \neq 0$, but not in dom $\overline{B}$; see Proposition 7.2.4), it follows that $n_\pm(\overline{A}) < n_\pm(\overline{B})$ (because $n_\pm(\overline{B}) < \infty$) and the unique possibility is then $n_-(A) = 0 = n_+(A)$, and so $\overline{A}$ is self-adjoint.

Let $\psi, \varphi \in$ dom H^*. Pick $\psi_c, \varphi_c \in C_0^\infty(a, b)$ so that both functions $\psi_2 := \psi + \psi_c$, $\varphi_2 := \varphi + \varphi_c$ vanish at c. Then, $\psi_2, \varphi_2 \in$ dom $\overline{A}$ and in view of $W_c[\psi_2, \varphi_2] = 0$ one finds

$$\begin{aligned} W_a[\psi, \varphi] &= W_a[\psi_2 - \psi_c, \varphi_2 - \varphi_c] = W_a[\psi_2, \varphi_2] \\ &= W_a[\psi_2, \varphi_2] - W_c[\psi_2, \varphi_2] = -\Gamma_{\overline{A}}(\psi_2, \varphi_2) = 0, \end{aligned}$$

since $\overline{A}$ is self-adjoint (see Lemma 7.1.7). Similar arguments show that $W_b[\psi, \varphi] = 0$, so that Γ_{H^*} vanishes identically on dom H^* and H^* is self-adjoint. Thereby the proof is complete. □

Exercise 7.2.14. Show that H has deficiency indices $n_+ = n_- = 1$ iff it is limit circle at one end and limit point at the other.

Example 7.2.15. If V is a real polynomial and $H\psi = -\psi'' + V\psi$, dom $H = C_0^\infty(a, b)$ and (a, b) a bounded interval, then both ends are regular and so $n_+ = n_- = 2$. Note that such a conclusion holds also for any continuous potential in $[a, b]$, including the free particle in the interval, that is, $V = 0$ (cf. Example 2.6.8).

Example 7.2.16. Let $V(x) = \kappa \ln(\gamma x)$, $\kappa \neq 0, \gamma > 0$, and dom $H = C_0^\infty(0, 1)$. Since V is regular at both end points, it follows that $n_- = n_+ = 2$.

Exercise 7.2.17. Show that the deficiency indices of H in $(0, 1)$ with potential $V(x) = \kappa(\ln x)^2$ are equal to 2. Generalize for $V(x) = \kappa(\ln x)^m$, for any $\kappa \in \mathbb{R}, m \in \mathbb{N}$.

Example 7.2.18. Let $V(x) = \kappa/x^2$, $\kappa \neq 0$, and H with dom $H = C_0^\infty(0, 1)$. By Proposition 2.3.20, dom $H^* = \{\psi \in \mathrm{L}^2(0, 1) : \psi, \psi' \in \mathrm{AC}(0, 1), (-\psi'' + \kappa/x^2\psi) \in$

$L^2(0,1)\}$. The end point 1 is regular, while 0 is not; so H is limit circle at 1. For the end point 0 one needs to determine the solutions of the $K_\mp$-equation

$$H^*\psi = -\psi'' + \frac{\kappa}{x^2}\psi = \pm i\psi;$$

if one searches for solutions in the form $\psi(x) = x^a$, it follows that

$$-a(a-1)x^a + \kappa x^a \mp ix^{a+2} = 0,$$

so that, whether for $x \to 0$ the term x^{a+2} could be ignored in comparison with the other terms, then one has approximately $-a(a-1)+\kappa = 0$, whose solutions are $a_\pm = 1/2(1 \pm \sqrt{1+4\kappa})$. If $-1/4 < \kappa < 3/4$ both solutions are independent and L^2 near 0 (so limit circle), whereas for $\kappa \geq 3/4$ only one of them is in L^2 near 0 (so limit point). Hence, $n_- = n_+ = 1$ if $\kappa \geq 3/4$ and $n_- = n_+ = 2$ if $-1/4 < \kappa < 3/4$.

Now a justification of the above procedure for $x \to 0$. If $\psi \in \operatorname{dom} H^*$, then

$$u = H^*\psi = -\psi'' + \frac{\kappa}{x^2}\psi \ \in L^2(0,1);$$

this may be thought of as a nonhomogeneous second-order linear differential equation for ψ. Note that the independent solutions of the homogeneous equation are exactly the above $\psi_+(x) = x^{a_+}$ and $\psi_-(x) = x^{a_-}$. By the well-known variation of parameters technique one obtains the general solution, that is,

$$\begin{aligned}\psi(x) = {} & b_+\psi_+(x) + b_-\psi_-(x) \\ & + \left[\psi_+(x)\int_0^x \frac{\psi_-(t)u(t)}{W_t[\overline{\psi_+},\psi_-]}dt - \psi_-(x)\int_0^x \frac{\psi_+(t)u(t)}{W_t[\overline{\psi_+},\psi_-]}dt\right],\end{aligned}$$

for some constants $b_\pm$. A direct calculation gives $W_t[\overline{\psi_+},\psi_-] = -\gamma$, $\forall t$, with $\gamma = \sqrt{1+4\kappa}$. Write $\|u\|_{2,x} = \left(\int_0^x |u(t)|^2 dt\right)^{1/2}$ and note that $\|u\|_{2,x} \to 0$ as $x \to 0^+$. The absolute value of the term in square brackets is estimated from above by using Cauchy-Schwarz,

$$\begin{aligned}&\frac{\|u\|_{2,x}}{\gamma} \times \left(|\psi_+(x)|\left(\int_0^x |\psi_-(t)|^2\right)^{1/2} + |\psi_-(x)|\left(\int_0^x |\psi_+(t)|^2\right)^{1/2}\right) \\ &\qquad \leq \frac{4}{|4-\gamma^2|}\frac{\|u\|_{2,x}}{\gamma}x^{3/2}, \qquad -\frac{1}{4} < \kappa < \frac{3}{4}.\end{aligned}$$

The case $\kappa = 3/4$ is left as an exercise. Since such a term is in L^2 near 0, the final analysis of ψ near 0 is left to the solutions of the homogeneous equation $\psi_+(x) = x^{a_+}$ and $\psi_-(x) = x^{a_-}$, which is exactly the analysis performed above.

Exercise 7.2.19. Discuss the case $\kappa = 3/4$ in Example 7.2.18 (see also Exercise 7.2.23).

Exercise 7.2.20. For $\psi \in \operatorname{dom} H^*$ in Example 7.2.18, find the behavior of $\psi'(x)$ for $x \to 0^+$.

Example 7.2.21. This is the potential of Example 7.2.18, but on the half-line. Let $V(x) = \kappa/x^2$, $\kappa \neq 0$, and H with dom $H = C_0^\infty(0,\infty)$. The same conclusions about the end point 0 as in Example 7.2.18 are obtained. For the other end point consider the K_--equation

$$-x^2\psi'' + \kappa\psi = ix^2\psi;$$

for $x \to \infty$ its solutions are governed by the equation $-\psi'' = i\psi$ whose solutions are $u_\pm(x) = e^{\pm(1\pm i)x/\sqrt{2}}$; since only one of them is in L^2 near ∞ (analogously to the K_+-equation), one concludes that H is in the limit point at ∞ for all $\kappa \neq 0$. Therefore, if $\kappa \geq 3/4$ the operator H is essentially self-adjoint, whereas $n_- = n_+ = 1$ if $-1/4 < \kappa < 3/4$.

For the justification of the above argument in case $x \to \infty$, apply Proposition 7.5.3 and Exercise 7.5.6.

Exercise 7.2.22. Check that

$$u_1(x) = \sqrt{x}\,\cos(t\ln x)/\sqrt{t}, \qquad u_2(x) = \sqrt{x}\,\sin(t\ln x)/\sqrt{t},$$

with $t = \sqrt{-\kappa - 1/4}$, $\kappa < -1/4$, are solutions of $-\psi'' + \frac{\kappa}{x^2}\psi = 0$.

Exercise 7.2.23. Show that the deficiency indices of dom $H = C_0^\infty(0,\infty)$, $H\psi = -\psi'' - \psi/(4x^2)$ are $n_- = 1 = n_+$. Note that $\psi_+(x) = \sqrt{x}$ and $\psi_-(x) = \sqrt{x}\ln x$ are solutions of $H^*\psi = 0$.

7.3 Regular Examples

In this section boundary triples will be used to get explicitly self-adjoint extensions of H with regular end points. The ideas can be adapted to other situations.

Example 7.3.1. [Free particle on a half-line] The initial energy operator is $H\psi = -\psi''$, dom $H = C_0^\infty(0,\infty)$; by Example 2.3.19, $n_- = n_+ = 1$. Also dom $H^* = \mathcal{H}^2[0,\infty)$ and the boundary form, for $\psi, \varphi \in$ dom H^*, is readily seem to be

$$\Gamma(\psi,\varphi) = W_\infty[\psi,\varphi] - W_0[\psi,\varphi] = \overline{\psi'(0)}\varphi(0) - \overline{\psi(0)}\varphi'(0),$$

since the elements of dom H^* vanish at infinity. Now define the vector spaces $X := \{\Psi = \psi(0) - i\psi'(0) : \psi \in \text{dom } H^*\}$ and the map $Y = \rho(X) := \{\rho(\Psi) = \psi(0) + i\psi'(0) : \Psi \in X\}$, and observe that

$$\langle\Psi,\Phi\rangle - \langle\rho(\Psi),\rho(\Phi)\rangle = 2i\Gamma(\psi,\varphi)$$

(of course $\Phi = \varphi(0) - i\varphi'(0)$), so that a boundary triple was found (with respect to Definition 7.1.11, think of $X = \rho_1(\text{dom } H^*)$ and $Y = \rho_2(\text{dom } H^*) = \rho(X)$).

Now, according to Theorem 7.1.13, a domain $\mathcal{D}$ so that $H^*|_\mathcal{D}$ is self-adjoint is characterized by unitary maps between X and Y. Since X and Y are unidimensional, such unitary maps are multiplication by $e^{i\theta}$ for some $0 \leq \theta < 2\pi$. Therefore, the domain of self-adjoint extensions of H are so that $\Psi = e^{i\theta}\rho(\Psi)$ for all $\Psi \in X$. Writing out such a relation

$$\psi(0) - i\psi'(0) = e^{i\theta}\left(\psi(0) + i\psi'(0)\right),$$

and so $(1-e^{i\theta})\psi(0) = i(1+e^{i\theta})\psi'(0)$; if $\theta \neq 0$ one has

$$\psi(0) = \lambda\psi'(0), \qquad \lambda = i\frac{(1+e^{i\theta})}{(1-e^{i\theta})} \in \mathbb{R}.$$

Therefore the self-adjoint extensions H_λ of H are characterized by the following boundary conditions

$$\text{dom } H_\lambda = \{\psi \in \mathcal{H}^2[0,\infty) : \psi(0) = \lambda\psi'(0)\}, \qquad H_\lambda\psi = -\psi'',$$

for each $\lambda \in \mathbb{R}\cup\{\infty\}$. The value $\lambda = \infty$ is for including $\theta = 0$, which corresponds to Neumann boundary condition $\psi'(0) = 0$. A Dirichlet boundary condition occurs for $\lambda = 0$. Exercises 7.3.2 and 11.6.11 discuss the spectra of such operators.

Exercise 7.3.2. Show that the self-adjoint operators H_λ in Example 7.3.1 have an eigenvalue E iff $\lambda < 0$ and $E = -1/\lambda^2$, whose eigenfunction is $\psi_E(x) = e^{x/\lambda}$. The existence of a negative value in the spectrum can be considered rather unexpected, since the actions of H_λ indirectly suggest they are positive operators; the question is the boundary condition choice. Maybe, someone could discard such possibilities on the basis of physical arguments.

Exercise 7.3.3. Check that if in Example 7.2.21 one takes $\kappa = 0$, then Example 7.3.1 is recovered.

Example 7.3.4. [Free particle on an interval] The initial energy operator is $H\psi = -\psi''$, dom $H = C_0^\infty(0,1)$; by Example 7.2.15, $n_- = n_+ = 2$. Also dom $H^* = \mathcal{H}^2[0,1]$ and the boundary form is, for $\psi,\varphi \in$ dom H^*,

$$\begin{aligned}\Gamma(\psi,\varphi) &= W_1[\psi,\varphi] - W_0[\psi,\varphi]\\ &= \overline{\psi(1)}\varphi'(1) - \overline{\psi'(1)}\varphi(1) - \overline{\psi(0)}\varphi'(0) + \overline{\psi'(0)}\varphi(0).\end{aligned}$$

Based on Example 7.3.1, define the two-dimensional vector spaces of elements

$$\Psi = \begin{pmatrix}\psi'(0) - i\psi(0)\\ \psi'(1) + i\psi(1)\end{pmatrix}, \qquad \rho(\Psi) = \begin{pmatrix}\psi'(0) + i\psi(0)\\ \psi'(1) - i\psi(1)\end{pmatrix},$$

for $\psi \in$ dom H^*. A direct evaluation of inner products leads to

$$\langle\Psi,\Phi\rangle - \langle\rho(\Psi),\rho(\Phi)\rangle = -2i\Gamma(\psi,\varphi),$$

and a boundary triple was found.

By Theorem 7.1.13, a domain $\mathcal{D}$ so that $H^*|_{\mathcal{D}}$ is self-adjoint is characterized by a unitary 2×2 matrix $\hat{U}$ so that $\Psi = \hat{U}\rho(\Psi)$ for all Ψ; recall that the general form of such matrices is

$$\hat{U} = e^{i\theta}\begin{pmatrix} a & -\bar{b}\\ b & \bar{a}\end{pmatrix}, \qquad \theta \in [0,2\pi),\ a,b \in \mathbb{C}, |a|^2 + |b|^2 = 1.$$

Writing out such a relation one obtains the boundary conditions

$$\left(\mathbf{1}-\hat{U}\right)\begin{pmatrix}\psi'(0)\\ \psi'(1)\end{pmatrix} = -i\left(\mathbf{1}+\hat{U}\right)\begin{pmatrix}-\psi(0)\\ \psi(1)\end{pmatrix}$$

and the domain of the corresponding self-adjoint extension $H_{\hat{U}}$ of H is composed of the elements $\psi \in \mathcal{H}^2[0,1]$ so that the above boundary conditions are satisfied; also $H_{\hat{U}}\psi = -\psi''$. Some particular choices of $\hat{U}$ appear in exercises.

In case $(\mathbf{1}+\hat{U})$ is invertible (similarly if $(\mathbf{1}-\hat{U})$ is invertible) one can write the above boundary conditions as

$$A\begin{pmatrix}\psi'(0)\\ \psi'(1)\end{pmatrix} = \begin{pmatrix}-\psi(0)\\ \psi(1)\end{pmatrix}, \qquad A = i\left(\mathbf{1}+\hat{U}\right)^{-1}\left(\mathbf{1}-\hat{U}\right),$$

with A a self-adjoint 2×2 matrix. By allowing some entries of A that take the value ∞, it is possible to recover some cases $\left(\mathbf{1}+\hat{U}\right)$ that are not invertible; nevertheless, it is not always a simple task to recover all such cases, so that the boundary conditions in terms of $\hat{U}$ seem preferable.

Exercise 7.3.5. Show that A above is actually a self-adjoint matrix. Note that it recalls the inverse Cayley transform.

Exercise 7.3.6. Check that the choices for the matrix $\hat{U}$

$$\text{a) } \mathbf{1}, \qquad \text{b) } -\mathbf{1}, \qquad \text{c) } \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \qquad \text{d) } \begin{pmatrix}0 & -1\\ -1 & 0\end{pmatrix},$$

impose, respectively, the boundary conditions: a) $\psi(0) = 0 = \psi(1)$ (Dirichlet); b) $\psi'(0) = 0 = \psi'(1)$ (Neumann); c) $\psi(0) = \psi(1)$ and $\psi'(0) = \psi'(1)$ (periodic); d) $\psi(0) = -\psi(1)$ and $\psi'(0) = -\psi'(1)$ (antiperiodic).

Exercise 7.3.7. With respect to Exercise 7.3.6, find the spectra of all those operators by solving the corresponding eigenvalue equations; confirm that they are formed solely of eigenvalues. Check that cases a) and b) have the same spectra, except for $E = 0$ that is an eigenvalue only in case b) and, in both cases, all eigenvalues are simple. Note that the multiplicity of all eigenvalues in case d) is two.

Example 7.3.8. If the potential V is such that both end points $0, 1$ are regular, then the deficiency indices of $H\psi = -\psi'' + V\psi$, dom $H = C_0^\infty(0,1)$, are equal to 2, and for any $\psi \in$ dom H^* the boundary values $\psi(0), \psi(1), \psi'(0), \psi'(1)$ are well defined. Thus, its self-adjoint extensions can be characterized in the same way as in Example 7.3.4, through the same boundary conditions. Particular cases are

$$V(x) = \kappa \ln x, \qquad V(x) = \kappa/x^\alpha, \qquad \alpha < 1,\ \kappa \in \mathbb{R}.$$

Example 7.3.9. Let $V(x)$ be continuous and lower bounded with $|V(x)| \le |x|^{-\alpha}$, for some $0 < \alpha < 1/2$, and $H\psi = -\psi'' + V\psi$, dom $H = C_0^\infty(\mathbb{R})$. By Theorem 6.2.23, H is in the limit point case at both end points $-\infty, +\infty$, so that H^* is self-adjoint, with dom $H^* = \mathcal{H}^2(\mathbb{R})$ and $H^*\psi = -\psi'' + V\psi$.

7.4 Singular Examples and All That

For singular endpoints the limit values of ψ, ψ' could not exist, so that the strategy presented in the examples in Section 7.3 is not guaranteed to work. However, in some cases it is possible to properly adapt that strategy in order to get self-adjoint extensions. This will be illustrated in this section through a series of examples, including some point interactions.

Example 7.4.1. The self-adjoint extensions of $\mathrm{dom}\, H = C_0^\infty(0,1)$,

$$(H\psi)(x) = -\psi''(x) - \frac{1}{4x^2}\psi(x), \qquad \psi \in \mathrm{dom}\, H,$$

will be found (cf., Example 7.2.18 and Exercise 7.2.23). If $\psi \in \mathrm{dom}\, H^* = \{\psi \in \mathrm{L}^2(0,1) : \psi, \psi' \in \mathrm{AC}(0,1), (-\psi'' - \psi/(4x^2)) \in \mathrm{L}^2(0,1)\}$ one has

$$u = H^*\psi = -\psi'' - \frac{1}{4x^2}\psi \in \mathrm{L}^2(0,1),$$

which is a nonhomogeneous second-order linear differential equation for ψ; the general solution of the corresponding homogeneous equation $H^*\psi = 0$ is $b_1\psi_1(x) + b_2\psi_2(x)$, $b_1, b_2 \in \mathbb{C}$, with $\psi_1(x) = \sqrt{x}$ and $\psi_2(x) = \sqrt{x}\,\ln x$, whose wronskian is $W_x[\overline{\psi_1}, \psi_2] = 1$, $\forall x \in [0,1]$. Introduce $\varphi = \psi/\sqrt{x}$ so that

$$\sqrt{x}\,\varphi'' + \frac{1}{\sqrt{x}}\varphi' = -u,$$

or

$$(x\varphi')' = x\varphi'' + \varphi' = -\sqrt{x}u,$$

and since $\sqrt{x}u \in \mathrm{L}^1[0,1]$, on integrating one gets

$$\varphi'(x) = \frac{b_2}{x} - \frac{1}{x}\int_0^x \sqrt{s}\,u(s)\,ds.$$

By Cauchy-Schwarz, the function $x \mapsto \frac{1}{x}\int_0^x \sqrt{s}u(s)\,ds$ is also integrable in $[0,1]$, so that

$$\varphi(x) = b_1 + b_2 \ln x - \int_0^x \frac{ds}{s}\int_0^s \sqrt{t}\,u(t)\,dt$$

and, finally, $\psi(x) = b_1\sqrt{x} + b_2\sqrt{x}\,\ln x + v_\psi(x)$, (note that $b_j = b_j(\psi)$, $j = 1,2$) with v_ψ denoting the differentiable function

$$v_\psi(x) = -\sqrt{x}\int_0^x \frac{ds}{s}\int_0^s \sqrt{t}\,u(t)\,dt.$$

By Cauchy-Schwarz again,

$$\begin{aligned}|v_\psi(x)| &\le \sqrt{x}\int_0^x \frac{ds}{s}\left|\int_0^s \sqrt{t}\,u(t)\right| dt \\ &\le \sqrt{x}\int_0^x \frac{ds}{s}\frac{s}{\sqrt{2}}\,\|u\|_2 = \frac{x^{3/2}}{\sqrt{2}}\,\|u\|_2,\end{aligned}$$

so that $v_\psi(x) \sim x^{3/2}$, $v_\psi'(x) \sim x^{1/2}$ as $x \to 0$.

The boundary form of H is, for $\psi, \varphi \in \text{dom } H^*$,

$$\psi(x) = b_1(\psi)\sqrt{x} + b_2(\psi)\sqrt{x}\,\ln x + v_\psi(x)$$

and

$$\varphi(x) = b_1(\varphi)\sqrt{x} + b_2(\varphi)\sqrt{x}\,\ln x + v_\varphi(x),$$

$$\begin{aligned}\Gamma(\psi,\varphi) &= W_1[\psi,\varphi] - W_0[\psi,\varphi] \\ &= \overline{\psi(1)}\varphi'(1) - \overline{\psi'(1)}\varphi(1) + \lim_{x\to 0^+}\left(-\overline{\psi(x)}\varphi'(x) + \overline{\psi'(x)}\varphi(x)\right) \\ &= \overline{\psi(1)}\varphi'(1) - \overline{\psi'(1)}\varphi(1) - \overline{b_1(\psi)}b_2(\varphi) + b_1(\varphi)\overline{b_2(\psi)}.\end{aligned}$$

Remark 7.4.2. The above procedure, to deal with functions in dom H^*, was an alternative to the use of the variation of parameters formula employed in Example 7.2.18.

Based on Example 7.3.1, define the two-dimensional vector spaces of elements

$$\Psi = \begin{pmatrix} b_2(\psi) - ib_1(\psi) \\ \psi'(1) + i\psi(1) \end{pmatrix}, \qquad \rho(\Psi) = \begin{pmatrix} b_2(\psi) + ib_1(\psi) \\ \psi'(1) - i\psi(1) \end{pmatrix},$$

for $\psi \in \text{dom } H^*$. A direct evaluation of inner products leads to

$$\langle \Psi, \Phi\rangle - \langle \rho(\Psi), \rho(\Phi)\rangle = -2i\Gamma(\psi,\varphi),$$

and a boundary triple for H was found. The self-adjoint extensions $H_{\hat{U}}$ of H are associated with 2×2 unitary matrices $\hat{U}$ that entail the boundary conditions

$$\left(\mathbf{1} - \hat{U}\right)\begin{pmatrix} b_2(\psi) \\ \psi'(1) \end{pmatrix} = -i\left(\mathbf{1} + \hat{U}\right)\begin{pmatrix} -b_1(\psi) \\ \psi(1) \end{pmatrix},$$

that is, the domain of the self-adjoint extension $H_{\hat{U}}$ of H is composed of the elements $\psi \in \text{dom } H^*$ so that the above boundary conditions are satisfied; also $H_{\hat{U}}\psi = H^*\psi$, $\forall \psi \in \text{dom } H_{\hat{U}}$. The reader can play with different choices of $\hat{U}$ in order to get explicit self-adjoint extensions. What about some with $b_2 = 0$?

7.4.1 One-dimensional H-Atom

The operator with domain dom $H = C_0^\infty(\mathbb{R}\setminus\{0\})$ and action

$$H = -d^2/dx^2 - \kappa/|x|, \qquad \kappa > 0, \quad x \in \mathbb{R}\setminus\{0\},$$

is known as the (initial) one-dimensional hydrogen atom hamiltonian. It easily follows that H is hermitian and the question is to determine its self-adjoint extensions. In the way of finding such extensions, some typical difficulties encountered when dealing with more realistic potentials will appear. This model has a controversial history which can be traced through the references in the article [LoCdO06].

First the deficiency indices will be handled. Write

$$C_0^\infty(\mathbb{R}\setminus\{0\}) = C_0^\infty(-\infty,0)\oplus C_0^\infty(0,\infty)$$

and set $H_1 = H|_{C_0^\infty(-\infty,0)}$ and $H_2 = H|_{C_0^\infty(0,\infty)}$, so that $H = H_1 \oplus H_2$. By Proposition 2.3.20, dom $H_1^* = \{\psi \in \mathrm{L}^2(-\infty,0) : \psi,\psi' \in \mathrm{AC}(-\infty,0), (-\psi'' - \kappa/|x|\psi) \in \mathrm{L}^2(-\infty,0)\}$, dom $H_2^* = \{\psi \in \mathrm{L}^2(0,\infty) : \psi,\psi' \in \mathrm{AC}(0,\infty), (-\psi'' - \kappa/|x|\psi) \in \mathrm{L}^2(0,\infty)\}$ and

$$(H_j^*\psi)(x) = -\psi''(x) - \frac{\kappa}{|x|}\psi(x), \qquad \psi \in \mathrm{dom}\ H_j^*, \quad j = 1,2.$$

Hence, dom $H^* = \{\psi \in \mathrm{L}^2(\mathbb{R}) : \psi,\psi' \in \mathrm{AC}(\mathbb{R}\setminus\{0\}), (-\psi'' - \kappa/|x|\psi) \in \mathrm{L}^2(\mathbb{R})\}$ and H^* with the same action as H.

By using Whittaker functions [GraR80] (solutions of a particular confluent hypergeometric equation) in [Mos93] it was shown that for $\psi \in$ dom H^* the lateral limits $\psi(0^\pm) := \lim_{x\to 0^\pm}\psi(x)$ are finite while $\psi'(x)$ has logarithmic divergences as $x \to 0^\pm$. Furthermore, $\lim_{x\to\pm\infty}\psi(x) = 0$, $\lim_{x\to\pm\infty}\psi'(x) = 0$. With such information, a characterization of $\psi'(0^\pm)$ is possible. The following lemma is an alternative way of getting such information.

Lemma 7.4.3. *If $\psi \in$ dom H^*, then the lateral limits $\psi(0^\pm) = \lim_{x\to 0^\pm}\psi(x)$ and*

$$\tilde{\psi}(0^\pm) := \lim_{x\to 0^\pm}\left(\psi'(x) \pm \kappa\psi(x)\ln(|\kappa x|)\right)$$

exist and are finite.

Proof. We will discuss the case $x > 0$; the other $x < 0$ is similar. For $\psi \in$ dom H^* one has

$$-H^*\psi = \frac{d^2\psi}{dx^2} + \frac{\kappa}{x}\psi := u \in \mathrm{L}^2(0,\infty),$$

and one can write $\psi = \psi_1 + \psi_2$ with $\psi_1'' = u$, $\psi_1(0^+) = 0$ and $\psi_2'' + \kappa/x\psi = 0$. Since $\psi_j \in \mathcal{H}^2(\varepsilon,\infty)$, $j = 1,2$, for all $\varepsilon > 0$, and $u \in \mathrm{L}^2$, it follows that these functions are of class $C^1(0,\infty)$.

Consider an interval $[x,c]$, $0 < x < c < \infty$; c will be fixed later on. Since

$$\psi_1'(x) - \psi_1'(c) = \int_x^c u(s)\,ds,$$

$\psi_1'(x)$ has a lateral limit

$$\psi_1'(0^+) = \psi'(c) + \int_0^c u(s)\,ds.$$

On integrating successively twice over the interval $[x,c]$ one gets

$$\psi_2'(c) - \psi_2'(x) = -\kappa\int_x^c \frac{\psi(s)}{s}\,ds,$$

and then

$$\psi_2(x) = \psi_2(c) - (c-x)\psi_2'(c) - \kappa \int_x^c dv \int_v^c ds \, \frac{\psi(s)}{s}$$
$$= \psi_2(c) - (c-x)\psi_2'(c) - \kappa \int_x^c ds \, \psi(s) \, \frac{s-x}{s},$$

and since $0 \le (s-x)/s < 1$, by dominated convergence the last integral converges to $\int_0^1 \psi(s)$ as $x \to 0^+$. Therefore $\psi_2(0^+)$ exists and

$$\psi_2(0^+) = \psi_2(c) - c\psi_2'(c) - \kappa \int_0^c \psi(s) \, ds.$$

Now,

$$\left|\psi_2(x) - \psi_2(0^+)\right| \le x|\psi_2'(c)| + \kappa \int_0^x |\psi(s)| \, ds + \kappa x \int_x^c ds \, \frac{|\psi(s)|}{s}.$$

Taking into account that ψ is bounded, say $|\psi(x)| \le C$, $\forall x$, Cauchy-Schwarz in L^2 implies

$$\int_0^x |\psi(s)| ds = \int_0^x 1 \, |\psi(s)| ds \le C\sqrt{x},$$

and so, for $0 < x$ small enough and fixing $c = 1$,

$$\int_x^c ds \frac{\psi(s)}{s} \le C \left(c|\ln c| + x|\ln x|\right) \le \tilde{C}\sqrt{x},$$

for some constant $\tilde{C}$. Such inequalities imply $\psi(x) = \psi(0^+) + O(\sqrt{x})$, and on substituting this into

$$\psi'(x) = \psi'(1) + \kappa \int_x^1 \frac{\psi(s)}{s} \, ds$$

(recall that $\psi_1'(0^+)$ is finite) it is found that there is b so that, as $x \to 0^+$,

$$\psi'(x) = \psi'(1) - \kappa\psi(0^+) \ln(\kappa x) + b + o(1);$$

thus, the derivative ψ' has a logarithmic divergence as $r \to 0$ and the statement in the lemma also follows. □

By means of Whittaker's functions [Mos93] one gets the values $n_-(H_1) = 1 = n_+(H_1)$ and $n_-(H_2) = 1 = n_+(H_2)$, so that $n_-(H) = 2 = n_+(H)$. Similarly to Example 7.3.4, taking into account that ψ, ψ' vanish at $\pm\infty$, it follows that

$$\Gamma(\psi, \varphi) = W_{0^+}[\psi, \varphi] - W_{0^-}[\psi, \varphi]$$
$$= \lim_{x \to 0^+} \left(\overline{\psi(x)}\varphi'(x) - \overline{\psi'(x)}\varphi(x)\right) + \lim_{x \to 0^-} \left(\overline{\psi'(x)}\varphi(x) - \overline{\psi(x)}\varphi'(x)\right).$$

Though the right-hand side is finite, each lateral limit may diverge. However, invoking Lemma 7.4.3 and since one readily checks that

$$\Gamma(\psi,\varphi) = \overline{\psi(0^+)}\tilde{\varphi}(0^+) - \overline{\tilde{\psi}(0^+)}\varphi(0^+) + \overline{\tilde{\psi}(0^-)}\varphi(0^-) - \overline{\psi(0^-)}\tilde{\varphi}(0^-),$$

but now each lateral limit is finite, again by following Example 7.3.4 a boundary triple was constructed. The self-adjoint extensions $H_{\hat{U}}$ of H are associated with 2×2 unitary matrices $\hat{U}$ that entail the boundary conditions

$$\left(\mathbf{1} - \hat{U}\right) \begin{pmatrix} \tilde{\psi}(0^-) \\ \tilde{\psi}(0^+) \end{pmatrix} = -i \left(\mathbf{1} + \hat{U}\right) \begin{pmatrix} -\psi(0^-) \\ \psi(0^+) \end{pmatrix},$$

and the domain of the self-adjoint extension $H_{\hat{U}}$ of H is composed of the elements $\psi \in \operatorname{dom} H^*$ so that the above boundary conditions are satisfied; also $H_{\hat{U}}\psi = H^*\psi$. Dirichlet boundary conditions $\psi(0^-) = 0 = \psi(0^+)$ are obtained by choosing $\hat{U} = \mathbf{1}$. Some boundary conditions mix the right and left half-lines, which are interpreted as quantum permeability of the singularity at the origin, that is, the particle is allowed to pass through the origin; see more details in Exercise 14.4.10 and [deOV08]. The above discussion also holds for $\kappa < 0$.

Exercise 7.4.4. Based on the arguments used to conclude Corollary 7.2.5, find the closure of the initial operator for the one-dimensional H-atom, that is, $H = -d^2/dx^2 - \kappa/|x|$ with domain $C_0^\infty(\mathbb{R} \setminus \{0\})$.

7.4.2 Some Point Interactions

Roughly speaking, *point interactions* are a kind of potential concentrated on a single point of $\mathbb{R}^n$, which are also called *zero-range potentials* and *delta-function potentials*. Often they are properly defined via the choice of domains and boundary conditions at the point in question, and it is a possible way to describe a hamiltonian with a Dirac δ potential.

Physically, the main consequence of extracting a point of $\mathbb{R}^n$ is that translation invariance is lost, which has impressive consequences on some quantum observables (i.e., operators) since the unique self-adjointness can also be lost (at least in dimensions $n \le 3$).

Different approaches for associating self-adjoint operators to point interactions are discussed in [Zor80]; more information can be obtained from the books [AGKH05] and [AlK00]. In those references, in case of $\mathbb{R}^n$, $n \le 3$, self-adjoint extensions of hermitian (Schrödinger) operators with point interactions are characterized and their spectral properties explicitly computed. Hence, point interactions have been called “solvable models” and used to approximately study physical systems with “very short range” potentials.

Here a few of the simplest cases will be discussed; Example 4.4.9 can be considered the first instance of point interaction in this book.

Example 7.4.5. Let $T = -id/dx$ with

$$\text{dom } T = C_0^\infty(\mathbb{R} \setminus \{0\}) = C_0^\infty(-\infty, 0) \oplus C_0^\infty(0, \infty).$$

One point was removed and the self-adjoint extensions are obtained from dom T^* through suitable matching conditions at the origin (recall that in case the domain is $C_0^\infty(\mathbb{R})$ the operator T is essentially self-adjoint; see Section 3.3). Set $T_1 = T|_{C_0^\infty(-\infty,0)}$ and $T_2 = T|_{C_0^\infty(0,\infty)}$, so that $T = T_1 \oplus T_2$. One has dom $T^* = \{\psi \in \mathrm{AC}(\mathbb{R} \setminus \{0\}) : \psi' \in \mathrm{L}^2(\mathbb{R})\}$, $T^*\psi = -i\psi'$.

Exercise 7.4.6. Check that

$$\text{dom } T_1^* = \{\psi \in \mathrm{AC}(-\infty, 0) : \psi' \in \mathrm{L}^2(-\infty, 0]\},$$
$$\text{dom } T_2^* = \{\psi \in \mathrm{AC}(0, \infty) : \psi' \in \mathrm{L}^2[0, \infty)\},$$

and verify that T^* is the above operator.

In order to determine the deficiency indices consider the $\mathrm{K}_\pm$-equations

$$(T_2^* \pm i\mathbf{1})\psi_\pm = 0,$$

whose solutions are proportional to $\psi_\pm(x) = e^{\pm x}$. Similarly for T_1. Hence $n_-(T_1) = 0 = n_+(T_2)$, $n_-(T_2) = 1 = n_+(T_1)$, and combining these values one obtains $n_-(T) = 1 = n_+(T)$.

Exercise 7.4.7. Follow the proof of Lemma 7.4.3 to show that, for $\psi \in$ dom T^*, the lateral limits $\psi(0^-), \psi(0^+)$, exist.

Now, for $\psi, \varphi \in$ dom T^* the boundary form is found (on integrating by parts):

$$\begin{aligned}\Gamma(\psi, \varphi) &= \langle T^*\psi, \varphi\rangle - \langle \psi, T^*\varphi\rangle \\ &= \left(\int_{-\infty}^{0^-} + \int_{0^+}^{\infty}\right) dx\ \left((\overline{-i\psi'(x)})\varphi(x) - \overline{\psi(x)}(-i\varphi'(x))\right) \\ &= i\left(\overline{\psi(0^+)}\varphi(0^+) - \overline{\psi(0^-)}\varphi(0^-)\right).\end{aligned}$$

Introduce the one-dimensional vector spaces $X = \{\psi(0^+) : \psi \in \text{dom } T^*\}$ and $Y = \{\psi(0^-) = \rho(\psi(0^+) : \psi \in \text{dom } T^*\}$ and note that $\Gamma(\psi, \varphi) = 0$ is equivalent to the equality of inner products

$$\langle \psi(0^+), \varphi(0^+)\rangle = \langle \rho(\psi(0^+)), \rho(\varphi(0^+))\rangle.$$

Self-adjoint extensions are obtained on domains $\mathcal{D} \subset$ dom T^* so that $\Gamma(\psi, \varphi) = 0$, $\forall \psi, \varphi \in \mathcal{D}$, that is, X and Y are related by unitary maps $e^{i\theta}$, $0 \le \theta < 2\pi$; explicitly $\psi(0^+) = e^{i\theta}\psi(0^-)$.

Therefore, the family of operators

$$\begin{aligned}\text{dom } T_\theta &= \left\{\psi \in \mathrm{AC}(\mathbb{R} \setminus \{0\}) : \psi' \in \mathrm{L}^2(\mathbb{R}), \psi(0^+) = e^{i\theta}\psi(0^-)\right\}, \\ T_\theta\psi &= -i\frac{d\psi}{dx},\end{aligned}$$

constitutes the self-adjoint extensions of T. The case $\theta = 0$ agrees with the momentum operator P (see Example 2.3.11 and Section 3.3) defined without point interaction, that is, with initial domain $C_0^\infty(\mathbb{R})$.

Exercise 7.4.8. Find the self-adjoint extensions of the hermitian operator $\operatorname{dom} T = C_0^\infty(\mathbb{R} \setminus \{0\})$, $T\psi = -\psi''$. Show that its deficiency indices are $n_- = n_+ = 2$.

Exercise 7.4.9. A circumference with one point removed can be considered a segment, say $[0,1]$, with the ends identified. Write $0 = 0^+$ and $1 = 0^-$, and construct the possible hamiltonians of a free particle on this circumference as self-adjoint extensions of $\operatorname{dom} H = C_0^\infty(0^+, 0^-)$, $H\psi = -\psi''$.

Example 7.4.10. This should be compared with Example 7.4.5. It is another possible way to define self-adjoint realizations of $T = -i\frac{d}{dx}$ in $\mathrm{L}^2(\mathbb{R})$ with the origin removed. Here one takes $\operatorname{dom} T = \{\psi \in \mathcal{H}^1(\mathbb{R}) : \psi(0) = 0\}$. It also illustrates another way of finding self-adjoint extensions. By using Fourier transform, this operator (see Section 3.3) is rewritten as a specific multiplication operator $S = \mathcal{F}^{-1}T\mathcal{F}$ so that

$$\operatorname{dom} S = \left\{\phi \in \operatorname{dom} P = \mathcal{H}^1(\hat{\mathbb{R}}) : 0 = \int_{\mathbb{R}} \phi(p)\, dp\right\}, \quad (S\phi)(p) = p\phi(p).$$

Recall that for $\psi \in \mathcal{H}^1(\mathbb{R})$ one has $\psi(0) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{\psi}(p)\, dp$, whose integral means $\lim_{M\to\infty} \int_{-M}^{M} \hat{\psi}(p)\, dp$; this explains $\operatorname{dom} S$.

Exercise 7.4.11. Show that S (and so T) is a hermitian operator.

Lemma 7.4.12. a) *S is a closed operator.*

b) *The solutions $u \in \mathrm{L}^2_{\mathrm{loc}}(\hat{\mathbb{R}})$ (or $\mathrm{L}^1_{\mathrm{loc}}(\hat{\mathbb{R}})$) of $\int_{\mathbb{R}} \phi(p)u(p)\, dp = 0$, $\forall \phi \in \operatorname{dom} S$, are the constant functions.*

Proof. a) Let $\psi_n \to \psi$ and $S\psi_n \to \phi$, $\psi_n \in \operatorname{dom} S$. For each $M > 0$ one has $\|\psi_n - \psi\| < 1/M$ if n is large enough. By Cauchy-Schwarz,

$$\left|\int_{-M}^{M} (\psi - \psi_n)\, dx\right| \le (2M)^{1/2} \|\psi_n - \psi\| < \sqrt{\frac{2}{M}}.$$

Since $\int_{\mathbb{R}} \psi_n\, dx = 0$, $\forall n$, choose n so that $\left|\int_{-M}^{M} \psi_n\, dx\right| < \sqrt{2/M}$; thus

$$\left|\int_{-M}^{M} \psi\, dx\right| \le \left|\int_{-M}^{M} (\psi - \psi_n)\, dx\right| + \left|\int_{-M}^{M} \psi_n\, dx\right| < 2\sqrt{\frac{2}{M}}$$

and it follows that $\int_{\mathbb{R}} \psi\, dx = 0$. Denote $|||\varphi|||_M := \left(\int_{M}^{M} |\varphi|^2\, dx\right)^{1/2}$. Pick n so large that $\|S\psi_n - \phi\| < 1/M^{1/2}$, and $\|\psi - \psi_n\| < 1/M$; then

$$\begin{aligned} |||p\psi|||_M &\le |||p(\psi - \psi_n)|||_M + |||p\psi_n - \phi|||_M + |||\phi|||_M \\ &\le M^{1/2} |||\psi - \psi_n|||_M + |||S\psi_n - \phi|||_M + \|\phi\| \\ &\le M^{1/2} \|\psi - \psi_n\| + \|S\psi_n - \phi\| + \|\phi\| < \frac{2}{M^{1/2}} + \|\phi\|, \end{aligned}$$

and for $M \to \infty$ one obtains $\|S\psi\| \le \|\phi\|$, consequently $\psi \in \mathrm{dom}\ S$. Similarly, by picking n large enough so that $\|\psi - \psi_n\| < 1/M$ and $\|S\psi_n - \phi\| < 1/M^{1/2}$, one gets

$$\begin{aligned}|||S\psi - \phi|||_M &\le |||S\psi - S\psi_n|||_M + |||S\psi_n - \phi|||_M \\ &\le M^{1/2}\|\psi - \psi_n\| + \|S\psi_n - \phi\| < \frac{2}{M^{1/2}}.\end{aligned}$$

Therefore $S\psi = \phi$ and S is a closed operator.

b) Note that the problem has no nonzero solution $u \in \mathrm{L}^2(\hat{\mathbb{R}})$, since such u would be orthogonal to the dense set dom S. Further, dom S contains the derivative ϕ' of all $\phi \in C_0^\infty(\mathbb{R})$ (since $\int \phi'\, dx = 0$), and so the distributional derivative u' of any solution u is null; the result then follows by applying Lemma 2.3.9. □

The deficiency spaces are $\mathrm{K}_\pm(S) = \mathrm{rng}\ (S \mp i\mathbf{1})^\perp$. Thus, for $u_\pm \in \mathrm{K}_\pm(S)$ one has, for all $\phi \in \mathrm{dom}\ S$,

$$\begin{aligned}0 &= \langle (S \mp i\mathbf{1})\phi, u_\pm\rangle = \int_{\mathbb{R}} \overline{(p \mp i)\phi(p)}\, u_\pm(p)\, dp \\ &= \int_{\mathbb{R}} \overline{\phi(p)}\, (p \pm i) u_\pm(p)\, dp \Longrightarrow u_\pm(p) = \frac{1}{p \pm i}.\end{aligned}$$

Lemma 7.4.12 was employed and, actually, the above $u_\pm$ linearly spans $\mathrm{K}_\pm(S)$, so that $n_- = n_+ = 1$; note that $\|u_-\| = \|u_+\|$. Thus the self-adjoint extensions S_θ of S are parametrized by $e^{i\theta}$, $0 \le \theta < 2\pi$, and given by (see Proposition 2.5.8)

$$\begin{aligned}\mathrm{dom}\ S_\theta &= \{\phi_\theta = \phi + c(u_- - e^{i\theta}u_+) : \phi \in \mathrm{dom}\ S, c \in \mathbb{C}\}, \\ (S_\theta\phi_\theta)(p) &= p\phi(p) + ci\left(u_-(p) + e^{i\theta}u_+(p)\right).\end{aligned}$$

By recalling of Section 3.3, the following question naturally arises: For which values of θ do S_θ act as multiplication by p? Since $u_\pm(p) = 1/(p \pm i)$ one has

$$S_\theta(u_- - e^{i\theta}u_+)(p) = i\frac{p(1 + e^{i\theta}) + i(1 - e^{i\theta})}{1 + p^2},$$

and by imposing that it equals $p(u_- - e^{i\theta}u_+)(p)$, it follows that $\theta = 0$. Surely S_0 corresponds to the usual multiplication operator $\mathcal{M}_p$ acting in $\mathrm{L}^2(\hat{\mathbb{R}})$, which is the usual momentum operator P (see Example 2.3.11 and Section 3.3), clearly a self-adjoint extension of T.

Exercise 7.4.13. Apply the procedure in Example 7.4.10 to find all self-adjoint extensions of $T\psi = -\Delta\psi$, dom $T = \{\psi \in \mathcal{H}^2(\mathbb{R}^n) : \psi(0) = 0\}$, for $n \in \mathbb{N}$. Note that there is a problem for $n \ge 4$, since by Sobolev embedding the functions in dom T are not ensured to be continuous; in any event, for all n the following operators obtained after Fourier transforming are well defined:

$$\mathrm{dom}\ S = \left\{\phi \in \mathrm{dom}\ P : 0 = \int_{\mathbb{R}^n} \phi(p)\, dp\right\}, \qquad (S\phi)(p) = p^2\phi(p).$$

What is it possible to conclude about the operator S for $n \geq 4$? See Remark 7.4.14 for related issues.

Remark 7.4.14. In [Far75], page 33, it is shown that the set $C_0^\infty(\mathbb{R}^n \setminus \{0\})$ is dense in $\mathcal{H}^2(\mathbb{R}^n)$ iff $n \geq 4$. From this it follows that $\dot{H} = -\Delta$, dom $\dot{H} = C_0^\infty(\mathbb{R}^n \setminus \{0\})$, is essentially self-adjoint iff $n \geq 4$, and in this case its unique self-adjoint extension is $H_0 = -\Delta$, dom $H_0 = \mathcal{H}^2(\mathbb{R}^n)$. As a matter of fact, clearly H_0 is a self-adjoint extension of $\dot{H}$, and since the graph norm of H_0 is equivalent to the norm of $\mathcal{H}^2(\mathbb{R}^n)$, $C_0^\infty(\mathbb{R}^n \setminus \{0\})$ is a core of H_0 iff this set is dense in $\mathcal{H}^2(\mathbb{R}^n)$; so, iff $n \geq 4$.

Remark 7.4.15. The procedures discussed in Examples 7.4.5 and 7.4.10 to remove the origin are not equivalent in general. When applied to the operator $T\psi = -\psi''$ in $\mathbb{R}$ (see Exercises 7.4.8 and 7.4.13), the former procedure results in deficiency indices $n_- = 2 = n_+$, whereas the latter in $n_- = 1 = n_+$.

7.5 Spherically Symmetric Potentials

A potential $v : \mathbb{R}^n \to \mathbb{R}$ is *spherically symmetric* (also called *radial* or *central*) if its values depend only on $r = |x|$, that is, if there exists $V : [0, \infty) \to \mathbb{R}$ so that $v(x) = V(r)$.

It is convenient to exclude the origin and take as the initial hamiltonian operator

$$H = -\Delta + V(r), \qquad \text{dom } H = C_0^\infty(\mathbb{R}^n \setminus \{0\}).$$

It is natural to introduce the radius r and $n-1$ angle variables $\Omega = \{\omega_1, \dots, \omega_{n-1}\}$ for the description of the system. For instance, if $n = 3$ one passes from cartesian $x = (x_1, x_2, x_3)$ to spherical (r, φ, θ) coordinates $x_1 = r \sin\theta \cos\varphi$, $x_2 = r \sin\theta \cos\varphi$, $x_3 = r\cos\theta$, so that $\mathrm{L}^2(\mathbb{R}^3)$ is unitarily equivalent to

$$E^3 = \mathrm{L}^2_{r^2dr}([0,\infty)) \otimes \mathrm{L}^2_{d\Omega}(S^2),$$

with S^2 denoting the unit sphere in $\mathbb{R}^3$ and $d\Omega = \sin\theta d\theta d\varphi$. If $n = 2$ polar coordinates $x_1 = r\cos\varphi$, $x_2 = r\sin\varphi$ are introduced so that $\mathrm{L}^2(\mathbb{R}^2)$ is unitarily equivalent to

$$E^2 = \mathrm{L}^2_{rdr}([0,\infty)) \otimes \mathrm{L}^2_{d\varphi}(S^1),$$

with S^1 denoting the unit circumference in $\mathbb{R}^2$. Here only $n = 2, 3$ will be considered, although many results have straight counterparts in higher dimensions; see, e.g., [Mu66].

By Lemma 1.4.8 the set of finite linear combinations of the functions $R(r)\Phi(\theta, \varphi) \in E^3$ (resp. $R(r)\Phi(\varphi) \in E^2$) is dense in $\mathrm{L}^2(\mathbb{R}^3)$ (resp. $\mathrm{L}^2(\mathbb{R}^2)$) and the spherical harmonics $Y_{lm}(\theta, \varphi)$, $l \in \mathbb{N} \cup \{0\}$, $-l \leq m \leq l$, (resp. $e_m(\varphi) = e^{im\varphi}/\sqrt{2\pi}$, $m \in \mathbb{Z}$) form an orthonormal basis of $\mathrm{L}^2(S^2)$ (resp. $\mathrm{L}^2(S^1)$). For functions $R(r)Y_{lm}(\theta, \varphi)$, $R \in C_0^\infty(0, \infty)$, in case $n = 3$, the well-known expression of the laplacian Δ in spherical coordinates implies that (see, e.g., [Will03])

$$H(RY_{lm}) = \left(-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + \frac{l(l+1)}{r^2} + V(r) \right) RY_{lm},$$

and after the unitary transformation $u_3 : \mathrm{L}^2_{r^2dr}([0,\infty)) \to \mathrm{L}^2_{dr}([0,\infty))$, $(u_3R)(r) = rR(r)$, one obtains for $u_3Hu_3^{-1}$ restricted to the subspace spanned by Y_{lm} (note that $u_3(C_0^\infty(0,\infty)) \subset C_0^\infty(0,\infty))$

$$\hat{H}_{lm} = -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + V(r), \qquad \mathrm{dom}\ \hat{H}_{lm} = C_0^\infty(0,\infty).$$

For $n = 2$ one has

$$H(Re_m) = \left(-\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{m^2}{r^2} + V(r)\right) Re_m,$$

and after the unitary transformation $u_2 : \mathrm{L}^2_{rdr}([0,\infty)) \to \mathrm{L}^2_{dr}([0,\infty))$, with $(u_2R)(r) = \sqrt{r}R(r)$, one obtains for $u_2Hu_2^{-1}$ restricted to the subspace spanned by e_m,

$$\hat{H}_m = -\frac{d^2}{dr^2} + \frac{m^2 - 1/4}{r^2} + V(r), \qquad \mathrm{dom}\ \hat{H}_m = C_0^\infty(0,\infty).$$

In both cases, i.e., $n = 2, 3$, the original problem is reduced to the study of infinitely many Schrödinger operators on the half-line $[0,\infty)$ with suitable effective potentials $\hat{V}_m$ or $\hat{V}_{l,m}$; e.g., in the two-dimensional case,

$$\hat{V}_m(r) = (m^2 - 1/4)/r^2 + V(r), \qquad m \in \mathbb{Z}.$$

The previous discussions in this chapter, about Schrödinger operators on intervals, apply to $\hat{H}_m$ and $\hat{H}_{lm}$.

Remark 7.5.1. Note that the *radial momentum operator* $-id/dr$ is not defined as a physical quantity on $C_0^\infty(0,\infty)$, since it has no self-adjoint extensions (see Example 2.3.17 and an intuitive digression in Remark 5.4.7).

Exercise 7.5.2. Consider $\hat{H}_{lm}$ and $\hat{H}_m$ in $\mathbb{R}^3$ and $\mathbb{R}^2$, respectively, for the free particle, i.e., $V = 0$ identically. Use results of this chapter to show that $\hat{H}_{lm}$ (resp. $\hat{H}_m$) is not essentially self-adjoint only if $l = 0$ (resp. $m = 0$). Find the corresponding deficiency indices. What can be said about $H = -\Delta$, $\mathrm{dom}\ H = C_0^\infty(\mathbb{R}^n \setminus \{0\})$, $n = 2, 3$? Cf. Exercise 7.4.8.

Now some particular cases of minimal operators $\mathrm{dom}\ H = C_0^\infty(0,\infty)$, $H\psi = -\psi'' + V(r)\psi$ will be discussed (think of the above notation with $\hat{V}$ replaced by V). In the remainder of this section, H always denotes this operator.

Proposition 7.5.3. *If $V \in \mathrm{L}^2(0,\infty)$, then $n_-(H) = 1 = n_+(H)$ and*

$$\Gamma_{H^*}(\psi,\varphi) = -W_0[\psi,\varphi], \qquad \forall \psi,\varphi \in \mathrm{dom}\ H^*.$$

Lemma 7.5.4. *Fix $c > 0$. If $V \in \mathrm{L}^2(0,\infty)$, then for each $\psi \in \mathrm{dom}\ H^*$ there exists $0 \le C < \infty$ so that*

$$\left|\frac{\psi'(x)}{\sqrt{x}}\right| \le C, \qquad \forall x > c.$$

Proof. For $\psi \in \operatorname{dom} H^*$ one has $-\psi'' + V\psi = u \in \mathrm{L}^2(0,\infty)$; integrating u and taking into account that $V\psi \in \mathrm{L}^1(0,\infty)$ one obtains ($x > c$)

$$\psi'(x) = \psi'(c) + \int_c^x dt\, V(t)\psi(t) - \int_c^x dt\, u(t),$$

and by Cauchy-Schwarz,

$$\begin{aligned}|\psi'(x)| &\le |\psi'(c)| + \int_c^x dt\, |V(t)\psi(t)| + \int_c^x dt\, |u(t)| \\ &\le |\psi'(c)| + \|V\psi\|_1 + \left(\int_c^x dt\, |u(t)|^2\right)^{1/2} \left(\int_c^x dt\right)^{1/2} \\ &\le |\psi'(c)| + \|V\psi\|_1 + \|u\|_2 \sqrt{x-c}.\end{aligned}$$

Hence,

$$\begin{aligned}\left|\frac{\psi'(x)}{\sqrt{x}}\right| &\le \frac{|\psi'(c)| + \|V\psi\|_1}{\sqrt{x}} + \frac{\|u\|_2 \sqrt{x-c}}{\sqrt{x}} \\ &\le \frac{|\psi'(c)| + \|V\psi\|_1}{\sqrt{c}} + \|u\|_2 := C, \qquad x > c.\end{aligned}$$

The lemma is proved. □

Proof. **[Proposition 7.5.3]** Since 0 is a regular point of H it is in the limit circle case (and $\psi(0), \psi'(0)$ take finite values). So the deficiency indices are equal either to 1 or to 2. It will be checked that $W_\infty[\psi,\varphi] = 0$, $\forall \psi,\varphi \in \operatorname{dom} H^*$, so that $\Gamma_{H^*}(\psi,\varphi) = -W_0[\psi,\varphi] = \varphi(0)\overline{\psi'(0)} - \varphi'(0)\overline{\psi(0)}$ and, as in Example 7.3.1, the self-adjoint extensions of H are parametrized by the complex numbers $e^{i\theta}$; thus the deficiency indices of H are equal to 1. As a subproduct it follows that H is in the limit point case at ∞.

Let $\psi \in \operatorname{dom} H^*$; it is known that $W_\infty[\psi,\varphi]$ is finite. Suppose $x > c$; by Lemma 7.5.4,

$$\frac{1}{\sqrt{x}}\, |W_x[\psi,\varphi]| = \left|\overline{\psi(x)}\frac{\psi'(x)}{\sqrt{x}} - \frac{\overline{\psi'(x)}}{\sqrt{x}}\psi(x)\right| \le 2C\, |\psi(x)|\,,$$

so that the right-hand side belongs to $\mathrm{L}^2(c,\infty)$, but the left-hand side does not belong to $\mathrm{L}^2(c,\infty)$ if $W_\infty[\psi,\varphi] \ne 0$. Hence, $W_\infty[\psi,\varphi] = 0$, $\forall \psi \in \operatorname{dom} H^*$. □

Exercise 7.5.5. If $V \in \mathrm{L}^2(0,\infty)$, find all self-adjoint extensions of H (see Example 7.3.1).

Exercise 7.5.6. Show that if the potential $V \in \mathrm{L}^2_{\mathrm{loc}}(0,\infty)$ is in L^2 near ∞, then $\Gamma_{H^*}(\psi,\varphi) = -W_0[\psi,\varphi]$, $\forall \psi,\varphi \in \operatorname{dom} H^*$. Conclude that if V is regular at 0, then the deficiency indices of H are equal to 1.

Remark 7.5.7. As discussed in [Win47], for a class of negative potentials $V(x)$, $x \in \mathbb{R}$, satisfying a technical condition and $\lim_{x\to\infty} V(x) = -\infty$, the differential operator H is limit circle at infinity iff, for some $x_0 > 0$, $\int_{x_0}^{\infty} (-V(x))^{-1/2}\, dx < \infty$. In case of $V(x) = -\kappa x^\alpha$, $x > 0$ and $\kappa > 0, \alpha > 0$, H is then limit point at ∞ iff $\alpha \le 2$ (this case is included in Wintner's class).

This characterization of limit point at infinity has a counterpart in classical mechanics that is worth mentioning (and appreciating). For a classical particle of mass m and total mechanical energy E under this potential $V(x)$, the travel time from the initial position $x_0 > 0$ to ∞ is

$$\tau_\infty = \sqrt{\frac{m}{2}} \int_{x_0}^{\infty} \frac{dx}{\sqrt{E - V(x)}}.$$

This follows from conservation of mechanical energy (check this!). If $x_0 \gg 1$ so that $|V(x)| \gg E$, $\forall x \ge x_0$ (since $\lim_{x\to\infty} V(x) = -\infty$), one has

$$\tau_\infty \approx \sqrt{\frac{m}{2}} \int_{x_0}^{\infty} \frac{dx}{\sqrt{-V(x)}},$$

that is, the condition $\tau_\infty = \infty$ coincides with the limit point criterion, which, in its turn, is a necessary condition for the existence of just one self-adjoint extension of H. Hence, for such potentials, a finite travel time to reach infinity in classical mechanics is reflected in the quantum limit circle at infinity, inferring the quantum ambiguity of more than one self-adjoint extension of H. However, there are counterexamples to this correspondence between essential self-adjointness and finite travel time to infinity [RaR73].

A discussion, from a physical point of view, of the unitary evolution group generated by H with negative potentials so that $\tau_\infty < \infty$ can be found in [CFGM90].

Additional criteria for limit point and limit circle can be found in [Na69], [ReeS75] and [DuS63]. See also [BaZG04].

7.5.1 A Multiply Connected Domain

Some self-adjoint extensions of a hermitian operator with infinite deficiency index will be found. It will combine the spherical symmetry with the topological property of multiply connectedness. Some specific results on Sobolev traces will be invoked; see [Bre99, Ad75] and Chapters 1 and 2 of the first volume of [LiM72]. Nevertheless we think the set of presented results will make this subsection worthwhile; except for Section 10.5, they will not be needed for other parts of the text.

Let $\Lambda = \mathbb{R}^2 \setminus \overline{B}(0; a)$, $a > 0$ (i.e., the plane with a circular hole), and its closure $\overline{\Lambda} = \mathbb{R}^2 \setminus B(0; a)$; its boundary $\partial\Lambda$ is the circumference $S = \{(x_1, x_2) \in$

$\mathbb{R}^2 : r = (x_1^2 + x_2^2)^{\frac{1}{2}} = a\}$. The potential will be a bounded continuous $V : \overline{\Lambda} \to \mathbb{R}$, with $V(x) = V(r)$, and the initial hamiltonian is the hermitian operator

$$H = -\Delta + V, \qquad \mathrm{dom}\, H = C_0^\infty(\Lambda).$$

What are the self-adjoint extensions of H?

As above, polar coordinates $x_1 = r\cos\varphi$, $x_2 = r\sin\varphi$ are introduced so that $\mathrm{L}^2(\overline{\Lambda})$ is unitarily equivalent to $\mathrm{L}^2_{rdr}([a,\infty)) \otimes \mathrm{L}^2_{d\varphi}(S)$, and consider the functions $e_m(\varphi) = e^{im\varphi}/\sqrt{2\pi}$, $0 \le \varphi \le 2\pi, m \in \mathbb{Z}$, so that

$$H(Re_m) = \left(-\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{m^2}{r^2} + V(r)\right) Re_m.$$

After performing the unitary transformation $u_2 : \mathrm{L}^2_{rdr}([a,\infty)) \to \mathrm{L}^2_{dr}([a,\infty))$, $(u_2R)(r) = \sqrt{r}R(r)$, the operator $u_2Hu_2^{-1}$ restricted to the subspace spanned by e_m takes the form

$$\hat{H}_m = -\frac{d^2}{dr^2} + \frac{m^2 - 1/4}{r^2} + V(r), \qquad \mathrm{dom}\, \hat{H}_m = C_0^\infty(a,\infty).$$

The original problem is thus reduced to the study of infinitely many Schrödinger operators on $[a,\infty)$ with potentials

$$\hat{V}_m(r) = (m^2 - 1/4)/r^2 + V(r), \qquad m \in \mathbb{Z}.$$

One then easily checks that, for all m, the deficiency indices of H_m are equal to 1 (the point here is that $a > 0$, instead of $a = 0$ previously discussed), so that $n_+(H) = \infty = n_-(H)$.

The subject now is to recall Sobolev traces in a convenient way. Although a $\psi(r,\varphi) \in \mathcal{H}^1(\Lambda)$ is not necessarily continuous, it is possible to give a meaning to the restriction $\psi(a,\varphi) = \psi|_{\partial\Lambda}(\varphi) \in \mathrm{L}^2(S)$ via the so-called *Sobolev trace* of ψ (see below), that is, the trace of ψ is interpreted as its value on the boundary of Λ.

Let $\mathcal{R}C_0^1(\mathbb{R}^2)$ be the restriction of $C_0^1(\mathbb{R}^2)$ to $C_0^1(\overline{\Lambda})$ (see the references for details); it turns out that there is a continuous linear map $\gamma : \mathcal{R}C_0^1(\mathbb{R}^2) \subset \mathcal{H}^1(\Lambda) \to \mathrm{L}^2(S)$, $\gamma(\phi(r,\varphi)) = \phi(a,\varphi)$, that is, there is $C > 0$ so that

$$\|\gamma\phi\|_{\mathrm{L}^2(S)} = \|\phi(a,\varphi)\|_{\mathrm{L}^2(S)} \le C\,\|\mathcal{R}\phi\|_{\mathcal{H}^1(\Lambda)}, \qquad \phi \in C_0^1(\mathbb{R}^2).$$

Note that for $\phi \in C_0^1(\mathbb{R}^2)$ the boundary values $\phi(a,\varphi)$ are well defined for any angular value φ. By density, this map has a unique continuous extension (keeping the same notation) $\gamma : \mathcal{H}^1(\Lambda) \to \mathrm{L}^2(S)$, called the *Sobolev trace map*, and one defines the trace of ψ as $\psi(a,\varphi) := \gamma(\psi)$ for all $\psi \in \mathcal{H}^1(\Lambda)$. The essential characteristics here are smoothness and compactness of the boundary $\partial\Lambda$ [Bre99]; some important properties of the trace are as follows.

i) For $\psi \in \mathcal{H}^1(\Lambda)$ the trace is not defined in a pointwise manner, only as a function in $\mathrm{L}^2(S)$. General elements of $\mathrm{L}^2(\Lambda)$ do not have a trace defined.

ii) rng γ is dense in $\mathrm{L}^2(S)$ and the Green formula

$$\int_\Lambda \frac{\partial \psi(x)}{\partial x_j} \phi(x)\, dx + \int_\Lambda \psi(x) \frac{\partial \phi(x)}{\partial x_j}\, dx = a \int_0^{2\pi} \psi(a,\varphi)\phi(a,\varphi)\, d\varphi$$

holds for all $\psi, \phi \in \mathcal{H}^1(\Lambda)$, $j = 1, 2$.

iii) The kernel of the trace operator is

$$\mathcal{H}_0^1(\Lambda) := \{\psi \in \mathcal{H}^1(\Lambda) : \gamma(\psi) = \psi(a,\varphi) = 0\},$$

which is a Hilbert space that can also be defined as the closure of $C_0^\infty(\Lambda)$ in $\mathcal{H}^1(\Lambda)$.

iv) In a similar way, if $\psi \in \mathcal{H}^2(\Lambda)$ one has a well-defined trace $\gamma(\partial\psi/\partial r)$, which will be denoted by $\partial\psi/\partial r(a,\varphi)$, which stands for the normal derivative with respect to $\partial\Lambda$ (this is used in the adaptation to more general Λ) and belongs to $\mathrm{L}^2(\partial\Lambda)$.

v) The ranges of both trace maps $\mathcal{H}^2(\Lambda) \ni \psi \mapsto \psi(a,\varphi)$ and $\mathcal{H}^2(\Lambda) \ni \psi \mapsto \partial\psi/\partial r(a,\varphi)$ are dense in $\mathrm{L}^2(S)$, and the Green formula

$$\int_\Lambda \Delta\psi(x)\phi(x)\, dx + \int_\Lambda \nabla\psi(x)\nabla\phi(x)\, dx = a \int_0^{2\pi} \frac{\partial\psi}{\partial r}(a,\varphi)\phi(a,\varphi)\, d\varphi$$

holds for all $\psi, \phi \in \mathcal{H}^2(\Lambda)$.

Now a subtlety must be mentioned. At first sight one could (wrongly) guess that the domain of the adjoint H^* is $\mathcal{H}^2(\Lambda)$. However, for open sets $\Omega \subset \mathbb{R}^n$, $\Omega \neq \mathbb{R}^n$ and $n \geq 2$, there are functions $\psi \in \mathrm{L}^2(\Omega)$ with distributional laplacian $\Delta\psi \in \mathrm{L}^2(\Omega)$ that do not belong to $\mathcal{H}^2(\Omega)$; the point is that other derivatives, as first derivatives, of ψ need not exist as functions! It turns out that

$$\mathrm{dom}\ H^* = \left\{\psi \in \mathrm{L}^2(\Lambda) : (-\Delta\psi + V\psi) \in \mathrm{L}^2(\Lambda)\right\}$$

and $H^*\psi = -\Delta\psi + V\psi$, $\psi \in \mathrm{dom}\ H^*$, and this domain is strictly larger than $\mathcal{H}^2(\Lambda)$. See [Gru06], [Gru08] and references therein.

By using the above characterization of H^*, some self-adjoint extensions of H will be found via suitable restrictions of H^*. The boundary form of H, for $\psi, \phi \in \mathrm{dom}\ H^*$, is

$$\Gamma(\psi,\phi) := \langle(-\Delta + V)\psi, \phi\rangle - \langle\psi, (-\Delta + V)\phi\rangle.$$

By restricting to those self-adjoint extensions whose domains are contained in $\mathcal{H}^2(\Lambda)$, Sobolev traces can be invoked, the continuity of the potential guarantees that $V|_{\partial\Lambda} = V(a)$ is well posed and the above Green formula can be used to compute, for $\psi, \phi \in \mathcal{H}^2(\Lambda)$,

$$\Gamma(\psi,\phi) = a \int_0^{2\pi} \left(\overline{\psi(a,\varphi)}\, \frac{\partial\phi}{\partial r}(a,\varphi) - \overline{\frac{\partial\psi}{\partial r}(a,\varphi)}\, \phi(a,\varphi)\right) d\varphi.$$

Introduce $\rho_j : \mathcal{H}^2(\Lambda) \to \mathrm{L}^2(S)$, $j = 1, 2$, by

$$\rho_1(\psi) = \psi(a,\varphi) + i\frac{\partial\psi}{\partial r}(a,\varphi),$$
$$\rho_2(\psi) = \psi(a,\varphi) - i\frac{\partial\psi}{\partial r}(a,\varphi),$$

and so

$$(2i/a)\,\Gamma(\psi,\phi) = \langle\rho_1(\psi),\rho_1(\phi)\rangle_{\mathrm{L}^2(S)} - \langle\rho_2(\psi),\rho_2(\phi)\rangle_{\mathrm{L}^2(S)}\,.$$

Exercise 7.5.8. Verify the above two expressions for the boundary form $\Gamma(\psi,\phi)$ of H, for $\psi,\phi \in \mathcal{H}^2(\Lambda)$.

A boundary triple for H in the Sobolev space $\mathcal{H}^2(\Lambda)$ has been found with $\mathbf{h} = \mathrm{L}^2(S)$. As before (i.e., by Theorem 7.1.13), from this boundary triple the self-adjoint extensions H_U of H in $\mathcal{H}^2(\Lambda)$ are characterized by unitary operators $U : \mathrm{L}^2(S) \hookleftarrow$ so that $\rho_1(\psi) = U\rho_2(\psi)$, $\forall\psi \in \mathrm{dom}\ H_U$, and $H_U\psi = H^*\psi$. After writing out this relation one finds

$$(\mathbf{1} - U)\,\psi(a,\varphi) = -i(\mathbf{1} + U)\frac{\partial\psi}{\partial r}(a,\varphi).$$

Therefore, all self-adjoint extensions of H with domain in $\mathcal{H}^2(\Lambda)$ were found and they are realized through suitable boundary conditions on $\partial\Lambda$; such boundary conditions are in terms of traces of elements of $\mathcal{H}^2(\Lambda)$. Below some explicit self-adjoint extensions are described.

1. $U = -\mathbf{1}$.

   In this case

   $$\mathrm{dom}\ H_U = \{\psi \in \mathcal{H}^2(\Lambda) : \psi(a,\varphi) = 0\} = \mathcal{H}^2(\Lambda) \cap \mathcal{H}^1_0(\Lambda),$$

   $H_U\psi = (-\Delta + V)\psi$, $\psi \in \mathrm{dom}\ H_U$. This is the so-called Dirichlet realization (of the laplacian if $V = 0$) in Λ.

2. $U = \mathbf{1}$.

   In this case $\mathrm{dom}\ H_U = \{\psi \in \mathcal{H}^2(\Lambda) : \partial\psi/\partial r(a,\varphi) = 0\}$, $H_U\psi = (-\Delta + V)\psi$. This is the so-called Neumann realization.

3. $(\mathbf{1} + U)$ is invertible.

   In this case one gets that for each self-adjoint operator $A : \mathrm{dom}\ A \sqsubseteq \mathrm{L}^2(S) \to \mathrm{L}^2(S)$ corresponds a self-adjoint extension H^A. In fact, first pick a unitary operator U_A so that $A = -i(\mathbf{1} - U_A)(\mathbf{1} + U_A)^{-1}$, $\mathrm{dom}\ A = \mathrm{rng}\ (\mathbf{1}+U_A)$ and $\mathrm{rng}\ A = \mathrm{rng}\ (\mathbf{1}-U_A)$; recall the Cayley transform in Chapter 2. Now, $\mathrm{dom}\ H^A$ is the set of $\psi \in \mathcal{H}^2(\Lambda)$ with "$\partial\psi/\partial r(a,\cdot) = A\psi(a,\cdot)$," prudently understood in the sense that

   $$(\mathbf{1} - U_A)\,\psi(a,\varphi) = -i(\mathbf{1} + U_A)\frac{\partial\psi}{\partial r}(a,\varphi),$$

   in order to avoid domain questions. Of course the quotation marks can be removed in case the operator A is bounded.

Similarly, for each self-adjoint B acting in $\mathrm{L}^2(S)$ there corresponds a unitary U_B, and if $(\mathbf{1} - U_B)$ is invertible, then there corresponds the self-adjoint extension H^B of H with dom H^B the set of $\psi \in \mathcal{H}^2(\Lambda)$ so that "$\psi(a,\cdot) = B\frac{\partial\psi}{\partial r}r(a,\cdot)$," in the sense that

$$(\mathbf{1} - U_B)\,\psi(a,\varphi) = -i(\mathbf{1} + U_B)\frac{\partial\psi}{\partial r}(a,\varphi).$$

Again the quotation marks can be removed in case the operator B is bounded.

Note that 4 below is, in fact, particular cases of 3 in which $A = \mathcal{M}_f$ and $B = \mathcal{M}_g$.

4. U is a multiplication operator.

   Given a real-valued (measurable) function $u(\varphi)$ put $U = \mathcal{M}_{e^{iu(\varphi)}}$. If $\{\varphi : \exp(iu(\varphi)) = -1\}$ has measure zero, then

$$f(\varphi) = -i\frac{1 - e^{iu(\varphi)}}{1 + e^{iu(\varphi)}}$$

   is (measurable) well defined and real valued. The domain of the corresponding self-adjoint extension is

$$\operatorname{dom} H_U = \left\{\psi \in \mathcal{H}^2(\Lambda) : \partial\psi/\partial r(a,\varphi) = f(\varphi)\psi(a,\varphi)\right\}.$$

   Similarly, if $\{\varphi : \exp(iu(\varphi)) = 1\}$ has measure zero,

$$g(\varphi) = i\frac{1 + e^{iu(\varphi)}}{1 - e^{iu(\varphi)}}$$

   is real valued and the domain of the subsequent self-adjoint extension is

$$\operatorname{dom} H_U = \{\psi \in \mathcal{H}^2(\Lambda) : \psi(a,\varphi) = g(\varphi)\partial\psi/\partial r(a,\varphi)\}.$$

   Special cases are given by constant functions f, g.

5. $A = -id/d\varphi$ with domain $\mathcal{H}^1(S) = \{u \in \mathcal{H}^1(0, 2\pi) : u(0) = u(2\pi)\}$. The corresponding self-adjoint extension has domain

$$\left\{\psi \in \mathcal{H}^2(\Lambda) : \psi(a,\varphi) \in \mathcal{H}^1(S),\ \text{``}\frac{\partial\psi}{\partial r}(a,\varphi) = -i\frac{d\psi}{d\varphi}(a,\varphi)\text{''}\right\}.$$

Exercise 7.5.9. Show that $A = -id/d\varphi$ in 5 above is self-adjoint.

Since the deficiency indices of H are infinite, there is a plethora of self-adjoint extensions of the laplacian in the multiply connected domain $\Lambda = \mathbb{R}^2 \setminus \overline{B}(0; a)$. Some of them can be quite unusual and hard to understand from the physical and mathematical points of view.

Remark 7.5.10. The choice of $\Lambda = \mathbb{R}^2 \setminus \overline{B}(0;a)$ was for notational convenience. In a similar way one finds expressions for the boundary form of $H = -\Delta + V$ with domain $C_0^\infty(\mathbb{R}^2 \setminus \overline{\Omega})$, with $\Omega \subset \mathbb{R}^2$ an open set with compact boundary $\partial\Omega$ of class C^1; when restricted to domains in $\mathcal{H}^2(\mathbb{R}^2 \setminus \Omega)$, Sobolev traces are properly defined in this setting, and one can also consider $\mathbb{R}^n$, $n \geq 2$. For such more general multiply connected regions, one must consider the normal derivative $\partial\psi/\partial\mathbf{n}$ at the boundary $\partial\Omega$, instead of $\partial\psi/\partial r$, and also the corresponding modifications in the expressions of Green formulae [Bre99], [LiM72].

Remark 7.5.11. The above approach to the self-adjoint extensions of the laplacian in $\mathcal{H}^2(\Lambda)$ was borrowed from [deO08], as well as the variation of the concept of boundary triple. However, by using a continuous extension of the trace maps to the dual Sobolev spaces $\mathcal{H}^{-1/2}(\partial\Lambda)$ and $\mathcal{H}^{-3/2}(\partial\Lambda)$, in [Gru06] one finds references and comments to her previous works on all self-adjoint extensions of the laplacian in terms of self-adjoint operators from closed subspaces of $\mathcal{H}^{-1/2}(\partial\Lambda)$.

Exercise 7.5.12. Let $0 < a < b < \infty$ and

$$\Lambda_{ab} = \left\{ (x_1, x_2) \in \mathbb{R}^2 : a < (x_1^2 + x_2^2)^{\frac{1}{2}} < b \right\}$$

be an annulus in $\mathbb{R}^2$. Find the self-adjoint extensions of the laplacian $H_0 = -\Delta$, $\operatorname{dom} H_0 = C_0^\infty(\Lambda_{ab})$, whose domains are contained in $\mathcal{H}^2(\Lambda_{ab})$.

Chapter 8

Spectral Theorem

A discussion of the spectral theorem for self-adjoint operators is presented, including details of the resolution of the identity and functions of self-adjoint operators. Although a complete proof of this theorem for a given operator is not presented, different approaches to the proof are indicated. Spectral measures of some simple examples are discussed. Chapter 9 is devoted to some consequences of the spectral theorem. $\mathcal{A}$ denotes the σ-algebra of Borel sets in $\mathbb{R}$.

8.1 Compact Self-Adjoint Operators

In this section the particular case of compact self-adjoint operators on a Hilbert space $\mathcal{H}$ is considered. The spectral theorem for such operators will be presented; besides its own interest, it will serve as a motivating guide for the noncompact case discussed ahead. With a little additional effort compact normal operators will also be discussed.

Lemma 8.1.1. *Every nonzero compact and self-adjoint operator $T \in \mathrm{B}(\mathcal{H})$ has a nonzero eigenvalue, since either $-\|T\|$ or $\|T\|$ is an eigenvalue of T.*

Proof. The spectrum of T is real and by Proposition 2.1.12, its spectral radius is $\|T\|$, so either $-\|T\|$ or $\|T\|$ belongs to the spectrum of T. By the compactness of T it will follow that one of them is an eigenvalue, which is equivalent to finding $0 \neq \zeta \in \mathcal{H}$ with $(T^2 - \|T\|^2\mathbf{1})\zeta = 0$.

Let (ξ_n), $\|\xi_n\| = 1, \forall n$, so that $\|T\xi_n\| \to \|T\|$. Since T is compact, there exists a convergent subsequence of $(T\xi_n)$, also denoted by $(T\xi_n)$; since T is continuous, $(T^2\xi_n)$ also converges.

The estimate

$$\begin{aligned} 0 &\leq \left\|T^2\xi_n - \|T\xi_n\|^2\xi_n\right\|^2 = \|T^2\xi_n\|^2 - \|T\xi_n\|^4 \\ &\leq \|T\|^2\|T\xi_n\|^2 - \|T\xi_n\|^4 \ \longrightarrow 0 \ \text{ as } \ n \to \infty, \end{aligned}$$

shows that the sequence $\eta_n = T^2\xi_n - \|T\xi_n\|^2\xi_n$ converges to zero and so

$$\xi_n = \left(T^2\xi_n - \eta_n\right)/\|T\xi_n\|^2$$

converges to a vector ζ with $\|\zeta\| = 1$. Therefore, denoting $\lambda = \|T\|$ and recalling that T is continuous, $0 = T^2\zeta - \|T\|^2\zeta = T_\lambda T_{-\lambda}\zeta$. Hence either $T_{-\lambda}\zeta = 0$ and $-\|T\|$ is an eigenvalue of T, or $T_{-\lambda}\zeta \neq 0$ and $\|T\|$ is an eigenvalue of T. □

Theorem 8.1.2 (Hilbert-Schmidt). *Let $T \in \mathrm{B}_0(\mathcal{H})$ be compact and self-adjoint and Λ the set of eigenvalues of T. Then*

$$\mathcal{H} = \left[\bigoplus_{0\neq\lambda\in\Lambda} \mathrm{N}(T_\lambda)\right] \oplus \mathrm{N}(T).$$

Proof. Since T is self-adjoint $\mathrm{N}(T_\lambda) \perp \mathrm{N}(T_\mu)$ if $\lambda \neq \mu$, and the direct sum above is well defined (recall that $T_\lambda = T_\lambda \mathbf{1}$). Set $E = \bigoplus_{0\neq\lambda\in\Lambda} \mathrm{N}(T_\lambda)$; if $\eta \in E^\perp$, then for all $\xi_\lambda \in \mathrm{N}(T_\lambda)$ one has $\langle T\eta, \xi_\lambda\rangle = \langle \eta, T\xi_\lambda\rangle = \lambda\langle \eta, \xi_\lambda\rangle = 0$, and so $T\eta \in \mathrm{N}(T_\lambda)^\perp$. Since this occurs for all $\lambda \in \Lambda$, then $T\eta \in E^\perp$, that is, $E^\perp$ is invariant under T; further $\mathcal{H} = E \oplus E^\perp$.

Note that $E^\perp \supset \mathrm{N}(T)$; the proof ends by showing that $E^\perp = \mathrm{N}(T)$. Since E is also invariant under T, then $S = T|_{E^\perp}$, the restriction of T to $E^\perp$, is well defined and is a self-adjoint compact operator. If $S \neq 0$, by Lemma 8.1.1 there exists an eigenvector $0 \neq \zeta$ of S with nonzero eigenvalue; thus, by construction, $\zeta \in E$ and $\zeta \in E^\perp$, and necessarily $\zeta = 0$. Then $S = 0$, that is, $E^\perp = \mathrm{N}(T)$. □

Corollary 8.1.3. *Let $T \in \mathrm{B}_0(\mathcal{H})$ be self-adjoint and Λ the set of eigenvalues of T. Then $\mathcal{H}$ has an orthonormal basis of eigenvectors of T.*

Proof. For each eigenvalue $\lambda \neq 0$ of T, denote by $d_\lambda = \dim \mathrm{N}(T_\lambda) < \infty$ and pick an orthonormal basis $\{\xi_j^\lambda\}_{j=1}^{d_\lambda}$ of $\mathrm{N}(T_\lambda)$. Let $\{\eta_j\}_{j\in J}$ be an orthonormal basis of the kernel of T. By Theorem 8.1.2,

$$\left[\bigcup_{0\neq\lambda\in\Lambda} \{\xi_j^\lambda\}_{j=1}^{d_\lambda}\right] \cup \{\eta_j\}_{j\in J}$$

is an orthonormal basis of $\mathcal{H}$. □

Theorem 8.1.4 (Spectral Theorem for Compact Operators). *Let T be a (nonzero) self-adjoint compact operator on $\mathcal{H}$, $\{\lambda_j\} \subset \mathbb{R}$ the nonzero eigenvalues of T and P_j the orthogonal projections onto $\mathrm{N}(T_{\lambda_j})$, $\forall j$ (recall that $\dim \mathrm{N}(T_{\lambda_j}) < \infty$). Then*

$$T = \sum_j \lambda_j P_j,$$

and the series converges in the norm of $\mathrm{B}(\mathcal{H})$.

Proof. Let P_0 be the orthogonal projection onto $\mathrm{N}(T)$. By Corollary 8.1.3 one has $\mathbf{1} = P_0 + \sum_j P_j$; thus, for all $\xi \in \mathcal{H}$,

$$T\xi = TP_0\xi + T\sum_j P_j\xi = \sum_j T(P_j\xi) = \sum_j \lambda_j P_j\xi.$$

From this and $P_jP_k = 0$, $j \neq k$, it is found that (with j running over $\mathbb{N}$, for simplicity)

$$\begin{aligned}\left\|(T - \sum_{j=1}^{n} \lambda_j P_j)\xi\right\|^2 &= \sum_{j=n+1}^{\infty} |\lambda_j|^2 \|P_j\xi\|^2 \\ &\leq \left(\max_{j\geq n+1} |\lambda_j|^2\right) \sum_{j=n+1}^{\infty} \|P_j\xi\|^2 \leq \left(\max_{j\geq n+1} |\lambda_j|^2\right) \|\xi\|^2.\end{aligned}$$

Therefore, $\|T - \sum_{j=1}^{n} \lambda_j P_j\|^2 \leq \max_{j\geq n+1} |\lambda_j|^2$. Since λ_j constitutes a sequence that vanishes as $j \to \infty$, then $T = \lim_{n\to\infty} \sum_{j=1}^{n} \lambda_j P_j$ in $B(\mathcal{H})$. □

Corollary 8.1.5. *If $T \in \mathrm{B}_0(\mathcal{H})$ is positive, then there exists a compact positive operator S so that $S^2 = T$ (S is called a square root operator of T, and often denoted by $T^{1/2}$ or $\sqrt{T}$).*

Proof. Since T is positive, then it is self-adjoint with all nonzero eigenvalues $\lambda_j > 0$. By the spectral theorem $T = \sum_j \lambda_j P_j$. Define the operator S by $S = \sum_j \sqrt{\lambda_j} P_j$, which is compact since $\lambda_j \to 0$ for $j \to \infty$, and S can be approximated by finite rank operators in $\mathrm{B}(\mathcal{H})$ (explicitly by $\sum_{j=1}^{n} \sqrt{\lambda_j} P_j$). The property $S^2 = T$ is left as an exercise; for uniqueness see Section 8.3. □

Exercise 8.1.6. Let $T \in \mathrm{B}_0(\mathcal{H})$ be positive. Find the spectrum of $\sqrt{T}$?

Remark 8.1.7. Let $T \in \mathrm{B}_0(\mathcal{H})$ be self-adjoint. For each bounded function $f : \sigma(T) \to \mathbb{C}$, one defines the operator $f(T) := \sum_j f(\lambda_j) P_j$. Which is the spectrum of $f(T)$?

A specific class of functions of a compact self-adjoint operator T is ($\Lambda \in \mathcal{A}$, that is, it is a Borel set in $\mathbb{R}$)

$$P^T(\Lambda) = \chi_\Lambda(T) := \sum_{\lambda_j \in \Lambda} P_j,$$

which has properties similar to a measure, but projection-valued. E.g., $P^T(\mathbb{R}) = \mathbf{1}$, if $\Lambda_1 \cap \Lambda_2 = \emptyset$, then $P^T(\Lambda_1 \cap \Lambda_2) = 0 = P^T(\Lambda_1)P^T(\Lambda_2)$ (null operator) and $P^T(\Lambda_1 \cup \Lambda_2) = P^T(\Lambda_1) + P^T(\Lambda_2)$. A possibility is to reverse the construction, that is, to use P^T to build an operator-valued integration theory of functions f and then define $f(T)$. This program will be described in other sections of this chapter; see in particular Definition 8.2.1 and the whole Section 8.2.

8.1.1 Compact Normal Operators

It is a small step to generalize Corollary 8.1.3 to compact normal operators, and it will be used in future chapters. Nevertheless, the spectral theorem in the general case will be restricted to self-adjoint operators, by far the most important case to quantum mechanics.

Lemma 8.1.8. *If $R, S \in \mathrm{B}_0(\mathcal{H})$ are self-adjoint and commuting, then $\mathcal{H}$ has an orthonormal basis of simultaneous eigenvectors of R and S.*

Proof. For each eigenvalue λ of S, $S\xi^\lambda = \lambda\xi^\lambda$, one has $S(R\xi^\lambda) = R(S\xi^\lambda) = \lambda R\xi^\lambda$, and $\mathrm{N}(S_\lambda)$ is invariant under R (as well as its orthogonal complement). Since the restriction operator $R|_{\mathrm{N}(S_\lambda)}$ is self-adjoint and compact, pick an orthonormal basis of $\mathrm{N}(S_\lambda)$ (as in Corollary 8.1.3) composed of eigenvectors of R and, of course, also eigenvectors of S. Taking the union over all eigenvalues of S the result follows, again by Corollary 8.1.3. □

Corollary 8.1.9. *If $T \in \mathrm{B}_0(\mathcal{H})$ is normal, then $\mathcal{H}$ has an orthonormal basis of eigenvectors of T and the decomposition of $\mathcal{H}$ as in Hilbert-Schmidt Theorem* 8.1.2 *holds.*

Proof. It is enough to recall that $T = T_R + iT_I$, with T_R, T_I self-adjoint and compact (since T^* is also compact by Corollary 1.3.27) and since T is normal T_R commutes with T_I, and then apply Lemma 8.1.8. Note that if $T\xi^\lambda = \lambda\xi^\lambda$, then $T_R\xi^\lambda = (\mathrm{Re}\ \lambda)\xi^\lambda$ and $T_I\xi^\lambda = (\mathrm{Im}\ \lambda)\xi^\lambda$, and those eigenvectors corresponding to different eigenvalues are orthogonal. □

Exercise 8.1.10. Enunciate and prove a version of Theorem 8.1.4 for compact normal operators. Verify, furthermore, that the corresponding operator is self-adjoint if, and only if, $\{\lambda_j\} \subset \mathbb{R}$.

Exercise 8.1.11. Let $T \in \mathrm{B}(\mathcal{H})$, with $\dim \mathcal{H} = \infty$. Show that if there exists $C > 0$ with $\|T\xi\| \geq C\|\xi\|$ for all $\xi \in \mathcal{H}$, then T is not compact.

Exercise 8.1.12 (Fredholm alternative). Let $T \in \mathrm{B}_0(\mathcal{H})$ be a normal operator. Consider the equation $T\xi - \lambda\xi = \eta$, $\lambda \in \mathbb{C}$, $\eta \in \mathcal{H}$, and the subsequent homogeneous equation $T\xi - \lambda\xi = 0$. Show that for each $\lambda \neq 0$, one, and only one, of the following possibilities occurs (note that, in this case, uniqueness implies the existence of a solution!):

i) The homogeneous equation has only the trivial solution and the original equation has a unique solution for each $\eta \in \mathcal{H}$.
ii) The homogeneous equation has $0 < \dim \mathrm{N}(T_\lambda) < \infty$ linearly independent solutions, and the original equation either has infinite many solutions or no solution at all.

Exercise 8.1.13. Let $0 \neq \varphi \in \mathrm{L}^2[0,1]$ and $K(t,s) = \varphi(t)\overline{\varphi(s)}$, $t, s \in [0,1]$. Show that $\lambda = \|\varphi\|_2^2$ is the unique nonzero eigenvalue of the operator $T_K : \mathrm{L}^2[0,1] \hookleftarrow$, $(T_K\psi)(t) = \int_0^1 K(t,s)\psi(s)\, ds$. Find the corresponding eigenfunction (note that it is usual for the term *eigenfunction* to designate an eigenvector in a function vector space). Determine also the eigenfunctions corresponding to the zero eigenvalue.

Exercise 8.1.14. Fix $\eta \in \mathcal{H}$ with $\|\eta\| = 1$. Let $T_\eta : \mathcal{H} \to \mathcal{H}$ defined by $T_\eta \xi = \langle \eta, \xi \rangle \eta$, $\xi \in \mathcal{H}$. Determine the spectrum and the spectral radius of T_η.

Exercise 8.1.15. Let $T : l^2(\mathbb{Z}) \to l^2(\mathbb{Z})$ given by

$$(T\xi)_n = -i\,(\xi_{n+1} - \xi_{n-1}),$$

with $\xi = (\dots, \xi_{-2}, \xi_{-1}, \xi_0, \xi_1, \xi_2, \dots)$. Show that T is bounded and self-adjoint; then find its spectral radius.

Exercise 8.1.16. Let $U \in \mathrm{B}(\mathcal{H})$ be unitary, so normal. Show that if it is compact then $\dim \mathcal{H} < \infty$.

Remark 8.1.17. It was F. Riesz who developed most of the spectral theory of compact operators on Hilbert and Banach spaces around 1920.

8.2 Resolution of the Identity

The spectral theorem for self-adjoint operators gives a complete description of such operators, and it is a sophisticated infinite-dimensional analogue of the fact that hermitian matrices in finite-dimensional Hilbert spaces can be diagonalized. This theorem also reduces many questions about self-adjoint operators to questions about multiplication operators, where the situation can be more transparent.

As discussed in Chapter 13, the characterization of self-adjoint operators via spectral measures (see below) is an important step to suitable spectral classification and its relation to the dynamical behavior of solutions of the corresponding Schrödinger equation for large times.

Another consequence directly related to the spectral theorem is the possibility of defining functions of self-adjoint operators, as discussed in Section 3.4 for momentum and free hamiltonian operators; there, the main tool was the Fourier transform, a unitary operator on $\mathrm{L}^2(\mathbb{R}^n)$.

Write $\mathrm{Proj}(\mathcal{H})$ for the set of orthogonal projection operators on the Hilbert space $\mathcal{H}$, that is, $P_0 \in \mathrm{Proj}(\mathcal{H})$ iff $P_0 \in \mathrm{B}(\mathcal{H})$, is self-adjoint and $P_0^2 = P_0$ (and so $\mathrm{rng}\, P_0$ is a closed subspace of $\mathcal{H}$). $\mathcal{A}$ denotes the Borel σ-algebra in $\mathbb{R}$ and for pairwise disjoint sets Λ_j the symbol $\sum_j \Lambda_j$ indicates their union. Finally, χ_A denotes the characteristic function of the set A.

Definition 8.2.1. A (*spectral*) *resolution of the identity* on $\mathcal{H}$ is a map

$$P : \mathcal{A} \to \mathrm{Proj}(\mathcal{H})$$

so that

i) $P(\mathbb{R}) = \mathbf{1}$, and

ii) If $\Lambda = \sum_{j=1}^\infty \Lambda_j$, with $\Lambda_j \in \mathcal{A}$, $\forall j$, then one has the strong limit

$$P(\Lambda) = \mathrm{s} - \lim_{n\to\infty} \sum_{j=1}^{n} P(\Lambda_j).$$

Remark 8.2.2. A resolution of the identity is also called *spectral family*, *spectral decomposition*, *spectral resolution* and *projection-valued measure*.

Exercise 8.2.3. Verify:

a) $P(\mathbb{R}\setminus\Lambda) = \mathbf{1} - P(\Lambda)$ and $P(\emptyset) = 0$ (null operator).
b) $P(\Lambda_1 \cup \Lambda_2) + P(\Lambda_1 \cap \Lambda_2) = P(\Lambda_1) + P(\Lambda_2)$.
c) $P(\Lambda_1)P(\Lambda_2) = P(\Lambda_1 \cap \Lambda_2)$.

For item c) consider first $\Lambda_1 \cap \Lambda_2 = \emptyset$ and use b).

Given a resolution of the identity P, to each $\xi \in \mathcal{H}$ one associates a finite positive Borel measure μ_ξ in $\mathbb{R}$ by

$$\mathcal{A} \ni \Lambda \mapsto \mu_\xi(\Lambda) := \langle \xi, P(\Lambda)\xi \rangle;$$

note that $\mu_\xi(\Lambda) = \langle \xi, P(\Lambda)P(\Lambda)\xi\rangle = \|P(\Lambda)\xi\|^2$ and $\mu_\xi(\mathbb{R}) = \|\xi\|^2$. To each pair $\xi, \eta \in \mathcal{H}$ one associates the complex Borel measure

$$\mu_{\xi,\eta}(\Lambda) := \langle \xi, P(\Lambda)\eta \rangle,$$

and by polarization

$$\mu_{\xi,\eta}(\Lambda) = \frac{1}{4}\left[\mu_{\xi+\eta}(\Lambda) - \mu_{\xi-\eta}(\Lambda) + i\left(\mu_{\xi-i\eta}(\Lambda) - \mu_{\xi+i\eta}(\Lambda)\right)\right].$$

Clearly $\mu_\xi = \mu_{\xi,\xi}$ and $|\mu_{\xi,\eta}(\Lambda)| \le \|\xi\|\,\|\eta\|$.

Definition 8.2.4. The above μ_ξ and $\mu_{\xi,\eta}$ are called *spectral measures* of the resolution of the identity P associated with ξ and the pair $\xi, \eta \in \mathcal{H}$, respectively.

It is important to recognize that all spectral measures μ_ξ are *regular*, that is, $\mu_\xi(\Lambda) = \inf\{\mu_\xi(U) : U \subset \mathbb{R} \text{ is open}, \Lambda \subset U\}$ and $\mu_\xi(\Lambda) = \sup\{\mu_\xi(K) : \text{K is compact}, K \subset \Lambda\}$, for all $\Lambda \in \mathcal{A}$ [Ru74].

With such spectral measures at hand one can integrate functions and so define the integral with respect to P; different notations will be used to indicate this integral. For a measurable simple function $f = \sum_{j=1}^n a_j \chi_{\Lambda_j}$ one defines

$$P(f) = \int_{\mathbb{R}} f(t)\, dP(t) = \int f\, dP := \sum_{j=1}^n a_j P(\Lambda_j).$$

Note that $P(\chi_\Lambda) = P(\Lambda)$, which gives grounds for keeping the same notation P for the resolution of identity and subsequent integrals. This map $f \mapsto P(f)$ is linear and satisfies

$$\langle \xi, P(f)\xi\rangle = \int_{\mathbb{R}} f(t)\, d\mu_\xi(t),$$

and since

$$\|P(f)\xi\|^2 = \int_{\mathbb{R}} |f(t)|^2\, d\mu_\xi(t) = \|f\|^2_{\mathrm{L}^2_{\mu_\xi}} \le \left(\sup_{t\in\mathbb{R}} |f(t)|^2\right) \|\xi\|^2,$$

it follows that the linear map P :{simple functions}→ $\mathrm{B}(\mathcal{H})$ is continuous (the simple functions with the sup norm).

Let $B^\infty(\mathbb{R})$ denote the vector space of bounded Borel functions on $\mathbb{R}$ with the norm $\|f\|_\infty := \sup_{t\in\mathbb{R}} |f(t)|$. Since the simple functions constitute a dense set in $B^\infty(\mathbb{R})$, there exists a unique extension of P to a bounded linear operator (and using the same notation) $P : B^\infty(\mathbb{R}) \to \mathrm{B}(\mathcal{H})$, so that, for all $f \in B^\infty(\mathbb{R})$,

$$\langle \xi, P(f)\eta\rangle = \int f(t)\, d\mu_{\xi,\eta}(t)$$

and

$$\|P(f)\xi\|^2 = \int |f(t)|^2\, d\mu_\xi(t) \le \left(\sup_{t\in\mathbb{R}} |f(t)|^2\right) \|\xi\|^2,$$

with strong convergence on the left-hand side and uniform convergence of functions on the right one.

Exercise 8.2.5. By first considering simple functions and then taking limits, verify that for $f, g \in B^\infty(\mathbb{R})$ and any $\xi, \eta \in \mathcal{H}$, one has

i) $d\mu_{P(g)\xi,P(f)\eta} = \overline{g} f\, d\mu_{\xi,\eta}(t)$.
ii) $\langle P(g)\xi, P(f)\eta\rangle = \int \overline{g(t)} f(t)\, d\mu_{\xi,\eta}(t)$.
iii) $P(fg) = P(f)P(g) = P(g)P(f)$.
iv) $P(\overline{f}) = P(f)^*$ (and so for a real-valued function $f \in B^\infty(\mathbb{R})$ the operator $P(f)$ is bounded and self-adjoint).
v) $P(f)^*P(f) = P(|f|^2) = P(f)P(f)^*$ (and so $P(f)$ is a normal operator for any $f \in B^\infty(\mathbb{R})$).
vi) $P(1) = \mathbf{1}$ (1 denotes the constant function: $1(t) = 1, \forall t \in \mathbb{R}$) and if f is invertible with $f^{-1} \in B^\infty(\mathbb{R})$, then $P(f^{-1}) = P(f)^{-1}$.

Lemma 8.2.6. *If P is a resolution of the identity, consider the map $P : B^\infty(\mathbb{R}) \to \mathrm{B}(\mathcal{H})$. If $(f_n) \subset B^\infty(\mathbb{R})$ with $(\|f_n\|_\infty)$ a bounded sequence with pointwise convergence $f_n \to f$, then $f \in B^\infty(\mathbb{R})$ and*

$$\mathrm{s} - \lim_{n\to\infty} P(f_n) = P(f).$$

Proof. A direct verification shows that $f \in B^\infty(\mathbb{R})$. If $\xi \in \mathcal{H}$,

$$\begin{aligned}\|P(f_n)\xi - P(f)\xi\|^2 &= \|(P(f_n) - P(f))\xi\|^2\\ &= \int_{\mathbb{R}} |f_n(t) - f(t)|^2\, d\mu_\xi(t) \longrightarrow 0\end{aligned}$$

as $n \to \infty$ by the dominated convergence theorem. Note that if $f_n \to f$ in the norm of $B^\infty(\mathbb{R})$, i.e., uniform convergence, the result would be immediate. □

The next step is to extend the map P to unbounded Borel functions $f : \mathbb{R} \to \mathbb{C}$. Define

$$\text{dom } f := \left\{ \xi \in \mathcal{H} : f \in \mathrm{L}^2_{\mu_\xi}(\mathbb{R}) \right\} = \left\{ \xi \in \mathcal{H} : \int |f|^2 d\mu_\xi < \infty \right\},$$

which is a vector space, since $\mu_{a\xi}(\Lambda) = |a|^2 \mu_\xi(\Lambda)$ and by using the triangular inequality $\mu_{\xi+\eta}(\Lambda) \leq 2(\mu_\xi(\Lambda) + \mu_\eta(\Lambda))$ (to get it use the relation $0 \leq \langle (\xi - \eta), P(\Lambda)(\xi - \eta) \rangle$).

Set

$$\Lambda_n = \Lambda_n(f) := \{t \in \mathbb{R} : |f(t)| \leq n\}, \qquad f_n := f\, \chi_{\Lambda_n},$$

and for $\xi \in \text{dom } f$ this sequence of functions converges to f in $\mathrm{L}^2_{\mu_\xi}(\mathbb{R})$ by dominated convergence. Hence (f_n) is a Cauchy sequence in $\mathrm{L}^2_{\mu_\xi}(\mathbb{R})$. Since $f_n \in B^\infty(\mathbb{R})$ and

$$\|P(f_n)\xi\|^2 = \int |f_n|^2 \, d\mu_\xi = \|f_n\|^2_{\mathrm{L}^2_{\mu_\xi}},$$

it follows that $(P(f_n)\xi)_n$ is a Cauchy sequence in $\mathcal{H}$, so that it converges to a vector $P(f)\xi$, which defines the desired extension with $\text{dom } P(f) = \text{dom } f$. Note that such extension $f \mapsto P(f)$ is linear, continuous and, with the notation $P(f) := \int f\, dP$, by taking $n \to \infty$ in the above equality

$$\|P(f)\xi\|^2 = \int |f|^2 \, d\mu_\xi = \|f\|^2_{\mathrm{L}^2_{\mu_\xi}}.$$

Exercise 8.2.7. Show that for any $(g_n) \subset B^\infty(\mathbb{R})$ with $g_n \to f$ in $\mathrm{L}^2_{\mu_\xi}(\mathbb{R})$, one has $P(g_n)\xi \to P(f)\xi$, for any $\xi \in \text{dom } f$, so that $P(f)$ above, for $f \in \mathrm{L}^2_{\mu_\xi}(\mathbb{R})$, is well defined.

Lemma 8.2.8. *For every Borel function $f : \mathbb{R} \to \mathbb{C}$ one has* dom $f \sqsubseteq \mathcal{H}$. *Thus the adjoint $P(f)^*$ is well posed.*

Proof. Let Λ_n be as above. If $\xi \in \mathcal{H}$, by considering $\xi_n = P(\Lambda_n)\xi$ one has $\mu_{\xi_n} = \chi_{\Lambda_n}\mu_\xi$. Thus

$$\int_{\mathbb{R}} |f(t)|^2 \, d\mu_{\xi_n}(t) = \int_{\Lambda_n} |f(t)|^2 \, d\mu_\xi(t) \leq n^2 \|\xi\|^2 < \infty,$$

and so $\xi_n \in \text{dom } f$. Since $\chi_{\Lambda_n} \to 1$ in $\mathrm{L}^2_{\mu_\xi}(\mathbb{R})$, and

$$\|\xi - \xi_n\|^2 = \int_{\mathbb{R}} |1 - \chi_{\Lambda_n}(t)|^2 \, d\mu_\xi,$$

one obtains that $\xi_n \to \xi$ in $\mathcal{H}$ by dominated convergence. This shows that dom f is dense in $\mathcal{H}$. ☐

Definition 8.2.9. A linear operator $T : \text{dom } T \sqsubseteq \mathcal{H} \to \mathcal{H}$ is *normal* if $\text{dom } T = \text{dom } T^*$ and $\|T\xi\| = \|T^*\xi\|$, $\forall \xi \in \text{dom } T$.

Lemma 8.2.10.

a) *Any normal operator is closed.*
b) *If T is a normal operator, then $T^*T = TT^*$ (where both compositions are defined).*

Proof. a) Since T^* is closed $(\text{dom } T^*, \|\cdot\|_{T^*})$ is a complete space. Since T is normal, then the norms $\|\cdot\|_T = \|\cdot\|_{T^*}$ coincide on dom T, so $(\text{dom } T, \|\cdot\|_T)$ is complete as well, and then T is also closed.

b) If T is normal then, by polarization,

$$\langle T\xi, T\eta\rangle = \langle T^*\xi, T^*\eta\rangle, \qquad \forall \xi, \eta \in \text{dom } T.$$

Since T is closed, $T = \overline{T} = T^{**}$; so if

$$\xi \in \text{dom } (T^*T) \cap \text{dom } (T^{**}T^*) = \text{dom } (T^*T) \cap \text{dom } (TT^*),$$

then

$$\langle T^*T\xi, \eta\rangle = \langle T^{**}T^*\xi, \eta\rangle = \langle TT^*\xi, \eta\rangle, \qquad \forall \eta \in \text{dom } T,$$

so that $T^*T\xi = TT^*\xi$; consequently $T^*T = TT^*$. □

Remark 8.2.11. Bounded normal operators were introduced in Definition 2.1.7.

Exercise 8.2.12. Show that a normal operator has no proper normal extension.

Exercise 8.2.13. If T is normal, show that $T - z\mathbf{1}$ is also normal for any $z \in \mathbb{C}$.

Theorem 8.2.14. *Every normal operator has nonempty spectrum.*

Exercise 8.2.15. Adapt the proof of Theorem 2.4.4 to conclude Theorem 8.2.14.

Proposition 8.2.16. *Let P be a resolution of the identity.*

a) *For every Borel function $f : \mathbb{R} \to \mathbb{C}$ the operator $P(f)$ is normal (so closed) and $P(f)^* = P(\overline{f})$.*
b) *For every real-valued Borel function $f : \mathbb{R} \to \mathbb{R}$ the operator $P(f)$ is self-adjoint.*

Proof. b) follows straightly from a).

a) If $f_n = f\,\chi_{\Lambda_n}$, Λ_n as defined on page 208, it follows that $f_n \in B^\infty(\mathbb{R})$, $f_n \to f$ in $\mathrm{L}^2_{\mu_\xi}(\mathbb{R})$, $P(f_n)^* = P(\overline{f_n})$ (see Exercise 8.2.5) and, thus, $\langle \xi, P(f_n)\eta\rangle = \langle P(\overline{f_n})\xi, \eta\rangle$, $\forall \xi, \eta \in \mathcal{H}$.

If $\forall \xi, \eta \in \text{dom } P(f)$, by the dominated convergence theorem $P(f_n)\eta \to P(f)\eta$, $P(\overline{f_n})\xi \to P(\overline{f})\xi$ and, by continuity of the inner product

$$\langle \xi, P(f)\eta\rangle = \langle P(\overline{f})\xi, \eta\rangle,$$

and so $P(\overline{f}) \subset P(f)^*$.

Now, if $\xi \in \text{dom } P(f)^*$ there is $\eta \in \mathcal{H}$ with

$$\langle \xi, P(f)\zeta \rangle = \langle \eta, \zeta \rangle, \qquad \forall \zeta \in \text{dom } P(f).$$

By considering f_n again, for $m \geq n$,

$$\begin{aligned}\langle P(\overline{f_n})\xi, \zeta \rangle &= \langle \xi, P(f_n)\zeta \rangle = \langle \xi, P(f_n \chi_{\Lambda_n})\zeta \rangle = \langle \xi, P(f_m \chi_{\Lambda_n})\zeta \rangle \\ &= \lim_{m\to\infty} \langle \xi, P(f_m)P(\Lambda_n)\zeta \rangle = \langle \xi, P(f)P(\Lambda_n)\zeta \rangle \\ &= \langle P(\Lambda_n)P(f)^*\xi, \zeta \rangle,\end{aligned}$$

consequently $P(\overline{f_n})\xi = P(\Lambda_n)P(f)^*\xi$. The limit $\lim_{n\to\infty} \|P(\Lambda_n)P(f)^*\xi\|^2$ exists by Lemma 8.2.6; thus

$$\begin{aligned}\|P(f)^*\xi\|^2 &= \lim_{n\to\infty} \|P(\Lambda_n)P(f)^*\xi\|^2 = \lim_{n\to\infty} \|P(\overline{f_n})\xi\|^2 \\ &= \lim_{n\to\infty} \int_{\mathbb{R}} |f_n(t)|^2 \, d\mu_\xi(t) = \int_{\mathbb{R}} |f(t)|^2 \, d\mu_\xi(t),\end{aligned}$$

and $f \in \mathrm{L}^2_{\mu_\xi}(\mathbb{R})$, that is, $\xi \in \text{dom } P(\overline{f})$. Therefore, $\text{dom } P(f)^* \subset \text{dom } P(\overline{f})$ and so $P(\overline{f}) = P(f)^*$. If $\xi \in \text{dom } f$, then

$$\|P(f)\xi\|^2 = \int |f|^2 \, d\mu_\xi = \|P(\overline{f})\xi\|^2$$

which implies $\text{dom } P(f) = \text{dom } P(\overline{f})$. Hence $P(f)$ is normal. □

It is worth emphasizing the following characterization:

Lemma 8.2.17. *A vector* $\xi \in \text{dom } P(f)$ *iff*

$$\|P(f)\xi\|^2 = \int_{\mathbb{R}} |f(t)|^2 \, d\mu_\xi(t) < \infty.$$

Proof. It is a direct consequence of the definition of $P(f)$, Proposition 8.2.16 and its proof. □

Exercise 8.2.18. Let f_n and f be as in the proof of Proposition 8.2.16. Clearly one has the pointwise convergence $f_n \to f$. Show that $f_n \to f$ in $\mathrm{L}^2_{\mu_\xi}(\mathbb{R})$ too.

Lemma 8.2.19. *Let P be a resolution of the identity, $f, g : \mathbb{R} \to \mathbb{C}$ be Borel functions and a, b complex numbers. Then*

a) $aP(f) + bP(g) \subset P(af + bg)$, *with* $\text{dom } (aP(f) + bP(g)) = \text{dom } P(f) \cap \text{dom } P(g)$.
b) $P(f)P(g) \subset P(fg)$, *with* $\text{dom } (P(f)P(g)) = \text{dom } P(g) \cap \text{dom } P(fg)$. *Note that if* $\text{dom } P(g) \supset \text{dom } P(fg)$, *then* $P(f)P(g) = P(fg) = P(gf) = P(g)P(f)$ *with domain* $\text{dom } P(fg)$.

Proof. Let Λ_n and f_n be as defined on page 208 and g_n the corresponding functions for g. Recall that if $f, g \in B^\infty(\mathbb{R})$, then $P(f)P(g) = P(fg)$ and $P(f+g) = P(f) + P(g)$.

a) If $\xi \in \text{dom } (aP(f) + bP(g)) = \text{dom } P(f) \cap \text{dom } P(g) \Rightarrow f, g \in \mathrm{L}^2_{\mu_\xi}(\mathbb{R}) \Rightarrow (af + bg) \in \mathrm{L}^2_{\mu_\xi}(\mathbb{R}) \Rightarrow \xi \in \text{dom } P(af + bg)$. Thus,

$$\begin{aligned} P(af+bg)\xi &= \lim_{n\to\infty} P(af_n + bg_n)\xi \\ &= \lim_{n\to\infty} (aP(f_n)\xi + bP(g_n)\xi) = aP(f)\xi + bP(g)\xi. \end{aligned}$$

b) For Borel functions f, g, if $\xi \in \text{dom } (P(f)P(g))$ then $\xi \in \text{dom } P(g)$ and $P(g)\xi \in \text{dom } P(f)$. Since $f_n, g_n \in B^\infty(\mathbb{R})$ and $f_n g_k \to f_n g$ in $\mathrm{L}^2_{\mu_\xi}(\mathbb{R})$ as $k \to \infty$, one has

$$\begin{aligned} P(f)P(g)\xi &= \lim_{n\to\infty} P(f_n) \lim_{k\to\infty} P(g_k)\xi = \lim_{n\to\infty}\lim_{k\to\infty} P(f_n)P(g_k)\xi \\ &= \lim_{n\to\infty}\lim_{k\to\infty} P(f_n g_k)\xi = \lim_{n\to\infty} P(f_n g)\xi; \end{aligned}$$

thus the last limit exists and so the sequence $(f_n g)_n$ is Cauchy in $\mathrm{L}^2_{\mu_\xi}(\mathbb{R})$. As the pointwise convergence $f_n g \to fg$ holds, it follows that $fg \in \mathrm{L}^2_{\mu_\xi}(\mathbb{R})$ and so $\xi \in \text{dom } P(fg)$,

$$P(f)P(g)\xi = \lim_{n\to\infty} P(f_n g)\xi = P(fg)\xi.$$

Hence $P(f)P(g) \subset P(fg)$ and $\text{dom } (P(f)P(g)) \subset \text{dom } P(g) \cap \text{dom } P(fg)$.

Now if $\xi \in \text{dom } P(g) \cap \text{dom } P(fg)$ one has

$$\begin{aligned} P(fg)\xi &= \lim_{n\to\infty}\lim_{k\to\infty} P(f_n g_k)\xi \\ &= \lim_{n\to\infty}\lim_{k\to\infty} P(f_n)P(g_k)\xi = \lim_{n\to\infty} P(f_n)P(g)\xi \end{aligned}$$

so that $f \in \mathrm{L}^2_{\mu_{P(g)\xi}}(\mathbb{R})$. Hence $P(g)\xi \in \text{dom } P(f)$ and therefore $\xi \in \text{dom } (P(f)P(g))$. The equality $\text{dom } (P(f)P(g)) = \text{dom } P(f) \cap \text{dom } P(fg)$ is proved. □

8.3 Spectral Theorem

Given a spectral family P and $\xi \in \mathcal{H}$, denote

$$\mathcal{H}_\xi := \left\{ P(f)\xi : f \in \mathrm{L}^2_{\mu_\xi}(\mathbb{R}) \right\}.$$

Exercise 8.3.1. Check that $\mathcal{H}_\xi$ is a closed vector subspace of $\mathcal{H}$.

Definition 8.3.2. $\mathcal{H}_\xi$ is called the *cyclic subspace* spanned by ξ for P, and if $\mathcal{H}_\xi = \mathcal{H}$ then ξ is called a *cyclic vector* for P.

Given $\xi \in \mathcal{H}$ and P, consider the operator

$$U_\xi : \mathcal{H}_\xi \to \mathrm{L}^2_{\mu_\xi}(\mathbb{R}), \qquad U_\xi(P(f)\xi) := f.$$

Since

$$\|U_\xi(P(f)\xi)\|^2_{\mathrm{L}^2_{\mu_\xi}} = \int |f|^2 \, d\mu_\xi = \|P(f)\xi\|^2,$$

U_ξ is an isometry onto $\mathrm{L}^2_{\mu_\xi}(\mathbb{R})$, so a unitary operator between such spaces. Furthermore, for $\eta \in \mathcal{H}_\xi$, there exists a $g \in \mathrm{L}^2_{\mu_\xi}(\mathbb{R})$ with $\eta = P(g)\xi$, hence (since $P(f)P(g) \subset P(fg)$; see Lemma 8.2.19)

$$\left(U_\xi P(f) U_\xi^{-1}\right) g = U_\xi P(f)P(g)\xi = U_\xi P(fg)\xi = fg = \mathcal{M}_f g,$$

that is,

$$U_\xi P(f) U_\xi^{-1} = \mathcal{M}_f,$$

with $\mathrm{dom}\ \mathcal{M}_f = U_\xi \mathrm{dom}\ (P(f) \cap \mathcal{H}_\xi) = \{f \in \mathrm{L}^2_{\mu_\xi}(\mathbb{R}) : fg \in \mathrm{L}^2_{\mu_\xi}(\mathbb{R})\}$, and $P(f)$ is unitarily equivalent to the multiplication operator $\mathcal{M}_f$ acting in $\mathrm{L}^2_{\mu_\xi}(\mathbb{R})$ (see Section 2.3.2). Write 1 for the constant function $1(t) = 1$, $\forall t \in \mathbb{R}$, so that $U_\xi \xi = U_\xi P(1)\xi = 1$, which is cyclic in $\mathrm{L}^2_{\mu_\xi}(\mathbb{R})$ in the sense that $\{\mathcal{M}_f 1 = f : f \in \mathrm{dom}\ (1) = \mathrm{L}^2_{\mu_\xi}(\mathbb{R})\} = \mathrm{L}^2_{\mu_\xi}(\mathbb{R})$. Summing up:

Theorem 8.3.3. *If the resolution of the identity P has a cyclic vector $\xi \in \mathcal{H}$, then there is a unitary operator $U_\xi : \mathcal{H} \to \mathrm{L}^2_{\mu_\xi}(\mathbb{R})$ so that $U_\xi P(f) U_\xi^{-1} = \mathcal{M}_f$. Further, $U_\xi(\xi) = 1$ is a cyclic vector for P in $\mathrm{L}^2_{\mu_\xi}(\mathbb{R})$.*

What if there is no cyclic vector for P?

Definition 8.3.4. A maximal orthogonal family of vectors $\{\xi_j\}_{j\in J} \subset \mathcal{H}$ with $\mathcal{H}_{\xi_j} \perp \mathcal{H}_{\xi_k}$, if $j \neq k$, is called a *spectral basis* of P. P has *simple spectrum* if it has a cyclic vector.

Remark 8.3.5. By Zorn's Lemma, independently of the Hilbert dimension of $\mathcal{H}$, a spectral basis always exists and, if $\{\xi_j\}_{j\in J}$ is a spectral basis, then $\mathcal{H} = \bigoplus_{j\in J} \mathcal{H}_{\xi_j}$.

Remark 8.3.6. If $(\xi_j)_{j=1}^N$, with $N \in \mathbb{N} \cup \{\infty\}$, is an orthonormal countable (since $\mathcal{H}$ is supposed separable) spectral basis of P, define the measure

$$\mu := \sum_{j=1}^N \frac{1}{2^j} \mu_{\xi_j},$$

so that $\mathrm{L}^2_\mu(\mathbb{R} \times \{1, 2, 3, \ldots, N\}) = \bigoplus_{j=1}^N \mathrm{L}^2_{\mu_{\xi_j}}(\mathbb{R})$.

Since the direct sum of unitary operators is unitary and the direct sum of multiplication operators is also a multiplication operator (check this!), one has

Theorem 8.3.7. *For each resolution of the identity P, on the separable Hilbert space $\mathcal{H}$, there exists a countable spectral basis $(\xi_j)_{j=1}^N$, with $N \in \mathbb{N} \cup \{\infty\}$ and $\|\xi_j\| = 1/2^j$, so that $\mathcal{H} = \bigoplus_{j=1}^N \mathcal{H}_{\xi_j}$ and the unitary operator*

$$U := \bigoplus_{j=1}^{N} U_{\xi_j} : \mathcal{H} \to \bigoplus_{j=1}^{N} \mathrm{L}^2_{\mu_{\xi_j}}(\mathbb{R}),$$

satisfies

$$UP(f)U^{-1} = \tilde{\mathcal{M}}_f,$$

with $\tilde{\mathcal{M}}_f = \bigoplus_{j=1}^N \mathcal{M}_f$ a multiplication operator acting in $\bigoplus_{j=1}^N \mathrm{L}^2_{\mu_{\xi_j}}(\mathbb{R})$, for all Borel $f : \mathbb{R} \to \mathbb{C}$.

Let P be a resolution of the identity on $\mathcal{H}$. Among the self-adjoint operators defined via $P(f)$, a special role is played by

$$T := \int_{\mathbb{R}} t \, dP(t),$$

that is, it is an expression of $T = P(h)$ for $h(t) = t$. One of the forms of the spectral theorem is to show that such relation is one-to-one:

Theorem 8.3.8 (Spectral Theorem). *To each self-adjoint operator $T : \mathrm{dom}\, T \sqsubseteq \mathcal{H} \to \mathcal{H}$ corresponds a unique resolution of the identity P^T on $\mathcal{H}$, so that $T = \int t \, dP^T(t)$.*

Thus, each self-adjoint operator T is unitarily equivalent to the multiplication operator $\mathcal{M}_h$, $h(t) = t$, acting in $\mathrm{L}^2_\mu(\mathbb{R} \times \{1, 2, 3, \ldots, N\})$, μ a probability measure, and

$$\mathrm{dom}\, T = \left\{ \xi \in \mathcal{H} : \int t^2 \, d\mu_\xi^T(t) < \infty \right\},$$

where $\mu_{\xi,\eta}^T$ are the spectral measures of the resolution of the identity P^T.

Definition 8.3.9. The spectral measures $\mu_{\xi,\eta}^T$ defined by means of P^T, are called the *spectral measures* of T. Further, T is said to have simple spectrum if P^T has simple spectrum.

This structure of T as a multiplication operator is called *spectral representation*. Basically, by changing the self-adjoint operator, what changes in the spectral representation are the spectral measures μ_ξ^T, so that they carry fundamental information about T.

The spectral theorem allows one to define measurable functions of T through $f(T) := P^T(f)$. P^T is called the *resolution of the identity of* T. Instead of proving the spectral theorem, it was opted to discuss different strategies of proofs in Section 8.5.

Proposition 8.3.10. *Let P be a spectral resolution on $\mathcal{H}$. If $f:\mathbb{R}\to\mathbb{C}$ is the polynomial $f(t)=\sum_{j=0}^n a_j t^j$, $a_j\in\mathbb{C},\forall j$, then $P(f)=\sum_{j=0}^n a_j T^j$, where $T:=P(h)$ with $h(t)=t$.*

Proof. Induction. For $n=0$ one has $P(a_0)=a_0\mathbf{1}$. Assume now it holds for all polynomials of degree $\le (n-1)$. Thus, if $g(t)=\sum_{j=1}^n a_j t^{j-1}$ and $h(t)=t$, one has $f(t)=h(t)g(t)+a_0$ and, by Lemma 8.2.19,

$$P(f)\supset P(h)P(g)+P(a_0)=\sum_{j=0}^n a_j T^j.$$

Since for $n\ge 1$ one has dom $P(h)\supset$ dom $P(hg)$, by Lemma 8.2.19 again,

$$\text{dom } P(f)=\text{dom } P(hg)=\text{dom } (P(h)P(g))$$

and it follows that $P(f)=P(h)P(g)+P(a_0)=\sum_{j=0}^n a_j T^j$. □

Given a self-adjoint operator T, Proposition 8.3.10 validates the notation

$$f(T)=P^T(f)$$

for Borel functions $f:\mathbb{R}\to\mathbb{C}$. For Borel sets $\Lambda\subset\mathbb{R}$ one has $P^T(\Lambda)=\chi_\Lambda(T)$, and such operators are orthogonal projections called the *spectral projections* of T. Note that if T is bounded and $f(T)$ can be defined by convergent power series, then this definition via series coincides with the one given by the spectral theorem, since the partial series sums are the same operators in both approaches.

In a very short statement: measurable functions $f(t)$ are approximated by simple functions $\sum_{j=1}^n a_j\chi_{\Lambda_j}(t)$, whereas normal operators $f(T)$ are approximated by the corresponding linear combinations of projections $\sum_{j=1}^n a_j\chi_{\Lambda_j}(T)$.

Example 8.3.11. Let T be a compact self-adjoint operator and $\{\lambda_j\}$ the set of its eigenvalues. Let $d_j=\dim \mathrm{N}(T-\lambda_j\mathbf{1})<\infty$ be the corresponding multiplicity and pick an orthonormal basis $\{\xi_j^{k_j}\}_{k_j=1}^{d_j}$ of $\mathrm{N}(T-\lambda_j\mathbf{1})$. From the discussion in Section 8.1, it is found for ξ_j^k, $k=1,\dots,d_j$, (strictly, the index should be k_j) the spectral measures

$$\mu^T_{\xi_j^k}=\delta_{\lambda_j}$$

(δ_λ is the Dirac measure at λ_j). On the space $\mathrm{L}^2_\mu(\mathbb{R})$, with ($k$ fixed)

$$\mu=\sum_j\frac{1}{2^j}\,\mu^T_{\xi_j^k}=\sum_j\frac{1}{2^j}\,\delta_{\lambda_j},$$

whose elements $\psi(t)$ are determined by sequences $(\psi(\lambda_j))_j$, the operator T acts as a multiplication by $\mathcal{M}_h(t), h(t)=t$, that is,

$$T\psi=(\lambda_j\psi(\lambda_j)),$$

which is a consequence of the decomposition $T = \sum_j \lambda_j P_j$ presented in Theorem 8.1.4. Note that for the spectral representation, for each $d_j > 1$ one needs $d_j - 1$ additional copies of $\mathbb{R}$ (so just one copy of $\mathbb{R}$ suffices iff all eigenvalues are simple, i.e., $d_j = 1$, $\forall j$). See also Subsection 8.4.2.

Remark 8.3.12. It was concluded that a linear operator T is self-adjoint iff it is unitarily equivalent to a multiplication operator $\mathcal{M}_\varphi$ (with real-valued φ) acting in some $\mathrm{L}^2_\mu(E)$, with finite μ. More precisely, by the spectral theorem one can take $\varphi = h$, $h(t) = t$, acting in the space $\mathrm{L}^2_\mu(\mathbb{R} \times \{1, 2, 3, \dots, N\})$. However, in many situations most information on the operator T can be extracted if (hopefully!) some φ – not necessarily equal to h above – can be found. For an example, see Subsection 8.4.1, in particular the discussion about the free hamiltonian.

Theorem 8.3.13. *If T is self-adjoint, then its spectrum is the support of the resolution of identity P^T, that is,*

$$\sigma(T) = \left\{ t \in \mathbb{R} : P^T(t-\varepsilon, t+\varepsilon) = \chi_{(t-\varepsilon, t+\varepsilon)}(T) \neq 0, \, \forall \varepsilon > 0 \right\}.$$

Furthermore, $P^T(\sigma(T)) = \chi_{\sigma(T)}(T) = \mathbf{1}$ and $P^T(\rho(T) \cap \mathbb{R}) = 0$ (which will also simply be denoted by $P^T(\rho(T)) = 0$).

Proof. If $P^T(t_0 - \varepsilon, t_0 + \varepsilon) \neq 0$ for all $\varepsilon > 0$, then there exists a normalized sequence (ξ_j) with

$$\xi_j \in P^T\left(t_0 - \frac{1}{j}, t_0 + \frac{1}{j}\right) \mathcal{H}, \qquad \forall j \in \mathbb{N}.$$

Hence $P^T\left(t_0 - \frac{1}{j}, t_0 + \frac{1}{j}\right) \xi_j = \xi_j$ and since

$$\mu_{\xi_j}(\Lambda) = \left\langle \xi_j, P^T(\Lambda) \, P^T\left(t_0 - \frac{1}{j}, t_0 + \frac{1}{j}\right) \xi_j \right\rangle,$$

it follows that $\mu_{\xi_j}\left(\mathbb{R} \setminus (t_0 - \frac{1}{j}, t_0 + \frac{1}{j})\right) = 0$. Thus, by Lemma 8.2.17,

$$\begin{aligned} \|(T - t_0\mathbf{1})\xi_j\|^2 &= \int_{(t_0 - \frac{1}{j}, t_0 + \frac{1}{j})} (t - t_0)^2 \, d\mu_{\xi_j}(t) \\ &\leq \frac{1}{j^2} \|\xi_j\|^2 = \frac{1}{j^2} \overset{j \to \infty}{\longrightarrow} 0, \end{aligned}$$

that is, (ξ_j) is a Weyl sequence for T at t_0, and so $t_0 \in \sigma(T)$ by Corollary 2.4.9.

Assume now that for $t_0 \in \mathbb{R}$ there exists $\varepsilon_0 > 0$ so that the projection $P^T(t_0 - \varepsilon_0, t_0 + \varepsilon_0) = 0$. Then $\mu_\xi((t_0 - \varepsilon_0, t_0 + \varepsilon_0)) = 0$, $\forall \xi \in \mathcal{H}$. If (ξ_j) is a normalized sequence in $\mathcal{H}$, then

$$\begin{aligned} \|(T - t_0\mathbf{1})\xi_j\|^2 &= \int_{\mathbb{R}} (t - t_0)^2 \, d\mu_{\xi_j}(t) \\ &= \int_{\mathbb{R} \setminus (t_0 - \varepsilon_0, t_0 + \varepsilon_0)} (t - t_0)^2 \, d\mu_{\xi_j}(t) \geq \varepsilon_0^2 \, \|\xi_j\|^2 = \varepsilon_0^2. \end{aligned}$$

Therefore there is no Weyl sequence for T at t_0, consequently $t_0 \in \rho(T)$.

Since $\rho(T)\cap\mathbb{R}$ is an open set in $\mathbb{R}$, it can be written as a countable union of disjoint intervals

$$\rho(T)\cap\mathbb{R} = \sum_j (a_j, b_j),$$

and, as just discussed, $P^T(a_j,b_j) = 0, \forall j$, so that $P^T(\rho(T)) = 0$. Finally, $\sigma(T) = \mathbb{R}\setminus\rho(T)$ and $P^T(\mathbb{R}) = \mathbf{1}$, and it immediately follows that $P^T(\sigma(T)) = \mathbf{1}$. □

Remark 8.3.14. Let T be self-adjoint and $t_0 \in \mathbb{R}$. Then $t_0 \in \rho(T)$ iff the map $\mathbb{R}\ni t \mapsto P^T(-\infty, t]$ is constant in a neighbourhood of t_0, that is, there is $\varepsilon > 0$ so that $P^T(-\infty,t] = P^T(-\infty,s]$ for all $t,s\in(t_0-\varepsilon, t_0+\varepsilon)$.

Exercise 8.3.15. Prove the statement in Remark 8.3.14.

Theorem 8.3.13 justifies why P^T is called the spectral projections of T; it also correctly indicates that $P^T(\Lambda) = \chi_\Lambda(T)$ will play a distinguished role in spectral issues in this and other chapters. Now a simple but useful result.

Lemma 8.3.16. *Let T be a self-adjoint operator.*

a) *If Λ is a bounded Borel set in $\mathbb{R}$, then* rng $\chi_\Lambda(T)\subset$ dom T.

b) *If $\int_{\mathbb{R}} t\, d\mu_\xi^T(t) \ge 0$ for all $\xi\in$ dom T, then $\mu_\xi^T(-\infty,0) = 0$, $\forall\xi\in$ dom T.*

Proof. a) If $\xi\in\mathcal{H}$ then

$$\begin{aligned}\|T\chi_\Lambda(T)\xi\|^2 &= \int_{\mathbb{R}} t^2\, d\mu_{\chi_\Lambda(T)\xi}(t)\\ &= \int_\Lambda t^2\, d\mu_\xi(t) \le \mu_\xi^T(\Lambda)\sup_{\lambda\in\Lambda}\lambda^2 < \infty\end{aligned}$$

since Λ is bounded. Hence, $\chi_\Lambda(T)\xi\in$ dom T, $\forall\xi\in\mathcal{H}$.

b) Suppose $\mu_\xi^T(-\infty,0) > 0$; then there exists a bounded interval $(a,b)\subset(-\infty,0)$ with $b<0$ and $\mu_\xi^T(a,b)>0$, and also a vector $\xi\in$ dom T so that $0\ne\eta = P^T(a,b)\xi$, and $\eta\in$ dom T by a). Since $P^T(a,b)\eta = \eta$,

$$\begin{aligned}\mu_\eta^T(\Lambda) &= \langle\eta, P^T(\Lambda)\eta\rangle = \langle\eta, P^T(\Lambda)P^T(a,b)\eta\rangle\\ &= \langle\eta, P^T(\Lambda\cap(a,b))\eta\rangle = \mu_\eta^T(\Lambda\cap(a,b)),\end{aligned}$$

and so $\mu_\eta^T(\mathbb{R}\setminus(a,b)) = 0$. Thus,

$$\int_{\mathbb{R}} t\, d\mu_\eta^T(t) = \int_{(a,b)} t\, d\mu_\eta^T(t) \le b\int_{(a,b)} d\mu_\eta^T(t) = b\|\eta\|^2 < 0.$$

This contradiction proves the lemma. □

Corollary 8.3.17. *Let T be self-adjoint in $\mathcal{H}$. Then:*

a) *For each Borel function $f:\mathbb{R}\to\mathbb{C}$,*

$$f(T) = \int_{\sigma(T)} f\, dP^T := P^T(\chi_{\sigma(T)} f);$$

particularly, for $\xi\in$ dom $f(T)$, one has $\langle\xi, f(T)\xi\rangle = \int_{\sigma(T)} f\, d\mu_\xi^T$.

b) *A real number* $t_0 \in \rho(T)$ *iff there exists* $\varepsilon_0 > 0$ *so that*

$$\mu_\xi^T(t_0 - \varepsilon_0, t_0 + \varepsilon_0) = 0, \qquad \forall \xi \in \text{dom } T.$$

Proof. a) Since $\chi_{\sigma(T)} \in B^\infty(\mathbb{R})$, Lemma 8.2.19 implies that dom $P^T(\chi_{\sigma(T)} f) =$ dom f and

$$P^T(\chi_{\sigma(T)} f) = P^T(\chi_{\sigma(T)}) P^T(f) = \mathbf{1} P^T(f) = P^T(f).$$

Therefore, $f(T) = \int_{\sigma(T)} f \, dP^T$. If $\xi \in \mathcal{H}$, then

$$\begin{aligned} \mu_\xi^T(\Lambda) = \langle \xi, P^T(\Lambda)\xi \rangle &= \langle \xi, P^T(\Lambda) P^T(\sigma(T))\xi \rangle \\ &= \langle \xi, P^T(\Lambda \cap \sigma(T))\xi \rangle = \mu_\xi^T(\Lambda \cap \sigma(T)), \end{aligned}$$

hence

$$\langle \xi, f(T)\xi \rangle = \int_{\sigma(T)} f \, d\mu_\xi^T, \qquad \forall \xi \in \text{dom } f(T).$$

b) By Theorem 8.3.13, $t_0 \in \rho(T) \cap \mathbb{R}$ iff $P^T(t_0 - \varepsilon_0, t_0 + \varepsilon_0) = 0$ for some $0 < \varepsilon_0$ iff for all $\xi \in \mathcal{H}$,

$$\begin{aligned} 0 = \|P^T(t_0 - \varepsilon_0, t_0 + \varepsilon_0)\xi\|^2 &= \langle \xi, P^T(t_0 - \varepsilon_0, t_0 + \varepsilon_0)\xi \rangle \\ &= \mu_\xi^T(t_0 - \varepsilon_0, t_0 + \varepsilon_0). \end{aligned}$$

This proves b). □

Exercise 8.3.18. Show that the spectrum of T is the smallest closed set Λ for which $P^T(\Lambda) = \mathbf{1}$.

Corollary 8.3.19 (functional calculus). *Let T be self-adjoint in $\mathcal{H}$. Then there is a unique linear map $B^\infty(\mathbb{R}) \to \mathrm{B}(\mathcal{H})$, $f \mapsto f(T)$, so that the items a) to f) below are satisfied:*

a) $fg \mapsto f(T)g(T) = g(T)f(T)$.
b) $\overline{f}(T) = f(T)^*$.
c) $\|f(T)\| \le \|f\|_\infty$.
d) *If* $z \in \rho(T)$, *then* $\frac{1}{t-z} \mapsto R_z(T)$ *and*

$$\langle \xi, R_z(T)\xi \rangle = \int_{\sigma(T)} \frac{1}{t-z} \, d\mu_\xi^T(t).$$

e) *If* support$(f) \cap \sigma(T) = \emptyset$, *then* $f(T) = 0$.
f) *If* f_n *is a bounded sequence in* $B^\infty(\mathbb{R})$ *and* $f_n \to f$ *pointwise, then* $\mathrm{s} - \lim_{n\to\infty} f_n(T) = f(T)$.

Furthermore,

1) *If* $f \ge 0$ *then* $f(T) \ge 0$ *(so, if* $f \ge g$ *then* $f(T) \ge g(T)$*).*
2) *If* $T\xi_\lambda = \lambda\xi_\lambda$ *and* f *is continuous, then* $f(T)\xi_\lambda = f(\lambda)\xi_\lambda$.

Proof. Note that a), b), c), e) and f) (e.g., for f) see Lemma 8.2.6) were already discussed in some way. The uniqueness follows by the spectral theorem, since by taking $f = \chi_\Lambda$ the unique resolution of identity P^T is obtained.

d) By Proposition 8.3.10 one has $P^T(t-z) = T - z\mathbf{1}$, and using Lemma 8.2.19b) with $f(t) = t - z$ and $g(t) = 1/(t-z)$,

$$\begin{aligned}\mathbf{1} = P^T(1) &= P^T\left((t-z)\frac{1}{t-z}\right) \\ &= P^T(t-z)P^T\left(\frac{1}{t-z}\right) = (T - z\mathbf{1})P^T\left(\frac{1}{t-z}\right).\end{aligned}$$

It is then found that $P^T\left(\frac{1}{t-z}\right) = R_z(T)$.

1) For $f \geq 0$

$$\langle \xi, f(T)\xi \rangle = \int_{\sigma(T)} f(t)\, d\mu_\xi^T(t) \geq 0.$$

Hence, $f(T) \geq 0$.

2) Since, by Lemma 8.2.17,

$$0 = \|(T - \lambda\mathbf{1})\xi_\lambda\|^2 = \int_{\sigma(T)} |t-\lambda|^2\, d\mu_\xi^T(t),$$

there is a positive constant c so that $\mu_{\xi_\lambda} = c\delta_\lambda$, where δ_λ is the Dirac measure concentrated at λ, that is, $\delta_\lambda(\Lambda) = 1$ if $\lambda \in \Lambda$ and 0 otherwise. In view of $\langle \xi_\lambda, \xi_\lambda \rangle = \int_{\sigma(T)} d\mu_{\xi_\lambda}$, it follows that $c = \|\xi_\lambda\|^2$. Thus, again by Lemma 8.2.17 (with $P(f) = f(T)$ in this case),

$$\begin{aligned}\|f(T)\xi_\lambda - f(\lambda)\xi_\lambda\|^2 &= \int_{\sigma(T)} |f(t) - f(\lambda)|^2\, d\mu_\xi^T(t) \\ &= c\int_{\sigma(T)} |f(t) - f(\lambda)|^2\, d\delta_\lambda(t) = 0,\end{aligned}$$

and so $f(T)\xi_\lambda = f(\lambda)\xi_\lambda$. □

Exercise 8.3.20. Verify that items b), e), 1) and 2) of Corollary 8.3.19 hold for unbounded Borel functions f.

Proposition 8.3.21. *Let T be self-adjoint and recall that $\chi_\Lambda(T) = P^T(\Lambda)$. Then:*

a) *$T \geq \beta\mathbf{1}$, that is, $\langle \xi, T\xi \rangle \geq \beta\|\xi\|^2$, $\forall \xi \in \operatorname{dom} T$, iff $\chi_\Lambda(T) = 0$ for any Borel set $\Lambda \subset (-\infty, \beta)$. Similarly in case $\langle \xi, T\xi \rangle \leq \gamma\|\xi\|^2$.*
b) *$T \in \mathrm{B}(\mathcal{H})$ iff there are $\beta, \gamma \in \mathbb{R}$ so that $\chi_\Lambda(T) = 0$ for any Borel set $\Lambda \subset ((-\infty, \beta) \cup (\gamma, \infty))$ (i.e., $\chi_{[\beta,\gamma]}(T) = \mathbf{1}$).*
c) *$T \in \mathrm{B}(\mathcal{H})$ iff $\sigma(T)$ is a bounded set in $\mathbb{R}$.*
d) *If $f : \mathbb{R} \to \mathbb{R}$ is Borel, then $\chi_\Lambda(f(T)) = \chi_{f^{-1}(\Lambda)}(T)$ for any Borel set $\Lambda \subset \mathbb{R}$.*

Proof. a) Since dom T is dense in $\mathcal{H}$:

$$\begin{aligned}
&\langle \xi, T\xi\rangle \geq \beta\|\xi\|^2,\ \forall \xi \in \operatorname{dom} T\\
\iff &\int_{\mathbb{R}} t\, d\mu_\xi^T(t) \geq \beta \int_{\mathbb{R}} d\mu_\xi^T(t),\ \forall \xi \in \operatorname{dom} T\\
\iff &\int_{\mathbb{R}} (t-\beta)\, d\mu_\xi^T(t) \geq 0,\ \forall \xi \in \operatorname{dom} T\\
\iff &\text{(by Lemma 8.3.16b))}\\
&0 = \mu_\xi^T((-\infty,\beta)) = \|P^T(-\infty,\beta)\xi\|^2,\ \forall \xi \in \operatorname{dom} T\\
\iff &P^T(-\infty,\beta) = 0.
\end{aligned}$$

b) Note that

$$\|T\xi\|^2 \leq C^2\|\xi\|^2,\ \forall \xi \in \mathcal{H} \iff \int_{\mathbb{R}} (t^2 - C^2)\, d\mu_\xi^T(t) \leq 0,\ \forall \xi \in \mathcal{H}.$$

The former relation is equivalent to T being bounded while the latter (by a variation of Lemma 8.3.16) to $\mu_\xi^T(\mathbb{R} \setminus [-C,C]) = 0$, $\forall \xi \in \mathcal{H}$, that is $\chi_{[-C,C]}(T) = \mathbf{1}$ (see the proof of item a)).

c) is equivalent to b).

d) This is a direct consequence of the relation $\chi_\Lambda(f(t)) = \chi_{f^{-1}(\Lambda)}(t)$, which is valid for complex-valued functions. □

Exercise 8.3.22. Let T be self-adjoint and $\xi \in \operatorname{dom} T$. Use the spectral theorem to show that the family $\xi_t := e^{-itT}\xi$, $t \in \mathbb{R}$, is uniformly continuous in the space $(\operatorname{dom} T, \|\cdot\|_T)$; note that, by the functional calculus, the unitary evolution group $e^{-itT} = f_t(T)$ with $f_t(x) = e^{-itx}$.

Exercise 8.3.23. Let T be self-adjoint, λ an isolated point of the spectrum of T (so an eigenvalue) and $\sigma(T) \neq \{\lambda\}$. Show that there is a bounded operator $S \neq 0$ such that $S\chi_{\{\lambda\}}(T) = 0 = \chi_{\{\lambda\}}(T)S$ and $(T - \lambda\mathbf{1})S = \mathbf{1} - \chi_{\{\lambda\}}(T)$.

8.4 Examples

This section is devoted to some examples of resolutions of the identity. A practical and simple recipe for finding explicitly the resolutions of identity for most self-adjoint operators is certainly a dream of many people!

8.4.1 Multiplication Operator

Consider the self-adjoint operator $\mathcal{M}_\varphi$, for $\varphi : E \to \mathbb{R}$, acting in $\mathrm{L}^2_\mu(E)$, defined in Subsection 2.3.2. In the following it will be verified that the map

$$\mathcal{A} \ni \Lambda \mapsto P(\Lambda) := \chi_{\varphi^{-1}(\Lambda)}$$

is a resolution of the identity.

Since characteristic functions can assume only the real values 1 and 0, it follows that the just defined $P(\Lambda)$ are bounded self-adjoint operators and also $P(\Lambda)^2 = P(\Lambda)$, i.e., they are orthogonal projections acting on $\mathrm{L}^2_\mu(E)$. As $\varphi^{-1}(\mathbb{R}) = E$, $\chi_E(x) = 1$, $\forall x \in E$, it follows that $P(\mathbb{R}) = \mathbf{1}$; in fact, for all $\psi \in \mathrm{L}^2_\mu(E)$,

$$\|P(\mathbb{R})\psi - \psi\|^2 = \int_E |\chi_E(x) - 1|^2 \, |\psi(x)|^2 \, d\mu(x) = 0.$$

Now, if $\Lambda = \sum_{j=1}^\infty \Lambda_j$, due to the pointwise convergence $\sum_{j=1}^n \chi_{\varphi^{-1}(\Lambda_j)}(x) \to \chi_{\varphi^{-1}(\Lambda)}(x)$, as $n \to \infty$, for any $\psi \in \mathrm{L}^2_\mu(E)$,

$$\begin{aligned} &\left\| \sum_{j=1}^n P(\Lambda_j)\psi - P(\Lambda)\psi \right\|^2 \\ &= \int_E \left| \sum_{j=1}^n \chi_{\varphi^{-1}(\Lambda_j)}(x) - \chi_{\varphi^{-1}(\Lambda)}(x) \right|^2 \, |\psi(x)|^2 \, d\mu(x) \end{aligned}$$

which vanishes as $n \to \infty$ by dominated convergence. Hence

$$\sum_{j=1}^n P(\Lambda_j)\psi \to P(\Lambda)\psi,$$

and so P is a resolution of the identity. For a Borel function $f : \mathbb{R} \to \mathbb{C}$ one has the normal operator $f(\mathcal{M}_\varphi) = \mathcal{M}_{f\circ\varphi}$.

Position Operator. In the particular case $E = \mathbb{R}$ with $d\mu = dx$ (i.e., Lebesgue measure), one has the position operator $q(x) = \mathcal{M}_x$ acting in $\mathrm{L}^2(\mathbb{R})$ (Example 2.3.31). Then the above construction leads to the resolution of the identity $\mathcal{A} \ni \Lambda \mapsto P^q(\Lambda) = \chi_\Lambda$, so that

$$\langle \psi, P^q(\Lambda)\psi \rangle = \int_\Lambda |\psi(x)|^2 \, dx, \qquad \psi \in \mathrm{L}^2(\mathbb{R}),$$

and

$$\langle \psi, q\psi \rangle = \int_{\mathbb{R}} x|\psi(x)|^2 \, dx, \qquad \psi \in \mathrm{dom}\; q.$$

Consequently, the spectral measures of the position operator are

$$d\mu_\psi(x) = |\psi(x)|^2 \, dx.$$

Note that they are absolutely continuous with respect to Lebesgue measure, for $|\psi(x)|^2 \in \mathrm{L}^1(\mathbb{R})$. It is worth observing that actually

$$\mathrm{dom}\; q = \{\psi : q \in \mathrm{L}^2_{\mu_\psi}(\mathbb{R})\} = \left\{ \psi : \int_{\mathbb{R}} x^2 |\psi(x)|^2 \, dx < \infty \right\}.$$

Given a Borel function $f : \mathbb{R} \to \mathbb{C}$ one has the normal operator $f(q) = \mathcal{M}_{f(x)}$. Such construction generalizes at once to the components of the position operator in $\mathrm{L}^2(\mathbb{R}^n)$.

Momentum Operator. Recall the momentum operator in $L^2(\mathbb{R})$ (see Section 3.3), here denoted by $\mathcal{P}$, and given by dom $\mathcal{P} = \mathcal{F}^{-1}\mathcal{H}^1(\hat{\mathbb{R}})$,

$$(\mathcal{F}\mathcal{P}\mathcal{F}^{-1})\hat{\psi}(p) = p\hat{\psi}(p), \qquad (P\psi)(x) = (\mathcal{F}^{-1}p\mathcal{F})\psi(x).$$

Hence, based on the above construction for the position operator, the spectral resolution of the momentum is $P^{\mathcal{P}}(\Lambda)\psi(x) = \mathcal{F}^{-1}\chi_\Lambda(p)\hat{\psi}(p)$, and for the spectral measures consider

$$\begin{aligned}\langle\psi, P^{\mathcal{P}}(\Lambda)\psi\rangle &= \langle\psi, \mathcal{F}^{-1}\chi_\Lambda(p)\hat{\psi}(p)\rangle \\ &= \langle\hat{\psi}(p), \chi_\Lambda(p)\hat{\psi}(p)\rangle = \int_\Lambda |\hat{\psi}(p)|^2\, dp,\end{aligned}$$

so that its spectral measures are $d\mu_\psi(p) = |\hat{\psi}(p)|^2\, dp$, again absolutely continuous with respect to Lebesgue measure. For a Borel function $f : \mathbb{R} \to \mathbb{C}$ one has the normal operator $f(\mathcal{P}) = \mathcal{F}^{-1}\mathcal{M}_{f(p)}\mathcal{F}$, in accord with the discussion in Section 3.4.

Kinetic Energy Operator. The free hamiltonian H_0 in $L^2(\mathbb{R}^n)$ (Section 3.4) is

$$(H_0\psi)(x) := -\Delta\psi(x) = \mathcal{F}^{-1}[\mathcal{M}_{p^2}\hat{\psi}(p)](x), \qquad \psi \in \text{dom } H_0,$$

dom $H_0 = \mathcal{H}^2(\mathbb{R}^n)$, that is, H_0 is unitarily equivalent to the multiplication operator by the function $\varphi(p) = p^2$ in $L^2(\hat{\mathbb{R}}^n)$. Therefore, its resolution of identity is

$$\mathcal{A} \ni \Lambda \mapsto P^{H_0}(\Lambda) = \mathcal{F}^{-1}\chi_{\varphi^{-1}(\Lambda)}\mathcal{F};$$

note the simple expression $\varphi^{-1}(\Lambda) = \{p \in \hat{\mathbb{R}}^n : p^2 \in \Lambda\}$. From this and Parseval's identity, it is found for its spectral measures

$$\mu_\psi(\Lambda) = \langle\psi, P^{H_0}(\Lambda)\psi\rangle = \int_{p^2\in\Lambda} |\hat{\psi}(p)|^2\, dp,$$

which are also absolutely continuous with respect to Lebesgue measure and only Borel sets $\Lambda \subset [0, \infty)$ can have nonzero spectral measures.

For simplicity consider $n = 1$. If $\psi \in$ dom H_0 write

$$\langle\psi, H_0\psi\rangle = \int_{\mathbb{R}} p^2|\hat{\psi}(p)|^2\, dp = \int_{-\infty}^0 p^2|\hat{\psi}(p)|^2\, dp + \int_0^\infty p^2|\hat{\psi}(p)|^2\, dp,$$

and introduce the variable $t = p^2$ (i.e., $p = -\sqrt{t}$ and $p = \sqrt{t}$, in the first and second integrals, respectively) so that

$$\langle\psi, H_0\psi\rangle = \int_0^\infty t\left(\left|\hat{\psi}(-\sqrt{t})\right|^2 + \left|\hat{\psi}(\sqrt{t})\right|^2\right)\frac{dt}{2\sqrt{t}}.$$

If $\hat{\psi}$ is an odd or even function one has

$$\langle\psi, H_0\psi\rangle = \int_0^\infty t\left|\hat{\psi}(\sqrt{t})\right|^2\frac{dt}{\sqrt{t}}.$$

Introduce the Hilbert spaces L_+ (resp. L_-) of functions $\psi \in \mathrm{L}^2(\mathbb{R})$ so that $\hat{\psi}$ are even (resp. odd) functions, both with the inner product

$$[\phi, \psi] := \int_0^\infty \overline{\hat{\phi}(\sqrt{t})}\, \hat{\psi}(\sqrt{t})\, \frac{dt}{\sqrt{t}},$$

and on each of such subspaces H_0 becomes the multiplication operator $\mathcal{M}_h$, $h(t) = t$. Since every function $\hat{\psi} = \hat{\psi}_+ \oplus \hat{\psi}_-$, with $\hat{\psi}_+$ even and $\hat{\psi}_-$ odd functions and (by using the same change of variable above)

$$\|\psi\|^2 = \|\hat{\psi}\|^2 = \int_0^\infty \left|\hat{\psi}_-(\sqrt{t})\right|^2 \frac{dt}{\sqrt{t}} + \int_0^\infty \left|\hat{\psi}_+(\sqrt{t})\right|^2 \frac{dt}{\sqrt{t}},$$

the direct sum $L_+ \oplus L_-$ is isomorphic to $\mathrm{L}^2(\mathbb{R})$ and the space where H_0 acts as $\mathcal{M}_h$ was made explicit. Further, for $\psi \in \mathrm{dom}\, f(H_0)$, in $L_\pm$ one has

$$\langle \psi, f(H_0)\psi \rangle = \int_0^\infty f(t) \left|\hat{\psi}(\sqrt{t})\right|^2 \frac{dt}{\sqrt{t}}.$$

By considering $f = \chi_\Lambda$, it is found that the spectral measures of H_0 at ψ can be written in the form (one can consider $t \in \mathbb{R}$)

$$d\mu_\psi^{H_0}(t) = \chi_{(0,\infty)}(t) \left|\hat{\psi}(\sqrt{t})\right|^2 \frac{dt}{\sqrt{t}},$$

which are clearly absolutely continuous with respect to Lebesgue measure. Note the presence of two subspaces in this decomposition, indicating that the spectrum of H_0 is not simple.

Exercise 8.4.1. Spectral measures of the free hamiltonian H_0 in $\mathrm{L}^2(\mathbb{R}^3)$. Introduce spherical coordinates $(\hat{r}, \hat{\Omega})$, $\hat{r} = |p|, \hat{\Omega} = (\hat{\theta}, \hat{\varphi})$ in the momentum space $\hat{\mathbb{R}^3}$, so that $\mathrm{L}^2(\hat{\mathbb{R}^3}) = \mathrm{L}^2_{\hat{r}^2 dr}[0,\infty)) \otimes \mathrm{L}^2_{d\hat{\Omega}}(\hat{S}^2)$, where $\hat{S}^2$ is the unit sphere in $\hat{\mathbb{R}^3}$ and $d\hat{\Omega} = \sin\hat{\theta}\, d\hat{\theta} d\hat{\varphi}$. Write

$$\langle \psi, H_0\psi \rangle = \int_{\mathbb{R}} p^2 \left|\hat{\psi}(p)\right|^2 dp = \int_0^\infty d\hat{r}\, \hat{r}^4 \int_{\hat{S}^2} \left|\hat{\psi}(\hat{r}, \hat{\Omega})\right|^2 d\hat{\Omega},$$

perform the change of variable $t = \hat{r}^4$ and conclude that

$$\langle \psi, H_0\psi \rangle = \int_{\mathbb{R}} t\, d\mu_\psi^{H_0}(t),$$

where $\mu_\psi^{H_0}$ is given by

$$d\mu_\psi^{H_0}(t) = \left(\int_{\hat{S}^2} d\hat{\Omega} \left|\hat{\psi}(t^{\frac{1}{4}}, \hat{\Omega})\right|^2 \right) \chi_{(0,\infty)}(t)\, \frac{dt}{4t^{\frac{3}{4}}}.$$

Exercise 8.4.2. Find the spectral measures $\mu_{\xi,\eta}$ for the position, momentum and kinetic energy operators in $\mathrm{L}^2(\mathbb{R})$.

8.4.2 Purely Point Operators

The discussion in this subsection is directly related, especially, to compact self-adjoint operators discussed in Section 8.1 and to standard Schrödinger operators $H = -\Delta + V$, with lower bounded and unbounded potentials V, considered in Section 11.5.

Let T be a self-adjoint operator in $\mathcal{H}$ and $(\xi_j)_j$ an orthonormal basis of $\mathcal{H}$ composed of eigenvectors of T corresponding to the eigenvalues λ_j, that is, $T\xi_j = \lambda_j \xi_j$, $\|\xi_j\| = 1$. Such operators are called *purely point operators* and will be considered in later chapters. Suppose that $\lambda_j \neq \lambda_k$ if $j \neq k$ (that is, all eigenvalues are simple) and denote by P_j the orthogonal projection onto the one-dimensional subspace generated by ξ_j. For a Borel set $\Lambda \subset \mathbb{R}$ the map (infinite sums are understood as strong limits)

$$P^T(\Lambda) = \sum_{\lambda_j \in \Lambda} P_j$$

defines the resolution of the identity of T. In fact, since $P_j P_k = \delta_{k,j} P_j$ it follows that $P^T(\Lambda)$ is an orthogonal projection. Every $\xi \in \mathcal{H}$ can be written as $\xi = \sum_j a_j \xi_j$, with $\|\xi\|^2 = \sum_j |a_j|^2$, so that $P_j \xi = a_j \xi_j$ and if $\xi \in \operatorname{dom} T$ one has $T\xi = \sum_j \lambda_j a_j \xi_j = \sum_j \lambda_j P_j \xi$ (since T is closed). Thus

$$T = \sum_j \lambda_j P_j = \int_{\mathbb{R}} t \, dP^T(t).$$

For a continuous function $f : \mathbb{R} \to \mathbb{C}$ one has (see Corollary 8.3.19)

$$f(T) = \sum_j f(\lambda_j) P_j, \qquad f(T)\xi = \sum_j f(\lambda_j) a_j \xi_j,$$

and

$$\xi \in \operatorname{dom} f(T) \Longleftrightarrow \sum_j |f(\lambda_j)|^2 |a_j|^2 < \infty.$$

Especially, $T = f(h)$, $h(t) = t$, which confirms that the above resolution of identity is actually the resolution of identity of T. The spectral measures are

$$\mu_\xi^T(\Lambda) = \langle \xi, P^T(\Lambda)\xi \rangle = \sum_{\lambda_j \in \Lambda} |a_j|^2 \, \delta_{\lambda_j} = \sum_j |a_j|^2 \, \delta_{\lambda_j}(\Lambda),$$

with δ_{λ_j} denoting the Dirac measure at λ_j. Thus,

$$\mu_\xi^T = \sum_j |a_j|^2 \, \delta_{\lambda_j},$$

and for the eigenvectors ξ_j one has $\mu_{\xi_j}^T = \delta_{\lambda_j}$. Such spectral measures are not absolutely continuous with respect to Lebesgue measure (they are called *purely point measures* or *atomic measures*).

Exercise 8.4.3. Find the resolution of the identity and spectral measures for the harmonic oscillator energy operator, Example 2.3.3.

Exercise 8.4.4. Find the resolution of the identity and spectral measures of the identity operator $\mathbf{1} : \mathcal{H} \to \mathcal{H}$, $\mathbf{1}\xi = \xi$, $\forall \xi \in \mathcal{H}$.

Exercise 8.4.5. Discuss the adaptations needed in the above construction if there are eigenvalues that are not simple, that is, with multiplicity greater than 1.

Exercise 8.4.6. Show that every operator $\sum_j \lambda_j P_j$, with $\lambda_j \in \mathbb{R}$, P_j orthogonal projections onto pairwise orthogonal finite-dimensional spaces, with $\sum_j P_j = \mathbf{1}$ and $\lim_{j\to\infty} \lambda_j = 0$, is compact and self-adjoint.

Exercise 8.4.7. Find the resolution of identity and spectral measures of self-adjoint operators on a Hilbert space of finite dimension.

8.4.3 Tight-Binding Kinetic Energy

The *tight-binding* Schrödinger kinetic energy operator h_0 (also called *discrete* kinetic energy) acting on the Hilbert space of sequences $l^2(\mathbb{Z})$ is

$$(h_0 u)_j = u_{j+1} + u_{j-1}, \qquad u = (u_j) \in l^2(\mathbb{Z}).$$

It is a bounded self-adjoint operator. It is a specific case of operators acting on ℓ^2 spaces and called *Jacobi matrices*, which have been extensively considered in the framework of random Schrödinger operators [CaL90].

By means of Fourier series it is possible to translate h_0 as a multiplication operator. Recall that the Fourier series $\mathrm{F} : \mathrm{L}^2[-\pi, \pi] \to l^2(\mathbb{Z})$,

$$(\mathrm{F}\psi)_j = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} e^{-ijx} \psi(x)\, dx,$$

is a unitary operator and that $(\mathrm{F}^{-1}u)(x) = \sum_j u_j e^{ijx}/\sqrt{2\pi}$. If $e_k = (\delta_{j,k})_{k\in\mathbb{Z}}$ denotes an element of canonical basis of $l^2(\mathbb{Z})$, then $(\mathrm{F}^{-1}e_k)(x) = e^{ikx}/\sqrt{2\pi}$ and $(e^{ikx}/\sqrt{2\pi})_{k\in\mathbb{Z}}$ is an orthonormal basis of $\mathrm{L}^2[-\pi, \pi]$. A direct calculation leads to

$$(\mathrm{F}^{-1} h_0 \mathrm{F})\psi(x) = \mathcal{M}_{2\cos x} \psi(x).$$

Hence h_0 is unitarily equivalent to the multiplication operator $\mathcal{M}_{2\cos x}$ in $\mathrm{L}^2[-\pi, \pi]$, so that (see Section 2.3.2) $\sigma(h_0) = [-2, 2]$, and it has no eigenvalues. Again by Fourier series, if $\psi = \mathrm{F}^{-1}u$, $\|u\| = 1$, with the change of variable $t = 2\cos x$ one gets

$$\begin{aligned}
\langle u, h_0 u\rangle_{l^2} &= \langle \psi, \mathrm{F}^{-1} h_0 \mathrm{F}\psi\rangle_{\mathrm{L}^2} \\
&= \int_{-\pi}^{0} 2\cos x\, |\psi(x)|^2\, dx + \int_0^{\pi} 2\cos x\, |\psi(x)|^2\, dx \\
&= \int_{-2}^{2} t \left|\psi\left(\arccos\frac{t}{2}\right)\right|^2 \frac{dt}{\sqrt{4-t^2}} + \int_{-2}^{2} t \left|\psi\left(\arccos\frac{t}{2}\right)\right|^2 \frac{dt}{\sqrt{4-t^2}},
\end{aligned}$$

so that $l^2(\mathbb{Z})$ is isomorphic to $\mathrm{L}^2[-\pi,\pi] = \mathrm{L}^2[-\pi,0] \oplus \mathrm{L}^2[0,\pi]$ which in its turn is isomorphic to

$$\mathrm{L}^2_\mu[-2,2] \oplus \mathrm{L}^2_\mu[-2,2], \qquad d\mu(t) = \frac{dt}{\sqrt{4-t^2}},$$

and in this space h_0 acts as the multiplication operator $\mathcal{M}_h$, $h(t) = t$.

Exercise 8.4.8. Show that h_0 is self-adjoint and $\|h_0\| = 2$.

8.5 Comments on Proofs

Instead of a detailed proof of the spectral theorem, a short discussion of ideas involved in different proofs will be presented. The expectation is that the reader could get an overall flavor of different strategies, and what follows should be considered just a guide to different presentations. A few historical remarks will also be inserted and references to complete proofs are of course provided. As it should be clear from the discussion of purely point operators in Subsection 8.4.2, the chief difficulty is the presence of continuous spectra.

The spectral theorem has many nuances spread among different presentations in the literature. A nice discussion about various aspects can be found in the first volume of the Reed-Simon books [ReeS81], and additional information including the Hahn-Hellinger theorem and multiplicity function of spectral measures can also be found in [Sun97] and [Hel86].

Given a self-adjoint operator T, often the main point is the construction of the resolution of identity P^T, and so spectral measures and integration theory follow by standard arguments (including functions $f(T)$). Also, by standard arguments of integration theory, it is enough to define $P^T((a,b])$ for intervals $(a,b]$ in $\mathbb{R}$ and imposing a strong continuity from the right, i.e., $P^T((a,b]) = \mathrm{s}-\lim_{\varepsilon\to 0^+} P^T((a,b+\varepsilon])$.

There are two general approaches to proofs of the spectral theorem:

- A1 Proofs that consider first bounded self-adjoint operators. Then it is extended to a version for unitary operators. The unbounded self-adjoint case is obtained by means of a Cayley transform (Definition 2.2.1); this approach was pioneered by von Neumann.
- A2 Proofs that work directly for both bounded and unbounded operators.

The version of the spectral theorem for unitary operators expresses that they are equivalent to multiplication operators $\mathcal{M}_{e^{it}}$ on some suitable spaces $\mathrm{L}^2_\nu[-\pi,\pi]$.

The first general proofs of the spectral theorem were due to independent works by von Neumann, Stone and F. Riesz; the first version on unbounded operators was published around 1930. Since then other proofs have appeared, and the most important proposals are mentioned below. E. Schmidt was the first to note that a restriction to self-adjoint operators was necessary, and T. Carleman (around 1920) had a first version of this theorem for some singular integral operators with symmetric kernels. The proof by Stone relies on some ideas developed in such works of Carleman. There is in fact a version of the spectral theorem for unbounded normal operators; in this case the resolution of identity is a function on the Borel sets in the complex plane; see [Con85].

In some sense, the history of the spectral theorem began with the problem of finding the principal axes of an ellipsoid; in modern language, the problem of diagonalizing symmetric matrices.

Via Resolvent Operator. This approach to the proof of the spectral theorem applies to bounded as well as unbounded self-adjoint operators. The main ideas have appeared in a proof due to Doob and Koopman of 1934. Given a self-adjoint operator T and $\xi \in \mathcal{H}$, consider the matrix element of the resolvent $R_z(T)$,

$$F_\xi(z) := \langle \xi, R_z(T)\xi \rangle, \qquad z \in \rho(T),$$

which is a holomorphic function on $\rho(T)$, satisfies $\overline{F_\xi(z)} = F_\xi(\overline{z})$, and

$$|F_\xi(z)| \le \frac{\|\xi\|^2}{\text{Im } z}, \qquad \text{Im } F_\xi(z) = \text{Im } z \, \|R_z(T)\xi\|^2,$$

so that the complex upper half-plane is invariant under F_ξ. Such function is an instance of the so-called Herglotz functions and so it is the Borel transform of a Borel positive measure μ_ξ on $\mathcal{A}$, that is,

$$F_\xi(z) := \int_{\mathbb{R}} \frac{1}{t-z} \, d\mu_\xi(t).$$

A related argument gives the measure μ_ξ via the (inversion) formula

$$\mu_\xi((a,b]) = \lim_{\delta\to 0^+} \lim_{\varepsilon \to 0^+} \frac{1}{\pi} \int_{a+\delta}^{b+\delta} \text{Im } F_{t+i\varepsilon}(T)\, dt.$$

The measures μ_ξ are actually spectral measures of T from which the resolution of identity P^T can be defined by

$$\langle \xi, P^T(\Lambda)\xi \rangle = \int_{\mathbb{R}} \chi_\Lambda(t)\, d\mu_\xi(t).$$

Since the measures μ_ξ follow uniquely from the resolvent $R_z(T)$, the construction of P^T is unique.

Proofs along these lines appear, for example, in [Wei80] and [Te08].

Via Polar Decomposition. This proof can be classified in A2 above and has become a standard one; see [Kat80]. First it is shown that every positive self-adjoint operator T has a positive square root $T^{1/2}$, i.e., $T^{1/2}$ is a positive self-adjoint operator so that $T^{1/2}T^{1/2} = T$; this is not an easy task. The second step is to show that every self-adjoint operator T admits a polar decomposition, i.e., $T = W|T|$, where $|T|$ is a positive operator and $W : \text{rng } |T| \to \text{rng } T$ is unitary. Explicitly $|T| = (T^*T)^{1/2}$ (note that T^*T is positive).

Now for each $t \in \mathbb{R}$ consider the self-adjoint operator

$$T_t := T - t\mathbf{1} = W_t|T_t|,$$

where $W_t|T_t|$ is the polar decomposition of T_t. Finally, define

$$P^T((-\infty, t]) := \mathbf{1} - \frac{1}{2}\left(W_t + W_t^2\right),$$

and it is possible to check that P^T is actually the resolution of identity of T. The motivation for such choices comes from the position operator on $\mathrm{L}^2(\mathbb{R})$, $\mathcal{M}_x$, for which $P((-\infty, t])$ is just the projection onto $x \le t$. In this particular case

$$\mathcal{M}_x - t\mathbf{1} = W_t(x)|x-t|, \qquad W_t(x) = \begin{cases} -\mathbf{1}, & \text{if } x \le t \\ \mathbf{1}, & \text{if } x > t \end{cases}.$$

Then, since $W_t(x)^2 = \mathbf{1}$,

$$P^T((-\infty, t]) = \mathbf{1} - \frac{1}{2}\left(W_t(x) - W_t(x)^2\right) = \frac{1}{2}\left(\mathbf{1} - W_t(x)\right) = \chi_{(-\infty,t]}(x),$$

and the expected projection operator is obtained. There are small variations of this program, and in case it is first carried out to bounded self-adjoint operators, the Cayley transform is used to transfer the results to the unbounded case; a detailed proof along these lines can be found in [Kr78].

In Chapter 9 the square root and polar decomposition will be derived as consequences of the spectral theorem. This is valid since this theorem can be obtained by means of different arguments.

Via C^*-Algebras. For bounded self-adjoint operators there is a proof of the spectral theorem based on representations of abelian C^*-algebras, which was first developed by I.M. Gel'fand and M.A. Naimark beginning in 1943. It is a beautiful approach that gives more information than just the theorem itself and, with little additional effort, can be extended to normal operators. Very briefly, the involved ideas go as follows: if T is bounded and self-adjoint, the construction begins with the set J'_T of polynomials $p(T)$, and its closure J_T in $\mathrm{B}(\mathcal{H})$, which is an abelian C^*-algebra with identity $\mathbf{1}$ (obtained from the constant polynomial $p(t) = 1$). A fundamental step is the proof that there is a unique isomorphism of C^*-algebras between J_T and $C(\sigma(T))$, that is, the set of continuous functions defined on the spectrum of T with the sup norm, so that $p(T)$ is mapped to $p(t)$. Thus, elements of J_T are interpreted as continuous functions $f(T)$. The analogous to the cyclic subspaces $\mathcal{H}_\xi$ above can be defined as the closure of

$$\{p(T)\xi : p \text{ a polynomial function}\},$$

and if the latter equals $\mathcal{H}$ then ξ is said to be cyclic. In case a cyclic vector exists, the just mentioned isomorphism can be combined with the Riesz-Markov theorem to provide spectral measures, which then allow the definition of $f(T)$ for some measurable functions; in particular for $\chi_\Lambda(T)$, i.e., the resolution of identity

P^T emerges. If no cyclic vector exists, direct sums should be considered as in Theorem 8.3.7.

If T is normal and bounded, then polynomials $p(T, T^*)$ are well posed since $TT^* = T^*T$, and the results for normal operators follow similar lines as the ones just sketched.

Such a point of view has other advantages, for instance, it is a natural setting for discussions about *complete systems of observables* in quantum mechanics as well as the Hahn-Hellinger theorem.

See detailed proofs in [Sun97] and [Con85].

Via Bochner Theorem. First a proof for unitary operators is presented, and then Cayley transform is used to get a version for the self-adjoint case. If U is unitary, then for each $\xi \in \mathcal{H}$ the sequence $t_n = \langle \xi, U^n \xi \rangle$, $n \in \mathbb{Z}$, is positive definite (see Exercise 5.3.10) and so by the Bochner theorem there is a finite positive measure ν_ξ so that

$$\langle \xi, U^n \xi \rangle = \int_0^{2\pi} e^{isn}\, d\nu_\xi(s), \qquad \forall n \in \mathbb{Z}.$$

The unitary analogue to $\mathcal{H}_\xi$ is the closure of $\{U^n \xi : n \in \mathbb{Z}\}$, and a construction shows that U is unitarily equivalent to the multiplication operator $\mathcal{M}_{e^{it}}$ on some space $\mathrm{L}^2_\nu[-\pi, \pi]$, and so on. Given T self-adjoint, such a construction can be transferred from its Cayley transform $U(T)$ to T itself, so that spectral measures of T as well as P^T follow. See, for instance, [AkG93], [Que87] and [Hel86].

Leinfelder's Geometric Proof. In 1935 Lengyel and Stone presented a proof of the spectral theorem for bounded self-adjoint operators which used only intrinsic properties of Hilbert spaces [LenS36]; the main point was the consideration of suitable invariant subspaces, and so the term "geometric proof." In [Lei79] that proof was generalized to the unbounded case.

As an illustration of how the spectral projections arise, the case of positive operators will be mentioned. Let T be a closed hermitian operator, $D^\infty(T) = \cap_{n\geq 1} \mathrm{dom}\, T^n$ and, for $\lambda \geq 0$,

$$F(T, \lambda) = \{\xi \in D^\infty(T) : \|T^n \xi\| \leq \lambda^n \|\xi\|, n = 1, 2, \dots\}.$$

It is then shown that $F(T, \lambda)$ is a closed invariant subspace, and $\cup_{n\geq 1} F(T, n)$ is dense in $\mathcal{H}$ iff T is self-adjoint.

In case T is self-adjoint, let $Q(T, \lambda)$ denote the orthogonal projection onto $F(T, \lambda)$. If also $T \geq 0$, then it is shown that $P^T(-\infty, \lambda] = Q(T, \lambda)$, $\lambda \geq 0$, and $P^T(-\infty, \lambda] = 0$ if $\lambda < 0$ (of course!); for general self-adjoint operators a limiting process is needed.

Via the Helffer-Sjöstrand Formula. This is a rather new proof based on a formula, deduced by Helffer and Sjöstrand in 1989, which gives smooth functions $f(T)$ as an integral over resolvents, and can be extended to a somewhat large class of functions f. It works for bounded as well as unbounded self-adjoint operators. Details and references can be found in [Dav95].

Chapter 9

Applications of the Spectral Theorem

Several applications of the spectral theorem will be discussed in this chapter; some are as strong as simple to get, thanks to the functional calculus. Additional applications will appear in other chapters. Recall that $\mathcal{A}$ denotes the Borel σ-algebra in $\mathbb{R}$.

9.1 Quantum Interpretation of Spectral Measures

Strictly speaking, this is not an application of the spectral theorem, but an interpretation based on quantum postulates. Given a self-adjoint operator T representing a quantum observable and $\Lambda \in \mathcal{A}$, according to quantum mechanics, if the system is in the state $\xi \in \operatorname{dom} T \subset \mathcal{H}$, then the quantities

$$\langle \xi, \chi_\Lambda(T)\xi \rangle, \qquad \langle \xi, T\xi \rangle,$$

are the probability that a measurement of T results in a value in Λ and the expectation valued of T, respectively (see a discussion on page 132). By the spectral theorem such quantities are written in terms of the spectral measure of T at ξ, that is,

$$\langle \xi, \chi_\Lambda(T)\xi \rangle = \mu_\xi^T(\Lambda), \qquad \langle \xi, T\xi \rangle = \int_{\sigma(T)} t \, d\mu_\xi^T(t).$$

Therefore, $t \mapsto \mu_\xi^T((-\infty, t])$ is the probability distribution of the possible values of the observable represented by T when the system is in the state ξ. Note that since $\mu_\eta^T(\mathbb{R} \setminus \sigma(T)) = 0$, for all $\eta \in \mathcal{H}$, actually all measurements of T result in values in the spectrum of T.

It is interesting to have a closer look at the case T is pure point, discussed in Subsection 8.4.2. Let $(\xi_j)_j$ be an orthonormal basis of $\mathcal{H}$ composed of eigenvectors of T corresponding to the eigenvalues λ_j, that is, $T\xi_j = \lambda_j\xi_j$, $\|\xi_j\| = 1$. If the system is in the normalized state $\xi \in \operatorname{dom} T$, one has $\xi = \sum_j a_j\xi_j$, with $1 = \|\xi\|^2 = \sum_j |a_j|^2$ and

$$T\xi = \sum_j a_j\lambda_j\xi_j.$$

The spectral measure is

$$\mu_\xi^T = \sum_j |a_j|^2 \, \delta_{\lambda_j}.$$

If $\lambda_k \in \Lambda$ and if $\lambda_j \notin \Lambda$ for $j \neq k$, then the probability of a measurement of T resulting in a value in Λ is $\mu_\xi^T(\Lambda) = |a_k|^2$, in other words, $|a_k|^2$ is the probability of λ_k being the measured value of T. It is also interpreted as the probability of the system being found in the state ξ_j upon measurement; this is called a *quantum reduction* of the state ξ to ξ_j, one of the many mysteries of quantum mechanics! Note that such interpretation is compatible with the expression

$$\sum_j \lambda_j|a_j|^2$$

for the expectation value of T. More generally, $\sum_j f(\lambda_j)|a_j|^2$ is the expectation value of $f(T)$.

Remark 9.1.1. Another interesting interpretation related to spectral measures appears in Section 14.2.

9.2 Proof of Theorem 5.3.1

As an application of the spectral theorem the proof of Theorem 5.3.1 will be presented.

Proof. Let T be self-adjoint. For each $t \in \mathbb{R}$ let $f_t(x) = e^{-itx}$ and define $U(t) := f_t(T)$, which will also be denoted by e^{-itT}. By the functional calculus, Corollary 8.3.19, these are bounded normal operators and for all $s, t \in \mathbb{R}$,

$$U(t)U(s) = U(t+s), \qquad U(t)^* = U(-t) = U(t)^{-1},$$

(since $f_s(x)f_t(x) = f_{s+t}(x)$; note that $U(0) = \mathbf{1}$) so that $t \mapsto U(t)$ is a unitary evolution group. The next step is to show that this map is strongly continuous. If $\xi \in \mathcal{H}$, then

$$\|U(h)\xi - \xi\|^2 = \int_{\sigma(T)} \left|e^{-ihx} - 1\right|^2 \, d\mu_\xi^T(x)$$

which vanishes as $h \to 0$ by dominated convergence. Hence $t \mapsto U(t)$ is strongly continuous.

If $\eta \in \mathcal{H}$ and $h \neq 0$, then

$$\left\| \frac{i}{h}(U(h) - \mathbf{1})\eta \right\|^2 = \int_{\sigma(T)} \left| \frac{1}{h}(e^{-ihx} - 1) \right|^2 \, d\mu_\eta^T(x).$$

Since

$$\left| \frac{i}{h}(e^{-ihx} - 1) \right| \leq |x|$$

and for $h \to 0$ one has the pointwise limit

$$\frac{i}{h}\left(e^{-ihx} - 1\right) \to x,$$

the above integral converges as $h \to 0$ iff the function $f(x) = x$, $x \in \mathbb{R}$, belongs to $\mathrm{L}^2_{\mu_\eta^T}(\mathbb{R})$. In fact, if $f \in \mathrm{L}^2_{\mu_\eta^T}(\mathbb{R})$, then the convergence holds by dominated convergence, and if $f \notin \mathrm{L}^2_{\mu_\eta^T}(\mathbb{R})$ it does not converge by Fatou's lemma. Hence, it converges iff $\eta \in \operatorname{dom} T$, since $T = f(x)$ for $f(x) = x$. The same argument also implies, for $\eta \in \operatorname{dom} T$,

$$\left\| \frac{i}{h}(U(h) - \mathbf{1})\eta - T\eta \right\|^2 = \int_{\sigma(T)} \left| \frac{i}{h}(e^{-ihx} - 1) - x \right|^2 \, d\mu_\eta^T(x) \xrightarrow{h\to 0} 0,$$

and T is actually the infinitesimal generator of $U(t)$. □

Exercise 9.2.1. Present details of the following alternative proof of Theorem 5.3.1. If T is self-adjoint, by the spectral theorem it is unitarily equivalent to $\mathcal{M}_h$, $h(x) = x$, acting in some L^2_μ. Define $U(t) = \mathcal{M}_{e^{-itx}}$ and use Example 5.1.6.

9.3 Form Domain of Positive Operators

First the square root operator must be addressed.

Proposition 9.3.1. *Let $T \geq 0$ be a self-adjoint operator. Then, for each $n \in \mathbb{N}$, there exists a unique self-adjoint operator $S \geq 0$ so that $S^n = T$. Such S is denoted by $S = T^{1/n}$.*

Proof. For the existence consider the function $f(x) = x^{\frac{1}{n}}$, $x \geq 0$, and zero for $x < 0$, and define $S = f(T)$, which is a positive operator since, by Proposition 8.3.21, $\sigma(T) \subset \mathbb{R}_+ = [0, \infty)$ and

$$\langle \xi, S\xi \rangle = \int_{\sigma(T)} x^{\frac{1}{n}} \, d\mu_\xi^T(x) \geq 0, \qquad \forall \xi \in \operatorname{dom} S.$$

By Proposition 8.3.10, $S^n = T$. Moreover, since on $\mathbb{R}_+$ the function f is one-to-one, for any Borel set $\Lambda \in \mathcal{A}$, $\Lambda \subset \mathbb{R}_+$,

$$\chi_\Lambda(S) = \chi_{f^{-1}(\Lambda)}(T),$$

and $\chi_\Lambda(S) = 0$ if $\Lambda \subset (-\infty, 0)$.

For uniqueness, consider a self-adjoint operator $A \geq 0$ obeying $A^n = T$; then,

$$\chi_\Lambda(T) = \chi_\Lambda(A^n) = \chi_{f(\Lambda)}(A), \qquad \Lambda \subset \mathbb{R}_+,$$

and $\chi_\Lambda(T) = 0$ if $\Lambda \subset (-\infty, 0)$. Since on $\mathbb{R}_+$ the function f is one-to-one,

$$\chi_\Lambda(A) = \chi_{f^{-1}(\Lambda)}(T), \qquad \Lambda \in \mathcal{A},$$

so that $\chi_\Lambda(A) = \chi_\Lambda(S)$, $\forall \Lambda \in \mathcal{A}$. By the uniqueness of the resolution of the identity, $S = A$. □

Remark 9.3.2. In case $n = 2$ in Proposition 9.3.1 one gets the (positive) square root operator of T, also denoted by $\sqrt{T}$. If A is closed and densely defined, by Proposition 4.3.9, A^*A is self-adjoint and positive, and the *absolute value of* A, denoted by $|A|$, is defined by $|A| := \sqrt{A^*A}$.

Remark 9.3.3. If $T \geq 0$ is compact, by uniqueness the square root $T^{1/2}$ coincides with the operator described in Corollary 8.1.5 and it is also compact.

Exercise 9.3.4. If $T \geq 0$ is invertible and self-adjoint, show that $T^{\frac{1}{n}}$ is also invertible.

Proposition 9.3.5. *If* $T \geq 0$ *is self-adjoint, then* $\operatorname{dom} T \sqsubseteq \operatorname{dom} T^{\frac{1}{2}}$*, with the latter equipped with both the graph norm* $\|\cdot\|_{T^{1/2}}$ *and the norm of* $\mathcal{H}$*, and so* $\operatorname{dom} T$ *is a core of* $T^{1/2}$*. See also Example* 4.4.1.

Proof. Since $\operatorname{dom} T \subset \operatorname{dom} T^{\frac{1}{2}}$ and both are densely defined in $\mathcal{H}$, it is clear that $\operatorname{dom} T \sqsubseteq \operatorname{dom} T^{\frac{1}{2}}$ with the norm of $\mathcal{H}$. The other statement is a direct consequence of Proposition 4.3.11, since $T^{\frac{1}{2}}$ is self-adjoint and $T = \left(T^{\frac{1}{2}}\right)^2$. □

In the study of sesquilinear forms in Chapter 4, it was considered that $b^T(\xi, \eta) = \langle \xi, T\eta \rangle$ for a self-adjoint operator $T \geq 0$, $\xi, \eta \in \operatorname{dom} T$, and (see Examples 4.1.11 and 4.2.4)

$$\langle \xi, \eta \rangle_+ = \langle \xi, T\eta \rangle + \langle \xi, \eta \rangle,$$

as well as its completion $(\mathcal{H}^T_+, b^T_+)$. Note that

$$\langle \xi, \eta \rangle_+ = \left\langle T^{\frac{1}{2}}\xi, T^{\frac{1}{2}}\eta \right\rangle + \langle \xi, \eta \rangle = \langle \xi, \eta \rangle_{T^{\frac{1}{2}}}, \qquad \xi, \eta \in \operatorname{dom} T,$$

and since $T^{\frac{1}{2}}$ is self-adjoint (so closed), $\operatorname{dom} T \subset \operatorname{dom} T^{\frac{1}{2}}$ and $\operatorname{dom} T$ is dense in $\operatorname{dom} T^{\frac{1}{2}}$ with the graph norm $\|\cdot\|_{T^{\frac{1}{2}}}$ (Proposition 9.3.5), one concludes that $\|\xi\|_+ = \langle \xi, \eta \rangle_+^{\frac{1}{2}}$ coincides with the graph norm of $T^{\frac{1}{2}}$ restricted to $\operatorname{dom} T$, whose completion is then

$$\mathcal{H}^T_+ = \operatorname{dom} T^{\frac{1}{2}}, \qquad b^T_+(\cdot, \cdot) = \langle \cdot, \cdot \rangle_{T^{\frac{1}{2}}},$$

and so $(\mathcal{H}_+^T, b_+^T)$ has been uncovered. Hence, for positive self-adjoint operators T it is natural to consider the form generated by T, i.e., b^T (see Definition 4.1.12), extended from dom T to

$$b^T(\xi,\eta) = \left\langle T^{\frac{1}{2}}\xi, T^{\frac{1}{2}}\eta \right\rangle, \qquad \xi,\eta \in \mathrm{dom}\ T^{\frac{1}{2}}.$$

The same notation b^T was kept and this extension is also called "the form generated by T."

Conversely:

Proposition 9.3.6. *Let b be a positive closed hermitian form and $T_b \geq 0$ the self-adjoint operator associated with b (Definition 4.2.5). Then,* dom b = dom $T_b^{1/2}$ *and $b(\xi,\eta) = \langle T_b^{1/2}\xi, T_b^{1/2}\eta\rangle$, $\forall \xi,\eta \in$ dom b.*

Proof. Given b and so T_b, define the hermitian form

$$\mathrm{dom}\ b_0 = \mathrm{dom}\ T_b^{1/2}, \quad b_0(\xi,\eta) := \left\langle T_b^{1/2}\xi, T_b^{1/2}\eta \right\rangle,$$

which is closed and positive, since $T_b^{1/2}$ is closed. By Theorem 4.2.6, dom T_b is a core of b, and since dom T_b is a core of $T^{\frac{1}{2}}$ (Proposition 9.3.5), it follows that it is also a core of b_0.

To finish the proof, it is enough to note that

$$b(\xi,\eta) = \langle \xi, T_b\eta\rangle = \left\langle T_b^{1/2}\xi, T_b^{1/2}\eta \right\rangle = b_0(\xi,\eta), \qquad \forall \xi,\eta \in \mathrm{dom}\ T_b,$$

that is, b and b_0 are closed and coincide on a common core; thus $b = b_0$. □

In summary:

Theorem 9.3.7. *There is a one-to-one correspondence between the set of positive closed hermitian forms b and the set of positive self-adjoint operators T, in the following sense:*

- *Given $b \geq 0$, it corresponds to $T = T_b$, i.e., the operator associated with b, so that* dom b = dom $T_b^{1/2}$ *and $b(\xi,\eta) = \langle T_b^{1/2}\xi, T_b^{1/2}\eta\rangle$.*
- *Given $T \geq 0$, it corresponds to $b = b^T$, i.e., the form generated by T, so that* dom b^T = dom $T^{1/2}$ *and $b^T(\xi,\eta) = \langle T^{1/2}\xi, T^{1/2}\eta\rangle$.*

This discussion adapts also to Theorem 4.2.6 and its lower-bounded operator T_b; it also reveals why the form b is asked to be lower bounded, for if $T - \beta\mathbf{1} \geq 0$ then $(T-\beta\mathbf{1})^1/2 \geq 0$ is well defined and the above discussion applies.

Remark 9.3.8. If $T \geq 0$ is self-adjoint, then dom b^T = dom $T^{\frac{1}{2}}$. By Remark 4.3.12, dom b^T = dom T iff T is bounded. In other words, if T is unbounded, then dom T is a proper subset of its form domain dom b^T.

Example 9.3.9. This is Example 4.2.11 revisited. Let dom $H_0 = \mathcal{H}^2(\mathbb{R})$, $H_0\psi = -\psi''$ and dom $P = \mathcal{H}^1(\mathbb{R})$, $P\psi = -i\psi'$ be the free hamiltonian and momentum operators on $\mathbb{R}$. By using Fourier transform one has $\|H_0^{1/2}\psi\| = \|P\psi\|$ for any $\psi \in \mathrm{dom}\ b^{H_0} = \mathrm{dom}\ H_0^{1/2}$; since the converse also holds, and $P^2 = H_0$, dom $P = \mathcal{H}^1(\mathbb{R})$, $P\psi = -i\psi'$ (by Proposition 4.3.9, $P^2 \subset H_0$, but since both are self-adjoint the equality follows), the form domain of H_0 is dom $b^{H_0} = \mathcal{H}^1(\mathbb{R})$ and

$$b^{H_0}(\psi, \varphi) = \langle \psi', \varphi' \rangle, \qquad \forall \psi, \varphi \in \mathrm{dom}\ b^{H_0}.$$

Note that functions in the form domain of the kinetic energy operator H_0 on $\mathbb{R}$ are continuous. Similarly, in $\mathbb{R}^n$ one has dom $b^{H_0} = \mathcal{H}^1(\mathbb{R}^n)$ and $b^{H_0}(\psi, \varphi) = \langle \nabla\psi, \nabla\varphi \rangle$.

As another application of the fact that the form domain of $T \geq 0$ is dom $T^{1/2}$, it will be shown that such a subspace is invariant under the unitary evolution group generated by T.

Proposition 9.3.10. *Let $T \geq 0$ be self-adjoint and $\mathcal{H}_+^T$ the form domain of T. Then $e^{-itT}\mathcal{H}_+^T \subset \mathcal{H}_+^T$ for all $t \in \mathbb{R}$.*

Proof. Recall that e^{-itT} is unitary and $\xi \in \mathcal{H}_+^T$ iff $\|T^{1/2}\xi\| < \infty$. Since dom $e^{-itT} = \mathcal{H}$, for every $\xi \in \mathcal{H}_+^T$ Lemma 8.2.19b) implies that

$$\infty > \|T^{1/2}\xi\| = \|e^{-itT}T^{1/2}\xi\| = \|T^{1/2}e^{-itT}\xi\|;$$

hence $e^{-itT}\xi \in \mathcal{H}_+^T$, $\forall t$. □

As mentioned before, for positive hermitian sesquilinear forms b, it is sometimes convenient to assume that $b(\xi) = +\infty$ if $\xi \notin \mathrm{dom}\ b$; see, for instance, Theorem 9.3.11. Recall that a function $f : \mathcal{N} \to \mathbb{R} \cup \{\infty\}$, defined on a normed space $\mathcal{N}$, is lower semicontinuous if for each $t \in \mathbb{R}$ the set $\{\xi : f(\xi) > t\}$ is open, which is equivalent to $f(\xi) \leq \liminf_{\eta \to \xi} f(\eta)$, $\forall \xi \in \mathcal{N}$. An important consequence of the definition is that the supremum of a collection of lower semicontinuous functions is also lower semicontinuous; clearly, every continuous function is lower semicontinuous. The next result was adapted from [Dav95].

Theorem 9.3.11. *If b is a hermitian positive sesquilinear form with* dom $b \sqsubseteq \mathcal{H}$, *then the following assertions are equivalent:*

i) *b is closed.*
ii) *b is the sesquilinear form generated by a positive self-adjoint operator T, that is, $b(\xi, \eta) = \langle T^{1/2}\xi, T^{1/2}\eta \rangle$, $\xi, \eta \in$* dom b = dom $T^{1/2}$.
iii) *$\mathcal{H} \ni \xi \mapsto b(\xi)$ is a lower semicontinuous function (recall that $b(\xi) = +\infty$ if $\xi \notin$* dom b).

Proof. i) ⇒ ii) follows by Theorem 4.2.6 and the above discussion.

ii) ⇒ iii) Since $-n \in \rho(T)$, $n \in \mathbb{N}$, by the spectral theorem and dominated convergence one has, for $n \to \infty$,

$$\langle nTR_{-n}(T)\xi, \xi\rangle = \int_{[0,\infty)} \frac{nx}{x+n}\, d\mu_\xi^T(x) \longrightarrow \int_{[0,\infty)} x\, d\mu_\xi^T(x)$$
$$= \|T^{\frac{1}{2}}\xi\|^2 = b(\xi,\xi), \qquad \forall \xi \in \mathrm{dom}\ b,$$

so $b(\xi)$ is the limit of a monotonically increasing sequence of continuous functions (since $TR_{-n}(T) \in \mathrm{B}(\mathcal{H})$) and hence b is lower semicontinuous.

iii) ⇒ i) If (ξ_n) in dom b is a Cauchy sequence with respect to the inner product $\langle \xi, \eta\rangle_+ = b(\xi,\eta) + \langle \xi, \eta\rangle$, given $\varepsilon > 0$ there exists N so that

$$\|\xi_n - \xi_m\|_+^2 = b(\xi_n - \xi_m) + \|\xi_n - \xi_m\|^2 < \varepsilon^2, \qquad \forall m, n \geq N.$$

Thus it is also a Cauchy sequence in $\mathcal{H}$ and so $\xi_n \to \xi$ in $\mathcal{H}$. Since b is lower semicontinuous, it follows that $b(\xi_n - \xi) \leq \liminf_{m\to\infty} b(\xi_n - \xi_m)$ (accepting the possible value $+\infty$) and the above inequality implies

$$b(\xi_n - \xi) + \|\xi_n - \xi\|^2 \leq \varepsilon^2, \qquad n \geq N,$$

which shows that $(\xi - \xi_n) \in \mathrm{dom}\ b$, $\xi = [(\xi - \xi_n) + \xi_n] \in \mathrm{dom}\ b$ and $\lim_{n\to\infty} b(\xi_n - \xi) = 0$. Therefore b is closed by Lemma 4.1.9. □

Corollary 9.3.12. *Let $(T_j)_{j=1}^N$, $N < \infty$, be positive self-adjoint operators so that*

$$\mathcal{D} := \bigcap_{j=1}^N \mathrm{dom}\ T_j^{\frac{1}{2}}$$

is dense in $\mathcal{H}$. Then there is a unique positive and self-adjoint operator T so that dom $T \sqsubseteq$ dom $T^{\frac{1}{2}} = \mathcal{D}$ *and*

$$b^T(\xi,\eta) = \left\langle T^{\frac{1}{2}}\xi, T^{\frac{1}{2}}\eta \right\rangle := \sum_{j=1}^N \left\langle T_j^{\frac{1}{2}}\xi, T_j^{\frac{1}{2}}\eta \right\rangle, \qquad \forall \xi, \eta \in \mathcal{D}.$$

Proof. A finite sum of lower semicontinuous functions is lower semicontinuous, so the sum on the right-hand side defines a (densely defined) positive closed sesquilinear form (assume $\langle T_j^{\frac{1}{2}}\xi, T_j^{\frac{1}{2}}\xi\rangle = \infty$ in case $\xi \notin \mathrm{dom}\ T_j^{\frac{1}{2}}$). The result then follows by Theorem 9.3.11. □

Remark 9.3.13. (a) The operator T constructed in Corollary 9.3.12 is the *form sum of T_j's* and denoted by

$$T = T_1 \dot{+} T_2 \dot{+} \cdots \dot{+} T_N;$$

see also page 106. It can happen that $\cap_j \text{dom}\, T_j = \{0\}$, consequently the form sum can become useful in order to define "generalized sum of operators;" see Subsection 9.3.1 for the domain of $T_1 \dot{+} T_2$ in some situations.

(b) Sometimes it is possible to adapt this result for $N = \infty$ even though $\overline{\mathcal{D}}$ is a proper subspace of $\mathcal{H}$, as discussed in Subsection 10.4.1.

Exercise 9.3.14. Let $T = T_1 \dot{+} T_2$. Show that $\text{dom}\, T_1 \cap \text{dom}\, T_2 \subset \text{dom}\, T$, and if $\xi \in \text{dom}\, T_1 \cap \text{dom}\, T_2$, then $T\xi = T_1\xi \dot{+} T_2\xi$.

Example 9.3.15. Let $\mathcal{H} = \mathrm{L}^2(\mathbb{R}^n)$ and $0 \le V \in \mathrm{L}^1_{\text{loc}}(\mathbb{R}^n)$. Then $C_0^\infty(\mathbb{R}^n) \subset \text{dom}\, H_0^{1/2} \cap \text{dom}\, V^{1/2}$ and this intersection is dense in $\mathcal{H}$. By Corollary 9.3.12 the operator $H_f = H_0 \dot{+} V$ is self-adjoint and positive. See details in Subsection 9.3.1.

9.3.1 Domain of Form Sum of Operators

In this subsection Kato's inequality will be used to find the domain of some form sum of standard Schrödinger operators in $\mathrm{L}^2(\mathbb{R}^n)$. Let $V \in \mathrm{L}^1_{\text{loc}}(\mathbb{R}^n)$ be a positive potential (the argument can be adapted to lower bounded potentials). The goal is to give a meaning to the expression "$H_0 + V$" and to determine its domain, even though $V\phi$ is not necessarily in $\mathrm{L}^2(\mathbb{R}^n)$ for $\phi \in C_0^\infty(\mathbb{R}^n)$; below, this is the main technical point to be dealt with.

Since both H_0 and V are positive self-adjoint operators, one can construct the self-adjoint realization $H_f := -\Delta \dot{+} V$, given by the form sum in Corollary 9.3.12, whose domain

$$\text{dom}\, H_f \subset \mathcal{D} = \text{dom}\, H_0^{\frac{1}{2}} \cap \text{dom}\, V^{\frac{1}{2}}.$$

According to Corollary 9.3.12, the sesquilinear form b^{H_f} generated by H_f is

$$b^{H_f}(\psi, \phi) = \langle \nabla\psi, \nabla\phi \rangle + \langle V^{\frac{1}{2}}\psi, V^{\frac{1}{2}}\phi \rangle, \qquad \forall \psi, \phi \in \mathcal{D},$$

and note that for $\psi \in \text{dom}\, H_f$ one has $V^{1/2}\psi \in \mathrm{L}^2(\mathbb{R}^n)$ and, since $V^{1/2} \in \mathrm{L}^2_{\text{loc}}(\mathbb{R}^n)$, it follows that $V\psi = V^{1/2}\left(V^{1/2}\psi\right) \in \mathrm{L}^1_{\text{loc}}(\mathbb{R}^n)$.

For $\psi \in \text{dom}\, H_f$ and $\phi \in C_0^\infty(\mathbb{R}^n)$, by writing out the inner products as integrals,

$$\begin{aligned} b^{H_f}(\psi, \phi) &= \langle \psi, -\Delta\phi \rangle + \langle V^{\frac{1}{2}}\psi, V^{\frac{1}{2}}\phi \rangle \\ &= \int_{\mathbb{R}^n} \overline{\psi(x)}(-\Delta + V)\phi(x)\, dx. \end{aligned}$$

Since $b^{H_f}(\psi, \phi) = \langle H_f\psi, \phi \rangle$, for all $\psi \in \text{dom}\, H_f$ and all $\phi \in C_0^\infty(\mathbb{R}^n)$,

$$\int_{\mathbb{R}} \overline{H_f\psi(x)}\, \phi(x)\, dx = \int_{\mathbb{R}^n} \overline{\psi(x)}\, (-\Delta + V)\phi(x)\, dx,$$

and so $H_f\psi = (-\Delta + V)\psi$ in the sense of distributions.

Theorem 9.3.16. *Let* $0 \le V \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$ *and* H_f *be as above. Then* $\mathrm{dom}\, H_f = D_f$, *with*

$$D_f = \left\{\psi \in \mathrm{L}^2(\mathbb{R}^n) : (V\psi) \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n), (-\Delta + V)\psi \in \mathrm{L}^2(\mathbb{R}^n)\right\},$$

and the $(-\Delta + V)\psi$ *in the sense of distributions.*

Proof. The above discussion showed that $\mathrm{dom}\, H_f \subset D_f$. Now, let h be the operator $\mathrm{dom}\, h = D_f$, $h\psi = (-\Delta\psi + V)\psi$, $\psi \in D_f$, so that $H_f \subset h$. Since $H_f \ge 0$, one has $-1 \in \rho(H_f)$ and so $\mathrm{rng}\,(H_f + \mathbf{1}) = \mathrm{L}^2(\mathbb{R}^n)$. Thus, given $\zeta \in D_f$, there exists $\psi \in \mathrm{dom}\, H_f$ with

$$(h + \mathbf{1})\zeta = (H_f + \mathbf{1})\psi = (h + \mathbf{1})\psi,$$

and so $(h + \mathbf{1})(\zeta - \psi) = 0$. By denoting $u = \zeta - \psi$, one finds

$$-\Delta u = hu - Vu = -(u + Vu) \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n).$$

Hence it is possible to apply Kato's inequality, Theorem 6.3.3, to get

$$\Delta|u| \ge \mathrm{Re}\ (\mathrm{sgn}\, u)\Delta u = \mathrm{Re}\ [(\mathrm{sgn}\, u)(u + Vu)] = (V + \mathbf{1})|u| \ge 0.$$

The same arguments used at the end of the proof of Corollary 6.3.5 imply that $u = 0$, consequently $\psi = \zeta$ and $\zeta \in \mathrm{dom}\, H_f$. Therefore, $D_f \subset \mathrm{dom}\, H_f$ and the theorem is proved. □

Corollary 9.3.17. *Let* V *be a positive potential with* $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$, *and consider the initial operator*

$$\mathrm{dom}\, H = C_0^\infty(\mathbb{R}^n), \qquad H\psi = -\Delta\psi + V\psi.$$

Then H *is essentially self-adjoint and its unique self-adjoint extension is given by* (*as before, with distributional operation*)

$$\mathrm{dom}\, \overline{H} = \left\{\psi \in \mathrm{L}^2(\mathbb{R}^n) : (-\Delta + V)\psi \in \mathrm{L}^2(\mathbb{R}^n)\right\},$$
$$\overline{H}\psi = (-\Delta + V)\psi, \qquad \psi \in \mathrm{dom}\, \overline{H}.$$

Proof. Apply some known facts: $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ implies the operator sum H is defined on $C_0^\infty(\mathbb{R}^n)$, it is essentially self-adjoint (Corollary 6.3.5) and its unique self-adjoint extension is its closure $\overline{H}$; since $\mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n) \subset \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$ (check this!), this extension coincides with the form sum extension H_f given by Theorem 9.3.16; since in this case $(V\psi) \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$ for all $\psi \in \mathrm{L}^2(\mathbb{R}^n)$, this condition may be omitted in $\mathcal{D}_f$ and the form extension H_f is exactly the operator in the statement of the corollary. □

Remark 9.3.18. If the potential $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ (not necessarily bounded from below), then it is possible to show that (see Chapter VII of [EdE87]) the adjoint of the standard energy operator $\mathrm{dom}\, H = C_0^\infty(\mathbb{R}^n)$, $H\psi = H_0\psi + V\psi$, has the same action as H but with $\mathrm{dom}\, H^* = \{\psi \in \mathrm{L}^2(\mathbb{R}^n) : V\psi \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n),\ (H_0\psi + V\psi) \in \mathrm{L}^2(\mathbb{R}^n)\}$. In case V is bounded from below, according to Corollary 9.3.17, the adjoint H^* is the only self-adjoint extension of H.

9.4 Polar Decomposition

This is the analogue, for closed operators, of the well-known decomposition $z = e^{i\theta}|z|$ for complex numbers. In order to motivate what follows, let T be a closed operator; then $|z| = (\bar{z}z)^{1/2}$ should correspond to $|T| = (T^*T)^{1/2}$ and $e^{i\theta} = z/|z|$ to $W = T(T^*T)^{-1/2}$. Although $|T|$ is actually well defined, one still has to understand W. In any event, the formal computation

$$\begin{aligned}\|W\xi\|^2 &= \left\langle T(T^*T)^{-1/2}\xi, T(T^*T)^{-1/2}\xi\right\rangle \\ &= \left\langle \xi, (T^*T)^{-1/2}T^*T(T^*T)^{-1/2}\xi\right\rangle = \|\xi\|^2\end{aligned}$$

suggests that W is an isometry.

Definition 9.4.1. A bounded linear operator $W : \mathcal{H}_1 \to \mathcal{H}_2$ is a *partial isometry* if it is an isometry on the orthogonal complement of its kernel $\mathrm{N}(W)$. The space $\mathrm{N}(W)^\perp$ is called the *initial space* of the partial isometry W.

Exercise 9.4.2. Show that if $W : \mathcal{H}_1 \to \mathcal{H}_2$ is a partial isometry then W^*W is the projection onto $\mathrm{rng}\, W^*W$. Give conditions on W so that it is a unitary operator.

Proposition 9.4.3. *Let $T : \mathrm{dom}\, T \sqsubseteq \mathcal{H} \to \mathcal{H}$ be a closed operator. Then T has a unique decomposition in the form $T = W\,S$, with S a positive self-adjoint operator (in fact $S = |T|$) and $W \in \mathrm{B}(\mathcal{H})$ a partial isometry with initial space $\overline{\mathrm{rng}\, S}$ and range $\overline{\mathrm{rng}\, T}$ (and $W\xi = 0$ if $\xi \in (\overline{\mathrm{rng}\, S})^\perp$).*

Proof. Since T is closed, by Proposition 4.3.9 the operator $T^*T \geq 0$ is self-adjoint and so $|T| = \sqrt{T^*T}$ is well defined.

Uniqueness: If $T = WS$, then the partial isometry W is uniquely determined by $WS\xi = T\xi$, $\xi \in \mathrm{dom}\, T$. If $\xi, \eta \in \overline{\mathrm{rng}\, S}$, since W is a partial isometry,

$$\langle \xi, \eta\rangle = \langle W\xi, W\eta\rangle = \langle \xi, W^*W\eta\rangle,$$

or $\langle \xi, (\mathbf{1} - W^*W)\eta\rangle = 0$, $\forall \xi \in \overline{\mathrm{rng}\, S}$, and so $(\mathbf{1} - W^*W)\eta \in (\overline{\mathrm{rng}\, S})^\perp$. On the other hand, $\mathrm{rng}\, W^* \subset \overline{\mathrm{rng}\, S}$ (check this!) and it follows that

$$(\mathbf{1} - W^*W)\eta \in (\overline{\mathrm{rng}\, S})^\perp \cap \overline{\mathrm{rng}\, S} = \{0\};$$

thus $W^*W\eta = \eta$ and W^*W is the orthogonal projection onto $\overline{\mathrm{rng}\, S}$.

Now $T^*T = S^*W^*WS = S^2$ (because S is self-adjoint and W^*W is the orthogonal projection onto $\overline{\mathrm{rng}\, S}$) and, since $S \geq 0$, $S = |T|$ by Proposition 9.3.1. The uniqueness follows.

Existence: Note first that $|T|^2 = |T|\,|T| = T^*T$. If $\xi \in \mathrm{dom}\, |T|^2 = \mathrm{dom}\,(T^*T)$, then

$$\||T|\xi\|^2 = \langle |T|\xi, |T|\xi\rangle = \langle |T|^2\xi, \xi\rangle = \langle T^*T\xi, \xi\rangle = \|T\xi\|^2.$$

By Proposition 4.3.9, the graph norms $\|\cdot\|_T$ and $\|\cdot\|_{|T|}$ coincide in $\mathrm{dom}\,(T^*T)$, which is a core of both $|T|$ and T (Proposition 4.3.11). Hence $\mathrm{dom}\,|T| = \mathrm{dom}\, T$ and $\||T|\xi\| = \|T\xi\|$, $\forall \xi \in \mathrm{dom}\, T$.

Thus, the map $W' : \text{rng } |T| \to \text{rng } T$ defined by

$$W'(|T|\xi) := T\xi$$

is an isometry that has a unique isometric extension $W'' : \overline{\text{rng } |T|} \to \overline{\text{rng } T}$. Define

$$W(\xi + \eta) := W''\xi, \qquad \xi \in \overline{\text{rng } |T|},\ \eta \in \left(\overline{\text{rng } |T|}\right)^{\perp},$$

so that $W|T| = T$ with W a partial isometry. □

Definition 9.4.4. If T is closed then $T = W|T|$, as in Proposition 9.4.3, is called the *polar decomposition* of T.

Example 9.4.5. Let $T : \mathcal{H} \to \mathcal{H}$ be the operator of rank 1,

$$T\xi = \langle \eta, \xi \rangle \zeta, \qquad \|\eta\| = \|\zeta\| = 1.$$

Then $T^*\xi = \langle \zeta, \xi \rangle \eta$ and $(T^*T)(\xi) = \langle \eta, \xi \rangle \eta$. In this case $|T|\xi = \langle \eta, \xi \rangle \eta$, since it is self-adjoint, $\langle \xi, |T|\xi \rangle = |\langle \eta, \xi \rangle|^2 \geq 0$ and $|T|^2 = T^*T$. Since $\text{rng } |T| = \text{Lin}(\{\eta\})$ and $\text{rng } T = \text{Lin}(\{\zeta\})$, the polar decomposition of T is

$$T = W|T|,$$

with $W : \text{Lin}(\{\eta\}) \to \text{Lin}(\{\zeta\})$, $W(a\eta) = a\zeta$, $a \in \mathbb{C}$. Remember $W\xi = 0$ if $\xi \in \text{Lin}(\{\zeta\})^{\perp}$.

Exercise 9.4.6. Discuss the alterations in Example 9.4.5 if ζ and η are not normalized.

Exercise 9.4.7. Let $S_r : l^2(\mathbb{Z}) \hookleftarrow$ be the right shift operator in Example 1.1.12. Find $|S_r|$ and its polar decomposition. What does happen for $S_r : l^2(\mathbb{N}) \hookleftarrow$?

Remark 9.4.8. The reader should be aware that, even for 2×2 real matrices T, S, it is possible that $|T + S| \leq |T| + |S|$ does not hold! Try to find an example.

9.4.1 Trace-Class Operators

The polar decomposition allows one to introduce some subspaces of compact operators $\mathrm{B}_0(\mathcal{H})$. If T is a compact operator, then $|T|$ is compact and self-adjoint; the nonzero eigenvalues $0 < \varpi_j = \varpi_j(T)$ of $|T|$ are called the *singular numbers* of $T = W|T|$ (this is the polar decomposition of T). By the spectral theorem for compact self-adjoint operators, if ζ_j are the corresponding eigenvectors, i.e., $|T|\zeta_j = \varpi_j \zeta_j$, $\forall j$, one has

$$|T|\xi = \sum_j \varpi_j \langle \zeta_j, \xi \rangle \zeta_j,$$

and so

$$T\xi = W|T|\xi = \sum_j \varpi_j \langle \zeta_j, \xi \rangle \xi_j, \qquad \xi_j = W\zeta_j.$$

This expression is called the *canonical form of* T.

Definition 9.4.9. The trace of the positive operator $Q \in \mathrm{B}(\mathcal{H})$ is

$$\operatorname{tr} Q := \sum_j \langle e_j, Q e_j \rangle = \sum_j \|Q^{1/2} \xi_j\|^2,$$

where $\{e_j\}_j$ is an orthonormal basis of $\mathcal{H}$. An operator $B \in \mathrm{B}(\mathcal{H})$ is *trace class* if $\operatorname{tr}|B| < \infty$.

By Proposition 1.4.2 the above trace of positive operators is well defined since $\operatorname{tr} Q = \|Q^{1/2}\|_{\mathrm{HS}}$ and the Hilbert-Schmidt norm is independent of the chosen orthonormal basis.

Proposition 9.4.10. *If an operator B is trace class, then it is compact, Hilbert-Schmidt and*

$$\operatorname{tr}|B| = \sum_j \varpi_j(B).$$

Further, $|B|^{1/2}$ is also Hilbert-Schmidt.

Proof. Since B is trace class it is immediate that $|B|^{1/2}$ is Hilbert-Schmidt, so compact. Thus, $|B| = |B|^{1/2}|B|^{1/2}$ is compact by Proposition 1.3.7ii). Let $(\xi_j)_j$ be the set of normalized eigenvectors of $|B|$; then

$$\operatorname{tr}|B| = \sum_j \langle \xi_j, |B| \xi_j \rangle = \sum_j \varpi_j(B).$$

On the other hand,

$$\begin{aligned} \|B\|_{\mathrm{HS}}^2 &= \sum_j \|B\xi_j\|^2 = \sum_j \|\,|B|\,\xi_j\|^2 \\ &= \sum_j \varpi_j(B)^2. \end{aligned}$$

Therefore, since $\operatorname{tr}|B| < \infty$ one has $\varpi_j < 1$ for large j, so $\varpi_j^2 < \varpi_j$ and the convergence of the sum $\|B\|_{\mathrm{HS}}^2 < \infty$ follows. □

Proposition 9.4.11. *$B \in \mathrm{B}(\mathcal{H})$ is trace class iff it is a product of two Hilbert-Schmidt operators.*

Proof. If B is trace class, then $|B|^{1/2}$ and $W|B|^{1/2}$ are Hilbert-Schmidt and $B = W|B|^{1/2}|B|^{1/2}$ is the product of two elements of $\mathrm{HS}(\mathcal{H})$.

Now, if $B_1, B_2 \in \mathrm{HS}(\mathcal{H})$, use polar decomposition to write $B_1 B_2 = W|B_1 B_2|$ and note that $B_1^* W \in \mathrm{HS}(\mathcal{H})$ (Proposition 1.3.7). Pick an orthonormal basis $(e_j)_j$ of $\mathcal{H}$ and make use of Cauchy-Schwarz inequality and then of Hölder inequality to get

$$\begin{aligned}
\operatorname{tr}|B_1B_2| &= \sum_j \langle e_j, |B_1B_2|e_j\rangle = \sum_j \langle e_j, W^*B_1B_2e_j\rangle \\
&= \sum_j |\langle B_1^*We_j, B_2e_j\rangle| \le \sum_j (\|B^*We_j\|\,\|B_2e_j\|) \\
&\le \left(\sum_j \|B_1^*We_j\|^2 \sum_n \|B_2e_n\|^2\right)^{\frac{1}{2}} \\
&= \|B_1^*W\|_{\mathrm{HS}}\,\|B_2\|_{\mathrm{HS}} < \infty.
\end{aligned}$$

Hence B_1B_2 is trace class. □

Exercise 9.4.12. If B is trace class, define its trace by $\operatorname{tr} B = \sum_j \langle e_j, Be_j\rangle$ and show that this series is absolutely convergent and independent of the orthonormal basis $(e_j)_j$ (hint: write $B = B_1^*B_2$, $B_1, B_2 \in \mathrm{HS}(\mathcal{H})$, and argue as for HS operators).

Exercise 9.4.13. Let B be a trace-class operator. Show that $\operatorname{tr}(BU) = \operatorname{tr}(UB)$ for any unitary operator U and use Proposition 9.5.12 to conclude that $\operatorname{tr}(BT) = \operatorname{tr}(TB)$ for any $T \in \mathrm{B}(\mathcal{H})$ (use $\operatorname{tr}(A+B) = \operatorname{tr} A + \operatorname{tr} B$).

Exercise 9.4.14. Check that any finite rank operator is trace class. Find those projections P that has $\operatorname{tr} P = 1$.

Remark 9.4.15. In statistical mechanics (and in other settings as well) one usually does not know exactly what is the state of a system. This lack of information about the system is taken into account by means of a *density matrix*, which is a positive trace-class operator ρ on $\mathcal{H}$ with $\operatorname{tr}\rho = 1$. In this case its singular values coincide with its eigenvalues p_j and $\sum_j p_j = 1$. A density matrix is used to describe mixed states and, given a bounded self-adjoint operator T, the average measured value of T over many realizations of the system is assumed to be $\operatorname{tr}(\rho T)$. For instance, if $(\xi_j)_j$ is an orthonormal basis of $\mathcal{H}$, P_{ξ_j} the projection onto $\mathrm{Lin}(\{\xi_j\})$, and the system is supposed to be prepared in ξ_j with probability p_j, $\sum_j p_j = 1$, then on physical grounds the average expectation value of T is

$$\sum_j p_j\, \mathcal{E}^T_{\xi_j} = \sum_j p_j\, \langle \xi_j, T\xi_j\rangle\,,$$

and in this situation an effective description is given in terms of the density matrix $\rho = \sum_j p_j P_{\xi_j}$, since $\rho\xi_j = p_j\xi_j$, $\forall j$, and

$$\operatorname{tr}(\rho T) = \sum_j \langle \rho\xi_j, T\xi_j\rangle = \sum_j p_j \mathcal{E}^T_{\xi_j}.$$

For other results related to trace-class operators, generalizations and applications see [Scha60] and [Sim05].

9.5 Miscellanea

Throughout this section T is a self-adjoint operator acting in the Hilbert space $\mathcal{H}$. Some relations involving integrals of operator quantities and spectral measures will be presented. Lemmas 8.2.6 and 8.2.17 as well as the dominated convergence theorem will be often invoked. As customary, the use of the spectral theorem means the use of any related results presented in Chapter 8.

The following lemma will be employed ahead, sometimes implicitly, and its proof illustrates the usual arguments for passing from functions to operators.

Lemma 9.5.1. *Let $J \subset \mathbb{R}$ be an interval and $g : J \times \mathbb{R} \to \mathbb{C}$ be a (uniformly) bounded Borel function such that for each x the function $t \mapsto g(t,x)$ is integrable with respect to Lebesgue measure. If $G(x) := \int_J g(t,x)\,dt$, then*

$$G(T) = \int_J g(t,T)\,dt.$$

Proof. Since g is a bounded function, $g(t,T)$ is a bounded (normal) operator for any $t \in J$. For any $\xi, \eta \in \mathcal{H}$, by continuity of the inner product,

$$\begin{aligned}
\left\langle \xi, \int_J g(t,T)\,dt\,\eta \right\rangle &= \int_J \langle \xi, g(t,T)\,\eta\rangle \; dt \\
&= \int_J \int_{\sigma(T)} g(t,x)\,d\mu^T_{\xi,\eta}(x)\,dt \\
&\overset{\text{Fubini}}{=} \int_{\sigma(T)} \int_J g(t,x)\,dt\,d\mu^T_{\xi,\eta}(x) \\
&= \int_{\sigma(T)} G(x)\,\mu^T_{\xi,\eta}(x) = \langle \xi, G(T)\eta\rangle\,.
\end{aligned}$$

Hence, $G(T) = \int_J g(t,T)\,dt$. □

Resolvent and Distance to the Spectrum. For quite general operators S, that is, if both $\sigma(S)$ and $\rho(S)$ are nonempty, Corollary 1.5.15 provides a simple proof that

$$\|R_\lambda(S)\| \geq 1/d(\lambda, \sigma(S)), \qquad \forall \lambda \in \rho(S);$$

recall that $d(\lambda,\sigma(S)) := \inf_{\mu\in\sigma(S)} |\mu - \lambda|$. For self-adjoint operators T the spectral theorem can be used to prove a complement to this result, i.e., another proof of Corollary 2.4.5.

Proposition 9.5.2. *If T is self-adjoint, then*

$$\|R_\lambda(T)\| = 1/d(\lambda, \sigma(T))$$

for all $\lambda \in \rho(T)$.

Proof. Note that $R_\lambda(T)=r_\lambda(T)$, with $r_\lambda(x)=(x-\lambda)^{-1}$. For $\xi\in\mathcal{H}$ Lemma 8.2.17 implies

$$\begin{aligned}\|R_\lambda(T)\xi\|^2 &= \int_{\sigma(T)} |r_\lambda(x)|^2\, d\mu_\xi^T(x)\\ &\le \int_{\sigma(T)} \frac{1}{d(\lambda,\sigma(T))^2}\, d\mu_\xi^T(x) \le \frac{1}{d(\lambda,\sigma(T))^2}\|\xi\|^2.\end{aligned}$$

Hence,

$$\|R_\lambda(T)\| \le 1/d(\lambda,\sigma(T)),$$

and the result follows by combining with Corollary 1.5.15. □

Exercise 9.5.3. Let T be self-adjoint and $z\in\rho(T)$. Use the spectral theorem to recover the known results

$$\|R_z(T)\| \le \frac{1}{|\text{Im } z|},\ \text{Im } z\ne 0, \qquad \text{and} \qquad TR_z(T)\in \mathrm{B}(\mathcal{H}).$$

Find un upper bound of the norm of $TR_z(T)$.

Exercise 9.5.4. Let T be self-adjoint.

(a) Show that for any $\xi\in\text{dom } T$ one has $\|(T-\lambda\mathbf{1})\xi\|\ge d(\lambda,\sigma(T))\|\xi\|$, for all $\lambda\in\mathbb{C}$.

(b) Let $\varepsilon>0$. If for some $\mu\in\mathbb{C}$ there is a $0\ne\xi\in\text{dom } T$ with $\|(T-\mu\mathbf{1})\xi\|<\varepsilon\|\xi\|$, show that there is a $\lambda\in\sigma(T)$ so that $|\lambda-\mu|<\varepsilon$.

Spectral Projection onto a Single Point. For $t,t_0\in\mathbb{R}$, $\varepsilon>0$ let

$$u_{t_0+i\varepsilon}(t)=\frac{-i\varepsilon}{t-(t_0+i\varepsilon)}.$$

Since

$$\lim_{\varepsilon\to 0}\frac{-i\varepsilon}{t-(t_0+i\varepsilon)}=\chi_{\{t_0\}}(t),$$

then by the spectral theorem one obtains the relation

$$\text{s}-\lim_{\varepsilon\to 0} -i\varepsilon R_{t_0+i\varepsilon}(T)=\chi_{\{t_0\}}(T),$$

that is, the spectral projection of T at the point t_0. Indeed, note that $u_{t_0+i\varepsilon}(T)=-i\varepsilon R_{t_0+i\varepsilon}(T)$ and for any $\xi\in\mathcal{H}$,

$$\left\|-i\varepsilon R_{t_0+i\varepsilon}(T)\xi-\chi_{\{t_0\}}(T)\xi\right\|^2=\int_{\sigma(T)}\left|u_{t_0+i\varepsilon}(t)-\chi_{\{t_0\}}(t)\right|^2\, d\mu_\xi^T(t)$$

which vanishes as $\varepsilon\to 0$ by dominated convergence. The relation is proved. It is worth mentioning that, by Theorem 11.2.1, $\chi_{\{t_0\}}(T)$ is the orthogonal projection onto the eigenspace associated with t_0.

Boundary Values of the Borel Transform. The *Borel transform* of a finite (positive) measure μ on $\mathcal{A}$ is the map

$$F_\mu(z) := \int_{\mathbb{R}} \frac{d\mu(t)}{t-z}, \qquad z \in \mathbb{C} \setminus \mathbb{R}.$$

In the specific case of spectral measures μ_ξ^T, for $\varepsilon > 0$ and $t_0 \in \mathbb{R}$ one has

$$\begin{aligned} F_{\mu_\xi^T}(t_0 + i\varepsilon) = \langle \xi, R_{t_0+i\varepsilon}(T)\xi \rangle &= \int_{\mathbb{R}} \frac{d\mu_\xi^T(t)}{t-(t_0+i\varepsilon)} \\ &= \int_{\mathbb{R}} \frac{t-t_0}{(t-t_0)^2+\varepsilon^2}\, d\mu_\xi^T(t) + i\varepsilon \int_{\mathbb{R}} \frac{d\mu_\xi^T(t)}{(t-t_0)^2+\varepsilon^2}. \end{aligned}$$

Hence, by dominated convergence, the following boundary values are obtained:

$$\lim_{\varepsilon \to 0^+} \varepsilon \,\mathrm{Re}\, F_{\mu_\xi^T}(t_0 + i\varepsilon) = 0$$

and

$$\lim_{\varepsilon \to 0^+} \varepsilon \,\mathrm{Im}\, F_{\mu_\xi^T}(t_0 + i\varepsilon) = \mu_\xi^T(\{t_0\}).$$

Note that the relation $\|R_{t_0+i\varepsilon}(T)\| \le 1/|\varepsilon|$ shows that the resolvent $R_{t_0+i\varepsilon}(T)$ cannot have limits in $\mathrm{B}(\mathcal{H})$ as $\varepsilon \to 0$.

Stone Formula. For $-\infty < a < b < \infty$ and $\varepsilon > 0$, consider the function defined on $\mathbb{R}$

$$v_\varepsilon(x) = \frac{1}{2\pi i} \int_a^b \left(\frac{1}{x-(t+i\varepsilon)} - \frac{1}{x-(t-i\varepsilon)} \right) dt,$$

which is uniformly bounded as a function of ε and the following pointwise convergence holds

$$\lim_{\varepsilon \to 0^+} v_\varepsilon(x) = \begin{cases} 0 & \text{if } x \notin [a,b] \\ \frac{1}{2} & \text{if } x \in \{a,b\} \\ 1 & \text{if } x \in (a,b) \end{cases}.$$

By Lemma 9.5.1 one gets the *Stone formula*

$$\frac{1}{2}\left(\chi_{[a,b]}(T) + \chi_{(a,b)}(T)\right) = \mathrm{s-}\lim_{\varepsilon \to 0^+} \frac{1}{2\pi i} \int_a^b \left(R_{t+i\varepsilon}(T) - R_{t-i\varepsilon}(T)\right) dt.$$

Exercise 9.5.5. Show that

$$\chi_{(a,b)}(T) = \mathrm{s-}\lim_{\delta \to 0^+} \mathrm{s-}\lim_{\varepsilon \to 0^+} \frac{1}{2\pi i} \int_{a+\delta}^{b-\delta} \left(R_{t+i\varepsilon}(T) - R_{t-i\varepsilon}(T)\right) dt.$$

Mean Ergodic Theorem. This relation is due to von Neumann and known as the *mean ergodic theorem*. Since for $t_0, x \in \mathbb{R}$,

$$\lim_{M\to\infty} \frac{1}{M} \int_0^M e^{ist_0} e^{-isx}\, ds = \chi_{\{t_0\}}(x),$$

by the spectral theorem and Lemma 9.5.1,

$$\chi_{\{t_0\}}(T) = \mathrm{s} - \lim_{M\to\infty} \frac{1}{M} \int_0^M e^{ist_0} e^{-isT}\, ds.$$

This is a relation between the spectral projection of T at the point t_0 and the unitary evolution group e^{-isT} whose infinitesimal generator is T (by Theorem 11.2.1, $\chi_{\{t_0\}}(T)$ is the orthogonal projection onto the eigenspace associated with t_0).

Exercise 9.5.6. Verify that the average in the mean ergodic theorem can be taken as $\frac{1}{2M}\int_{-M}^{M}$.

Evolution Group and Resolvent. Again Fubini's Theorem and Lemma 9.5.1 will be invoked. Let $z \in \mathbb{C}$ with $\mathrm{Im}\, z > 0$. Since for $x \in \mathbb{R}$,

$$\frac{1}{x-z} = -i \int_0^\infty e^{isz} e^{-isx}\, ds,$$

then for all $\xi, \eta \in \mathcal{H}$ one has

$$\begin{aligned}
\langle \xi, R_z(T)\eta\rangle &= \int_{\sigma(T)} \frac{1}{x-z}\, d\mu^T_{\xi,\eta}(x) \\
&= \int_{\sigma(T)} \left(-i \int_0^\infty e^{isz} e^{-isx}\, ds \right) d\mu^T_{\xi,\eta}(x) \\
&\overset{\text{Fubini}}{=} -i \int_0^\infty e^{isz} \left(\int_{\sigma(T)} e^{-isx}\, d\mu^T_{\xi,\eta}(x) \right) ds \\
&= -i \int_0^\infty e^{isz} \langle \xi, e^{-isT}\eta\rangle\, ds = \left\langle \xi, \left(-i \int_0^\infty e^{isz} e^{-isT}\, ds \right) \eta \right\rangle,
\end{aligned}$$

and the following relation between the resolvent operator and the unitary evolution group is obtained,

$$R_z(T) = -i \int_0^\infty e^{isz} e^{-isT}\, ds.$$

Exercise 9.5.7. What changes in the above relation if $\mathrm{Im}\, z < 0$?

Exercise 9.5.8. Let $\xi \in \mathcal{H}$. Since the map

$$z \mapsto \langle \xi, R_z(T)\xi\rangle, \qquad z \in \mathbb{C} \setminus \mathbb{R},$$

is holomorphic, show that

$$R_z(T)^2 = \int_0^\infty s e^{isz} e^{-isT}\, ds, \qquad \mathrm{Im}\, z > 0.$$

Riesz Projections. Assume that Λ is a (nonempty) compact subset of $\sigma(T)$, and Γ a closed piecewise smooth Jordan curve in the complex plane $\mathbb{C}$ (positively oriented) whose intersection of its interior with $\sigma(T)$ is Λ, and also $\Gamma \cap \sigma(T) = \emptyset$. Hence Λ is separated by a gap from the remainder of the spectrum of T.

Proposition 9.5.9. *The following equality holds,*

$$\chi_\Lambda(T) = \frac{i}{2\pi} \oint_\Gamma R_z(T)\, dz.$$

The right-hand side is called the Riesz projection *onto* Λ.

Proof. Let (a,b) be the (bounded) open interval obtained by the intersection of the interior of Γ with the real axis (the proof is almost the same if more than one such interval is present); so $\Lambda \subset (a,b)$. For $\xi \in \mathcal{H}$ the spectral theorem and Fubini imply

$$\begin{aligned} Z := \left\langle \xi, \frac{1}{2\pi i} \oint_\Gamma R_z(T)\, dz\, \xi \right\rangle &= \frac{1}{2\pi i} \oint_\Gamma \langle \xi, R_z(T)\xi \rangle \, dz \\ &= \frac{1}{2\pi i} \oint_\Gamma \int_{\sigma(T)} \frac{1}{t-z}\, d\mu_\xi^T(t)\, dz \\ &= - \int_{\sigma(T)} \left[\frac{1}{2\pi i} \oint_\Gamma \frac{dz}{z-t} \right] d\mu_\xi^T(t). \end{aligned}$$

By the Cauchy integral formula, the term given in brackets equals 1 if $t \in (a,b)$ and zero if $t \in \mathbb{R} \setminus [a,b]$. Thus, the term in brackets is the characteristic function $\chi_{(a,b)}$. Hence

$$\begin{aligned} Z &= - \int_{\sigma(T)} \chi_{(a,b)}(t)\, d\mu_\xi^T(t) = -\langle \xi, \chi_{(a,b)}(T)\xi \rangle \\ &= -\langle \xi, \chi_\Lambda(T)\xi \rangle. \end{aligned}$$

An application of Lemma 1.1.44 implies the proposition. □

An especially interesting case is of an isolated (with respect to the spectrum) eigenvalue t_0 of T. Then, for $0 < r$ small enough, if $S(t_0; r)$ is the sphere, in the complex plane, of radius r and centered at t_0, the orthogonal projection onto the eigenspace associated with t_0 is

$$\chi_{\{t_0\}}(T) = \frac{i}{2\pi} \oint_{S(t_0;r)} R_z(T)\, dz;$$

see also Theorem 11.2.1 and Corollary 11.2.3. Note that if the eigenvalue t_0 is not isolated in the spectrum of T, it is not possible to construct $\chi_{\{t_0\}}(T)$ as a Riesz projection.

Exercise 9.5.10. Let Λ, Γ and T be as in Proposition 9.5.9, and $f : \mathbb{C} \to \mathbb{C}$ an entire function. Show the following characterization of the operator $\chi_\Lambda(T) f^{(n)}(T)$ ($f^{(n)}$ is the nth derivative of f)

$$\chi_\Lambda(T) f^{(n)}(T) = \frac{(-1)^{n+1} n!}{2\pi i} \oint_\Gamma f(z) R_z(T)^{n+1}\, dz,$$

for all $n \in \mathbb{N}$.

Perturbation of Bounded from Below Operators. Let B be a hermitian and T-bounded operator with $N_T(B) < 1$. Then, by the Kato-Rellich theorem, the operator $T + B$ with dom $(T + B) =$ dom T is self-adjoint.

Proposition 9.5.11. *Under the above conditions, if* $T \geq \beta \mathbf{1}$*, then there exists* $\gamma \in \mathbb{R}$ *so that* $T + B \geq \gamma \mathbf{1}$*. In particular if* $\sigma(T) \subset [\beta, \infty)$*, then* $\sigma(T + B) \subset [\gamma, \infty)$*.*

Proof. By hypotheses, T is self-adjoint and there exist $0 \leq a < 1$ and $b \geq 0$ obeying

$$\|B\xi\| \leq a\|T\xi\| + b\|\xi\|, \qquad \forall \xi \in \text{dom}\, T.$$

By Proposition 8.3.21, $\sigma(T) \subset [\beta, \infty)$. Let $\lambda < \beta$; for all $\xi \in \mathcal{H}$,

$$\|TR_\lambda(T)\xi\|^2 = \int_{[\beta,\infty)} \frac{t^2}{(t-\lambda)^2}\, d\mu_\xi^T(t) \leq \int_{[\beta,\infty)} d\mu_\xi^T(t) = \|\xi\|^2,$$

so that $\|TR_\lambda(T)\| \leq 1$ (see also Exercise 6.1.7) and, by Proposition 9.5.2, $\|R_\lambda(T)\| \leq 1/|\beta - \lambda|$.

Such inequalities imply, for all $\xi \in \mathcal{H}$,

$$\|BR_\lambda(T)\xi\| \leq a\|TR_\lambda(T)\xi\| + b\|R_\lambda(T)\xi\| \leq \left(a + \frac{b}{|\beta - \lambda|}\right)\|\xi\|$$

and for large $|\lambda|$ one has $\|BR_\lambda(T)\| < 1$. Finally, from the relation

$$T + B - \lambda\mathbf{1} = (\mathbf{1} + BR_\lambda(T))\,(T - \lambda\mathbf{1})$$

it follows that

$$R_\lambda(T + B) = R_\lambda(T)\,(\mathbf{1} + BR_\lambda(T))^{-1}$$

belongs to $\mathrm{B}(\mathcal{H})$ and so $\lambda \in \rho(T + B)$. Therefore there exists $\gamma \in \mathbb{R}$ so that $(-\infty, \gamma) \subset \rho(T + B)$. The proposition is proved. □

Characterization of Bounded Operators

Proposition 9.5.12. *Any* $S \in \mathrm{B}(\mathcal{H})$ *is expressible as the linear combination of no more than two self-adjoint operators and also of no more than four unitary operators.*

Proof. If S is the zero operator it is self-adjoint and equals $(U - U)$ for any unitary U, and the conclusions follow in this specific case. Assume that $S \neq 0$. Write $S = S_1 + S_2$, with

$$S_1 = \frac{1}{2}(S + S^*), \qquad S_2 = \frac{i}{2}\, i(S^* - S),$$

so that S is a linear combination of two bounded self-adjoint operators. To finish the proof it is enough to show that any bounded self-adjoint operator is the linear combination of no more than two unitary operators.

If $0 \neq T$ is bounded and self-adjoint, then by considering $T/\|T\|$ one can suppose that $\|T\| = 1$, so that $(\mathbf{1} - T^2) \geq 0$. Then, if $f_\pm(t) = t \pm i(1 - t^2)^{1/2}$, $-1 \leq t \leq 1$, the bounded operators

$$T_\pm := T \pm i \left(\mathbf{1} - T^2\right)^{\frac{1}{2}} = f_\pm(T)$$

satisfy $T = \frac{1}{2}(T_+ + T_-)$. Such operators $T_\pm$ are invertible, since if $T_-\xi = 0$ (similarly for T_+) then $T\xi = i(\mathbf{1} - T^2)^{1/2}\xi$ and so

$$\begin{aligned} T^2\xi &= i(\mathbf{1} - T^2)^{1/2} T\xi = i(\mathbf{1} - T^2)^{1/2} i(\mathbf{1} - T^2)^{1/2}\xi \\ &= -\xi + T^2\xi \Longrightarrow \xi = 0. \end{aligned}$$

Since $T_\pm^* = \overline{f}_\pm(T) = f_\mp(T) = T_\mp$, it follows that $T_\pm^* T_\pm = \mathbf{1} = T_\pm T_\pm^*$, and these operators are actually unitary. □

9.6 Spectral Mapping

The next result generalizes item 2) in Proposition 8.3.19 and it is often called *spectral mapping*; sometimes this terminology is used for the restricted set of polynomial functions.

Proposition 9.6.1 (Spectral Mapping Theorem). *Let T be self-adjoint and $f \in C(\sigma(T))$. Then* (*the bar indicates closure*)

$$\sigma(f(T)) = \overline{f(\sigma(T))} := \overline{\{f(\lambda) : \lambda \in \sigma(T)\}}.$$

Proof. Since the spectrum of two unitarily equivalent operators are the same, by the spectral theorem it is possible to assume that $T = \mathcal{M}_h$, $h(t) = t$, $t \in \mathbb{R}$, a multiplication operator acting in some $\mathrm{L}^2_\mu(E)$. Hence $f(T) = \mathcal{M}_{f(t)}$.

Recall that, by Proposition 2.3.27, $\lambda \in \sigma(\mathcal{M}_\varphi(t))$ iff for all open neighbourhood V of λ in $\mathbb{C}$ one has $\mu(\varphi^{-1}(V)) > 0$.

If $\lambda \in \sigma(T)$ and $y = f(\lambda)$, then for all open neighbourhoods V of y one has $\mu(f^{-1}(V)) \neq 0$, since $f^{-1}(V)$ is an open neighbourhood of λ; thus $y \in \sigma(\mathcal{M}_{f(t)}) = \sigma(f(T))$. Hence $f(\sigma(T)) \subset \sigma(f(T))$. Since $\sigma(f(T))$ is a closed set,

$$\overline{f(\sigma(T))} \subset \sigma(f(T)).$$

Now let $z \in \rho(f(T)) = \rho(\mathcal{M}_{f(t)})$. Then there exists an open neighbourhood V of z so that $\mu(f^{-1}(V)) = 0$; but this implies that $f^{-1}(V) \subset \rho(T)$, and so $z \in f(\rho(T))$. Thus

$$\rho(f(T)) \subset f(\rho(T)).$$

The above two inclusions infer that $\sigma(f(T)) = \overline{f(\sigma(T))}$. □

Corollary 9.6.2. *If in Proposition* 9.6.1 *the operator T is bounded and f is continuous, then*

$$\sigma(f(T)) = f(\sigma(T)).$$

Proof. If T is bounded then $\sigma(T)$ is a compact set; since f is continuous $f(\sigma(T))$ is also compact, so closed. Thus $\overline{f(\sigma(T))} = f(\sigma(T))$. Apply Proposition 9.6.1. □

Corollary 9.6.3. *Let $U(t)$ be a strongly continuous unitary evolution group on $\mathcal{H}$. If T is its infinitesimal generator, then for each $t \in \mathbb{R}$ one has*

$$\sigma(U(t)) = \text{closure}\,\{e^{-it\sigma(T)}\}.$$

Exercise 9.6.4. Use the spectral mapping theorem to show that if T is an idempotent self-adjoint operator and $T \neq 0, \mathbf{1}$, then $\sigma(T) = \{0, 1\}$.

Exercise 9.6.5. Let T be self-adjoint and $f : \mathbb{C} \to \mathbb{C}$ continuous. Give necessary and sufficient conditions so that the equation

$$f(T)\xi = \eta,$$

has unique solution $\xi = \xi(\eta)$, for each $\eta \in \mathcal{H}$, that depends continuously on η.

9.7 Duhamel Formula

Let T be self-adjoint and B a hermitian operator so that $T + B$ is self-adjoint with

$$\text{dom}\,(T + B) \subset \text{dom}\,T \cap \text{dom}\,B.$$

Then the evolution groups e^{-itT} and $e^{-it(T+B)}$ are well defined (see Section 9.2) and the task here is to compare them. It is a kind of perturbation of the unitary evolution group when the infinitesimal generator is perturbed.

Let $\xi \in \text{dom}\,(T + B)$. First note that $e^{-it(T+B)}\xi \in \text{dom}\,T \cap \text{dom}\,B$, $\forall t \in \mathbb{R}$, so the following manipulations are justified (see Proposition 5.1.3). Begin with the derivative

$$\begin{aligned}\frac{d}{dt}\left(e^{itT}e^{-it(T+B)}\xi\right) &= iTe^{itT}e^{-it(T+B)}\xi - ie^{itT}(T + B)e^{-it(T+B)}\xi \\ &= -ie^{itT}Be^{-it(T+B)}\xi,\end{aligned}$$

then integrate between 0 and t, to obtain

$$e^{itT}e^{-it(T+B)}\xi - \xi = -i\int_0^t e^{iuT}Be^{-iu(T+B)}\xi\,du,$$

and finally the so-called *Duhamel formula* follows

$$e^{-it(T+B)}\xi = e^{-itT}\xi - i\int_0^t e^{-iT(t-u)}Be^{-iu(T+B)}\xi\,du.$$

Note that this formula is a direct consequence of the fundamental theorem of calculus in this context!

In case B is also a bounded operator, one gets

$$\begin{aligned}\left\|e^{-it(T+B)}\xi - e^{-itT}\xi\right\| &\le \left|\int_0^t \left\|Be^{-iu(T+B)}\xi\right\|\,du\right| \\ &\le |t|\,\|B\|\|\xi\|,\end{aligned}$$

which could be useful for small $|t|$.

Exercise 9.7.1. Deduce

$$e^{itT}e^{-it(T+B)}\xi - e^{isT}e^{-is(T+B)}\xi = -i\int_s^t e^{iuT}Be^{-iu(T+B)}\xi\,du\,.$$

9.8 Reducing Subspaces

Let T be a self-adjoint operator acting in $\mathcal{H}$. The main goal of this section is to present some important subspaces E of $\mathcal{H}$ invariant under T, i.e., $T\xi \in E$ if $\xi \in E \cap \operatorname{dom} T$.

Let E be a closed subspace of $\mathcal{H}$ and P_E the orthogonal projection onto E; thus

$$\mathcal{H} = E \oplus E^\perp, \qquad \mathbf{1} = P_E + P_{E^\perp}.$$

Next a preparation for introducing important concepts in Definition 9.8.1. If $A : \operatorname{dom} A \subset \mathcal{H} \to \mathcal{H}$ is a linear operator, then

$$\operatorname{dom} A = P_E(\operatorname{dom} A) + P_{E^\perp}(\operatorname{dom} A).$$

If $P_E(\operatorname{dom} A) \subset \operatorname{dom} A$, then $P_{E^\perp}(\operatorname{dom} A) = (\mathbf{1} - P_E)\operatorname{dom} A \subset \operatorname{dom} A$ and so

$$A(\operatorname{dom} A) = AP_E(\operatorname{dom} A) + AP_{E^\perp}(\operatorname{dom} A),$$

that is $A\xi = AP_E\xi + AP_{E^\perp}\xi$ for all $\xi \in \operatorname{dom} A$.

Definition 9.8.1. The closed subspace E is called a *reducing subspace* of the operator A, or E *reduces* A, if

$$P_E(\text{dom } A) \subset \text{dom } A, \quad AP_E(\text{dom } A) \subset E, \quad \text{and} \quad AP_{E^\perp}(\text{dom } A) \subset E^\perp.$$

In this case the restriction operators $A_E := A|_E = AP_E$ and $A_{E^\perp} := A|_{E^\perp} = AP_{E^\perp}$ are well defined.

Exercise 9.8.2. Show that E reduces A iff $E^\perp$ reduces A, and in this case $(\text{dom } A|_E) \perp (\text{dom } A|_{E^\perp})$ and $\text{dom } A = \text{dom } A_E + \text{dom } A_{E^\perp}$.

The next theorem summarizes important properties of some reducing subspaces of self-adjoint operators. Its proof will be postponed to the end of this section.

Theorem 9.8.3. *Let T be a self-adjoint operator and $E \subset \mathcal{H}$ a closed subspace.*

a) *If E reduces T, then T_E and $T_{E^\perp}$ are self-adjoint operators, and in this case one writes $T = T_E \oplus T_{E^\perp}$.*
b) *For any Borel set $\Lambda \in \mathcal{A}$ the subspace* $\text{rng } \chi_\Lambda(T)$ *reduces T.*

Now some (preparatory) results of independent interest, which will be used in other chapters.

Lemma 9.8.4. *Let E be a closed subspace of $\mathcal{H}$ and $A : \text{dom } A \sqsubseteq \mathcal{H} \to \mathcal{H}$ a linear operator.*

a) *E reduces A iff $P_E A \subset AP_E$.*
b) *If A is hermitian, then E reduces A iff*

$$P_E(\text{dom } A) \subset \text{dom } A \qquad \text{and} \qquad AP_E(\text{dom } A) \subset E.$$

Proof. a) If E reduces A, for each $\xi \in \text{dom } A$ one has $P_E\xi \in \text{dom } A$, $AP_E\xi \in E$ and $AP_{E^\perp}\xi = A(\mathbf{1} - P_E)\xi \in E^\perp$; thus

$$(\mathbf{1} - P_E)AP_E\xi = 0 = P_E AP_{E^\perp}\xi = P_E A(\mathbf{1} - P_E)\xi$$

and so $AP_E\xi = P_E A\xi$, that is, $P_E A \subset AP_E$.

Assume now that $P_E A \subset AP_E$; so $P_{E^\perp} A = A - P_E A \subset A - AP_E = AP_{E^\perp}$. Hence $P_E(\text{dom } A) \subset \text{dom } A$ and $P_{E^\perp}(\text{dom } A) \subset \text{dom } A$ (see the above discussion). If $\xi \in \text{dom } A$ one has $AP_E\xi = P_E A\xi \in E$, and so $AP_E(\text{dom } A) \subset E$. Analogously to $E^\perp$.

b) Assume that A is hermitian. If E reduces A then the statement in the lemma follows immediately. Suppose that

$$P_E(\text{dom } A) \subset \text{dom } A \quad \text{and} \quad AP_E(\text{dom } A) \subset E;$$

then for $\xi \in \text{dom } A$ one has $AP_E\xi \in E$ and so $P_E AP_E\xi = AP_E\xi$. Thus, for all $\eta \in \text{dom } A$,

$$\langle P_E AP_E\xi, \eta\rangle = \langle \xi, P_E AP_E\eta\rangle = \langle \xi, AP_E\eta\rangle = \langle P_E A\xi, \eta\rangle,$$

and since dom A is dense in the Hilbert space $P_E A P_E \xi = P_E A\xi$. Since $AP_E\xi \in E$, it follows that $AP_E\xi = P_E A\xi$, that is, $AP_E \supset P_E A$. By item a), E reduces A. □

Proposition 9.8.5. *Let T be self-adjoint and $E \subset \mathcal{H}$ a closed subspace. Then E reduces T iff*

$$P_E\chi_{(a,b)}(T) = \chi_{(a,b)}(T)P_E$$

for all open intervals $(a,b) \subset \mathbb{R}$ with $-\infty < a < b < \infty$.

Proof. If $P_E\chi_{(a,b)}(T) = \chi_{(a,b)}(T)P_E$, for all bounded $(a,b) \subset \mathbb{R}$, it follows that $P_E\chi_\Omega(T) = \chi_\Omega(T)P_E$ for all open sets $\Omega \subset \mathbb{R}$, since every bounded open set is a countable pairwise disjoint union of such intervals and for an unbounded interval one takes a limit procedure, e.g., $\chi_{(a,\infty)}(T) = \mathrm{s} - \lim_{n\to\infty} \chi_{(a,n)}(T)$.

If $\xi \in \operatorname{dom} T$, then

$$\begin{aligned}\mu^T_{P_E\xi}(\Omega) &= \|\chi_\Omega(T)P_E\xi\|^2 = \|P_E\chi_\Omega(T)\xi\|^2 \\ &\le \|\chi_\Omega(T)\xi\|^2 = \mu^T_\xi(\Omega),\end{aligned}$$

and since the spectral measures are regular (recall that every finite Borel measure over $\mathbb{R}$ is regular) it is found that

$$\mu^T_{P_E\xi}(\Lambda) \le \mu^T_\xi(\Lambda), \qquad \forall \Lambda \in \mathcal{A}.$$

Therefore,

$$\|TP_E\xi\|^2 = \int_{\sigma(T)} t^2\, d\mu^T_{P_E\xi}(t) \le \int_{\sigma(T)} t^2\, d\mu^T_\xi(t) = \|T\xi\|^2 < \infty,$$

and so $P_E\xi \in \operatorname{dom} T$. Since P_E is a bounded operator, $\operatorname{dom}(TP_E) \supset \operatorname{dom} T = \operatorname{dom}(P_E T)$.

Let $h(t) = t$, $t \in \mathbb{R}$. By Lemma 9.8.6 ahead, there is a sequence (f_n) of simple functions with $f_n \to h$ in $\mathrm{L}^2_{\mu_\xi}(\mathbb{R})$ so that $P_E f_n(T) = f_n(T)P_E$; the above inequality between spectral measures implies that $f_n \to h$ in $\mathrm{L}^2_{\mu_{P_E\xi}}(\mathbb{R})$ as $n \to \infty$. Thus, for $\xi \in \operatorname{dom} T$,

$$\begin{aligned}P_E T\xi &= P_E h(T)\xi = P_E \lim_{n\to\infty} f_n(T)\xi = \lim_{n\to\infty} P_E f_n(T)\xi \\ &= \lim_{n\to\infty} f_n(T)P_E\xi = TP_E\xi,\end{aligned}$$

that is, $P_E T \subset TP_E$ and, by Lemma 9.8.4, it is found that E is a reducing subspace of T.

Suppose now that E reduces T. Then $P_E T \subset TP_E$ and for all $z \in \rho(T)$ one has

$$R_z(T)P_E = R_z(T)P_E(T - z\mathbf{1})R_z(T) \subset R_z(T)(T - z\mathbf{1})P_E R_z(T) = P_E R_z(T),$$

and since $\operatorname{dom}(R_z(T)P_E) = \mathcal{H}$ one has $R_z(T)P_E = P_E R_z(T)$. Since $\chi_{(a,b)}(T)$ is a continuous operator, by using the Stone formula (see Exercise 9.5.5) it is found that $P_E\chi_{(a,b)}(T) = \chi_{(a,b)}(T)P_E$. This finishes the proof. □

Lemma 9.8.6. *Let $h(t) = t$, $t \in \mathbb{R}$, T be self-adjoint and the projection P_E so that*

$$P_E \chi_{(a,b)}(T) = \chi_{(a,b)}(T) P_E,$$

for all open intervals $(a, b) \subset \mathbb{R}$ with $-\infty < a < b < \infty$. Then there is a sequence (f_n) of simple functions with $f_n \to h$ in $\mathrm{L}^2_{\mu_\xi}(\mathbb{R})$, as $n \to \infty$, for any $\xi \in \operatorname{dom} T$, and further

$$P_E f_n(T) = f_n(T) P_E, \qquad \forall n.$$

Proof. First note the pointwise limit $\chi_{(a,b]}(t) = \lim_{n\to\infty} \chi_{(a,b+1/n)}(t)$, which implies

$$\chi_{(a,b]}(T)\xi = \lim_{n\to\infty} \chi_{(a,b+1/n)}(T)\xi, \qquad \forall \xi \in \mathcal{H}.$$

Thus, since P_E is bounded, for all $\xi \in \mathcal{H}$,

$$\begin{aligned} P_E \chi_{(a,b]}(T)\xi &= P_E \lim_{n\to\infty} \chi_{(a,b+1/n)}(T)\xi \\ &= \lim_{n\to\infty} \chi_{(a,b+1/n)}(T) P_E \xi = \chi_{(a,b]}(T) P_E \xi, \end{aligned}$$

that is, $\chi_{(a,b]}(T) P_E = P_E \chi_{(a,b]}(T)$. Similar arguments show that

$$\chi_J(T) P_E = P_E \chi_J(T)$$

for all intervals $J \subset \mathbb{R}$ (bounded or not).

For $n \in \mathbb{N}$ and $-n2^n + 1 \le j \le n2^n$, define

$$A_n = (-\infty, -n), \quad B_n = [n, \infty), \quad J_{n,j} = [\frac{j-1}{2^n}, \frac{j}{2^n}),$$

and set

$$f_n(t) = -n\chi_{A_n}(t) + \sum_{-n2^n+1}^{n2^n} \chi_{J_{n,j}}(t) + n\chi_{B_n}(t).$$

Note that f_n are simple functions, $f_n(t) \to h(t)$ as $n \to \infty$ for every $t \in \mathbb{R}$, and since P_E commutes with each term in the (finite) sum

$$f_n(T) = -n\chi_{A_n}(T) + \sum_{-n2^n+1}^{n2^n} \chi_{J_{n,j}}(T) + n\chi_{B_n}(T),$$

it follows that $P_E f_n(T) = f_n(T) P_E, \forall n.$ □

Exercise 9.8.7. Give the arguments to conclude that

$$\chi_J(T) P_E = P_E \chi_J(T)$$

for all intervals $J \subset \mathbb{R}$, which was used in the proof of Lemma 9.8.6.

Exercise 9.8.8. Show that E reduces the self-adjoint operator T iff

$$P_E\chi_{(-\infty,t]}(T) = \chi_{(-\infty,t]}(T)P_E, \quad \forall t \in \mathbb{R}.$$

Finally the proof of Theorem 9.8.3 will be presented.

Proof. **[Theorem 9.8.3]** Let T be a self-adjoint operator.

a) Let E be a reducing subspace of T. Then T_E and $T_{E^\perp}$ are hermitian and $T_E^* : \text{dom } T_E^* \sqsubseteq E \to E$. If $\eta \in \text{dom } T_E^*$ and $\xi \in \text{dom } T$, then, since $TP_{E^\perp}\xi \in E^\perp$,

$$\begin{aligned} \langle \eta, T\xi\rangle &= \langle \eta, TP_E\xi\rangle + \langle \eta, TP_{E^\perp}\xi\rangle = \langle \eta, TP_E\xi\rangle \\ &= \langle \eta, T_E\xi\rangle = \langle T_E^*\eta, \xi\rangle, \end{aligned}$$

hence $\eta \in (\text{dom } T^* \cap E) = (\text{dom } T \cap E) = \text{dom } T_E$ (by definition). Therefore, $\text{dom } T_E^* = \text{dom } T_E$ and T_E is self-adjoint. In a similar way one checks that $T_{E^\perp}$ is self-adjoint.

b) If $E = \text{rng } \chi_\Lambda(T)$, then $P_E = \chi_\Lambda(T)$ and $P_E\chi_{(a,b)}(T) = \chi_{(a,b)}(T)P_E$. Apply Proposition 9.8.5. ☐

Exercise 9.8.9. If E is a closed subspace that reduces the self-adjoint operator T, then is E a spectral subspace of T, that is, is there $\Lambda \in \mathcal{A}$ such that $E = \text{rng } \chi_\Lambda(T)$?

9.9 Sequences and Evolution Groups

In this section T denotes a self-adjoint operator.

Evolution Group via Power Series. Let $P^T(\Lambda)$ be the resolution of identity of T. By Lemma 8.3.16a), for each $\xi \in \mathcal{H}$ one has $P^T([-M,M])\xi \in \text{dom } T$, $\forall M > 0$, and since

$$\lim_{M\to\infty} P^T([-M,M])\xi = \xi,$$

it follows that

$$Z = \bigcup_{M=1}^{\infty} P^T([-M,M])\mathcal{H},$$

is dense in $\mathcal{H}$ and $Z \subset \text{dom } T$. Further, if $\eta \in Z$, then there exists M so that $\eta \in P^T([-M,M])\mathcal{H}$; by Theorem 9.8.3, $P^T([-M,M])\mathcal{H}$ reduces T and since on such subspace T is a bounded operator (see the proof of Lemma 8.3.16a)), then – see also Theorem 5.2.3 –

$$e^{-itT}\eta = \sum_{j=0}^{\infty} \frac{(-itT)^j}{j!}\eta.$$

Note that the convergence is in fact uniform on $P^T([-M,M])\mathcal{H}$. Therefore, even though T is unbounded, on a dense set of vectors $Z \sqsubseteq \mathcal{H}$ this unitary evolution group can be obtained via the power series of the exponential.

Evolution Group via a Bounded Sequence. It will be checked that for each fixed real t the sequence of bounded (resolvent) operators

$$\left(1 + it\frac{T}{n}\right)^{-n}$$

strongly converges to the unitary evolution group e^{-itT}. This sequence can be a starting point of a proof of Theorem 5.3.1 without using the spectral theorem [Am81].

Recall that for each $x \in \mathbb{R}$ the sequence of functions $\left(1 + it\frac{x}{n}\right)^{-n}$ pointwise converges to e^{-itx} as $n \to \infty$. If $\xi \in \mathcal{H}$, by the spectral theorem,

$$\left\|\left(1 + it\frac{T}{n}\right)^{-n} \xi - e^{-itT}\xi\right\|^2 = \int_{\sigma(T)} \left|\left(1 + it\frac{x}{n}\right)^{-n} - e^{-itx}\right|^2 \, d\mu_\xi^T(x)$$

which vanishes as $n \to \infty$ by dominated convergence. Hence

$$\mathrm{s} - \lim_{n\to\infty} \left(1 + it\frac{T}{n}\right)^{-n} = e^{-itT}.$$

Exercise 9.9.1. Verify that $\left\|\left(1 + it\frac{T}{n}\right)^{-n}\right\| \leq 1$ for any $n \in \mathbb{N}$.

Exercise 9.9.2. Assume that $T \geq 0$.

(a) Show that for any $t > 0$ (see Subsection 5.5.1)

$$e^{-tT} = \mathrm{s} - \lim_{n\to\infty} \left(1 + t\frac{T}{n}\right)^{-n}.$$

(b) Use the spectral theorem to show that, for any $\lambda, s > 0$,

$$R_{-\lambda}(T)^s = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} e^{-t\lambda} e^{-tT} \, dt,$$

with $\Gamma(s) = \int_0^\infty t^{s-1} e^{-t} \, dt$ denoting the usual gamma function.

Trotter Product Formula. There is a version of Trotter product formula, discussed in Section 5.6, for real exponential of bounded from below operators. Follow the proof of Theorem 5.6.2 to solve the following exercise.

Exercise 9.9.3. Let T, S and $T + S$ be as in Theorem 5.6.2. Assume that T and S are bounded from below.

a) Show that for each $t \geq 0$ the operators e^{-tT}, e^{-tS} and $e^{-t(T+S)}$ are bounded.

b) Show that

$$e^{-t(T+S)} = \mathrm{s} - \lim_{n\to\infty} \left(e^{-\frac{t}{n}T} e^{-\frac{t}{n}S}\right)^n, \qquad \forall t \geq 0.$$

Chapter 10

Convergence of Self-Adjoint Operators

In this chapter T_n and T denote (usually unbounded) self-adjoint operators acting in $\mathcal{H}$. Due to domain intricacies, alternative concepts of operator convergence are introduced. The strong convergences in the resolvent and dynamical senses are shown to be equivalent. Some relations with spectrum are also discussed. Convergence to operators with shrinking domains are discussed with the help of sesquilinear forms, with application to the Aharonov-Bohm effect.

10.1 Resolvent and Dynamical Convergences

It is not a simple task to give a precise definition of a sequence of unbounded Schrödinger operators T_n approaching another one T. For instance, the simple adaptation of the strong convergence of operators $\|T_n\xi - T\xi\| \to 0$ is only meaningful for $\xi \in \cap_n \text{dom } T_n$, which could consist only of the null vector! A common procedure when dealing with unbounded operators is to rest the concepts upon the corresponding resolvents $R_z(T_n)$ ($z \in \mathbb{C} \setminus \mathbb{R}$) and/or unitary evolution groups e^{-itT_n}, which are bounded operators and defined everywhere. This seems natural because it is expected that two self-adjoint operators are "close" if their resolvents are close and/or their unitary evolution groups are close. This approach has become traditional and fruitful and is followed here; it will be supported by a series of properties and examples presented in this chapter.

Definition 10.1.1.

a) T_n converges to T in the *strong resolvent sense* (SR) if $R_i(T_n) \stackrel{\text{s}}{\longrightarrow} R_i(T)$, and this will be denoted by $T_n \stackrel{\text{SR}}{\longrightarrow} T$.

b) T_n converges to T in the *strong dynamical sense* (SD) if, for each $t \in \mathbb{R}$, $e^{-itT_n} \xrightarrow{\text{s}} e^{-itT}$, and this will be denoted by $T_n \xrightarrow{\text{SD}} T$.

Remark 10.1.2. The definitions of convergence in the *weak resolvent sense* (WR), *norm resolvent sense* (NR), *weak dynamical sense* (WD) and *norm dynamical sense* (ND) are similar; it is enough to exchange strong convergence in Definition 10.1.1 by the appropriate convergence type. For instance, $T_n \xrightarrow{\text{WD}} T$ indicates that, for each $t \in \mathbb{R}$, $e^{-itT_n} \xrightarrow{\text{w}} e^{-itT}$, and norm convergence refers to convergence in $\mathrm{B}(\mathcal{H})$. Each of such convergences is also called *generalized convergence*.

Remark 10.1.3. The norm resolvent convergence is also called *uniform resolvent convergence*. Most definitions and results on convergence of sequences of operators discussed in this chapter hold for convergence with respect to a parameter $\lambda \in \mathbb{R}$, e.g., for $\lambda \to \lambda_0$. The reader will find no special difficulty in adapting the arguments.

Exercise 10.1.4. Let S, Q be two linear operators with domain in $\mathcal{H}$ and codomain $\mathcal{H}$. Show that if $R_z(T) = R_z(S)$, for some $z \in \rho(T) \cap \rho(S)$, then $T = S$. Conclude that the above limits in the resolvent sense are unique. What about the uniqueness of the limits in the dynamical sense?

The relations among the above defined types of convergence of self-adjoint operators are summarized in Theorems 10.1.15 and 10.1.16.

Lemma 10.1.5. *$T_n \xrightarrow{\text{SR}} T$ iff $R_{-i}(T_n) \xrightarrow{\text{s}} R_{-i}(T)$.*

Proof. Since $R_i(T) = r(T)$, for $r(t) = (t - i)^{-1}$, which is a bounded normal operator (see Definition 8.2.9) and $R_i(T)^* = R_{-i}(T)$, one has

$$\|R_i(T)\xi\| = \|R_i(T)^*\xi\| = \|R_{-i}(T)\xi\|, \qquad \forall \xi \in \mathcal{H}.$$

Hence,

$$\|(R_i(T_n) - R_i(T))\xi\| = \|(R_i(T_n) - R_i(T))^*\xi\| = \|(R_{-i}(T_n) - R_{-i}(T))\xi\|$$

$\forall \xi \in \mathcal{H}$, and the result follows. □

Exercise 10.1.6. Let $B_n, B \in \mathrm{B}(\mathcal{H})$ be normal operators; show that $B_n \xrightarrow{\text{s}} B$ iff $B_n^* \xrightarrow{\text{s}} B^*$.

Exercise 10.1.7. Show that

a) $T_n \xrightarrow{\text{NR}} T$ iff $R_{-i}(T_n) \to R_{-i}(T)$ in $\mathrm{B}(\mathcal{H})$.

b) $T_n \xrightarrow{\text{WR}} T$ iff $R_{-i}(T_n) \xrightarrow{\text{w}} R_{-i}(T)$.

One of the goals of this chapter is to prove the following equivalence, related to strong convergences and due to H. Trotter in 1958. Theorem 10.1.15 presents an extension of this result. Such equivalence may not happen in case of norm convergence, as illustrated by Example 10.3.1.

Proposition 10.1.8. $T_n \xrightarrow{\text{SR}} T$ *iff* $T_n \xrightarrow{\text{SD}} T$.

Proof. By a relation between the resolvent operator and the evolution group in Section 9.5, for any $\xi \in \mathcal{H}$ one obtains

$$\begin{aligned}\|R_i(T_n)\xi - R_i(T)\xi\| &= \left\| -i \int_0^\infty e^{-s} \left(e^{-isT_n}\xi - e^{-isT}\xi \right) ds \right\| \\ &\le \int_0^\infty e^{-s} \left\| e^{-isT_n}\xi - e^{-isT}\xi \right\| ds.\end{aligned}$$

Since $\left\| e^{-isT_n}\xi - e^{-isT}\xi \right\| \le 2\|\xi\|$, the dominated convergence theorem implies that if $T_n \xrightarrow{\text{SD}} T$, then $T_n \xrightarrow{\text{SR}} T$.

The converse relation will follow from the fact that if $T_n \xrightarrow{\text{SR}} T$ then $f(T_n) \xrightarrow{\text{s}} f(T)$ for all bounded and continuous $f : \mathbb{R} \to \mathbb{C}$, proved in Proposition 10.1.9. Indeed, for fixed t, just take $f(x) = e^{-itx}$ to conclude that if $T_n \xrightarrow{\text{SR}} T$, then $T_n \xrightarrow{\text{SD}} T$. □

Proposition 10.1.9. $T_n \xrightarrow{\text{SR}} T$ *iff* $f(T_n) \xrightarrow{\text{s}} f(T)$ *for all bounded and continuous* $f : \mathbb{R} \to \mathbb{C}$.

Proof. Let $r : \mathbb{R} \to \mathbb{C}$ denote the function $r(t) = (t - i)^{-1}$. So $\overline{r}(t) = (t + i)^{-1}$,

$$R_i(T) = r(T) \qquad \text{and} \qquad R_{-i}(T) = \overline{r}(T).$$

Since r is a bounded continuous function one implication in the proposition is trivial.

Suppose then that $T_n \xrightarrow{\text{SR}} T$; the task is to pass from r to all bounded continuous functions. Note that r separates points of $\mathbb{R}$ (i.e., if $t, s \in \mathbb{R}$, $t \ne s$, then $r(t) \ne r(s)$) and $\lim_{|t|\to\infty} r(t) = 0$. Thus, by the Stone-Weierstrass theorem [Simm63] the set of polynomials $p_\varepsilon(r(t), \overline{r}(t))$ in the variables $r(t)$ and $\overline{r}(t)$ is dense in the space $C_\infty(\mathbb{R})$, that is, the space of continuous functions that vanish at infinity with the sup norm $\|\cdot\|_\infty$ (i.e., if $\psi \in C_\infty(\mathbb{R})$, then for each $\varepsilon > 0$ there is $M > 0$ so that $|\psi(x)| < \varepsilon$ if $|x| \ge M$).

Hence, if $\phi \in C_\infty(\mathbb{R})$, for each $\varepsilon > 0$ there exists a polynomial $p_\varepsilon(r(t), \overline{r}(t))$ with

$$\|\phi - p_\varepsilon\|_\infty < \varepsilon,$$

and by the spectral theorem (see Corollary 8.3.19) the two inequalities

$$\|\phi(T) - p_\varepsilon(R_i(T), R_{-i}(T))\| < \varepsilon,$$

and

$$\|\phi(T_n) - p_\varepsilon(R_i(T_n), R_{-i}(T_n))\| < \varepsilon, \qquad \forall n,$$

hold simultaneously. If $T_n \xrightarrow{\text{SR}} T$, then $R_i(T_n) \xrightarrow{\text{s}} R_i(T)$ and $R_{-i}(T_n) \xrightarrow{\text{s}} R_{-i}(T)$, and one concludes that

$$p_\varepsilon(R_i(T_n), R_{-i}(T_n)) \xrightarrow{\text{s}} p_\varepsilon(R_i(T), R_{-i}(T)), \qquad n \to \infty.$$

By collecting these inequalities together with the triangle inequality, it follows that $\phi(T_n) \xrightarrow{\text{s}} \phi(T)$ for all $\phi \in C_\infty(\mathbb{R})$.

Let $f : \mathbb{R} \to \mathbb{C}$ be bounded and continuous. By the spectral theorem $\|f(T)\| \le \|f\|_\infty$ and $\|f(T_n)\| \le \|f\|_\infty$, $\forall n$. Pick a monotone increasing sequence ϕ_j in $C_0^\infty(\mathbb{R})$ with $0 \le \phi_j \le 1$ with $\phi_j(t) \uparrow 1$, $\forall t \in \mathbb{R}$, as $j \to \infty$. Thus, $\phi_j(T) \xrightarrow{\text{s}} \mathbf{1}$ and $\phi_j(T_n) \xrightarrow{\text{s}} \mathbf{1}$, $\forall n$.

Since the product function $f(t)\phi_j(t) \in C_\infty(\mathbb{R})$ one has

$$f(T_n)\phi_j(T_n) \xrightarrow{\text{s}} f(T)\phi_j(T), \qquad \forall j.$$

If $\xi \in \mathcal{H}$ it follows that

$$\begin{aligned} \|f(T_n)\xi - f(T)\xi\| \le{}& \|f(T_n)\xi - f(T_n)\phi_j(T)\xi\| \\ &+ \|f(T_n)\phi_j(T)\xi - f(T_n)\phi_j(T_n)\xi\| \\ &+ \|f(T_n)\phi_j(T_n)\xi - f(T)\phi_j(T)\xi\| + \|f(T)\phi_j(T)\xi - f(T)\xi\| \\ &\le \|f(T_n)\| \left(\|\xi - \phi_j(T)\xi\| + \|\phi_j(T)\xi - \phi_j(T_n)\xi\|\right) \\ &+ \|f(T_n)\phi_j(T_n)\xi - f(T)\phi_j(T)\xi\| + \|f(T)\|\|\phi_j(T)\xi - \xi\|. \end{aligned}$$

Given $\varepsilon > 0$, take j so that $\|\xi - \phi_j(T)\xi\| < \varepsilon/\|f\|_\infty$. Then, for n large enough, one has $\|\phi_j(T)\xi - \phi_j(T_n)\xi\| < \varepsilon/\|f\|_\infty$ and

$$\|f(T_n)\phi_j(T_n)\xi - f(T)\phi_j(T)\xi\| < \varepsilon.$$

Hence,

$$\|f(T_n)\xi - f(T)\xi\| < 4\varepsilon.$$

Since $\varepsilon > 0$ was arbitrary, $f(T_n)\xi \to f(T)\xi$. Thereby the proof of the proposition is complete. □

Remark 10.1.10. Note that the definition of SR and/or SD convergence could be defined as $f(T_n) \xrightarrow{\text{s}} f(T)$ for all bounded and continuous $f : \mathbb{R} \to \mathbb{C}$; this is an important support to the use of resolvents in convergence of operators, as in Definition 10.1.1. What makes the resolvent work here is its property related to the Stone-Weierstrass theorem.

Exercise 10.1.11. Verify that

$$p_\varepsilon(R_i(T_n), R_{-i}(T_n)) \xrightarrow{\text{s}} p_\varepsilon(R_i(T), R_{-i}(T)), \qquad n \to \infty,$$

used in the proof of Proposition 10.1.9.

Exercise 10.1.12. Use Proposition 10.1.9 to show that if $T_n \xrightarrow{\text{SR}} T$, then

$$R_z(T_n) \xrightarrow{\text{s}} R_z(T), \qquad \forall z \in \mathbb{C} \setminus \mathbb{R}.$$

See Exercise 10.1.17 for a generalization.

The next result confirms that strong convergence in the resolvent and dynamical senses are adequate generalizations of strong convergence of bounded self-adjoint operators. This is also in favor of the concepts introduced in Definition 10.1.1.

Proposition 10.1.13. *Let $T_n, T \in \mathrm{B}(\mathcal{H})$ be self-adjoint.*

a) *If $T_n \xrightarrow{\text{s}} T$, then $T_n \xrightarrow{\text{SR}} T$.*

b) *If $\sup_n \|T_n\| < \infty$ and $T_n \xrightarrow{\text{SR}} T$, then $T_n \xrightarrow{\text{s}} T$.*

Proof. a) By Theorem 2.2.17 (or Exercise 9.5.3) $\|R_i(T_n)\| \le 1$ for all n. Then, for each $\xi \in \mathcal{H}$ the second resolvent identity implies

$$R_i(T_n)\xi - R_i(T)\xi = R_i(T_n)(T - T_n)R_i(T)\xi$$

and so

$$\|R_i(T_n)\xi - R_i(T)\xi\| \le \|(T - T_n)\eta\|, \qquad \eta = R_i(T)\xi,$$

which vanishes as $n \to \infty$ since $T_n \xrightarrow{\text{s}} T$. a) follows.

b) Let $M = \sup_n \|T_n\| < \infty$. Write

$$T_n - T = (T_n - i\mathbf{1})(R_i(T) - R_i(T_n))(T - i\mathbf{1}).$$

For each $\xi \in \mathcal{H}$ denote $\eta = (T - i\mathbf{1})\xi$; so

$$\|T_n\xi - T\xi\| \le (M + 1)\,\|(R_i(T) - R_i(T_n))\eta\|,$$

which vanishes as $n \to \infty$ since $T_n \xrightarrow{\text{SR}} T$. b) follows. Note that in this case necessarily $T \in \mathrm{B}(\mathcal{H})$ by Banach-Steinhaus 1.1.33.

□

Exercise 10.1.14. Let T_n, T be self-adjoint. Show that:
a) If $T_n, T \in \mathrm{B}(\mathcal{H})$, then $T_n \xrightarrow{\text{NR}} T$ iff $T_n \to T$ in $\mathrm{B}(\mathcal{H})$.
b) If $T_n \xrightarrow{\text{NR}} T$, then $\|f(T_n) - f(T)\| \to 0$, $\forall f \in C_\infty(\mathbb{R})$. See also Remark 10.2.7.

Theorem 10.1.15. *For self-adjoint operators T_n, T, the following assertions are equivalent:*

i) $T_n \xrightarrow{\text{SR}} T$. ii)$T_n \xrightarrow{\text{WR}} T$. iii) $T_n \xrightarrow{\text{SD}} T$ iv) $T_n \xrightarrow{\text{WD}} T$.

Proof. • i) ⇒ ii) is clear.

• i) ⇔ iii) is Proposition 10.1.8.

• iii) ⇔ iv) Since all the operators involved in the convergence are unitary, the weak convergence is equivalent to strong convergence (see the proof of Proposition 5.1.7), and so iii) is equivalent to iv).

• ii) ⇒ i) Suppose $T_n \xrightarrow{\text{WR}} T$. If $\xi \in \mathcal{H}$, one has

$$\begin{aligned}\|R_i(T_n)\xi - R_i(T)\xi\|^2 &= \|R_i(T_n)\xi\|^2 + \|R_i(T)\xi\|^2 \\ &\quad - \langle R_i(T_n)\xi, R_i(T)\xi\rangle - \langle R_i(T)\xi, R_i(T_n)\xi\rangle.\end{aligned}$$

Both sequences $\langle R_i(T_n)\xi, R_i(T)\xi\rangle$ and $\langle R_i(T)\xi, R_i(T_n)\xi\rangle$ converge to $\|R_i(T)\xi\|^2$ as $n \to \infty$. Thus, the task becomes to check that

$$\|R_i(T_n)\xi\|^2 \to \|R_i(T)\xi\|^2$$

if $\mathrm{w} - \lim_{n\to\infty} R_i(T_n)\xi = R_i(T)\xi$. Indeed, by the first resolvent identity (and Exercise 10.1.14)

$$\begin{aligned}
\|R_i(T_n)\xi\|^2 &= \langle R_i(T_n)\xi, R_i(T_n)\xi\rangle = \langle \xi, R_{-i}(T_n)R_i(T_n)\xi\rangle \\
&= \left\langle \xi, \frac{1}{2i}\left(R_{-i}(T_n) - R_i(T_n)\right)\xi \right\rangle \\
&= \frac{1}{2i}\left(\langle R_i(T_n)\xi, \xi\rangle - \langle \xi, R_i(T_n)\xi\rangle\right) \\
&\overset{\mathrm{n}\to\infty}{\longrightarrow} \left\langle \xi, \frac{1}{2i}\left(R_{-i}(T) - R_i(T)\right)\xi \right\rangle = \langle R_i(T)\xi, R_i(T))\xi\rangle \\
&= \|R_i(T)\xi\|^2.
\end{aligned}$$

Therefore $\|R_i(T_n)\xi - R_i(T)\xi\| \to 0$ and i) follows. □

Theorem 10.1.16. *The* ND *and* NR *convergences of self-adjoint operators are not equivalent in general, although* ND *convergence implies* NR *convergence.*

Proof. Let T_n, T be self-adjoint operators. If $T_n \xrightarrow{\mathrm{ND}} T$, from the proof of Proposition 10.1.8 one has, for all $\xi \in \mathcal{H}$,

$$\begin{aligned}
\|R_i(T_n)\xi - R_i(T)\xi\| &\le \int_0^\infty e^{-s}\left\|e^{-isT_n}\xi - e^{-isT}\xi\right\| ds \\
&\le \left(\int_0^\infty e^{-s}\left\|e^{-isT_n} - e^{-isT}\right\| ds\right)\|\xi\|.
\end{aligned}$$

Since $\left\|e^{-isT_n} - e^{-isT}\right\| \le 2$, $\forall s \in \mathbb{R}$, if $T_n \xrightarrow{\mathrm{ND}} T$, by dominated convergence the above integral vanishes as $n \to \infty$, which implies that $T_n \xrightarrow{\mathrm{NR}} T$.

Example 10.3.1 shows the NR convergence does not necessarily imply ND convergence. □

Exercise 10.1.17. If $z_0 \in \mathbb{C} \setminus \mathbb{R}$ and T is self-adjoint, recall that

$$R_z(T) = \sum_{j=0}^{\infty} (z - z_0)^j R_{z_0}(T)^{j+1},$$

and since $\|R_{z_0}(T)\| \le 1/|\mathrm{Im}\ z_0|$, this series is convergent if $|z - z_0| < |\mathrm{Im}\ z_0|$. Use these facts to show that if $R_{z_0}(T_n) \xrightarrow{\mathrm{s}} R_{z_0}(T)$ (or in norm), then $R_z(T_n) \xrightarrow{\mathrm{s}} R_z(T)$ (in norm, resp.) for any $z \in \mathbb{C} \setminus \mathbb{R}$. Discuss the implications of this result to the convergence of self-adjoint operators.

It can be a nontrivial task to compute resolvents of linear operators. So the next result, in which the operators themselves intervene, can be quite useful.

Proposition 10.1.18. *Let $\mathcal{D}$ be a core of the self-adjoint operator T. If T_n are self-adjoint, $\mathcal{D} \subset \operatorname{dom} T_n$, $\forall n$, and $T_n\xi \to T\xi$, $\forall \xi \in \mathcal{D}$, then $T_n \xrightarrow{\text{SR}} T$.*

Proof. First note that $\mathcal{C} = (T - i\mathbf{1})\mathcal{D}$ is a dense set in $\mathcal{H}$ (since the deficiency indices of $T|_\mathcal{D}$ are zero). For each $\xi \in \mathcal{D}$ denote $\eta_\xi = (T - i\mathbf{1})\xi \in \mathcal{C}$. Thus, by Theorem 2.2.17 and the second resolvent identity, for all η_ξ in the dense set $\mathcal{C}$,

$$\begin{aligned}\|(R_i(T_n) - R_i(T))\,\eta_\xi\| &= \|R_i(T_n)\,(T_n - T)\,\xi\| \\ &\le \|(T_n - T)\xi\| \to 0, \qquad n \to \infty.\end{aligned}$$

Since the set of such resolvent operators is uniformly bounded, i.e.,

$$\sup\{\|R_i(T)\|, \|R_i(T_n)\|\} \le 1,$$

the convergence in the dense set $\mathcal{C}$ can be extended to $\mathcal{H}$, that is, $(R_i(T_n) - R_i(T))\eta \to 0$ for all $\eta \in \mathcal{H}$. The proposition is proved. □

Example 10.1.19. Let S be an unbounded self-adjoint operator and $T_n = S/n$, so that $T_n\xi \to 0$ for any $\xi \in \operatorname{dom} S$. Since $\operatorname{dom} S$ is dense in the Hilbert space, it is a core of the bounded operator $T = 0$; by Proposition 10.1.18, $T_n \xrightarrow{\text{SR}} T$. This is an instance of a sequence of unbounded operators that converges in the SR sense to a bounded one. See also Example 10.3.4.

Remark 10.1.20. The conditions in Proposition 10.1.18 are not necessary for SR convergence, as shown by an example in [Gol72].

Exercise 10.1.21. Let $V_n, V \in \mathrm{L}^\infty(\mathbb{R}^n)$ be real-valued so that there is $C > 0$ with $\|V_n\|_\infty \le C, \forall n$, and $V_n(x) \to V(x)$ pointwise a.e. Show that $H_0 + V_n \xrightarrow{\text{SR}} H_0 + V$.

Exercise 10.1.22. a) Inspect the proof of Proposition 10.1.18 and show that if $\mathcal{D} \subset \operatorname{dom} T$ is a core of T, and for each $\xi \in \mathcal{D}$ there exists m so that $\xi \in \operatorname{dom} T_n$ if $n \ge m$, and $T_n\xi \to T\xi$, then that $T_n \xrightarrow{\text{SR}} T$.
b) Use Proposition 10.1.18 to show that T_n, T are bounded and $T_n \xrightarrow{\text{s}} T$, then $T_n \xrightarrow{\text{SR}} T$.

Finally, a word in case the convergence of the resolvents of self-adjoint operators is known for a point in the real line.

Proposition 10.1.23. *If T_j, T are self-adjoint operators in a Hilbert space $\mathcal{H}$ with $R_\lambda(T_j) \xrightarrow{\text{s}} R_\lambda(T)$ in $\mathcal{H}$ for some real λ, then $T_j \xrightarrow{\text{SR}} T$ (λ is supposed to belong to the resolvent set of all involved operators).*

Proof. It is a direct application of the third resolvent identity (Proposition 1.5.11) with $z_0 = \lambda$ and $z = \pm i$. Note that, by the Uniform Boundedness Principle 1.1.31, $\sup_j \|R_\lambda(T_j)\| < \infty$, an ingredient used to complete this proof. □

10.2 Resolvent Convergence and Spectrum

If T_n and T are self-adjoint and $T_n \to T$ via resolvent or unitary evolution groups, a natural question is about the relation between the spectra of T and its approximating T_n. This section discusses some of such relations.

Theorem 10.2.1 (Rellich-Sz.-Nagy). *Let T_n and T be self-adjoint. If $T_n \xrightarrow{\text{SR}} T$ and $\Lambda \subset \mathbb{R}$ is an open set with*

$$\Lambda \subset \bigcap_{n \geq N} \rho(T_n),$$

for some N, then $\Lambda \subset \rho(T)$.

Proof. Note that it is enough to consider intervals $\Lambda = (a,b)$. For $\varepsilon > 0$ small enough, put $\Lambda_\varepsilon = (a-\varepsilon, b-\varepsilon)$. Let $f_\varepsilon \in C_0^\infty(\mathbb{R})$ with $0 \leq \chi_{\Lambda_\varepsilon} \leq f_\varepsilon \leq \chi_{(a,b)}$; thus, by Theorem 8.3.13, for $n \geq N$ one has

$$0 = \chi_{(a,b)}(T_n) \geq f_\varepsilon(T_n).$$

By Proposition 10.1.9, $f_\varepsilon(T_n) \xrightarrow{\text{s}} f_\varepsilon(T)$. Thus $f_\varepsilon(T) = 0$.

Since $0 \leq \chi_{\Lambda_\varepsilon}(T) \leq f_\varepsilon(T) = 0$, by Theorem 8.3.13 again, $\Lambda_\varepsilon \subset \rho(T)$. As $\varepsilon > 0$ was arbitrarily small, $(a,b) \subset \rho(T)$. □

Corollary 10.2.2. *Let T_n and T be self-adjoint. If $T_n \xrightarrow{\text{SR}} T$ and $t_0 \in \sigma(T)$, then there exists a sequence $(t_n) \subset \mathbb{R}$, with $t_n \in \sigma(T_n), \forall n$, so that $t_n \to t_0$.*

Proof. If $t_0 \in \sigma(T)$, then by Theorem 10.2.1, for all $j \geq 1$ the interval $(t_0 - 1/j, t_0 + 1/j)$ is not a subset of

$$W_N := \cap_{n \geq N}\, \rho(T_n), \qquad \forall N.$$

Thus, for all j, N,

$$\begin{aligned} \emptyset \neq & \,(t_0 - 1/j, t_0 + 1/j) \,\cap\, (\mathbb{R} \setminus W_N) \\ = & \,(t_0 - 1/j, t_0 + 1/j) \,\cap\, (\cup_{n \geq N} \sigma(T_n)). \end{aligned}$$

Hence there is $t_{n_j} \in \sigma(T_{n_j})$ so that $t_{n_j} \to t_0$.

Suppose now that the subsequence t_{n_j} can not be replaced by the full sequence t_n, $t_n \in \sigma(T_n)$, $\forall n$, and with $t_n \to t_0$. Then there is a subsequence (n_k) so that no choice $t_{n_k} \in \sigma(T_{n_k})$ does converge to t_0; set $\tilde{W} = \cap_{n_k}\, \rho(T_{n_k})$. Thus there is $\varepsilon > 0$, so that (take a subsequence if necessary)

$$\emptyset = (t_0 - \varepsilon, t_0 + \varepsilon) \,\cap\, (\cup_{n_k} \sigma(T_{n_k})),$$

then

$$(t_0 - \varepsilon, t_0 + \varepsilon) \subset \mathbb{R} \setminus (\cup_{n_k} \sigma(T_{n_k})) = \tilde{W}.$$

Since $T_{n_k} \xrightarrow{\text{SR}} T$, Theorem 10.2.1 implies that $t_0 \in \rho(T)$. This contradiction finishes the proof of the proposition. □

It is common to refer to the result of Corollary 10.2.2 as "the spectrum does not increase under strong resolvent limits."

Exercise 10.2.3. If for all n one has $T_n \geq \beta\mathbf{1}$ and $T_n \xrightarrow{\text{SR}} T$, show that $T \geq \beta\mathbf{1}$. Use this to give another proof that if T_n is a uniformly bounded sequence in $\mathrm{B}(\mathcal{H})$ and $T_n \xrightarrow{\text{SR}} T$, then $T \in \mathrm{B}(\mathcal{H})$.

Proposition 10.2.4. *If $T_n \xrightarrow{\text{NR}} T$, then:*

a) *If $t_0 \in \sigma(T)$, then there is a sequence $t_n \to t_0$ with $t_n \in \sigma(T_n)$.*
b) *If $t_0 \in \rho(T)$, then $t_0 \in \rho(T_n)$ for all n sufficiently large.*

Proof. a) follows by Corollary 10.2.2, since convergence in the NR sense implies convergence in the SR sense and with the same limit.

b) It is possible to restrict the discussion to $t_0 \in \mathbb{R}$. If $t_0 \in \rho(T)$ take $\varepsilon > 0$ so that $\Lambda_{2\varepsilon} := (t_0 - 2\varepsilon, t_0 + 2\varepsilon) \subset \rho(T)$. Pick $f_\varepsilon \in C_0^\infty(\mathbb{R})$ so that

$$\chi_{\Lambda_\varepsilon} \leq f_\varepsilon \leq \chi_{\Lambda_{2\varepsilon}}.$$

Hence

$$0 \leq \chi_{\Lambda_\varepsilon}(T) \leq f_\varepsilon(T) \leq \chi_{\Lambda_{2\varepsilon}}(T) = 0.$$

By Exercise 10.1.14, $f_\varepsilon(T_n) \to f_\varepsilon(T) = 0$ uniformly, so for n large enough one has $\|f_\varepsilon\|_\infty < 1$.

Thus, for all $\xi \in \mathcal{H}$, $\|\xi\| = 1$, Cauchy-Schwarz implies

$$\begin{aligned}\|\chi_{\Lambda_\varepsilon}(T_n)\xi\|^2 &= \langle \xi, \chi_{\Lambda_\varepsilon}(T_n)\xi \rangle \\ &\leq \langle \xi, f_\varepsilon(T_n)\xi \rangle \leq \|f_\varepsilon(T_n)\|,\end{aligned}$$

and $\|\chi_{\Lambda_\varepsilon}(T_n)\| < 1$ for large n. Since $\chi_{\Lambda_\varepsilon}(T_n)$ are projection operators, it follows that $\chi_{\Lambda_\varepsilon}(T_n) = 0$ and so $t_0 \in \rho(T_n)$ for all n large enough. This finishes the proof. Note that the norm convergence was crucial in the argument. □

The conclusions of Proposition 10.2.4b) may not hold if only strong convergence is required. See Examples 10.3.3 and 10.3.4.

Corollary 10.2.5. *Let $T_n \xrightarrow{\text{NR}} T$. Then:*

a) *If $(a, b) \subset \rho(T)$, then $\chi_{(a,b)}(T_n) = 0$ for n sufficiently large.*
b) *$\sigma(T)$ is the set of $t_0 \in \mathbb{R}$ for which there is a sequence $t_n \to t_0$ with $t_n \in \sigma(T_n)$.*
c) *If $\{a, b\} \subset \rho(T)$, then $\chi_{(a,b)}(T_n) \to \chi_{(a,b)}(T)$ in $\mathrm{B}(\mathcal{H})$.*

Proof. a) was presented in the proof of Proposition 10.2.4.

b) is just a restatement of Proposition 10.2.4.

c) Since $\rho(T)$ is an open set, there is $\varepsilon > 0$ so that $(a, a + \varepsilon)$ and $(b - \varepsilon, b)$ are subsets of $\rho(T)$. Let $\Omega_\varepsilon = [a + \varepsilon, b - \varepsilon]$ and $f_\varepsilon \in C_0^\infty(\mathbb{R})$ with

$$\chi_{\Omega_\varepsilon} \leq f_\varepsilon \leq \chi_{(a,b)}.$$

Thus $\chi_{(a,b)}(T) = f_\varepsilon(T)$ and by a) one has $\chi_{(a,b)}(T_n) = f_\varepsilon(T_n)$ for n sufficiently large. Hence

$$\|\chi_{(a,b)}(T) - \chi_{(a,b)}(T_n)\| = \|f_\varepsilon(T_n) - f_\varepsilon(T)\|$$

which vanishes as $n \to \infty$ (see Exercise 10.1.14). □

Exercise 10.2.6. If $T_n \xrightarrow{\text{NR}} T$ and $\{a, b\} \subset \rho(T)$, show that $\mu_\xi^{T_n}(a, b) \to \mu_\xi^T(a, b)$, $\forall \xi \in \mathcal{H}$.

Remark 10.2.7. With respect to these types of convergences of self-adjoint operators, it is found that weak/strong can be combined with resolvent/dynamical sense resulting in equivalent concepts. However, in general norm resolvent convergence is not equivalent to strong resolvent convergence and, as Example 10.3.1 shows, convergence in the NR sense is not equivalent to ND sense either.

Remark 10.2.8. There are other notions of convergence of unbounded operators, e.g., graph convergence, usually related to convergence in the resolvent sense. See [Kat80],[ReeS81] and [Dav80].

10.3 Examples

Example 10.3.1. let $\mathcal{H} = \mathrm{L}^2(\mathbb{R})$. Consider $T_n = \mathcal{M}_{x - x/n}$ and $T = \mathcal{M}_x$, $x \in \mathbb{R}$. A simple calculation shows that

$$R_i(T_n) - R_i(T) = \mathcal{M}_{\varphi_n},$$

with

$$\varphi_n(x) = \frac{1}{n} \, \frac{x}{(1 - \frac{1}{n})x^2 - 1 + ix(\frac{1}{n} - 2)},$$

which converges uniformly to the zero function for $n \to \infty$. Hence, $T_n \xrightarrow{\text{NR}} T$. However, since for any $t \in \mathbb{R}$ (see Example 1.1.16),

$$\left\| e^{-itT} - e^{-itT_n} \right\| = \left\| e^{-itx} - e^{-itx(1-1/n)} \right\|_\infty = 2, \qquad \forall n,$$

convergence in the norm dynamical sense does not take place. Therefore, the NR convergence does not infer ND convergence.

Exercise 10.3.2. Show that NR convergence implies SD convergence (cf. Example 10.3.1).

Example 10.3.3. Let (ξ_n) be an orthonormal basis of $\mathcal{H}$, $\dim \mathcal{H} = \infty$, and P_n the orthogonal projection onto the subspace spanned by the vectors $\{\xi_1, \ldots, \xi_n\}$; then $P_n \xrightarrow{\text{s}} \mathbf{1}$ and so $P_n \xrightarrow{\text{SR}} \mathbf{1}$ (Proposition 10.1.13). Now, $\sigma(P_n) = \{0, 1\}$, $\forall n$, while $\sigma(\mathbf{1}) = \{1\}$.

Example 10.3.4. Consider the multiplication operators $T_n = \mathcal{M}_{x/n}$ and $T = 0$ in $\mathrm{L}^2(\mathbb{R})$. By Example 10.1.19, $T_n \xrightarrow{\text{SR}} T$. Now, $\sigma(T_n) = \mathbb{R}$, $\forall n$, while $\sigma(T) = \{0\}$; thus, by Proposition 10.2.4, T_n does not converge in the norm resolvent sense to T.

Remark 10.3.5. The above examples show that $T_n \xrightarrow{\text{SR}} T$ does not ensure the strong convergence of spectral projections $\chi_\Lambda(T_n) \xrightarrow{\text{s}} \chi_\Lambda(T)$ (cf. Prop. 10.1.9).

Exercise 10.3.6. Let $T = \mathcal{M}_x$ in $\mathrm{L}^2(\mathbb{R})$ and $T_n(x) = \chi_{[-n,n]}(x)\mathcal{M}_x$. Show that, for each $\psi \in \mathrm{L}^2(\mathbb{R})$,

$$R_i(T_n)\psi - R_i(T)\psi \to 0, \qquad n \to \infty.$$

It is a sequence T_n of bounded operators that converges in the strong resolvent sense to an unbounded operator T. Discuss the relation between the spectra of T_n and T.

Exercise 10.3.7. Let T be a self-adjoint operator and $T(\lambda) = \lambda T$, $\lambda \in \mathbb{R}$. Show that, in the strong resolvent sense, $T(\lambda)$ converges to the null operator as $\lambda \to 0$ and that it does not converge to any operator as $|\lambda| \to \infty$.

Example 10.3.8 (Perturbation of a self-adjoint operator). Let T be self-adjoint and $\mathcal{D}$ a core of T. Let B be symmetric with $\mathcal{D} \subset \operatorname{dom} B$. Suppose that $T + \lambda B$ is self-adjoint, for all real λ in a neighborhood of zero, with $\mathcal{D} \subset \operatorname{dom}\,(T + \lambda B)$.

Proposition 10.3.9. *Under the above conditions one has*

i) $(T + \lambda B) \xrightarrow{\text{SR}} T$ *as* $\lambda \to 0$.

ii) *If* $B \in \mathrm{B}(\mathcal{H})$, *then* $(T + \lambda B) \xrightarrow{\text{NR}} T$ *as* $\lambda \to 0$.

Proof. Note first that $W := (T - i\mathbf{1})\mathcal{D}$ is dense in $\mathcal{H}$ (the deficiency indices of $T|_{\mathcal{D}}$ are zero). For $\eta \in W$ one has $\eta = (T - i\mathbf{1})\xi$, $\xi \in \mathcal{D}$, and by the second resolvent identity,

$$\begin{aligned} R_i(T)\eta - R_i(T + \lambda B)\eta &= \lambda R_i(T + \lambda B) B R_i(T)\eta \\ &= \lambda R_i(T + \lambda B) B\xi. \end{aligned}$$

i) Since $\|R_i(T + \lambda B)\| \le 1$, $\forall\lambda$ (including $\lambda = 0$):

$$\|R_i(T)\eta - R_i(T + \lambda B)\eta\| \le |\lambda|\,\|B\xi\|$$

which vanishes as $\lambda \to 0$. Since these resolvent operators are uniformly bounded, this strong convergence on the dense set W extends to $\mathcal{H}$ and i) follows.

ii) Similarly to i) one gets

$$\|R_i(T) - R_i(T + \lambda B)\| \le |\lambda|\,\|R_i(T + \lambda B)\|\,\|B\|\,\|R_i(T)\| \le |\lambda|\,\|B\|,$$

which vanishes as $\lambda \to 0$ and ii) follows. □

Corollary 10.3.10. *Under the conditions in Proposition* 10.3.9*:*

i) *If* $t_0 \in \sigma(T)$, *then there exists* $t_\lambda \in \sigma(T + \lambda B)$ *with*

$$t_0 = \lim_{\lambda \to 0} t_\lambda.$$

ii) *For all continuous and bounded functions* $f : \mathbb{R} \to \mathbb{C}$ *one has*

$$f(T)\xi = \lim_{\lambda\to 0} f(T + \lambda B)\xi, \qquad \forall \xi \in \mathcal{H}.$$

This holds, in particular, for the evolution groups

$$\lim_{\lambda\to 0} e^{-it(T+\lambda B)}\xi = e^{-itT}\xi, \qquad \forall \xi \in \mathcal{H},$$

for each fixed $t \in \mathbb{R}$*.*

In case B is T-bounded with $N_T(B) < 1$, the Kato-Rellich Theorem 6.1.8 holds and so the above results apply. In particular if $T = H_0$ in $\mathrm{L}^2(\mathbb{R}^n)$, $n \le 3$ (the free energy), and $B \in \mathrm{L}^2(\mathbb{R}^n) + \mathrm{L}^\infty(\mathbb{R}^n)$ (see Kato's Theorem 6.2.2).

Example 10.3.11. Consider the free energy operator H_0 in $\mathrm{L}^2(\mathbb{R})$ and $V_\lambda(x) = \lambda x^2$. The Schwartz space $\mathcal{S}(\mathbb{R})$ is a core of H_0 (Proposition 3.4.1) and is in the domain of V_λ for all $\lambda \in \mathbb{R}$. The "perturbed" operator

$$(H_\lambda\psi)(x) = (H_0\psi)(x) + (V_\lambda\psi)(x) = -\psi''(x) + \lambda x^2\psi(x)$$

is a harmonic oscillator (Example 2.3.3) if $\lambda > 0$. By Proposition 10.3.9 it follows that

$$H_\lambda \xrightarrow{\mathrm{SR}} H_0, \qquad \lambda \to 0, \qquad \lambda \in \mathbb{R}.$$

Recall that $\sigma(H_0) = [0, \infty)$ while for $\lambda > 0$,

$$\sigma(H_\lambda) = \{\sqrt{\lambda}\,(2j+1) : j = 0, 1, 2, \dots\}.$$

Note the interesting changing of the spectrum of H_λ at $\lambda = 0$ and its relation to Corollary 10.3.10.

Exercise 10.3.12. Based on Example 2.3.3, confirm the above spectrum $\sigma(H_\lambda)$ for $\lambda > 0$.

Example 10.3.13. Let $\operatorname{dom} H_D = \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = 0 = \psi(1)\}$, $\operatorname{dom} H_N = \{\psi \in \mathcal{H}^2[0,1] : \psi'(0) = 0 = \psi'(1)\}$ and both operators with the same action $\psi \mapsto -\psi''$. Both are self-adjoint operators (see, for instance, Example 7.3.1).

By Example 4.4.3, the self-adjoint Friedrichs extension of the operator sum $H = H_N + H_D$, $\operatorname{dom} H = \operatorname{dom} H_D \cap \operatorname{dom} H_N = \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = \psi'(0) = 0 = \psi(1) = \psi'(1)\}$, $H\psi = -\psi''$, is the operator H_D.

If $(H_N + \lambda H_D)_F$ denotes the Friedrichs extension of $H_N + \lambda H_D$, then the above remark implies that for any $\lambda > 0$,

$$(H_N + \lambda H_D)_F = (1 + \lambda)\, H_D;$$

by Proposition 10.1.18 (or Proposition 10.3.9), it is found that

$$(H_N + \lambda H_D)_F \xrightarrow{\mathrm{SR}} H_D, \qquad \lambda \to 0.$$

This example illustrates how "fragile" the sum of operators via sesquilinear forms can be!

10.3.1 Nonrelativistic Limit of Dirac Operator

Consider the one-dimensional free Dirac operator $D_0 = D_0(c)$ that has appeared in Exercise 2.6.12, where $c > 0$ denotes the speed of light. D_0 is self-adjoint, acting on some two-component functions (the meaning of the notation should be clear) given by

$$\text{dom } D_0 = \mathcal{H}^1(\mathbb{R};\mathbb{C}^2) \sqsubseteq \mathcal{H} := \mathrm{L}^2(\mathbb{R};\mathbb{C}^2) = \mathrm{L}^2(\mathbb{R}) \oplus \mathrm{L}^2(\mathbb{R}),$$

independent of $c > 0$, and action

$$D_0 := -ic\frac{d}{dx}\sigma_1 + mc^2\sigma_3,$$

with

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \text{and} \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

denoting standard Pauli matrices and m the mass of the particle. Note that Planck's constant $\hbar = 1$. If $P = -id/dx$ denotes the momentum operator on $\mathbb{R}$ (see Example 2.3.11 and Section 3.3), in a compact form one has

$$D_0(c) = \begin{pmatrix} mc^2 & -ic\frac{d}{dx} \\ -ic\frac{d}{dx} & -mc^2 \end{pmatrix} = \begin{pmatrix} mc^2 & cP \\ cP & -mc^2 \end{pmatrix}.$$

The Dirac operator is a relativistic version of the Schrödinger operator for particles of spin 1/2; details can be found, for instance, in [Tha92]. Dirac's original arguments [Dir58] to get his operator is a masterpiece in physics.

The question here is the *nonrelativistic limit* of $D_0(c)$, which is characterized by taking $c \to \infty$ (try directly from the action of D_0!) and relating it to the free Schrödinger operator H_0 via convergence in the resolvent sense. Some pertinent notation is introduced:

$$\mathbf{1}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad F_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad F_- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

are the 2×2 identity matrix and the projections $F_\pm$ onto the upper ("positive energy") and lower ("negative energy") components of vectors in $\mathrm{L}^2(\mathbb{R};\mathbb{C}^2)$, respectively. Write also

$$W = P\sigma_1 \qquad \text{and} \qquad \tilde{D}_0(c) = D_0 - mc^2\mathbf{1}_2.$$

Since mc^2 is the particle rest energy, a pure relativistic factor, it must be subtracted from D_0 before taking $c \to \infty$, so the importance of considering the operator $\tilde{D}_0$.

Introduce the operators

$$A_\pm = \tilde{D}_0 \pm i\mathbf{1}_2 = cW \pm 2mc^2F_\pm \pm i\mathbf{1}_2,$$

and check that

$$A_+A_- = A_-A_+ = c^2W^2 - \big(2mc^2 i - 1\big)\,\mathbf{1}_2.$$

Since $R_{\mp i}(\tilde{D}_0) = A_\pm^{-1} = A_\mp\,(A_\pm A_\mp)^{-1}$, one gets

$$R_{\mp i}(\tilde{D}_0) = \frac{1}{2mc^2} A_\mp \left(\frac{1}{2m}W^2 - \left(i - \frac{1}{2mc^2}\right)\mathbf{1}_2\right)^{-1}.$$

Using the relation

$$(A+B)^{-1} = (\mathbf{1} + A^{-1}B)^{-1}A^{-1}$$

with

$$A = \frac{1}{2m}W^2 - i\mathbf{1}_2, \qquad B = \frac{1}{2mc^2}\mathbf{1}_2,$$

it follows that the resolvent operator can be put in the form

$$\begin{aligned} R_i\left(\tilde{D}_0\right) &= \frac{1}{2mc^2}A_+\left(\mathbf{1} - \frac{R_i(h)}{2mc^2}\right)^{-1}\left(\frac{W^2}{2m} - i\mathbf{1}\right)^{-1} \\ &= \left(F_+ + \frac{cW - i\mathbf{1}_2}{2mc^2}\right)\left(\mathbf{1} + \frac{1}{2mc^2}R_i(h)\right)^{-1} R_i(h), \end{aligned}$$

where

$$h = \frac{1}{2m}W^2 = \begin{pmatrix} H_0 & 0 \\ 0 & H_0 \end{pmatrix},$$

with $H_0 = -\Delta/(2m)$ denoting the self-adjoint (nonrelativistic) free hamiltonian operator on $\mathbb{R}$ with domain $\mathcal{H}^2(\mathbb{R})$ (see Section 3.4) and explicit mass term $1/(2m)$.

Since h is self-adjoint $\|R_i(h)\| \le 1$ and so, in the norm of $\mathrm{B}(\mathcal{H})$, one obtains

$$\lim_{c\to\infty}\left(\mathbf{1} + \frac{1}{2mc^2}R_i(h)\right)^{-1} = \mathbf{1}.$$

Now, by the spectral theorem one has $\|WR_i(W^2)\| \le 1$; consequently, in $\mathrm{B}(\mathcal{H})$,

$$\lim_{c\to\infty}\frac{cW - i\mathbf{1}_2}{2mc^2}R_i(h) = 0.$$

Therefore,

$$\lim_{c\to\infty} R_i\left(\tilde{D}_0(c)\right) = F_+R_i\,(h)\,.$$

Similarly one gets $R_{-i}\left(\tilde{D}_0(c)\right) \to F_+R_{-i}\,(h)$. Such results can be interpreted as the convergence of $\tilde{D}_0(c)$ to the positive energy component of h in the norm resolvent sense. This supports the nonrelativistic theory, since it means that the free Dirac $D_0(c)$ has the free Schrödinger operator H_0 as the limiting case of light travelling at infinite speed.

Remark 10.3.14. If $\hat{D}_0(c) = D_0 + mc^2\mathbf{1}_2$ is considered, one gets that $R_i(\hat{D}_0(c))$ converges to $F_- R_i\,(-h)$ in the norm as $c \to \infty$; to some extent, the interpretations of such positive and negative components of the free energy in Dirac theory are as controversial as interesting, but will not be discussed here [Tha92]. The presence of some potentials (i.e., $D(c) = D_0(c) + V\mathbf{1}_2$), instead of just the free case, as well as Dirac operators in $\mathbb{R}^n$, $n \geq 1$, are allowed and nonrelativistic limits dealt with in a somewhat similar way.

Remark 10.3.15. Readers are recommended to check the traditional (and formal) prescription for the nonrelativistic limit of the Dirac operator in textbooks on quantum mechanics for physicists.

Exercise 10.3.16. Verify the relation

$$(A + B)^{-1} = (\mathbf{1} + A^{-1}B)^{-1}A^{-1}$$

used in the above nonrelativistic limit.

Exercise 10.3.17. If T is self-adjoint, show that $\|TR_i(T^2)\| \leq 1$.

10.4 Sesquilinear Form Convergence

In some cases of monotone sequences of positive self-adjoint operators, it is possible to conclude convergence in the strong resolvent sense from the convergence of the corresponding generated sesquilinear forms. Such an approach has the advantage that sometimes nondense domains in the underlying Hilbert space $\mathcal{H}$ are allowed! This phenomenon will be illustrated by a physical application in Section 10.5. Most of the results reported here have their roots in [Kat80], [Dav80], [Rob71] and [Sim78].

10.4.1 Nondecreasing Sequences

Let b be a closed positive sesquilinear form with domain $\operatorname{dom} b \subset \mathcal{H}$ and $\mathcal{H}_0 = \overline{\operatorname{dom} b}$, which does not necessarily coincide with $\mathcal{H}$. Thus, by Theorem 4.2.6, b is the sesquilinear form associated with a positive self-adjoint operator T with $\operatorname{dom} T \sqsubseteq \mathcal{H}_0$. If P_0 denotes the orthogonal projection onto $\mathcal{H}_0$, for $\lambda > 0$ one defines the *pseudoresolvent operator* $\tilde{R}_{-\lambda}(T)$ on $\mathcal{H}$ by

$$\langle \tilde{R}_{-\lambda}(T)\xi, \eta\rangle := \left\langle (T + \lambda\mathbf{1})^{-1} P_0\xi, P_0\eta \right\rangle, \qquad \xi, \eta \in \mathcal{H}.$$

Definition 10.4.1. Let $\mathcal{H}_0$ be a closed subspace of $\mathcal{H}$, P_0 the orthogonal projection onto $\mathcal{H}_0$, T_j, T be positive self-adjoint operators with $\operatorname{dom} T_j \sqsubseteq \mathcal{H}$ and $\operatorname{dom} T \sqsubseteq \mathcal{H}_0$. The expression "$T_j$ converges in the strong convergence sense to T in $\mathcal{H}_0$" (or in symbols "$T_j \xrightarrow{\text{SR}} T$ in $\mathcal{H}_0$") will indicate that

$$\lim_{j\to\infty} R_{-\lambda}(T_j)P_0\xi = \tilde{R}_{-\lambda}(T)\xi, \qquad \forall\xi \in \mathcal{H}, \forall\lambda > 0.$$

Similarly for other types of convergence, e.g., NR in $\mathcal{H}_0$. $\tilde{R}_{-\lambda}(T_j)$ will be a shorthand for $R_{-\lambda}(T_j)P_0$.

The main result in this section, i.e., Theorem 10.4.2, is related to the following setting. Suppose (T_j) is a nondecreasing sequence of positive self-adjoint operators with dom $T_j \sqsubseteq \mathcal{H}$ so that dom $T_j \supset$ dom T_{j+1}, and $T_j \leq T_{j+1}$ (i.e., $\langle T_j\xi, \xi\rangle \leq \langle T_{j+1}\xi, \xi\rangle$, $\forall \xi \in$ dom T_{j+1}), $\forall j \in \mathbb{N}$. Write $b^j = b^{T_j}$ for the sesquilinear form generated by T_j (see Section 9.3), that is,

$$b^j(\xi, \eta) = \left\langle T_j^{\frac{1}{2}}\xi, T_j^{\frac{1}{2}}\eta \right\rangle, \qquad \xi, \eta \in \operatorname{dom} b^j = \operatorname{dom} T_j^{\frac{1}{2}},$$

and set

$$\mathcal{D} := \left\{ \xi \in \bigcap_j \operatorname{dom} b^j : \lim_{j\to\infty} b^j(\xi) < \infty \right\},$$

and let $\mathcal{H}_0$ be the closure of $\mathcal{D}$ in $\mathcal{H}$; $\mathcal{D}$ is not supposed to be dense in $\mathcal{H}$. For sesquilinear forms the relation $b^j \leq b^{j+1}$ means $b^j(\xi) \leq b^{j+1}(\xi)$, $\forall \xi \in \mathcal{H}$ (recall that $b(\xi) = \infty$ if $\xi \notin$ dom b); note that this automatically implies dom $b^{j+1} \subset$ dom b^j.

Theorem 10.4.2 (Kato-Robinson). *Let (T_j), $\mathcal{D}$, $\mathcal{H}$ and $\mathcal{H}_0$ be as described above. Then, there is a positive self-adjoint operator T with* dom $T \sqsubseteq \mathcal{H}_0$, dom $T^{\frac{1}{2}} = \mathcal{D}$, *so that $T_j \xrightarrow{\text{SR}} T$ in $\mathcal{H}_0$ and the form generated by T is given by the limit*

$$b^T(\xi) := \left\langle T^{\frac{1}{2}}\xi, T^{\frac{1}{2}}\xi \right\rangle = \lim_{j\to\infty} \left\langle T_j^{\frac{1}{2}}\xi, T_j^{\frac{1}{2}}\xi \right\rangle, \qquad \forall \xi \in \mathcal{D}.$$

First some preparatory facts for the proof of this theorem.

Lemma 10.4.3. *Let $S, Q \in \mathrm{B}(\mathcal{H})$ be (self-adjoint) positive and invertible in $\mathrm{B}(\mathcal{H})$. If $Q \geq S \geq 0$, then $S^{-1} \geq Q^{-1} \geq 0$.*

Proof. Introduce the self-adjoint operator $C := Q^{-1/2}SQ^{-1/2}$. Then $C \leq \mathbf{1}$, since for all $\xi \in \mathcal{H}$,

$$\langle \xi, C\xi\rangle = \left\langle Q^{-1/2}\xi, SQ^{-1/2}\xi \right\rangle \leq \left\langle Q^{-1/2}\xi, QQ^{-1/2}\xi \right\rangle = \langle \xi, \mathbf{1}\xi\rangle .$$

By the spectral theorem (see Proposition 8.3.21), $\langle \xi, C\xi\rangle = \int_{[0,1]} x \, d\mu_\xi^C(x)$ and so

$$\left\langle \xi, C^{-1}\xi \right\rangle = \int_{[0,1]} \frac{1}{x} \, d\mu_\xi^C(x) \geq \int_{[0,1]} 1 \, d\mu_\xi^C(x) = \langle \xi, \mathbf{1}\xi\rangle,$$

that is, $Q^{1/2}S^{-1}Q^{1/2} = C^{-1} \geq \mathbf{1}$. Now,

$$\begin{aligned} \left\langle \xi, S^{-1}\xi \right\rangle &= \left\langle Q^{-1/2}\xi, C^{-1}Q^{-1/2}\xi \right\rangle \\ &\geq \left\langle Q^{-1/2}\xi, Q^{-1/2}\xi \right\rangle = \left\langle \xi, Q^{-1}\xi \right\rangle, \qquad \forall \xi \in \mathcal{H}, \end{aligned}$$

and $S^{-1} \geq Q^{-1}$. □

Lemma 10.4.4. *Let T_1, T_2 be two positive self-adjoint operators with domains dense in the closed subspace $\mathcal{H}_0$ of $\mathcal{H}$, and b^1, b^2 the sesquilinear forms generated by T_1, T_2, respectively. Then, for any $\lambda > 0$, $b^1 \le b^2$ iff $\tilde{R}_{-\lambda}(T_2) \le \tilde{R}_{-\lambda}(T_1)$.*

Proof. Since $\lambda > 0$ the resolvent operators in the statement of the lemma are bounded, self-adjoint and positive. Assume first that $\tilde{R}_{-\lambda}(T_2) \le \tilde{R}_{-\lambda}(T_1)$ and denote by P_0 the orthogonal projection onto $\mathcal{H}_0$. Since

$$\tilde{R}_{-\lambda}(T_2) + \frac{1}{n}\mathbf{1} \le \tilde{R}_{-\lambda}(T_1) + \frac{1}{n}\mathbf{1}, \qquad \forall n,$$

by Lemma 10.4.3 one has the inequality

$$0 \le \left(\tilde{R}_{-\lambda}(T_1) + \frac{1}{n}\mathbf{1}\right)^{-1} \le \left(\tilde{R}_{-\lambda}(T_2) + \frac{1}{n}\mathbf{1}\right)^{-1},$$

and the functional calculus implies, for $j = 1, 2$,

$$\begin{aligned}\lim_{n\to\infty} & \left\langle \left(\tilde{R}_{-\lambda}(T_j) + \frac{1}{n}\mathbf{1}\right)^{-1} \xi, \xi \right\rangle \\ &= \lim_{n\to\infty} \left[\langle n\,(T_j + \lambda\mathbf{1}) R_{-\lambda-n}(T_j) P_0\xi, P_0\xi\rangle + n\,\langle(\mathbf{1} - P_0)\xi, \xi\rangle\right] \\ &= (b^j + \lambda)(\xi, \xi), \qquad \forall \xi \in \mathcal{H}.\end{aligned}$$

Recall that $(b^j + \lambda)(\xi, \eta) := b^j(\xi, \eta) + \lambda\langle\xi, \eta\rangle$ and $b^j(\xi) = \infty$ iff $\xi \notin \operatorname{dom} b^j$, $j = 1, 2$. Together with the above inequality, it follows that $b^1 \le b^2$ (the motivation for considering the operator in the above square brackets comes from $(1/(x+\lambda) + 1/n)^{-1} = n(x+\lambda)/(x+n+\lambda)$).

Now assume that $b^1 \le b^2$, which implies that $\operatorname{dom} T_2 \subset \operatorname{dom} T_1$. For $\xi \in \mathcal{H}_0$ set $\xi_j = \tilde{R}_{-\lambda}(T_j)\xi$, $j = 1, 2$, and note that $\xi_1, \xi_2 \in \operatorname{dom} T_1 \subset \mathcal{H}_0$. By Cauchy-Schwarz (Exercise 4.1.5),

$$\begin{aligned}\left\langle \tilde{R}_{-\lambda}(T_2)\xi, \xi \right\rangle^2 &= \langle \xi_2, (T_1 + \lambda\mathbf{1})\xi_1\rangle^2 = \left((b^1 + \lambda)(\xi_2, \xi_1)\right)^2 \\ &\le (b^1 + \lambda)(\xi_2)\,(b^1 + \lambda)(\xi_1) \\ &\le (b^2 + \lambda)(\xi_2)\,(b^1 + \lambda)(\xi_1) \\ &= \left\langle \tilde{R}_{-\lambda}(T_2)\xi, \xi \right\rangle \left\langle \tilde{R}_{-\lambda}(T_1)\xi, \xi \right\rangle,\end{aligned}$$

and so $\left\langle \tilde{R}_{-\lambda}(T_2)\xi, \xi \right\rangle \le \left\langle \tilde{R}_{-\lambda}(T_1)\xi, \xi \right\rangle$, $\forall \xi \in \mathcal{H}_0$. This also holds for $\xi \in \mathcal{H}$ since both sides vanish as $\xi \in \mathcal{H}_0^\perp$. This proves $\tilde{R}_{-\lambda}(T_2) \le \tilde{R}_{-\lambda}(T_1)$. □

Proof. [**Theorem 10.4.2**] Define the positive form b by the monotone increasing limit

$$b(\xi) := \lim_{j\to\infty} b^j(\xi), \qquad \forall \xi \in \mathcal{H}.$$

Note that $b(\xi) < \infty$ iff $\xi \in \mathcal{D}$, so that $\mathcal{D} = \operatorname{dom} b$. By Theorem 9.3.11, each function $\xi \mapsto b^j(\xi)$ is lower semicontinuous, so that b is also positive and lower semicontinuous; define $b(\xi, \eta)$ by polarization (Exercise 4.1.1). Again by Theorem 9.3.11, b is the form generated by a positive self-adjoint operator T with $\operatorname{dom} T \sqsubseteq \mathcal{H}_0$, and so the notation $b = b^T$ will be used.

Since $b^j \leq b^{j+1} \leq b^T$, $\forall j$, by Lemma 10.4.4, for any $\lambda > 0$ one has $\tilde{R}_{-\lambda}(T) \leq \tilde{R}_{-\lambda}(T_{j+1}) \leq \tilde{R}_{-\lambda}(T_j)$, $\forall j$, so

$$\lim_{j\to\infty} \left\langle \tilde{R}_{-\lambda}(T_j)\xi, \xi \right\rangle = \inf_j \left\langle \tilde{R}_{-\lambda}(T_j)\xi, \xi \right\rangle \geq \left\langle \tilde{R}_{-\lambda}(T)\xi, \xi \right\rangle$$

and the limit is finite for $\xi \in \mathcal{H}_0$; note that

$$\left\langle \tilde{R}_{-\lambda}(T_j)\xi, \xi \right\rangle = \left\langle \tilde{R}_{-\lambda}(T_j)^{1/2}\xi, \tilde{R}_{-\lambda}(T_j)^{1/2}\xi \right\rangle = \left\| \tilde{R}_{-\lambda}(T_j)^{1/2}\xi \right\|^2 .$$

Hence, by polarization, there exists the limit

$$t(\xi, \eta) := \lim_{j\to\infty} \left\langle \tilde{R}_{-\lambda}(T_j)\xi, \eta \right\rangle, \qquad \forall \xi, \eta \in \mathcal{H}_0,$$

which defines a positive (hermitian) sesquilinear form t, and since

$$t(\xi, \xi) \leq \lim_{j\to\infty} \|\tilde{R}_{-\lambda}(T_j)\| \|\xi\|^2 \leq \frac{1}{\lambda} \|\xi\|^2,$$

t is bounded and $\|t\| \leq 1/\lambda$. By Proposition 4.1.3 there is a unique bounded and self-adjoint operator $C = C(\lambda) \in B(\mathcal{H}_0)$ so that $\|C\| \leq 1/\lambda$ and $\langle C\xi, \eta\rangle = t(\xi, \eta)$, $\forall \xi, \eta \in \mathcal{H}_0$. Explicitly

$$\langle C\xi, \eta\rangle = \lim_{j\to\infty} \left\langle \tilde{R}_{-\lambda}(T_j)\xi, \eta \right\rangle,$$

and $\tilde{R}_{-\lambda}(T_j)$ converges weakly to C. Note the following properties of C:

- $\langle C\xi, \xi\rangle \geq \left\langle \tilde{R}_{-\lambda}(T)\xi, \xi \right\rangle$, for all $\xi \in \mathcal{H}_0$.
- C is invertible. To check this, suppose $C\xi = 0$ for some $\xi \in \mathcal{H}_0$; then $0 = \langle C\xi, \xi\rangle \geq \left\langle \tilde{R}_{-\lambda}(T)\xi, \xi \right\rangle$. Write $\eta = \tilde{R}_{-\lambda}(T)\xi$; since T is positive, one has $0 \geq \langle \eta, (T + \lambda\mathbf{1})\eta\rangle \geq \lambda\|\eta\|^2$, so $\eta = 0$ and then $\xi = 0$. Hence C is invertible.

If b^S is the sesquilinear form generated by $S = C^{-1} - \lambda\mathbf{1}$, from the relation $\tilde{R}_{-\lambda}(T_j) \geq C \geq \tilde{R}_{-\lambda}(T)$ and Lemma 10.4.4 one finds $b^j \leq b^S \leq b^T$, and since $b^T = \lim_j b^j$ it follows that $b^S = b^T$, so $T = S$ and $C = \tilde{R}_{-\lambda}(T)$. Therefore, $\tilde{R}_{-\lambda}(T_j)$ converges weakly to $\tilde{R}_{-\lambda}(T)$ in $\mathcal{H}_0$.

Lemma 10.4.5. *For all $\lambda > 0$, $\tilde{R}_{-\lambda}(T_j)$ converges strongly to $\tilde{R}_{-\lambda}(T)$ in $\mathcal{H}_0$.*

Proof. All arguments are restricted to $\mathcal{H}_0$. Since $\tilde{R}_{-\lambda}(T_j)$ is a uniformly bounded sequence of self-adjoint operators (by Proposition 9.5.2, $\|\tilde{R}_{-\lambda}(T_j)\| \le 1/|\lambda|$), it follows that $A_j := \tilde{R}_{-\lambda}(T_j) - \tilde{R}_{-\lambda}(T)$ is a positive sequence of bounded self-adjoint operators that converges weakly to zero. Let $a^j(\xi,\eta) = \langle \xi, A_j\eta\rangle$, $\xi,\eta \in \mathcal{H}_0$, be the positive sesquilinear form generated by A_j; note that $\|a_j\| \le 2/|\lambda|$, $\forall j$. By Cauchy-Schwarz (Exercise 4.1.5),

$$\begin{aligned}\|A_j\xi\|^4 &= |a^j(A_j\xi,\xi)|^2 \le |a^j(\xi)|\,|a^j(A_j\xi)| \\ &\le |\langle A_j\xi,\xi\rangle|\,\|a_j\|\,\|A_j\xi\|^2 \le \frac{2}{|\lambda|}|\langle A_j\xi,\xi\rangle|\,\|A_j\xi\|^2,\end{aligned}$$

consequently

$$\|A_j\xi\|^2 \le \frac{2}{|\lambda|}\,|\langle A_j\xi,\xi\rangle| \stackrel{j\to\infty}{\longrightarrow} 0, \qquad \forall \xi \in \mathcal{H}_0.$$

This proves the lemma. □

Combine Proposition 10.1.23 and Lemma 10.4.5 to get the convergence $T_j \stackrel{\text{SR}}{\longrightarrow} T$ in $\mathcal{H}_0$. □

Exercise 10.4.6. Adapt the proof of Lemma 10.4.5 to show that if a sequence of uniformly bounded and positive self-adjoint operators converges weakly to zero, then it actually converges strongly to zero.

Exercise 10.4.7. Use Hellinger-Toeplitz (Proposition 2.1.27) to show that the operator C, defined in the proof of Theorem 10.4.2 as the weak limit of $\tilde{R}_{-\lambda}(T_j)$, is bounded, that is, $C \in \mathrm{B}(\mathcal{H}_0)$.

Remark 10.4.8. Note that a solution to Exercise 10.4.6 can be obtained as a consequence of Theorem 10.1.15. The alternative proof that relies on Lemma 10.4.5 is of independent interest.

This subsection ends with a sufficient condition for norm resolvent convergence in the Kato-Robinson Theorem.

Proposition 10.4.9. *Let T_j, T be as in Theorem* 10.4.2. *If for some $\lambda > 0$ the operators $\tilde{R}_{-\lambda}(T_j) - R_{-\lambda}(T)$ are compact in $\mathcal{H}_0$, $\forall j$, then $T_j \stackrel{\text{NR}}{\longrightarrow} T$ in $\mathcal{H}_0$.*

Proof. By Kato-Robinson, the sequence of bounded self-adjoint and positive operators

$$C_j := \tilde{R}_{-\lambda}(T_j) - R_{-\lambda}(T) \ge 0$$

converges strongly to zero in $\mathcal{H}_0$; also $C_j \ge C_{j+1}$, $\forall j$. Since C_1 is compact, given $\varepsilon > 0$ the spectral theorem for compact operators, Theorem 8.1.4, and Proposition 1.6.6 imply that there is a finite-dimensional subspace E_ε that reduces C_1 and $\|C_1\eta\| < \varepsilon\|\eta\|$ for all $\eta \in E_\varepsilon^\perp$.

For $\xi \in \mathcal{H}_0$ write $\xi = \xi_\varepsilon + \xi_\varepsilon^\perp$, with $\xi_\varepsilon \in E_\varepsilon$ and $\xi_\varepsilon^\perp \in E_\varepsilon^\perp$. Thus

$$\begin{aligned}0 \le \langle C_j\xi, \xi\rangle &= \left\| C_j^{1/2}(\xi_\varepsilon + \xi_\varepsilon^\perp)\right\|^2 \le \left(\left\|C_j^{1/2}\xi_\varepsilon\right\| + \left\|C_j^{1/2}\xi_\varepsilon^\perp\right\|\right)^2 \\ &= \left\|C_j^{1/2}\xi_\varepsilon\right\|^2 + \left\|C_j^{1/2}\xi_\varepsilon^\perp\right\|^2 + 2\left\|C_j^{1/2}\xi_\varepsilon\right\| \left\|C_j^{1/2}\xi_\varepsilon^\perp\right\| \\ &\le 2\left\|C_j^{1/2}\xi_\varepsilon\right\|^2 + 2\left\|C_j^{1/2}\xi_\varepsilon^\perp\right\|^2 = 2\langle C_j\xi_\varepsilon, \xi_\varepsilon\rangle + 2\langle C_j\xi_\varepsilon^\perp, \xi_\varepsilon^\perp\rangle.\end{aligned}$$

For all j one has $0 \le \langle C_j\xi_\varepsilon^\perp, \xi_\varepsilon^\perp\rangle \le \langle C_1\xi_\varepsilon^\perp, \xi_\varepsilon^\perp\rangle \le \varepsilon\|\xi_\varepsilon^\perp\|^2$. On the other hand, since E_ε is finite dimensional, the convergence of the restriction $C_j|_{E_\varepsilon} \to 0$ is uniform; so there is $N > 0$ with $\|C_j\xi_\varepsilon\| \le \varepsilon\|\xi_\varepsilon\|$, $\forall\xi_\varepsilon$, if $j \ge N$. Summing up

$$\begin{aligned}0 \le \langle C_j\xi, \xi\rangle &\le 2\left(\langle C_j\xi_\varepsilon, \xi_\varepsilon\rangle + \left\langle C_j\xi_\varepsilon^\perp, \xi_\varepsilon^\perp\right\rangle\right) \\ &\le 2\left(\varepsilon\|\xi_\varepsilon\|^2 + \varepsilon\|\xi_\varepsilon^\perp\|^2\right) = 2\varepsilon\|\xi\|^2, \qquad \forall\xi \in \mathcal{H}_0.\end{aligned}$$

Now, by Proposition 2.1.13, $\|C_j\| \le 2\varepsilon$ for $j \ge N$ and so $C_j \to 0$ in the norm of the space $\mathrm{B}(\mathcal{H}_0)$. □

10.4.2 Nonincreasing Sequences

The main result in this section is related to the following setting. Suppose (T_j) is a sequence of positive self-adjoint operators acting in $\mathcal{H}$ with $T_{j+1} \le T_j$, i.e., $\mathrm{dom}\, T_j \subset \mathrm{dom}\, T_{j+1} \subset \mathcal{H}$ and $0 \le \langle T_{j+1}\xi, \xi\rangle \le \langle T_j\xi, \xi\rangle$, $\forall\xi \in \mathrm{dom}\, T_j$. The results are easily adapted for a uniformly lower bounded (nonincreasing) sequence of operators, i.e., there is $\beta \in \mathbb{R}$ so that $T_j \ge \beta\mathbf{1}$, $\forall j$.

Write b^j for the sesquilinear form generated by T_j, that is,

$$b^j(\xi, \eta) = \left\langle T_j^{1/2}\xi, T_j^{1/2}\eta\right\rangle, \qquad \forall\xi, \eta \in \mathrm{dom}\, b^j = \mathrm{dom}\, T_j^{1/2};$$

thus $b^{j+1} \le b^j$. Set $\mathcal{D} := \cup_j \mathrm{dom}\, b^j$, which is dense in $\mathcal{H}$.

Theorem 10.4.10. *Let (T_j) be as above. There is a positive self-adjoint operator T, with* $\mathrm{dom}\, T \subset \mathcal{D}$, *so that* $T_j \xrightarrow{\mathrm{SR}} T$.

Remark 10.4.11. Evidently one could begin with a nonincreasing sequence of positive and closed forms b^j, associate T_j to them and then conclude the existence of T as in Theorem 10.4.10.

Lemma 10.4.12. *Let $\emptyset \ne \Lambda \subset \mathbb{C}$ and $S : \Lambda \to \mathrm{B}(\mathcal{H})$, $\lambda \mapsto S_\lambda$, be a linear map satisfying the first resolvent identity*

$$S_\omega - S_\lambda = (\omega - \lambda)S_\omega S_\lambda, \qquad \forall\omega, \lambda \in \Lambda,$$

and suppose that S_{λ_0} is injective for some $\lambda_0 \in \Lambda$. Then, there exists a unique closed operator T, with $\mathrm{dom}\, T \subset \mathcal{H}$, *so that $\Lambda \subset \rho(T)$ and $R_\lambda(T) = S_\lambda$, $\forall\lambda \in \Lambda$.*

Proof. The above equation for the family S_λ implies $S_\lambda S_\omega = S_\omega S_\lambda$, $\forall\lambda,\omega\in\Lambda$, and that there are subspaces $\mathcal{I}, N\subset\mathcal{H}$ so that for the range and kernel os S_λ one has

$$\operatorname{rng} S_\lambda = \mathcal{I}, \qquad \mathrm{N}(S_\lambda) = N, \qquad \forall\lambda\in\Lambda.$$

The hypothesis S_{λ_0} is injective implies $N=\{0\}$, and so all S_λ are injective. Thus, for $\eta\in\mathcal{I}$ fixed, there is a unique $\xi_\lambda\in\mathcal{H}$ so that $\eta = S_\lambda\xi_\lambda$ for each $\lambda\in\Lambda$; hence $\xi_\lambda = S_\lambda^{-1}\eta$. By the first resolvent identity,

$$S_\lambda S_\omega\left(\xi_\omega-\xi_\lambda\right) = S_\lambda\eta - S_\omega\eta = (\lambda-\omega)S_\lambda S_\omega\eta,$$

and

$$S_\lambda S_\omega\left[\xi_\omega-\xi_\lambda-(\lambda-\omega)\eta\right] = 0,$$

so that $\xi_\lambda+\lambda\eta = \xi_\omega+\omega\eta$, $\forall\lambda,\omega\in\Lambda$. Thus, the linear operator $T:\mathcal{I}\to\mathcal{H}$, $T\eta := \xi_\lambda+\lambda\eta$, is well posed and it also follows that

$$(T-\lambda\mathbf{1})\eta = \xi_\lambda = S_\lambda^{-1}\eta, \qquad \forall\eta\in\mathcal{I}.$$

Therefore $S_\lambda = R_\lambda(T)$. Since $S_\lambda\in\mathrm{B}(\mathcal{H})$, by Proposition 1.2.13, it is a closed operator, so its inverse is also closed; this implies T is closed. Uniqueness is immediate. □

Exercise 10.4.13. Check that in the proof of Lemma 10.4.12 one has $\operatorname{rng} S_\lambda = \mathcal{I}$, $\mathrm{N}(S_\lambda) = N$, $\forall\lambda\in\Lambda$.

Exercise 10.4.14. With respect to Lemma 10.4.12, discuss the particular case in which Λ has just one element.

Exercise 10.4.15. Let $(S_j),(Q_j)$ be uniformly bounded sequences in $\mathrm{B}(\mathcal{H})$. If $S_j\xrightarrow{\text{s}}S$ and $Q_j\xrightarrow{\text{s}}Q$, with $S,Q\in\mathrm{B}(\mathcal{H})$, show that $S_jQ_j\xrightarrow{\text{s}}SQ$.

Proof. **[Theorem 10.4.10]** Since the sequence of sesquilinear forms b^j is nonincreasing and for $\lambda>0$ the sequence of self-adjoint operators $R_{-\lambda}(T_j)$ is uniformly bounded $\|R_{-\lambda}(T_j)\|\le 1/|\lambda|$, $\forall j$, by Lemma 10.4.4 one has

$$0\le R_{-\lambda}(T_j)\le R_{-\lambda}(T_{j+1})\le\frac{1}{|\lambda|}\mathbf{1}, \qquad \forall j.$$

Hence, as in the proof of Theorem 10.4.2 (combined with Exercise 10.4.6) one concludes that $R_{-\lambda}(T_j)$ strongly converges to a bounded self-adjoint operator $S_{-\lambda}$ and $0\le R_{-\lambda}(T_j)\le S_{-\lambda}$. Since for each j the bounded operators $R_{-\lambda}(T_j)$ satisfy the first resolvent identity, the strong limit imposes that (see Exercise 10.4.15)

$$S_{-\omega}-S_{-\lambda} = (-\omega+\lambda)S_{-\omega}S_{-\lambda}, \qquad \forall\omega,\lambda>0.$$

If $S_{-\lambda}\xi = 0$, fix j_0 and set $R_{-\lambda}(T_{j_0})\xi = \eta$. Since $R_{-\lambda}(T_{j_0})$ is positive and self-adjoint,

$$\begin{aligned}0 &= \langle S_{-\lambda}\xi,\xi\rangle \ge \langle R_{-\lambda}(T_{j_0})\xi,\xi\rangle\\ &= \left\langle R_{-\lambda}(T_{j_0})^{\frac12}\xi, R_{-\lambda}(T_{j_0})^{\frac12}\xi\right\rangle = \left\|R_{-\lambda}(T_{j_0})^{\frac12}\xi\right\|^2,\end{aligned}$$

hence $R_{-\lambda}(T_{j_0})\xi = R_{-\lambda}(T_{j_0})^{\frac{1}{2}} R_{-\lambda}(T_{j_0})^{\frac{1}{2}}\xi = 0$ and so $\xi = 0$; it follows that $S_{-\lambda}$ is injective. By Lemma 10.4.12, the family $S_{-\lambda}$ is the resolvent of a closed linear operator T at $-\lambda$, that is, $S_{-\lambda} = (T + \lambda\mathbf{1})^{-1}$, and since $S_{-\lambda}$ is self-adjoint, by Lemma 2.4.1, T is self-adjoint. Further, T is positive since $-\lambda \in \rho(T)$ for all $\lambda > 0$. Note that dom $T =$ rng $S_{-\lambda} \subset \mathcal{D}$, for otherwise the corresponding form would be infinity, a contradiction with the nonincreasing hypothesis on b^j. This concludes the proof. □

Example 10.4.16. Let $H_0\psi = -\psi''$, dom $H_0 = \mathcal{H}^2(\mathbb{R})$ so that dom $b^{H_0} = \mathcal{H}^1(\mathbb{R})$, $b^{H_0}(\psi, \varphi) = \langle H_0^{1/2}\psi, H_0^{1/2}\varphi\rangle$ (see Example 9.3.9). Let $V(x) = 1/|x|$ and b^V be the subsequent generated positive sesquilinear form, whose action is

$$b^V(\psi, \varphi) = \int_{\mathbb{R}} \frac{1}{|x|}\overline{\psi(x)}\varphi(x)\,dx.$$

Since each $\psi \in$ dom b^{H_0} is continuous, if $\psi \in \mathcal{Q} :=$ dom $b^{H_0} \cap$dom b^V the condition

$$b^V(\psi) = \int_{\mathbb{R}} \frac{|\psi(x)|^2}{|x|}\,dx < \infty$$

implies $\psi(0) = 0$, i.e., Dirichlet boundary condition at the origin.

For each $n \in \mathbb{N}$ let H_n be the operator associated with the closure of the positive form, dom $b^{H_0 + \frac{1}{n}V} = \mathcal{Q}$,

$$b^{H_0 + \frac{1}{n}V}(\psi, \varphi) = b^{H_0}(\psi, \varphi) + b^{\frac{1}{n}V}(\psi, \varphi),$$

that is, H_n is the Friedrichs extension of $H_0 + \frac{1}{n}V$. This sequence is nonincreasing and so, by Theorem 10.4.10, there is a positive self-adjoint operator T so that $H_n \stackrel{\text{SR}}{\longrightarrow} T$ as $n \to \infty$. By an adaptation of the arguments in Example 4.4.5 (see a hint in Exercise 10.4.17), it is found that the Dirichlet boundary condition at the origin is imposed on dom H_n, $\forall n$, in fact imposed on the completion $\mathcal{H}_+^{H_n}$ and so also on

$$\text{dom } T \subset \mathcal{D} = \bigcup_n \mathcal{H}_+^{H_n}.$$

Thus, the elements of dom T vanish at the origin. Since such a condition does not appear on dom H_0, it follows that for $n \to \infty$ one has

$$\left(H_0 + \frac{1}{n}V\right)_F \stackrel{\text{SR}}{\longrightarrow} T \neq H_0.$$

Exercise 10.4.17. Let $a > 0$ be sufficiently large. For $\psi \in \mathcal{H}^1(\mathbb{R})$, integrate $\psi'(t)/(1+t)^a$ by parts to check that

$$\psi(0) = a\int_0^\infty \frac{\psi(t)}{(1+t)^{1+a}}\,dt - \int_0^\infty \frac{\psi'(t)}{(1+t)^a}\,dt,$$

and so, by Cauchy-Schwarz, that there is $C > 0$ for which ($\forall \psi \in \text{dom } b^V$, V the potential in Example 10.4.16)

$$\begin{aligned}|\psi(0)|^2 &\leq C\,(\|\psi\| + \|\psi'\|)^2 \leq 2C\,\left(\|\psi\|^2 + \|\psi'\|^2\right)\\ &\leq 2C\left(\|\psi\|^2 + \|\psi'\|^2 + \frac{1}{n}\int_{\mathbb{R}} \frac{1}{|x|}|\psi(x)|^2\,dx\right)\\ &= 2C\langle\psi,\psi\rangle_+.\end{aligned}$$

Hence $|\psi(0)| \leq \sqrt{2C}\,\langle\psi,\psi\rangle_+^{1/2}$ and use this inequality to conclude that all elements $\psi \in \mathcal{H}_+^{H_n}$, H_n as in Example 10.4.16, vanish at the origin, that is, the Dirichlet boundary condition at the origin is imposed on the completion $\mathcal{H}_+^{H_n}$, $\forall n$.

Remark 10.4.18. In Theorem 10.4.10 the limiting form is not ensured to be closed (see Example 10.4.19), so there is less information when compared with Theorem 10.4.2; in the latter the nondecreasing property imposed that the limiting form was lower semicontinuous and so closed by Theorem 9.3.11. See Example 10.4.19.

Example 10.4.19. Consider the sequence of forms b_j with domain $\mathcal{H}^1(\mathbb{R})$,

$$b_j := \frac{1}{j} b^{H_0} + b_\delta,$$

discussed in Example 6.2.16. Such forms are closed, since b^{H_0} is closed and the b^{H_0}-bound of b_δ is zero; apply Lemma 6.1.16. As $j \to \infty$ this sequence is decreasing to b_δ which is not closable (Example 4.1.15); in particular b_δ is not closed.

Remark 10.4.20. Let T_j be the operator associated with b_j in Example 10.4.19. By using the notion of a regular part of a hermitian form, introduced in [Sim78], it is possible to show that T_j converges to the zero operator in the strong resolvent sense. That is, the operator T in Theorem 10.4.10 is the zero operator. What about taking the verification of this convergence as a small challenging project?

10.5 Application to the Aharonov-Bohm Effect

Let $\mathbf{A} = (A_1, A_2, A_3)$, $A_j : \mathbb{R}^3 \to \mathbb{R}$, be a continuous function for $j = 1, 2, 3$, and $V = \chi_C$ the characteristic function of the closed cylindric $C = \{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_1^2 + x_2^2 \leq 1\}$ of radius 1. The interest is in the investigation of the limiting operator H_∞ of

$$H_n = \left(-i\nabla - \frac{e}{c}\mathbf{A}\right)^2 + nV = \sum_{j=1}^{3}\left(-i\frac{\partial}{\partial x_j} - \frac{e}{c}A_j\right)^2 + nV,$$

as $n \to \infty$; a precise formulation appears below. For $n = 0$ the corresponding operator describes the hamiltonian of a charged particle in $\mathbb{R}^3$ under a magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$, i.e., the curl of the vector field $\mathbf{A}$, which is the so-called *vector* *potential* in electrodynamics. Recall that in classical mechanics the magnetic field is an agent that changes the momentum particle, so the way the vector potential appears in H_n and in other magnetic hamiltonian operators. The letters e,c denote the charge of the particle and speed of light, respectively, and in what follows in this section both are set to 1.

A particular choice $\mathbf{A} = \mathbf{A}_{\mathrm{S}}$ ahead yields the magnetic field $\mathbf{B}_{\mathrm{S}}$ of an infinitely long (cylindrical) solenoid given by the border of C. The potential nV represents a barrier to the particle motion, and for $n \to \infty$ an impenetrable solenoid is modeled. Explicitly, from electrodynamics one has (write $r^2 = x_1^2 + x_2^2$)

$$\mathbf{A}_{\mathrm{S}}(x_1, x_2, x_3) = \begin{cases} \frac{B}{2}(-x_2, x_1, 0), & 0 \le r \le 1 \\ \frac{B}{2r^2}(-x_2, x_1, 0), & 1 \le r \end{cases},$$

with B a constant, which turns out to be the intensity of the magnetic field inside the solenoid

$$\mathbf{B}_{\mathrm{S}}(x_1, x_2, x_3) = \begin{cases} (0, 0, B), & 0 \le r < 1 \\ (0, 0, 0), & 1 < r \end{cases}.$$

In what follows $\mathbf{A} = \mathbf{A}_{\mathrm{S}}$.

An interesting point in the physical context is that $\mathbf{A}_{\mathrm{S}}$ yields a nonzero magnetic field only inside the impenetrable region C. Whereas in classical mechanics a null magnetic field imposes a null force, in 1959 Y. Aharonov and D. Bohm proposed that in quantum mechanics the vector potentials should play a key role so that some measurable effects should be imputed exclusively to them; this is called the *Aharonov-Bohm effect* (in spite of the fact that related questions had been considered previously by W. Ehrenberg and R.E. Siday in 1949 and W. Franz in 1939) and it is directly related to the acceptance of H_∞ below as the quantum model of such a situation. As the expression of H_n above indicates, the source of the (possible) effect is the presence of the vector potential $\mathbf{A}$ in the energy operator, instead of the magnetic field $\mathbf{B}$ itself.

There is a vast literature about this Aharonov-Bohm effect, with debates and conflicting views; it is one of the most widely discussed topics of quantum mechanics. The interested reader is referred to the article [MaVG95] for an interesting discussion and as a starting point for tracking references; the application that follows was borrowed from that work.

In order to precisely define H_n consider the self-adjoint momentum operators (see Section 3.3) P_j given by the closure of dom $\tilde{P}_j = C_0^\infty(\mathbb{R}^3)$, $\tilde{P}_j\psi = -i\partial\psi/\partial x_j$, and

$$\mathrm{dom}\ T_j = \mathrm{dom}\ P_j, \qquad T_j\psi := P_j\psi - A_j\psi, \qquad j = 1, 2, 3,$$

which are self-adjoint since A_j are bounded continuous functions (so bounded multiplication operators). Note that $\cap_j \mathrm{dom}\ P_j = \mathcal{H}^1(\mathbb{R}^3)$.

By a simple variation of Proposition 4.3.9, the operator $H = \sum_{j=1}^3 T_j^2$, dom $H = \{\psi \in \mathcal{H}^1(\mathbb{R}^3) : T_j\psi \in \mathrm{dom}\ T_j, j = 1, 2, 3\} = \mathcal{H}^2(\mathbb{R}^3)$, is self-adjoint and the sesquilinear form generated by H is

$$b^H(\psi, \varphi) = \sum_{j=1}^{3} \langle T_j \psi, T_j \varphi \rangle, \qquad \text{dom } b^H = \mathcal{H}^1(\mathbb{R}^3).$$

Note that from this expression (see also Section 9.3) the form b^H is automatically closed and positive, since it is a sum of three positive closed forms. Now, for each n the potential $nV = n\chi_C$ is bounded, so

$$H_n \psi := H\psi + nV\psi, \qquad \text{dom } H_n = \text{dom } H = \mathcal{H}^2(\mathbb{R}^3),$$

is a nondecreasing sequence of positive self-adjoint operators whose quadratic forms are (write $b^n = b^{H_n}$)

$$b^n(\psi) = b^H(\psi) + n \int_C |\psi(x)|^2 \, d^3x, \qquad \text{dom } b^n = \mathcal{H}^1(\mathbb{R}^3).$$

To apply Theorem 10.4.2, introduce

$$\mathcal{D} := \left\{ \varphi \in \cap_n \text{dom } b^n : \lim_{n \to \infty} b^n(\varphi) < \infty \right\}$$

and note that $\psi \in \mathcal{D}$ iff

$$\sup_{n \geq 1} b^n(\psi) = \sup_{n \geq 1} \left(b^H(\psi) + n \int_C |\psi(x)|^2 \, d^3x \right) < \infty,$$

so that $\mathcal{D} = \left\{ \psi \in \mathcal{H}^1(\mathbb{R}^3) : \psi(x) = 0 \text{ a.e. in } C \right\}$, and so

$$\mathcal{H}_0 := \overline{\mathcal{D}} = \mathrm{L}^2(\mathbb{R}^3 \setminus C) \neq \mathcal{H} = \mathrm{L}^2(\mathbb{R}^3).$$

Note that $\mathcal{H}_0$ is the space $\mathcal{H}_0^1(\mathbb{R}^3 \setminus C)$ mentioned in Subsection 7.5.1 and this space realizes, in the sense of Sobolev traces, Dirichlet boundary conditions on the solenoid border.

By Theorem 10.4.2, there exists a self-adjoint operator H_∞ with $H_n \xrightarrow{\text{SR}} H_\infty$ in $\mathcal{H}_0$ whose quadratic form is

$$\begin{aligned} b^\infty(\psi) &= \left\langle H_\infty^{1/2} \psi, H_\infty^{1/2} \psi \right\rangle := \lim_{n \to \infty} b^n(\psi) \\ &= b^H(\psi) = \sum_{j=1}^{3} \langle T_j \psi, T_j \varphi \rangle, \qquad \psi \in \text{dom } b^\infty = \text{dom } H_\infty^{1/2} = \mathcal{D}. \end{aligned}$$

Since dom $H_\infty \subset$ dom $H_\infty^{1/2}$, H_∞ also carries Dirichlet boundary conditions; moreover, it is possible to give an explicit action of this operator.

Since T_j with domain $\{\psi \in \text{dom } P_j : \psi(x) = 0 \text{ a.e. in } C\}$ is closed (check this!), by Proposition 4.3.9, $T_j^* T_j$ is self-adjoint and one obtains

$$H_\infty \psi = \sum_{j=1}^{3} T_j^* T_j \psi = (-i\nabla - \mathbf{A})^2 \psi,$$
$$\text{dom } H_\infty = \left\{\psi \in \mathcal{D} : T_j \psi \in \text{dom } T_j^*, j = 1, 2, 3\right\}.$$

Therefore Dirichlet boundary conditions have been naturally assigned to the limiting operator H_∞, which should describe the quantum motion of a particle outside an impenetrable and infinitely long solenoid carrying a constant magnetic field inside. Finally, note that everything works in case no magnetic field is present, as well as for other shapes of region C.

Remark 10.5.1. A more realistic modeling would be considering penetrable (i.e., $n < \infty$) solenoids of finite length $L > 0$, so that there is a nonzero magnetic field outside the solenoid, and then take both limits $L \to \infty, n \to \infty$. This was carried out in [deOPe08] and it was shown that both limits commute and also lead to H_∞ above.

Remark 10.5.2. It is intriguing that the convergence of the limiting processes to H_∞ has led different authors to extremely opposite conclusions: whereas Magni and Valz-Gris ([MaVG95], pp. 185–186) concluded that “The way of coming to that hamiltonian, however, makes it clear that there is no cogent reason to attribute vector potentials any physical activity. . . ,” Berry [Ber86] argues that similar limits justify the exclusive quantum role of potentials!

Chapter 11

Spectral Decomposition I

In this chapter the decomposition of a self-adjoint operator in discrete and essential parts is discussed, with an important application to the hydrogen atom hamiltonian. Other applications include the discrete spectrum in case of unbounded potentials in $\mathbb{R}^n$ and the comparison of the spectra of different self-adjoint extensions (in case of finite deficiency indices).

11.1 Spectral Reduction

Let T be self-adjoint, E a (closed) reducing subspace of T and P_E the orthogonal projection onto E, as discussed in Section 9.8. Recall that if E reduces T, then the restrictions $T_E = T|_E := TP_E : \mathrm{dom}\, T \cap E \to E$ and $T_{E^\perp} = T|_{E^\perp} := TP_{E^\perp} : \mathrm{dom}\, T \cap E^\perp \to E^\perp$ are well-defined self-adjoint operators.

Accompanying such operator decomposition $T = T_E \oplus T_{E^\perp}$, there is the following *spectral reduction*, which will play an important role in this and the next chapters.

Proposition 11.1.1. *Let T be self-adjoint and E a closed subspace of $\mathcal{H}$ that reduces T. Then*

$$\sigma(T) = \sigma(T_E) \cup \sigma(T_{E^\perp}).$$

Proof. If $\xi \in \mathrm{dom}\, T$ and $t \in \mathbb{R}$, then

$$\|(T - t\mathbf{1})\xi\|^2 = \|(T_E - t\mathbf{1})P_E\xi\|^2 + \|(T_{E^\perp} - t\mathbf{1})P_{E^\perp}\xi\|^2 .$$

If $t \in \sigma(T_E)$ there exists a Weyl sequence $(\xi_j^E) \subset \mathrm{dom}\, T_E$ for T_E at t (see Section 2.4); since $P_{E^\perp}\xi_j^E = 0, \forall j$, it follows that this sequence is also a Weyl sequence for T at t, and so $t \in \sigma(T)$. In a similar way one gets $\sigma(T_{E^\perp}) \subset \sigma(T)$. Hence, $\sigma(T) \supset \sigma(T_E) \cup \sigma(T_{E^\perp})$.

Now, if $t \in \sigma(T)$ and (ξ_j) is a Weyl sequence for T at t, then

$$1 = \|\xi_j\|^2 = \|P_E \xi_j\|^2 + \|P_{E^\perp} \xi_j\|^2$$

and one has, for each j,

$$1 \geq \max\left\{\|P_E \xi_j\|^2, \|P_{E^\perp} \xi_j\|^2\right\} \geq \frac{1}{2},$$

and there exists a subsequence of nonzero vectors of either $(P_E \xi_j)$ or $(P_{E^\perp} \xi_j)$. Say $P_E \xi_{j_k} \neq 0$ and with $\|P_E \xi_{j_k}\|^2 \geq 1/2$, $\forall k$ (similarly for the other possibility). Normalize it and define

$$\eta_k = \frac{P_E \xi_{j_k}}{\|P_E \xi_{j_k}\|}.$$

Again from the equality at the beginning of this proof, it is found that

$$2\,\|(T - t\mathbf{1})\xi_{j_k}\|^2 \geq \left\|(T - t\mathbf{1})\frac{\xi_{j_k}}{\|\xi_{j_k}\|}\right\|^2 = \|(T_E - t\mathbf{1})\eta_k\|^2$$

and so (η_k) is a Weyl sequence for T_E at t and $t \in \sigma(T_E)$. Hence $\sigma(T) \subset \sigma(T_E) \cup \sigma(T_{E^\perp})$. This finishes the proof. □

In case of infinitely many $(E_j)_{j=1}^\infty$ pairwise orthogonal reducing subspaces of the self-adjoint operator T, with $\mathcal{H} = \bigoplus_j E_j$, the following version of Proposition 11.1.1 holds:

Proposition 11.1.2. *Let T be self-adjoint and $\mathcal{H} = \bigoplus_j E_j$ as above. Then $\sigma(T) = \overline{\cup_{j=1}^\infty \sigma(T_{E_j})}$ (the bar indicates closure).*

Proof. As in the proof of Proposition 11.1.1 ,$\sigma(T_{E_j}) \subset \sigma(T)$, and since $\sigma(T)$ is closed $\sigma(T) \supset \overline{\cup_{j=1}^\infty \sigma(T_{E_j})}$. However, a new argument is needed for the other half of the proof; note that the argument here also applies to Proposition 11.1.1, and it is instructive to keep both proofs.

If $t \notin \overline{\cup_{j=1}^\infty \sigma(T_{E_j})}$, then there is $\varepsilon > 0$ such that

$$|t - \lambda| > \varepsilon, \qquad \forall \lambda \in \cup_{j=1}^\infty \sigma(T_{E_j}).$$

By Proposition 9.5.2, the resolvent operators $R_t(T_{E_j})$ form a uniformly bounded family with $\|R_t(T_{E_j})\| \leq 1/\varepsilon$, for all j. It then follows that

$$R_t(T) = \bigoplus_j R_t(T_{E_j})$$

is bounded. Therefore $t \in \rho(T)$, which finishes the proof. □

Exercise 11.1.3. Check that if E reduces T and λ is an eigenvalue of T_E, then λ is an eigenvalue of T.

11.2 Discrete and Essential Spectra

In this section T will always denote a self-adjoint operator. In this case it is known that $\lambda \in \sigma(T)$ iff $\chi_{(\lambda-\varepsilon,\lambda+\varepsilon)}(T) \neq 0$, $\forall \varepsilon > 0$ (Theorem 8.3.13). The spectral projections $\chi_\Lambda(T)$ can be used to introduce spectral decompositions of T, and the interest in such decompositions resides mainly in three aspects:

1. They help to better understand the spectrum.
2. Some kinds of spectra are invariant under suitable perturbations of T.
3. The behavior of the time evolution $e^{-itT}\xi$, for large values of time t, may be strongly dependent on the spectral type.

Theorem 11.2.1. *If T is self-adjoint, the following assertions are equivalent:*

i) *λ is an eigenvalue of T, i.e., there is $0 \neq \xi_\lambda \in \mathcal{H}$ so that $T\xi_\lambda = \lambda\xi_\lambda$.*

ii) *The spectral measure of T at λ is $\mu_{\xi_\lambda} = \|\xi_\lambda\|^2\delta_\lambda$ (δ_λ is the Dirac measure at λ and $\xi_\lambda \neq 0$).*

iii) *$\chi_{\{\lambda\}}(T) \neq 0$, and so there is $\xi_\lambda \neq 0$ obeying $\chi_{\{\lambda\}}(T)\xi_\lambda = \xi_\lambda$.*
Moreover, in this case $\operatorname{rng} \chi_{\{\lambda\}}(T) = \{\xi \in \mathcal{H} : \chi_{\{\lambda\}}(T)\xi = \xi\}$ *is the eigenspace corresponding to the eigenvalue λ, and its dimension is (by definition) the multiplicity of λ (if the multiplicity is 1 the eigenvalue is said to be simple).*

Proof. i) $\Rightarrow$ ii) If i) holds, then $\lambda \in \sigma(T)$,

$$0 = \|T\xi_\lambda - \lambda\xi_\lambda\|^2 = \int_{\sigma(T)} |t-\lambda|^2 \, d\mu_{\xi_\lambda}(t),$$

and so $\mu_{\xi_\lambda} = c\delta_\lambda$ for some $c \geq 0$. Since

$$\mu_{\xi_\lambda}(\sigma(T)) = \|\xi_\lambda\|^2 = c\delta_\lambda(\sigma(T)) = c,$$

item ii) follows.

ii) $\Rightarrow$ i) If ii) holds, then

$$\|T\xi_\lambda - \lambda\xi_\lambda\|^2 = \int_{\sigma(T)} |t-\lambda|^2 \, \|\xi_\lambda\|^2 d\delta_\lambda(t) = 0,$$

and so $T\xi_\lambda - \lambda\xi_\lambda = 0$.

ii) $\Rightarrow$ iii) Suppose that ii) holds; then

$$\|\xi_\lambda\|^2 = \mu_{\xi_\lambda}(\{\lambda\}) = \langle \xi_\lambda, \chi_{\{\lambda\}}(T)\xi_\lambda \rangle = \|\chi_{\{\lambda\}}(T)\xi_\lambda\|^2,$$

and so $\chi_{\{\lambda\}}(T) \neq 0$, and since this operator is a projection, by such equality it follows that $\chi_{\{\lambda\}}(T)\xi_\lambda = \xi_\lambda$ (check this!).

iii) $\Rightarrow$ ii) If the projection $\chi_{\{\lambda\}}(T) \neq 0$ there is $0 \neq \eta \in \mathcal{H}$ with $\chi_{\{\lambda\}}(T)\eta = \eta$. Thus

$$\mu_\eta(\mathbb{R}) = \|\eta\|^2 = \langle \eta, \chi_{\{\lambda\}}(T)\eta \rangle = \mu_\eta(\{\lambda\}).$$

Hence, $\mu_\eta(\mathbb{R} \setminus \{\lambda\}) = 0$, which implies $\mu_\eta = c\delta_\lambda$. As in the above argument for i) $\Rightarrow$ ii), it is found that $c = \|\eta\|^2$. Finally, set $\xi_\lambda = \eta$. □

Exercise 11.2.2. Verify that the relation

$$\text{rng } \chi_{\{\lambda\}}(T) = \left\{\xi \in \mathcal{H} : \chi_{\{\lambda\}}(T)\xi = \xi\right\} = \{\xi : T\xi = \lambda\xi\}$$

follows from the arguments in the proof of Theorem 11.2.1.

A very interesting consequence is

Corollary 11.2.3. *Let T be self-adjoint. If λ is an isolated point of $\sigma(T)$, then λ is an eigenvalue of T.*

Proof. Since λ is an isolated point of $\sigma(T)$ there exists $\varepsilon > 0$ so that

$$(\lambda - \varepsilon, \lambda + \varepsilon) \cap \sigma(T) = \{\lambda\}.$$

On the other hand, by Theorem 8.3.13,

$$0 \neq \chi_{(\lambda-\varepsilon,\lambda+\varepsilon)}(T) = \chi_{(\lambda-\varepsilon,\lambda)}(T) + \chi_{\{\lambda\}}(T) + \chi_{(\lambda,\lambda+\varepsilon)}(T),$$

and since $(\lambda-\varepsilon, \lambda)$ and $(\lambda, \lambda+\varepsilon)$ are subsets of $\rho(T)$, again by Theorem 8.3.13 it is found that $0 \neq \chi_{\{\lambda\}}(T)$. Therefore λ is an eigenvalue of T by Theorem 11.2.1. □

Exercise 11.2.4. If S is a closed operator in $\mathcal{H}$, show that λ is an eigenvalue of S iff there exists a Cauchy sequence $(\xi_n) \subset \text{dom } S$, $\|\xi_n\| = 1, \forall n$, with $(S - \lambda\mathbf{1})\xi_n \to 0$ as $n \to \infty$. This holds especially for self-adjoint operators.

The time is ripe for the first spectral decomposition alluded to in the title of this chapter.

Definition 11.2.5. Let T be a self-adjoint operator.

a) The *essential spectrum* of T is the set $\sigma_{\text{ess}}(T)$ of the accumulation points of $\sigma(T)$ together with the eigenvalues of T of infinite multiplicity.
b) The *discrete spectrum* of T is the set $\sigma_{\text{d}}(T) := \sigma(T) \setminus \sigma_{\text{ess}}(T)$, that is, the set of isolated eigenvalues of T, each of them of finite multiplicity.
c) If $\sigma_{\text{ess}}(T) = \emptyset$, then T is said to have *purely discrete spectrum*; if $\sigma_{\text{d}}(T) = \emptyset$, then T is said to have *purely essential spectrum*.

Clearly $\sigma_{\text{ess}}(T) \subset \sigma(T)$ since the latter is a closed set. Suppose that for a subset $\Lambda \subset \mathbb{R}$ one has $\sigma_{\text{ess}}(T) \cap \Lambda = \emptyset$ (resp. $\sigma_{\text{d}}(T) \cap \Lambda = \emptyset$), then the operator T is said to have *purely* discrete (resp. essential) spectrum in Λ. The above definitions of discrete and essential spectra apply to any linear operator, not necessarily self-adjoint.

Example 11.2.6. Suppose $\dim \mathcal{H} = \infty$. Then:

i) The operator $\mathbf{1}$ has purely essential spectra: $\sigma(\mathbf{1}) = \{1\}$ and 1 is an isolated eigenvalue of infinite multiplicity. Similarly for the null operator.

ii) $0 \in \sigma_{\text{ess}}(T)$ for any compact self-adjoint operator T; the other points in its spectrum belong to the discrete part. Refer to Section 1.6 for details.

The next result presents important characterizations of the essential spectrum, including one via particular Weyl sequences.

Theorem 11.2.7. *If T is self-adjoint, the following assertions are equivalent:*

i) $\lambda \in \sigma_{\text{ess}}(T)$.

ii) *There exists a normalized sequence* $(\xi_n) \subset \operatorname{dom} T$ *(i.e.,* $\|\xi_n\| = 1$, $\forall n$*) so that* $\mathrm{w} - \lim_{n\to\infty} \xi_n = 0$ *and*

$$(T - \lambda\mathbf{1})\xi_n \to 0, \qquad n \to \infty.$$

Such a sequence is called a singular Weyl sequence for T *at* λ.

iii) *For all* $\varepsilon > 0$, $\dim \operatorname{rng} \chi_{(\lambda-\varepsilon,\lambda+\varepsilon)}(T) = \infty$.

Proof. i) ⇒ ii) There are only two possibilities for $\lambda \in \sigma_{\text{ess}}(T)$:

- λ is an eigenvalue of T of infinite multiplicity. In this case there is an orthonormal sequence $(\xi_n^\lambda)_n \subset \operatorname{dom} T$ of eigenvectors $T\xi_n^\lambda = \lambda\xi_n^\lambda$ and ii) clearly holds.
- λ is an accumulation point of $\sigma(T)$. In this case there exists a sequence $(\lambda_n) \subset \sigma(T)$, $\lambda_n \neq \lambda_m$ if $n \neq m$, with $\lambda_n \to \lambda$ (and $\lambda \neq \lambda_n$). Pick $\varepsilon_n \to 0^+$ so that, for $n \neq m$,

$$(\lambda_n - \varepsilon_n, \lambda_n + \varepsilon_n) \cap (\lambda_m - \varepsilon_m, \lambda_m + \varepsilon_m) = \emptyset,$$

and since $P_n := \chi_{(\lambda_n-\varepsilon_n,\lambda_n+\varepsilon_n)}(T) \neq 0$, there exists $\xi_n \in \operatorname{rng} P_n \subset \operatorname{dom} T$ (Lemma 8.3.16) with $\|\xi_n\| = 1$, $\forall n$. For $n \neq m$ one has $P_n P_m = 0$; thus

$$\langle \xi_n, \xi_m\rangle = \langle P_n\xi_n, P_m\xi_m\rangle = \langle \xi_n, P_nP_m\xi_m\rangle = 0,$$

and (ξ_n) is an orthonormal sequence. Now, since

$$\mu_{\xi_n}(\mathbb{R} \setminus (\lambda_n - \varepsilon_n, \lambda_n + \varepsilon_n)) = 0,$$

it follows that

$$\begin{aligned}\|T\xi_n - \lambda\xi_n\|^2 &= \int_{(\lambda_n-\varepsilon_n,\lambda_n+\varepsilon_n)} |t-\lambda|^2 \, d\mu_{\xi_n}(t) \\ &\leq \int_{(\lambda_n-\varepsilon_n,\lambda_n+\varepsilon_n)} (|t-\lambda_n| + |\lambda_n - \lambda|)^2 \, d\mu_{\xi_n}(t) \\ &\leq (\varepsilon_n + |\lambda_n-\lambda|)^2 \, \|\xi_n\|^2 = (\varepsilon_n + |\lambda_n - \lambda|)^2,\end{aligned}$$

which vanishes as $n \to \infty$. Hence (ξ_n) is a singular Weyl sequence for T at λ.

ii) $\Rightarrow$ iii) Let (ξ_n) be as in ii). If there exists $\varepsilon_0 > 0$ so that

$$\dim \operatorname{rng} \chi_{(\lambda-\varepsilon_0,\lambda+\varepsilon_0)}(T) < \infty,$$

then $P_0(T) := \chi_{(\lambda-\varepsilon_0,\lambda+\varepsilon_0)}(T)$ is a compact operator since it has finite range; since (ξ_n) is orthonormal $\xi_n \xrightarrow{\text{w}} 0$ and by Proposition 1.3.22 one has $P_0(T)\xi_n \to 0$. Hence

$$\begin{aligned}
\|T\xi_n - \lambda\xi_n\|^2 &= \int_{\mathbb{R}} |t-\lambda|^2 \; d\mu_{\xi_n}(t) \\
&\geq \int_{\mathbb{R}\setminus(\lambda_n-\varepsilon_0,\lambda_n+\varepsilon_0)} |t-\lambda|^2 \; d\mu_{\xi_n}(t) \\
&= \int_{\mathbb{R}} (1-P_0(t)) \; |t-\lambda|^2 \; d\mu_{\xi_n}(t) \geq \varepsilon_0^2 \int_{\mathbb{R}} (1-P_0(t)) \, d\mu_{\xi_n}(t) \\
&= \varepsilon_0^2 \; \left(\|\xi_n\|^2 - \|P_0(T)\xi_n\|^2\right) = \varepsilon_0^2 \; \left(1 - \|P_0(T)\xi_n\|^2\right),
\end{aligned}$$

and $T\xi_n - \lambda\xi_n$ does not converge to zero as $n \to \infty$ (recall that $P_0(T)\xi_n \to 0$). This contradiction shows that iii) follows from ii).

iii) $\Rightarrow$ i) If iii) holds, by Theorem 11.2.1, λ may be an eigenvalue of T with infinity multiplicity, so an element of $\sigma_{\text{ess}}(T)$. If this is not the case, then for all $\varepsilon > 0$ either

$$\dim \operatorname{rng} \chi_{(\lambda-\varepsilon,\lambda)}(T) = \infty \qquad \text{or} \qquad \dim \operatorname{rng} \chi_{(\lambda,\lambda+\varepsilon)}(T) = \infty,$$

or both. In other words, there is a point of $\sigma(T)$, different from λ, and at a distance less then ε of λ. Since it holds for arbitrarily small $\varepsilon > 0$, then λ is an accumulation point of $\sigma(T)$ and $\lambda \in \sigma_{\text{ess}}(T)$. The proof is finished. □

Exercise 11.2.8. Verify that an orthonormal sequence $(\xi_n) \subset \operatorname{dom} T$ so that $(T - \lambda\mathbf{1})\xi_n \to 0$ works as a singular Weyl sequence of T at λ.

Exercise 11.2.9. Discuss the spectral possibilities if for all $\varepsilon > 0$ one has

$$\dim \operatorname{rng} \chi_{(\lambda-\varepsilon,\lambda+\varepsilon)}(T) > 0.$$

Corollary 11.2.10. *If T is self-adjoint, then $\sigma_{\text{ess}}(T)$ is a closed subset of $\mathbb{R}$.*

Proof. If $\lambda \notin \sigma_{\text{ess}}(T)$, then there exists ε_0 with

$$\dim \operatorname{rng} \chi_{(\lambda-\varepsilon_0,\lambda+\varepsilon_0)}(T) < \infty.$$

Thus, for each $t \in (\lambda - \varepsilon_0, \lambda + \varepsilon_0)$ one can choose $\varepsilon_t > 0$ so that

$$(t-\varepsilon_t, t+\varepsilon_t) \subset (\lambda-\varepsilon_0, \lambda+\varepsilon_0).$$

In view of

$$\dim \operatorname{rng} \chi_{(t-\varepsilon_t,t+\varepsilon_t)}(T) \leq \dim \operatorname{rng} \chi_{(\lambda-\varepsilon_0,\lambda+\varepsilon_0)}(T) < \infty,$$

it follows that $t \notin \sigma_{\text{ess}}(T)$, that is, $\mathbb{R} \setminus \sigma_{\text{ess}}(T)$ is an open set. □

Exercise 11.2.11. Let T be self-adjoint. Discuss if $\sigma_{\rm d}(T)$ is a closed subset of $\mathbb{R}$. What about compact operators?

Exercise 11.2.12. a) Show that if $0 < \dim \operatorname{rng} \chi_{(a,b)}(T) < \infty$, then

$$\sigma(T) \cap (a,b) \subset \sigma_{\rm d}(T).$$

b) Show that if $0 < \dim \operatorname{rng} \chi_{(a,b)}(T) = \infty$, then $\sigma_{\rm ess}(T) \cap [a,b] \neq \emptyset$.

11.3 Essential Spectrum and Compact Perturbations

Let T^0 be a self-adjoint operator and $\lambda^0 \in \sigma_{\rm d}(T^0)$; then λ^0 is an isolated eigenvalue of multiplicity $m < \infty$, and denote its eigenspace by $M = \operatorname{Lin}(\{\xi_1, \dots, \xi_m\})$, $T^0 \xi_j = \lambda^0 \xi_j$, $1 \le j \le m$. Thus $M = \operatorname{rng} \chi_{\{\lambda^0\}}(T^0)$. By Propositions 9.8.5 and 11.1.1, M reduces T^0 and

$$\sigma(T^0) = \sigma(T^0_M) \cup \sigma(T^0_{M^\perp}) = \{\lambda^0\} \cup \sigma(T^0_{M^\perp});$$

further, $\{\lambda^0\} \cap \sigma(T^0_{M^\perp}) = \emptyset$.

For $\varepsilon \in \mathbb{R}$, $|\varepsilon| < d(\lambda^0, \sigma(T^0_{M^\perp}))$, denote $\Lambda_\varepsilon = \mathbb{R} \setminus (\lambda^0 - \varepsilon, \lambda^0 + \varepsilon)$ so that $M^\perp = \operatorname{rng} \chi_{\Lambda_\varepsilon}(T^0)$. Consider the self-adjoint operator

$$T^\varepsilon = T^0 + \varepsilon \chi_{\{\lambda^0\}}(T^0).$$

Since $T^\varepsilon = f_\varepsilon(T^0)$, with $f_\varepsilon(t) = t + \varepsilon \chi_{\{\lambda^0\}}(t)$, one has $\chi_\Lambda(T^\varepsilon) = \chi_{f_\varepsilon^{-1}(\Lambda)}(T^0)$, for any Borel set $\Lambda \subset \mathbb{R}$. In view of $f_\varepsilon^{-1}(\Lambda_\varepsilon) = \Lambda_\varepsilon$, one has $\chi_{\Lambda_\varepsilon}(T^\varepsilon) = \chi_{\Lambda_\varepsilon}(T^0)$ and so, for any interval (a,b),

$$\chi_{\Lambda_\varepsilon}(T^0) \chi_{(a,b)}(T^\varepsilon) = \chi_{(a,b)}(T^\varepsilon) \chi_{\Lambda_\varepsilon}(T^0);$$

thus, by Proposition 9.8.5, $M^\perp$ reduces T^ε. This, together with $T^\varepsilon_{M^\perp} = T^0_{M^\perp}$, imply

$$\sigma(T^\varepsilon) = \sigma(T^\varepsilon_M) \cup \sigma(T^\varepsilon_{M^\perp}) = \{\lambda^0 + \varepsilon\} \cup \sigma(T^0_{M^\perp}).$$

Since λ^0 is an isolated point of $\sigma(T^0)$, if $0 \neq |\varepsilon|$ is small enough (as above) one has $\lambda_0 \notin \sigma(T^\varepsilon)$ and this point was "removed" from the spectrum of T^0 by a finite rank perturbation $\varepsilon \chi_{\{\lambda^0\}}(T^0)$ of arbitrarily small norm. In contrast to this discussion, it will be seen that the essential spectrum is invariant under any compact perturbation (the so-called Weyl criterion, i.e., Corollary 11.3.6 and Proposition 11.6.2)!

Exercise 11.3.1. If T is self-adjoint and $\lambda \in \sigma_{\rm d}(T)$, argue that there are self-adjoint finite rank perturbations $B \in \mathrm{B}_{\rm f}(\mathcal{H})$, with norm arbitrarily small, so that $\lambda \notin \sigma_{\rm d}(T + B)$, and also that there exists $\delta > 0$ for which

$$\sigma(T + B) \cap (\lambda - \delta, \lambda + \delta)$$

consists of a finite number of simple eigenvalues.

Definition 11.3.2. Let A, B be linear operators in $\mathcal{H}$ and $\rho(A) \neq \emptyset$. Then B is said to be *A-compact* (or *relatively compact with respect to A*) if dom $A \subset$ dom B and $BR_z(A)$ is a compact operator for some $z \in \rho(A)$.

Example 11.3.3. If B is a compact operator, then B is A-compact for all linear operators A with nonempty resolvent set.

Theorem 11.3.4. *Let T be self-adjoint and B a T-compact operator. Then:*

i) *$BR_z(T)$ is compact for all $z \in \rho(T)$.*
ii) *If B is also hermitian, then B is T-bounded with $N_T(B) = 0$.*
iii) *If B is also hermitian, then $T+B$ with* dom $(T+B) =$ dom T *is self-adjoint.*

Proof. i) If BR_{z_0} is compact for some $z_0 \in \rho(T)$, then if $z \in \rho(T)$ the first resolvent identity implies

$$BR_z(T) = BR_{z_0}(T) + (z - z_0)BR_{z_0}(T)R_z(T),$$

which is compact by Proposition 1.3.7, since $R_z(T)$ is a bounded operator.

ii) If $\lambda \in \mathbb{R}$, then

$$BR_{i\lambda}(T) = BR_i(T)(T - i\mathbf{1})R_{i\lambda}(T);$$

now $BR_i(T)$ is compact and since $(T - i\mathbf{1})R_{i\lambda}(T) \xrightarrow{\text{s}} 0$ as $\lambda \to \infty$ by the spectral theorem (write $(T - i\mathbf{1})R_{i\lambda}(T) = f(T)$ with $f(t) = (t-i)/(t-i\lambda)$) or Corollary 2.2.19, it follows that $\lim_{\lambda\to\infty} \|BR_{i\lambda}(T)\| = 0$ (by Proposition 1.3.29). Proposition 6.1.5 implies $N_T(B) = 0$.

iii) It follows by ii) and the Kato-Rellich Theorem 6.1.8. □

Exercise 11.3.5. Verify that Theorem 11.3.4i) holds even if T is not self-adjoint.

Corollary 11.3.6 (Weyl). *Let T be self-adjoint and B hermitian. If B is T-compact, then $\sigma_{\text{ess}}(T+B) = \sigma_{\text{ess}}(T)$.*

Proof. Let $\lambda \in \sigma_{\text{ess}}(T)$ and (ξ_n) a singular Weyl sequence for T at λ. Thus

$$\begin{aligned}(T + B - \lambda\mathbf{1})\xi_n &= (T - \lambda\mathbf{1})\xi_n + BR_{i+\lambda}(T)(T - (i+\lambda)\mathbf{1})\xi_n \\ &= (T - \lambda\mathbf{1})\xi_n + BR_{i+\lambda}(T)(T - \lambda\mathbf{1})\xi_n - iBR_{i+\lambda}(T)\xi_n\end{aligned}$$

which vanishes as $n \to \infty$ since $BR_{i+\lambda}(T)$ is a compact operator. Hence (ξ_n) is a singular Weyl sequence for $(T+B)$ at λ and so $\sigma_{\text{ess}}(T) \subset \sigma_{\text{ess}}(T+B)$.

In order to exchange the roles of T and $T+B$ in the above argument, it is necessary to show that B is also $(T+B)$-compact, and then use that $T = (T+B) - B$.

Pick $\lambda_0 \in \mathbb{R}$ obeying $\|BR_{i\lambda_0}(T)\| < 1$. Thus, from the relation

$$T + B - i\lambda_0\mathbf{1} = (\mathbf{1} + BR_{i\lambda_0}(T))(T - i\lambda_0\mathbf{1})$$

one gets

$$BR_{i\lambda_0}(T+B) = BR_{i\lambda_0}(T)\ (\mathbf{1} + BR_{i\lambda_0}(T))^{-1},$$

and so B is $(T+B)$-compact since $BR_{i\lambda_0}(T)$ is compact. Hence $\sigma_{\text{ess}}(T) \supset \sigma_{\text{ess}}(T+B)$. The corollary is proved. □

Corollary 11.3.7. *Let T be self-adjoint. If B is compact and self-adjoint, then $\sigma_{\text{ess}}(T+B) = \sigma_{\text{ess}}(T)$.*

Proof. If $z \in \mathbb{C} \setminus \mathbb{R}$ then $BR_z(T)$ is compact. The conclusion follows by Weyl's result 11.3.6. □

Exercise 11.3.8. If T is self-adjoint, B is hermitian and T-bounded with $N_T(B) < 1$ and K is T-compact, show that K is $(T+B)$-compact.

Exercise 11.3.9. Suppose $\dim \mathcal{H} = \infty$. Let T be self-adjoint with purely discrete spectrum. Show that T is not T-compact.

Exercise 11.3.10. If $T \in \mathrm{B}(\mathcal{H})$ is self-adjoint and $\dim \mathcal{H} = \infty$, show that $\sigma_{\text{ess}}(T) \neq \emptyset$.

Exercise 11.3.11. Show that if $R_{z_0}(T)$ is a compact operator for some $z_0 \in \rho(T)$, then $R_z(T)$ is compact for any $z \in \rho(T)$.

Exercise 11.3.12. If T is self-adjoint and E is a reducing subspace of T, show that $\sigma_{\text{ess}}(T_E) \subset \sigma_{\text{ess}}(T)$.

11.3.1 Operators With Compact Resolvent

The subject now is a characterization of the self-adjoint operators with empty essential spectrum; due to such a characterization these operators are also called *operators with compact resolvent.*

Theorem 11.3.13. *Let $T : \operatorname{dom} T \sqsubseteq \mathcal{H} \to \mathcal{H}$ be self-adjoint and assume that $\dim \mathcal{H} = \infty$. Then, the following assertions are equivalent:*

i) *$\sigma_{\text{ess}}(T) = \emptyset$.*
ii) *There is an orthonormal basis $(\xi_j)_{j=1}^{\infty}$ of $\mathcal{H}$ built of eigenvectors of T, $T\xi_j = \lambda_j \xi_j, \forall j$, with real eigenvalues λ_j, counting their multiplicities, satisfying $\lim_{j\to\infty} |\lambda_j| = \infty$ (and so each of them of finite multiplicity).*
iii) *$R_z(T)$ is a compact operator for some $z \in \rho(T)$ (and so for all $z \in \rho(T)$).*

Proof. i) ⇒ ii) If i) holds then $\sigma(T)$ is purely discrete and so consists of a sequence $\Lambda = (\lambda_j) \subset \mathbb{R}$ of eigenvalues of T of finite multiplicity $T\xi_j = \lambda_j \xi_j$, and one may assume that (ξ_j) is an orthonormal sequence. Thus, with multiplicities, there is a finite number of eigenvalues in $[-n, n]$ for all $n \in \mathbb{N}$, which implies $|\lambda_j| \to \infty$ as $j \to \infty$.

Note that the closed subspace $E := \operatorname{rng} \chi_\Lambda(T) = \overline{\operatorname{Lin}((\xi_j)_j)}$ reduces T and so

$$\sigma(T) = \sigma(T_E) \cup \sigma(T_{E^\perp}).$$

One has $\sigma_{\text{ess}}(T_E) = \emptyset$. If $E \neq \mathcal{H}$, there would exist additional eigenvalues of T outside Λ (those of $T_{E^\perp}$). This contradiction shows that (ξ_j) is an orthonormal basis of $\mathcal{H}$.

ii) $\Rightarrow$ i) Order each eigenvalue of T according to its distance to the origin. Since $|\lambda_j| \to \infty$, each λ_j has finite multiplicity and is isolated. Thus $\Lambda = \{\lambda_j : j \in \mathbb{N}\}$ is a discrete set and hence a closed subset of $\mathbb{R}$. By Theorem 2.2.10 one has $\sigma(T) = \overline{\Lambda} = \Lambda$. Therefore $\sigma_{\text{ess}}(T) = \emptyset$.

ii) $\Rightarrow$ iii) Since the eigenvalues of T are real, $\inf_j |\lambda_j - i| \geq 1$. Note that, by Corollary 8.3.19, for all j one has $R_i(T)\xi_j = 1/(\lambda_j - i)\xi_j$.

For each $n \in \mathbb{N}$ the operator $S_n : \mathcal{H} \hookleftarrow$ defined by

$$S_n\xi = \sum_{|\lambda_j| \leq n} \frac{\langle \xi_j, \xi\rangle}{\lambda_j - i}\xi_j,$$

is bounded and of finite rank, so compact. Since (see the proof of Theorem 2.2.10)

$$R_\lambda(T)\xi = \sum_j \frac{\langle \xi_j, \xi\rangle}{\lambda_j - i}\,\xi_j,$$

for all $\xi \in \mathcal{H}$ one has

$$\begin{aligned}\|R_i(T)\xi - S_n\xi\|^2 &\leq \left\| \sum_{|\lambda_j| > n} \frac{\langle \xi_j, \xi\rangle}{\lambda_j - i}\,\xi_j \right\|^2 \\ &\leq \frac{1}{n^2} \sum_{|\lambda_j| > n} |\langle \xi_j, \xi\rangle|^2 \leq \frac{1}{n^2}\|\xi\|^2.\end{aligned}$$

Therefore,

$$\|R_i(T) - S_n\| \leq \frac{1}{n} \to 0,$$

and $R_i(T)$ is compact by Corollary 1.3.14.

iii) $\Rightarrow$ ii) If $R_z(T)$ is compact for some fixed $z \in \rho(T)$, since it is also a normal operator, Corollary 8.1.9 implies the existence of an orthonormal basis (ξ_j) of $\mathcal{H}$ of eigenvectors of $R_z(T)$ whose corresponding eigenvalues z_j, i.e., $R_z(T)\xi_j = z_j\xi_j$, are of finite multiplicity and $z_j \to 0$ as $j \to \infty$. Further, all $z_j \neq 0$ since $R_z(T) = (T - z\mathbf{1})^{-1}$ is the inverse of a linear operator. Therefore,

$$\xi_j = (T - z\mathbf{1})R_z(T)\xi_j = (T\xi_j - z\xi_j)z_j,$$

consequently

$$T\xi_j = \left(z + \frac{1}{z_j}\right)\xi_j, \qquad \forall j.$$

This implies $\sigma_{\text{ess}}(T) = \emptyset$, for $(\xi_j)_j$ is a basis of $\mathcal{H}$. $\square$

Example 11.3.14. Consider the self-adjoint operator $T : \mathrm{dom}\, T \subset l^2(\mathbb{N}) \to l^2(\mathbb{N})$,

$$\mathrm{dom}\, T = \{\xi \in l^2(\mathbb{N}) : (T\xi) \in l^2(\mathbb{N})\},$$

given by

$$T(\xi_1, \xi_2, \xi_3, \dots) = (1\xi_1, 1\xi_2, 2\xi_3, 1\xi_4, 2\xi_5, 3\xi_6, 1\xi_7, 2\xi_8, 3\xi_9, 4\xi_{10}, 1\xi_{11}, \dots).$$

Its spectrum $\sigma(T) = \mathbb{N}$ is purely essential, and each point of $\mathbb{N}$ is an (isolated) eigenvalue of infinite multiplicity. For any compact self-adjoint operator K one has $\sigma(T + K) \supset \mathbb{N}$.

Example 11.3.15. The harmonic oscillator (Example 8.4.3) has purely discrete spectrum.

Exercise 11.3.16. Consider finite rank (hermitian) perturbations of the operator in Example 11.3.14 and discuss the possible spectral variations.

Exercise 11.3.17. If T is self-adjoint, show that T has purely discrete spectrum iff its Cayley transform $U(T)$ is a compact perturbation of the identity, i.e., $U(T) = \mathbf{1} + K$, with K a compact operator.

In Theorem 11.5.6 it will be shown that if $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ is bounded from below and $\lim_{|x|\to\infty} V(x) = \infty$, then the subsequent standard Schrödinger operator $-\Delta + V$ has purely discrete spectrum.

11.4 Applications

11.4.1 Eigenvalues of the H-Atom

Let $\mathrm{dom}\, H_0 = \mathcal{H}^2(\mathbb{R}^n)$, $H_0 = -\Delta$ be the usual free particle hamiltonian operator on $\mathbb{R}^n$ (see Section 3.4). If $f(p) = p^2$, recall that by using Fourier transform $\mathcal{F}$ one has

$$\left(\mathcal{F} H_0 \mathcal{F}^{-1}\right) \phi(p) = p^2 \phi(p) = \mathcal{M}_f \phi(p), \qquad \phi \in \mathrm{dom}\, p^2.$$

By the discussion in Chapter 3 (see also Proposition 2.3.27), one concludes

Proposition 11.4.1. $\sigma(H_0) = \sigma_{\mathrm{ess}}(H_0) = [0, \infty)$.

One of the goals of this section is to show that the Coulomb potential is H_0-compact and, by Weyl criterion, the essential spectrum of the hydrogen atom Schrödinger operator is $[0, \infty)$. For this a rather general sufficient condition for H_0-compactness of perturbations will be addressed.

If $f, g \in B^\infty(\mathbb{R}^n)$ (bounded Borel functions with the sup norm), denote by $f(x)$ the operator $\mathcal{M}_f$ on $\mathrm{L}^2(\mathbb{R}^n)$, by $g(p)$ the operator $\mathcal{M}_g$ on $\mathrm{L}^2(\hat{\mathbb{R}}^n)$ and by $f(x)g(p)$ and $g(p)f(x)$ the operators (both with domain $\mathrm{L}^2(\mathbb{R}^n)$)

$$\begin{aligned}(f(x)g(p)\psi)(x) &:= f(x)\mathcal{F}^{-1}\left[g(p)\hat{\psi}(p)\right](x),\\ (g(p)f(x)\psi)(x) &:= \mathcal{F}^{-1}\left[g(p)\mathcal{F}(f(x)\psi(x))\right](x),\end{aligned}$$

respectively. These operators are bounded, but with additional assumptions they become compact. Write $B^\infty_\infty(\mathbb{R}^n)$ for the elements of $B^\infty(\mathbb{R}^n)$ that vanish at infinity, that is, $f \in B^\infty(\mathbb{R}^n)$ for which given $\varepsilon > 0$ there is $r > 0$ so that $|f(x)| < \varepsilon$ if $|x| > r$.

Roughly speaking, Lemma 11.4.2 and Exercise 11.4.5 indicate that compact operators in $\mathrm{L}^2(\mathbb{R}^n)$ "vanish in phase space (x, p) as both $|p|, |x| \to \infty$."

Lemma 11.4.2. *Consider the functions $f, g : \mathbb{R}^n \to \mathbb{C}$ in $B^\infty(\mathbb{R}^n)$. If one of them belongs to $\mathrm{L}^2(\mathbb{R}^n)$ and the other to $\mathrm{L}^2(\mathbb{R}^n) + B^\infty_\infty(\mathbb{R}^n)$, then the operators $f(x)g(p)$ and $g(p)f(x)$ are compact.*

Proof. Note first that $g(p)f(x) = (\overline{f(x)}\,\overline{g(p)})^*$; thus, by Corollary 1.3.27, it is enough to show that $f(x)g(p)$ is compact. Assume, initially, that $f, g \in \mathrm{L}^2(\mathbb{R}^n)$. In this case, for any $\psi \in \mathrm{L}^2(\mathbb{R}^n)$ one has $g\hat{\psi} \in \mathrm{L}^1(\mathbb{R}^n)$ and so

$$\begin{aligned}(2\pi)^{(n/2)}(g(p)\psi)(x) &= \int_{\mathbb{R}^n} e^{iqx} g(q)\hat{\psi}(q)\, dq \\ &= \left\langle e^{-iqx}\overline{g(q)}, \hat{\psi}(q)\right\rangle = \left\langle \mathcal{F}^{-1} e^{-iqx}\overline{g(q)}, \psi(q)\right\rangle \\ &= \left\langle \overline{\check{g}(x-q)}, \psi(q)\right\rangle = \int_{\mathbb{R}^n} \check{g}(x-q)\psi(q)\, dq.\end{aligned}$$

Thus, $f(x)g(p)\psi(x) = \int_{\mathbb{R}^n} K(x, q)\psi(q)\, dq$ is an integral operator with kernel

$$K(x, q) = \frac{1}{(2\pi)^{n/2}} f(x)\check{g}(x-q),$$

which belongs to $\mathrm{L}^2(\mathbb{R}^n \times \mathbb{R}^n)$ and so $f(x)g(p)$ is a compact operator (see Example 1.4.9 and Theorem 1.4.6).

Now suppose that $f \in B^\infty_\infty(\mathbb{R}^n)$ and $g \in \mathrm{L}^2(\mathbb{R}^n)$. Then, for all $r > 0$ the function $f_r(x) := f(x)\chi_{\{|x|<r\}}(x)$ belongs to $\mathrm{L}^2(\mathbb{R}^n)$, and given $\varepsilon > 0$ there exists $r_\varepsilon > 0$ so that $|f(x)| < \varepsilon$ if $|x| \geq r_\varepsilon$. Thus, $\|f - f_{r_\varepsilon}\|_\infty \leq \varepsilon$ and for all $\psi \in \mathrm{L}^2(\mathbb{R}^n)$ one has

$$\begin{aligned}\|(f_{r_\varepsilon}(x)g(p) - f(x)g(p))\psi\|_2 &= \left\|\chi_{\{|x|\geq r_\varepsilon\}}(x)f(x)g(p)\psi\right\|_2 \\ &\leq \varepsilon\, \|g(p)\psi\|_2 \leq \varepsilon\, \|g\|_2\, \|\psi\|_2,\end{aligned}$$

and thus $\|f_{r_\varepsilon}(x)g(p) - f(x)g(p)\| \leq \varepsilon$. Hence $f(x)g(p)$ is a uniform limit (as $\varepsilon \to 0$) of compact operators $f_{r_\varepsilon}(x)g(p)$, so it is also compact by Theorem 1.3.13. Similarly one deals with the case $g \in B^\infty_\infty(\mathbb{R}^n)$ and $f \in \mathrm{L}^2(\mathbb{R}^n)$. The lemma is proved. ☐

Exercise 11.4.3. Verify that $g(p)f(x) = (\overline{f}(x)\,\overline{g}(p))^*$.

Exercise 11.4.4. Based on the proof of Lemma 11.4.2, show that $f(x)g(p)$ and $g(p)f(x)$ are in fact Hilbert-Schmidt operators if both $f, g \in \mathrm{L}^2(\mathbb{R}^n)$.

Exercise 11.4.5. By considering $f_r(x)g_r(p)$ (notation as in the proof of Lemma 11.4.2), show that the conclusions of Lemma 11.4.2 hold if $f, g \in B^\infty_\infty(\mathbb{R}^n)$.

Exercise 11.4.6. Let H_0 be the free hamiltonian in $\mathrm{L}^2(\mathbb{R}^n)$. Show that the operator $f(x)(H_0+\lambda\mathbf{1})^{-\gamma} = f(x)(p^2+\lambda)^{-\gamma}$ is compact for all $f \in B^\infty_\infty(\mathbb{R}^n)$ and $\lambda, \gamma > 0$.

Next an important application to standard Schrödinger operators with potentials that include the 3D hydrogen atom H_H energy operator.

Theorem 11.4.7. *Let $V \in \mathrm{L}^2(\mathbb{R}^3)+B^\infty_\infty(\mathbb{R}^3)$ be real-valued. Then V is H_0-compact, $H = H_0 + V$ with* dom H = dom H_0 *is self-adjoint and $\sigma_{\mathrm{ess}}(H) = [0,\infty)$.*

Proof. The operator H is self-adjoint by the Kato-Rellich theorem. By an application of Lemma 11.4.2, $VR_i(H_0) = f(x)g(p)$, with $f(x) = V(x)$ and $g(p) = \left(p^2 - i\right)^{-1}$, is a compact operator since $f \in \mathrm{L}^2(\mathbb{R}^3) + B^\infty_\infty(\mathbb{R}^3)$ and $g \in B^\infty_\infty(\mathbb{R}^3)$. Hence the potential V is H_0-compact and $\sigma_{\mathrm{ess}} = [0,\infty)$ by Corollary 11.3.6 and Proposition 11.4.1. □

Exercise 11.4.8. If $V \in B^\infty_\infty(\mathbb{R}^n)$, show that $H = H_0 + V$ is self-adjoint and $\sigma_{\mathrm{ess}}(H) = [0,\infty)$.

Note that such results apply to the Coulomb and Yukawa potentials in $\mathbb{R}^3$ (see Subsection 6.2.1). Now the Coulomb case

$$V(x) = -\frac{\kappa}{|x|}$$

will get a closer inspection. Fix $R > 0$ and write $V = V_2 + V_\infty$, with

$$V_2(x) = V(x)\chi_{[0,R)}(|x|), \qquad V_\infty(x) = V(x)\chi_{[R,\infty)}(|x|),$$

so that $V_2 \in \mathrm{L}^2(\mathbb{R}^3)$, $V_\infty \in B^\infty_\infty(\mathbb{R}^3)$, and Theorem 11.4.7 applies. By Corollary 6.2.9, if $\kappa < 0$ the operator

$$H_\kappa := H_0 - \frac{\kappa}{|x|}$$

has no eigenvalues, hence $\sigma(H_\kappa) = [0,\infty)$. For $\kappa > 0$ (which includes the Schrödinger operators for atoms with just one electron) all eigenvalues are negative and, since H_0 is lower bounded, it follows that H_κ is also lower bounded (Proposition 9.5.11) and so its eigenvalues belong to $[a, 0)$ for some $a < 0$. Hence $\chi_{(-\infty,0)}(H_\kappa) = \chi_{[a,0)}(H_\kappa)$; recall that rng $\chi_{[a,0)}(H_\kappa)$ reduces H_κ. Further, such eigenvalues belong to the discrete spectrum and so each of them is of finite multiplicity.

Remark 11.4.9. The 3D H-atom Schrödinger (energy) operator has a lowest spectral point, which is an eigenvalue in the discrete spectrum. In general quantum systems, the eigenvectors corresponding to the lowest possible energy (if they do exist) are called *ground states*. In physics it is assumed that, in practice, a system under small influence of its surroundings loses energy and in the limit it approaches a ground state; in many situations these are the only states of interest. In classical mechanics the coulombian system has no lowest energy and the electron could collapse onto the nucleus. The existence of a lowest possible quantum energy avoids this electron-nucleus "collision" and is then interpreted as stability of the H-atom, an outstanding achievement of quantum mechanics. Compare with Exercise 6.2.12.

Let $U_d(s)$ be the dilation unitary group in $\mathbb{R}^3$ of Example 5.4.8, that is,

$$(U_d(s)\psi)(x) = e^{-3s/2}\psi(e^{-s}x).$$

From the discussion on the Virial Theorem 6.2.8, if $\varphi \in C_0^\infty(\mathbb{R}^3)$, $\|\varphi\|_2 = 1$, and with support in $[1, 2]$, one has

$$\langle U_d(s)\varphi, H_\kappa U_d(s)\varphi\rangle = e^{-2s}\langle\varphi, H_0\varphi\rangle - \kappa e^{-s}\left\langle \varphi, \frac{1}{|x|}\varphi\right\rangle.$$

If $\kappa > 0$ this expression is negative for s large enough. Note that the support of $U_d(s)\varphi$ is in $[e^s, 2e^s]$; thus, by taking a sequence $s_j \to \infty$ so that the functions in the sequence $(U_d(s_j)\varphi)_j$ have pairwise disjoint supports, it follows that such a sequence is orthonormal and so $\dim \operatorname{rng} \chi_{(-\infty,0)}(H_\kappa) = \infty$; according to Theorem 11.2.1, this is the sum of the multiplicities of the eigenvalues of H_κ. Since the spectrum of H_κ in $[a, 0)$ is discrete and $0 \in \sigma_{\text{ess}}(H_\kappa)$, zero is the unique accumulation point of its eigenvalues. Summing up

Corollary 11.4.10. *Consider H_κ as above.*

i) *If $\kappa < 0$, then $\sigma(H_\kappa) = [0, \infty)$ and it has no eigenvalues.*
ii) *If $\kappa > 0$, then $\sigma(H_\kappa) = \{\lambda_j\}_{j=1}^\infty \cup [0, \infty)$, with $\lambda_1 < \lambda_2 < \lambda_3 < \cdots$, $\lambda_j \to 0$, and each λ_j is an eigenvalue of H_κ of finite multiplicity; finally, there are no positive eigenvalues.*

Remark 11.4.11. By solving explicitly the eigenvalue equation for H_κ, with $\kappa > 0$, one obtains $\lambda_j = -\left(\frac{\kappa}{2j}\right)^2$, $j \geq 1$. Most books on quantum mechanics present details of this calculation; see, for instance, [Will03], [LaL58]. The eigenvalues of 3D hydrogenic atoms, with physical constants included, are

$$\lambda_j = -\frac{m}{2}\left(\frac{Ze^2}{\hbar j}\right)^2, \qquad j \in \mathbb{N},$$

where Z is the atomic number (i.e., number of protons in the nucleus), m and e the electron mass and electric charge, respectively, and finally $\hbar$ denotes Planck's constant; further, the multiplicity of λ_j is j^2. It was Hermann Weyl who helped Schrödinger in the first calculation of such eigenvalues λ_j, and the subsequent agreement with the experimental spectral lines of the H-atom was very important to validate Schrödinger's proposal for his quantum energy operator.

Exercise 11.4.12. If (λ_j) are eigenvalues of a self-adjoint operator T and $\lambda_j \to \lambda$, use the corresponding eigenvectors to construct a Weyl singular sequence (see Theorem 11.2.7) for T at λ.

11.4.2 Embedded Eigenvalue

In Subsection 11.4.1 the virial was used to exclude eigenvalues embedded in the essential spectrum of some Schrödinger operators, including the hydrogen atom in $\mathbb{R}^3$. Now an example of an embedded eigenvalue in the essential spectrum will be presented; it has its roots in a paper by von Neumann and Wigner of 1929. Although for standard energy operators $-\Delta+V$, with vanishing potential at infinity, physically one should expect no eigenvalue embedded in the interior of the positive essential spectrum (see the discussion in the example ahead and Remark 13.6.12), and to prove it mathematically has been a difficult problem. Nevertheless, the absence of such embedded eigenvalues has been proved for a large class of "physically reasonable" potentials. For general results on embedding eigenvalues the reader is referred to [EaK82], [Sta96], [CrHM02] and references therein.

For each $a > 0$ define the potential in $\mathbb{R}^3$ (set $r = |x|, x \in \mathbb{R}^3$)

$$V^a(x) = V^a(r) = 32 \sin r \,\frac{(\sin r - (a + r)\cos r)}{(2a + 2r - \sin 2r)^2},$$

which has the following properties:

a) V^a is a bounded and continuous function.
b) For large r one has $V^a(r) \sim -4\sin(2r)/r$.
c) Given $\varepsilon > 0$ there is $m > 0$ so that $\|V^a\|_\infty < \varepsilon$ if $a > m$.

Thus, $V^a \in B^\infty_\infty(\mathbb{R}^3)$, V^a can be made arbitrarily small (take a large) and it is oscillating with decaying amplitude; in such a situation, the motion of a particle under V^a in classical mechanics with energy equal to 1 would be quite similar to a free motion, since V^a acts as a very small perturbation. In quantum mechanics, by Theorem 11.4.7, the operator

$$\mathrm{dom}\ H^a = \mathrm{dom}\ H_0, \qquad H^a = H_0 + V^a,$$

is self-adjoint and $\sigma_{\mathrm{ess}}(H^a) = [0,\infty)$, for all $a > 0$ (or by Proposition 11.4.15).

As discussed below, the operator H^a has an eigenvector corresponding to the eigenvalue 1 for all $a > 0$. Since the free energy operator H_0 has no eigenvalues and classically the motion with energy equal to 1 is quite similar to the free one, it is suggested that such an eigenvalue should not exist! The oscillations of the potential, even if of small amplitude (again for large a) and decaying for $r \to \infty$, are responsible for such an eigenvalue. Further, the dynamical behavior of eigenvectors is different from the dynamics of vectors in subspaces with no eigenvectors, as discussed in Chapter 13.

The function

$$\psi^a(x) = \psi^a(r) = \frac{2 \sin r}{r(2a + 2r - \sin 2r)}$$

is an element of dom H_0 and a direct calculation shows that

$$H^a \psi^a = \psi^a,$$

and ψ^a is an eigenvector of H^a corresponding to the eigenvalue 1. Note that it is convenient to use spherical coordinates and the unitary transformation u_3, discussed in Section 7.5, in order to perform such a calculation; also, ψ^a carries the values $l = m = 0$ so that the spherical harmonic Y_{00} is a constant function.

Exercise 11.4.13. Consider the potential

$$V(x) = 2\frac{3x^2 - 1}{(1 + x^2)^2}, \qquad x \in \mathbb{R}.$$

Check that $H = H_0 + V$, dom H = dom H_0, is self-adjoint, $\sigma_{\text{ess}}(H) = [0, \infty)$ and $\psi(x) = 1/(1 + x^2)$ is an eigenvector of H with eigenvalue zero.

11.4.3 Three Simple Classes of Potentials

In classical mechanics, if the potential V in $\mathbb{R}^n$ is lower bounded by β, i.e., $V(x) \geq \beta$, $\forall x \in \mathbb{R}^n$, then the mechanical energy $E = p^2 + V(x)$ of the particle clearly can not be smaller than β (otherwise $p^2 < 0$). Its quantum mechanical version is:

Proposition 11.4.14. *If $T \geq 0$ is a self-adjoint operator in* $\mathrm{L}^2(\mathbb{R}^n)$ *and* $V : \mathbb{R}^n \to [\beta, \infty)$ *is so that $T + V$ is self-adjoint with* dom $(T + V)$ = dom T, *then*

$$(-\infty, \beta) \subset \rho(T + V).$$

This holds, in particular, if $T = H_0$, i.e., the free particle hamiltonian.

Proof. Let $t < \beta$ and $\xi \in$ dom T with $\|\xi\| = 1$. Then,

$$\begin{aligned} \langle \xi, (T + V - t\mathbf{1})\xi\rangle &= \langle \xi, T\xi\rangle + \langle \xi, (V - t\mathbf{1})\xi\rangle \\ &\geq \langle \xi, (\beta - t)\xi\rangle = (\beta - t), \end{aligned}$$

and so

$$0 < (\beta - t) \leq \langle \xi, (T + V - t\mathbf{1})\xi\rangle \leq \|(T + V - t\mathbf{1})\xi\|.$$

Therefore, there is no Weyl sequence for $T + V$ at t. By Corollary 2.4.9, $t \in \rho(T + V)$. □

Proposition 11.4.15. *Let H_0 be the free particle Schrödinger operator in* $\mathrm{L}^2(\mathbb{R}^n)$ *and the potential* $V \in \mathrm{L}^2_{\text{loc}}(\mathbb{R}^n)$. *If H is a self-adjoint extension of $H_0 + V$,* dom $(H_0 + V) = C_0^\infty(\mathbb{R}^n)$, *and* $\lim_{|x|\to\infty} V(x) = a$, *then*

$$[a, \infty) \subset \sigma_{\text{ess}}(H).$$

Recall that if V is lower bounded, then $H_0 + V$ is essentially self-adjoint by Corollary 6.3.5.

Proof. A Weyl sequence for H at each $t > a$ will be constructed. Pick $t > a$ and $k \in \mathbb{R}^n$ obeying $k^2 = t - a$. Then $u_k(x) := e^{ikx}$ satisfies $(H_0 + a\mathbf{1})u_k(x) = tu_k(x)$ (since $H_0 u_k = -\Delta u_k$), and hence

$$\lim_{|x|\to\infty} (H_0 + V(x) - t\mathbf{1})\, u_k(x) = 0.$$

By considering $V(x) - a$ it is possible to assume that $a = 0$ in what follows. Note that $u_k \notin \mathrm{L}^2(\mathbb{R}^n)$. Pick $0 \neq \phi \in C_0^\infty(\mathbb{R}^n)$ with support in the closed ball $\overline{B}(0;1)$. For each $m = (m_1, \ldots, m_n) \in \mathbb{R}^n$ denote $|m| = |m_1 + \cdots + |m_n|$ and define, for $m \neq 0$,

$$\phi_m(x) = \phi\left(\frac{x-m}{\sqrt{|m|}}\right), \qquad \psi_m(x) = \frac{1}{\|\phi\|_2\, |m|^{n/4}}\, \phi_m(x)\, u_k(x).$$

The function $\psi_m \in \operatorname{dom} H$, for any self-adjoint extension H of $H_0 + V$, and it is normalized with support in the ball $B_m := \overline{B}(m; \sqrt{|m|})$. Note that there exists $C > 0$ so that

$$\|\nabla\phi_m\|_\infty \leq \frac{C}{\sqrt{|m|}}, \qquad \|H_0\phi_m\|_\infty \leq \frac{C}{|m|},$$

and if ℓ denotes Lebesgue measure, $\ell(B_m) \leq C|m|^{n/2}$. Further, given $\varepsilon > 0$, if $|m|$ is large enough then $|V(x)| \leq \varepsilon$ for all $x \in B_m$.

A direct computation leads to

$$\begin{aligned}(H - t\mathbf{1})\psi_m(x) &= (H_0 + V - t\mathbf{1})\psi_m(x)\\ &= \frac{u_k(x)}{\|\phi\|_2\, |m|^{n/4}}\left[(H_0+V)\phi_m(x) - ik\cdot(\nabla\phi_m)(x)\right],\end{aligned}$$

and so, for $|m|$ large enough,

$$\|(H_0 + V - t\mathbf{1})\psi_m\|_\infty \leq \frac{C}{\|\phi\|_2 |m|^{n/4}}\left[\frac{1}{|m|} + \varepsilon + |k|\frac{1}{|m|^{1/2}}\right].$$

Again for $|m|$ large enough,

$$\begin{aligned}\|(H_0 + V - t\mathbf{1})\psi_m\|_2^2 &\leq \|(H_0 + V - t\mathbf{1})\psi_m\|_\infty^2 \times \ell(B_m)\\ &\leq \frac{C^2}{\|\phi\|_2^2}\left[\frac{1}{|m|} + \varepsilon + |k|\frac{1}{|m|^{1/2}}\right]^2 \leq \frac{C^2}{\|\phi\|_2^2}\,(3\varepsilon)^2.\end{aligned}$$

This shows that (ψ_m) is a Weyl sequence for H at t, and so $t \in \sigma(H)$. Since the essential spectrum is closed, the result follows. □

Exercise 11.4.16. If $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R})$ and $\lim_{x\to\infty} V(x) = a$ (the behavior of V on the negative half-line does not matter!), show that $[a, \infty) \subset \sigma_{\mathrm{ess}}(H)$, for any self-adjoint extension H of $(H_0 + V)$ with dom $(H_0 + V) = C_0^\infty(\mathbb{R})$. Note that everything works in $\mathrm{L}^2[0, \infty)$. How to generalize this to $\mathbb{R}^n$?

Proposition 11.4.17. *Let h_0 be the tight-binding Schrödinger kinetic energy operator acting on $l^2(\mathbb{Z})$ and discussed in Subsection* 8.4.3. *If V is a real sequence that is nonzero only at a finite number of entries, then* $\sigma_{\text{ess}}(h_0 + V) = [-2, 2]$.

Proof. It is known that $\sigma(h_0) = [-2, 2]$. Since such V is a finite rank operator on $l^2(\mathbb{Z})$, it is compact. Therefore the result follows by Corollary 11.3.7. □

Exercise 11.4.18. Let $V(n)$ be a real-valued sequence in $l^2(\mathbb{Z})$. Show that $\sigma_{\text{ess}}(h_0 + V) = [-2, 2]$.

11.4.4 Existence of Negative Eigenvalues

In this subsection V is assumed to be an H_0-compact potential in $\mathbb{R}^n$ and $H = H_0 + V$ the subsequent self-adjoint operator with dom $H = \mathcal{H}^2(\mathbb{R}^n)$. Then, $\sigma_{\text{ess}}(H) = [0, \infty)$. A sufficient condition for the existence of negative eigenvalues of H will be given; such eigenvalues belong to $\sigma_{\text{d}}(H)$ and are important due to their physical meaning discussed in Chapter 13 and the possibility of existence of ground states. By Theorem 8.3.13, this goal is attained by showing that the projection $\chi_{(-\infty,0)}(H) \neq 0$; note that $\dim \operatorname{rng} \chi_{(-\infty,0)}(H)$ is exactly the number of negative eigenvalues, counted with multiplicities, since this subspace is spanned by the corresponding eigenvectors. In this subsection it will be used that, for $a > 0$, $g(a) = \int_{\mathbb{R}} e^{-ax^2} dx = \sqrt{\pi/a}$ and the derivatives $g^{(n)}(a) = (-1)^n \int_{\mathbb{R}} x^{2n} e^{-ax^2} dx$.

Theorem 11.4.19. *Let V be a potential in $\mathbb{R}^n$ as above. If there is $a > 0$ so that*

$$\int_{\mathbb{R}^n} V(x) e^{-2a^2x^2}\, dx < -na^{2-n} \left(\frac{\pi}{2}\right)^{n/2},$$

then H has (at least) one negative isolated eigenvalue of finite multiplicity.

Proof. $\chi_{(-\infty,0)}(H) \neq 0$ is equivalent to $\langle H\psi, \psi\rangle < 0$ for some $\psi \in \operatorname{dom} H$. Thus, the idea is to consider the trial function $\psi(x) = e^{-a^2x^2}$, $a > 0$, which belongs to dom H. Now, $\langle H\psi, \psi\rangle = \langle H_0\psi, \psi\rangle + \langle V\psi, \psi\rangle = \|\nabla\psi\|_2^2 + \langle V\psi, \psi\rangle$. By direct computation

$$\begin{aligned}
\langle H_0\psi, \psi\rangle = \|\nabla\psi\|_2^2 = \|i2a^2 e^{-a^2x^2} x\|_2^2 = 4a^4 \int_{\mathbb{R}^n} x^2 e^{-2a^2x^2}\, dx \\
= n4a^4 \int_{\mathbb{R}} t^2 e^{-2a^2t^2}\, dt \times \left(\int_{\mathbb{R}} e^{-2a^2t^2}\, dt\right)^{n-1} \\
= n4a^4 \times \frac{\sqrt{\pi/2}}{4a^3} \times \left(\frac{\sqrt{\pi/2}}{a}\right)^{n-1} = na^{2-n}\left(\frac{\pi}{2}\right)^{n/2}.
\end{aligned}$$

Hence

$$\langle H\psi, \psi\rangle = na^{2-n}\left(\frac{\pi}{2}\right)^{n/2} + \int_{\mathbb{R}^n} V(x) e^{-2a^2x^2}\, dx,$$

and the hypothesis in the theorem implies $\langle H\psi, \psi\rangle < 0$. □

This criterion is particularly useful in the one-dimensional case, since the condition on the potential reads

$$\int_{\mathbb{R}} V(x)e^{-2a^2x^2}\,dx < -a\sqrt{\frac{\pi}{2}},$$

and the right-hand side vanishes as $a \to 0$. This observation leads to the following consequences.

Corollary 11.4.20. *Let H be the above operator in $\mathrm{L}^2(\mathbb{R})$ with potential $V(x) \le 0$, $\forall x \in \mathbb{R}$.*

a) *If there is an interval $J \subset \mathbb{R}$ obeying $\int_J V(x)\,dx < 0$, then H has a negative eigenvalue.*
b) *If $\int_{\mathbb{R}} V(x)\,dx < 0$, then H has a negative eigenvalue.*

Proof. Note that b) follows at once from a). One has

$$\int_{\mathbb{R}} V(x)e^{-2a^2x^2}\,dx \le \int_J V(x)e^{-2a^2x^2}\,dx,$$

which converges to $\int_J V(x)\,dx < 0$ as $a \to 0$ by dominated convergence, and so, for a small enough,

$$\int_{\mathbb{R}} V(x)e^{-2a^2x^2}\,dx < -a\sqrt{\frac{\pi}{2}}$$

and the condition in Theorem 11.4.19 is satisfied. This proves a). □

Exercise 11.4.21. Check that, in the one-dimensional case, any (nonzero) continuous potential $V \le 0$ of compact support leads to a Schrödinger operator H with a negative eigenvalue.

Exercise 11.4.22. Give examples of potentials V in $\mathbb{R}^n$ so that H has a negative eigenvalue.

Remark 11.4.23. The idea in the proof of Theorem 11.4.19 can be elaborated in order to get conditions on V ensuring the existence of infinitely many negative eigenvalues as well as finitely many. For instance, in one-dimension, if there is c so that $V(x) \le 0$ for $x > c$ with $\int_{[c,\infty)} V(x)\,dx = -\infty$, then $\dim \operatorname{rng} \chi_{(-\infty,0)}(H) = \infty$ [Sche81]. See [BlaS], [DeK08], the book [ReeS78] and the review [Lie80] for additional information and references related to this vast area of research.

Remark 11.4.24. By a simple adaptation of Exercise 11.4.21, a nonzero continuous $V \le 0$ in $\mathbb{R}$ always produces a negative eigenvalue for H; it turns out that the same is true in $\mathbb{R}^2$. However, in $\mathbb{R}^n$, $n \ge 3$, there are cases of negative V with no negative eigenvalues for H; more explicitly, no such eigenvalue is present if $\int_{\mathbb{R}^n} |V(x)|^{n/2}\,dx$ is sufficiently small [Cw77, Lie80]. Interesting heuristic arguments can be found in Section 45 of the book [LaL58].

Exercise 11.4.25. In $\mathbb{R}^3$ let the radial potential $V(r) = -b\chi_{[0,a]}(r)$ ($r = |x|$, $a > 0$ and χ is a characteristic function) and $H = H_0 + V$, dom $H = \mathcal{H}^2(\mathbb{R}^3)$, a self-adjoint operator. Consider the eigenvalue equation $H\psi = \lambda\psi$ and show that if $b > 0$ is small enough, then H has no eigenvalues [LaL58].

Example 11.4.26. In case Planck's constant $\hbar > 0$ is taken into account one has $H = H(\hbar) = -\hbar^2\Delta + V$. Assume that the potential $V : \mathbb{R}^n \to \mathbb{R}$ is continuous, bounded from below, H_0-compact and that there is $x_0 \in \mathbb{R}^n$ with $V(x_0) = \min_{x\in\mathbb{R}^n} V(x) < 0$. Denote the unique self-adjoint extension of $H(\hbar)$ by the same symbol. Thus dom $H \supset C_0^\infty(\mathbb{R}^n)$ and $\sigma_{\text{ess}}(H(\hbar)) = [0, \infty)$. In spite of Remark 11.4.24, if $\hbar$ is small enough a negative eigenvalue is always present. In fact, let $\psi \in C_0^\infty(\mathbb{R}^n)$ with support S_ψ in a neighborhood of x_0 with $V(x) \le V(x_0)/2$, $\forall x \in S_\psi$; then

$$\begin{aligned}
\langle \psi, H(\hbar)\psi\rangle &= \hbar^2\|\nabla\psi\|^2 + \int_{\mathbb{R}^n} |\psi(x)|^2 V(x)\, dx \\
&= \hbar^2\|\nabla\psi\|^2 + \int_{S_\psi} |\psi(x)|^2 V(x)\, dx \\
&\le \hbar^2\|\nabla\psi\|^2 + \frac{1}{2}V(x_0)\|\psi\|^2
\end{aligned}$$

is negative for $\hbar$ small enough and a negative eigenvalue does exist (and it belongs to the discrete spectrum). The general study of small $\hbar$, including the limit $\hbar \approx 0$, is called the *semiclassical limit* of $H(\hbar)$. See also Section 14.5.

Exercise 11.4.27. By picking $\psi_j \in C_0^\infty(\mathbb{R}^n)$ with pairwise disjoint supports, show that given a positive integer k it is possible to take Planck's constant small enough so that $H(\hbar)$, in Example 11.4.26, has at least k negative eigenvalues.

In some cases it is possible to characterize the eigenvalues below the essential spectrum by means of a *variational approach* described in Proposition 11.4.28. Occasionally this characterization can be used to estimate the eigenvalues from above, as indicated in an exercise.

Proposition 11.4.28. *Let T be a bounded from below self-adjoint operator acting in $\mathcal{H}$. Suppose that, up to multiplicities, the eigenvalues of T are*

$$\lambda_0 < \lambda_1 < \lambda_2 < \cdots < \inf \sigma_{\text{ess}}(T).$$

Then

$$\begin{aligned}
\lambda_0 &= \inf_{0\neq\xi\in\text{dom } T} \langle \xi, T\xi\rangle/\|\xi\|^2, && E_0 := \mathrm{N}(T - \lambda_0\mathbf{1}), \\
\lambda_1 &= \inf_{0\neq\xi\in\text{dom } T\cap E_0^\perp} \langle \xi, T\xi\rangle/\|\xi\|^2, && E_1 := E_0 \oplus \mathrm{N}(T - \lambda_1\mathbf{1}), \\
\lambda_k &= \inf_{0\neq\xi\in\text{dom } T\cap E_{k-1}^\perp} \langle \xi, T\xi\rangle/\|\xi\|^2,
\end{aligned}$$

where $E_{k-1} := E_{k-2} \oplus \mathrm{N}(T - \lambda_{k-1}\mathbf{1})$.

Proof. The proof begins with λ_0 and then repeats the procedure. If $T\xi_0 = \lambda_0\xi_0$, $\xi_0 \neq 0$, then

$$\inf_{0\neq\xi\in\text{dom } T} \langle\xi, T\xi\rangle/\|\xi\|^2 \leq \langle\xi_0, T\xi_0\rangle/\|\xi_0\|^2 = \lambda_0.$$

Since λ_0 is the lower bound of the spectrum of T, then $T \geq \lambda_0\mathbf{1}$ and consequently

$$0 \leq \inf_{0\neq\xi\in\text{dom } T} \langle\xi, (T - \lambda_0\mathbf{1})\xi\rangle/\|\xi\|^2;$$

hence $\lambda_0 \leq \inf_{0\neq\xi\in\text{dom } T}\langle\xi, T\xi\rangle/\|\xi\|^2$, and the expression for λ_0 in the theorem follows.

Now, note that $\chi_{\{\lambda_0\}}(T)$ is the projection onto E_0 and it reduces T; so write $T = T_{E_0} \oplus T_{E_0^\perp}$ and, by Proposition 11.1.1,

$$\sigma(T_{E_0^\perp}) = \{\lambda_1, \lambda_2, \dots\} \cup \sigma_{\text{ess}}(T).$$

Apply the above steps to get the first eigenvalue of $T_{E_0^\perp}$, that is,

$$\begin{aligned}\lambda_1 &= \inf_{0\neq\xi\in\text{dom } T_{E_0^\perp}} \langle\xi, T_{E_0^\perp}\xi\rangle/\|\xi\|^2 \\ &= \inf_{0\neq\xi\in\text{dom } T\cap E_0^\perp} \langle\xi, T\xi\rangle/\|\xi\|^2.\end{aligned}$$

Note that $E_1 := E_0 \oplus \text{N}(T - \lambda_1\mathbf{1}) = \text{rng } \chi_{\{\lambda_0,\lambda_1\}}(T)$ and use the same procedure to get λ_2 as well as the remaining eigenvalues below the essential spectrum of T. $\square$

Exercise 11.4.29. Get an upper bound for the first eigenvalue of the operators $H_2\psi = -\psi'' + x^2$ and $H_4\psi = -\psi'' + x^4$ in $\text{L}^2(\mathbb{R})$ by considering the function $\psi_a(x) = e^{-ax^2}$, $a > 0$, and minimizing $\langle\psi_a, H_j\psi_a\rangle$, $j = 2, 4$, with respect to the parameter a (by Theorem 11.5.6, both operators are purely discrete).

Exercise 11.4.30. Let T be self-adjoint and $\mathcal{E}_\xi^T = \langle\xi, T\xi\rangle/\|\xi\|^2$ the expectation value of T with $0 \neq \xi \in \text{dom } T$ (see page 132 for a physical interpretation). If for all $\eta \in \text{dom } T$ one has

$$\frac{d}{ds}\mathcal{E}_{\xi+s\eta}^T\bigg|_{s=0} = 0,$$

show that $T\xi = \mathcal{E}_\xi^T\xi$, that is, ξ is an eigenvector of T whose corresponding eigenvalue is $\mathcal{E}_\xi^T$.

11.4.5 Resolvent Convergence and Essential Spectrum

In this subsection T_n, T denote self-adjoint operators.

Proposition 11.4.31. *Suppose* $T_n \xrightarrow{\text{NR}} T$.

i) *If* $\sigma(T_n)$ *is discrete in* (a, b) *for all* n*, then* $\sigma(T)$ *is discrete in* (a, b)*.*
ii) *If* $\sigma_{\text{ess}}(T_n) = [a, b]$*,* $-\infty \leq a \leq b \leq \infty$*,* $\forall n$*, then* $\sigma_{\text{ess}}(T) = [a, b]$*.*

The proof will make use of the following lemma which is of independent interest.

Lemma 11.4.32. *T has purely discrete spectrum in (a,b) iff $f(T)$ is a compact operator for all continuous f with support in (a,b).*

Proof. It is enough to assume that f has support $[\tilde{a},\tilde{b}] \subset (a,b)$. If T has discrete spectrum in (a,b), then the spectrum of T has only a finite number of eigenvalues $t_1,\dots,t_k$ in $[\tilde{a},\tilde{b}]$, each of them of finite multiplicity. Hence,

$$\chi_{[\tilde{a},\tilde{b}]}(T)T = \sum_{j=1}^{k} t_j \chi_{\{t_j\}}(T)$$

has finite rank and so is a compact operator. By noting that

$$f(T) = \chi_{[\tilde{a},\tilde{b}]}(T)f(T) = \sum_{j=1}^{k} f(t_j)\chi_{\{t_j\}}(T)$$

has also finite rank, it follows that $f(T)$ is compact.

Suppose now that every $f(T)$ is compact (f as in the lemma). Given $[\tilde{a},\tilde{b}] \subset (a,b)$ take a continuous function f so that

$$\chi_{[\tilde{a},\tilde{b}]} \le f \le \chi_{(a,b)}.$$

Then the projection $\chi_{[\tilde{a},\tilde{b}]}(T) = \chi_{[\tilde{a},\tilde{b}]}(T)f(T)$ is a compact operator, since it is the product of a bounded operator (itself) by the compact one $f(T)$. Necessarily a compact projection has finite rank, and so any $t \in [\tilde{a},\tilde{b}] \cap \sigma(T)$ is an isolated eigenvalue of T of finite multiplicity. Since this holds for any compact subinterval of (a,b), T has discrete spectrum in this interval. □

Proof. [**Proposition 11.4.31**] i) If f is continuous with support in (a,b), then $f(T_n) \to f(T)$ in $\mathrm{B}(\mathcal{H})$ (see Exercise 10.1.14). By Lemma 11.4.32, $f(T_n)$ is compact for any n, and Theorem 1.3.13 implies that $f(T)$ is compact. Apply Lemma 11.4.32 again.

ii) By Corollary 10.2.5, $[a,b] \subset \sigma_{\mathrm{ess}}(T)$. By i), $\mathbb{R} \setminus [a,b] \subset \sigma_{\mathrm{d}}(T)$. Combine these two statements. □

Exercise 11.4.33. Adapt the proof of Proposition 11.4.31ii) to the case $\sigma_{\mathrm{ess}}(T_n) = [a_n,b_n]$, $T_n \xrightarrow{\mathrm{NR}} T$, and conclude that $\sigma_{\mathrm{ess}}(T) = [a,b]$ for some $-\infty \le a \le b \le \infty$. Conclude also that necessarily one has $a = \lim_{n\to\infty} a_n$ and $b = \lim_{n\to\infty} b_n$.

Example 11.4.34. In case of just strong convergence in the resolvent sense, Example 10.3.4 shows that it may occur that $\sigma_{\mathrm{ess}}(T_n) = \mathbb{R}$, $\forall n$, and $\sigma_{\mathrm{ess}}(T) = \{0\}$.

11.5 Discrete Spectrum for Unbounded Potentials

The main goal of this section is to show that for potentials $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$, bounded from below $V(x) \geq \beta > -\infty$ and with

$$\lim_{|x|\to\infty} V(x) = \infty,$$

the corresponding Schrödinger operators H, given by the unique self-adjoint extension of $H_0 + V$ with domain $C_0^\infty(\mathbb{R}^n)$ (see Corollary 6.3.5), has purely discrete spectrum. An important especial case is given by the harmonic oscillator potential $V(x) = \kappa|x|^2$, $\kappa > 0$. By considering $V - \beta$, it is possible to assume that $V \geq 0$ in what follows, and this will be done.

Before proceeding to a detailed proof, a prominent decomposition of such unbounded potentials will be underlined. For any given $\lambda > 0$, define

$$V_\lambda(x) = \min\{V(x) - \lambda, 0\}, \qquad V^\lambda(x) = \max\{V(x) - \lambda, 0\},$$

so that $V - \lambda = V^\lambda + V_\lambda$, $V^\lambda \geq 0$ and the support of V_λ, denoted by $\Omega_\lambda = \{x \in \mathbb{R}^n : V_\lambda(x) \neq 0\}$, is a compact subset of $\mathbb{R}^n$ if $\lim_{|x|\to\infty} V(x) = \infty$. The latter property will be crucial in the proof of discrete spectrum.

Lemma 11.5.1. *Let $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$, $V(x) \geq 0$, and H the unique self-adjoint extension of $H_0 + V$,* dom $(H_0 + V) = C_0^\infty(\mathbb{R}^n)$. *Then:*

a) *The operator $H_0^{1/2} R_{-1}(H)^{1/2}$ is bounded with norm ≤ 1.*

b) *For each bounded borelian $\Lambda \subset \mathbb{R}$, the operator $\chi_\Lambda(x) R_{-1}(H_0^{1/2})$ is compact.*

Proof. Note that $H \geq 0$ and both $R_{-1}(H_0)$ and $R_{-1}(H)$ are bounded self-adjoint operators.

a) For $\psi \in C_0^\infty(\mathbb{R}^n)$,

$$\begin{aligned}\|H_0^{1/2}\psi\|^2 &= \langle \psi, H_0\psi\rangle \leq \langle \psi, H\psi\rangle \\ &\leq \langle \psi, (H+\mathbf{1})\psi\rangle = \|(H+\mathbf{1})^{1/2}\psi\|^2.\end{aligned}$$

Write $\psi = R_{-1}(H)^{1/2}\phi$; thus

$$\left\| H_0^{1/2} R_{-1}(H)^{1/2}\phi \right\| \leq \|\phi\|, \qquad \forall \phi \in \mathcal{D} = (H+\mathbf{1})^{1/2} C_0^\infty(\mathbb{R}^n).$$

Since dom H is a core of $H^{1/2}$ it follows that $\mathcal{D}$ is dense in $\mathrm{L}^2(\mathbb{R}^n)$, so the above inequality holds for all $\phi \in \mathrm{L}^2(\mathbb{R}^n)$. Therefore $\left\| H_0^{1/2} R_{-1}(H)^{1/2} \right\| \leq 1$.

b) It is a consequence of Lemma 11.4.2, with $f(x) = \chi_\Lambda(x)$ and $g(p) = (|p|+1)^{-1}$, since $f \in \mathrm{L}^2(\mathbb{R}^n)$ and $g \in B_\infty^\infty(\mathbb{R}^n)$. □

Exercise 11.5.2. Present details of the conclusion that the subspace $\mathcal{D}$ in the proof of Lemma 11.5.1 is dense in the Hilbert space; see Proposition 9.3.5.

Definition 11.5.3. A self-adjoint operator T, acting in $\mathrm{L}^2(\mathbb{R}^n)$, for which

$$\chi_\Lambda(x) R_z(T)$$

is a compact operator for some $z \in \rho(T)$ (and so for all $z \in \rho(T)$) and all bounded borelian $\Lambda \subset \mathbb{R}$ is called *locally compact.*

Example 11.5.4. $H_0^{1/2}$ and the operator H in Lemma 11.5.1 are locally compact.

Proof. The case of $H_0^{1/2}$ is immediate from Lemma 11.5.1. Now the operator H. For any bounded borelian $\Lambda \subset \mathbb{R}$ one has

$$\chi_\Lambda(x) R_{-1}(H) = \chi_\Lambda(x) R_{-1}(H)^{\frac{1}{2}}\, R_{-1}(H)^{\frac{1}{2}} = A\, B\, R_{-1}(H)^{\frac{1}{2}},$$

with, by Lemma 11.5.1, $A = \chi_\Lambda(x) R_{-1}(H_0^{1/2})$ a compact operator and $B = (H_0^{1/2} + \mathbf{1}) R_{-1}(H)^{1/2}$ a bounded operator. It follows that $\chi_\Lambda(x) R_{-1}(H)$ is compact by Proposition 1.3.7. □

Exercise 11.5.5. Show that H_0 is a locally compact operator.

Theorem 11.5.6. *Let* $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$*,* $V(x) \geq 0$*, and* H *the unique self-adjoint extension of* $H_0 + V$*,* dom $(H_0 + V) = C_0^\infty(\mathbb{R}^n)$*. If* $\lim_{|x|\to\infty} V(x) = \infty$*, then* H *has purely discrete spectrum.*

Proof. Let $\lambda > 0$ and H^λ the unique (see Corollary 6.3.5) self-adjoint extension of $H_0 + V^\lambda$ with dom $(H_0 + V^\lambda) = C_0^\infty(\mathbb{R}^n)$. V_λ is a bounded multiplication operator (see the beginning of this section for notation),

$$H - \lambda\mathbf{1} = H^\lambda + V_\lambda$$

and Ω_λ is a compact subset of $\mathbb{R}^n$. By Example 11.5.4, $\chi_{\Omega_\lambda}(x) R_{-1}(H^\lambda)$ is a compact operator. Thus

$$V_\lambda(x) R_{-1}(H^\lambda) = V_\lambda(x) \chi_{\Omega_\lambda}(x) R_{-1}(H^\lambda)$$

is also compact; hence, V_λ is H^λ-compact. Since $H^\lambda \geq 0$, by Weyl criterion, that is, Corollary 11.3.6,

$$\sigma_{\mathrm{ess}}(H - \lambda\mathbf{1}) = \sigma_{\mathrm{ess}}(H^\lambda) \subset [0, \infty),$$

and so

$$\sigma_{\mathrm{ess}}(H) \subset [\lambda, \infty).$$

Since this holds true for all $\lambda > 0$, it follows that $\sigma_{\mathrm{ess}}(H) = \emptyset$. □

Theorem 11.3.13 implies

Corollary 11.5.7. *Let* H *be as in Lemma* 11.5.1 *with* $\lim_{|x|\to\infty} V(x) = \infty$*. Then* $R_z(H)$ *is compact for all* $z \in \rho(H)$*.*

Example 11.5.8. If $V(x)$ is a real polynomial with $\lim_{|x|\to\infty} V(x) = \infty$, then the unique self-adjoint extension of $H_0 + V$ has purely discrete spectrum.

Exercise 11.5.9. The harmonic oscillator hamiltonian $H = H_0 + x^2$ in $\mathrm{L}^2(\mathbb{R})$, discussed in Example 2.3.3, has purely discrete spectrum and $\psi_0(x) = e^{-x^2/2}$ is an eigenfunction of H with $H\psi_0 = \psi_0$. Verify that $H_1 = H_0 + x^2 + \varepsilon|x|$ (resp. $H_4 = H_0 + x^2 + \varepsilon x^4$), $\varepsilon \geq 0$, are purely discrete operators and use Exercise 9.5.4 to show that H_1 (resp. H_4) has an eigenvalue in the interval $[1-\varepsilon a, 1+\varepsilon a]$, $a = \sqrt{\pi}/2$ (resp. $a = 105\sqrt{\pi}/16$).

Remark 11.5.10. The condition $\lim_{|x|\to\infty} V(x) = \infty$, with bounded below $V \in \mathrm{L}^2_{\mathrm{loc}}$, is not necessary for discrete spectrum, since oscillations are admissible. In $\mathrm{L}^2(\mathbb{R})$ a necessary and sufficient condition for discrete spectrum given in [Mol53] is

$$\lim_{|x|\to\infty} \int_a^{a+\varepsilon} V(x)dx = \infty, \qquad \forall \varepsilon > 0;$$

there are also conditions in $\mathrm{L}^2(\mathbb{R}^n)$. For corresponding conditions on operators with magnetic fields see [KoMS04].

Exercise 11.5.11. Let T_1, T_2 be positive self-adjoint operators and assume that $b^1 \leq b^2$, as in Lemma 10.4.4. Show that if T_1 has purely discrete spectrum, then T_2 is also purely discrete. Hint: For $\xi \in \mathrm{dom}\ T_2$, show that

$$\|R_{-1}(T_1)^{\frac{1}{2}}\xi\|^2 \leq \|R_{-1}(T_2)^{\frac{1}{2}}\xi\|^2,$$

and for $\eta \in \mathcal{H}$, write $\xi = R_{-1}(T_2)^{\frac{1}{2}}\eta$ and conclude that $A = (T_1 + \mathbf{1})^{\frac{1}{2}} R_{-1}(T_2)^{\frac{1}{2}}$ is bounded. Write $R_{-1}(T_2)^{\frac{1}{2}} = R_{-1}(T_1)^{\frac{1}{2}} A$ and conclude that $R_{-1}(T_2)$ is compact.

11.6 Spectra of Self-Adjoint Extensions

In this section some relations among the spectra of self-adjoint extensions of a given hermitian operator $S : \mathrm{dom}\ S \sqsubseteq \mathcal{H} \to \mathcal{H}$ will be discussed. It will be assumed that S is closed and with equal deficiency indices $n_+(S)$ and $n_-(S)$. In this case denote $d(S) := n_+(S) = n_-(S)$.

It is clear that the eigenvalues of an operator are preserved by its extensions. In the case of hermitian operators more can be said. Before the rigorous arguments, it is worth saying something at an intuitive level. If S is a closed hermitian operator, by Theorem 2.2.11,

$$\mathrm{dom}\ S^* = \mathrm{dom}\ S \oplus_{S^*} \mathrm{K}_+(S) \oplus_{S^*} \mathrm{K}_-(S),$$

so if T_1 and T_2 are self-adjoint extensions of S, then $X = T_1 - T_2$ is the zero operator on dom S; if $d(S) < \infty$, since both $T_1, T_2 \subset S^*$, the operator X can be nonzero only on a subspace of the finite-dimensional $\mathrm{K}_+(S) \oplus_{S^*} \mathrm{K}_-(S)$, so its spectrum should be discrete there. I.e., if this intuitive reasoning is correct, the multiplicity of each eigenvalue (including new ones) of T_1 and/or T_2 increases at most by a finite amount with respect to S, and the essential spectrum of T_1 and T_2 coincide. Now the correct statements and proofs.

Proposition 11.6.1. *Let S be hermitian and closed. If λ is an eigenvalue of S of multiplicity m, then λ is also an eigenvalue of each of its self-adjoint extensions T and of multiplicity $\leq m + d(S)$.*

Proof. By Proposition 2.5.8, $\dim(\text{dom } T/\text{dom } S) = d(S)$ (see also the remark that follows that proposition). Put

$$M(\lambda) := \mathrm{N}(T - \lambda\mathbf{1}) \cap \mathrm{N}(S - \lambda\mathbf{1})^{\perp},$$

and note that

$$\mathrm{N}(T - \lambda\mathbf{1}) = \mathrm{N}(S - \lambda\mathbf{1}) \oplus M(\lambda).$$

The task is to show that $d(S)$ is an upper bound to $\dim M(\lambda)$. Since $\mathrm{N}(S - \lambda\mathbf{1}) = \mathrm{N}(T - \lambda\mathbf{1}) \cap \text{dom } S$ it follows that $M(\lambda) \cap \text{dom } S = \{0\}$. Now $M(\lambda) \subset \text{dom } T$ and $\text{dom } S \subset \text{dom } T$, so

$$M(\lambda) + \text{dom } S := \{\xi + \eta : \xi \in M(\lambda), \eta \in \text{dom } S\} \subset \text{dom } T.$$

Hence, $\dim M(\lambda) \leq \dim(\text{dom } T/\text{dom } S) = d(S)$. □

For the discussion of the essential spectrum the following variation of Weyl's criterion 11.3.6 will be used.

Proposition 11.6.2. *Let T, S be self-adjoint operators. If $R_i(T) - R_i(S)$ is a compact operator, then $\sigma_{\text{ess}}(S) = \sigma_{\text{ess}}(T)$.*

Proof. Put $Q := R_i(T) - R_i(S)$. If $t \in \sigma_{\text{ess}}(T)$, then there exists a singular Weyl sequence (ξ_j) for T at t. Note that $Q\xi_j \to 0$, as $j \to \infty$, and

$$\begin{aligned} R_i(T)\xi_j - \frac{1}{t-i}\xi_j &= \frac{R_i(T)}{t-i}\left[(t-i)\mathbf{1} - (T - i\mathbf{1})\right]\xi_j \\ &= -\frac{R_i(T)}{t-i}\left(T - t\mathbf{1}\right)\xi_j \to 0, \end{aligned}$$

which implies

$$\lim_{j\to\infty} \|R_i(T)\xi_j\| = \frac{1}{|t-i|} > 0.$$

The goal is to show that $t \in \sigma_{\text{ess}}(S)$. Since

$$\lim_{j\to\infty} \|R_i(S)\xi_j\| = \lim_{j\to\infty} \|R_i(T)\xi_j - Q\xi_j\| = \frac{1}{|t-i|},$$

then for sufficiently large j one has

$$\|R_i(S)\xi_j\| \geq \frac{1}{2|t-i|}$$

and the sequence

$$\eta_j := \frac{R_i(S)\xi_j}{\|R_i(S)\xi_j\|}$$

is normalized with $\eta_j \xrightarrow{\mathrm{w}} 0$; in fact, for any $\zeta \in \mathcal{H}$,

$$\langle \eta_j, \zeta \rangle = \frac{1}{\|R_i(S)\xi_j\|} \langle \xi_j, R_{-i}(S)\zeta \rangle$$

which vanishes for $j \to \infty$ since $\xi_j \xrightarrow{\mathrm{w}} 0$ and $\|R_i(S)\xi_j\| \to 1/|t-i|$.

Next it will be checked that $(S - t\mathbf{1})\eta_j \to 0$, so that, by Exercise 11.2.8, (η_j) is a singular Weyl sequence for S at t and $t \in \sigma_{\mathrm{ess}}(S)$. Indeed,

$$\begin{aligned}(S - t\mathbf{1})\eta_j &= (S - i\mathbf{1})\eta_j + (i - t)\eta_j \\ &= \frac{t-i}{\|R_i(S)\xi_j\|} \left(\frac{\xi_j}{t-i} - R_i(S)\xi_j \right) \\ &= \frac{t-i}{\|R_i(S)\xi_j\|} \left(\frac{\xi_j}{t-i} - R_i(T)\xi_j + Q\xi_j \right) \to 0.\end{aligned}$$

Hence $\sigma_{\mathrm{ess}}(T) \subset \sigma_{\mathrm{ess}}(S)$. Exchange the roles of S and T to get $\sigma_{\mathrm{ess}}(S) \subset \sigma_{\mathrm{ess}}(T)$. The proposition is proved. ☐

Exercise 11.6.3. Show that i in Proposition 11.6.2 can be replaced by any $z \in \rho(T) \cap \rho(S)$.

Exercise 11.6.4. Show that if $(T-S)$ is T-compact, then $R_z(T) - R_z(S)$ is compact for any $z \in \rho(T) \cap \rho(S)$. Thus, in principle, Proposition 11.6.2 is a generalization of Weyl criterion 11.3.6.

Lemma 11.6.5. *If T_1 and T_2 are two self-adjoint extensions of the closed and hermitian operator S, then $Q := R_i(T_1) - R_i(T_2)$ is an operator of rank $\le d(S)$.*

Proof. First note that $Q\,(\mathrm{rng}\ (S - i\mathbf{1})) = 0$; by continuity of the operator Q one has $Q(\overline{\mathrm{rng}\ (S - i\mathbf{1})}) = 0$, and so

$$\mathrm{rng}\ Q = Q\,[\mathrm{rng}\ (S - i\mathbf{1})]^{\perp} = Q\mathrm{K}_+,$$

where K_+ is a deficiency subspace of S. Since $\dim \mathrm{K}_+ = d(S)$, the rank of Q is $\le d(S)$. ☐

Theorem 11.6.6. *If T_1 and T_2 are two self-adjoint extensions of the closed and hermitian operator S with $d(S) < \infty$, then $\sigma_{\mathrm{ess}}(T_1) = \sigma_{\mathrm{ess}}(T_2)$.*

Proof. By Lemma 11.6.5, $R_i(T_1) - R_i(T_2)$ is a finite rank operator, so compact. Apply Proposition 11.6.2. ☐

Corollary 11.6.7. *If a self-adjoint extension of a closed and hermitian operator S, with $d(S) < \infty$, has purely discrete spectrum, then this holds for all self-adjoint extensions of S.*

Remark 11.6.8. If the deficiency indices $n_- = n_+ = \infty$, there are many possibilities for the spectra of the corresponding self-adjoint extensions. Based on the intuitive discussion on page 307, since in this case self-adjoint extensions differ on their action on the infinite-dimensional deficiency subspaces, a richness of spectral possibilities should be expected. For precise results see [BraN96].

11.6.1 Green Function and a Free Compact Resolvent

In this subsection the Green function of a particular self-adjoint extension H_N of the free energy operator on $[0,1]$ (see Example 7.3.4) will be computed, and the corresponding resolvent operator shown to be compact. It will follow, by Theorem 11.3.13, that this operator H_N has purely discrete spectrum and, by Corollary 11.6.7, that all self-adjoint extensions $H_{\hat{U}}$ have empty essential spectra. This simple example illustrates quite well the involved ideas and, as a subproduct, the eigenvalues of this self-adjoint extension H_N are found.

Recall that the initial energy operator is $H\psi = -\psi''$, dom $H = C_0^\infty(0,1)$, $n_- = n_+ = 2$, dom $H^* = \mathcal{H}^2[0,1]$ and its self-adjoint extensions $H_{\hat{U}}$ are labeled by the 2×2 unitary matrix $\hat{U}$. The dom $H_{\hat{U}}$ is the subspace of $\psi \in \mathcal{H}^2[0,1]$ so that

$$\left(\mathbf{1} - \hat{U}\right) \begin{pmatrix} \psi'(0) \\ \psi'(1) \end{pmatrix} = -i \left(\mathbf{1} + \hat{U}\right) \begin{pmatrix} -\psi(0) \\ \psi(1) \end{pmatrix},$$

and $H_{\hat{U}}\psi = -\psi''$.

For $z \in \mathbb{C}$ and $\psi \in \mathrm{L}^2[0,1]$, write $R_z(H_{\hat{U}})\psi = \phi \in \mathrm{dom}\, H_{\hat{U}}$ so that

$$(H_{\hat{U}} - z\mathbf{1})\phi(x) = -\phi''(x) - z\phi(x) = \psi(x),$$

which is a second-order linear differential equation for ϕ. For $z \neq 0$, the solutions of the homogeneous equation are linearly spanned by $\phi_\pm(x) = \exp\left(\pm i\sqrt{z}\, x\right)$; fix, say, Im $\sqrt{z} \geq 0$. Note that $\psi \in \mathrm{L}^1[0,1]$.

The wronskian $W_x[\overline{\phi_+}, \phi_-] = -2i\sqrt{z}$ and, by the variation of parameters technique (see page 180), there are constants $b_\pm$ so that

$$\begin{aligned} \phi(x) &= b_+\phi_+(x) + b_-\phi_-(x) \\ &\quad - \frac{1}{2i\sqrt{z}} \int_0^x \left(e^{i\sqrt{z}\,(x-s)} - e^{-i\sqrt{z}\,(x-s)}\right) \psi(s)\, ds \\ &= b_+\phi_+(x) + b_-\phi_-(x) - \frac{1}{\sqrt{z}} \int_0^x \sin\left(\sqrt{z}\,(x-s)\right)\, \psi(s)\, ds. \end{aligned}$$

Thus,

$$\phi'(x) = i\sqrt{z}\,(b_+\phi_+ - b_-\phi_-) - \int_0^x \cos(\sqrt{z}\,(x-s))\, \psi(s)\, ds.$$

Up to this point no specific self-adjoint extension was selected; by choosing the Neumann boundary condition $\phi'(0) = 0 = \phi'(1)$, i.e., $\hat{U} = -\mathbf{1}$ above, and denoting

$H_N = H_{\hat{U}=-\mathbf{1}}$, it follows that

$$b_+ = b_- = -\frac{1}{2\sqrt{z}\,\sin\sqrt{z}} \int_0^1 \cos(\sqrt{z}\,(1-s))\,\psi(s)\,ds.$$

Hence

$$\begin{aligned}\phi(x) &= -\frac{1}{\sqrt{z}}\left[\frac{\cos\sqrt{z}x}{\sin\sqrt{z}}\int_0^1 \cos(\sqrt{z}(1-s))\psi(s)ds\right.\\ &\quad \left.+\int_0^x \sin\left(\sqrt{z}\,(x-s)\right)\,\psi(s)\,ds\right]\\ &= \int_0^1 G(x,s;z)\,\psi(s)\,ds = (R_z(H_N)\psi)(x),\end{aligned}$$

where $G(x, s; z)$ is the *Green function* of such a self-adjoint extension, which is given by (recall $z \neq 0$)

$$G(x,s;z) = \begin{cases} \frac{-1}{\sqrt{z}}\left[\frac{\cos\sqrt{z}x}{\sin\sqrt{z}}\cos(\sqrt{z}(1-s)) + \sin(\sqrt{z}\,(x-s))\right], & s < x \\ \frac{-\cos\sqrt{z}x}{\sqrt{z}\sin\sqrt{z}}\ \cos(\sqrt{z}(1-s)), & s > x \end{cases}.$$

Similarly, for $z = 0$ one gets $\phi_+(x) = 1$, $\phi_-(x) = x$,

$$\phi(x) = b_+ + b_- x + \int_0^x s\psi(s)\,ds - x\int_0^x \psi(s)\,ds,$$

$\phi'(x) = b_- - \int_0^x \psi(s)\,ds$, and imposing Neumann conditions it follows that $b_- = 0$, and $0 = \phi'(1) = -\int_0^1 \psi(s)\,dx$, so that $\phi(1) = b_+ + \int_0^1 s\psi(s)\,ds$. Since this holds for all $b_+ \in \mathbb{C}$, and ϕ is a continuous function, the resolvent operator is not defined for $z = 0$; in fact, the constant function $\psi(x) = 1$ is an eigenvector of H_N with zero eigenvalue and $0 \in \sigma(H_N)$ (check this!).

Thus the resolvent operator $R_z(H_N)$ is an integral operator whose kernel is the Green function; note that for $z = 1$ (or take any value $z \in \mathbb{C}\setminus\mathbb{R}$) the function $G(x, s; 1) \in \mathrm{L}^2([0, 1] \times [0, 1])$, and so, by Example 1.4.9, it is a Hilbert-Schmidt operator, in particular a compact one. By applying successively Theorems 11.3.13 and 11.6.6 it follows that all self-adjoint extensions $H_{\hat{U}}$ have purely discrete spectra.

Furthermore, in case of Neumann conditions dealt with above, by including the eigenvalue $\lambda_0 = 0$, one sees that the Green function is not defined (it has poles) at λ_n so that $\sin\sqrt{\lambda_n} = 0$, that is, $\lambda_n = n^2\pi^2$, $n = 0, 1, 2, \ldots$. Therefore, each λ_n belongs to the spectrum of this self-adjoint operator H_N; since they are isolated points in the spectrum, $\sigma(H_N) = \{\lambda_n\}$, and Corollary 11.2.3 implies they are eigenvalues.

Exercise 11.6.9. Redo the above analysis for the Dirichlet self-adjoint extension $H_D = H_{\hat{U}=\mathbf{1}}$, and check that the Green function is well defined for $z = 0$, so that zero belongs to the resolvent of H_D.

Exercise 11.6.10. Compute the Green function and spectra of all self-adjoint extensions for the momentum operator on the interval $[0, 1]$, as discussed in Example 2.6.5. Check that such Green functions are Hilbert-Schmidt operators.

Exercise 11.6.11. Show that for any $\lambda \in \mathbb{R} \cup \{\infty\}$ the free energy operator H_λ on $[0, \infty)$, discussed in Example 7.3.1, has $\sigma_{\mathrm{ess}}(H_\lambda) = [0, \infty)$. Note that it is enough to consider a fixed value of λ, say $\lambda = \infty$, check that, for $z > 0$, for any $0 \neq \psi \in \mathrm{L}^2[0, \infty)$ one has $R_z(H_\lambda)\psi \notin \mathrm{L}^2[0, \infty)$, so that $z \in \sigma(H_\lambda)$ for any $z > 0$, and combine this with Corollary 11.6.7 and Exercise 7.3.2.

Exercise 11.6.12. Let T be self-adjoint and $\lambda_0 \in \sigma_{\mathrm{d}}(T)$ with eigenfunction ψ_0. Use Corollary 1.5.14 to show that the function

$$\mathbb{C} \ni z \mapsto \langle \psi_0, R_z(T)\psi_0 \rangle$$

is meromorphic on a neighbourhood of λ_0 with a pole at λ_0.

Chapter 12

Spectral Decomposition II

The prominent spectral decomposition of a self-adjoint operator into a point part, an absolutely continuous part, and a singular continuous part is discussed in detail. Some basic criteria are presented. At the end of the chapter, the Weyl-von Neumann and wonderland theorems are proved. Dynamical consequences of this spectral decomposition are described in Chapter 13.

12.1 Point, Absolutely Continuous and Singular Continuous Subspaces

Given two (finite) measures μ, ν, the standard notations

$$\mu \perp \nu \qquad \text{and} \qquad \mu \ll \nu$$

indicate that μ and ν are mutually singular and that μ is absolutely continuous with respect to ν, respectively. In case $\mu \ll \nu$ the respective Radon-Nikodym derivative will be denoted by $d\mu/d\nu$, as usual.

Let ℓ denote the Lebesgue measure over the Borel sets $\mathcal{A}$ of $\mathbb{R}$. Recall that, by Lebesgue decomposition, a Borel measure μ over $\mathbb{R}$ can be (uniquely) decomposed as $\mu = \mu_{\mathrm{p}} + \mu_{\mathrm{c}}$, with μ_{c} and μ_{p} denoting its continuous part (that is, $\mu_{\mathrm{c}}(\{t\}) = 0$, $\forall t \in \mathbb{R}$) and point part (that is, there is a countable set Ω so that $\mu_{\mathrm{p}}(\mathbb{R} \setminus \Omega) = 0$), respectively. Note that $\mu_{\mathrm{p}} \perp \ell$, that is, they are mutually singular measures. By Lebesgue decomposition one has (uniquely) $\mu_{\mathrm{c}} = \mu_{\mathrm{ac}} + \mu_{\mathrm{sc}}$, with $\mu_{\mathrm{ac}} \ll \ell$ and $\mu_{\mathrm{sc}} \perp \ell$, so that

$$\mu = \mu_{\mathrm{p}} + \mu_{\mathrm{ac}} + \mu_{\mathrm{sc}}.$$

μ_{ac} is called the absolutely continuous component of μ (with the complement "with respect to Lebesgue measure" being understood), while μ_{sc} is the singular continuous component of μ. Such decompositions will be used to perform corresponding decompositions of self-adjoint operators, via their respective spectral measures, since their spectra are nonempty and real.

In this chapter $T : \mathrm{dom}\, T \sqsubseteq \mathcal{H} \to \mathcal{H}$ will always denote a self-adjoint operator acting in the separable Hilbert space $\mathcal{H}$ and $\mu_\xi = \mu_\xi^T$ the spectral measures of T at $\xi \in \mathcal{H}$.

Definition 12.1.1. The *point subspace* of T is $\mathcal{H}_\mathrm{p} = \mathcal{H}_\mathrm{p}(T) \subset \mathcal{H}$ given by the closure of the linear subspace spanned by the eigenvectors of T. Its orthogonal complement $\mathcal{H}_\mathrm{c} = \mathcal{H}_\mathrm{c}(T) := \mathcal{H}_\mathrm{p}(T)^\perp$ is the *continuous subspace* of T. P_p^T and P_c^T will denote the respective orthogonal projection operators.

Theorem 12.1.2. *Let T be self-adjoint.*

i) *There exists a countable set $\Lambda \subset \mathbb{R}$ so that*

$$\mathcal{H}_\mathrm{p}(T) = \{\xi \in \mathcal{H} : \mu_\xi(\mathbb{R} \setminus \Lambda) = 0\}.$$

Λ can be taken as the set of eigenvalues of T.

ii) $\mathcal{H}_\mathrm{c}(T) = \{\xi \in \mathcal{H} : \mu_\xi(\{t\}) = 0, \forall t \in \mathbb{R}\}$, *that is, the function* $t \mapsto \|\chi_{(-\infty,t]}(T)\xi\|$ *is continuous.*

iii) $\mathcal{H} = \mathcal{H}_\mathrm{p}(T) \oplus \mathcal{H}_\mathrm{c}(T)$ *and both* $\mathcal{H}_\mathrm{p}(T)$ *and* $\mathcal{H}_\mathrm{c}(T)$ *reduce* T.

Proof. Let $\Lambda = \{\lambda_j\}_j$ be the set of eigenvalues of T, i.e., $T\xi_j = \lambda_j\xi_j$, $\|\xi_j\| = 1$, $\xi_j \in \mathrm{dom}\, T$, $\forall j$.

i) If $\xi \in \mathcal{H}_\mathrm{p}$, then $\xi = \sum_j a_j\xi_j$, $\sum_j |a_j|^2 = \|\xi\|^2$. Thus $\chi_\Lambda(T)\xi = \xi$ and $\mu_\xi(\mathbb{R} \setminus \Lambda) = 0$.

Now, if for $\xi \in \mathcal{H}$ there exists a countable set $\Omega = \{t_j\}_j$, $t_j \neq t_k$ if $j \neq k$, with $\mu_\xi(\mathbb{R} \setminus \Omega) = 0$, one has

$$\xi = \chi_\Omega(T)\xi = \sum_j \chi_{\{t_j\}}(T)\xi.$$

By Theorem 11.2.1, for each t_j so that $\chi_{\{t_j\}}(T)\xi \neq 0$, the vector $\chi_{\{t_j\}}(T)\xi$ is an eigenvector of T with eigenvalue t_j, so it follows that $t_j \in \Lambda$ and $\xi \in \mathcal{H}_\mathrm{p}(T)$.

ii) By definition $\mathcal{H}_\mathrm{c}(T)$ contains no eigenvector of T, so if $\xi \in \mathcal{H}_\mathrm{c}$ one has $\chi_{\{t\}}(T)\xi = 0$ for all $t \in \mathbb{R}$. Thus, $\mu_\xi(\{t\}) = \langle \xi, \chi_{\{t\}}(T)\xi\rangle = 0$.

If $\mu_\xi(\{t\}) = 0$ for all $t \in \mathbb{R}$, then if $T\eta = \lambda\eta$ it follows that

$$\langle \eta, \xi\rangle = \langle \chi_{\{\lambda\}}(T)\eta, \xi\rangle = \langle \eta, \chi_{\{\lambda\}}(T)\xi\rangle = 0,$$

and so $\xi \in \mathcal{H}_\mathrm{p}(T)^\perp = \mathcal{H}_\mathrm{c}(T)$.

iii) Let $\xi \in \mathcal{H}$. Then $P_\mathrm{p}^T\xi \in \mathcal{H}_\mathrm{p}(T)$ and by i) one has $\chi_\Lambda(T)P_\mathrm{p}^T\xi = P_\mathrm{p}^T\xi$. Thus, for any Borel set $\Omega \in \mathcal{A}$,

$$\chi_\Omega(T)P_\mathrm{p}^T\xi = \chi_\Omega(T)\chi_\Lambda(T)P_\mathrm{p}^T\xi = \chi_\Lambda(T)\chi_\Omega(T)P_\mathrm{p}^T\xi \in \mathcal{H}_\mathrm{p}(T).$$

Hence (from the left-hand side of this relation) $\chi_\Omega(T)P_{\rm p}^T = P_{\rm p}^T\chi_\Omega(T)P_{\rm p}^T$. By taking the adjoint of this equality it follows that

$$\chi_\Omega(T)P_{\rm p}^T = P_{\rm p}^T\chi_\Omega(T), \qquad \forall\Omega \in \mathcal{A},$$

and so, by Proposition 9.8.5, $\mathcal{H}_{\rm p}(T)$ reduces T. Since $P_{\rm c}^T = \mathbf{1} - P_{\rm p}^T$, it is immediate that $\mathcal{H}_{\rm c}(T) = \mathcal{H}_{\rm p}(T)^\perp$ also reduces T. □

Due to Theorem 12.1.2ii) $\mathcal{H}_{\rm p}(T)$ is also called the *discontinuous subspace* of T. One then has the decomposition

$$T = T_{\rm p} \oplus T_{\rm c}, \qquad T_{\rm p} := TP_{\rm p}^T,\ T_{\rm c} := TP_{\rm c}^T,$$

as in Theorem 9.8.3.

Definition 12.1.3. The *point spectrum* of T is $\sigma_{\rm p}(T) := \sigma(T_{\rm p})$, and the *continuous spectrum* of T is $\sigma_{\rm c}(T) := \sigma(T_{\rm c})$.

Note that $T_{\rm c}$ has no eigenvalues and, by Proposition 11.1.1,

$$\sigma(T) = \sigma_{\rm p}(T) \cup \sigma_{\rm c}(T).$$

These sets are not necessarily disjoint.

Example 12.1.4. Let $\mathcal{H} = \mathbb{C} \oplus \mathrm{L}^2[-1,1]$, $h : [-1,1] \hookleftarrow$ be the function $h(t) = t$, and $T : \mathcal{H} \hookleftarrow$ given by $T(z,\psi) := (0, \mathcal{M}_h\psi)$, $z \in \mathbb{C}$ and $\psi \in \mathrm{L}^2[-1,1]$. Then, since $\mathcal{M}_h$ has no eigenvalues and $T(z,0) = 0$, it is found that $\sigma_{\rm p}(T) = \{0\}$, $\sigma_{\rm c}(T) = \sigma(\mathcal{M}_h) = [-1,1]$ and $\sigma_{\rm p}(T) \cap \sigma_{\rm c}(T) \neq \emptyset$.

Definition 12.1.5. Let T be self-adjoint.

i) The *singular subspace* of T is

$$\mathcal{H}_{\rm s}(T) := \{\xi \in \mathcal{H} : \mu_\xi \perp \ell\}.$$

So, $\mathcal{H}_{\rm p}(T) \subset \mathcal{H}_{\rm s}(T)$.

ii) The *absolutely continuous subspace* of T is

$$\mathcal{H}_{\rm ac}(T) := \{\xi \in \mathcal{H} : \mu_\xi \ll \ell\}.$$

So, $\mathcal{H}_{\rm ac}(T) \subset \mathcal{H}_{\rm c}(T)$.

iii) The *singular continuous subspace* of T, denoted by $\mathcal{H}_{\rm sc}(T)$, is the set of $\xi \in \mathcal{H}$ so that $\mu_\xi(\mathbb{R} \setminus \Omega) = 0$ for some Borel set $\Omega \subset \mathbb{R}$ with $\ell(\Omega) = 0$ and $\mu_\xi(\Lambda) = 0$ for all countable sets $\Lambda \subset \mathbb{R}$. Hence, μ_ξ is a singular continuous measure. So, $\mathcal{H}_{\rm sc}(T) \subset \mathcal{H}_{\rm c}(T) \cap \mathcal{H}_{\rm s}(T)$.

Exercise 12.1.6. Check that $\mathcal{H}_{\rm p}(T) \subset \mathcal{H}_{\rm s}(T)$, $\mathcal{H}_{\rm ac}(T) \subset \mathcal{H}_{\rm c}(T)$ and $\mathcal{H}_{\rm sc}(T) \subset \mathcal{H}_{\rm c} \cap \mathcal{H}_{\rm s}(T)$.

Lemma 12.1.7. *$\mathcal{H}_{\rm s}(T)$, $\mathcal{H}_{\rm ac}(T)$ and $\mathcal{H}_{\rm sc}(T)$ are closed vector subspaces of $\mathcal{H}$. The respective orthogonal projections will be denoted by $P^T_{\rm s}, P^T_{\rm ac}$ and $P^T_{\rm sc}$.*

Proof. The proof will be in three steps.

- If $\xi, \eta \in \mathcal{H}_{\rm s}(T)$ there exist Borel sets Ω_ξ and Ω_η with $\ell(\Omega_\xi) = 0 = \ell(\Omega_\eta)$ and $\chi_{\Omega_\xi}(T)\xi = \xi$, $\chi_{\Omega_\eta}(T)\eta = \eta$. Thus, for any $a, b \in \mathbb{C}$, $\chi_{\Omega_\xi \cup \Omega_\eta}(T)(a\xi + b\eta) = a\xi + b\eta$ and so $(a\xi + b\eta) \in \mathcal{H}_{\rm s}(T)$; therefore, $\mathcal{H}_{\rm s}(T)$ is a vector subspace.

  Take a sequence $(\xi_j) \subset \mathcal{H}_{\rm s}(T)$ with $\xi_j \to \xi$; then there exist Borel sets $\Omega_j \in \mathcal{A}$ with $\ell(\Omega_j) = 0$ and $\chi_{\Omega_j}(T)\xi_j = \xi_j$, $\forall j$. Put $\Omega = \cup_j \Omega_j$ and note that $\ell(\Omega) = 0$ and
  $$\chi_\Omega(T)\xi = \lim_{j\to\infty} \chi_\Omega(T)\xi_j = \lim_{j\to\infty} \xi_j = \xi,$$
  so that $\xi \in \mathcal{H}_{\rm s}(T)$ and this subspace is closed.
- In view of $\mathcal{H}_{\rm sc}(T) \subset \mathcal{H}_{\rm c}(T)$ (so $\mathcal{H}_{\rm sc} \cap \mathcal{H}_{\rm p} = \{0\}$), the proof that $\mathcal{H}_{\rm sc}(T)$ is a closed subspace follows the same lines as above.
- If $\xi, \eta \in \mathcal{H}_{\rm ac}(T)$, then for $a \in \mathbb{C}$ one has $\mu_{a\xi} = |a|^2 \mu_\xi \ll \ell$, and $a\xi \in \mathcal{H}_{\rm ac}(T)$. Now, for all $\Omega \in \mathcal{A}$ one has
  $$\langle (\xi + \eta), \chi_\Omega(T)(\xi + \eta)\rangle = \mu_\xi(\Omega) + \mu_\eta(\Omega) + \mu_{\eta,\xi}(\Omega) + \mu_{\xi,\eta}(\Omega).$$

  Since $|\mu_{\xi,\eta}(\Omega)| \le \|\xi\| \, \|\chi_\Omega(T)\eta\| = \|\xi\| \, \mu_\eta(\Omega)^{1/2}$, it follows that if $\ell(\Omega) = 0$ then $\mu_{\xi,\eta}(\Omega) = 0$; hence $\mu_{\xi+\eta}(\Omega) = 0$ and so $(\xi + \eta) \in \mathcal{H}_{\rm ac}(T)$. Therefore, $\mathcal{H}_{\rm ac}(T)$ is a vector space.

  Suppose $(\xi_j) \subset \mathcal{H}_{\rm ac}(T)$ with $\xi_j \to \xi$. Let $\Omega \in \mathcal{A}$. Then,
  $$\begin{aligned} \left|\mu_{\xi_j}(\Omega) - \mu_\xi(\Omega)\right| &= |\langle \xi_j, \chi_\Omega(T)\xi_j\rangle - \langle \xi, \chi_\Omega(T)\xi\rangle| \\ &= |\langle (\xi_j - \xi), \chi_\Omega(T)\xi_j\rangle + \langle \xi, \chi_\Omega(T)(\xi_j - \xi)\rangle| \\ &\le \|\xi_j - \xi\| \left(\|\xi_j\| + \|\xi\|\right) \longrightarrow 0 \end{aligned}$$
  as $j \to \infty$, consequently $\mu_{\xi_j}(\Omega) \to \mu_\xi(\Omega)$. If $\ell(\Omega) = 0$, then
  $$\mu_\xi(\Omega) = \lim_{j\to\infty} \mu_{\xi_j}(\Omega) = 0$$
  and $\mu_\xi \ll \ell$. Therefore, $\mathcal{H}_{\rm ac}(T)$ is a closed subspace.

Thereby the proof is complete. □

Theorem 12.1.8. *Let T be self-adjoint.*

i) $\mathcal{H}_{\rm s}(T) = \mathcal{H}_{\rm p}(T) \oplus \mathcal{H}_{\rm sc}(T)$.
ii) $\mathcal{H}_{\rm c}(T) = \mathcal{H}_{\rm ac}(T) \oplus \mathcal{H}_{\rm sc}(T)$.
iii) $\mathcal{H} = \mathcal{H}_{\rm p}(T) \oplus \mathcal{H}_{\rm ac}(T) \oplus \mathcal{H}_{\rm sc}(T)$.
iv) *Each of these subspaces, i.e., $\mathcal{H}_\kappa(T)$ with $\kappa \in \{\rm s, c, p, ac, sc\}$, reduces the operator T. Denote the corresponding orthogonal projections P^T_κ and define the self-adjoint restrictions $T_\kappa := TP^T_\kappa$.*

Proof. Recall that $\mathcal{H} = \mathcal{H}_{\rm p}(T) \oplus \mathcal{H}_{\rm c}(T)$ and every measure can be uniquely written as $\mu = \mu_{\rm p} + \mu_{\rm ac} + \mu_{\rm sc}$. Hence, from $\mathcal{H}_{\rm sc} \subset \mathcal{H}_{\rm c}$ and $\mathcal{H}_{\rm ac} \subset \mathcal{H}_{\rm c}$ one has $\mathcal{H}_{\rm p}(T) \perp \mathcal{H}_{\rm ac}(T)$ and $\mathcal{H}_{\rm p}(T) \perp \mathcal{H}_{\rm sc}(T)$.

If $\xi \in \mathcal{H}_{\rm sc}(T)$ there exists a (Lebesgue) measure zero set $\Lambda \subset \mathbb{R}$ with $\chi_\Lambda(T)\xi = \xi$; thus, if $\eta \in \mathcal{H}_{\rm ac}(T)$ one has $\chi_\Lambda(T)\eta = 0$ and

$$\langle \xi, \eta \rangle = \langle \chi_\Lambda(T)\xi, \eta \rangle = \langle \xi, \chi_\Lambda(T)\eta \rangle = 0,$$

and so $\mathcal{H}_{\rm sc}(T) \perp \mathcal{H}_{\rm ac}(T)$.

i) If $\xi \in \mathcal{H}_{\rm s} \cap \mathcal{H}_{\rm p}{}^\perp$, then $\mu_\xi \perp \ell$ and $\mu_\xi(\Lambda) = 0$ for all countable sets $\Lambda \subset \mathbb{R}$. Therefore, due to the decomposition of measures mentioned above, μ_ξ is purely singular continuous and $\xi \in \mathcal{H}_{\rm sc}(T)$, that is, i) follows.

ii) If $\xi \in \mathcal{H}_{\rm c} \cap \mathcal{H}_{\rm ac}{}^\perp$, then the point part of μ_ξ is zero and $\mu_\xi \perp \ell$. Therefore, μ_ξ is a singular continuous measure and $\xi \in \mathcal{H}_{\rm sc}(T)$, that is, ii) follows.

iii) follows straightly from ii) and the definitions of $\mathcal{H}_{\rm p}$ and $\mathcal{H}_{\rm c}$.

iv) It is known that $\mathcal{H}_{\rm p}(T)$ is a reducing subspace of T. Due to the above relations, it is enough to show that $\mathcal{H}_{\rm s}(T)$ reduces T. But this proof is quite similar to that for $\mathcal{H}_{\rm p}(T)$ in Theorem 12.1.2, just take Λ as a set with $\ell(\Lambda) = 0$ instead of a countable set. □

Exercise 12.1.9. Present the details of the proof of Theorem 12.1.8iv).

By Theorem 12.1.8 one has the decomposition

$$T = T_{\rm p} \oplus T_{\rm ac} \oplus T_{\rm sc}$$

alluded in the title of this chapter.

Definition 12.1.10. The *absolutely continuous spectrum* of T is $\sigma_{\rm ac}(T) := \sigma(T_{\rm ac})$ and the *singular continuous spectrum* of T is $\sigma_{\rm sc}(T) := \sigma(T_{\rm sc})$.

Hence $\sigma(T) = \sigma_{\rm p}(T) \cup \sigma_{\rm ac}(T) \cup \sigma_{\rm sc}(T)$. Now some additional nomenclature: The operator T has *purely point spectrum* if $\sigma_{\rm ac}(T) = \emptyset = \sigma_{\rm sc}(T)$; *purely absolutely continuous spectrum* if $\sigma_{\rm p}(T) = \emptyset = \sigma_{\rm sc}(T)$; *purely singular continuous spectrum* if $\sigma_{\rm ac}(T) = \emptyset = \sigma_{\rm p}(T)$. It is also common to say that T is pure point, and so on. The concept of pure point (and so on) spectrum in a set Λ, similar to the ones on page 286, will also be employed.

Remark 12.1.11. Note that $\sigma_{\rm p}(T)$, $\sigma_{\rm ac}(T)$ and $\sigma_{\rm sc}(T)$ are closed subsets of $\mathbb{R}$, since they are the spectra of self-adjoint operators (i.e., convenient restrictions of T). Note also that $\sigma_{\rm p}(T)$ is the closure of the set of its eigenvalues; see Example 12.2.2.

Remark 12.1.12. Up to the 1970s, the singular continuous spectrum was considered a pathology in quantum mechanics and was occasionally named *exotic* in the literature; currently they appear, for instance, related to models of quasicrystals. See Example 12.2.13 for a purely singular continuous operator (one that should be kept in mind when thinking of such kind of spectrum) and Section 12.6 for an existential result.

Exercise 12.1.13. Show that:

a) $\sigma_{\mathrm{d}}(T) \subset \sigma_{\mathrm{p}}(T)$.
b) $\sigma_{\mathrm{ess}}(T) = \sigma_{\mathrm{c}}(T) \cup \{\sigma_{\mathrm{p}}(T) \setminus \sigma_{\mathrm{d}}(T)\}$.

Conclude then that $\sigma_{\mathrm{c}}(T) \subset \sigma_{\mathrm{ess}}(T)$.

Exercise 12.1.14. Show that for any Borel set $\Omega \subset \mathbb{R}$ one has

$$\chi_\Omega(T_\kappa) = P_\kappa^T \chi_\Omega(T),$$

for $\kappa \in \{\mathrm{p}, \mathrm{s}, \mathrm{c}, \mathrm{ac}, \mathrm{sc}\}$.

Exercise 12.1.15. If T, S are two unitarily equivalent self-adjoint operators, show that $\sigma_\kappa(T) = \sigma_\kappa(S)$ for $\kappa \in \{\mathrm{p}, \mathrm{s}, \mathrm{c}, \mathrm{ac}, \mathrm{sc}, \mathrm{d}, \mathrm{ess}\}$.

12.2 Examples

Example 12.2.1. If T is a self-adjoint and compact operator, then T is pure point.

Example 12.2.2. If $\{q_j\}_j$ is an enumeration of the rational numbers in $[-1, 1]$, then $T : l^2(\mathbb{Z}) \hookleftarrow$, $Te_j = q_j e_j$ ($\{e_j\}_j$ is the canonical basis of $l^2(\mathbb{Z})$) is self-adjoint, bounded, pure point and, since the spectrum is a closed set,

$$\sigma(T) = \sigma_{\mathrm{p}}(T) = \sigma_{\mathrm{ess}}(T) = [-1, 1].$$

Note that this operator has point spectrum larger than the set of its eigenvalues.

Example 12.2.3. The hydrogen atom Schrödinger operator H_H, discussed in Subsection 11.4.1, has continuous spectrum $\sigma_{\mathrm{c}}(H_H) = [0, \infty)$, nonempty discrete spectrum $\sigma_{\mathrm{d}}(H_H) \subset (-\infty, 0)$ and point spectrum $\sigma_{\mathrm{p}}(H_H) = \sigma_{\mathrm{d}}(H_H) \cup \{0\}$. Note that zero is a common element of the point and continuous spectra of this operator. See Remark 12.3.19.

Example 12.2.4. [Position operator in $\mathbb{R}$] Let $T = \mathcal{M}_h$ in $\mathrm{L}^2(\mathbb{R})$, $h : \mathbb{R} \hookleftarrow$, $h(t) = t$. Then, for all $\psi \in \mathrm{L}^2(\mathbb{R})$ and Borel sets $\Lambda \subset \mathbb{R}$, one has

$$\mu_\psi(\Lambda) = \langle \psi, \chi_\Lambda(T)\psi \rangle = \int_{\mathbb{R}} \chi_\Lambda(t) \, |\psi(t)|^2 \, dt = \int_\Lambda |\psi(t)|^2 \, dt,$$

so that the spectral measures $\mu_\psi \ll \ell$ with $\frac{d\mu_\psi}{d\ell} = |\psi(t)|^2$, a positive function in $\mathrm{L}^1(\mathbb{R})$. Therefore T is purely absolutely continuous and $\sigma(T) = \sigma_{\mathrm{ac}}(T) = \mathbb{R}$.

Exercise 12.2.5. Show that the momentum operator in $\mathrm{L}^2(\mathbb{R})$ (see Example 2.3.11 and Section 3.3) has purely absolutely continuous spectrum.

Example 12.2.6. [Free fall] The potential $V(x) = -gx$, $x \in \mathbb{R}$, describes a constant gravitational field of intensity $g > 0$. The total energy in this case, for a particle of unity mass and other convenient units, is $p^2 - gx$, implying the formal action $-\psi''(x) - gx\psi(x)$ for the quantum energy operator. In this case it is convenient to use Fourier transform (see Chapter 3) to precisely define the energy operator.

Beginning with dom $\tilde{H} = C_0^\infty(\hat{\mathbb{R}})$, $(\tilde{H}\psi)(p) = p^2\psi(p) - gi\psi'(p)$ (the prime indicates derivative with respect to p), it is found that its adjoint $H = \tilde{H}^*$ is given by

$$\text{dom } H = \{\psi \in \mathrm{L}^2(\hat{\mathbb{R}}) : \psi \in \mathrm{AC}(\hat{\mathbb{R}}), (p^2\psi(p) - gi\psi'(p)) \in \mathrm{L}^2(\hat{\mathbb{R}})\},$$
$$(H\psi)(p) = p^2\psi(p) - gi\psi'(p), \qquad \psi \in \text{dom } H.$$

An integration by parts shows that this operator is symmetric, so, by Theorem 2.1.24, it is self-adjoint and $\tilde{H}$ is essentially self-adjoint. H is the Schrödinger operator describing the free fall in a constant gravitational field.

Now let $\psi_\lambda \in \text{dom } H$ be an eigenvector $H\psi_\lambda = \lambda\psi_\lambda$, for some $\lambda \in \mathbb{R}$. Then

$$p^2\psi_\lambda(p) - gi\psi'_\lambda(p) = \lambda\psi_\lambda(p),$$

whose solutions are $\psi_\lambda(p) = c\exp(i(\lambda p - p^3/3)/g)$, $c \in \mathbb{R}$, and since $\psi_\lambda \in \mathrm{L}^2(\hat{\mathbb{R}})$ iff $c = 0$, it follows that H has purely continuous spectrum. Example 12.3.15 complements this result.

Exercise 12.2.7. Based on Example 2.3.11 and Proposition 2.3.20, confirm the adjoint operator $\tilde{H}^*$ in Example 12.2.6.

Example 12.2.8. Let $\mathcal{T}^2$ denote the two-dimensional torus, i.e., the square $[-\pi, \pi] \times [-\pi, \pi]$ with the usual identifications $(-\pi, y) \sim (\pi, y)$, $\forall y$, and $(x, -\pi) \sim (x, \pi)$, $\forall x$. A continuous function $f : \mathbb{R}^2 \to \mathbb{C}$ is 2π-periodic if $f(x + 2\pi, y) = f(x, y)$ and $f(x, y + 2\pi) = f(x, y)$, $\forall x, y \in \mathbb{R}$; its restriction to $\mathcal{T}^2$ will simply be abbreviated to $f : \mathcal{T}^2 \to \mathbb{C}$. It is known that the Sobolev space $\mathcal{H}^1(\mathcal{T}^2)$ is dense in $\mathcal{H} = \mathrm{L}^2(\mathcal{T}^2)$.

Let $\alpha \in \mathbb{R}$ and $V : \mathcal{T}^2 \to \mathbb{R}$ be a continuous and real 2π-periodic function. Consider the self-adjoint operator $T_V = T_V(\alpha)$ given by

$$T_V\psi := -i\alpha\frac{\partial}{\partial x}\psi - i\frac{\partial}{\partial y}\psi + V(x, y)\psi, \qquad \psi \in \text{dom } T_V,$$

where dom $T_V = \mathcal{H}^1(\mathcal{T}^2)$.

The standard orthonormal basis of $\mathcal{H}$ is

$$\{\phi_{n,m}(x, y) = e^{-i(nx+my)}/(2\pi) : n, m \in \mathbb{Z}\},$$

and any $\psi \in \mathcal{H}$ has the Fourier series expansion

$$\psi(x, y) = \sum_{n,m} a_{n,m}\, \phi_{n,m}(x, y), \qquad \|\psi\|_2^2 = \sum_{n,m} |a_{n,m}|^2.$$

If $V = 0$ (null function), then

$$T_0\, \phi_{n,m} = (n\alpha + m)\phi_{n,m},$$

and T_0 has purely point spectrum. Note that if $\alpha \in \mathbb{Q}$, then each eigenvalue is isolated and of infinite multiplicity, while if α is an irrational number, then its eigenvalues are simple but they form a dense set in $\mathbb{R}$, so that $\sigma(T_0) = \mathbb{R}$. In both cases the spectra are purely essential.

Proposition 12.2.9. *Let $\alpha \in \mathbb{R} \setminus \mathbb{Q}$ and V as above. If $\sigma_{\mathrm{p}}(T_V) \neq \emptyset$, then T_V is a purely point operator and $\sigma(T_V) = \mathbb{R}$.*

Proof. By hypothesis there exists an eigenvalue $\lambda \in \mathbb{R}$ of T_V, that is, there exists $0 \neq \psi_\lambda \in \mathrm{dom}\, T_V$ with $T_V \psi_\lambda = \lambda \psi_\lambda$. Thus

$$-i\alpha \frac{\partial}{\partial x}\psi_\lambda - i\frac{\partial}{\partial y}\psi_\lambda + V(x,y)\psi_\lambda = \lambda\psi_\lambda,$$
$$i\alpha \frac{\partial}{\partial x}\overline{\psi_\lambda} + i\frac{\partial}{\partial y}\overline{\psi_\lambda} + V(x,y)\overline{\psi_\lambda} = \lambda\overline{\psi_\lambda},$$

and after multiplying the first of these equations by $\overline{\psi_\lambda}$, the second by ψ_λ and subtracting the first from the second, one gets

$$\left(\alpha\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\right)\varphi = 0, \qquad \varphi := |\psi_\lambda|^2.$$

Note that $\varphi \in \mathrm{L}^1(\mathcal{T})$ and so it can be expressed by Fourier series

$$\varphi(x,y) = \sum_{n,m} a_{n,m}\, \phi_{n,m}(x,y);$$

after inserting this into the above equation one gets

$$-i\sum_{n,m}(\alpha n + m)\, a_{n,m}\, \phi_{n,m}(x,y) = 0,$$

so that $(\alpha n + m)\, a_{n,m} = 0$, $\forall (n,m)$. Since α is an irrational number $(\alpha n + m) = 0$ iff $n = m = 0$, consequently $a_{n,m} = 0$ if $(n,m) \neq (0,0)$. Hence $\varphi(x,y) = a_{0,0}$ and it is a constant function.

Therefore the eigenfunction ψ_λ has constant modulus and by assuming $|\psi_\lambda(x,y)| = 1$, $\forall (x,y)$, the multiplication operator $\Xi : \mathcal{H} \hookleftarrow$, $(\Xi\psi)(x,y) = \psi_\lambda(x,y)\,\psi(x,y)$, is unitary and a direct calculation shows that

$$\Xi^{-1} T_V \Xi = T_0 + \lambda\mathbf{1},$$

that is, T_V is unitarily equivalent to $T_0 + \lambda\mathbf{1}$, and since the latter is pure point, so is T_V. Thereby the proof is complete. □

In what follows a characterization of some potentials V so that T_V has purely point spectrum will be presented. For this α will be supposed to be a *diophantine number*, that is, there are $\gamma, \sigma > 0$ so that

$$\left|\alpha - \frac{n}{m}\right| > \frac{\gamma}{|m|^\sigma}, \qquad \forall \frac{n}{m} \in \mathbb{Q}\,.$$

Proposition 12.2.10. *If V is a C^r function, $r > 3$, and α is a diophantine number with $\sigma < r - 2$, then T_V has purely point spectrum and its eigenvalues are precisely those of T_0 plus the average $V_{0,0} = \int_{\mathcal{T}} V(x,y)dxdy$.*

Proof. Note that $T_V = T_0 + V$. The idea is to find a continuously differentiable real function $g(x, y)$ so that $e^{-ig}T_V e^{ig} = T_0 + \lambda\mathbf{1}$; since multiplication by e^{ig} is a unitary operator on $\mathcal{H}$, if one also shows that $\lambda = V_{0,0}$, then the spectral assertions follow.

By imposing that

$$(T_0 + \lambda\mathbf{1})\psi = e^{-ig}T_V e^{ig}\psi = T_0\psi + i\,(\alpha\partial_x g + \partial_y g + V)\,\psi,$$

for $\psi \in \operatorname{dom} T_V$, one obtains

$$(\alpha\partial_x g + \partial_y g) = -V + \lambda,$$

that is, a differential equation for g. By using Fourier series, write

$$g(x,y) = \sum_{n,m} g_{n,m}\, e^{i(mx+ny)}, \qquad V(x,y) = \sum_{n,m} V_{n,m}\, e^{i(mx+ny)}$$

and insert these expressions into the above differential equation to get

$$\sum_{n,m} \left[i(m\alpha + n)\, g_{m,n} + V_{m,n}\right] e^{i(mx+ny)} = \lambda.$$

Hence, $\lambda = V_{0,0}$ (the average of V) and

$$g_{m,n} = i\frac{V_{m,n}}{\alpha m + n}, \qquad (m,n) \neq (0,0).$$

Since V is a C^r function, there is $C > 0$ so that $|V_{m,n}| \leq C/(|m|+|n|)^r$, $\forall (m,n) \neq (0,0)$, and taking into account the diophantine condition on α with $\sigma < r - 2$,

$$\begin{aligned} |g_{m,n}| = \frac{|V_{m,n}|}{|m|\,|\alpha + n/m|} &\leq \frac{1}{|m|} \times \frac{C}{(|m|+|n|)^r} \times \frac{|m|^\sigma}{\gamma} \\ &= \frac{C}{\gamma}\frac{|m|^{\sigma-1}}{(|m|+|n|)^r} \leq \frac{C}{\gamma}\frac{|m|^{r-3}}{(|m|+|n|)^r} \\ &\leq \frac{C}{\gamma}\frac{1}{(|m|+|n|)^3}. \end{aligned}$$

Such decaying properties of the Fourier coefficients $g_{m,n}$ imply g is continuously differentiable and all manipulations above are justified, including $e^{-ig}T_V e^{ig} = T_0 + V_{00}\mathbf{1}$. □

Under additional assumptions on α and differentiability of V, more information about T_V can be obtained.

Corollary 12.2.11. *If $\sigma > 2$ and $r > \sigma + 2$, then T_V in Proposition* 12.2.10 *has purely point spectrum for α in a set of full Lebesgue measure over $\mathbb{R}$.*

Proof. Fix $\sigma > 2$. Note that it is possible to restrict the argument for $0 < \alpha < 1$ and $0 < n/m < 1$. Let A^γ be the set of such α that the diophantine condition does not hold with γ; if A^γ_m, $m \geq 1$, is the set of $0 < \alpha < 1$ such that there exists $n \in \{0, 1, \dots, m-1\}$ with

$$\left| \alpha - \frac{n}{m} \right| \leq \frac{\gamma}{m^\sigma},$$

then $A^\gamma = \cup_{m \geq 1} A^\gamma_m$. Hence

$$\ell(A^\gamma_m) \leq \sum_{n=0}^{m} \frac{2\gamma}{m^\sigma} = \frac{2\gamma}{m^{\sigma-1}},$$

and so $\ell(A^\gamma) \leq \sum_{m=1}^\infty \ell(A^\gamma_m) = 2\gamma \sum_{m=1}^\infty 1/m^{\sigma-1} := \gamma C(\sigma)$ is convergent since $\sigma > 2$. Therefore, the set of $\alpha \in (0,1)$ so that the diophantine condition holds with $\gamma > 0$ containing $(0,1) \setminus A^\gamma$; now

$$\ell((0,1) \setminus A^\gamma) = 1 - \ell(A^\gamma) \geq 1 - \gamma C(\sigma).$$

Since this must hold for all $\gamma > 0$, it follows that the set of diophantine numbers in $(0,1)$, with $\sigma > 2$, has full Lebesgue measure there. If additionally $V \in C^r$, with $r > \sigma + 2$, then Proposition 12.2.10 infers that $T_V(\alpha)$ is pure point for α in a set of full Lebesgue measure. □

To close the discussion of Example 12.2.8, note that (for irrational α) Proposition 12.2.10 deals with perturbations of operators with dense point spectrum, often a difficult question!

Exercise 12.2.12. With respect to Example 12.2.8, check that Ξ is a unitary operator and that $\Xi^{-1} T_V \Xi = T_0 + \lambda \mathbf{1}$. Check also that g in the proof of Proposition 12.2.10 is continuously differentiable.

Example 12.2.13. [Purely singular continuous operator] Let

$$J = [0, 1/3] \cup [2/3, 1], \qquad c : [0,1] \to \mathbb{R},\ c(t) := \chi_J(t),$$

so that if $\mathcal{C}$ is the well-known ternary Cantor set, one has for its characteristic function

$$\chi_{\mathcal{C}}(t) = \prod_{j=0}^{\infty} c(3^j t \ (\mathrm{mod}\, 1)) .$$

Recall that $\ell(\mathcal{C}) = 0$ and that $\mathcal{C}$ is nonempty, compact, with empty interior and it has no isolated points; also, it has the same cardinality as $\mathbb{R}$.

By defining

$$c_j(t) = \frac{3}{2} c(3^j t \ (\mathrm{mod}\, 1)) ,$$

one has $\int_0^1 \prod_{j=0}^n c_j(t)\, dt = 1$, $\forall n$, and if $I \subset [0,1]$ is an interval, then

$$n \mapsto \int_I \left(\prod_{j=0}^{n} c_j(t) \right) dt$$

is a nonincreasing sequence so that there exists a positive measure $\mu^{\mathcal{C}}$ defined on intervals by

$$\mu^{\mathcal{C}}(I) := \lim_{n\to\infty} \int_I \prod_{j=0}^{n} c_j(t)\, dt,$$

and we can apply the standard procedure for extending $\mu^{\mathcal{C}}$ from intervals I to measurable sets Λ. This measure is, intuitively, "the measure uniformly distributed over $\mathcal{C}$."

$\mu^{\mathcal{C}}$ is singular (with respect to Lebesgue), since $\mu^{\mathcal{C}}([0,1]\setminus\mathcal{C}) = 0$ and $\ell(\mathcal{C}) = 0$, and it is also continuous, since for every interval I_k with $\ell(I_k) \le 1/3^k$ one has $\mu^{\mathcal{C}}(I_k) \le 1/2^k$, so that $\mu^{\mathcal{C}}(\{t\}) = 0$ for every $t \in [0,1]$. Therefore, $\mu^{\mathcal{C}}$ is singular continuous.

Consider now the operator $T = \mathcal{M}_h : \mathrm{L}^2_{\mu^{\mathcal{C}}}[0,1] \hookleftarrow$, with $h(t) = t$. Then T is purely singular continuous since for every $\psi \in \mathrm{L}^2_{\mu^{\mathcal{C}}}[0,1]$ the corresponding spectral measure μ^T_ψ of T is

$$\mu^T_\psi(\Lambda) = \|\chi_\Lambda(T)\psi\|^2 = \int_\Lambda |\psi|^2\, d\mu^{\mathcal{C}},$$

that is, $\mu^T_\psi = |\psi|^2 d\mu^{\mathcal{C}}$, which is a singular continuous measure (in fact, $\mu^T_\psi([0,1]\setminus\mathcal{C}) = 0$ and $\mu^T_\psi(\{t\}) = 0$ for every $t \in [0,1]$). Further, by Proposition 2.3.27, $\sigma(T) = \sigma_{\mathrm{sc}}(T) = \mathcal{C}$.

Exercise 12.2.14. Set $C_j(x) = \int_0^x c_j(t)\, dt$. Show that:

a) $C_j(0) = 0$, $C_j(1) = 1, \forall j$, and $t \mapsto C_j(t)$ is nondecreasing for all t.

b) If $E_k = \{t \in [0,1] : c_k(t) = 1\}$, i.e., the k-th subset in the well-known construction of the ternary Cantor set $\mathcal{C}$, then if $t \notin E_k$ one has $C_k(t) = C_{k+j}(t)$, $\forall j \ge 0$, and derivative $C_k'(t) = 0$.

c) The map $t \mapsto C_k(t)$ is continuous and there exists a continuous $C : [0,1] \hookleftarrow$ so that $C_k \to C$ uniformly as $k \to \infty$, and $C(0) = 0$, $C(1) = 1$, $C'(t) = 0$ for $t \notin \mathcal{C}$, $C' \in \mathrm{L}^1[0,1]$ and

$$\int_0^x C'(t)\, dt = 0 < 1 = C(1) - C(0).$$

Conclude that C is a singular continuous function, the so-called *ternary Cantor function*. Conclude also that $C(x) = \mu^{\mathcal{C}}([0,x])$.

The ternary Cantor function is a standard example of a continuous function in a compact interval, differentiable a.e. with respect to Lebesgue measure, but not absolutely continuous.

Example 12.2.15. The operator $\mathcal{M}_h$ on $\mathrm{L}^2_\nu[0,1]$, with $h(t) = t$ and $\nu = \mu^{\mathcal{C}} + \ell + \delta_{1/2}$ ($\delta_{1/2}$ is a Dirac measure) has mixed spectrum, since $\sigma_{\mathrm{ac}}(\mathcal{M}_h) = [0,1]$, $\sigma_{\mathrm{sc}}(\mathcal{M}_h) = \mathcal{C}$ and $\sigma_{\mathrm{p}}(\mathcal{M}_h) = \{\frac{1}{2}\}$.

Exercise 12.2.16. Verify the details in Example 12.2.15.

Remark 12.2.17. A sophisticated and interesting construction that recalls of Example 12.2.13 appears in [Pea78a]; Pearson considered measures

$$\mu_n(I) = \int_I \prod_{j=0}^{n} (1 + g_j \sin(N_j t))\, dt$$

in $[0,1]$, with $0 < g_j < 1$ and $g_j \to 0$. For subintervals $I \subset [0,1]$ define $\mu(I) = \lim_{n\to\infty} \mu_n(I)$. Then, if N_j increase sufficiently rapidly, it was shown that

1. μ is singular continuous provided $\sum_{j=1}^{\infty} g_j^2 = \infty$,
2. μ is absolutely continuous provided $\sum_{j=1}^{\infty} g_j^2 < \infty$.

Remark 12.2.18. Most examples of singular continuous spectrum are obtained rather indirectly, i.e., through proofs of absence of absolutely continuous and absence of point spectra.

12.3 Some Absolutely Continuous Spectra

For all n the Lebesgue measure over (subsets of) $\mathbb{R}^n$ will be denoted by the same symbol ℓ.

12.3.1 Multiplication Operators

The discussion that follows is closely related to examples in Subsection 8.4.1. Initially a general result about spectral measures.

Proposition 12.3.1. *Let T be self-adjoint in $\mathcal{H}$.*

i) *If $\xi \in \mathcal{H}_\kappa(T)$, $\kappa \in \{\mathrm{p}, \mathrm{s}, \mathrm{c}, \mathrm{ac}, \mathrm{sc}\}$, and $\eta \in \mathcal{H}$, then*

$$|\mu_{\xi,\eta}(\Lambda)|^2 \le \mu_\xi(\Lambda)\, \mu_{P_\kappa^T \eta}(\Lambda), \quad \forall \Lambda \in \mathcal{A}.$$

ii) *If $\xi \in \mathcal{H}_{\mathrm{ac}}(T)$ and $\eta \in \mathcal{H}$, then $\mu_{\xi,\eta} \ll \ell$.*

iii) *If $\xi \in \mathcal{H}_{\mathrm{c}}(T)$ and $\eta \in \mathcal{H}$, then $\mu_{\xi,\eta}$ is a continuous measure.*

Proof. i) In view of $\chi_\Lambda(T)^2 = \chi_\Lambda(T)$, $(P_\kappa^T)^2 = P_\kappa^T$, both are self-adjoint, $P_\kappa^T \chi_\Lambda(T) = \chi_\Lambda(T) P_\kappa^T$ and, by hypothesis, $P_\kappa^T \xi = \xi$, one has

$$\begin{aligned} |\mu_{\xi,\eta}(\Lambda)| &= |\langle \chi_\Lambda(T)\xi, \eta\rangle| = |\langle \chi_\Lambda(T)^2 P_\kappa^T \xi, \eta\rangle| \\ &= |\langle \chi_\Lambda(T) P_\kappa^T \xi, \chi_\Lambda(T)\eta\rangle| = |\langle \chi_\Lambda(T)\xi, P_\kappa^T \chi_\Lambda(T)\eta\rangle| \\ &\le \|\chi_\Lambda(T)\xi\|\, \|\chi_\Lambda(T) P_\kappa^T \eta\| = \left(\mu_\xi(\Lambda)\, \mu_{P_\kappa^T \eta}(\Lambda)\right)^{1/2}. \end{aligned}$$

ii) and iii) follow by i) since if $\xi \in \mathcal{H}_{\mathrm{ac}}(T)$ then $\mu_\xi \ll \ell$ and if $\xi \in \mathcal{H}_{\mathrm{c}}(T)$ then $\mu_\xi(\{t\}) = 0$, $\forall t \in \mathbb{R}$. □

Theorem 12.3.2. *Let $E \subset \mathbb{R}^n$ be a Borel set with $\ell(E) > 0$ and $\varphi : E \to \mathbb{R}$ a measurable function. Consider the multiplication operator $\mathcal{M}_\varphi$ in $\mathrm{L}^2(E)$. Then, if $\ell(A) = 0$ implies $\ell(\varphi^{-1}(A)) = 0$ ($A \in \mathcal{A}$), then $\mathcal{M}_\varphi$ is purely absolutely continuous.*

Proof. If $\psi \in \mathrm{L}^2(E)$, for every Borel set $A \subset \mathbb{R}$, one has

$$\begin{aligned}\mu_\psi(A) &= \langle \psi, \chi_A(\mathcal{M}_\varphi)\psi \rangle \\ &= \int_E \chi_A(\varphi(x))\, |\psi(x)|^2 dx = \int_{\varphi^{-1}(A)} |\psi(x)|^2 dx;\end{aligned}$$

so, if $\ell(A) = 0 \Rightarrow \ell(\varphi^{-1}(A)) = 0$, then $\mu_\psi(A) = 0$ and $\mu_\psi \ll \ell$. □

Corollary 12.3.3. *The free particle hamiltonian H_0 in $\mathrm{L}^2(\mathbb{R}^n)$ has purely absolutely continuous spectrum and $\sigma_{\mathrm{ac}}(H_0) = [0, \infty)$.*

Proof. Since $(\mathcal{F}^{-1}H_0\mathcal{F})(p) = p^2 = \sum_{j=1}^n p_j^2$ in $\mathrm{L}^2(\hat{\mathbb{R}}^n)$, the results follow by Theorem 12.3.2 and Proposition 11.4.1. □

Remark 12.3.4. The same argument in Corollary 12.3.3 shows that the operators $\mathcal{M}_{x^k}$ and $\mathcal{M}_{p^k}$, $k \in \mathbb{N}$ (which includes the position and momentum operators), in $\mathrm{L}^2(\mathbb{R}^n)$ have purely absolutely continuous spectrum. It is interesting to note that, in spite of the absolutely continuous spectra of x^2 and p^2, the sum $H = p^2 + x^2$ acting in $\mathrm{L}^2(\mathbb{R})$ (i.e., the harmonic oscillator hamiltonian – Example 11.3.15) is purely discrete!

Now the free particle in $\mathbb{Z}$, discussed in Subsection 8.4.3, will be considered. The corresponding tight-binding Schrödinger operator is $h_0 : l^2(\mathbb{Z}) \hookleftarrow$,

$$h_0 := S_l + S_r, \qquad (S_l u)_j = u_{j+1}, \qquad (S_r u)_j = u_{j-1},$$

for $u = (u_j) \in l^2(\mathbb{Z})$, so that h_0 is bounded, self-adjoint and $\|h_0\| = 2$. By means of Fourier series (see Subsection 8.4.3 for notation) one has $\left(\mathrm{F}^{-1}S_l\mathrm{F}\right)(x) = \mathcal{M}_{e^{-ix}}$, $\left(\mathrm{F}^{-1}S_r\mathrm{F}\right)(x) = \mathcal{M}_{e^{ix}}$, so that

$$\left(\mathrm{F}^{-1}h_0\mathrm{F}\right)(x) = \mathcal{M}_{2\cos x}, \qquad x \in [-\pi, \pi].$$

Hence, by Theorem 12.3.2 one concludes the

Corollary 12.3.5. *The free particle operator h_0 in $l^2(\mathbb{Z})$ has purely absolutely continuous spectrum and $\sigma(h_0) = \sigma_{\mathrm{ac}}(h_0) = [-2, 2]$.*

Exercise 12.3.6. Use Fourier series to show that for every $m \in \mathbb{N}$, and every $e_k = (\delta_{j,k})_{j\in\mathbb{Z}}$, that is, the elements of canonical basis of $l^2(\mathbb{Z})$,

$$\langle e_k, (h_0)^m e_k \rangle = \frac{2}{\pi} \int_0^\pi (2\cos(x))^m \, dx = \int_{-2}^2 \frac{s^m}{\pi} \frac{ds}{\sqrt{4 - s^2}}.$$

Conclude that $\mu_{e_k} \ll \ell$ with Radon-Nikodym derivative

$$\frac{d\mu_{e_k}}{d\ell}(s) = \begin{cases} \left(\pi\sqrt{4-s^2}\right)^{-1} & |s| < 2 \\ 0 & |s| \geq 2 \end{cases}.$$

Exercise 12.3.7. Show that the operator $T = \cos(-id/dx)$ in $\mathrm{L}^2(\mathbb{R})$ has spectrum $[-1, 1]$ and it is purely absolutely continuous. This operator is related to the continuous Harper equation.

12.3.2 Putnam Commutator Theorem

Two technical conditions, related to boundary values in $\mathbb{R}$ of the resolvent operator, that guarantee the presence of absolutely continuous spectrum will be discussed. Then a result due to Putnam (around 1960) will be derived.

Proposition 12.3.8. *Let T be self-adjoint and $(a, b) \subset \mathbb{R}$. If for some $\xi \in \mathcal{H}$ there exists $0 \leq c(\xi) < \infty$ so that*

$$\liminf_{\varepsilon \to 0^+} \sup_{t \in (a,b)} \varepsilon \left\| R_{t+i\varepsilon}(T)\xi \right\|^2 \leq c(\xi),$$

then $\chi_{(a,b)}(T)\xi \in \mathcal{H}_{\mathrm{ac}}(T)$.

Proof. Consider bounded intervals $[\tilde{a}, \tilde{b}] \subset (a, b)$. By the Stone formula (see Section 9.5) and the first resolvent identity,

$$\begin{aligned} \mu_\xi((\tilde{a}, \tilde{b})) &= \langle \xi, \chi_{(\tilde{a},\tilde{b})}(T)\xi \rangle \\ &\leq \lim_{\varepsilon \to 0^+} \frac{\varepsilon}{\pi} \int_{(\tilde{a},\tilde{b})} \langle \xi, R_{t-i\varepsilon}(T) R_{t+i\varepsilon}(T)\xi \rangle \, dt \\ &= \lim_{\varepsilon \to 0^+} \frac{\varepsilon}{\pi} \int_{(\tilde{a},\tilde{b})} \left\| R_{t+i\varepsilon}(T)\xi \right\|^2 \, dt \leq \frac{1}{\pi} c(\xi)\, \ell((\tilde{a}, \tilde{b})). \end{aligned}$$

Since every open set in $\mathbb{R}$ can be expressed as a countable disjoint union of open intervals, this inequality holds for any open set $\Lambda \subset (a, b)$. By regularity of the spectral measure it follows that

$$\mu_\xi(\Lambda) \leq \frac{1}{\pi} c(\xi)\, \ell(\Lambda), \qquad \forall \Lambda \subset (a, b),\ \Lambda \in \mathcal{A}.$$

Therefore, $\mu_{(\chi_{(a,b)}(T)\xi)}(\cdot) = \mu_\xi((a, b) \cap \cdot) \ll \ell$. □

Recall that

$$F_{\mu_\xi}(t + i\varepsilon) = \langle \xi, R_{t+i\varepsilon}(T)\xi \rangle$$

is the Borel transform of the spectral measure μ_ξ at $t + i\varepsilon$, as introduced in Section 9.5.

Corollary 12.3.9. *Let T be self-adjoint and (a,b) a bounded interval in $\mathbb{R}$. If for some $p>1$ one has*

$$u_{a,b} := \sup_{0<\varepsilon<1} \int_{(a,b)} \left|\text{Im } F_{\mu_\xi}(t+i\varepsilon)\right|^p \, dt < \infty,$$

then $\chi_{(a,b)}(T)\xi \in \mathcal{H}_{\text{ac}}(T)$.

Proof. By the second resolvent identity

$$\begin{aligned}\text{Im } F_{\mu_\xi}(t+i\varepsilon) &= \frac{1}{2i}(F_{\mu_\xi}(t+i\varepsilon) - F_{\mu_\xi}(t-i\varepsilon)) \\ &= \langle \xi, \varepsilon R_{t-i\varepsilon}(T) R_{t+i\varepsilon}(T)\xi\rangle\,,\end{aligned}$$

and, as in the proof of Proposition 12.3.8,

$$\begin{aligned}\mu_\xi((\tilde{a},\tilde{b})) &= \langle \xi, \chi_{(\tilde{a},\tilde{b})}(T)\xi\rangle \\ &\le \lim_{\varepsilon\to 0^+} \frac{1}{\pi} \int_{(\tilde{a},\tilde{b})} \text{Im } F_{\mu_\xi}(t+i\varepsilon)\, dt.\end{aligned}$$

If $1/q + 1/p = 1$, by Hölder inequality,

$$\begin{aligned}\mu_\xi((\tilde{a},\tilde{b})) &\le \lim_{\varepsilon\to 0^+} \frac{1}{\pi} \left(\int_{(\tilde{a},\tilde{b})} \left|\text{Im } F_{\mu_\xi}(t+i\varepsilon)\right|^p \, dt \right)^{1/p} \ell((\tilde{a},\tilde{b}))^{1/q} \\ &\le \frac{1}{\pi} u_{a,b}^{1/p}\, \ell((\tilde{a},\tilde{b}))^{1/q},\end{aligned}$$

and the proof can be finished as the proof of Proposition 12.3.8. □

Theorem 12.3.10 (Putnam). *If T and S are bounded self-adjoint operators so that*

$$i(TS - ST) = B^* B,$$

for some invertible operator $B \in \mathrm{B}(\mathcal{H})$, then T is purely absolutely continuous.

Proof. Since B is invertible one has $\mathrm{N}(B) = \{0\}$ and so $(\text{rng } B^*)^\perp = \mathrm{N}(B^{**}) = \mathrm{N}(B) = \{0\}$ and rng B^* is a dense set in $\mathcal{H}$. For $\xi = B^*\eta$, $\eta \in \mathcal{H}$, $\varepsilon > 0$, by Propositions 2.1.12a) and 2.1.6,

$$\begin{aligned}\varepsilon\|R_{t+i\varepsilon}(T)\xi\|^2 &= \varepsilon\|R_{t+i\varepsilon}(T)B^*\eta\|^2 \le \varepsilon\|R_{t+i\varepsilon}(T)B^*\|^2\|\eta\|^2 \\ &= \varepsilon\|R_{t+i\varepsilon}(T)B^*BR_{t-i\varepsilon}(T)\|\,\|\eta\|^2 \\ &= \varepsilon\|R_{t-i\varepsilon}(T)B^*BR_{t+i\varepsilon}(T)\|\,\|\eta\|^2.\end{aligned}$$

On account of Proposition 12.3.8, the goal is to find a (finite) uniform upper bound for

$$\begin{aligned}C(\varepsilon) &:= \varepsilon\, \|R_{t-i\varepsilon}(T)B^*BR_{t+i\varepsilon}(T)\| \\ &= \varepsilon\, \|R_{t-i\varepsilon}(T)(TS-ST)R_{t+i\varepsilon}(T)\|\,.\end{aligned}$$

By Theorem 2.2.17,

$$\begin{aligned}C(\varepsilon) &= \varepsilon\,\|[\mathbf{1} + (t - i\varepsilon)R_{t-i\varepsilon}(T)]\,SR_{t+i\varepsilon}(T)\\ &\quad -R_{t-i\varepsilon}(T)S\,[\mathbf{1} + (t + i\varepsilon)R_{t+i\varepsilon}(T)]\,\|\\ &= \varepsilon\,\|SR_{t+i\varepsilon}(T) - 2i\varepsilon\,R_{t-i\varepsilon}(T)SR_{t+i\varepsilon}(T) - R_{t-i\varepsilon}(T)S\|\\ &\le \varepsilon\,\|S\|\frac{1}{\varepsilon} + \frac{2}{\varepsilon^2}\,\varepsilon^2\|S\| + \varepsilon\|S\|\frac{1}{\varepsilon} = 4\|S\|, \qquad \forall \varepsilon > 0, t \in \mathbb{R}.\end{aligned}$$

Now apply Proposition 12.3.8 with any interval $(a, b) \subset \mathbb{R}$. □

Remark 12.3.11. In Theorem 12.3.10, given T one has to determine S so that their commutator times i is a positive operator B^*B. Although it is hard to get immediate applications of this result, it is related to interesting developments due to Mourre on absence of singular continuous spectra [Mou81], [Mou83]. Such developments were applied to somewhat involved situations as N-body Schrödinger operators.

Exercise 12.3.12. If B in Theorem 12.3.10 is not invertible, conclude that $\operatorname{rng} B^* \subset \mathcal{H}_{\mathrm{ac}}(T)$.

Exercise 12.3.13. Show that the closure of the set of $\xi \in \mathcal{H}$ so that there exists $0 < c(\xi) < \infty$ for which $\|R_{t+i\varepsilon}(T)\xi\| \le c(\xi)/\sqrt{\varepsilon}$ for all $z = t + i\varepsilon \in \mathbb{C}$, $t \in \mathbb{R}$ and $0 < \varepsilon < 1$, is contained in $\mathcal{H}_{\mathrm{ac}}(T)$.

Remark 12.3.14. The condition in Exercise 12.3.13 is also necessary for $\xi \in \mathcal{H}_{\mathrm{ac}}(T)$, as discussed in [GuJ74]. Compare with the condition for point spectrum presented in [AleM78]: if (λ_k) are the eigenvalues of T, then T is a purely point operator iff

$$\sum_{\lambda_k} \lim_{\varepsilon\to 0^+} \varepsilon^2\|R_{\lambda_k+i\varepsilon}(T)\xi\|^2 = \|\xi\|^2, \qquad \forall \xi \in \mathcal{H}.$$

Example 12.3.15. It will be shown that for all gravitational intensity $g > 0$ the free fall Schrödinger operator $(H\psi)(p) = p^2\psi(p) - gi\psi'(p)$, $\psi \in \operatorname{dom} H$, introduced in Example 12.2.6, has purely absolutely continuous spectrum and $\sigma_{\mathrm{ac}}(H) = \mathbb{R}$. Two different proofs will be provided. First a representation of the resolvent of H at $z \in \mathbb{C} \setminus \mathbb{R}$, as an integral operator, will be derived.

(1) For $\psi \in C_0^\infty(\hat{\mathbb{R}})$, let $\phi(p) = (R_z(H)\psi)(p)$ so that $(H - z\mathbf{1})\phi(p) = \psi(p)$, which is a differential equation for ϕ whose solution one searches in terms of an integral operator representation.

The function $\mathbb{R} \ni r \mapsto v(r) := 1/(r - z)$ is square integrable and so its Fourier transform (defined via limit in the mean – see Section 3.1)

$$\hat{v}_z(p) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \frac{dr}{r - z}\, e^{-irp}$$

is well defined and $\hat{v}_z \in \mathrm{L}^2(\hat{\mathbb{R}})$. Now it will be checked that

$$\phi_z(p) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} ds\, \hat{v}_z\left(\frac{s - p}{g}\right)\, e^{-i(p^3 - s^3)/(3g)}\,\psi(s)$$

equals $R_z(H)\psi_z(p)$, that is $\phi_z(p) = R_z(H)\psi(p)$. Indeed,

$$\begin{aligned}(H - z\mathbf{1})\phi_z(p) &= \left(-ig\frac{d}{dp} + p^2 - z\mathbf{1}\right)\phi_z(p) \\ &= \frac{1}{2\pi}\int_{\mathbb{R}} ds \int_{\mathbb{R}} \frac{dr}{r-z}\left[-ig\left(\frac{i}{g}r - \frac{i}{g}p^2\right) + p^2 - z\right] \\ &\quad \times e^{ir(p-s)/g}\, e^{-i(p^3-s^3)/(3g)}\, \psi(s) \\ &= \int_{\mathbb{R}} ds \left(\frac{1}{2\pi}\int_{\mathbb{R}} dr\, e^{ir(p-s)/g}\right) e^{-i(p^3-s^3)/(3g)}\, \psi(s) = \psi(p),\end{aligned}$$

after using the distributional identity

$$\frac{1}{2\pi}\int_{\mathbb{R}} dr\, e^{ir(p-s)/g} = \delta((p-s)/g).$$

By Fubini's theorem,

$$\begin{aligned}|\phi_z(p)| &= \frac{1}{2\pi}\left|\int_{\mathbb{R}} dr\, \frac{e^{irp/g}}{r-z}\int_{\mathbb{R}} ds\, e^{-irs/g} e^{-i(p^3-s^3)/(3g)}\, \psi(s)\right| \\ &\le \frac{1}{2\pi}\left|\int_{\mathbb{R}} dr\, \frac{e^{irp/g}}{r-z}\right| \|\psi\|_1 = \frac{g}{2\pi}\left|\int_{\mathbb{R}} dr\, \frac{e^{irp}}{gr-z}\right| \|\psi\|_1,\end{aligned}$$

and for $z = t + i\varepsilon$, $\varepsilon > 0$, by the Plancherel theorem (note the presence of the inverse Fourier transform of $r \mapsto 1/(gr - z)$),

$$\begin{aligned}\|R_z(H)\psi\|^2 = \|\phi_z(p)\|^2 &= \int_{\mathbb{R}} dp\, |\phi_z(p)|^2 \\ &\le \left(\frac{g\|\psi\|_1}{2\pi}\right)^2 \int_{\mathbb{R}} dr\, \frac{1}{|gr-z|^2} \\ &= \left(\frac{g\|\psi\|_1}{2\pi}\right)^2 \int_{\mathbb{R}} dr\, \frac{1}{(gr-t)^2 + \varepsilon^2} \\ &= \frac{g}{\varepsilon\, 8\pi}\|\psi\|_1^2, \qquad \forall t \in \mathbb{R}.\end{aligned}$$

Therefore, for any interval (a, b) one has

$$\sup_{t\in(a,b)} \varepsilon\, \|R_{t+i\varepsilon}(T)\psi\|^2 \le \frac{g}{8\pi}\|\psi\|_1^2,$$

and $\psi \in \mathcal{H}_{\rm ac}(H)$ by Proposition 12.3.8. Since $C_0^\infty(\hat{\mathbb{R}}) \sqsubseteq \mathrm{L}^2(\hat{\mathbb{R}})$ and this holds for all intervals (a, b), it follows that $\mathcal{H}_{\rm ac}(H) = \mathrm{L}^2(\mathbb{R})$ and $\sigma_{\rm ac}(H) = \mathbb{R}$. Finally, note that all arguments can be easily adapted for $g < 0$.

(2) Now a shorter argument for $\mathcal{H}_{ac}(H) = L^2(\mathbb{R})$, which does not use the above distributional identity, will be presented. Let x and P denote the position and momentum operator on $\mathbb{R}$ and consider the unitary evolution group $U_s = e^{-isP^3}$, $s \in \mathbb{R}$. Set $o(s) := U_{-s} x U_s$ with dom $o(s) = \mathcal{S}(\mathbb{R})$. Note that $o(0) = x$ and

$$\frac{d}{ds} o(s) = iU_{-s}\left(P^3 x - xP^3\right) U_s = 3P^2,$$

so, on $\mathcal{S}(\mathbb{R})$ one has $o(s) = o(0) + 3sP^2 = x + 3sP^2$. By Example 12.2.6, for all $s \in \mathbb{R}$ the operator $o(s)$ is essentially self-adjoint, and with the choice $s = s_g = -1/(3g)$,

$$-\frac{1}{g}P^2 + x = U_{-s_g} x U_{s_g} \Longrightarrow P^2 - gx = U_{-s_g}(-gx)U_{s_g},$$

and the free fall operator $P^2 - gx$ is unitarily equivalent to the operator $-gx$. Since x is purely absolutely continuous with $\sigma_{ac}(x) = \mathbb{R}$, the result follows.

Exercise 12.3.16. Let $g > 0$. For $n \in \mathbb{N}$, $n \geq 2$, consider the operator dom $\tilde{H}_n = C_0^\infty(\hat{\mathbb{R}})$, $(\tilde{H}_n \psi)(p) = p^{n-1}\psi(p) - gi\psi'(p)$. Show that its adjoint $H_n = \tilde{H}_n^*$ is given by dom $H_n = \{\psi \in L^2(\hat{\mathbb{R}}) : \psi \in AC(\hat{\mathbb{R}}), (p^{n-1}\psi(p) - gi\psi'(p)) \in L^2(\hat{\mathbb{R}})\}$,

$$(H_n\psi)(p) = p^{n-1}\psi(p) - gi\psi'(p), \qquad \psi \in \text{dom } H,$$

and that this operator is hermitian, so that it is self-adjoint and $\tilde{H}_n$ is essentially self-adjoint. Check explicitly that $\sigma_p(H_n) = \emptyset$. Then verify that for $z \in \mathbb{C} \setminus \mathbb{R}$, $\psi \in C_0^\infty(\hat{\mathbb{R}})$ and $\hat{v}_z$ as in Example 12.3.15, one has

$$R_z(H_n)\psi(p) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} ds\, \hat{v}_z\left(\frac{s-p}{g}\right) e^{-i[p^n - s^n]/(ng)}\, \psi(s),$$

and finally, that H_n is purely absolutely continuous with $\sigma_{ac}(H_n) = \mathbb{R}$.

Remark 12.3.17. Note that in Example 12.3.16 and Exercise 12.3.16 the Green functions of some Schrödinger operators were found.

Exercise 12.3.18. Let x and P denote, respectively, the position and momentum operator on $\mathbb{R}^n$. By considering $o(s) = U_{-s}x^2 U_s$, $U_s = e^{-iP^2 s}$, acting on the Schwartz space $\mathcal{S}(\mathbb{R}^n)$, show that the perturbation of the harmonic oscillator

$$H = -4s^2\Delta^2 + x^2 + i2s(x\nabla + \nabla x), \qquad s \in \mathbb{R},$$

is essentially self-adjoint on $\mathcal{S}(\mathbb{R}^n)$ and its unique self-adjoint extension is purely absolutely continuous with spectrum $[0, \infty)$, $\forall n$.

Remark 12.3.19. There is an extension of the dilation evolution group which, in conjunction with Proposition 12.3.8, can be applied to conclude that the essential spectrum $[0, \infty)$ of the H-atom Schrödinger operator is, in fact, absolutely continuous. Details can be found in [BaC71],[Thi81], and a variation that uses Mourre estimates in [CyFKS87].

12.3.3 Scattering and Kato-Rosenblum Theorem

Some tools of scattering theory will be used to discuss the presence of an absolutely continuous spectrum. General references to the mathematics of scattering theory are [AmJS77], [ReeS79], [Ya92]. Most quantum mechanics textbooks present a detailed picture of basic scattering processes [LaL58], [AmJS77].

Let T and B be two self-adjoint operators in $\mathcal{H}$, with $B \in \mathrm{B}(\mathcal{H})$ (this is just to simplify technicalities, e.g., dom $(T+B) =$ dom T and $T+B$ is self-adjoint), and P_{ac}^{T}, P_{ac}^{T+B} the corresponding projections onto their absolutely continuous subspaces $\mathcal{H}_{\mathrm{ac}}(T)$, $\mathcal{H}_{\mathrm{ac}}(T+B)$. The motivating aim of scattering theory is to compare the large time behavior of the "free" time evolution $e^{-itT}\xi_\pm$ with the "perturbed" time evolution $e^{-it(T+B)}\xi$. Under some conditions, it is physically expected that for "scattering states ξ" the time evolution $e^{-it(T+B)}\xi$ should behave as free vectors $\xi_\pm$, that is, as $e^{-itT}\xi_\pm$, as time $t \to \pm\infty$. So one writes

$$\left\| e^{-it(T+B)}\xi - e^{-itT}\xi_\pm \right\| = \left\| \xi - e^{it(T+B)}e^{-itT}\xi_\pm \right\|$$

and defines:

Definition 12.3.20. The *wave operators* are the strong limits

$$\mathcal{W}_\pm(T+B,T) := \mathrm{s} - \lim_{t\to\pm\infty} e^{it(T+B)}e^{-itT}P_{\mathrm{ac}}^{T},$$

if they exist. Their domains are maximal, that is,

$$\mathrm{dom}\ \mathcal{W}_\pm(T+B,T) = \left\{ \xi \in \mathcal{H} : \exists \lim_{t\to\pm\infty} e^{it(T+B)}e^{-itT}P_{\mathrm{ac}}^{T}\xi \right\}.$$

Wave operators were introduced in a purely physical context by Møller in 1945; sometimes they are called *Møller operators* and here the shorthand notation $\mathcal{W}_\pm$ will also be used. A possibility of violation of such asymptotic free conditions would be an event in which a free particle as $t \to -\infty$ gets captured by the scatter, e.g., by an eigenstate of $T+B$ for $t \geq 0$.

On writing $\xi \in$ dom $\mathcal{W}_\pm$ it will be implicitly assumed that $\xi \in \mathcal{H}_{\mathrm{ac}}(T)$, since on $\mathcal{H}_{\mathrm{ac}}(T)^\perp$ the wave operators $\mathcal{W}_\pm(T+B,T)$ act as the null operator. The interpretations are as follows:

- dom $\mathcal{W}_-$ is the set of incoming asymptotic states.
- dom $\mathcal{W}_+$ is the set of outgoing asymptotic states.
- rng $\mathcal{W}_-$ is the set of the states that have an incoming free asymptotic state.
- rng $\mathcal{W}_+$ is the set of the states that have an outgoing free asymptotic state.

Definition 12.3.21. The wave operators $\mathcal{W}_\pm(T+B,T)$ are said to be *complete* if dom $\mathcal{W}_\pm(T+B,T) = \mathcal{H}_{\mathrm{ac}}(T)$ and rng $\mathcal{W}_\pm(T+B,T) = \mathcal{H}_{\mathrm{ac}}(T+B)$, that is, if the set of free states is $\mathcal{H}_{\mathrm{ac}}(T)$ and the set of states that have both incoming and outgoing free asymptotic states is exactly $\mathcal{H}_{\mathrm{ac}}(T+B)$.

Since for $\xi \in \operatorname{dom} \mathcal{W}_\pm$ one has

$$\|\mathcal{W}_\pm \xi\| = \lim_{t\to\pm\infty} \left\| e^{it(T+B)} e^{-itT} P^T_{\rm ac} \xi \right\| = \|\xi\|,$$

it follows that $\mathcal{W}_\pm : \operatorname{dom} \mathcal{W}_\pm \to \operatorname{rng} \mathcal{W}_\pm$ are partial isometries.

Exercise 12.3.22. Show that $\operatorname{dom} \mathcal{W}_\pm(T+B,T)$ are closed subspaces (hint: if $\xi \in \overline{\operatorname{dom} \mathcal{W}_\pm}$ show that $t \mapsto e^{it(T+B)}e^{-itT}\xi$ is Cauchy). Since these operators are isometries, conclude that $\operatorname{rng} \mathcal{W}_\pm$ are also closed.

Remark 12.3.23. A similar theory of scattering can be developed if in Definition 12.3.20 $P^T_{\rm ac}$ is replaced by a general projection P that commutes with the "free" time evolution e^{-itT}, provided it is possible to describe the asymptotic behavior of such vectors. In $\mathrm{L}^2(\mathbb{R}^n)$ a convincing choice would be the projection onto $\mathcal{H}_{\rm scatt}(T)$ introduced in Definition 13.6.1! Besides the results ahead, the option $P^T_{\rm ac}$ here is mainly guided by the standard (purely absolutely continuous) free hamiltonian H_0 in $\mathrm{L}^2(\mathbb{R}^n)$ so that one expects that the general "free" dynamics should be governed by this spectral type.

Thus $\mathcal{W}_\pm \mathcal{W}_\pm^*$ are the projections onto $\operatorname{rng} \mathcal{W}_\pm$, and restricted to these spaces $\mathcal{W}_\pm^* = \mathcal{W}_\pm^{-1}$. Further, if $\xi \in \operatorname{dom} \mathcal{W}_\pm$, then for any $t \in \mathbb{R}$,

$$\lim_{s\to\pm\infty} e^{is(T+B)} e^{-isT} e^{-itT}\xi = \lim_{s\to\pm\infty} e^{-it(T+B)} e^{i(t+s)(T+B)} e^{-i(t+s)T}\xi$$

so that

$$\mathcal{W}_\pm e^{-itT}\xi = e^{-it(T+B)}\mathcal{W}_\pm \xi, \qquad \forall \xi \in \operatorname{dom} \mathcal{W}_\pm(T+B,T),$$

also $e^{-itT}\operatorname{dom} \mathcal{W}_\pm \subset \operatorname{dom} \mathcal{W}_\pm$ and $e^{-it(T+B)}\operatorname{rng} \mathcal{W}_\pm \subset \operatorname{rng} \mathcal{W}_\pm$. By Proposition 5.3.9 and its proof, it follows that $\operatorname{dom} \mathcal{W}_\pm(T+B,T)$ reduces T while $\operatorname{rng} \mathcal{W}_\pm(T+B,T)$ reduces $T+B$. Upon differentiating the above equality with respect to t one finds the so-called *intertwining property* of the wave operators, that is, for all $\xi \in \operatorname{dom} \mathcal{W}_\pm \cap \operatorname{dom} T$,

$$\mathcal{W}_\pm(T+B,T)T\xi = (T+B)\mathcal{W}_\pm(T+B,T)\xi.$$

This relation implies

Proposition 12.3.24. *If $\mathcal{W}_\pm(T+B,T)$ are complete, then $T_{\rm ac}$ and $(T+B)_{\rm ac}$ are unitarily equivalent (so they have the same absolutely continuous spectra).*

Exercise 12.3.25. Let $\xi \in \operatorname{dom} T$ be an eigenvector of T. Show that the limit $\lim_{t\to\infty} e^{it(T+B)}e^{-itT}\xi$ exists iff ξ is an eigenvector of $T+B$ with the same eigenvalue. Conclude that $B\xi = 0$. This is one reason to include $P^T_{\rm ac}$ in the definition of wave operators.

The operator $S := \mathcal{W}_+^* \mathcal{W}_-$ connects free asymptotic states in the remote past with free asymptotic states in the remote future, and it is called a *scattering operator* or *S-matrix*.

Lemma 12.3.26. *For all* $z \in \mathbb{C} \setminus \mathbb{R}$,

$$\mathcal{W}_\pm(T+B,T)R_z(T) = R_z(T+B)\mathcal{W}_\pm(T+B,T),$$

and for any open set $\Lambda \subset \mathbb{R}$,

$$\mathcal{W}_\pm(T+B,T)\chi_\Lambda(T) = \chi_\Lambda(T+B)\mathcal{W}_\pm(T+B,T),$$

with both relations acting on dom $\mathcal{W}_\pm(T+B,T)$.

Proof. Write $\mathcal{W}_\pm = \mathcal{W}_\pm(T+B,T)$. According to the spectral theorem (see page 245), for $\xi \in \text{dom } W_\pm$ and $\text{Im } z > 0$,

$$\begin{aligned}\mathcal{W}_\pm R_z(T)\xi &= -i\int_0^\infty e^{isz}\mathcal{W}_\pm e^{-isT}\xi\, ds \\ &= -i\int_0^\infty e^{isz}e^{-is(T+B)}\mathcal{W}_\pm\xi\, ds \\ &= R_z(T+B)\mathcal{W}_\pm\xi.\end{aligned}$$

Similarly if $\text{Im } z < 0$. By the Stone formula (see Exercise 9.5.5) it follows that $\mathcal{W}_\pm\chi_{(a,b)}(T) = \chi_{(a,b)}(T+B)\mathcal{W}_\pm$ for all bounded intervals (a,b) in $\mathbb{R}$; the final result follows by taking strong limits and recalling that any open set in $\mathbb{R}$ is a countable union of pairwise disjoint open intervals. □

Lemma 12.3.27. *Assume that* $\mathcal{W}_\pm(T+B,T)$ *exist with domain* $\mathcal{H}_{\text{ac}}(T)$*. Then such wave operators are complete iff* $\mathcal{W}_\pm(T,T+B)$ *exist with domain* $\mathcal{H}_{\text{ac}}(T+B)$*.*

Proof. If $\xi \in \mathcal{H}_{\text{ac}}(T)$, then

$$\eta_\pm = \lim_{t\to\pm\infty} e^{it(T+B)}e^{-itT}\xi = \mathcal{W}_\pm\xi$$

is equivalent to

$$\lim_{t\to\pm\infty} \|e^{-itT}\xi - e^{-it(T+B)}\eta_\pm\| = 0$$

which is equivalent to

$$\xi = \lim_{t\to\pm\infty} e^{itT}e^{-it(T+B)}\eta_\pm = \mathcal{W}_\pm^*\eta_\pm = \mathcal{W}_\pm(T,T+B)\eta_\pm.$$

By Lemma 12.3.26, for all open sets $\Lambda \subset \mathbb{R}$,

$$\begin{aligned}\mu_{\eta_\pm}^{T+B}(\Lambda) &= \langle \eta_\pm, \chi_\Lambda(T+B)\eta_\pm\rangle \\ &= \left\langle \eta_\pm, \mathcal{W}_\pm\chi_\Lambda(T)\mathcal{W}_\pm^*\eta_\pm\right\rangle \\ &= \langle \xi, \chi_\Lambda(T)\xi\rangle = \mu_\xi^T(\Lambda),\end{aligned}$$

and so the equality $\mu_{\eta_\pm}^{T+B}(\Lambda) = \mu_\xi^T(\Lambda)$ extends to all Borel sets $\Lambda \in \mathcal{A}$ (e.g., use the regularity of such measures). This shows that the spectral measures $\mu_{\eta_\pm}^{T+B}$ are absolutely continuous since μ_ξ^T is, and so $\eta_\pm \in \mathcal{H}_{\text{ac}}(T+B)$. Thus, for $\xi \in \mathcal{H}_{\text{ac}}(T)$ the limits $\mathcal{W}_\pm(T,T+B)\xi$ exist iff $\xi \in \text{rng } \mathcal{W}_\pm(T+B,T)$, but the above calculation shows that this range is in $\mathcal{H}_{\text{ac}}(T+B)$. This proves the lemma. □

From the proof of Lemma 12.3.27 follows the

Corollary 12.3.28. rng $W_\pm(T+B,T) \subset \mathcal{H}_{\mathrm{ac}}(T+B)$.

Theorem 12.3.29 (Kato-Rosenblum). *Let T and B be self-adjoint. If B is trace class, then the wave operators $\mathcal{W}_\pm(T+B,T)$ exist and are complete. Hence T and $T+B$ have the same absolutely continuous spectra.*

Proof. This proof will make use of some facts discussed in Chapter 13 and the proof will be for $\mathcal{W}_+(T+B,T)$; the discussion on $\mathcal{W}_-(T+B,T)$ being similar. Write $W(t) = e^{it(T+B)}e^{-iT}$. It will be shown that $W(t)P^T_{\mathrm{ac}}\xi$ is Cauchy, and since $W(t)$ is unitary for all $t \in \mathbb{R}$, it is enough to check this for all $\xi \in \mathcal{H}_{\mathrm{ac}}(T)$ such that the Radon-Nikodym derivative $d\mu^T_\xi/d\ell$ is bounded, since by Exercise 13.5.4 this is a dense subset of $\mathcal{H}_{\mathrm{ac}}(T)$. In the following ξ is supposed to belong to this set and we write $|||\xi||| := \|d\mu^T_\xi/d\ell\|_\infty$.

By noting that

$$\|(W(t)-W(s))\,\xi\|^2 = \langle W(t)\xi,(W(t)-W(s))\xi\rangle - \langle W(s)\xi,(W(t)-W(s))\xi\rangle,$$

it follows that it is enough to show that $\langle \xi, W(t)^*(W(t)-W(s))\xi\rangle$ vanishes as $t,s\to\infty$; with no loss it will be assumed that $t \ge s$.

Introduce $G(u) := e^{iuT}W(t)^*W(s)e^{-iuT}$, $u \in \mathbb{R}$ is an auxiliary parameter, and check that (hint: add and subtract B to T in the expression of Y)

$$\frac{dG}{du}(u) = e^{iuT}Y(t,s)e^{-iuT},$$

with $Y(t,s) = -i\left[e^{itT}Be^{-i(t-s)(T+B)}e^{-isT} - e^{itT}e^{-i(t-s)(T+B)}Be^{-isT}\right]$, and upon integrating

$$W(t)^*W(s) = e^{i\tau T}W(t)^*W(s)e^{-i\tau T} - \mathcal{I}_\tau[Y(t,s)],$$

where

$$\mathcal{I}_\tau[X] := \int_0^\tau e^{iuT}Xe^{-iuT}\,du, \qquad \tau \ge 0.$$

Hence

$$\begin{aligned}\langle \xi, W(t)^*(W(t)-W(s))\xi\rangle& \\ &= \langle W(t)e^{-i\tau T}\xi,(W(t)-W(s))e^{-i\tau T}\xi\rangle\\ &+ \langle \xi, \mathcal{I}_\tau[Y(t,s)]\xi\rangle.\end{aligned}$$

Since B is trace class it is compact, and so (as in the Duhamel formula, differentiate and then integrate $W(t)$)

$$W(t)-W(s) = i\int_s^t e^{iu(T+B)}Be^{-iuT}\,du$$

is also compact. Taking $\tau \to \infty$ one has $(W(t) - W(s))e^{-i\tau T}\xi \to 0$ by RAGE Theorem 13.4.1ii), and this result consequently shows that

$$\langle \xi, W(t)^*(W(t) - W(s))\xi\rangle = \langle \xi, \mathcal{I}_\infty[Y(t,s)]\,\xi\rangle,$$

with well-posed limit $\tau \to \infty$.

Note that $\langle \xi, \mathcal{I}_\infty[Y(t,s)]\xi\rangle$ is a sum of terms of the form

$$\langle \xi, \mathcal{I}_\infty[Z(t,s)Be^{-isT}]\,\xi\rangle$$

with $Z(t,s) = e^{itT}e^{-i(t-s)(T+B)}$, and their complex conjugates, and $Z(t,s)$ are unitary operators. Hence, the proof finishes if one shows that (recall that $s \le t$)

$$\lim_{s\to\infty} \left\langle \xi, \mathcal{I}_\infty[Z(t,s)Be^{-isT}]\,\xi\right\rangle = 0.$$

Write $B(\cdot) = \sum_j \varpi_j \langle \eta_j, \cdot\rangle \xi_j$, with $\{\eta_j\}_j$ and $\{\xi_j\}_j$ orthonormal sets in $\mathcal{H}$ and $\sum_j |\varpi_j| < \infty$, that is, the canonical form of the trace-class operator B. Thus, by Cauchy-Schwarz inequality,

$$\begin{aligned}
&\left|\left\langle \xi, \mathcal{I}_\infty[Z(t,s)Be^{-isT}]\,\xi\right\rangle\right|^2 \\
&= \left| \sum_j \varpi_j \int_0^\infty \left\langle \eta_j, e^{-i(u+s)T}\xi\right\rangle \left\langle e^{-iuT}\xi, Z(t,s)\xi_j\right\rangle\, du \right|^2 \\
&\le \left(\int_s^\infty du \sum_j |\varpi_j| \left|\left\langle \eta_j, e^{-iuT}\xi\right\rangle\right|^2 \right) \left(\sum_j |\varpi_j| \int_{\mathbb{R}} du \left|\left\langle Z(t,s)\xi_j, e^{-iuT}\xi\right\rangle\right|^2 \right)
\end{aligned}$$

and by Exercise 13.5.4,

$$\begin{aligned}
&\sum_j |\varpi_j| \int_{\mathbb{R}} du \left|\left\langle Z(t,s)\xi_j, e^{-iuT}\xi\right\rangle\right|^2 \\
&\le 2\pi \|Z(t,s)\|^2 \left(\sum_j |\varpi_j|\right) |||\xi|||^2 = 2\pi\, \mathrm{tr}\,|B|\, |||\xi|||^2
\end{aligned}$$

so that

$$\begin{aligned}
&\left|\left\langle \xi, \mathcal{I}_\infty[Z(t,s)Be^{-isT}]\,\xi\right\rangle\right|^2 \\
&\le 2\pi \left(\int_s^\infty du \sum_j |\varpi_j| \left|\left\langle \eta_j, e^{-iuT}\xi\right\rangle\right|^2 \right) \mathrm{tr}\,|B|\, |||\xi|||^2,
\end{aligned}$$

and since $\sum_j |\varpi_j| \left|\left\langle \eta_j, e^{-iuT}\xi\right\rangle\right|^2$ belongs to $\mathrm{L}^1(\mathbb{R})$ (once more by Exercise 13.5.4), the above right-hand side vanishes as $s \to \infty$. This proves that $\mathcal{W}_+(T+B,T)$ does exist.

The same proof works for $\mathcal{W}_\pm(T, T+B)$ since $T-(T+B)=-B$ is also trace class. Combining with Lemma 12.3.27, the completeness of such wave operators follows. □

Remark 12.3.30. If instead of trace-class perturbations one considers Hilbert-Schmidt perturbations, then the conclusions of the Kato-Rosenblum theorem are false by the Weyl-von Neumann Theorem 12.5.2; see also Remark 12.5.5.

Remark 12.3.31. In an interesting work [How86] it was shown that the Kato-Rosenblum theorem has no simple generalization to a singular spectrum; for instance, if B is compact and the subsequent singular parts T_{s} and $(T+B)_{\mathrm{s}}$ are unitarily equivalent for every self-adjoint T, then $B=0$. In fact, much more is concluded in that work.

Remark 12.3.32. The original proof of Theorem 12.3.29 was published in [Kat57] and [Ros57]; the above proof is based on a useful generalization of the Kato-Rosenblum theorem in [Pea78b]. There is also a version of this theorem for unitary operators in [BiK62].

Of particular interest is the case of the free particle hamiltonian $T=H_0$ in $\mathrm{L}^2(\mathbb{R}^n)$, so that for any trace-class perturbation B, the absolutely continuous part of H_0+B is unitarily equivalent to H_0. However, if $B=V$, that is, multiplication by a potential function, the Kato-Rosenblum theorem does not apply, since it assumes that the perturbation is a trace-class operator, so compact. In any event, there are generalizations that are powerful in standard quantum mechanics, e.g., it is enough that $R_i(H_0)-R_i(H)$ is trace class [Sim05].

For potential V scattering one must have $V(x)\to 0$ sufficiently fast as $|x|\to\infty$, so that states leave the region of influence of the potential and move asymptotically as free ones and scattering occurs (the so-called short-range potentials). However, the important Coulomb potential influences particles even far away, and a modification of the wave operators is necessary; this modification was introduced in [Doll64] and a detailed discussion appears in [AmJS77].

While talking about scattering in quantum mechanics it becomes imperative to mention at least a version of the so-called Cook's lemma [Coo57]; this reference can be considered the genesis of mathematical scattering theory. The proof of Theorem 12.3.33 is a simple version of Cook's approach to existence of wave operators for potentials V in $\mathbb{R}^3$.

Theorem 12.3.33. *Let $V\in\mathrm{L}^2(\mathbb{R}^3)$, H_0 the free hamiltonian and $H=H_0+V$ with domain $\mathcal{H}^2(\mathbb{R}^3)$. Then the strong limits*

$$\mathcal{W}_\pm(H,H_0)=\mathrm{s}-\lim_{t\to\pm\infty} e^{itH}e^{-itH_0}$$

exist in $\mathrm{L}^2(\mathbb{R}^3)$.

Proof. First note that $P_{\rm ac}^{H_0} = \mathbf{1}$ and, by Theorem 6.2.2, H is self-adjoint. By the Duhamel formula, if $\psi \in \operatorname{dom} H$ and $t > s$,

$$\left\|e^{itH}e^{-itH_0}\psi - e^{isH}e^{-isH_0}\psi\right\|_2 = \left\| i\int_s^t e^{iuH}Ve^{-iuH_0}\psi\, du\right\|_2$$
$$\leq \int_s^t \left\|Ve^{-iuH_0}\psi\right\|_2 du$$
$$\leq \|V\|_2 \int_s^t \|e^{-iuH_0}\psi\|_\infty\, du.$$

If $\psi \in D = \mathcal{H}^2(\mathbb{R}^3) \cap \mathrm{L}^1(\mathbb{R}^3)$, by Corollary 5.5.5 the function $u \mapsto \|e^{-iuH_0}\psi\|_\infty$ is integrable over $\mathbb{R}$, consequently $t \mapsto e^{itH}e^{-itH_0}\psi$ is Cauchy as $t \to \pm\infty$. Hence the limits $\mathcal{W}_\pm(H, H_0)\psi$ exist for any $\psi \in D$. Since D is dense in $\mathrm{L}^2(\mathbb{R}^3)$ and $e^{itH}e^{-itH_0}$ is an isometry for any t, $\mathcal{W}_\pm(H, H_0)\psi$ exist for any $\psi \in \mathrm{L}^2(\mathbb{R}^3)$. □

Corollary 12.3.34. *Let $V \in \mathrm{L}^2(\mathbb{R}^3)$. The hamiltonian $H = H_0 + V$ with domain $\mathcal{H}^2(\mathbb{R}^3)$ has nonempty absolutely continuous spectrum.*

Proof. By Theorem 12.3.33, $\mathcal{W}_\pm(H, H_0)$ exist with domain $\mathrm{L}^2(\mathbb{R}^3)$. Since the wave operators are isometries, one has $\{0\} \neq \operatorname{rng} \mathcal{W}_\pm(H, H_0) \subset \mathcal{H}_{\rm ac}(H)$. □

Remark 12.3.35. A simple condition to state, although not immediate to prove, that guarantees the existence and completeness of wave operators in case of $\mathrm{L}^2(\mathbb{R})$ and $l^2(\mathbb{Z})$, is whether the potential $V \in \mathrm{L}^1(\mathbb{R}) \cap \mathrm{L}^2(\mathbb{R})$ or $V \in l^1(\mathbb{Z})$, respectively. For example, $\sigma_{\rm ac}(H_0 + V) = \sigma_{\rm ac}(H_0) = [0, \infty)$ if V is continuous and $|V(x)| \leq C/(1 + |x|)^a$, $a > 1$. Similarly for the discrete case. For references and results in this direction refer to [Rem98]. Sufficient conditions on V for absolutely continuous spectra of $H = H_0 + V$ in $\mathrm{L}^2(\mathbb{R}^3)$ appear, for instance, in [Pea88] and [ReeS78].

12.4 Magnetic Field: Landau Levels

The Schrödinger operator corresponding to a charged particle in a homogeneous magnetic field of intensity $\mathbf{B}$ will be considered; homogeneous means that the magnetic field is the same at all points of space (usually the term "constant magnetic field" means that $\mathbf{B}$ does not depend on time, so "homogeneous" is employed).

First suppose that the particle motion is restricted to $\mathbb{R}^2$, with coordinates x, y, and $\mathbf{B}$ perpendicular to this plane. As in Section 10.5 the vector potential $\mathbf{A}$ is the quantity that appears in the hamiltonian operator; in this case a convenient choice is $\mathbf{A} = (A_x, A_y) = (-By, 0)$ so that $B = \partial A_y/\partial x - \partial A_x/\partial y$. The Hilbert space is $\mathrm{L}^2(\mathbb{R}^2)$ and it will be interesting to make explicit some physical constants, such as the mass m of the particle, speed of light c and electric charge e; Planck's constant will be set $\hbar = 1$. The intention here is just to provide a flavor of the vast area of magnetic phenomena.

Remark 12.4.1. In case of $\mathbb{R}^3$ (or $\mathbb{R}^2$) with a homogeneous magnetic field $\mathbf{B}$, a popular choice of the vector potential is $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{x}$, with $\mathbf{x} = (x, y, z)$ and "$\times$" indicates vector product. Recall that $\mathbf{B} = \nabla \times \mathbf{A}$.

The initial energy operator $H = H(\mathbf{A})$ is dom $H = \mathcal{S}(\mathbb{R}^2)$ (the Schwartz space; see Section 3.1),

$$\begin{aligned}(H\psi)(x,y) &= \frac{1}{2m}\left(-i\nabla - \frac{e}{c}\mathbf{A}\right)^2 \psi(x,y) \\ &= \frac{1}{2m}\left[\left(-i\frac{\partial}{\partial x} + \frac{eB}{c}y\right)^2 - \frac{\partial^2}{\partial y^2}\right]\psi(x,y), \qquad \psi \in \operatorname{dom} H.\end{aligned}$$

Apply Fourier transform $\mathcal{F}_x$ in the variable x, going to the space $\mathrm{L}^2(\hat{\mathbb{R}} \times \mathbb{R})$, $\hat{\psi}(p_1, y) := \mathcal{F}_x\psi(x,y) \in \mathcal{S}(\hat{\mathbb{R}} \times \mathbb{R})$, and

$$\begin{aligned}(\hat{H}\hat{\psi})(p_1,y) &:= (\mathcal{F}_x H \mathcal{F}_x^{-1})\hat{\psi}(p_1,y) \\ &= \frac{1}{2m}\left(p_1 + \frac{eB}{c}y\right)^2 \hat{\psi}(p_1,y) - \frac{1}{2m}\frac{\partial^2}{\partial y^2}\hat{\psi}(p_1,y) \\ &= -\frac{1}{2m}\frac{\partial^2}{\partial y^2}\hat{\psi}(p_1,y) + \frac{m\omega^2}{2}\left(y + \frac{cp_1}{eB}\right)^2 \hat{\psi}(p_1,y),\end{aligned}$$

with $\omega = eB/(mc)$. This operator acts as a multiplication operator in the variable p_1 and as a harmonic oscillator with frequency ω in the variable $y - cp_1/(eB)$; in fact, $\hat{H}$ is a direct integral of some one-dimensional operators. By Example 2.3.3, for any $\phi \in \mathcal{S}(\hat{\mathbb{R}})$ the operator $\hat{H}$ has eigenfunctions

$$\hat{\psi}_j(p_1,y) := \psi_j\left(y + \frac{cp_1}{eB}\right)\phi(p_1), \qquad \hat{H}\hat{\psi}_j = \omega\left(j + \frac{1}{2}\right)\hat{\psi}_j,$$

where $\psi_j(y)$ are the usual Hermite functions for $j = 0, 1, 2, \ldots$, i.e., eigenfunctions of the harmonic oscillator.

Since ϕ is quite general (e.g., consider functions in $C_0^\infty(\mathbb{R}^2)$ with pairwise disjoint support), each eigenvalue has infinite multiplicity; it was crucial that the eigenvalues do not depend on p_1. Note also that even a constant $\phi(p_1) = 1$ can be considered, since the very $\psi_j\,(y + cp_1/(eB)) \in \mathcal{S}(\hat{\mathbb{R}} \times \mathbb{R})$; in this case physicists like to relate the infinite multiplicity of eigenvalues to different choices of momentum p_1 (the analogy with classical mechanics is mentioned ahead).

Since the set of all possible $\hat{\psi}_j$ is dense in $\mathrm{L}^2(\hat{\mathbb{R}} \times \mathbb{R})$ (see Theorem 2.2.10), it follows that $\hat{H}$, and so also its unitarily equivalent H, are essentially self-adjoint and their closures have the same spectra, i.e.,

$$\sigma(\overline{H}) = \{(j + 1/2)\,\omega : j = 0, 1, 2, \ldots\},$$

which is pure point and also pure essential. These eigenvalues are called *Landau levels*, named after L. Landau who found them in 1930; since they were also discussed by Fock two years before Landau, maybe it would be correct to say Fock-Landau levels. Note that the ground state energy (i.e., the lowest eigenvalue) is $\omega/2$ and has infinite multiplicity.

Remark 12.4.2. In case the vector potential components A_x, A_y belong to $C^\infty(\mathbb{R}^2)$ and the magnetic field tends to a nonzero constant as $x^2 + y^2 \to \infty$, in [Iwa83] it was shown that the corresponding Schrödinger operator has also purely essential and also purely point spectra.

In classical mechanics the planar motion of a particle under such homogeneous $\mathbf{B}$ corresponds to a circumference of fixed center which, of course, depends on the initial conditions $(x_0, p_{x,0}, y_0, p_{y,0})$; the y component of the center of this circumference is given by $y_0 - cp_{x,0}/(eB)$, which is directly related to the quantity the variable y represents in the above quantum eigenfunctions (i.e., the center of the gaussian in the Hermite functions). It is then interpreted that the infinite multiplicity of eigenvalues is related to different classical (circular) motions.

A natural question is about the role played by the x components of such centers; why they did not show up here? The answer is the choice of vector potential $\mathbf{A}$; other choices are possible, e.g., $\mathbf{A} = (0, xB)$, since they generate the same homogeneous magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$. The latter choice would have led to the appearance of the x component of the center of classical orbits in the quantum energy eigenfunctions.

To be more precise, consider the case of three dimensions (the two-dimensional case is similar); two vector potentials $\mathbf{A^1}$ and $\mathbf{A^2}$ generate the same $\mathbf{B}$ iff $\nabla \times (\mathbf{A^1} - \mathbf{A^2}) = 0$, which amounts to

$$\mathbf{A^1} = \mathbf{A^2} + \nabla\chi,$$

that is, the addition of the gradient of some real-valued smooth function $\chi : \mathbb{R}^3 \to \mathbb{R}$. Each χ is known as a *gauge function* which generates a *gauge transformation* defined as the passage from $\mathbf{A^2}$ to $\mathbf{A^1}$ via $\nabla\chi$, and classical physics is clearly invariant under gauge transformations, since only the magnetic fields appear in the expression of Lorenz force $(e/c)\mathbf{v} \times \mathbf{B}$. The next exercise clarifies the situation in quantum mechanics. For some controversial situations see the discussion in Section 10.5. General discussions about quantum magnetic gauge transformations are found in [Lei83].

Exercise 12.4.3. Let $\mathbf{A^1} = \mathbf{A^2} + \nabla\chi$, with both defining self-adjoint hamiltonians $H(\mathbf{A^1})$ and $H(\mathbf{A^2})$ (see general results in [LeiS81]).

Show that $e^{-ie\chi(x)/c}\mathrm{dom}\, H(\mathbf{A^1}) = \mathrm{dom}\, H(\mathbf{A^2})$ and

$$\left(-i\nabla - \frac{e}{c}\mathbf{A^1}\right)^2 = e^{ie\chi/c}\left(-i\nabla - \frac{e}{c}\mathbf{A^2}\right)^2 e^{-ie\chi/c},$$

that is, the energy operators corresponding to two vector potentials that differ by a gauge transformation are unitarily equivalent, so physically equivalent. Sometimes, by proper selections of χ one can impose suitable conditions on vector potentials $\mathbf{A}$, for instance, the so-called Coulomb gauge for which the divergent $\nabla \cdot \mathbf{A} = 0$.

Exercise 12.4.4. Repeat the above discussion on quantum eigenfunctions for a charged quantum particle in $\mathbb{R}^2$, but now with the gauge selection $\mathbf{A} = (0, xB)$.

The corresponding problem in $\mathbb{R}^3$, with variables (x,y,z) and $\mathbf{A}=(-yB,0,0)$, generates the homogeneous magnetic field $\mathbf{B} = (0, 0, B)$, and the initial hamiltonian is

$$H_3\psi = \frac{1}{2m}\left(-i\frac{\partial}{\partial x} + \frac{eB}{c}y\right)^2 \psi - \frac{1}{2m}\frac{\partial^2}{\partial y^2}\psi - \frac{1}{2m}\frac{\partial^2}{\partial z^2}\psi,$$

with $\psi \in \mathcal{S}(\mathbb{R}^3)$. One then gets the same problem in $\mathbb{R}^2$, but with an additional term corresponding to a free particle in the z direction. It turns out that the spectrum will be formed by the addition of the same eigenvalues of the two-dimensional case with the absolutely continuous part $[0, \infty)$ coming from the free motion. Thus, the resulting spectrum is $[\omega/2, \infty)$, absolutely continuous with embedded eigenvalues of infinite multiplicity. The classical motion is formed by helical orbits, which are composed by uniform rotation in the plane (x, y) and uniform translations in the z direction (i.e., the direction parallel to the homogeneous magnetic field).

Remark 12.4.5. A detailed verification of the spectral properties of the above magnetic Schrödinger operator H_3 in $\mathbb{R}^3$ involves the concept of *tensor products* [ReeS81]. Think of a small challenging project: consider a Fourier transform in the variables x and z, and follow the proof of Proposition 11.1.1 as a starting way to check the missing technical details with respect to the spectrum of H_3.

Exercise 12.4.6. Consider the operator $(-id/dx - eA(x)/c)^2$ in $\mathbb{R}$, with a continuous function A. If $\chi(x) = -\int_0^x A(s)\,ds$, verify that

$$e^{ie\chi/c}\left(-i\frac{d}{dx} - eA(x)/c\right)^2 e^{-ie\chi/c} = -\frac{d^2}{dx^2},$$

that is, the "vector potential A can be removed by a gauge transformation." This is interpreted as absence of magnetic phenomena in $\mathbb{R}$ – see also Example 12.4.8.

Exercise 12.4.7. Use the construction in Exercise 12.4.6 to present another solution to Exercise 12.3.18 (that is, select a proper gauge).

Example 12.4.8. Although magnetic phenomena are absent in $\mathbb{R}$, it is present in the unit circumference $S^1 = \{(x, y) \in \mathbb{R}^2 : x^2 + y^2 = 1\}$, which is also a one-dimensional system. The simplest case is a constant magnetic vector potential A (think of a restriction to S^1 of a radial vector potential $\mathbf{A}(x, y) = \mathbf{A}(r)$, $r = \sqrt{x^2 + y^2}$). If φ is the polar angle that parametrizes S^1, $0 \le \varphi \le 2\pi$, the Schrödinger operator is the unique self-adjoint extension of (set $A = \mathbf{A}(1)$)

$$H = \left(-i\frac{d}{d\varphi} - \frac{e}{c}A\right)^2, \qquad \text{dom } H = C^\infty(S^1).$$

This operator is essentially self-adjoint since $e_m(\varphi) = e^{im\varphi}$, $m \in \mathbb{Z}$, form an orthogonal basis of $\mathrm{L}^2(S^1)$ and $He_m = (m - eA/c)^2 e_m$ (see Theorem 2.2.10).

The effect of A can be measured in the eigenvalues; if $0 \le eA/c \le 1/2$ the *ground state* (i.e., the lowest eigenvalue) is $(eA/c)^2$ which has multiplicity 1 except for $A = c/(2e)$, where the multiplicity is 2. What is the ground state for general $A \in \mathbb{R}$?

Example 12.4.9. It is possible to have a purely point spectrum in case of planar magnetic fields that vanish at infinity. This can be illustrated by the vector potential (set $r = \sqrt{x^2 + y^2}$)

$$\mathbf{A} = \left(\frac{y}{(1+r)^\gamma}, \frac{-x}{(1+r)^\gamma} \right), \qquad 0 < \gamma < 1,$$

so that the subsequent Schrödinger operator is

$$H = \left(-i\frac{\partial}{\partial x} - \frac{y}{(1+r)^\gamma} \right)^2 + \left(-i\frac{\partial}{\partial y} + \frac{x}{(1+r)^\gamma} \right)^2 .$$

It will be argued that H, with domain $C_0^\infty(\mathbb{R}^2)$, is essentially self-adjoint and its unique self-adjoint extension is pure point. The magnetic field intensity is

$$B(x,y) = B(r) = \frac{2}{(1+r)^\gamma} + \frac{r}{(1+r)^{1+\gamma}},$$

and clearly $\lim_{r\to\infty} B(r) = 0$.

By passing to polar coordinates (r, φ) and expanding H one gets

$$H = H_0 + \frac{r^2}{(1+r)^{2\gamma}} + \frac{2}{(1+r)^\gamma} L,$$

where $H_0 = -\Delta$ is the usual free hamiltonian and

$$L = -i\frac{\partial}{\partial \varphi} = -i(x\partial/\partial y - y\partial/\partial x).$$

Consider the realization of L with periodic boundary conditions (similar to Example 2.6.5 with $\alpha = 1$), so that it is self-adjoint with discrete spectrum $\sigma(L) = \mathbb{Z}$ (see Section 7.5), and eigenfunctions $e_m(\varphi) = e^{im\varphi}$, $m \in \mathbb{Z}$.

Restricted to the subspace spanned by $e_m(\varphi)$, which is invariant under H, one obtains the operator

$$H_m = H_0 + \frac{r^2}{(1+r)^{2\gamma}} + \frac{2m}{(1+r)^\gamma} = H_0 + V_m(r),$$

which is a Schrödinger operator with effective potential $V_m(r)$ (and $H = \oplus_m H_m$). Since $V_m \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^2)$ and is lower bounded with $\lim_{r\to\infty} V_m(r) = \infty$, Theorem 11.5.6 implies H_m is essentially self-adjoint and with discrete spectrum, for all m. Therefore, H is essentially self-adjoint (with $\operatorname{dom} H = C_0^\infty(\mathbb{R})$) and its closure $\overline{H}$ has purely point spectrum by Proposition 11.1.2. Other values of γ give different spectral properties, as discussed in [MiS80].

12.4.1 Magnetic Resolvent Convergence

In this subsection, the convergence of H with a homogeneous magnetic field $\mathbf{B}$ to H_0, as $\mathbf{B} \to 0$, will be discussed; then the limit of very intense vector potentials.

Theorem 12.4.10. *Let* $\mathbf{A}$ *be a vector potential in* $\mathbb{R}^2$ *corresponding to a homogeneous magnetic field of intensity* B*; denote* $H(B) = H(\mathbf{A})$ *and* $H_0 = H(0) = -\Delta$*. Then, as* $B \to 0$*:*

i) $H(B) \xrightarrow{\text{SR}} H_0$.
ii) $H(B)$ *does not converge to* H_0 *in the norm resolvent sense.*

Proof. Fix the gauge $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{x}$, so that

$$H(B) = H_0 + \frac{B^2}{4}(x^2 + y^2) - BL,$$

L as in Example 12.4.9.

i) Recall that $\mathcal{S}(\mathbb{R}^2)$ is a core of both $H(B)$ and H_0. If $\psi \in \mathcal{S}(\mathbb{R}^2)$, then a direct computation leads to $\|H(B)\psi - H_0\psi\| \to 0$ as $B \to 0$, and so Proposition 10.1.18 implies $H(B) \xrightarrow{\text{SR}} H_0$.

ii) Restricted to the subspace spanned by $e_m(\varphi) = e^{im\varphi}$, which is invariant under both $H(B)$ and H_0, one obtains the operator

$$H(B)|_m = H_0|_m + \frac{B^2}{4}(x^2 + y^2) - Bm,$$

which is a standard Schrödinger operator with effective potential

$$V_m(B; x, y) = \frac{B^2}{4}(x^2 + y^2) - Bm.$$

For $B \neq 0$ this operator has compact resolvent (see Theorem 11.5.6), while for $B = 0$ it is purely absolutely continuous (Corollary 12.3.3) and so its resolvent is not compact. Hence, by Theorem 1.3.13, $R_i(H(B))$ does not converge in norm to $R_i(H_0)$ as $B \to 0$. □

Exercise 12.4.11. Let $V(x)$ be a real polynomial in $\mathbb{R}^n$ with $\lim_{|x|\to\infty} V(x) = \infty$ and $H(\lambda)$, $\lambda > 0$, the unique self-adjoint extension of $H_0 + \lambda V$; see Example 11.5.8. Show that, $H(\lambda) \xrightarrow{\text{SR}} H_0$ as $\lambda \downarrow 0$, but does not converge in the norm resolvent sense. A particular case is the unidimensional harmonic oscillator $V(x) = x^2/2$.

The next result discusses the limit of very intense vector potentials. Rather unexpected, in case of intense homogeneous vector potentials the hamiltonian converges to the zero operator in the strong resolvent sense, even though they lead to zero magnetic fields! Since through a gauge transformation such homogeneous vector potentials can be put to zero, the "correct gauge choices" are still left to be investigated; see discussions in [HemH95].

Proposition 12.4.12. *For a homogeneous* $\mathbf{A} \neq 0$ *in* $\mathbb{R}^3$ *and* $\lambda \in \mathbb{R}$, *write* $H(\lambda\mathbf{A}) = (-i\nabla - \lambda\mathbf{A})^2$. *Then* $H(\lambda\mathbf{A}) \xrightarrow{\text{SR}} 0$ *as* $\lambda \to \infty$.

Proof. The resolvent of the zero operator at -1 is $R_{-1}(0) = \mathbf{1}$. For $\psi \in C_0^\infty(\mathbb{R}^3)$,

$$\|R_{-1}(H(\lambda\mathbf{A}))\psi - \mathbf{1}\psi\| \leq \left\|R_{-1}(H(\lambda\mathbf{A}))\psi - \left((\lambda\mathbf{A})^2 + 1\right)^{-1}\psi\right\| + \left\|\left((\lambda\mathbf{A})^2 + 1\right)^{-1}\psi - \psi\right\|,$$

and the second term on the right-hand side vanishes as $\lambda \to \infty$. By expanding the square in $H(\lambda\mathbf{A})$, using the second resolvent identity and taking into account that $\mathbf{A}$ is homogeneous, the first term gets the expression

$$R_{-1}(H(\lambda\mathbf{A}))\psi - \left((\lambda\mathbf{A})^2 + 1\right)^{-1}\psi = \frac{(-\Delta\psi - 2\lambda\mathbf{A}\cdot\nabla\psi)}{(\lambda\mathbf{A})^2 + 1}$$

which also vanishes in the Hilbert space as $\lambda \to \infty$.

Hence $\|R_{-1}(H(\lambda\mathbf{A}))\psi - \mathbf{1}\psi\| \to 0$ as $\lambda \to \infty$ in $C_0^\infty(\mathbb{R}^3)$; since this subspace is dense in $\mathrm{L}^2(\mathbb{R}^3)$ and the involved operators form a uniformly bounded family, the proposition is proved. □

Exercise 12.4.13. If $\mathbf{A}$ is homogeneous, find a gauge transformation so that the new vector potential is null. Based on Proposition 12.4.12, conclude that the strong resolvent convergence for operators with vector potentials is not "well behaved" under unitary transformations performed through gauge transformations.

Remark 12.4.14. In higher dimensions $\mathbb{R}^n$, $n > 3$, it is convenient to define the vector potential as the one-form

$$\mathbf{A} = \sum_{j=1}^{n} A_j(x)\, dx_j,$$

and the magnetic field is then defined by the two-form

$$\mathbf{B} = d\mathbf{A} = \sum_{j<k} (\partial_j A_k - \partial_k A_j)\, dx_j \wedge dx_k.$$

Clearly this also works for $n = 2, 3$.

Remark 12.4.15. An important result, first proved in [AvHS78], states that if the lower bounded potential V is such that $H(0) + V$ is purely discrete, then $H = H(\mathbf{A}) + V$ has also purely discrete spectrum for quite general vector potentials $\mathbf{A}$.

12.5 Weyl-von Neumann Theorem

A consequence of the Weyl-von Neumann theorem, presented in this section, is that any operator with purely continuous spectrum can be (in some sense) approximated by operators with purely point spectrum. More precisely, the original operator is perturbed by arbitrarily small Hilbert-Schmidt operators and the resulting operators have point spectra dense in the continuous spectrum of the unperturbed one. Such a result – and the wonderland theorem in Section 12.6 – gives an indication of how intricate perturbations of continuous spectra can be.

Exercise 12.5.1. In case of strong convergence of bounded operators there is a somewhat direct argument to get some approximations by purely point operators. Let $T \in \mathrm{B}(\mathcal{H})$ be self-adjoint with $\sigma(T) = [-\|T\|, \|T\|]$, $\{\xi_j\}$ an orthonormal basis of $\mathcal{H}$ and P_n the orthogonal projection onto $\mathrm{Lin}(\{\xi_1, \ldots, \xi_n\})$. If $\{q_j\}$ is the set of rational numbers in $[-\|T\|, \|T\|]$, define the self-adjoint operator $S \in \mathrm{B}(\mathcal{H})$ by $S\xi_j = q_j \xi_j$, for all j. Finally, write

$$T_n := P_n T P_n + (\mathbf{1} - P_n) S (\mathbf{1} - P_n).$$

Show that T_n is self-adjoint with purely point spectrum $\sigma_{\mathrm{p}}(T_n) = [-\|T\|, \|T\|]$, and $T_n \xrightarrow{\mathrm{s}} T$. Generalize to the case $\sigma(T) \subset [-\|T\|, \|T\|]$.

If S is a self-adjoint Hilbert-Schmidt operator (see Section 1.4), its normalized eigenvectors $\{\xi_j\}_j$, $S\xi_j = \lambda_j \xi_j$, can be taken as an orthonormal basis of $\mathcal{H}$ and consequently its HS-norm is given by

$$\|S\|_{\mathrm{HS}} = \left(\sum_j |\lambda_j|^2 \right)^{\frac{1}{2}}.$$

Recall Theorem 1.4.6, that is, $\mathrm{HS}(\mathcal{H}) \subset \mathrm{B}_0(\mathcal{H})$.

Theorem 12.5.2 (Weyl-von Neumann). *Let T be self-adjoint. For any $\varepsilon > 0$ there exists a self-adjoint Hilbert-Schmidt operator S, with $\|S\|_{\mathrm{HS}} < \varepsilon$, so that $T + S$ has purely point spectrum.*

If T has purely continuous spectrum, then $\sigma(T)$ has no isolated points and, since S in Theorem 12.5.2 is compact, the invariance of the essential spectrum implies that $\sigma(T) \subset \sigma(T + S)$ (see Corollary 11.3.7) and the spectrum of $T + S$ is pure point. For instance, if H_0 denotes the free hamiltonian in $\mathbb{R}^n$, it is known that it has purely absolutely continuous spectrum and $\sigma_{\mathrm{ac}}(H_0) = [0, \infty)$; then, by the Weyl-von Neumann theorem, for any $\varepsilon > 0$, there is a self-adjoint operator $B \in \mathrm{HS}(\mathrm{L}^2(\mathbb{R}^n))$ with $\|B\|_{\mathrm{HS}} < \varepsilon$ and $H_0 + B$ is pure point, hence a subset of its eigenvalues is dense in $[0, \infty)$.

Now a preliminary result for the proof of the Weyl-von Neumann theorem.

Lemma 12.5.3. *Let T be self-adjoint. For any $\xi \in \mathcal{H}$ and $\varepsilon > 0$, there exist a finite-dimensional subspace $E \subset \mathcal{H}$ and a self-adjoint Hilbert-Schmidt operator S so that $\|S\|_{\mathrm{HS}} < \varepsilon$, $\|(\mathbf{1} - P_E)\xi\| < \varepsilon$ and E reduces $T + S$.*

Proof. [**Theorem 12.5.2**] The idea is to use Lemma 12.5.3 to find finite-dimensional subspaces E_j that reduce $T + S$ and so that $\mathcal{H} = \oplus_j E_j$. Since the restrictions $(T + S)|_{E_j}$ are pure point, the result follows.

First fix some notations: if E_n is a closed subspace of $\mathcal{H}$, P_n will denote the corresponding orthogonal projection, $P_n^\perp = \mathbf{1} - P_n$; so if $E_n \perp E_m$, then $(P_n + P_m)^\perp = \mathbf{1} - (P_n + P_m)$.

Pick $\varepsilon > 0$. Let $\{\xi_j\}$ be a dense set in $\mathcal{H}$ and put $\mathcal{H}_1 = \mathcal{H}$. Apply Lemma 12.5.3 to $T, \xi_1, \mathcal{H}_1, \varepsilon/2^1$, then resulting in $E_1 \subset \mathcal{H}_1$, $S_1 \in \mathrm{HS}(\mathcal{H}_1)$ so that $\|S_1\|_{\mathrm{HS}} < \varepsilon/2^1$, $\|P_1^\perp \xi_1\| < \varepsilon/2^1$ and E_1 reduces $T + S_1$. Write $\mathcal{H}_2 = P_1^\perp \mathcal{H}$.

Now apply Lemma 12.5.3 to $T + S_1, P_1^\perp \xi_2, \mathcal{H}_2, \varepsilon/2^2$, then resulting in $E_2 \subset \mathcal{H}_2$, $S_2 \in \mathrm{HS}(\mathcal{H}_2)$, and extend S_2 and P_2 by zero to $\mathcal{H}$, so that $\|S_2\|_{\mathrm{HS}} < \varepsilon/2^2$, $\|P_2^\perp P_1^\perp \xi_2\| = \|(P_1 + P_2)^\perp \xi_2\| < \varepsilon/2^2$ and both E_1 and E_2 reduce $T + S_1 + S_2$ (note that $E_1 \perp E_2$). Denote $\mathcal{H}_3 = (P_1 + P_2)^\perp \mathcal{H}$.

After constructing E_{n-1}, $\mathcal{H}_n = (P_1 + \cdots + P_{n-1})^\perp \mathcal{H}$ and S_{n-1}, the nth step is an application of Lemma 12.5.3 to

$$T + S_1 + \cdots + S_{n-1}, (P_1 + \cdots + P_{n-1})^\perp \xi_n, \mathcal{H}_n, \varepsilon/2^n,$$

then resulting in $E_n \subset \mathcal{H}_n$, $S_n \in \mathrm{HS}(\mathcal{H}_n)$. Extend S_n and P_n by zero to $\mathcal{H}$, so that $\|S_n\|_{\mathrm{HS}} < \varepsilon/2^n$, $\|(P_1 + \cdots + P_n)^\perp \xi_n\| < \varepsilon/2^n$ and all the subspaces $E_1, \ldots, E_n$ reduce $T + S_1 + \cdots + S_n$.

One has $E_j = P_j \mathcal{H}$ and $\mathcal{H} = \oplus_j E_j$, which is equivalent to the strong limit $\sum_j P_j = \mathbf{1}$. In order to check this, let $\eta \in \mathcal{H}$ and pick ξ_n with $\|\eta - \xi_n\| < \varepsilon/2^n$ (recall that $\{\xi_j\}$ is dense in $\mathcal{H}$); thus

$$\begin{aligned}
\|\eta - (P_1 + \cdots + P_n)\eta\| &= \|(P_1 \cdots + P_n)^\perp \eta\| \\
&\le \|(P_1 \cdots + P_n)^\perp (\eta - \xi_n)\| + \|(P_1 \cdots + P_n)^\perp \xi_n\| \\
&< \|\eta - \xi_n\| + \frac{\varepsilon}{2^n} < \frac{\varepsilon}{2^{n-1}}.
\end{aligned}$$

This implies $\eta = \sum_j P_j \eta$, as required.

Define $S := \sum_j S_j$, which is convergent in $\mathrm{HS}(\mathcal{H})$ since (S_j) is a Cauchy sequence in this space (exercise for the reader), so S is also Hilbert-Schmidt and $\|S\|_{\mathrm{HS}} \le \sum_j \|S_j\|_{\mathrm{HS}} < \varepsilon$.

Assume that each $E_j = P_j \mathcal{H}$ reduces $T + S$. Since E_j is finite dimensional, the spectrum of $T + S$ restricted to E_j is pure point, and since $\mathcal{H} = \oplus_j E_j$ the eigenvectors of $T + S$ can be arranged in order to form an orthonormal basis of $\mathcal{H}$. Hence $T + S$ is pure point.

To see that E_j reduces $T + S$, note that E_j is a finite-dimensional subspace of $(P_1 + \cdots + P_{j-1})^\perp \mathcal{H}$ which reduces $T + S_1 + \cdots + S_j$, and in this setting it amounts to $P_j(T + S_1 + \cdots + S_j)P_j = (T + S_1 + \cdots + S_j)P_j$. Since $S = \sum_n S_n$ and $P_j S_n = 0 = S_n P_j$ for $n > j$, it follows that $P_j(T + S)P_j = (T + S)P_j$ and so E_j reduces $T + S$. □

Lemma 12.5.4. *If $S \in \mathrm{B_f}(\mathcal{H})$ is a self-adjoint finite rank operator, of rank m, then $\|S\|_{\mathrm{HS}} \le \sqrt{m}\, \|S\|$.*

Proof. Let $\lambda_1, \dots, \lambda_m$ be the nonzero eigenvalues of S and

$$t = \max\{|\lambda_1|, \dots, |\lambda_m|\}.$$

By Proposition 2.1.12, its spectral radius $r_\sigma(S) = \|S\| = t$. Hence

$$\|S\|^2 = t^2 = \sum_{j=1}^{m} \frac{t^2}{m} \geq \sum_{j=1}^{m} \frac{|\lambda_j|^2}{m} = \frac{1}{m}\|S\|_{\mathrm{HS}}^2,$$

and the result follows. □

Proof. **[Lemma 12.5.3]** Given $\xi \in \mathcal{H}$ and $\varepsilon > 0$, take $a > 0$ so that

$$\|\xi - \chi_{[-a,a)}(T)\xi\| < \varepsilon.$$

For $n \in \mathbb{N}$ set (some dependences on n will be kept implicit)

$$\Omega_j = \left[\left(\frac{2(j-1)}{n} - 1\right) a, \left(\frac{2j}{n} - 1\right) a\right), \qquad j = 1, 2, \dots, n,$$

and $E_j = \operatorname{rng} \chi_{\Omega_j}(T)$.

If $\chi_{\Omega_j}(T)\xi \neq 0$, set $\eta_j = \chi_{\Omega_j}(T)\xi / \|\chi_{\Omega_j}(T)\xi\|$; such η_j constitute an orthonormal set and let $E := \operatorname{Lin}(\{\eta_1, \dots, \eta_n\})$, with $\eta_j = 0$ in case $\chi_{\Omega_j}(T)\xi = 0$. For simplicity, from now on it is assumed that all $\eta_j \neq 0$, and note that E does not necessarily coincide with the subspace spanned by the set of all E_j. Thus

$$0 = (\mathbf{1} - P_E) \sum_{j=1}^{n} \|\chi_{\Omega_j}(T)\xi\| \eta_j = (\mathbf{1} - P_E)\chi_{[-a,a)}(T)\xi$$

and so, since $\|\mathbf{1} - P_E\| \leq 1$,

$$\begin{aligned} \|(\mathbf{1} - P_E)\xi\| &= \left\|(\mathbf{1} - P_E)\left(\mathbf{1} - \chi_{[-a,a)}(T)\right)\xi\right\| \\ &\leq \left\|\left(\mathbf{1} - \chi_{[-a,a)}(T)\right)\xi\right\| < \varepsilon. \end{aligned}$$

This last step is fundamental, since it shows that in the relation $\|\xi - \chi_{[-a,a)}(T)\xi\| < \varepsilon$ the operator $\chi_{[-a,a)}(T)$ "can be replaced" by a finite-dimensional projection P_E.

Now introduce the self-adjoint operator

$$S := -(\mathbf{1} - P_E)TP_E - P_E T(\mathbf{1} - P_E)$$

of rank n, and note that

$$\begin{aligned} T &= (\mathbf{1} - P_E + P_E)T(\mathbf{1} - P_E + P_E) \\ &= P_E T P_E + (\mathbf{1} - P_E)T(\mathbf{1} - P_E) - S. \end{aligned}$$

The term $P_E T P_E + (\mathbf{1} - P_E)T(\mathbf{1} - P_E)$ is reduced by E, and so is $T + S$. To finish the proof it will be shown that, for n large enough, $\|S\|_{\mathrm{HS}} < \varepsilon$.

The following facts will be used:

1. For any $t \in \Omega_j$, by the spectral theorem,

$$\|(T - t\mathbf{1})\eta_j\|^2 = \int_{\Omega_j} |x-t|^2 \, d\mu^T_{\eta_j}(x) \leq \left(\frac{2a}{n}\right)^2.$$

2. In view of $(\mathbf{1} - P_E)\eta_j = 0$, one has,

$$\begin{aligned}\|(\mathbf{1} - P_E)T\eta_j\| &= \|(\mathbf{1} - P_E)(T - t\mathbf{1})\eta_j\| \\ &\leq \|(T - t\mathbf{1})\eta_j\| \leq \frac{2a}{n}, \qquad \forall t \in \Omega_j.\end{aligned}$$

3. For $j \neq k$, $\langle (\mathbf{1} - P_E)T\eta_j, (\mathbf{1} - P_E)T\eta_k\rangle = 0$. In fact, since $E_j \perp E_k$, $j \neq k$, E_j reduces T and $T\eta_j \in E_j$, $\forall j$, it follows that $(\mathbf{1} - P_E)T\eta_j \in E_j$, and so this orthogonality follows.

Now, for any $\eta \in \mathcal{H}$, $P_E\eta = \sum_j \langle \eta_j, \eta\rangle\, \eta_j$, by 3 and 2 above, and then Bessel inequality,

$$\begin{aligned}\|(\mathbf{1} - P_E)TP_E\eta\|^2 &= \left\|\sum\nolimits_j \langle \eta_j, \eta\rangle (\mathbf{1} - P_E)T\eta_j\right\|^2 \\ &= \sum\nolimits_j |\langle \eta_j, \eta\rangle|^2 \, \|(\mathbf{1} - P_E)T\eta_j\|^2 \leq \frac{4a^2}{n^2}\|\eta\|^2,\end{aligned}$$

i.e., $\|(\mathbf{1} - P_E)TP_E\| \leq 2a/n$. By Lemma 12.5.4,

$$\|(\mathbf{1} - P_E)TP_E\|_{\mathrm{HS}} \leq \sqrt{n}\, \|(\mathbf{1} - P_E)TP_E\| \leq \frac{2a}{\sqrt{n}}.$$

Since $P_ET(\mathbf{1} - P_E) = ((\mathbf{1} - P_E)TP_E)^*$ and this operator is also of rank n, one has $\|P_ET(\mathbf{1} - P_E)\|_{\mathrm{HS}} \leq 2a/\sqrt{n}$. Hence, by choosing n large enough, the very definition of S and triangle inequality imply that $\|S\|_{\mathrm{HS}} \leq 4a/\sqrt{n} < \varepsilon$. ☐

Remark 12.5.5. Theorem 12.5.2 can be generalized by considering the so-called p-Schatten norm [Scha60]

$$\|S\|_p = \left(\sum_j |\varpi_j(S)|^p\right)^{\frac{1}{p}}, \qquad 1 < p < \infty,$$

where $\varpi_j(S)$ are the singular numbers of S (see Subsection 9.4.1). $p = 1$, the trace-norm, must in fact be excluded by the Kato-Rosenblum Theorem 12.3.29. Kuroda has shown that this theorem holds if the Hilbert-Schmidt norm is replaced by any cross-norm not equivalent to the trace-norm [Ku58].

Exercise 12.5.6. If S is a self-adjoint finite rank operator, of rank m, generalize Lemma 12.5.4 by showing that $\|S\|_p \leq m^{\frac{1}{p}}\|S\|$. With such information, is it possible to replace the Hilbert-Schmidt norm by $\|\cdot\|_p$, $p > 1$, in the Weyl-von Neumann Theorem? What about $p = 1$?

12.6 Wonderland Theorem

This is an existential result due to B. Simon who named it "wonderland" [Sim95]. Given a complete metric space (X, d) of self-adjoint operators, acting in the separable Hilbert space $\mathcal{H}$, under certain conditions it guarantees that operators in X whose spectrum is purely singular continuous is *generic*, that is, a dense G_δ set (recall that a set is a G_δ if it is the countable intersection of open sets). So, on the basis of the Baire category theorem, there is a strong indication that in some situations such kind of spectrum is not a pathology, as it was usually considered in the 1960s and 1970s. At that time a singular continuous spectrum was also "undesirable" in the mathematical theory of quantum mechanics.

The proof relies on two technical results (that is, Propositions 12.6.1 and 12.6.2) that have independent interest; although the proof of one of them (a version that appeared in [DeBF98]) will make use of a result of Chapter 13, it seems that here is the right place for presenting this set of results.

To be more precise, in this section (X, d) is assumed to be a complete metric space of self-adjoint operators, acting in the infinite-dimensional Hilbert space $\mathcal{H}$, such that metric d convergence implies strong resolvent convergence.

Proposition 12.6.1. *The set $Y := \{T \in X : \sigma_{\mathrm{p}}(T) = \emptyset\}$ is a G_δ in X.*

Proof. Given a self-adjoint operator $T : \operatorname{dom} T \sqsubseteq \mathcal{H} \to \mathcal{H}$, denote the average return probability

$$\left\langle p_\xi^T \right\rangle(t) = \frac{1}{t} \int_0^t \left|\left\langle \xi, e^{-isT}\xi \right\rangle\right|^2 ds, \qquad \xi \in \mathcal{H}.$$

By Theorem 10.1.15, strong resolvent convergence is equivalent to strong dynamical convergence, so for each $\xi \in \mathcal{H}$, $t > 0$, the map $X \ni T \mapsto \left\langle p_\xi^T \right\rangle(t)$ is continuous and $\{T \in X : \langle p_\xi^T\rangle(t) < 1/n\}$ is an open set in X.

Let $(\xi_j)_{j\geq 1}$ be an orthonormal basis of $\mathcal{H}$. By Theorem 13.3.7, $\sigma_{\mathrm{p}}(T) = \emptyset$ iff $\lim_{t\to\infty} \langle p_{\xi_j}^T\rangle(t) = 0$ for each ξ_j (the limit does exist). Since

$$Y = \bigcap_{j,n\in\mathbb{N}} \bigcap_{t\in\mathbb{N}} \left\{T \in X : \left\langle p_{\xi_j}^T \right\rangle(t) < 1/n \right\},$$

it follows that Y is a G_δ. □

Proposition 12.6.2. *The set $W := \{T \in X : \sigma_{\mathrm{ac}}(T) = \emptyset\}$ is a G_δ in X.*

Lemma 12.6.3. *A finite (positive) Borel measure $0 \neq \mu$ in $\mathbb{R}$ and Lebesgue measure ℓ are mutually singular (in symbols $\mu \perp \ell$) iff there exists a sequence of continuous functions $f_n : \mathbb{R} \to [0, 1]$, $n \geq 1$, so that*

$$\text{i)} \int_{\mathbb{R}} f_n \, d\ell < \frac{1}{2^n} \qquad \textit{and} \qquad \text{ii)} \int_{\mathbb{R}} f_n \, d\mu > \mu(\mathbb{R}) - \frac{1}{2^n}.$$

Proof. Assume that such a sequence of continuous functions exists. Put $C_n = \{x \in \mathbb{R} : f_n(x) > 1/2\}$. Thus

$$\ell(C_n) = 2\int_{C_n} \frac{1}{2} d\ell \le 2\int_{\mathbb{R}} f_n\, d\ell \overset{\text{i)}}{<} \frac{1}{2^{n-1}};$$

so $\ell(C_n) < 2^{-(n-1)}$ and

$$\begin{aligned}\mu(\mathbb{R}\setminus C_n) &= \mu(\mathbb{R}\setminus C_n) - \int_{\mathbb{R}\setminus C_n} f_n\, d\mu + \int_{\mathbb{R}\setminus C_n} f_n\, d\mu \\ &= \int_{\mathbb{R}\setminus C_n} (1-f_n)\, d\mu + \int_{\mathbb{R}\setminus C_n} f_n\, d\mu \\ &\overset{\text{ii)}}{<} \frac{1}{2^n} + \frac{\mu(\mathbb{R}\setminus C_n)}{2},\end{aligned}$$

hence $\mu(\mathbb{R}\setminus C_n) < 2^{-(n-1)}$. Set $C = \cap_{m\ge 1} \cup_{n\ge m} C_n$ so that $\mathbb{R}\setminus C = \cup_{m\ge 1} \cap_{n\ge m} (\mathbb{R}\setminus C_n)$. Since $(\cup_{n\ge m} C_n)_m$ is a nonincreasing sequence and $\ell(\cup_{n\ge 1} C_n) < \infty$, one has

$$\ell(C) = \lim_{m\to\infty} \ell(\cup_{n\ge m} C_n) \le \lim_{m\to\infty} \sum_{n\ge m} \frac{1}{2^{n-1}} = 0,$$

while

$$\mu\left(\cap_{n\ge m}(\mathbb{R}\setminus C_n)\right) \le \lim_{m\to\infty} \mu(\mathbb{R}\setminus C_m) = \lim_{m\to\infty} \frac{1}{2^{m-1}} = 0,$$

so that $\mu(\mathbb{R}\setminus C) = 0$; this shows that $C \ne \emptyset$ and, together with $\ell(C) = 0$, also that $\mu \perp \ell$.

Assume now that $\mu \perp \ell$, that is, there is a Borel set $C \subset \mathbb{R}$ with $\ell(C) = 0$ and $\mu(\mathbb{R}\setminus C) = 0$. Since such measures are regular, there exist sequences of compact sets $(K_n)_{n\ge 1}$ and open sets $(O_n)_{n\ge 1}$ with

$$K_n \subset C \subset O_n, \qquad \ell(O_n) < \frac{1}{2^n} \qquad \text{and} \qquad \mu(\mathbb{R}\setminus K_n) < \frac{1}{2^n}.$$

By the Uryshon lemma, there exists a sequence of continuous functions $f_n : \mathbb{R} \to [0,1]$ with $f_n(x) = 1$, $\forall x \in K_n$ and $f_n(x) = 0$ for all $x \in \mathbb{R}\setminus O_n$. Thus

$$\int_{\mathbb{R}} f_n\, d\ell \le \ell(O_n) < \frac{1}{2^n} \qquad \text{and} \qquad \int_{\mathbb{R}} (1-f_n)\, d\mu < \mu(\mathbb{R}\setminus K_n) < \frac{1}{2^n}.$$

Therefore i) and ii) hold. □

Proof. **[Proposition 12.6.2]** For $\xi \in \mathcal{H}$ set $Q(\xi) := \{T \in X : \mu_\xi^T \perp \ell\}$. If $f : \mathbb{R} \to [0,1]$ is continuous, write

$$\mathcal{U}_n(f,\xi) := \left\{ T \in X : \langle \xi, (\mathbf{1} - f(T))\xi\rangle = \mu_\xi^T(\mathbb{R}) - \int_{\mathbb{R}} f\, d\mu_\xi^T < \frac{1}{2^n} \right\};$$

finally denote by D_n the set of continuous $f : \mathbb{R} \to [0,1]$ with $\int_{\mathbb{R}} f\, d\ell < 2^{-n}$.

By Lemma 12.6.3,

$$Q(\xi) = \bigcap_{n\geq 2} \bigcup_{f\in D_n} \mathcal{U}_n(f,\xi)$$

and if $(\xi_j)_{j\geq 1}$ is an orthonormal basis of $\mathcal{H}$ one has $W = \cap_j Q(\xi_j)$. To complete the proof it will suffice to verify that given $\xi \in \mathcal{H}$ the set $\mathcal{U}_n(f,\xi)$ is open, $\forall n$, which is equivalent to show that the complement of $\mathcal{U}_n(f,\xi)$, i.e.,

$$\mathcal{U}_n(f,\xi)^c = \left\{ T \in X : \langle \xi, (\mathbf{1} - f(T))\xi\rangle \geq \frac{1}{2^n} \right\},$$

is a closed set for any $f \in D_n$.

Let T_k be a sequence in $\mathcal{U}_n(f,\xi)^c$ with $T_k \to T$ in X. By hypothesis $T_k \xrightarrow{\text{SR}} T$ and, by Proposition 10.1.9, $f(T_k) \xrightarrow{\text{s}} f(T)$ for all $f \in D_n$. Since the inner product is continuous

$$\frac{1}{2^n} \leq \langle \xi, (\mathbf{1} - f(T_k))\xi\rangle \longrightarrow \langle \xi, (\mathbf{1} - f(T))\xi\rangle$$

so that $T \in \mathcal{U}_n(f,\xi)^c$, that is, $\mathcal{U}_n(f,\xi)^c$ is closed. □

Theorem 12.6.4 (Wonderland). *Let (X,d) be as before. If both sets*

- *C_{p} of $T \in X$ with purely point spectrum, and*
- *C_{ac} of $T \in X$ with purely absolutely continuous spectrum,*

are dense in X, then the set C_{sc} of $T \in X$ with purely singular continuous spectrum is generic in X.

Proof. Since $C_{\mathrm{p}} \subset W$, by Proposition 12.6.2, W is generic. Since $C_{\mathrm{ac}} \subset Y$, by Proposition 12.6.1, Y is generic. Now it is enough to observe that $C_{\mathrm{sc}} = Y \cap W$, which is also generic (by the Baire theorem a countable intersection of generic sets is also generic). □

In applications one has to prove the presence of operators with purely point and purely absolutely continuous spectra in dense sets. Sometimes the Weyl-von Neumann theorem can be used to get purely point operators, and the absolutely continuous ones by some kind of periodicity ("periodic operators" have a tendency to absolutely continuous spectrum; see [ReeS78]) or other techniques not discussed in this text. For interesting applications of the wonderland theorem the reader is referred to the original paper [Sim95].

Example 12.6.5. Just as an illustration, consider the operator

$$T_V(\alpha)\psi := -i\alpha\frac{\partial}{\partial x}\psi - i\frac{\partial}{\partial y}\psi + V(x,y)\psi, \qquad \psi \in \mathrm{dom}\ T_V(\alpha),$$

discussed in Example 12.2.8. Fix V of class C^r with r large enough and $\sigma > 2$, and consider $T_V(\alpha)$ as function of the real parameter α. This forms a complete metric space $X(V)$ with distance $d(T_V(\alpha), T_V(\beta)) := |\alpha-\beta|$. Since dom $T_V(\alpha) = \mathcal{H}^1(\mathcal{T}^2)$, $\forall\alpha$,

$$\|T_V(\alpha)\psi - T_V(\beta)\psi\| = |\alpha - \beta| \, \|\partial\psi/\partial x\|,$$

by Proposition 10.1.18, it follows that convergence in the metric d implies convergence in the strong resolvent sense in $X(V)$.

By Corollary 12.2.11, $T_V(\alpha)$ is purely point in a dense set of parameters α; on the other hand, it is shown in [GeH97] (see also [Bell85]) that for a large set of choices of V (under the above conditions) the operator $T_V(\alpha)$ has a purely absolutely continuous spectrum iff $\alpha \in \mathbb{Q}$, so for a dense set of operators. Hence, for each V in a "large set," the wonderland theorem ensures the presence of purely singular continuous spectrum for a generic set of $T_V(\alpha)$'s in $X(V)$ (another argument appears in [deO93]).

Example 12.6.6. Fix $\mathcal{H}$ and let X_{01} be the subset of $\mathrm{B}(\mathcal{H})$ of self-adjoint operators T with $\sigma(T) = [0,1]$. It will be argued that the set of operators with purely singular continuous spectrum is generic in X_{01}.

Exercise 12.6.7. Based on Proposition 10.2.4 and Exercise 10.1.14, show that X_{01} is a closed subset of $\mathrm{B}(\mathcal{H})$. Conclude that it is a complete metric space with distance $d(T,S) = \|T - S\|$, $T, S \in X_{01}$, which implies convergence in the strong resolvent sense.

Given $T \in X_{01}$ and $\varepsilon > 0$, by the Weyl-von Neumann theorem there is $T_1 \in \mathrm{HS}(\mathcal{H})$ so that $T+T_1$ has purely point spectrum and $\|T_1\| \le \|T_1\|_{\mathrm{HS}} < \varepsilon$. Although $T+T_1$ may have eigenvalues in $(-\varepsilon, 0) \cup (1, 1+\varepsilon)$, one changes such eigenvalues to 0 or 1 by adding a self-adjoint operator T_2 with $\|T_2\| < \varepsilon$. Hence $T+T_1+T_2 \in X_{01}$ has purely point spectrum and $d(T, T+T_1+T_2) \le \|T_1\| + \|T_2\| < 2\varepsilon$. Therefore, the set of operators in X_{01} with purely point spectrum is dense in X_{01}.

In order to check that the set of purely absolutely continuous operators is dense in X_{01}, it is enough to show that in X_{01} purely point operators can be arbitrarily approximated by operators with purely absolutely continuous spectrum. If $T \in X_{01}$ has purely point spectrum, $T\xi_k = \lambda_k \xi_k$, (ξ_k) an orthonormal basis of $\mathcal{H}$, for each n let $J_j = [j/2^n, (j+1)/2^n)$, $j = 0, 1, \ldots, 2^n - 2$, $J_{2^n-1} = [1 - 1/2^n, 1]$ and $\mathcal{H}_j := \mathrm{rng}\ \chi_{J_j}(T)$. Since $\sigma(T) = [0,1]$, the set of eigenvalues (λ_k) of T is dense in $[0,1]$ and so $\dim \mathcal{H}_j = \infty$, $\forall j$, that is, $\chi_{J_j}(T)$ is the identity operator on the infinite-dimensional subspace $\mathcal{H}_j$. Further, $\sum_j \chi_{J_j}(T) = \mathbf{1}$, that is, $\mathcal{H} = \oplus_j \mathcal{H}_j$. Let $c_j = j/2^n$ denote the left end of J_j.

Define the self-adjoint operator $S_n : \bigoplus_j \mathcal{H}_j \to \mathcal{H}$ by

$$S_n = \bigoplus_{j=0}^{2^n-1} c_j \, \chi_{J_j}(T)$$

and note that the restriction $S_n|_{\mathcal{H}_j}$ is the multiple of the identity $c_j\,\mathbf{1}$ on $\mathcal{H}_j$, so that $S_n\xi_k = c_j\xi_k$, if $\lambda_k \in J_j$, and $\|S_n - T\| \le 2^{-n}$.

Now, if $A_j \in \mathrm{B}(\mathcal{H}_j)$ is a self-adjoint operator with purely absolutely continuous spectrum $[0, 1/2^n]$, then $\|A_j\| = 1/2^n$, $\forall j$, and the operator

$$K_n := \bigoplus_{j=0}^{2^n-1} \big(c_j\, \chi_{J_j}(T) + A_j\big)$$

belongs to X_{01}, has purely absolutely continuous spectrum and

$$\begin{aligned}\|T - K_n\| &\leq \|T - S_n\| + \|S_n - K_n\| \\ &\leq \frac{1}{2^n} + \max_j \|A_j\| \leq \frac{1}{2^{n-1}}.\end{aligned}$$

Since n is arbitrarily large, the set of absolutely continuous operators is dense in X_{01}. Therefore, by the wonderland theorem, the set of operators in X_{01} with purely singular continuous spectrum is generic in X_{01}.

Exercise 12.6.8. Verify that, for any j, the operators

$$\big(c_j\, \chi_{J_j}(T) + A_j\big) = c_j \mathbf{1} + A_j \in \mathrm{B}(\mathcal{H}_j),$$

is purely absolutely continuous. Conclude that K_n in Example 12.6.6 is purely absolutely continuous and belongs to X_{01}.

Exercise 12.6.9. Adapt Example 12.6.6 for the set of self-adjoint operators $X_{ab} \subset \mathrm{B}(\mathcal{H})$ with spectrum $[a, b]$, $a < b$.

Chapter 13

Spectrum and Quantum Dynamics

Different spectral subspaces of a self-adjoint operator T in general entail different behaviors of the unitary evolution group e^{-itT} (particularly as $|t| \to \infty$). In this chapter many such dynamical issues are discussed; the main motivation is when T corresponds to the Schrödinger operator of a quantum system. Some related physical concepts, such as quantum return probability and test operators, are used to probe the large-time behaviors. The cornerstones of such results are the concepts of precompactness, almost periodicity and the Wiener and Riemann-Lebesgue lemmas.

13.1 Point Subspace: Precompact Orbits

Fix a self-adjoint operator T in the Hilbert space $\mathcal{H}$. It will be seen that even the time evolution of linear combinations of eigenstates of T can present rich behavior.

Definition 13.1.1. The *orbit* of $\xi \in \mathcal{H}$ under T is the set

$$\mathcal{O}(\xi) = \left\{ e^{-itT}\xi : t \in \mathbb{R} \right\},$$

and its *trajectory* is the map $\mathbb{R} \ni t \mapsto \xi(t) = e^{-itT}\xi$.

Lemma 13.1.2. *Every trajectory is uniformly continuous.*

Proof. Since the unitary evolution group e^{-itT} is strongly continuous, then every trajectory $\xi(t)$ is continuous, and so continuous at the origin $t = 0$. Thus, given $\varepsilon > 0$, there is $\delta > 0$ so that $\|\xi(r) - \xi\| < \varepsilon$ for all $|r| < \delta$. Now, for any $t \in \mathbb{R}$ one has $\|\xi(t+r) - \xi(t)\| = \|\xi(r) - \xi\| < \varepsilon$ if $|r| < \delta$, and $\xi(t)$ is uniformly continuous. $\square$

Note that if ξ^λ is an eigenvector of T, i.e., $T\xi^\lambda = \lambda\xi^\lambda$, then its orbit

$$\mathcal{O}(\xi^\lambda) = \{e^{-it\lambda}\xi^\lambda : t \in \mathbb{R}\} = \{e^{-it\lambda}\xi^\lambda : t \in [0, 2\pi/\lambda]\}$$

is a compact subset of $\mathcal{H}$, since it is a continuous image of the compact set $[0, 2\pi/\lambda]$ (the case $\lambda = 0$ is trivial). This remark motivates the

Definition 13.1.3. $\mathcal{H}_{\rm pc}(T)$ will denote the vector subspace (check!) of $\xi \in \mathcal{H}$ with precompact orbit $\mathcal{O}(\xi)$, i.e., $\overline{\mathcal{O}(\xi)}$ is a compact subset of $\mathcal{H}$.

Recall that in a complete metric space a subset A is precompact iff A is totally bounded iff every sequence in A has a Cauchy subsequence.

Lemma 13.1.4. *$\mathcal{H}_{\rm pc}(T)$ is a closed subspace of $\mathcal{H}$.*

Proof. Let $(\xi_n) \subset \mathcal{H}_{\rm pc}$ with $\xi_n \to \xi$. For $\varepsilon_n \to 0^+$ choose ξ_n (or a subsequence if necessary) so that $\|\xi_n - \xi\| < \varepsilon_n/4$. Since $\mathcal{O}(\xi_1)$ is precompact, there exists an increasing sequence $t_j^1 \subset \mathbb{R}$ so that $(e^{-it_j^1 T}\xi_1)_j$ is a Cauchy sequence. So, there is M_1 so that

$$\left\| e^{-it_j^1 T}\xi_1 - e^{-it_k^1 T}\xi_1 \right\| < \frac{\varepsilon_1}{2}, \qquad \forall t_j^1, t_k^1 \geq M_1.$$

Since $\mathcal{O}(\xi_2)$ is precompact, there exists a Cauchy subsequence $(e^{-it_j^2 T}\xi_2)_j$ of $(e^{-it_j^1 T}\xi_2)_j$, consequently there is $M_2 > M_1$ (choose $M_2 \in (t_j^2)_j$) with

$$\left\| e^{-it_j^2 T}\xi_2 - e^{-it_k^2 T}\xi_2 \right\| < \frac{\varepsilon_2}{2}, \qquad \forall t_j^2, t_k^2 \geq M_2.$$

Follow this pattern and construct $(t_j^n)_j$, a subsequence of $(t_j^{n-1})_j$, and M_n accordingly, for all $n \in \mathbb{N}$.

Consider the sequence $(e^{-iM_n T}\xi) \subset \mathcal{O}(\xi)$. It then follows that, for $k, n \geq m$,

$$\begin{aligned} \left\| e^{-iM_n T}\xi - e^{-iM_k T}\xi \right\| &\leq \left\| e^{-iM_n T}(\xi - \xi_m) \right\| \\ &\quad + \left\| e^{-iM_n T}\xi_m - e^{-iM_k T}\xi_m \right\| + \left\| e^{-iM_k T}(\xi_m - \xi) \right\| \\ &< \frac{\varepsilon_m}{4} + \frac{\varepsilon_m}{2} + \frac{\varepsilon_m}{4} = \varepsilon_m. \end{aligned}$$

Hence $\mathcal{O}(\xi)$ has a Cauchy subsequence and so it is precompact. □

Lemma 13.1.5. *If $\xi \in \mathcal{H}_{\rm pc}(T)$, then for all $\varepsilon > 0$ there exists an orthogonal projection F_ε, onto a finite-dimensional subspace of $\mathcal{H}$, so that*

$$\left\| (\mathbf{1} - F_\varepsilon)e^{-itT}\xi \right\| < \varepsilon, \qquad \forall t \in \mathbb{R}.$$

Proof. Since e^{-itT} is a unitary operator for every $t \in \mathbb{R}$, it follows that $\mathcal{O}(\xi)$ is a subset of the sphere centered at the origin and radius $\|\xi\|$, so a bounded set. It is then possible to assume that $\|\xi\| = 1$ (the case $\xi = 0$ is trivial). Let $(\eta_j)_{j=1}^\infty$ be an orthonormal sequence in $\mathcal{O}(\xi)$ and P_n the orthogonal projection onto $\mathrm{Lin}(\{\eta_1, \ldots, \eta_n\})$. If such a sequence does not exist (i.e., it is finite), then $\mathcal{O}(\xi)$ is a subset of a finite-dimensional subspace and the result is immediate. Assume that it exists and put

$$M_n := \sup\{\|\eta\| : \eta \in (\mathbf{1} - F_n)\mathcal{O}(\xi)\}.$$

The proof ends if it is shown that $M_n \to 0$ as $n \to \infty$.

If M_n does not vanish, there exist $\varepsilon_0 > 0$ and an orthogonal sequence (ξ_{n_k}) so that

$$\xi_{n_k} \in \mathcal{O}(\xi) \cap \mathrm{rng}\,(\mathbf{1} - P_{n_k}), \qquad \|\xi_{n_k}\| \ge \varepsilon_0, \ \forall n_k.$$

Since by construction the sequence (ξ_{n_k}) is bounded and orthogonal, it converges weakly to zero, $\xi_{n_k} \xrightarrow{\mathrm{w}} 0$ (like orthonormal sequences). Further, (ξ_{n_k}) has a convergent subsequence (denoted with the same symbols) in $\mathcal{H}$ since it is a subset of the orbit of ξ, a precompact set. Hence, $\xi_{n_k} \to 0$, which is a contradiction with the above lower bound $\|\xi_{n_k}\| \ge \varepsilon_0$. This finishes the proof of the lemma. □

For the proof of the main result of this section, i.e., Theorem 13.1.6, RAGE Theorem 13.4.1 will be employed.

Theorem 13.1.6. *If T is self-adjoint, then $\mathcal{H}_{\mathrm{p}}(T) = \mathcal{H}_{\mathrm{pc}}(T)$.*

Proof. Since the orbit of each eigenvector of T is compact and $\mathcal{H}_{\mathrm{pc}}(T)$ is a closed subspace, it follows that $\mathcal{H}_{\mathrm{p}}(T) \subset \mathcal{H}_{\mathrm{pc}}(T)$.

Now pick $\xi \in \mathcal{H}_{\mathrm{pc}}(T)$. Given $\varepsilon > 0$, let F_ε be as in Lemma 13.1.5. For each $\eta \in \mathcal{H}_{\mathrm{c}}(T)$ one has (assume $t > 0$ for simplicity)

$$\begin{aligned}\langle \eta, \xi\rangle &= \frac{1}{t}\int_0^t \langle \eta, \xi\rangle\, ds = \frac{1}{t}\int_0^t \left\langle (F_\varepsilon + \mathbf{1} - F_\varepsilon)\, e^{-isT}\eta, e^{-isT}\xi\right\rangle\, ds\\ &= \frac{1}{t}\int_0^t \left\langle F_\varepsilon e^{-isT}\eta, e^{-isT}\xi\right\rangle\, ds + \frac{1}{t}\int_0^t \left\langle e^{-isT}\eta, (\mathbf{1} - F_\varepsilon) e^{-isT}\xi\right\rangle\, ds.\end{aligned}$$

Thus,

$$|\langle \eta, \xi\rangle| \le \frac{\|\xi\|}{t}\int_0^t \left\|F_\varepsilon e^{-isT}\eta\right\|\, ds + \frac{\|\eta\|}{t}\int_0^t \left\|(\mathbf{1} - F_\varepsilon) e^{-isT}\xi\right\|\, ds,$$

and by Cauchy-Schwarz and RAGE Theorem 13.4.1, for t sufficiently large,

$$\frac{1}{t}\int_0^t 1 \times \left\|F_\varepsilon e^{-isT}\eta\right\|\, ds \le \left(\frac{1}{t}\int_0^t \left\|F_\varepsilon e^{-isT}\eta\right\|^2\, ds\right)^{1/2} < \varepsilon.$$

This inequality and an appropriate choice of F_ε in Lemma 13.1.5 imply

$$|\langle \eta, \xi\rangle| \le \varepsilon\, (\|\xi\| + \|\eta\|)\,.$$

Since this holds for arbitrarily $\varepsilon > 0$ one has $\langle \eta, \xi\rangle = 0$. It was then shown that $\mathcal{H}_{\mathrm{pc}}(T) \perp \mathcal{H}_{\mathrm{c}}(T)$, that is, $\mathcal{H}_{\mathrm{pc}}(T) \subset \mathcal{H}_{\mathrm{p}}(T)$. This finishes the proof of the theorem. □

The interpretation of this result is that the elements of the point subspace $\mathcal{H}_p(T)$ are those whose trajectories, up to any given "small error" ε, spend long times in finite-dimensional subspaces of $\mathcal{H}$. It will be seen that the trajectories of elements of $\mathcal{H}_c(T)$ escape, in time average, from all finite-dimensional subspaces (see page 363). This is an attractive way of viewing the orthogonality $\mathcal{H}_p(T) \perp \mathcal{H}_c(T)$.

13.2 Almost Periodic Trajectories

Let T be a self-adjoint operator acting in the Hilbert space $\mathcal{H}$.

Definition 13.2.1. Let $\xi \in \mathcal{H}$ and $\mathbb{R} \ni t \mapsto \xi(t) := e^{-itT}\xi$ its trajectory.

a) Given $\varepsilon > 0$, an *ε-almost period* of $\xi(t)$ is a $\tau \in \mathbb{R}$ so that

$$\|\xi(t+\tau) - \xi(t)\| < \varepsilon, \qquad \forall t \in \mathbb{R}.$$

b) $\xi(t)$ is *almost periodic* if, for all $\varepsilon > 0$, there exists $L = L(\varepsilon) > 0$ so that for each $s \in \mathbb{R}$ the interval $[s, s+L] \subset \mathbb{R}$ contains an ε-almost period of $\xi(t)$.

It is also convenient to denote by ξ_τ the trajectory $\xi_\tau(t) := \xi(t+\tau)$, and so τ is an ε-almost period iff $\sup_t \|\xi_\tau(t) - \xi(t)\| \leq \varepsilon$.

Example 13.2.2.

a) $\tau = 0$ is always an ε-almost period of $\xi(t)$.

b) If $\xi(t)$ is periodic with period r, that is, $\xi(t) = \xi_r(t)$, $\forall t \in \mathbb{R}$, then r is an ε-almost period for all $\varepsilon > 0$. Thus, every periodic trajectory is almost periodic, since nr is an ε-almost period for all $n \in \mathbb{Z}$ (that is, $L(\varepsilon) = |r|$, $\forall \varepsilon > 0$).

The next result is a main motivation for considering almost periodic trajectories in this context.

Proposition 13.2.3. *If $T\xi^\lambda = \lambda\xi^\lambda$, then $\xi^\lambda(t)$ is periodic and so almost periodic. If $\lambda \neq 0$, the period is $2\pi/\lambda$.*

Proof. If $\lambda = 0$ the trajectory is constant, and so periodic. If $\lambda \neq 0$, then $\xi^\lambda(t) = e^{-i\lambda t}\xi^\lambda = \xi^\lambda(t + 2\pi/\lambda)$, $\forall t$. □

Lemma 13.2.4. *τ is an ε-almost period of $\xi(t)$ iff*

$$\|(\mathbf{1} - e^{-i\tau T})\xi\| < \varepsilon.$$

If $\xi(t)$ is almost periodic it is uniformly continuous and recurrent, that is, there exists a sequence $t_j \to \infty$ with $\lim_{j\to\infty} e^{-it_jT}\xi = \xi$.

Proof. τ is an ε-almost period of $\xi(t)$ iff, for all $t \in \mathbb{R}$,

$$\varepsilon > \|\xi(t+\tau) - \xi(t)\| = \|e^{-i(t+\tau)T}\xi - e^{-itT}\xi\| = \|e^{-i\tau T}\xi - \xi\|,$$

since e^{-itT} is a unitary operator.

$\xi(t)$ is uniformly continuous by Lemma 13.1.2. Finally, take a sequence $\varepsilon_j \to 0^+$ and $\tau_j > \tau_{j-1} + 1$ a corresponding sequence of ε_j-almost periods. Then $\tau_j \to \infty$ and, for each j one has

$$\|(\mathbf{1} - e^{-i\tau_j T})\xi\| < \varepsilon_j;$$

hence $\xi(t)$ is recurrent. □

The main result of this section is another characterization of the point subspace of a self-adjoint operator.

Theorem 13.2.5. *The trajectory $\xi(t)$ is almost periodic iff the orbit $\mathcal{O}(\xi)$ is precompact.*

Corollary 13.2.6. $\mathcal{H}_{\rm p}(T) = \{\xi \in \mathcal{H} : \xi(t) \text{ is almost periodic}\}$.

Proof. It follows directly from Theorems 13.1.6 and 13.2.5. □

Proof. [**Theorem 13.2.5**] Suppose that $\xi(t)$ is almost periodic; then given $\varepsilon > 0$ let $L = L(\varepsilon)$ be an ε-almost period. By Lemma 13.2.4, $\xi(t)$ is uniformly continuous and so there exists a finite set

$$F := \{t_1, \ldots, t_N\} \subset [-L(\varepsilon), 0], \qquad N < \infty,$$

so that $\bigcup_{j=1}^N B(\xi(t_j); \varepsilon)$ is an open cover of $\{\xi(t) : t \in [-L(\varepsilon), 0]\}$. It is claimed that $\bigcup_{j=1}^N B(\xi(t_j); 2\varepsilon)$ is an open cover of $\mathcal{O}(\xi)$, that is, that this orbit is totally bounded, thus precompact in $\mathcal{H}$.

If $s \in \mathbb{R}$ let $\tau = \tau(s, \varepsilon)$ be an ε-almost period of $\xi(t)$ in the interval $[s, s+L(\varepsilon)]$. Thus, since $(s - \tau) \in [-L(\varepsilon), 0]$ there exists $t_j \in F$ with $\|\xi(s-\tau) - \xi(t_j)\| < \varepsilon$. Therefore,

$$\begin{aligned}\|\xi(s) - \xi(t_j)\| &\le \|\xi(s) - \xi(s-\tau)\| + \|\xi(s-\tau) - \xi(t_j)\| \\ &< \|e^{-i\tau T}(\xi(s) - \xi(s-\tau))\| + \varepsilon = \|\xi(s+\tau) - \xi(s)\| + \varepsilon \\ &< \varepsilon + \varepsilon = 2\varepsilon.\end{aligned}$$

Since this holds for any $s \in \mathbb{R}$, the above claim follows. Hence $\mathcal{O}(\xi)$ is totally bounded.

Suppose now that $\mathcal{O}(\xi)$ is precompact; thus for each $\varepsilon > 0$ there are open balls

$$B(\xi(t_1); \varepsilon), \ldots, B(\xi(t_N); \varepsilon),$$

centered at points of $\mathcal{O}(\xi)$, whose union covers this orbit. It happens that every closed interval in $\mathbb{R}$ of length $M(\varepsilon) := 2\max_{1\le j\le N}|t_j|$ has an ε-almost period of $\xi(T)$; in fact, for each $s \in \mathbb{R}$ there is a t_j in $[s, s+M(\varepsilon)]$ with

$$\begin{aligned}\|\xi(t)-\xi(t+\tau)\| &= \|\xi(0)-\xi(\tau)\| = \|\xi(t_j)-\xi(t_j+\tau)\|\\ &= \|\xi(t_j)-\xi(s+M/2)\| < \varepsilon,\end{aligned}$$

that is, $\xi(t)$ is almost periodic. □

Remark 13.2.7. The following reasoning gives some insight into precompact orbits and almost periodic trajectories for vectors in the point subspace of T, i.e., $\xi = \sum_{j=1}^{\infty} a_j\xi_j$, $T\xi_j = \lambda_j\xi_j$, $\forall j$, and (ξ_j) orthonormal. By Example 5.4.10 its time evolution is $\xi(t) = \sum_{j=1}^{\infty} a_j e^{-it\lambda_j}\xi_j$.

1. For all $t \in \mathbb{R}$ one has

$$\|\xi(t)\|^2 = \sum_{j=1}^{\infty} |e^{-it\lambda_j} a_j|^2 = \sum_{j=1}^{\infty} |a_j|^2.$$

   Given $\varepsilon > 0$ there is N so that $\sum_{j=1}^{N} |e^{-it\lambda_j} a_j|^2 > (1-\varepsilon)$, $\forall t$, and a large part of the orbit lives in a finite-dimensional subspace (of dimension $\le N$). Compare with Lemma 13.1.5.

2. Note that in Hilbert space, $\xi(t) = \lim_{M\to\infty} \xi^M(t)$ with uniform convergence in t, where $\xi^M(t) = \sum_{j=1}^{M} a_j e^{-it\lambda_j}\xi_j$ is quasiperiodic, i.e., a linear combination of (finitely many) periodic trajectories. The almost periodicity "is obtained in the limit of infinitely many periods $M \to \infty$."

Remark 13.2.8. The equivalence between almost periodic trajectory and precompact orbit extends to time-periodic Schrödinger operators $H(t)$; however, there are counterexamples in case the time dependence of the Schrödinger operator $H(t)$ is quasiperiodic; these results are discussed in [deOS07b]. See [Katz76] and [Cor89] for a general treatment of almost periodic functions.

13.3 Quantum Return Probability

Let T be self-adjoint, $\eta, \xi \in \mathcal{H}$ and $\mu_\xi = \mu_\xi^T$, $\mu_{\xi,\eta} = \mu_{\xi,\eta}^T$ the corresponding spectral measures. Without loss of generality the initial condition of the Schrödinger equation

$$i\frac{d\xi}{dt}(t) = T\xi(t), \qquad \xi(0) = \xi \in \operatorname{dom} T,$$

will be supposed to be given at initial time $t_0 = 0$. The main quantities considered to probe the large time behavior of the dynamics $e^{-itT}\xi$ will be:

1. The (quantum) *return probability* to the initial condition ξ, at time t,
$$p_\xi(t) := \left|\left\langle \xi, e^{-itT}\xi\right\rangle\right|^2,$$
and more generally $p_{\eta,\xi}(t) := \left|\left\langle \eta, e^{-itT}\xi\right\rangle\right|^2$.
2. The *average return probability* up to time $t \neq 0$,
$$\langle p_\xi\rangle(t) := \frac{1}{t}\int_0^t p_\xi(s)\,ds,$$
and similarly one defines $\langle p_{\eta,\xi}\rangle(t)$.
3. The *total return probability* to the initial state ξ,
$$\int_{\mathbb{R}} p_\xi(t)\,dt,$$
also called *sojourn time* at the initial state.
4. A *test operator* is an unbounded self-adjoint operator $A \geq 0$ with compact resolvent, that is, with positive and purely discrete spectrum, so that $e^{-itT}\mathrm{dom}\, A \subset \mathrm{dom}\, A$, $\forall t \in \mathbb{R}$. One considers the expectation value of A in the state ξ at time t to be
$$\mathcal{E}_A^\xi(t) := \left\langle e^{-itT}\xi, Ae^{-itT}\xi\right\rangle.$$
5. The time average for A is
$$\left\langle \mathcal{E}_A^\xi\right\rangle(t) := \frac{1}{t}\int_0^t \mathcal{E}_A^\xi(s)\,ds.$$

Remark 13.3.1. It is important to notice that in both notations $\mathcal{E}_A^\xi(t)$ and $p_\xi(t)$ the self-adjoint operator T, the (infinitesimal) generator of the time unitary evolution group e^{-itT}, is not explicitly indicated.

A crucial relation for what follows comes from the spectral theorem
$$p_\xi(t) = |\hat{\mu}_\xi(t)|^2 := \left|\int_{\sigma(T)} e^{-itx}\,d\mu_\xi(x)\right|^2.$$
$\hat{\mu}_\xi(t) = \int_{\sigma(T)} e^{-it\lambda}\,d\mu_\xi(\lambda)$ is called the *Fourier transform of the measure* μ_ξ, so that the behavior of the return probability and expectation values of test operators are naturally related to spectral measures of T through $\left\langle \xi, e^{-itT}\xi\right\rangle = \hat{\mu}_\xi(t)$. Two general results on Borel measures over $\mathbb{R}$ are important here: the Riemann-Lebesgue lemma (around 1900) and the Wiener lemma (around 1935).

Lemma 13.3.2 (Riemann-Lebesgue). *If* $f \in \mathrm{L}^1(\mathbb{R})$ *and* $\hat{f}$ *denotes its Fourier transform, then* $\hat{f}$ *is continuous and* $\lim_{|p|\to\infty} \hat{f}(p) = 0$*; in other symbols* $\hat{f} \in C_\infty(\hat{\mathbb{R}})$.

Proof. The Fourier transform $\hat{f}$ is continuous by Lemma 3.2.8.

For a function $f \in \mathrm{L}^1(\mathbb{R})$, denote $f_h(t) = f(t+h)$. First note that for $\phi \in C_0^\infty(\mathbb{R})$ one has $\|\phi_h - \phi\|_1 \to 0$ as $h \to 0$ (by the uniform continuity of ϕ). Now since $C_0^\infty(\mathbb{R})$ is dense in $\mathrm{L}^1(\mathbb{R})$, given $\varepsilon > 0$ pick $\phi \in C_0^\infty(\mathbb{R})$ with $\|f-\phi\|_1 < \varepsilon$; by the invariance of Lebesgue measure under translations one has $\|f_h - \phi_h\|_1 = \|f-\phi\|_1 < \varepsilon$. Take $|h|$ sufficiently small so that $\|\phi_h - \phi\|_1 < \varepsilon$. Gathering these facts, one has

$$\|f_h - f\|_1 \le \|f_h - \phi_h\|_1 + \|\phi_h - \phi\|_1 + \|\phi - f\|_1 < 3\varepsilon.$$

This shows that $\|f_h - f\|_1 \to 0$ as $h \to 0$, $\forall f \in \mathrm{L}^1(\mathbb{R})$. Note that this property holds for all $\mathrm{L}^q(\mathbb{R})$, $1 \le q < \infty$; the proof is the same.

For $p \neq 0$ one has

$$\sqrt{2\pi}\,\hat{f}(p) = \int_{\mathbb{R}} e^{-ixp} f(x)\,dx = -\int_{\mathbb{R}} e^{-i(x+\pi/p)p} f(x)\,dx = -\int_{\mathbb{R}} e^{-ixp} f\left(x - \frac{\pi}{p}\right)dx,$$

and so

$$\begin{aligned} 2\sqrt{2\pi}\,|\hat{f}(p)| &= \left|\int_{\mathbb{R}} e^{-ixp}\left(f(x) - f\left(x - \frac{\pi}{p}\right)\right)dx\right| \\ &\le \left\| f(x) - f\left(x - \frac{\pi}{p}\right)\right\|_1, \end{aligned}$$

which vanishes as $|p| \to \infty$. □

Exercise 13.3.3. If $f(x) = \chi_{[a,b]}(x)$, write out its Fourier transform $\hat{f}(p)$ and check that $\lim_{|p|\to\infty} \hat{f}(p) = 0$. This is a seed of another proof of the Riemann-Lebesgue lemma.

Exercise 13.3.4. Follow the indicated steps to show that there are continuous functions $g \in C_\infty(\hat{\mathbb{R}})$ for which there is no $f \in \mathrm{L}^1(\mathbb{R})$ with $\hat{f} = g$. In other words, the bounded map $\mathcal{F} : \mathrm{L}^1(\mathbb{R}) \to C_\infty(\hat{\mathbb{R}})$ (see the proof of Proposition 10.1.9 for notation) is not onto.

1) Check that such map is invertible.
2) Assume it is onto. Since $C_\infty(\hat{\mathbb{R}})$ is a Banach space, conclude that $\mathcal{F}^{-1} : C_\infty(\hat{\mathbb{R}}) \to \mathrm{L}^1(\mathbb{R})$ is bounded by Corollary 1.2.6, i.e., the open mapping theorem.
3) For each $n \in \mathbb{N}$ pick $f_n \in C_0^\infty(\hat{\mathbb{R}})$ with $f_n(p) = 1$ if $|p| \le n$ and $f(p) = 0$ if $|p| \ge n + 1/n$, fast decaying in the gaps $(-n-1/n, -n)$ and $(n, n+1/n)$, so that $\|f_n\|_\infty = 1$ and
$$\sqrt{2\pi}\,\left\|\check{f}_n\right\|_1 \approx \int_{\mathbb{R}} \left|\int_{-n}^{n} dp\, e^{ixp} f_n(p)\right| dx = 2\int_{\mathbb{R}} dx \left|\frac{\sin nx}{x}\right|.$$
4) Conclude that $\left\|\check{f}_n\right\|_1$ diverges as $n \to \infty$, thus getting a contradiction with the boundedness of $\mathcal{F}^{-1}$, which implies rng $\mathcal{F}$ is a proper subset of $C_\infty(\hat{\mathbb{R}})$.

Lemma 13.3.5 (Wiener). *If μ is a finite Borel (real or complex) measure over $\mathbb{R}$, and $\Lambda = \{\lambda \in \mathbb{R} : \mu(\{\lambda\}) \neq 0\}$, then*

$$\lim_{t\to\infty} \frac{1}{t} \int_0^t |\hat{\mu}(s)|^2 \, ds = \sum_{\lambda \in \Lambda} |\mu(\{\lambda\})|^2 .$$

Proof. Since μ is finite, Λ is a countable set (check this!). Since $\hat{\mu}(t) = \int_{\mathbb{R}} e^{-itx} d\mu(x)$ one has, by the Fubini theorem, ($\overline{\mu}$ is the complex conjugate of μ)

$$\begin{aligned}\frac{1}{t}\int_0^t ds\, |\hat{\mu}(s)|^2 &= \frac{1}{t}\int_0^t ds \int\int d\mu(u)\, d\overline{\mu}(v)\, e^{-i(u-v)s} \\ &= \int\int d\mu(u)\, d\overline{\mu}(v)\, g(u,v,t),\end{aligned}$$

with $g(u,u,t) = 1$ and

$$g(u,v,t) = -i\frac{1-e^{-i(u-v)t}}{t(u-v)}, \qquad u \neq v.$$

Since $\lim_{t\to\infty} g(u,v,t) = \chi_{\{u\}}v)$, and this function is dominated by the constant function 1 which belongs to $\mathrm{L}^1_{\mu\times\bar{\mu}}(\mathbb{R}\times\mathbb{R})$, by dominated convergence one obtains

$$\begin{aligned}\lim_{t\to\infty}\frac{1}{t}\int_0^t ds\, |\hat{\mu}(s)|^2 &= \int\int d\mu(u)\, d\overline{\mu}v)\chi_{\{u\}}v) \\ &= \int \mu(\{v\})\, d\overline{\mu}v) = \sum_{v\in\Lambda} |\mu(\{v\})|^2 .\end{aligned}$$

The lemma is proved. □

Lemma 13.3.6. *If $\xi, \eta \in \mathcal{H}$, then there exists $g \in \mathrm{L}^2_{\mu_\xi}(\mathbb{R}) \cap \mathrm{L}^1_{\mu_\xi}(\mathbb{R})$ so that*

$$\langle \eta, e^{-itT}\xi\rangle = \int_{\sigma(T)} e^{-itx} g(x)\, d\mu_\xi(x).$$

Further, $\|g\|_{\mathrm{L}^2_{\mu_\xi}} \leq \|\eta\|$.

Proof. Let $\mathcal{H}_\xi$ be the cyclic subspace spanned by ξ, as discussed in Section 8.3. $\mathcal{H}_\xi$ reduces T and is unitarily equivalent to $\mathrm{L}^2_{\mu_\xi}(\mathbb{R})$. In this space T, that is, $T|_{\mathcal{H}_\xi}$, is represented by the multiplication operator $\mathcal{M}_h$, $h(x) = x$, the vector ξ is represented in $\mathrm{L}^2_{\mu_\xi}(\mathbb{R})$ by the constant function $1(x) = 1$ and the unitary evolution group e^{-itT} by $\mathcal{M}_{e^{-itx}}$.

If P_ξ is the orthogonal projection onto $\mathcal{H}_\xi$, then for $\eta \in \mathcal{H}$ the vector $P_\xi\eta$ is represented by a function $\overline{g} \in \mathrm{L}^2_{\mu_\xi}(\mathbb{R})$ (so $\|g\|_{\mathrm{L}^2_{\mu_\xi}} \leq \|\eta\|$). Thus, since $e^{-itT}\xi \in \mathcal{H}_\xi$,

$$\langle \eta, e^{-itT}\xi\rangle = \langle P_\xi\eta, e^{-itT}\xi\rangle = \langle \overline{g(x)}, e^{-itx}1\rangle_{\mathrm{L}^2_{\mu_\xi}} = \int_{\sigma(T)} g(x)e^{-itx}\, d\mu_\xi(x).$$

By taking $t = 0$ it follows that $g \in \mathrm{L}^1_{\mu_\xi}(\mathbb{R})$. □

Now a prominent result with respect to the large-time behavior of the return probability will be presented. Some dynamical differences between point and continuous subspaces are noteworthy.

Theorem 13.3.7. *Let T be self-adjoint.*

i) *For any $\xi \in \mathcal{H}$ the limit*

$$\mathfrak{X}_\xi := \lim_{t\to\infty} \langle p_\xi \rangle (t)$$

exists. Furthermore, $\mathfrak{X}_\xi = 0$ iff $\xi \in \mathcal{H}_{\rm c}(T)$.

ii) *If $\xi \in \mathcal{H}_{\rm ac}(T)$, then* $\lim_{t\to\infty} p_\xi(t) = 0$.

Proof. i) It follows immediately by the Wiener Lemma 13.3.5 and the crucial relation on page 359. In particular, $\mathfrak{X}_\xi = 0$ iff μ_ξ is a continuous measure and, by Theorem 12.1.2, iff $\xi \in \mathcal{H}_{\rm c}(T)$.

ii) One has $\xi \in \mathcal{H}_{\rm ac}(T)$ iff $\mu_\xi \ll \ell$ iff there exists $f \in \mathrm{L}^1(\mathbb{R})$, $f \geq 0$, with $\frac{d\mu_\xi}{d\ell} = f$. Thus

$$p_\xi(t) = \langle \xi, e^{-itT}\xi\rangle = \int_{\mathbb{R}} e^{-itx}\, d\mu_\xi(x) = \int_{\mathbb{R}} e^{-itx} f(x)\, dx,$$

which vanishes as $t \to \infty$ by Riemann-Lebesgue 13.3.2. □

Corollary 13.3.8. *Let T be self-adjoint.*

i) *$\xi \in \mathcal{H}_{\rm c}(T)$ iff* $\lim_{t\to\infty} \langle p_{\eta,\xi}\rangle(t) = 0$, $\forall \eta \in \mathcal{H}$.

ii) *If $\xi \in \mathcal{H}_{\rm ac}(T)$, then* $\lim_{t\to\infty} p_{\eta,\xi}(t) = 0$, $\forall \eta \in \mathcal{H}$, *in other words,*

$$\mathrm{w} - \lim_{t\to\infty} e^{-itT}\xi = 0.$$

Proof. If $\xi \in \mathcal{H}_{\rm c}(T)$, by Proposition 12.3.1, $\mu_{\xi,\eta}$ is a continuous measure and i) follows by the Wiener lemma and Theorem 13.3.7.

If $\xi \in \mathcal{H}_{\rm ac}(T)$ then $\mu_{\eta,\xi} \ll \ell$ and we write $d\mu_{\eta,\xi}(x) = f(x)dx$, $f \in \mathrm{L}^1(\mathbb{R})$; by Lemma 13.3.6,

$$\langle \eta, e^{-itT}\xi\rangle = \int_{\mathbb{R}} e^{-itx} g(x)\, d\mu_\xi(x) = \int_{\mathbb{R}} e^{-itx} g(x) f(x)\, dx.$$

By considering $t = 0$ it follows that $fg \in \mathrm{L}^1(\mathbb{R})$ and so

$$p_{\eta,\xi}(t) = \left| \int_{\mathbb{R}} e^{-itx} g(x) f(x)\, dx \right|^2 \longrightarrow 0, \qquad t \to \infty,$$

by Riemann-Lebesgue. □

Exercise 13.3.9. Show that

$$\frac{1}{t}\int_0^t \left|\langle \eta, e^{-isT}\xi\rangle\right| ds \leq \big(\langle p_{\eta,\xi}\rangle (t)\big)^{\frac{1}{2}}, \qquad \forall \eta \in \mathcal{H},$$

and conclude that $\xi \in \mathcal{H}_{\rm c}(T)$ iff $\lim_{t\to\infty} \frac{1}{t}\int_0^t \left|\langle \eta, e^{-isT}\xi\rangle\right| ds = 0$.

Such results are interpreted as follows. Under time evolution $e^{-itT}\xi$, any state η (in particular the initial state ξ) is completely abandoned in time average if $\xi \in \mathcal{H}_c(T)$, since $\langle p_{\eta,\xi}\rangle(t) \to 0$ as $t \to \infty$; for elements of $\mathcal{H}_{ac}(T)$ the time average is not necessary. Sometimes such properties are associated with instabilities, e.g., atomic ionization. On the other hand, for elements $\xi \in \mathcal{H}_p(T)$ one has $\mathfrak{X}_\xi > 0$ and so the initial state is not "forgotten," in accordance with their almost periodic trajectories, as discussed in Section 13.2.

Remark 13.3.10. All occurrences of $t \to \infty$ above can be replaced by $t \to -\infty$.

13.4 RAGE Theorem and Test Operators

The RAGE theorem is an important tool in the study of the time asymptotics of expectation values of test operators, which were introduced in Section 13.3.

Theorem 13.4.1 (RAGE). *Let T be a self-adjoint operator in $\mathcal{H}$.*

i) $\xi \in \mathcal{H}_c(T)$ *iff for every compact operator* $K : \mathcal{H} \hookleftarrow$,

$$\lim_{t\to\infty} \frac{1}{t}\int_0^t \left\|Ke^{-iTs}\xi\right\|^2 ds = 0.$$

ii) *If* $\xi \in \mathcal{H}_{ac}(T)$, *then for every compact operator* $K : \mathcal{H} \hookleftarrow$,

$$\lim_{t\to\infty} Ke^{-itT}\xi = 0.$$

Proof. K can be approximated in the norm of $\mathrm{B}(\mathcal{H})$ by finite-rank operators, and by induction and the triangle inequality, it is sufficient to consider rank-one operators

$$K\xi = \langle \eta, \xi\rangle\zeta,$$

for some $\eta, \zeta \in \mathcal{H}$. In this case

$$\|Ke^{-itT}\xi\| = \|\langle\eta, e^{-itT}\xi\rangle\zeta\| = \|\zeta\|\,|\langle\eta, e^{-itT}\xi\rangle|,$$

and the result follows by Corollary 13.3.8. □

Exercise 13.4.2. Discuss the missing details in the proof of Theorem 13.4.1.

Remark 13.4.3. The term RAGE comes from the initials of D. Ruelle, W.O. Amrein, V. Georgescu and V. Enss. The RAGE theorem has applications to localization in scattering theory in $\mathbb{R}^n$; see Section 13.6.

Important compact operators are the projections onto finite-dimensional subspaces of $\mathcal{H}$; so the elements of $\mathcal{H}_c(T)$ can be interpreted as those whose trajectories escape, in time average, from every finite-dimensional subspace (again, the average is not necessary for the absolutely continuous subspace). Compare with the corresponding remark about the point subspace on page 356.

Corollary 13.4.4. *Let T be self-adjoint and A a test operator. If $P_c(T)\xi \neq 0$ (i.e., ξ has a nonzero component in the continuous subspace of T), then*

i) *The function $t \mapsto \mathcal{E}_A^\xi(t)$ is unbounded.*

ii) $\lim_{|t|\to\infty}\langle\mathcal{E}_A^\xi\rangle(t) = \infty$.

Proof. Note that i) is a consequence of ii); then it will suffice to prove the latter assertion.

Let $0 \le \lambda_1 < \lambda_2 < \lambda_3 \cdots$ denote the eigenvalues of A and Q_N the orthogonal projection onto the subspaces spanned by the eigenvectors of A associated with its eigenvalues $\le \lambda_N$. Since A has purely discrete spectrum, $\lim_{j\to\infty}\lambda_j = \infty$. Then Q_N has finite rank, so is a compact operator, and $Q_N A = A Q_N$. Denote $\xi_c = P_c\xi$ and $\xi_p = P_p\xi$; by hypothesis $\xi_c \neq 0$.

Denote $\xi(t) = e^{-itT}\xi$ and similarly for $\xi_p(t)$ and $\xi_c(t)$. Thus

$$\begin{aligned}
\mathcal{E}_A^\xi(t) &= \langle\xi(t), A\xi(t)\rangle \\
&= \langle(\mathbf{1} - Q_N + Q_N)\xi(t), A(\mathbf{1} - Q_N + Q_N)\xi(t)\rangle \\
&= \langle Q_N\xi(t), AQ_N\xi(t)\rangle + \langle(\mathbf{1} - Q_N)\xi(t), A(\mathbf{1} - Q_N)\xi(t)\rangle \\
&\ge \langle(\mathbf{1} - Q_N)\xi(t), A(\mathbf{1} - Q_N)\xi(t)\rangle \ge \lambda_N\|Q_N\xi(t)\|^2 \\
&= \lambda_N\left(1 - \|Q_N\xi_c(t)\|^2 - \|Q_N\xi_p(t)\|^2\right) \\
&\ge \lambda_N\left(1 - \|Q_N\xi_c(t)\|^2 - \|\xi_p\|^2\right).
\end{aligned}$$

By RAGE Theorem 13.4,

$$\lim_{t\to\infty}\frac{1}{t}\int_0^t \|Q_N\xi_c(s)\|^2\,ds = 0,$$

and so

$$\liminf_{t\to\infty}\left\langle\mathcal{E}_A^\xi\right\rangle(t) \ge \lambda_N\left(1 - \|\xi_p\|^2\right) = \lambda_N\|\xi_c\|^2,$$

and since this holds for any N, ii) follows. □

By following the same kind of arguments, one obtains

Corollary 13.4.5. *If $P_{ac}(T)\xi \neq 0$, then* $\lim_{|t|\to\infty}\mathcal{E}_A^\xi(t) = \infty$.

Exercise 13.4.6. Prove Corollary 13.4.5.

Remark 13.4.7. Contrary to what could be expected on account of the above results, pure point spectrum does not guarantee that the function $t \mapsto \mathcal{E}_A^\xi(t)$ is bounded; under certain conditions the time evolution could push $\xi(t)$ to outside dom A as $|t| \to \infty$. The first (mathematically rigorous) example of an operator with purely point spectrum and unbounded $\mathcal{E}_A^\xi(t)$ has appeared in Section 9 of [delR96]; for a generalization in a framework of potentials generated by some dynamical systems and under short range perturbations, consult [deOPr07]. The same phenomenon was found in the random dimer model [JSBS03]. Corresponding results in case of time-periodic quantum systems have appeared in [deOS07a]. This is an interesting current area of research.

Exercise 13.4.8. Let T be self-adjoint in $\mathcal{H}$, K a compact operator and $B(t) \in \mathrm{B}(\mathcal{H})$ uniformly bounded, that is, there is $C > 0$ so that $\|B(t)\| \le C$, $\forall t \in \mathbb{R}$. Show that

$$\lim_{t\to\infty} \left\| \frac{1}{t} \int_0^t B(s) K e^{-isT} P_{\mathrm{c}}(T)\xi \, ds \right\| = 0, \qquad \forall \xi \in \mathcal{H}.$$

13.5 Continuous Subspace: Return Probability Decay

The main goal of this section is to present characterizations of the continuous subspaces, of a self-adjoint operator T, in terms of the decay rate of the return probability to zero as $|t| \to \infty$. Recall that $\mathcal{F}$ denotes the Fourier transform (see Chapter 3), ℓ is Lebesgue measure and $\mathcal{A}$ the Borel sets in $\mathbb{R}$. If the measures $\mu \ll \nu$, the Radon-Nikodym derivative is denoted by $d\mu/d\nu$.

First some technical preparation for the main results. Note that sometimes the results are formulated in terms of the return probability $p_{\eta,\xi}(t)$, and in other instances in terms of $\langle \eta, e^{-itT}\xi \rangle$.

Lemma 13.5.1. *Let T be self-adjoint. Let $\xi \in \mathcal{H}_{\mathrm{ac}}(T)$ and $\eta \in \mathcal{H}$. Then:*

i) $\langle \eta, e^{-itT}\xi \rangle = \sqrt{2\pi}\mathcal{F}\left(\frac{d\mu_{\eta,\xi}}{d\ell}\right)(t)$, *and hence*

$$p_{\eta,\xi}(t) = 2\pi \left| \mathcal{F}\left(\frac{d\mu_{\eta,\xi}}{d\ell}\right)(t) \right|^2 .$$

ii) *Lebesgue a.e.*

$$\left| \frac{d\mu_{\eta,\xi}}{d\ell} \right|^2 \le \frac{d\mu_\eta}{d\ell} \frac{d\mu_\xi}{d\ell}, \text{ with } \frac{d\mu_\eta}{d\ell} = 0 \text{ if } \eta \in \mathcal{H}_{\mathrm{ac}}(T)^\perp .$$

Proof. i) Since $\mu_{\eta,\xi} \ll \ell$ one has

$$\begin{aligned} \langle \eta, e^{-itT}\xi \rangle &= \int_{\mathbb{R}} e^{-itx} \, d\mu_{\eta,\xi}(x) = \int_{\mathbb{R}} e^{-itx} \frac{d\mu_{\eta,\xi}}{d\ell}(x) \, dx \\ &= \sqrt{2\pi}\, \mathcal{F}\left(\frac{d\mu_{\eta,\xi}}{d\ell}\right)(t). \end{aligned}$$

ii) If $\eta \in \mathcal{H}_{\mathrm{ac}}(T)^\perp$, then $\mu_{\eta,\xi} = 0$; thus it is possible to assume that $\eta \in \mathcal{H}_{\mathrm{ac}}(T)$ (alternatively work with $P_{\mathrm{ac}}(T)\eta$). For every Borel set $\Lambda \in \mathcal{A}$, Cauchy-Schwarz implies

$$\begin{aligned} |\mu_{\eta,\xi}(\Lambda)|^2 &= |\langle \eta, \chi_\Lambda(T)\xi \rangle|^2 = |\langle \chi_\Lambda(T)\eta, \chi_\Lambda(T)\xi \rangle|^2 \\ &\le \|\chi_\Lambda(T)\eta\|^2 \, \|\chi_\Lambda(T)\xi\|^2 \\ &= \langle \eta, \chi_\Lambda(T)\eta \rangle \, \langle \xi, \chi_\Lambda(T)\xi \rangle = \mu_\eta(\Lambda)\, \mu_\xi(\Lambda). \end{aligned}$$

By taking $\Lambda = J_x$, i.e., an open interval that contains x, one has

$$\left|\frac{\mu_{\eta,\xi}(J_x)}{\ell(J_x)}\right|^2 \leq \frac{\mu_\eta(J_x)}{\ell(J_x)}\,\frac{\mu_\xi(J_x)}{\ell(J_x)},$$

and for $\ell(J_x) \to 0$ it is found that ℓ-a.e. (see, e.g., [Ru74], Chapter 8)

$$\left|\frac{d\mu_{\eta,\xi}}{d\ell}\right|^2 \leq \frac{d\mu_\eta}{d\ell}\frac{d\mu_\xi}{d\ell},$$

since the involved functions are absolutely continuous. □

Lemma 13.5.2. *Let $\xi, \eta \in \mathcal{H}$. If the function $t \mapsto s(t) = \langle \eta, e^{-itT}\xi\rangle$ is an element of* $\mathrm{L}^2(\mathbb{R})$*, then the spectral measure $\mu_{\eta,\xi} \ll \ell$.*

Proof. Assume that $s \in \mathrm{L}^2(\mathbb{R})$. Then for all $\psi \in \mathrm{L}^2(\mathbb{R})$ the function $s(t)\psi(t) \in \mathrm{L}^1(\mathbb{R})$ and the linear map

$$\psi \mapsto L(\psi) := \int_{\mathbb{R}} \psi(t)\, s(t)\, dt$$

is bounded since $|L(\psi)| \leq \|s\|_2\, \|\psi\|_2$. By Riesz's Representation Theorem 1.1.40, there exists $\overline{\phi} \in \mathrm{L}^2(\mathbb{R})$ so that

$$\int_{\mathbb{R}} \overline{\phi}(t)\, \psi(t)\, dt = \langle \phi, \psi\rangle = L(\psi);$$

by Fubini's theorem,

$$\begin{aligned} L(\psi) &= \int_{\mathbb{R}} \psi(t) \left(\int_{\mathbb{R}} e^{-itx}\, d\mu_{\eta,\xi}(x)\right) dt \\ &= \sqrt{2\pi}\, \int_{\mathbb{R}} \hat{\psi}(x)\, d\mu_{\eta,\xi}(x) = \sqrt{2\pi}\, \langle \eta, \hat{\psi}(T)\xi\rangle. \end{aligned}$$

Given a bounded interval $(a,b) \subset \mathbb{R}$, take a sequence $0 \leq \hat{\psi}_n \in C_0^\infty(\hat{\mathbb{R}})$ so that pointwise $\hat{\psi}_n \uparrow \chi_{(a,b)}$; thus, by Lemma 8.2.6 and dominated convergence,

$$\begin{aligned} \sqrt{2\pi}\, \mu_{\eta,\xi}((a,b)) &= \sqrt{2\pi}\, \langle \eta, \chi_{(a,b)}(T)\xi\rangle \\ &= \sqrt{2\pi}\, \lim_{n\to\infty} \langle \eta, \hat{\psi}_n(T)\xi\rangle = \lim_{n\to\infty} L(\psi_n) \\ &= \lim_{n\to\infty} \int_{\mathbb{R}} \overline{\phi}(t)\, \psi_n(t)\, dt \\ &= \lim_{n\to\infty} \int_{\mathbb{R}} \hat{\overline{\phi}}(t)\, \hat{\psi}_n(t)\, dt = \int_{(a,b)} \hat{\overline{\phi}}(t)\, dt. \end{aligned}$$

Since this holds for all bounded (a,b) and $\mu_{\eta,xi}$ is finite (although in general it is complex), it follows that $\hat{\overline{\phi}} \in \mathrm{L}^1(\mathbb{R})$, $d\mu_{\eta,\xi}/d\ell = \hat{\overline{\phi}}$ and $\mu_{\eta,\xi} \ll \ell$. □

Theorem 13.5.3. *Let T be self-adjoint. Then $\xi \in \mathcal{H}_{\rm ac}(T)$ iff there exists a dense set $E(\xi) \sqsubseteq \mathcal{H}$ so that the function $t \mapsto p_{\eta,\xi}(t)$ is an element of $\mathrm{L}^1(\mathbb{R})$ for all $\eta \in E(\xi)$.*

Proof. Suppose such $E(\xi)$ exists. Then by Lemma 13.5.2 $\mu_{\eta,\xi} \ll \ell$ for each $\eta \in E(\xi)$. Thus, for any $\Lambda \in \mathcal{A}$,

$$\begin{aligned}\mu_{\eta,\xi}(\Lambda) &= \langle \eta, \chi_\Lambda(T)\xi\rangle \\ &= \langle \eta, \chi_\Lambda(T)P_{\rm ac}(T)\xi\rangle + \langle \eta, \chi_\Lambda(T)P_{\rm p}(T)\xi\rangle + \langle \eta, \chi_\Lambda(T)P_{\rm sc}(T)\xi\rangle,\end{aligned}$$

and since $\mu_{\eta,\xi} \ll \ell$ it follows, by Proposition 12.3.1,

$$\langle \eta, \chi_\Lambda(T)P_{\rm p}(T)\xi\rangle = \langle \eta, \chi_\Lambda(T)P_{\rm sc}(T)\xi\rangle = 0, \qquad \forall \eta \in E(\xi).$$

Hence, since $E(\xi)$ is dense in $\mathcal{H}$, $P_{\rm p}\xi = 0 = P_{\rm sc}\xi$ and so $\xi \in \mathcal{H}_{\rm ac}(T)$.

Suppose now that $\xi \in \mathcal{H}_{\rm ac}(T)$ and let $E(\xi)$ be defined as in the statement of the theorem, that is, the vectors η so that $t \mapsto p_{\eta,\xi}(t)$ is an element of $\mathrm{L}^1(\mathbb{R})$. It will be shown that $E(\xi)$ is dense in $\mathcal{H}$. If $\eta \in \mathcal{H}_{\rm p}(T) \oplus \mathcal{H}_{\rm sc}(T)$, then $p_{\eta,\xi}(t) = 0$, $\forall t$; hence it is enough to consider $\eta \in \mathcal{H}_{\rm ac}(T)$ and verify the result for η in a dense subset of $\mathcal{H}_{\rm ac}(T)$.

By Lemma 13.5.1i) and Plancherel, one has

$$p_{\eta,\xi} \in \mathrm{L}^1(\mathbb{R}) \Longleftrightarrow \frac{d\mu_{\eta,\xi}}{d\ell} \in \mathrm{L}^2(\mathbb{R}).$$

For each vector $\eta \in \mathcal{H}_{\rm ac}(T)$ that there exists $M = M(\eta) < \infty$ so that for ℓ-a.e.

$$0 \le \frac{d\mu_\eta}{d\ell}(x) \le M,$$

one has, by Lemma 13.5.1ii), that

$$\left\| \frac{d\mu_{\eta,\xi}}{d\ell} \right\|_2^2 \le M(\eta) \left\| \frac{d\mu_\xi}{d\ell} \right\|_1 < \infty.$$

Since such a set of η is dense in $\mathcal{H}_{\rm ac}(T)$ (see Exercise 13.5.4), the result follows. □

Exercise 13.5.4. For $\xi \in \mathcal{H}_{\rm ac}(T)$ set $\Omega_n := \{x \in \mathbb{R} : \frac{d\mu_\xi}{d\ell}(x) \le n\}$. Use dominated convergence to show that $\xi_n := \chi_{\Omega_n}(T)\xi \to \xi$ as $n \to \infty$ in $\mathcal{H}$. Conclude that

$$\left\{ \eta \in \mathcal{H}_{\rm ac}(T) : \frac{d\mu_\eta}{d\ell} \text{ is a bounded function} \right\} \sqsubseteq \mathcal{H}_{\rm ac}(T),$$

and for η in this set, $\int_{\mathbb{R}} p_{\zeta,\eta}(t)\, dt \le 2\pi \|\zeta\|^2 \|d\mu_\eta/d\ell\|_\infty^2$, for all $\zeta \in \mathcal{H}$.

The following interesting characterizations of the continuous subspaces, in terms of the time decay rate of the return probability, are consequences of the above results.

Corollary 13.5.5. *Let T be self-adjoint.*

i) $\mathcal{H}_{\mathrm{ac}}(T) = \overline{\{\xi \in \mathcal{H} : p_\xi(t) \in \mathrm{L}^1(\mathbb{R})\}}$.

ii) *If there exist $c, \varepsilon > 0$ so that for large $|t|$,*

$$p_\xi(t) \le \frac{c}{|t|^{1+\varepsilon}},$$

then $\xi \in \mathcal{H}_{\mathrm{ac}}(T)$.

Proof. i) By Lemma 13.5.2 the set

$$\Omega = \{\xi \in \mathcal{H} : p_\xi(t) \in \mathrm{L}^1(\mathbb{R})\} \subset \mathcal{H}_{\mathrm{ac}}(T),$$

and since $\mathcal{H}_{\mathrm{ac}}(T)$ is a closed subspace $\overline{\Omega} \subset \mathcal{H}_{\mathrm{ac}}(T)$. From the proof of Theorem 13.5.3 it follows that every $\eta \in \mathcal{H}_{\mathrm{ac}}(T)$ with bounded Radon-Nikodym derivative $\frac{d\mu_\eta}{d\ell}$ belongs to Ω, but this set is dense in $\mathcal{H}_{\mathrm{ac}}(T)$. Hence $\overline{\Omega} = \mathcal{H}_{\mathrm{ac}}(T)$.

ii) It is immediate from i) since in this case the given (bounded) function $t \mapsto p_\xi(t)$ belongs to $\mathrm{L}^1(\mathbb{R})$. □

Corollary 13.5.6. *Let T be self-adjoint.*

i) *$\xi \in \mathcal{H}_{\mathrm{c}}(T)$ with $P_{\mathrm{sc}}(T)\xi \neq 0$ iff $\mathfrak{X}_\xi = 0$ and there exists an open set $\emptyset \neq X(\xi) \subset \mathcal{H}$ so that*

$$\int_{\mathbb{R}} p_{\eta,\xi}(t)\, dt = \infty, \qquad \forall \eta \in X.$$

ii) *If $0 \neq \xi \in \mathcal{H}_{\mathrm{sc}}(T)$, then $\mathfrak{X}_\xi = 0$ and $\int_{\mathbb{R}} p_\xi(t)\, dt = \infty$.*

Proof. By Theorem 13.3.7, $\mathfrak{X}_\xi = 0$ iff $\xi \in \mathcal{H}_{\mathrm{c}}(T)$. Theorem 13.5.3 implies the existence of the open set $X(\xi)$, and i) follows. If $\xi \in \mathcal{H}_{\mathrm{sc}}(T)$, then $p_\xi \notin \mathrm{L}^1(\mathbb{R})$ by Corollary 13.5.5; this is ii). □

Note that if $\xi \in \mathcal{H}_{\mathrm{p}}(T)$, then $\int_{\mathbb{R}} p_\xi(t)\, dt = \infty$ but $\mathfrak{X}_\xi \neq 0$; this is obvious for eigenvectors, and the general case follows by Corollary 13.5.5i). The elements of the singular continuous subspace present a "weak time recurrence," characterized by a null average return probability $\mathfrak{X}_\xi = 0$ and infinite sojourn time (defined on page 359)!

Exercise 13.5.7. Define $\mathcal{H}_{\mathrm{w}}(T) := \{\xi \in \mathcal{H} : e^{-itT}\xi \xrightarrow{\mathrm{w}} 0 \text{ as } t \to \infty\}$. Show that:

a) $\mathcal{H}_{\mathrm{w}}(T) = \{\xi \in \mathcal{H} : p_\xi(t) \to 0 \text{ as } t \to \infty\}$.

b) $e^{-itT}\mathcal{H}_{\mathrm{w}}(T) = \mathcal{H}_{\mathrm{w}}(T)$, $\forall t \in \mathbb{R}$, and $\mathcal{H}_{\mathrm{ac}} \subset \mathcal{H}_{\mathrm{w}} \subset \mathcal{H}_{\mathrm{c}}$.

Remark 13.5.8.

i) There are examples [Sin77] of vectors $0 \neq \xi \in \mathcal{H}_{\mathrm{sc}}(T)$ so that, for large $|t|$,

$$p_\xi(t) \sim \frac{(\ln t)^4}{t},$$

and so "$p_\xi(t) \sim 1/t^{1-\varepsilon}$ for any $\varepsilon > 0$." Compare with Corollary 13.5.5.

ii) There are examples of singular continuous measures for which the time average is necessary in Wiener's lemma. For instance, some measures associated with Riesz products [Que87] or the autocorrelation measure of the Thue-Morse substitution sequence [AlMF95].

iii) The elements of $\mathcal{H}_{\mathrm{w}}(T)$ are those for which the conclusion of the Riemann-Lebesgue lemma holds for their spectral measures. Such measures are called Rajchman measures and in general $\mathcal{H}_{\mathrm{w}}(T)$ is strictly larger than $\mathcal{H}_{\mathrm{ac}}(T)$ [Sin77]. See [Pol01] for a discussion about stability of Rajchman spectral measures.

Exercise 13.5.9. Let μ be a Borel measure over $\mathbb{R}$.

i) If μ is continuous, show that

$$\frac{1}{t}\int_0^t \hat{\mu}(s)\,ds \to 0, \qquad t \to \infty.$$

ii) If $\mu \ll \ell$ and its support is a Cantor set (i.e., nonempty, closed with empty interior and no isolated points), show that $\hat{\mu}(t) \notin \mathrm{L}^1(\mathbb{R})$.

To summarize, roughly, i.e., up to accumulation points, one dynamically characterizes the spectral subspaces discussed above as:

- $\mathcal{H}_{\mathrm{p}}$ are the vectors $\xi \in \mathcal{H}$ with nonzero asymptotic return probability

$$\lim_{t\to\infty} p_\xi(t) \neq 0,$$

  including an infinite sojourn time $\int_{\mathbb{R}} p_\xi(t)\,dt = \infty$.
- $\mathcal{H}_{\mathrm{ac}}$ are the vectors $\xi \in \mathcal{H}$ with zero average return probability $\mathfrak{X}_\xi = 0$ and a finite sojourn time $\int_{\mathbb{R}} p_\xi(t)\,dt < \infty$.
- The "exotic" subspace $\mathcal{H}_{\mathrm{sc}}$ are the vectors $\xi \in \mathcal{H}$ with zero average return probability $\mathfrak{X}_\xi = 0$, but with an infinite sojourn time $\int_{\mathbb{R}} p_\xi(t)\,dt = \infty$. A possible quantum interpretation is that this case presents to the particle a barrier into which it particle may penetrate arbitrarily far but is eventually reflected.

Exercise 13.5.10. By using the expression of the free evolution group e^{-itH_0} discussed in Section 5.5, conclude that H_0 is purely absolutely continuous.

13.6 Bound and Scattering States in $\mathbb{R}^n$

As discussed in Example 12.2.3, $[0,\infty)$ is the continuous spectrum of the energy operator H_H of the hydrogen atom and its point spectrum is contained in $(-\infty, 0]$. Then, by following previous interpretations in this chapter, negative energy values of H_H should correspond to the electron linked to the nucleus, while positive energy values should correspond to an *ionized atom*. Definition 13.6.1 and Example 13.6.10 provide a rigorous geometrical version of such statements.

Note also that, in the case of Coulomb interaction between two particles with electric charges of the same sign, the parameter $\kappa < 0$ and, by Corollary 6.2.9, there is no point spectrum for the subsequent Schrödinger operator. I.e., it is a mathematical proof that the particle is not bound to the nucleus in such case, a physically expected result.

For a large class of Schrödinger operators in $L^2(\mathbb{R}^n)$ the above discussion has a geometrical appealing viewpoint. Throughout this section $\mathcal{H} = L^2(\mathbb{R}^n)$ and T is a self-adjoint operator in $\mathcal{H}$, and for $\psi \in \mathcal{H}$ its trajectory is $t \mapsto \psi(t) = e^{-itT}\psi$.

The idea is to investigate whether the time evolution of an (normalized) initial condition ψ remains localized in some ball $B(0;r)$ for large times t, or whether it leaves any of such balls as $t \to \infty$. Set

$$F_r(x) := \chi_{B(0;r)}(x),$$

which is a bounded multiplication operator on $\mathcal{H}$, in fact an orthogonal projection; so

$$|\langle \psi(t), F_r\psi(t)\rangle|^2 = \|F_r\psi(t)\|^2$$

is interpreted in quantum mechanics as the probability of finding the system, with initial state ψ, in the ball $B(0;r)$ at time t. If F_r is replaced by $\mathbf{1} - F_r$ in this expression, then one gets the probability of finding the system outside the ball $B(0;r)$. The following concepts have been introduced in the literature (see, for instance, [AmG73]).

Definition 13.6.1. With respect to the self-adjoint T in $L^2(\mathbb{R}^n)$, the elements of

$$\mathcal{H}_{\text{bound}}(T) = \left\{\psi \in \mathcal{H} : \lim_{r\to\infty} \sup_{t\in\mathbb{R}} \|(\mathbf{1} - F_r)\psi(t)\|^2 = 0\right\}$$

are called *bound states*, while the elements of

$$\mathcal{H}_{\text{scatt}}(T) = \left\{\psi \in \mathcal{H} : \lim_{\tau\to\infty} \frac{1}{2\tau}\int_{-\tau}^{\tau} \|F_r\psi(t)\|^2\, dt = 0,\ \forall r > 0\right\}$$

are called *scattering* or *evanescent states*.

Remark 13.6.2. The presence of time average in the definition of $\mathcal{H}_{\text{scatt}}(T)$ is directly related to the Wiener Lemma 13.3.5 and the singular continuous subspace. Of course it is possible to include a definition without time average and it would be related mainly to the absolutely continuous spectrum; the interested reader is referred to [AmG73],[Am81].

Exercise 13.6.3.

a) Check that $\text{s} - \lim_{r\to\infty} F_r = \mathbf{1}$.
b) If $\phi \in \mathcal{H}_{\text{scatt}}(T)$, show that for all bounded borelian $\Lambda \subset \mathbb{R}^n$,

$$\lim_{\tau\to\infty} \frac{1}{2\tau}\int_{-\tau}^{\tau} \|F_\Lambda\phi(t)\|^2\, dt = 0.$$

Exercise 13.6.4. Since for real numbers a, b one has $2ab \le a^2 + b^2$, use the triangle inequality to conclude that, if ξ, η are vectors in a Hilbert space, then $\|\xi + \eta\|^2 \le 2\|\xi\|^2 + 2\|\eta\|^2$.

Proposition 13.6.5. *Let T be self-adjoint in $\mathrm{L}^2(\mathbb{R}^n)$.*

i) *$\mathcal{H}_{\text{bound}}(T)$ and $\mathcal{H}_{\text{scatt}}(T)$ are closed subspaces of $\mathcal{H}$ and, for all $t \in \mathbb{R}$,*

$$e^{-itT}\mathcal{H}_{\text{bound}}(T) = \mathcal{H}_{\text{bound}}(T), \qquad e^{-itT}\mathcal{H}_{\text{scatt}}(T) = \mathcal{H}_{\text{scatt}}(T),$$

that is, both subspaces are invariant under time evolution.

ii) *$\mathcal{H}_{\text{bound}}(T) \perp \mathcal{H}_{\text{scatt}}(T)$.*

iii) *$\mathcal{H}_{\text{bound}}(T) \supset \mathcal{H}_{\text{p}}(T)$ and $\mathcal{H}_{\text{scatt}}(T) \subset \mathcal{H}_{\text{c}}(T)$.*

Proof. i) A simple use of the triangle inequality shows that both sets are linear subspaces and their invariances under time evolution follow at once from the corresponding definitions. Now suppose that $(\psi_j) \subset \mathcal{H}_{\text{bound}}(T)$ with $\psi_j \to \psi$. Let $\varepsilon > 0$. Thus

$$\|(\mathbf{1} - F_r)\psi(t)\|^2 \le 2\|(\mathbf{1} - F_r)(\psi(t) - \psi_j(t))\|^2 + 2\|(\mathbf{1} - F_r)\psi_j(t)\|^2;$$

since the time evolution is unitary, take j large so that

$$\begin{aligned}\sup_t \|(\mathbf{1} - F_r)(\psi(t) - \psi_j(t))\|^2 &\le \sup_t \|\psi(t) - \psi_j(t)\|^2 \\ &= \|\psi - \psi_j\|^2 < \varepsilon,\end{aligned}$$

and then r large enough so that $\sup_t \|(\mathbf{1} - F_r)\psi_j(t)\|^2 < \varepsilon$. Hence,

$$\sup_t \|(\mathbf{1} - F_r)\psi(t)\|^2 < 4\varepsilon$$

for r large enough. This shows that $\psi \in \mathcal{H}_{\text{bound}}(T)$, consequently $\mathcal{H}_{\text{bound}}(T)$ is closed. In a similar way one shows that $\mathcal{H}_{\text{scatt}}(T)$ is closed.

ii) Let $\psi \in \mathcal{H}_{\text{bound}}(T)$ and $\phi \in \mathcal{H}_{\text{scatt}}(T)$. Pick $\varepsilon > 0$. Since the time evolution is unitary,

$$\begin{aligned}|\langle \psi, \phi\rangle|^2 &= \frac{1}{2\tau}\int_{-\tau}^{\tau} |\langle \psi, \phi\rangle|^2\, dt = \frac{1}{2\tau}\int_{-\tau}^{\tau} |\langle \psi(t), \phi(t)\rangle|^2\, dt \\ &= \frac{1}{2\tau}\int_{-\tau}^{\tau} |\langle \psi(t), F_r\phi(t)\rangle + \langle \psi(t), (\mathbf{1} - F_r)\phi(t)\rangle|^2\, dt \\ &\le \frac{2\|\psi\|^2}{2\tau}\int_{-\tau}^{\tau} \|F_r\phi(t)\|^2\, dt + \frac{2\|\phi\|^2}{2\tau}\int_{-\tau}^{\tau} \|(\mathbf{1} - F_r)\psi(t)\|^2\, dt.\end{aligned}$$

For r large enough $\sup_t \|(\mathbf{1} - F_r)\psi(t)\|^2 < \varepsilon$ so we take τ large so that

$$1/(2\tau)\int_{-\tau}^{\tau} \|F_r\phi(t)\|^2\, dt < \varepsilon,$$

resulting in $|\langle \psi, \phi\rangle|^2 < 2\varepsilon(\|\psi\|^2 + \|\phi\|^2)$. It follows that $\langle \psi, \phi\rangle = 0$.

iii) If ψ_λ is an eigenfunction of T with $T\psi_\lambda = \lambda\psi_\lambda$, then $\psi_\lambda(t) = e^{-it\lambda}\psi_\lambda$ and so, for all $t \in \mathbb{R}$, $\|(\mathbf{1} - F_r)\psi_\lambda(t)\| = \|(\mathbf{1} - F_r)\psi_\lambda\|$ which vanishes for $r \to \infty$. Thus any eigenfunction of T belongs to $\mathcal{H}_{\rm bound}(T)$, and since this vector space is closed one obtains $\mathcal{H}_{\rm p}(T) \subset \mathcal{H}_{\rm bound}(T)$. By ii),

$$\mathcal{H}_{\rm scatt}(T) \subset \mathcal{H}_{\rm bound}(T)^\perp \subset \mathcal{H}_{\rm p}(T)^\perp = \mathcal{H}_{\rm c}(T),$$

and the proof is complete. □

Theorem 13.6.6. *If T is a (self-adjoint) locally compact operator in* $\mathrm{L}^2(\mathbb{R}^n)$ *(Definition* 11.5.3*), then* $\mathcal{H}_{\rm bound}(T) = \mathcal{H}_{\rm p}(T)$ *and* $\mathcal{H}_{\rm scatt}(T) = \mathcal{H}_{\rm c}(T)$.

Proof. Let $\phi \in \mathcal{D} := \mathcal{H}_{\rm c}(T) \cap \mathrm{dom}\, T$; so $(T - i\mathbf{1})\phi \in \mathcal{H}_{\rm c}(T)$. By hypothesis, the operator $F_r R_i(T)$ is compact and the RAGE Theorem 13.4.1 implies that, for each $r > 0$,

$$\begin{aligned} \lim_{\tau\to\infty} \frac{1}{2\tau} \int_{-\tau}^{\tau} \|F_r\phi(t)\|^2\, dt &= \lim_{\tau\to\infty} \frac{1}{2\tau} \int_{-\tau}^{\tau} \|F_r R_i(T)(T - i\mathbf{1})\phi(t)\|^2\, dt \\ &= \lim_{\tau\to\infty} \frac{1}{2\tau} \int_{-\tau}^{\tau} \|F_r R_i(T) e^{-itT}(T - i\mathbf{1})\phi\|^2\, dt = 0. \end{aligned}$$

Hence $\phi \in \mathcal{H}_{\rm scatt}(T)$ and, since $\mathcal{D}$ is dense in $\mathcal{H}_{\rm c}(T)$ and $\mathcal{H}_{\rm scatt}(T)$ is closed, it follows that $\mathcal{H}_{\rm c}(T) \subset \mathcal{H}_{\rm scatt}(T)$. Combine with Proposition 13.6.5 to get $\mathcal{H}_{\rm c}(T) = \mathcal{H}_{\rm scatt}(T)$.

Finally, again by Proposition 13.6.5,

$$\mathcal{H}_{\rm bound}(T) \subset \mathcal{H}_{\rm scatt}(T)^\perp = \mathcal{H}_{\rm c}(T)^\perp = \mathcal{H}_{\rm p}(T)$$

and $\mathcal{H}_{\rm p}(T) = \mathcal{H}_{\rm bound}(T)$ is found. □

Corollary 13.6.7. *If* $V \in \mathrm{L}^2_{\rm loc}(\mathbb{R}^n)$, $V \geq \beta > -\infty$, *and H is the unique self-adjoint extension of* $H_0 + V$, dom $(H_0 + V) = C_0^\infty(\mathbb{R}^n)$, *then* $\mathcal{H}_{\rm bound}(H) = \mathcal{H}_{\rm p}(H)$ *and* $\mathcal{H}_{\rm scatt}(H) = \mathcal{H}_{\rm c}(H)$.

Proof. Combine Example 11.5.4 and Theorem 13.6.6. □

Example 13.6.8. For the free hamiltonian H_0 one has $\mathcal{H}_{\rm scatt}(H_0) = \mathrm{L}^2(\mathbb{R}^n)$, while for $V \in \mathrm{L}^2_{\rm loc}(\mathbb{R}^n)$, $V \geq \beta > -\infty$ with $\lim_{|x|\to\infty} V(x) = \infty$, by Theorem 11.5.6, one has $\mathcal{H}_{\rm bound}(H) = \mathrm{L}^2(\mathbb{R}^n)$, where H is the unique self-adjoint extension of $H_0 + V$.

Corollary 13.6.9. *If* $n \leq 3$, $V \in \mathrm{L}^2(\mathbb{R}^n) + \mathrm{L}^\infty(\mathbb{R}^n)$, *and H is the unique self-adjoint extension of* $H_0 + V$, dom $(H_0 + V) = C_0^\infty(\mathbb{R}^n)$, *then* $\mathcal{H}_{\rm bound}(H) = \mathcal{H}_{\rm p}(H)$ *and* $\mathcal{H}_{\rm scatt}(H) = \mathcal{H}_{\rm c}(H)$.

Proof. Recall that, by Theorem 6.2.2, the self-adjoint operator H is well posed and dom $H = $ dom $H_0 = \mathcal{H}^2(\mathbb{R}^n)$. Let Λ be a bounded borelian subset of $\mathbb{R}^n$ and $F_\Lambda(x) := \chi_\Lambda(x)$. The second resolvent identity implies

$$F_\Lambda R_i(H) = F_\Lambda R_i(H_0) - F_\Lambda R_i(H_0) V R_i(H).$$

Since H_0 is locally compact and, by Exercise 6.1.12a), $VR_i(H) \in \mathrm{B}(\mathcal{H})$, it follows that $F_\Lambda R_i(H)$ is compact. Hence H is also locally compact and the result follows by Theorem 13.6.6. □

Example 13.6.10. For the hamiltonian H of the hydrogen atom in $\mathbb{R}^3$ (see Subsection 6.2.1 and Corollary 11.4.10) one has $\mathcal{H}_{\mathrm{bound}}(H) = \mathcal{H}_{\mathrm{p}}(H)$ and $\mathcal{H}_{\mathrm{scatt}}(H) = \mathcal{H}_{\mathrm{c}}(H)$. A parallel between classical and quantum mechanics of the hydrogen atom is particularly enlightening. The classical orbits with negative energy are ellipses (including the circumference), so they are bounded motions, whereas the orbits with positive energy are hyperbolas and parabolas, so they are unbounded motions. In quantum mechanics the negative part of the spectrum corresponds to $\mathcal{H}_{\mathrm{bound}}(H)$, while the positive to $\mathcal{H}_{\mathrm{scatt}}(H)$. How general such close classical-quantum correspondence holds is always an interesting question; see also Remark 13.6.11.

Remark 13.6.11. It is instructive to compare (a) and (b) below.

(a) The classical planar motions of a charged particle in a homogeneous magnetic field (perpendicular to the plane) is composed exclusively of circular motions, so one could expect pure point spectrum of the quantum energy operator. This was actually found in Section 12.4 with the Landau levels. Since for a fixed energy such circular motions are widespread over all $\mathbb{R}^2$, one has a classical interpretation of the quantum infinite multiplicity of Landau levels.

(b) For a "friendly" lower-bounded potential V with $V(x) \to \infty$ as $|x| \to \infty$ in $\mathbb{R}^n$, one gets only bounded classical motion so that purely point spectrum is expected for the quantum energy operator. Moreover, in contrast to the case of Landau levels, for a fixed energy the classical motions are restricted to a bounded set of $\mathbb{R}^n$, and one gets a classical interpretation of the found discrete spectrum proved in Theorem 11.5.6.

Remark 13.6.12. Recall that embedded eigenvalues are possible, as mentioned in Subsection 11.4.2. On account of the interpretations of $\mathcal{H}_{\mathrm{bound}}$ and $\mathcal{H}_{\mathrm{scatt}}$ one might guess that, from the physical point of view, eigenvalues embedded in the continuous spectrum should not occur; this makes the subject of embedded eigenvalues challenging and interesting.

Example 13.6.13. For some operators depending only on the position with purely continuous spectrum, say $T = \mathcal{M}_{x^2}$, since $F_r e^{-itx^2} = e^{-itx^2} F_r$ one has, for any $\psi \in \mathrm{L}^2(\mathbb{R}^n)$,

$$\|(\mathbf{1} - F_r)e^{-itT}\psi\| = \|e^{-itx^2}(\mathbf{1} - F_r)\psi\| = \|(\mathbf{1} - F_r)\psi\|$$

which vanishes as $r \to \infty$. Hence $\mathcal{H}_{\mathrm{bound}}(T) = \mathcal{H}_{\mathrm{c}}(T) = \mathrm{L}^2(\mathbb{R}^n)$. Consider the classical hamiltonian equations of motion (i.e., $\dot{x} = \partial T/\partial p, \dot{p} = -\partial T/\partial x$) corresponding to the hamiltonian $T(x,p) = x^2$ and "interpret this equality."

Exercise 13.6.14. Show that the conclusions in Example 13.6.13 hold for all $T = \mathcal{M}_\varphi$, with $\varphi : \mathbb{R}^n \to \mathbb{R}$ continuous.

13.7 α-Hölder Spectral Measures

At this point it is clear that there are sensible dynamical differences accomplished by point, absolutely and singular continuous spectra. Most of the results discussed so far are qualitative, in the sense of vanishing return probability or growth of expectation values of test operators (as defined in Section 13.3). Although some quantitative results (i.e., rate of vanishing or growth) have been discussed in Section 13.5, it should be interesting and useful to obtain more refined estimates; currently this is an active research area.

A way of getting such estimates is to assume specific hypotheses on spectral measures. Here, some dynamical consequences of an important ingredient, represented by the so-called uniformly α-Hölder measures (UαH, for short), will be discussed; related and more advanced material can be found in the references. In this section, several positive constants will be denoted by the same symbol C.

Definition 13.7.1. Let $\alpha \in [0,1]$. A (σ-finite positive) borelian measure μ over $\mathbb{R}$ is *uniformly α-Hölder* if there exists a constant $C > 0$ so that

$$\mu(I) \leq C\,\ell(I)^\alpha,$$

for any interval $I \subset \mathbb{R}$ with Lebesgue measure $\ell(I) < 1$.

Exercise 13.7.2. a) If μ is UαH, conclude that μ is UβH for any $0 \leq \beta < \alpha$.

b) Show that a purely point measure is UαH only for $\alpha = 0$.

c) If $\mu \ll \ell$ with bounded Radon-Nikodym derivative $d\mu/d\ell$, show that μ is U1H; this holds, in particular, for Lebesgue measure ℓ.

Exercise 13.7.2 indicates that, in some sense, the UαH measures μ interpolate between purely point measures ($\alpha = 0$) and absolutely continuous measures ($\alpha = 1$; at least for those with bounded density $d\mu/d\ell$). The point here is to assume that spectral measures μ_ξ^T of a self-adjoint operator T are UαH and so get "interpolated dynamical behavior" of $e^{-itT}\xi$. This idea was pioneered by Guarneri in a special case [Gua89], which was noticed by Combes to be directly related to a result in [Str90]; later on a simpler proof of the Strichartz result in case of finite measures appeared in [Las96] and is reproduced below.

Roughly speaking, UαH measures allow upper bounds of the decay rate of Fourier transforms of measures in Wiener's lemma. The time average of a function $u(t)$ of time t will be denoted by

$$\langle u\rangle(t) = \frac{1}{t}\int_0^t u(s)\,ds.$$

Theorem 13.7.3 (Strichartz). *If μ is a finite and* UαH *measure, then there is a constant $C_\mu > 0$ so that, for all $f \in \mathrm{L}^2_\mu(\mathbb{R})$,*

$$\left\langle \left| \int_{\mathbb{R}} e^{-ixs} f(x)\,d\mu(x) \right|^2 \right\rangle (t) \leq C_\mu\,\frac{\|f\|_2^2}{t^\alpha}, \qquad \forall t > 0.$$

Before proving Theorem 13.7.3, some application to the dynamics generated by a self-adjoint operator T, acting in $\mathcal{H}$, are discussed. The corresponding spectral measures will simply be denoted by μ_ξ, $\xi \in \mathcal{H}$.

Corollary 13.7.4. *If the spectral measure μ_ξ is absolutely continuous with respect to a* UαH *measure μ, with $d\mu_\xi/d\mu = f \in \mathrm{L}^2_\mu(\mathbb{R})$, then the average return probability satisfies*

$$\langle p_\xi \rangle(t) \le \frac{C}{t^\alpha},$$

for some $C > 0$ and all $t > 0$.

Proof. Since

$$p_\xi(t) = \left|\left\langle \xi, e^{-itT}\xi\right\rangle\right|^2 = \left|\int_{\mathbb{R}} e^{-itx}\, d\mu_\xi(x)\right|^2 = \left|\int_{\mathbb{R}} e^{-itx} f(x)\, d\mu_\xi(x)\right|^2$$

and μ_ξ is finite, the result follows immediately from Theorem 13.7.3, with $C = C_{\mu_\xi}\|f\|_2^2$. □

Corollary 13.7.5. *If μ_ξ is* UαH*, then there exists a constant $C = C(\xi) > 0$ so that for all $\eta \in \mathcal{H}$, $\|\eta\| = 1$, one has*

$$\langle p_{\xi,\eta} \rangle(t) \le \frac{C}{t^\alpha}, \qquad \forall t > 0.$$

Proof. By Lemma 13.3.6, for each $\eta \in \mathcal{H}$ there is $g \in \mathrm{L}^2_{\mu_\xi}(\mathbb{R}) \cap \mathrm{L}^1_{\mu_\xi}(\mathbb{R})$ so that $\|g\|_{\mathrm{L}^2_{\mu_\xi}} \le 1$ and

$$\langle \eta, e^{-itT}\xi \rangle = \int_{\sigma(T)} e^{-itx} g(x)\, d\mu_\xi(x).$$

An application of Theorem 13.7.3 completes the proof. □

Remark 13.7.6. a) If $\alpha > 0$, then Corollary 13.7.5 gives a more detailed version of the limit $\mathfrak{X}_\xi = 0$ in Theorem 13.3.7i).

b) In case of a purely point spectral measure one has $\alpha = 0$, and so Corollary 13.7.5 is consistent with the nonvanishing of the average return probability. Note that this can be used to give a solution to Exercise 13.7.2b).

In case of UαH spectral measures it is possible to say something about the growth rate of the expectation values of test operators A (see Section 13.3). Let $0 \le \lambda_1 < \lambda_2 < \lambda_3 \cdots$ denote the eigenvalues of the test operator A. For $s \in \mathbb{R}$ set $\lambda(s) := \lambda_{[s]}$, where $[s]$ indicates the integer part of s. First, a simple preparatory result.

Lemma 13.7.7. *Assume that μ_ξ is* UαH *and let $\xi(t) = e^{-itT}\xi$ be the orbit of ξ. Then there exists $C = C(\xi) > 0$ so that for any orthogonal projection P_F onto a finite-dimensional subspace F of $\mathcal{H}$, of dimension N, the time average*

$$\left\langle \|P_F\xi(t)\|^2 \right\rangle(t) \le \frac{CN}{t^\alpha}, \qquad \forall t > 0.$$

Proof. Let $\{\eta_1, \dots, \eta_N\}$ be an orthonormal basis of the subspace rng P_F, so that $P_F(\cdot) = \sum_{j=1}^N \langle \eta_j, \cdot \rangle \, \eta_j$. Thus,

$$\|P_F \xi(t)\|^2 = \langle \xi(t), P_F \xi(t) \rangle = \sum_{j=1}^N |\langle \eta_j, \xi(t) \rangle|^2 = \sum_{j=1}^N p_{\eta_j,\xi}(t).$$

Now take the time average and apply Corollary 13.7.5 to each $p_{\eta_j,\xi}$. □

Corollary 13.7.8. *Let T be the self-adjoint generator of a unitary time evolution group, and A a test operator. If μ_ξ is* UαH, *then there is a constant $C = C(\xi) > 0$ so that*

$$\left\langle \mathcal{E}_A^\xi \right\rangle (t) \geq \frac{1}{2} \lambda \left(C \, t^\alpha \right), \qquad \forall t > 1.$$

Proof. Let Q_N be the orthogonal projection onto the subspace spanned by the eigenvectors of A associated with its eigenvalues $\leq \lambda_N$. Since A has discrete spectrum, Q_N is a projection onto a finite-dimensional subspace; for simplicity of notation, assume that N is its dimension. Thus,

$$\begin{aligned} \langle \xi(t), A\xi(t) \rangle &= \langle Q_N \xi(t), A Q_N \xi(t) \rangle + \langle (\mathbf{1} - Q_N)\xi(t), A(\mathbf{1} - Q_N)\xi(t) \rangle \\ &\geq \lambda_N \langle (\mathbf{1} - Q_N)\xi(t), (\mathbf{1} - Q_N)\xi(t) \rangle \\ &= \lambda_N \|(\mathbf{1} - Q_N)\xi(t)\|^2 = \lambda_N \left[1 - \|Q_N \xi(t)\|^2 \right]. \end{aligned}$$

Taking the time average and using Lemma 13.7.7, it is found that

$$\left\langle \mathcal{E}_A^\xi \right\rangle (t) \geq \left(1 - \frac{CN}{t^\alpha} \right) \lambda_N = \left(1 - \frac{CN}{t^\alpha} \right) \lambda(N), \qquad \forall N.$$

Now choose $N = [t^\alpha/(2C)]$ and rename $1/(2C)$ as C. Thereby the proof is complete. □

Example 13.7.9. A typical application of the above results is to self-adjoint (tight-binding) hamiltonians $H : l^2(\mathbb{Z}) \to l^2(\mathbb{Z})$ and test operator $A = M$, the second *moment of the position operator*, that is, if $(e_j)_{j \in \mathbb{Z}}$ is the canonical basis of $l^2(\mathbb{Z})$, then

$$M(\cdot) = \sum_{j \in \mathbb{Z}} j^2 \langle e_j, \cdot \rangle \, e_j.$$

Assume $\|\xi\| = 1$; a large value of $M(\xi)$ means that the vector ξ is spread over large values of $|j|$ in $\mathbb{Z}$. The eigenvalues of M are the squares of integers and, except the null eigenvalue that is simple, the others have multiplicity 2. In this case, for $s > 0$, $\lambda(s) = [s]^2$, and if for an initial condition $\xi \in l^2(\mathbb{Z})$ the corresponding spectral measure is UαH, Corollary 13.7.8 implies

$$\left\langle \mathcal{E}_M^\xi \right\rangle (t) \geq C t^{2\alpha}.$$

This is a quantitative account, in case of a UαH spectral measure, of transport properties of $\xi(t)$ over $\mathbb{Z}$ as $t \to \infty$.

Remark 13.7.10. i) Note that the bounds in Corollaries 13.7.5 and 13.7.8 are quite suitable to numerical simulations; after the selection of a model, often one searches for a time exponent by plotting, for instance, $\ln[\langle \mathcal{E}_A^\xi \rangle(t)]$ as a function of $\ln t$.

ii) UαH measures are closely related to singular continuous and α-continuous measures, as well as to many "fractal-like dimensions" that have been proposed in the literature; see [Las96] and [Gua96]. For applications to specific models of one-dimensional quasicrystals see [DaL03] and references therein.

Remark 13.7.11. Some techniques have been proposed for the study of the growth of expectation values of test operators with no explicit mention of the spectral type; see the papers [GerKT04] and [DaT05].

Proof. **[Theorem 13.7.3]** Recall that, for $a > 0, b \in \mathbb{R}$,

$$\int_{\mathbb{R}} e^{-ax^2+ibx}\,dx = \sqrt{\frac{\pi}{a}}\,e^{-b^2/(4a)}$$

and that $\hat{\mu}$ denotes the Fourier transform of the measure μ. Note that the left-hand side of the inequality in Theorem 13.7.3 is $\left\langle |\widehat{f\mu}|^2 \right\rangle(t)$, that is, the time average of the Fourier transform of the measure $f\mu$.

Since $1 \le ee^{-s^2/t^2}$ for $0 \le s \le t$ and $f \in \mathrm{L}^2_\mu(\mathbb{R})$, one has a first estimate:

$$\begin{aligned}
\left\langle |\widehat{f\mu}|^2 \right\rangle(t) &= \frac{1}{t}\int_0^t |\widehat{f\mu}(s)|^2\,ds \le \frac{1}{t}\int_0^t ee^{-s^2/t^2}|\widehat{f\mu}(s)|^2\,ds \\
&\le \frac{e}{t}\int_{\mathbb{R}} ds\,e^{-s^2/t^2}|\widehat{f\mu}(s)|^2 \\
&= \frac{e}{t}\int_{\mathbb{R}} ds\,e^{-s^2/t^2}\int_{\mathbb{R}^2} d\mu(x)d\mu(y)\,f(x)\overline{f(y)}\,e^{-i(x-y)s} \\
&= \frac{e}{t}\int_{\mathbb{R}^2} d\mu(x)d\mu(y)\,f(x)\overline{f(y)}\int_{\mathbb{R}} ds\,e^{-s^2/t^2}e^{-i(x-y)s} \\
&= \frac{e}{t}\int_{\mathbb{R}^2} d\mu(x)d\mu(y)\,f(x)\overline{f(y)}\,\sqrt{\pi}\,t\,e^{-t^2(x-y)^2/4} \\
&= e\sqrt{\pi}\int_{\mathbb{R}^2} d\mu(x)d\mu(y)\,f(x)\overline{f(y)}\,e^{-t^2(x-y)^2/4} \\
&\le e\sqrt{\pi}\int_{\mathbb{R}^2} d\mu(x)d\mu(y)\,\left(|f(x)|e^{-t^2(x-y)^2/8}\right)\left(|f(y)|e^{-t^2(x-y)^2/8}\right) \\
&\overset{\text{CS}}{\le} e\sqrt{\pi}\left(\int_{\mathbb{R}^2} d\mu(x)d\mu(y)\,|f(x)|^2\,e^{-t^2(x-y)^2/4}\right)^{\frac{1}{2}} \\
&\quad\times\left(\int_{\mathbb{R}^2} d\mu(x)d\mu(y)\,|f(y)|^2\,e^{-t^2(x-y)^2/4}\right)^{\frac{1}{2}} \\
&= e\sqrt{\pi}\int_{\mathbb{R}} d\mu(x)\,|f(x)|^2\int_{\mathbb{R}} d\mu(y)\,e^{-t^2(x-y)^2/4};
\end{aligned}$$

CS stands for Cauchy-Schwarz inequality.

Now a second estimate. For fixed x, put

$$\Omega_n = \left\{ y \in \mathbb{R} : \frac{n}{t} \le |x-y| < \frac{n+1}{t} \right\}.$$

Since μ is UαH and for $t > 1$ one has $\ell(\Omega_n) \le 1/t < 1$, then

$$\begin{aligned}\int_{\mathbb{R}} d\mu(y)\, e^{-t^2(x-y)^2/4} &= \sum_{n=0}^{\infty} \int_{\Omega_n} d\mu(y)\, e^{-t^2(x-y)^2/4} \\ &\le \sum_{n=0}^{\infty} e^{-n^2/4} \int_{\Omega_n} d\mu(y) \le \sum_{n=0}^{\infty} e^{-n^2/4} \frac{C}{t^\alpha} \le \frac{C}{t^\alpha}.\end{aligned}$$

Together both estimates imply

$$\left\langle |\widehat{f\mu}|^2 \right\rangle (t) \le \frac{C}{t^\alpha} \|f\|_2^2, \qquad t > 1,$$

thereby completing the proof. □

Remark 13.7.12. If μ is a finite UαH measure, by taking $f = 1$ in the Strichartz theorem, the dynamical estimate

$$\langle |\hat{\mu}|^2 \rangle (t) \le \frac{C}{t^\alpha}$$

follows, and it implies some quantitative quantum estimates for the decay of the average return probability and lower bounds for expectation values of test operators. In [Las96] it is shown that such a dynamical estimate implies that μ is U$\frac{\alpha}{2}$H and not UβH for $\beta > \frac{\alpha}{2}$.

Chapter 14

Some Quantum Relations

Selected traditional quantum relations are discussed. The intention is roughly to complement a text connected to quantum dynamics with mathematical approaches to some quantum concepts; of course no exhaustive presentation should be expected and parallel reading of traditional books on quantum mechanics is highly recommended.

14.1 Hermitian $\times$ Self-Adjoint Operators

Starting with some quantum interpretations, in this short section a selection of arguments will be gathered together (maybe the best term should be "recalled") in order to justify the representation of quantum observables by self-adjoint operators, instead of just hermitian ones. It will consist of a combination of physical motivations and "reasonable assumptions," and the role played by the spectrum of such operators will arise in a rather natural way.

The usual space of quantum states of a particle is built of functions $\psi : \mathbb{R}^n \to \mathbb{C}$ (or defined on subsets of $\mathbb{R}^n$). If a certain particle system is in the state ψ and T is a linear operator that should represent a physical observable, according to quantum physics the quantities

$$\mathcal{E}_T^\psi := \langle \psi, T\psi \rangle \qquad \text{and} \qquad \mathrm{Prob}_\psi(\Lambda) = \int_\Lambda |\psi(x)|^2 \, dx$$

correspond, respectively, to the expectation value of measurements of T and the probability of finding the particle in the measurable set $\Lambda \subset \mathbb{R}^n$. Since the particle must be found somewhere in $\mathbb{R}^n$ (i.e., "it exists"), one has total probability

$$1 = \mathrm{Prob}_\psi(\mathbb{R}^n) = \int_{\mathbb{R}^n} |\psi(x)|^2 \, dx = \|\psi\|^2,$$

so the Hilbert space $L^2(\mathbb{R}^n)$ naturally appears and the states are supposed to be normalized $\|\psi\| = 1$. Since $\mathcal{E}_T^\psi$ is directly related to measurements in a laboratory (see a discussion on page 132), it should be a real number; so T is asked to be a hermitian operator, since in this case $\overline{\langle\psi, T\psi\rangle} = \langle T\psi, \psi\rangle = \langle\psi, T\psi\rangle$.

The time evolution of the initial state ψ is dictated by Schrödinger's equation

$$i\frac{\partial}{\partial t}\psi(x,t) = H\psi(x,t), \qquad \psi(x,0) = \psi,$$

with H the operator representing the total energy. Of course the normalization

$$\mathrm{Prob}_{\psi(x,t)}(\mathbb{R}^n) = \int_{\mathbb{R}^n} |\psi(x,t)|^2\, dx = 1$$

necessarily holds for all times t, and so the necessity of H being (besides hermitian) self-adjoint in order to have a unitary time evolution; see Chapter 5. Further, by the whole discussion regarding the spectral theorem, in case T is self-adjoint the values taken by $\mathcal{E}_T^\psi$ are computed from the spectrum $\sigma(T)$ of T (see also Exercise 2.4.18).

For an observable T with pure point spectrum and, say, eigenvalue $T\psi_\lambda = \lambda\psi_\lambda$, $\|\psi_\lambda\| = 1$, one has

$$\mathcal{E}_T^{\psi_\lambda} = \langle\psi_\lambda, T\psi_\lambda\rangle = \lambda\langle\psi_\lambda, \psi_\lambda\rangle = \lambda,$$

that is, the eigenvalues are especial expectation values, and in this particular case all measurements of T in the state ψ_λ will result in the value λ (transitions to states $\psi_{\lambda'}$ corresponding to different eigenvalues do not occur since $\langle\psi_\lambda, \psi_{\lambda'}\rangle = \delta_{\lambda,\lambda'}$). Since there are operators with no eigenvalues, it is assumed that the whole spectrum of a general observable is composed of possible measurable values. By Theorem 2.2.17, among closed hermitian operators the self-adjoint ones are exactly those with real spectrum, so self-adjointness is actually imposed to all observables; this is also supported by the fact that all spectral values of self-adjoint operators are approximate eigenvalues (Corollary 2.4.9). It is worth emphasizing that, as above, the particular case of eigenvalues has historically oriented the establishment of the role of the spectrum in quantum postulates.

Observe that expectation values do not necessarily belong to the spectrum. For example, if T is self-adjoint with two distinct eigenvalues λ_1, λ_2, $\lambda_1 < \lambda_2$, and corresponding normalized eigenvectors ξ_1, ξ_2, then $\xi = (\xi_1 + \xi_2)/\sqrt{2}$, is a possible normalized state of the system and (recall $\xi_1 \perp \xi_2$)

$$\mathcal{E}_T^\xi = \frac{1}{2}(\lambda_1 + \lambda_2),$$

and if $\sigma(T) \cap (\lambda_1, \lambda_2) = \emptyset$, then $\mathcal{E}_T^\xi \notin \sigma(T)$.

It was not the intention of the above discussion to begin with "first quantum principles" and logically deduce the mathematical foundations of quantum mechanics. Whether or not the discussion has illustrated that there is an attractive reciprocal link between the mathematical apparatus presented in this book and the physics of quantum mechanics, it was worthwhile!

14.2 Uncertainty Principle

In this section T and S are self-adjoint operators acting in the Hilbert space $\mathcal{H}$. Think of them as quantum observables. In general terms, the *uncertainty principle* states that if T, S do not commute, then in any experiment one can not measure both observables simultaneously with arbitrary precision. In what follows a quite general relation will be derived and then a specific case and physical consequences are discussed. The first version of the uncertainty principle was proposed by Heisenberg around 1925.

Theorem 14.2.1 (Uncertainty Principle). *For any $u, v \in \mathbb{R}$ and $\xi \in \text{dom}\,(ST) \cap \text{dom}\,(TS)$,*

$$\|(T - u\mathbf{1})\xi\| \; \|(S - v\mathbf{1})\xi\| \geq \frac{1}{2} \left|\langle (TS - ST)\xi, \xi\rangle\right|.$$

Equality occurs iff there is $a \in \mathbb{R} \cup \{\infty\}$ so that $(S - v\mathbf{1})\xi = ia(T - u\mathbf{1})\xi$.

Proof. Write $T - u = T - u\mathbf{1}$. A direct computation leads to

$$\begin{aligned}\langle (TS - ST)\xi, \xi\rangle &= \langle [(T-u)(S-v) - (S-v)(T-u)]\xi, \xi\rangle \\ &= \langle (S-v)\xi, (T-u)\xi\rangle - \langle (T-u)\xi, (S-v)\xi\rangle \\ &= 2i\; \text{Im}\; \langle (S-v)\xi, (T-u)\xi\rangle.\end{aligned}$$

Now,

$$\left|\langle (TS - ST)\xi, \xi\rangle\right| \leq 2 \left|\langle (S-v)\xi, (T-u)\xi\rangle\right|,$$

with equality iff $\langle (S-v)\xi, (T-u)\xi\rangle$ is a purely imaginary number and, by Cauchy-Schwarz,

$$2 \left|\langle (S-v)\xi, (T-u)\xi\rangle\right| \leq 2\|(S-v)\xi\| \; \|(T-u)\xi\|,$$

with equality iff the set $\{(S-v)\xi, (T-u)\xi\}$ is linearly dependent. Combining these inequalities and properties the result follows. □

Exercise 14.2.2. Discuss details of the case $a = \infty$, i.e., $1/a = 0$, in the uncertainty principle.

The purely quantum nature of such a "principle" is evident by the presence of the *commutator* $[T, S] := TS - ST$ (see Section 14.3), which is always null in classical mechanics (where compositions are defined).

The spectral theorem implies

$$\|(T - u\mathbf{1})\xi\| = \left(\int_{\sigma(T)} (x-u)^2 d\mu_\xi^T(x) \right)^{\frac{1}{2}},$$

which is the second moment (also called standard deviation) of the spectral measure at u and can be interpreted as how disperses T is around u. Note that this dispersion $\|(T - u\mathbf{1})\xi\|$ is zero iff ξ is an eigenvector of T with eigenvalue u.

A particularly interesting choice of u is the expectation value $u_0 = \mathcal{E}_T^\xi = \langle \xi, T\xi \rangle$ at the initial time zero (see page 359 and Section 14.1). The same for $v = v_0 = \mathcal{E}_S^\xi$ in case of the observable S. It is important to realize that such dispersion is physically obtained through the average of measured values of T over a large set of identical systems, all prepared in the initial state ξ.

With such understanding, it should be clear that the uncertainty principle refers to statistical statements with respect to dispersion of average quantities, e.g., $\|(T - u_0\mathbf{1})\xi\|$. More precisely, in case T, S do not commute, such a principle states that in quantum mechanics the dispersion of T around u and the dispersion of S around v may not be simultaneously arbitrarily small, so that their product has the lower bound $\frac{1}{2}|\langle (TS - ST)\xi, \xi\rangle|$ (note that this lower bound does not depend on u, v). Thus, the greater precision of observable T implies less precision of S and vice versa.

Exercise 14.2.3. Discuss the uncertainty principle in case $TS\xi_0 = ST\xi_0$ or $(TS\xi_0 - ST\xi_0) \perp \xi_0$ for a particular normalized vector ξ_0.

The failure to uncover simultaneous values of T and S in quantum mechanics is not interpreted as the lack of success of measuring the corresponding properties of the system, but rather that the system does not have such properties exactly! For instance, one should avoid the supposition that an electron always has simultaneously a position and a momentum (see Corollary 14.2.4). These properties are in clear contrast to classical mechanics, for which all observables can, in principle, be simultaneously measured with arbitrary precision.

Vectors ξ for which equality in Theorem 14.2.1 holds, that is, solutions of the equation $(T - u\mathbf{1})\xi = ia(S - v\mathbf{1})\xi$, are called *minimum uncertainty states*.

In case $T = x$ is the position operator in $\mathrm{L}^2(\mathbb{R})$ and $S = P = -i\hbar\frac{d}{dx}$, the momentum operator with Planck constant $\hbar$ included, the uncertainty principle is important due to physical interpretations as well as historically.

Corollary 14.2.4. *If $\psi \in \mathrm{dom}\ (xP) \cap \mathrm{dom}\ (Px)$, then for any $u, v \in \mathbb{R}$,*

$$\|(x - u\mathbf{1})\psi\|\,\|(P - v\mathbf{1})\psi\| \geq \frac{\hbar}{2}\|\psi\|^2,$$

with minimum uncertainty states $\psi_{u,v}(x) = Ce^{ivx/\hbar}e^{-a(x-u)^2/\hbar}$, for some $C \in \mathbb{C}$ and $a > 0$. Note that $\mathcal{S}(\mathbb{R}) \subset \mathrm{dom}\ (xP) \cap \mathrm{dom}\ (Px)$.

Proof. The inequality follows by Theorem 14.2.1 and $Px\psi - xP\psi = -i\hbar\psi$. Equality holds iff $ia(x - u)\psi = (P - v)\psi$, $a \in \mathbb{R}$, and since x and P do not have eigenvalues, $a \neq 0$ and $a \neq \infty$. Hence

$$\psi'(x) = -\frac{a}{\hbar}(x - u)\psi(x) + i\frac{v}{\hbar}\psi(x),$$

whose solutions are those in the statement of the corollary and belongs to $\mathrm{L}^2(\mathbb{R})$ iff $a > 0$. □

Remark 14.2.5. The realization of momentum in $\mathrm{L}^2(\mathbb{R})$ as $P = -id/dx$ with domain $\mathcal{H}^2(\mathbb{R})$, and position as multiplication operator by x, is called *Schrödinger representation*; it appeared through the "wave-particle duality" in the initial development of quantum mechanics. From the mathematical side, important steps for such representations were introduction of the formal commutation relation $Px - xP = -i\mathbf{1}$ by Dirac [Dir58], followed by its version in terms of the corresponding unitary evolution groups (see Example 5.6.1)

$$e^{-itP}e^{-isx} = e^{ist}e^{-isx}e^{-itP}, \qquad t, s \in \mathbb{R},$$

which are called the Weyl form of this canonical commutation relation and cause no domain problems; finally von Neumann proved that, up to multiplicities, all pairs $G(t), U(s)$ of unitary evolution groups that satisfy Weyl relations are unitarily equivalent to e^{-itP} and e^{-isx}, respectively [Su01]. This result is considered the rigorous justification of the Schrödinger representation.

Remark 14.2.6. i) Quantum mechanics should somehow approach classical mechanics as $\hbar \to 0$. Note that this formally agrees with Corollary 14.2.4 and quantum effects are expected to be disregarded as $\hbar \to 0$.

ii) Quantum mechanics did not show up earlier in physics, with explicit manifestation of noncommutativity, because

$$\hbar = 1.054 \times 10^{-34}\,\text{joule} \cdot \text{second}$$

is too small for such effects to be readily observable.

iii) The interpretation of the uncertainty principle in case of position-momentum operators is that if the particle position stays close to its average position, then the momentum will largely fluctuate. Recall that both operators x and P have purely absolutely continuous spectrum so that both $\|(x - u\mathbf{1})\psi\|$ and $\|(P - v\mathbf{1})\psi\|$ are never zero.

iv) The uncertainty principle for position-momentum operators comes from the fact that functions localized in space $\mathbb{R}^n$ are not localized in Fourier space $\hat{\mathbb{R}}^n$, and conversely.

v) Corollary 14.2.4 has a direct generalization to the components of position x_j and momentum $P_j = -i\hbar\frac{\partial}{\partial x_j}$ in $\mathrm{L}^2(\mathbb{R}^n)$. The resulting inequalities are called *Heisenberg relations*.

Exercise 14.2.7.

(a) Show that the inequality in the position-momentum uncertainty principle is equivalent to

$$\|x\psi\|^2 + \|P\psi\|^2 \geq \hbar\|\psi\|^2.$$

(b) Consider the harmonic oscillator hamiltonian $H = P^2 + x^2$, $P = -i\hbar\frac{d}{dx}$. If ψ is a normalized minimum uncertainty state in Corollary 14.2.4, use (a) to show that the expectation value $\mathcal{E}_H^\psi = \langle \psi, H\psi \rangle = \hbar$, exactly the first eigenvalue of H; cf. Example 2.3.3.

Exercise 14.2.8. Consider the position-momentum variables on the circumference parametrized by $0 \le x < 1$, $P = -i\frac{d}{dx}$. If $\psi \in \text{dom } P$, then it is an absolutely continuous function and so $\psi(0) = \psi(1)$. Show that $\|x\psi\| \le \|\psi\|$, $\forall\psi$, and for $\psi \in \text{dom } (xP) \cap \text{dom } (Px)$ one has $\psi(0) = \psi(1) = 0$. Verify the uncertainty relation (as in Corollary 14.2.4 with $u = v = 0$) for $\psi(x) = \sin(2\pi x)$. What about the eigenfunctions e^{imx}, $m \in \mathbb{Z}$, of this "angular" momentum operator P?

Remark 14.2.9. Weyl was the first to recognize that Heisenberg's uncertainty principle could be stated in terms of second moments, but in the particular case of position and momentum operators. Then, Wiener noted that Weyl's approach was a relation between functions and their Fourier transforms and, in 1933, Hardy quantified this by proving, among other results, Hardy's inequality (Lemma 4.4.16) which is sometimes called the *uncertainty principle lemma*.

Remark 14.2.10. There is in physics a time-energy uncertainty relation, usually written in the form

$$\Delta t \, \Delta E \ge \frac{\hbar}{2}.$$

However, there are controversies with respect to its interpretation and formalization. In fact, a complete quantum mechanical theory of time measurements has not yet been elaborated. Nevertheless, there is a "popular" interpretation of such an uncertainty relation: Δt is interpreted as the duration of a perturbation process and ΔE is the obtained uncertainty of the energy in the system; for example, for an exact measurement of energy E, an infinite interval of time Δt is necessary.

The nature of such a time-energy uncertainty relation is quite different from the position-momentum uncertainty relation, since while the latter comes from the noncommutation of the respective operators, time appears in the theory as a parameter and there is no "time operator" in quantum mechanics. So "t" is referred to as "external time," the one measured by a clock.

As already indicated, currently there is no satisfactory mathematical formulation of time-energy uncertainty. The interested reader may consult the review [Bus07] and references therein.

For a survey of different versions of the uncertainty principle in mathematics consult [FS97], and for general results close to the optimal localization of both position and momentum (simultaneously) in the uncertainty principle see [BeP06].

14.3 Commuting Observables

If ξ_0 is a simultaneous (normalized) eigenvector of both self-adjoint operators T, S,

$$T\xi_0 = u\xi_0, \qquad S\xi_0 = v\xi_0,$$

then the subsequent expectation values are $\mathcal{E}_T^{\xi_0} = u$, $\mathcal{E}_S^{\xi_0} = v$ and $TS\xi_0 = vT\xi_0 = vu\xi_0 = ST\xi_0$, and consequently

$$[T, S]\xi_0 = TS\xi_0 - ST\xi_0 = 0.$$

This and the uncertainty principle motivate one important physical aspect of quantum mechanics: two observables can be simultaneously measured if the corresponding operators commute. However, due to domain intricacies, the notion of commuting observables is not self-evident for unbounded operators.

The next goal is to give a precise definition of commuting observables that includes the case of unbounded self-adjoint operators. If T, S are bounded operators in $\mathrm{B}(\mathcal{H})$ the definition is clear: they commute if $TS\xi = ST\xi$, for all $\xi \in \mathcal{H}$; in what follows, this is the meaning whenever two bounded operators are said to commute. Now this definition will be written in a suitable form (Lemma 14.3.1) so that the extension to unbounded operators becomes feasible (Definition 14.3.2); then its plausibility will be discussed (Propositions 14.3.3 and 14.3.5).

Lemma 14.3.1.

i) $T, S \in \mathrm{B}(\mathcal{H})$ *commute iff* $R_\lambda(T), R_\mu(S)$ *commute for all* $\lambda \in \rho(T)$ *and all* $\mu \in \rho(S)$.

ii) *Let* T *be self-adjoint and* $S \in B(\mathcal{H})$. *If for some* $\lambda \in \rho(T)$ *the operators* $R_\lambda(T), S$ *commute, then* $S(\mathrm{dom}\ T) \subset \mathrm{dom}\ T$ *and* $ST\xi = TS\xi$, $\forall \xi \in \mathrm{dom}\ T$.

Proof. i) If T, S commute, then

$$(S - \mu\mathbf{1})(T - \lambda\mathbf{1}) = (T - \lambda\mathbf{1})(S - \mu\mathbf{1}),$$

and since inverses are defined in $B(\mathcal{H})$ one gets

$$R_\lambda(T)R_\mu(S) = R_\mu(S)R_\lambda(T).$$

Conversely, if $R_\lambda(T)R_\mu(S) = R_\mu(S)R_\lambda(T)$ it follows that

$$(S - \mu\mathbf{1})(T - \lambda\mathbf{1}) = (T - \lambda\mathbf{1})(S - \mu\mathbf{1}),$$

consequently $ST = TS$.

ii) If $\xi \in \mathrm{dom}\ T$ write $\xi = R_\lambda(T)\eta$, $\eta \in \mathcal{H}$. Thus

$$S\xi = SR_\lambda(T)\eta = R_\lambda(T)S\eta$$

and so $S\xi \in \mathrm{dom}\ T$; hence $S(\mathrm{dom}\ T) \subset \mathrm{dom}\ T$. Now

$$\begin{aligned} ST\xi &= S\left((T - \lambda\mathbf{1}) + \lambda\mathbf{1}\right)R_\lambda(T)\eta = S\eta + \lambda SR_\lambda(T)\eta \\ &= S\eta + \lambda R_\lambda(T)S\eta = (T - \lambda\mathbf{1})R_\lambda(T)S\eta + \lambda R_\lambda(T)S\eta \\ &= TR_\lambda(T)S\eta = TSR_\lambda(T)\eta = TS\xi. \end{aligned}$$

This concludes the proof of the lemma. □

Definition 14.3.2. Two (possible unbounded) self-adjoint operators T and S *commute* if $R_\lambda(T), R_\mu(S)$ commute for all $\lambda, \mu \in \mathbb{C} \setminus \mathbb{R}$, that is, if their (bounded) resolvents commute. In this case it is also said that T, S are *commuting observables*.

The definition of commuting observables has also a dynamical flavor, which supports this definition:

Proposition 14.3.3. *Let* T, S *be self-adjoint operators and* $U_t = e^{-itT}$, $V_s = e^{-isS}$, $t, s \in \mathbb{R}$, *the corresponding unitary evolution groups. Then,* T, S *commute iff* U_t, V_s *commute for all* $s, t \in \mathbb{R}$.

Proof. Recall that (see Section 9.9), for all $\xi \in \mathcal{H}$,

$$e^{-itT}\xi = \lim_{n\to\infty}\left(1 + it\frac{T}{n}\right)^{-n}\xi, \qquad e^{-isS}\xi = \lim_{n\to\infty}\left(1 + is\frac{S}{n}\right)^{-n}\xi.$$

These expressions immediately infer that U_t, V_s commute if T, S commute. The formula (see page 245)

$$R_z(T) = -i\int_0^\infty e^{isz}e^{-isT}\, ds$$

is valid for $\operatorname{Im} z > 0$, and an analogous formula for $\operatorname{Im} z < 0$, together with Fubini's theorem, imply that T, S commute if U_t, V_s commute. □

Exercise 14.3.4. Present the missing details in the proof of Proposition 14.3.3.

Proposition 14.3.5. *If* T, S *commute, then:*

i) $\chi_\Lambda(T), \chi_\Omega(S)$ *commute for all open sets* Λ, Ω *in* $\mathbb{R}$.
ii) $f(T), g(S)$ *commute for all bounded continuous functions* $f, g : \mathbb{R} \to \mathbb{C}$.

Proof. i) For bounded open intervals (a, b) one has, as a consequence of the Stone formula (see page 244),

$$\chi_{(a,b)}(T) = \mathrm{s}-\lim_{\delta\to 0^+}\mathrm{s}-\lim_{\varepsilon\to 0^+}\frac{1}{2\pi i}\int_{a+\delta}^{b-\delta}\left(R_{t+i\varepsilon}(T) - R_{t-i\varepsilon}(T)\right)dt.$$

This expression (along with one analogous to S) and Fubini's theorem prove i) for bounded intervals. Since every open set is a countable pairwise disjoint union of such intervals (for an unbounded interval take a limit procedure, e.g., $\chi_{(a,\infty)}(T) = \mathrm{s}-\lim_{n\to\infty}\chi_{(a,n)}(T)$), the general case follows.

ii) Some results deduced in the proof of Proposition 10.1.9 will be used. If $\phi, \psi \in C_\infty(\mathbb{R})$, there are sequences of polynomials

$$p_j^\phi(R_i(T), R_{-i}(T)), \quad p_k^\psi(R_i(S), R_{-i}(S)),$$

so that

$$\phi(T) = \lim_{j\to\infty} p_j^\phi(R_i(T), R_{-i}(T)), \qquad \psi(S) = \lim_{k\to\infty} p_k^\psi(R_i(S), R_{-i}(S))$$

with convergence in B($\mathcal{H}$). By hypothesis, p_j^ϕ, p_k^ψ commute for all j, k. Thus, for each k,

$$\phi(T)p_k^\psi = \lim_{j\to\infty} p_j^\phi p_k^\psi = p_k^\psi \lim_{j\to\infty} p_j^\phi = p_k^\psi \phi(T),$$

and taking $k \to \infty$ one gets $\phi(T)\psi(S) = \psi(S)\phi(T)$, since $\phi(T)$ is a bounded operator. Hence $\phi(T), \psi(S)$ commute in case $\phi, \psi \in C_\infty(\mathbb{R})$.

If f, g are bounded continuous functions, there exist sequences f_j, g_k in $C_\infty(\mathbb{R})$ with

$$f(T) = \mathrm{s} - \lim_{j\to\infty} f_j(T), \qquad g(S) = \mathrm{s} - \lim_{k\to\infty} g_k(S),$$

and $f_j(T), g_k(S)$ commute, $\forall j, k$. Repeat the above argument to interchange the strong limits to conclude that $f(T), g(S)$ commute. □

Note that Proposition 14.3.3 follows by Proposition 14.3.5ii). It is possible to generalize such results, as indicated in Exercise 14.3.6. This subject is directly related to the quantum concept of a complete set of observables; see [deO90] and references therein.

Exercise 14.3.6. If T, S commute, show that $\chi_{\{t_0\}}(T), \chi_{\{s_0\}}(S)$ also commute for all $t_0, s_0 \in \mathbb{R}$.

Remark 14.3.7. It is natural to speculate whether T, S commute in case there is a common core $\mathcal{D}$ (and invariant under) of T and S and $TS\xi = ST\xi$, $\forall \xi \in \mathcal{D}$. However this is false; see the famous Nelson counterexample in [ReeS81].

Proposition 14.3.3 has a nice application to conservation laws. Let H be a hamiltonian of a quantum system and suppose S is a self-adjoint operator that commutes with H. Given an initial condition $\xi \in \mathcal{H}$ and the resulting weak solution $\xi(t) = e^{-itH}\xi$ of the Schrödinger equation for H $id\xi(t)/dt = H\xi(t)$ (see Example 5.4.1), then for any $s \in \mathbb{R}$ the trajectory $\xi_s(t) := e^{-isS}\xi(t)$ is also a solution; indeed,

$$\xi_s(t) = e^{-isS}e^{-itH}\xi = e^{-itH}e^{-isS}\xi$$

and so $\xi_s(t)$ is the weak solution with initial condition $e^{-isS}\xi$. Another nomenclature of commuting observables is given in

Definition 14.3.8. A unitary evolution group e^{-isS} that commutes with e^{-itH}, $\forall s, t \in \mathbb{R}$, is called a *symmetry* of H, or a *symmetry* of the corresponding Schrödinger equation for H.

Exercise 14.3.9. If e^{-isS} is a symmetry of H, show that $e^{-itH}\mathrm{dom}\ S = \mathrm{dom}\ S$ for all $t \in \mathbb{R}$.

Theorem 14.3.10 (Noether Theorem). *Let e^{-isS} be a symmetry of the self-adjoint operator H. If $\xi \in \mathrm{dom}\ S$, then the expectation value*

$$\mathcal{E}_S^\xi(t) = \langle \xi(t), S\xi(t)\rangle = \mathcal{E}_S^\xi(0), \qquad \xi(t) = e^{-itH}\xi,$$

i.e., the expectation value of the infinitesimal generator of the symmetry is constant with respect to time (a "conservation law" was found).

Proof. Since $0 = e^{-isS}e^{-itH}\xi - e^{-itH}e^{-isS}\xi$, $\forall s,t$, one has

$$\begin{aligned} 0 &= \frac{d}{ds}\left(e^{-isS}e^{-itH}\xi - e^{-itH}e^{-isS}\xi\right) \\ &= -ie^{-isS}\left(S\xi(t) - e^{-itH}S\xi\right). \end{aligned}$$

Thus $S\xi(t) = e^{-itH\xi}S\xi$ for all t, and so

$$\mathcal{E}_S^\xi(t) = \langle \xi(t), S\xi(t)\rangle = \left\langle e^{-itH}\xi, e^{-itH}S\xi\right\rangle = \langle \xi, S\xi\rangle = \mathcal{E}_S^\xi(0).$$

The theorem is proved. □

Exercise 14.3.11. Let e^{-isS} be a symmetry of H. If ξ_λ is an eigenvector $H\xi_\lambda = \lambda\xi_\lambda$, show that for all $s \in \mathbb{R}$ the vectors $e^{-isS}\xi_\lambda$ are also eigenvectors of H corresponding to the same eigenvalue λ. This is a strategy to find eigenvalues of large multiplicity, so that often it is said that "symmetry implies repeated eigenvalues." What if ξ_λ is also an eigenvector of S?

14.4 Probability Current

In this section the Hilbert space is $\mathcal{H} = \mathrm{L}^2(\mathbb{R}^n)$ (or $\mathrm{L}^2(\Omega)$ with $\Omega \subset \mathbb{R}^n$) and H will denote a self-adjoint realization of $-\Delta + V(x)$ in $\mathcal{H}$ with dom $H \subset \mathcal{H}^2(\mathbb{R}^n)$, meaning the energy operator of a particle. If $\psi \in$ dom H is normalized, then the unique solution to the Schrödinger equation (see Example 5.4.1)

$$i\frac{\partial\psi}{\partial t}(x,t) = H\psi(x,t), \qquad \psi(x,0) = \psi(x),$$

is $\psi(x,t) = e^{-itH}\psi(x)$, and the probability of finding the particle in a measurable set $\Lambda \subset \mathbb{R}^n$ at time t is

$$\mathrm{Prob}_{\psi(t)}(\Lambda) = \int_\Lambda |\psi(x,t)|^2\, dx.$$

Since the time evolution is unitary, $\mathrm{Prob}_{\psi(t)}(\mathbb{R}^n) = \|\psi(x,t)\|^2 = 1$ for all $t \in \mathbb{R}$. This leads to two interesting remarks. First $x \mapsto |\psi(x,t)|^2$ is interpreted as a *probability density* at time t; second, in general the probability density changes with time t and position x and so some kind of "probability flux" should pass through the boundaries of sets Λ. The concept of probability current quantifies such flux.

Definition 14.4.1. The *probability current* (or *probability current density*) of $\psi \in$ dom H, with $H\psi = -\Delta\psi + V\psi$, is

$$\mathbf{j}(x,t) := -i\left(\overline{\psi}\nabla\psi - \psi\nabla\overline{\psi}\right)(x,t) = 2\mathrm{Re}\,\left(-i\overline{\psi}(x,t)\nabla\psi(x,t)\right).$$

Although not explicitly indicated, $\mathbf{j}$ does depend on ψ.

Proposition 14.4.2. *If $\psi \in \operatorname{dom} H$, then* $\mathbf{j}$ *satisfies the continuity equation*

$$\frac{\partial |\psi(x,t)|^2}{\partial t} + \nabla \cdot \mathbf{j}(x,t) = 0.$$

Proof. One has

$$\frac{\partial |\psi(x,t)|^2}{\partial t} = \overline{\frac{\partial \psi(x,t)}{\partial t}}\psi(x,t) + \overline{\psi(x,t)}\frac{\partial \psi(x,t)}{\partial t}.$$

Since $\psi(x,t)$ satisfies Schrödinger equation and

$$-i\frac{\partial \overline{\psi}}{\partial t}(x,t) = -\Delta\overline{\psi(x,t)} + V(x)\overline{\psi(x,t)},$$

it is found that

$$\begin{aligned}\frac{\partial |\psi(x,t)|^2}{\partial t} &= i\left(\overline{\psi(x,t)}\Delta\psi(x,t) - \psi(x,t)\Delta\overline{\psi(x,t)}\right)\\ &= i\nabla\cdot\left(\overline{\psi(x,t)}\nabla\psi(x,t) - \psi(x,t)\nabla\overline{\psi(x,t)}\right)\\ &= -\nabla\cdot\mathbf{j}(x,t).\end{aligned}$$

The proposition is proved. □

Thus the probability current satisfies a continuity equation, which has analogues in many areas of science, and has the following consequence. Consider a bounded volume Λ in $\mathbb{R}^3$ whose boundary is the "smooth" closed surface $\partial\Lambda$; then the probability that the particle will enter Λ per unit time is $d\mathrm{Prob}_{\psi(t)}(\Lambda)/dt$, which, by the Gauss divergence theorem,

$$\frac{d}{dt}\mathrm{Prob}_{\psi(t)}(\Lambda) = \int_\Lambda \frac{\partial}{\partial t}|\psi(x,t)|^2\,dx = -\int_\Lambda \nabla\cdot\mathbf{j}\,dx = -\int_{\partial\Lambda}\mathbf{j}\cdot d\mathbf{s}.$$

Hence the surface integral of $\mathbf{j}(x,t)$ is the probability that the particle will cross this surface per unit time. So, if $\hat{\mathbf{n}}(x)$ is the unit vector normal to the surface and pointing to the outside direction, then $\mathbf{j}(x,t)\cdot\hat{\mathbf{n}}(x)$ is the probability density of the particle crossing unit area of this surface (from inside to outside) per unit time, supporting the promised interpretation of the current probability density. This construction can be generalized to $\mathbb{R}^n$; for instance, in case of an interval $\Lambda = (a,b) \subset \mathbb{R}$ one has (since $\psi \in \mathcal{H}^2$)

$$\frac{d}{dt}\mathrm{Prob}_{\psi(t)}(a,b) = -\int_a^b \frac{\partial \mathbf{j}}{\partial x}(x,t)\,dx = \mathbf{j}(a,t) - \mathbf{j}(b,t).$$

Furthermore, since the momentum operator is $P = -i\nabla$, which can be thought of as a velocity operator (recall that in classical mechanics $P = mv$, v denoting the particle velocity and here the mass $m = 1$), one has

$$\mathbf{j}(x,t) = 2\mathrm{Re}\ \left(\overline{\psi}(x,t)P\psi(x,t)\right)$$

and the probability current looks like the velocity P times a probability density.

Remark 14.4.3. If $\mathbf{g}(x)$ is a vector field in $\mathbb{R}^3$ given by the curl of a continuously differentiable vector field $\mathbf{u}$, that is, $\mathbf{g} = \nabla\times\mathbf{u}$, then $\nabla\cdot\mathbf{g} = 0$ and $\mathbf{j}+\mathbf{g}$ also satisfies the continuity equation. Hence, $\mathbf{j}$ is not uniquely defined; one concludes that the flux of $\mathbf{j}$ through a (proper) piece of a surface $\partial\Lambda$ depends on the choice of $\mathbf{g}$ and so can not be a physical observable. Nevertheless, due to the Gauss divergence theorem, the probability of the particle crossing the whole closed surface $\partial\Lambda$, i.e., $\int_{\partial\Lambda}\mathbf{j}\cdot d\mathbf{s}$, does not depend on the choice of $\mathbf{g}$ and so it is a physical observable quantity. In summary, only variations of probability in volumes Λ are meaningful. Here $\mathbf{j}$ always means $\mathbf{j} = -i\left(\overline{\psi}\nabla\psi - \psi\nabla\overline{\psi}\right)$.

Exercise 14.4.4. Work out the one-dimensional version of Remark 14.4.3.

Exercise 14.4.5. If ψ_λ is an eigenfunction $H\psi_\lambda = \lambda\psi_\lambda$ in $\mathrm{L}^2(\mathbb{R}^3)$, show that the probability density $|\psi(x,t)|^2$ is constant in time, inferring null probability flux across all smooth closed surfaces $\partial\Lambda$, that is,

$$\int_{\partial\Lambda}\mathbf{j}\cdot d\mathbf{s} = 0.$$

Note that this is in accordance with the dynamical properties of states in the point subspace $\mathcal{H}_{\mathrm{p}}(H)$ that were discussed in Chapter 13.

Exercise 14.4.6. Check that $\mathbf{j} = 0$ if ψ is a real function.

Exercise 14.4.7. Show that, for $V \in \mathrm{L}^2_{\mathrm{loc}}(a,b)$, $-\infty \le a < b \le +\infty$, and H as above, the map $x \mapsto \mathbf{j}(x,t)$ is continuous for any $\psi \in \mathrm{dom}\, H$.

Sometimes the probability current $\mathbf{j}$ can be used to select some self-adjoint extensions of a hermitian operator, as the following example illustrates.

Example 14.4.8. The self-adjoint extensions of the operator $C_0^\infty(0,1) \ni \psi \mapsto H\psi = -\psi''$ were found in Example 7.3.4; the deficiency indices are equal to 2 and so there are infinitely many self-adjoint extensions. Such extensions are candidates for describing the free energy particle operator in the interval $(0,1)$.

From the discussion in Example 7.3.4, those self-adjoint extensions are characterized by vanishing boundary form (for suitable $\psi,\varphi \in \mathrm{dom}\, H^*$)

$$0 = \Gamma(\psi,\varphi) = \overline{\psi(1)}\varphi'(1) - \overline{\psi'(1)}\varphi(1) - \overline{\psi(0)}\varphi'(0) + \overline{\psi'(0)}\varphi(0).$$

Since in this one-dimensional case $\mathbf{j} = -i(\overline{\psi}\psi' - \psi\overline{\psi'})$, the vanishing of the boundary form $\Gamma(\psi,\psi)$ is equivalent to the physical condition of no net probability flux across the boundary (the set $\{0,1\}$ is the boundary of $(0,1)$), that is,

$$0 = -i\Gamma(\psi,\psi) = \mathbf{j}(1,t) - \mathbf{j}(0,t) = \int_0^1 \nabla\cdot\mathbf{j}\,dx.$$

What are the self-adjoint extensions of H that satisfy $\mathbf{j}(0,t) = 0 = \mathbf{j}(1,t)$, $\forall t$, for all ψ in their domains? This condition is equivalent to

$$\overline{\psi(0)}\psi'(0) - \psi(0)\overline{\psi'(0)} = 0 = \overline{\psi(1)}\psi'(1) - \psi(1)\overline{\psi'(1)}.$$

Thus, there are $\kappa, \gamma \in \mathbb{R} \cup \{\infty\}$ so that $\psi'(0) = \kappa\psi(0)$ and $\psi'(1) = \gamma\psi(1)$; the Dirichlet boundary condition at 0, say, corresponds to $\kappa = \infty$ (similarly for $\gamma = \infty$). Hence, these are necessary conditions on elements of the domains of the required self-adjoint extensions and actually they correspond to the self-adjoint extensions $H_{\kappa,\gamma}$ of H presented in the following.

For fixed κ, γ put

$$\text{dom } H_{\kappa,\gamma} = \{\psi \in \text{dom } H^* : \psi'(0) = \kappa\psi(0), \psi'(1) = \gamma\psi(1)\}$$

and $H_{\kappa,\gamma}\psi = -\psi''$. It is then found that $\Gamma(\psi, \varphi) = 0$ for all $\psi, \varphi \in \text{dom } H_{\kappa,\gamma}$, and these are the self-adjoint extensions for which $\mathbf{j}(0,t) = 0 = \mathbf{j}(1,t)$, as required. Note that such conditions hold true at any instant of time t, for the domain of each self-adjoint extension $H_{\kappa,\gamma}$ is invariant under the corresponding time evolution $e^{-itH_{\kappa,\gamma}}$.

Exercise 14.4.9. Check the existence of κ, γ in Example 14.4.8, and that $H_{\kappa,\gamma}$ are self-adjoint extensions as indicated therein.

Exercise 14.4.10. Consider the self-adjoint extensions $H_{\hat{U}}$ of the initial energy operator of the one-dimensional H-atom, discussed in Subsection 7.4.1. Show that:

1. $0 = \langle H_{\hat{U}}\varphi, \varphi\rangle = \langle \varphi, H_{\hat{U}}\varphi\rangle = i \lim_{\varepsilon\to 0}[j(\epsilon) - j(-\varepsilon)]$, $\forall \varphi \in \text{dom } H_{\hat{U}}$, and conclude that $j(0)$ can be defined so that j is continuous at the origin. Since $j(\pm\infty) = 0$,

$$j(0) = j(0^-) = \int_{-\infty}^{0} \nabla \cdot j \, dx$$

   and $j(0)$ represents the net probability flux leaving $(-\infty, 0)$; similarly it is concluded that $j(0)$ represents the net probability flux leaving $(0, \infty)$. Hence, a zero value of $j(0)$ means that the origin is *impermeable* so that the Coulomb singularity acts as a barrier that does not allow the electron to pass through it.

2. $j(0) = \lim_{x\to 0^\pm} \text{Im } [\overline{\varphi(x)}\varphi'(x)] = \lim_{x\to 0^\pm} \text{Im } [\overline{\varphi(x)}\tilde{\varphi}(x)]$.

3. In case $(\mathbf{1} - \hat{U})$ is invertible, write $A = i\left(\mathbf{1} + \hat{U}\right)^{-1}\left(\mathbf{1} - \hat{U}\right)$, a self-adjoint matrix, so it can be put in the form

$$A = \begin{pmatrix} a & z \\ \bar{z} & b \end{pmatrix}, \qquad a, b \in \mathbb{R}, z \in \mathbb{C},$$

   and

$$j(0) = \lim_{x\to 0^+} \text{Im } [z\tilde{\varphi}(x)\varphi'(x)], \qquad \varphi \in \text{dom } H_{\hat{U}}.$$

4. Conclude that if $z = 0$ then $j(0) = 0$ for all $\varphi \in \text{dom } H_{\hat{U}}$, that is, the origin is impermeable for such self-adjoint extensions.

Finally, discuss the analogous situation in case $(\mathbf{1} + \hat{U})$ is invertible.

Exercise 14.4.11. Write $\psi(x,t) = |\psi(x,t)|\, e^{i\theta(x,t)}$ and show that (suppose all operations are meaningful)

$$\mathbf{j}(x,t) = |\psi(x,t)|^2\, \nabla\theta(x,t).$$

Conclude that $\mathbf{j}$ points to the direction of maximum increasing phase θ.

Remark 14.4.12. With all physical constants included, the probability current density takes the form

$$\mathbf{j}(x,t) = -i\frac{\hbar}{2m}\left(\overline{\psi(x,t)}\nabla\psi(x,t) - \psi(x,t)\nabla\overline{\psi(x,t)}\right).$$

14.5 Ehrenfest Theorem

It is hard not to consider the relations between classical and quantum mechanics interesting. Quantum mechanics was, in fact, built on classical considerations, with suitable adaptations and innovative concepts; however, at first sight it does not sound natural that the laplacian $-\Delta$ plays the role of quantum kinetic energy in $\mathrm{L}^2(\mathbb{R}^n)$. The study of the classical-quantum relations, in one form or another, still occupies many people and with different types of results. Here a very few aspects will be mentioned in order to illustrate how such relations can emerge: the Ehrenfest theorem and the WKB approximation.

The force generated by a given potential $V : \mathbb{R}^n \to \mathbb{R}$ on a classical particle of mass m is $F(x) = -\nabla V(x)$. If P denotes the particle momentum, Newton's second law reads

$$\frac{dP}{dt}(t) = m\frac{d^2x}{dt^2}(t) = F(x(t)).$$

There is a quantum version of this law, the so-called Ehrenfest theorem, with the limitations naturally imposed by the uncertainty principle and quantum interpretations. In any event, it is a support for the Schrödinger equation and the usual operator correspondences for positions, momenta and energy in quantum mechanics.

Consider the expectation values

$$\mathcal{E}_x^\psi(t) = \langle\psi_t, x\psi_t\rangle, \qquad \mathcal{E}_P^\psi(t) = \langle\psi_t, P\psi_t\rangle, \qquad \mathcal{E}_F^\psi(t) = \langle\psi_t, F(x)\psi_t\rangle,$$

with $\psi_t = e^{-itH}\psi$ and H a self-adjoint realization of $\frac{1}{2m}P^2 + V(x)$ in $\mathrm{L}^2(\mathbb{R}^n)$ with initial domain $\mathcal{S}(\mathbb{R}^n)$; also assume that $V(\mathcal{S}(\mathbb{R}^n)) \subset \mathcal{S}(\mathbb{R}^n)$.

Theorem 14.5.1 (Ehrenfest Theorem). *If $\psi_t \in \mathcal{S}(\mathbb{R}^n)$ for all $t \in (a,b)$, then for t in such an interval the function $t \mapsto \mathcal{E}_P^\psi(t)$ is differentiable, $t \mapsto \mathcal{E}_x^\psi(t)$ is twice differentiable and the following relations hold*

$$\frac{d}{dt}\mathcal{E}_P^\psi(t) = \mathcal{E}_F^\psi(t), \qquad m\frac{d}{dt}\mathcal{E}_x^\psi(t) = \mathcal{E}_P^\psi(t), \qquad m\frac{d^2}{dt^2}\mathcal{E}_x^\psi(t) = \mathcal{E}_F^\psi(t).$$

Proof. Compute

$$\begin{aligned}\frac{d}{dt}\mathcal{E}_P^{\psi}(t) &= \langle -iH\psi_t, P\psi_t\rangle + \langle \psi_t, P(-iH)\psi_t\rangle \\ &= \langle \psi_t, i(HP-PH)\psi_t\rangle = \langle \psi_t, F(x)\psi_t\rangle,\end{aligned}$$

since $i(HP - PH) = -\nabla V(x) = F(x)$, and the first relation follows if such manipulations are justified. Note that the hypotheses on ψ_t imply that, for all $t \in (a, b)$, $\{x\psi_t, P\psi_t, H\psi_t\} \subset \mathcal{S}(\mathbb{R}^n)$ and so

$$\psi_t \in \text{dom } (HP - PH) \cap \text{dom } (Hx - xH), \qquad \forall t \in (a, b),$$

justifying the above manipulations. The second relation is obtained in a similar way, taking into account that $im(Hx - xH)\psi_t = P\psi_t$. The third relation follows by differentiating the second one. □

Therefore, it was found that under certain conditions Newton's law and the relation $mdx/dt = P$ have a quantum parallel in terms of expectation values.

Another way some traditional equations of classical mechanics show up in quantum mechanics is via the WKB approximation (after Wentzel, Kramers and Brillouin; sometimes the name of Jeffreys is added to this list). Since this approximation is a "semiclassical" one, the parameter $\hbar$ will appear explicitly. Here the derivations will have the general character of formal calculations and physical heuristic arguments. Write

$$\psi_t(x) = A(x,t)e^{iS(x,t)/\hbar}$$

in terms of two unknown real functions $A(x, t), S(x, t)$, and insert into the Schrödinger equation

$$-i\hbar\frac{\partial\psi}{\partial t}(x,t) = -\frac{\hbar^2}{2m}\Delta\psi(x,t) + V(x)\psi(x,t),$$

so that, after some algebra,

$$i\hbar\frac{\partial A}{\partial t} - A\frac{\partial S}{\partial t} = -\frac{\hbar^2}{2m}\left(\Delta A + 2\frac{i}{\hbar}\nabla A\cdot\nabla S + \frac{i}{\hbar}A\Delta S - \frac{1}{\hbar^2}A(\nabla S)^2\right) + VA.$$

Equating real and imaginary parts one finds two equations

$$\begin{aligned}\frac{\hbar^2}{2mA}\Delta A &= \frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 + V,\\ 0 &= \frac{\partial A}{\partial t} + \frac{A}{2m}\Delta S + \frac{1}{m}\nabla A\cdot\nabla S.\end{aligned}$$

Multiply the second of these equations by $2A$ and rewrite it as

$$\frac{\partial A^2}{\partial t} + \nabla\cdot\left(\frac{A^2}{m}\nabla S\right) = 0,$$

and one recognizes the continuity equation for the probability current discussed in Section 14.4 (note that $|\psi_t|^2 = A^2$; see Exercise 14.4.11). By looking at the first equation one sees that the left-hand side is proportional to $\hbar^2$, while this parameter does not appear on the right; by neglecting the term proportional to $\hbar^2$ the Hamilton-Jacobi equation of classical mechanics

$$\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 + V = 0$$

is obtained; hence S is identified with the classical action. Often, the use of these solutions is called the *semiclassical* approximation. In summary, in such an approximation the wave function phase S is calculated directly from solutions of the classical Hamilton-Jacobi equation of motion and the amplitude A from the continuity equation (in many situations A can be calculated from S through van Vleck formula!), and they provide a way to understand the transition from classical to quantum mechanics.

Customarily, the term semiclassical physics may refer to two different approaches to the classical-quantum connection. Starting from quantum mechanics one tries to recover the classical one when $\hbar \to 0$, whereas in the other procedure classical mechanics is used to get estimations of the quantum behaviour for small $\hbar$. Rather recently the search for a quantum counterpart of "chaotic motion" in classical mechanics has increased the interest in the subject; from the purely physical point of view see [Gut90] and [BraB03].

Different approaches to mathematical aspects of the semiclassical limit are exemplified with the references [Hag85], [Hel88] and [HiS96]; a recent approach that emphasizes pseudodifferential operators is discussed in [Ro98].

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