Valter Moretti

Fundamental Mathematical Structures of Quantum Theory

Spectral Theory, Foundational Issues, Symmetries, Algebraic Formulation

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Introduction

This book faithfully reflects and perfects the 63-h MSc course, *Mathematical Physics: Quantum and Quantum-Relativistic Theories*, I taught at Trento University in the academic year 2017–2018. (That course is a sweeping expansion of the mini-course held at the "XXIV International Fall Workshop on Geometry and Physics" in Zaragoza in September 2015.) The overall intention is to present the machinery needed to formalize and develop physics' ideas about quantum theories in Hilbert spaces both rigorously and in a concise and self-contained way. Notably, the last chapter eyes the C^*-algebra formulation and proves the basic relevant propositions of that theory. Chapter 5 addresses issues related to the philosophical foundations of quantum theories, such as realism, non-contextuality, and locality.

As a matter of fact, the reader is introduced to the beautiful web of mutual connections existing between logic, lattice theory, probability, and spectral theory, including the basic theory of von Neumann algebras that underpins the mathematics of quantum theories. This book should appeal to a dual readership: on one hand mathematicians who wish to acquire the tools that unlock the physical aspects of quantum theories and on the other physicists eager to solidify their understanding of the mathematical scaffolding of quantum theories. Several examples and solved exercises accompany the mathematical statements—most of which carefully demonstrated—and physical motivations are provided for every mathematical notion. That said, I must point out that *this is not a manual on (higher) quantum mechanics*. There are many (very good) books that treat standard or advanced material such as the Schrödinger equation using the proper machinery of PDEs, for which reason those topics are not found here.

Some of the present contents appear in [Mor18], other parts are completely new, for instance Chap. 5, the last section of Chap. 6, and some material in Chap. 8. Despite a good degree of ideological overlap, [Mor18] is more complete mathematically, but its 950+ pages do not make it suitable for a single Master course. Most of the proofs here are in fact novel, because they were developed autonomously to reflect the relative conciseness of the lectures to which this text is a companion.

The book is organized as follows.

Chapter 1 is a brisk review of elementary facts and properties typical of quantum systems, either of physical or mathematical nature. I have not explored the full depth of the mathematical details, but pointed out instead a number of technical issues that crop up even in a naive approach.

The closely related Chaps 2 and 3 present technical definitions and results of functional analysis and spectral theory on complex Hilbert spaces, H, including the classical theorems on the spectral decomposition of (unbounded) self-adjoint operators and bounded normal operators and the so-called measurable functional calculus. The proofs are unabridged and self-contained. This machinery is eventually put to use toward the elementary yet rigorous formulation of quantum mechanics (QM) in infinite-dimensional Hilbert spaces.

The mathematical structure of QM is investigated in Chap. 4 from a more sophisticated viewpoint, namely, through orthomodular lattices. The framework allows one to justify various basic assumptions of QM, like the mathematical nature of observables as self-adjoint operators or quantum states as trace-class operators. Thus, quantum theory turns out to be the theory of probability measures on the non-Boolean lattice $\mathscr{L}(\mathsf{H})$ of elementary observables. A key tool of that analysis is the theorem of Gleason that characterizes probability measures on $\mathscr{L}(\mathsf{H})$ in terms of trace-class operators, a special kind of compact operators.

Chapter 5 deals with the foundations of quantum theory. Some of the relevant issues are implications of Gleason's theorem and concern hidden-variable interpretations of QM such as the Kochen-Specker theorem and the related notions of *realism* and *non-contextuality*. We then examine the famous Bell (BCHSH) inequality and the entanglement phenomenon, in relation to locality, causality, and the less considered problem of contextuality.

After introducing von Neumann algebras, their properties and physical significance, in Chap. 6, we focus on the algebra of observables in the presence of superselection rules. Several physical technicalities are addressed with the help of this machinery, to name but a few, the notions of factor, maximal sets of compatible observables, and their use in the preparation of quantum states, superselection rules, and gauge groups.

Chapter 7 tackles quantum symmetries, illustrated in terms of the Wigner and Kadison theorems. We discuss basic facts about groups of quantum symmetries, especially in relation to the problem of their unitarization. We state Bargmann's condition and focus on strongly continuous one-parameter unitary groups. We prove von Neumann's theorem and the celebrated Stone theorem and highlight the latter's role in describing the time evolution of quantum systems. The quantum formulation of Noether's theorem closes this part. The chapter's final section introduces elementary results on continuous unitary representations of Lie groups: in particular, a theorem by Nelson proposes sufficient conditions for lifting (anti-)self-adjoint representations of Lie algebras to unitary representations of associated simply connected Lie groups.

To wrap up the book, Chap. 8 presents a circle of ideas about the so-called (C^*-)algebraic formulation of quantum theories, including important notions such as spontaneous symmetry breaking.

The mathematical prerequisites necessary to understand the proofs are *abstract measure theory* [Coh80, Rud86], basics on *complex Hilbert spaces* [Rud86, Mor18], and the Fourier(-Plancherel) transform. Acquaintance with undergraduate quantum mechanics would be preferable but is not strictly necessary. For Chap. 7, the reader should possess a basic knowledge of *Lie groups and their representations*. A compendium of what is relevant to physics can be found in [NaSt82], [Var84], (classical texts that emphasize the analytical aspects of the theory of Lie groups) and [HiNe13] (a recent and complete treatise on the subject). As modern general references on the mathematical foundations of quantum theories, I recommend [Tes14, Lan17, Mor18].

I am grateful to Antonio Lorenzin for helping me correct many mistakes of various nature that affected a preliminary version and to Nicolò Drago, Elio Fabri, Sonia Mazzucchi, Davide Pastorello, Nicola Pinamonti, Giovanni Stecca, Alex Strohmaier, and Chris Van de Ven for useful technical discussions and suggestions. I would like to thank Aldo Rampioni at Springer Publishing for the kind support. As usual, a big thanks goes to Simon Chiossi for revising the English text.

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Chapter 1
General Phenomenology of the Quantum World and Elementary Formalism

We quickly review in this chapter the most relevant common features of quantum systems. Readers interested in a concise introduction to the physics of Quantum Mechanics (QM) will profit from [SaTu94]: putting aside the mathematical rigour, it discusses Dirac's formulation of QM from a modern and smart perspective. Here the intention is to formalize in a simple way the ideas that will be developed in full in the subsequent chapters, after introducing the appropriate tools.

1.1 The Physics of Quantum Systems

This first section focuses on phenomenological aspects of quantum systems: in particular, when a physical system can be said to have a quantum nature and what are the basic features of this quantum nature.

1.1.1 When Is a Physical System a Quantum System?

Quantum Mechanics can be roughly defined as the physics of the microscopic world (elementary particles, atoms, molecules). This realm is characterized by a universal constant known as **Planck's constant** h. An associated constant—nowadays of more frequent use—is the **reduced Planck constant**

$$\hbar := \frac{h}{2\pi} = 1.054571726 \times 10^{-34}\,\mathrm{J\,s}\,.$$

The physical dimensions of h (or $\hbar$) are those of an *action*, i.e. *energy* $\times$ *time*. A simple but effective check on the appropriateness of a quantum physical description of the physical system under consideration consists in comparing the

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value of a characteristic action of the system with $\hbar$. Let us consider two examples. First take a macroscopic pendulum (of length, say, $\sim$1 m, mass $\sim$1 kg, maximum speed $\sim$1 ms^{-1}). By multiplying the maximum kinetic energy by the period of the oscillations we find a typical action of roughly 2 J s $\gg$ h. In this situation, quantum physics is definitely inappropriate, an expectation that is matched by our day-to-day experience. If instead we look at a hydrogen atom, the first *ionization energy* of the electron orbiting its proton multiplied the orbital period of rotation gives (using the classical formula with radius of order of 1 Å) a typical action comparable to h. Here Quantum Mechanics is necessary.

1.1.2 Basic Properties of Quantum Systems

A triple of features specific to Quantum Mechanics (QM), which seem to be very different from properties of Classical Mechanics (CM), is listed below. These remarkable general properties concern the physical quantities of physical systems. In QM physical quantities are called *observables*.

(1) **Randomness**. If we measure an observable of a quantum system, the outcomes appear to be *stochastic*: when measuring the same observable A on completely identical systems prepared in the *same* physical state, one generally finds different outcomes $a, a', a'' \ldots$.

If we refer to the standard interpretation of the formalism of QM (see [SEP] for a nice up-to-date account on the various interpretations), this randomness of measurement outcome should not be ascribed to an incomplete knowledge of the state of the system, as happens, for instance, in Classical Statistical Mechanics. Randomness, rather than *epistemic*, is *ontological*, and as such it is a fundamental property of quantum systems.

On the other hand, *QM allows to compute the* probability distribution *of all the outcomes of a given observable, once the state of the system is known*.

Moreover, it is always possible to prepare a state ψ_a in which a certain observable A is *defined* and where it takes the value a. That is, repeated measurements of A give rise to the same value a with probability 1. (Note that we can perform simultaneous measurements on identical systems all prepared in state ψ_a, or we can perform different subsequent measurements on the same system in state ψ_a. In the latter case these measurements have to be performed in rapid succession to prevent the system's state from evolving under Schrödinger evolution, see (3) below.) States where observables take definite values cannot be prepared for *all* observables simultaneously, as discussed in (2).

(2) **Compatible and Incompatible Observables**. The second standout feature of QM is the existence of *incompatible observables*. In contrast to CM, there are physical quantities which cannot be measured simultaneously since there is no physical instrument capable of such a task. If an observable A is *defined* in a

given state ψ—i.e. it attains a precise value a with probability 1 if measured—an observable B *incompatible* with A turns out to be *not defined* in the state ψ: it may attain *several different* values $b, b', b'' \ldots$, *none with probability* 1, in case of measurement. So, if we measure B we generally obtain a spectrum of values described by a distribution of frequencies, as mentioned in (1), by identifying the frequencies with corresponding a priori probabilities.
Incompatibility is *symmetric*: A is incompatible with B if and only if B is incompatible with A, though it is not *transitive*.
Compatible observables do exist and, by definition, they can be measured simultaneously. The component x of the position of a particle and the component y of its momentum are an example, if we refer to the rest space of a given inertial reference frame.
A popular instance of incompatible observables are pairs of *canonically conjugate observables*, like the position X and the momentum P of a particle along the same fixed axis of a reference frame. There is a lower bound for the product of the standard deviations—resp. ΔX_ψ, ΔP_ψ—for the outcomes of the measurements of these observables in a given state ψ. These measurements have to be performed on different identical systems all prepared in the same state ψ. The lower bound is independent of the state, and is encoded in the celebrated formula (a theorem in modern formulations)

$$\Delta X_\psi \Delta P_\psi \geq \hbar/2 \,, \tag{1.1}$$

which contains the Planck constant.

(3) **Collapse of the State**. Measurements of QM *usually change the state of the system* and give rise to a *post-measurement state* other that the state in which the measurement is performed. (We are considering rather idealized measurement procedures, which tend to be very often destructive.) Assuming ψ is the initial state, immediately after the measurement of an observable A that returns value a among a plethora of possible values $a, a', a'', \ldots$, the state settles in state ψ', in general different form ψ. Relative to ψ', the probabilities of the outcomes of A change to 1 for value a and 0 for all other values. In this sense A becomes *defined* in state ψ'.
If we measure a pair of incompatible observables A, B in alternation and repeatedly, the outcomes will interfere with each other: if the first outcome of A is a, after a measurement of B a subsequent measurement of A gives $a' \neq a$ in general. Instead, if A and B are compatible, the outcomes of subsequent measurements do not disturb one other.
Beside that, in CM there are measurements that, in practice, perturb and are perturbed by the state of the system. It is however theoretically possible to tweak this interference so to render it negligible. In QM this is not always possible, as manifested by (1.1).

Two types of time evolution of the state of a system exist in QM. One is due to the dynamics and is encoded in the famous *Schrödinger equation* we shall encounter in a short while. It is nothing but a quantum version of the classical *Hamiltonian evolution* [Erc15]. The other type is the sudden change of the state caused by the measuring procedure of an observable, which we outlined in (3): the *collapse of the state* (or of the *wavefunction*) of the system.

The physical nature of the second type of evolution remains, nowadays still, a source of animated debate in the community of physicists and philosophers of science. Several attempts have been made to reduce state collapse to a dynamical evolution of the whole physical system, including the measuring instruments and the environment by means of *de-coherence processes* [SEP, BGJ00]. None of these approaches seem to be completely satisfactory, however, at least until now [Lan17].

1.2 Elementary Quantum Formalism: The Finite-Dimensional Case

Remark 1.1 Unless said otherwise, we shall adopt a unit system where $\hbar = 1$ throughout the book. ■

We include here a number of technical details to complete the picture. We intend to show how (1)–(3) should be interpreted mathematically in practice (we shall swap (2) and (3) for convenience). A good part of the chapter is meant to justify and expand these ideas, and place them in a sound mathematical background.

In order to simplify, with the exception of Sect. 1.3 we shall indicate by H a *finite-dimensional* complex vector space endowed with a Hermitian scalar product $\langle\cdot|\cdot\rangle$. The linear entry is the second one. Given H, $\mathfrak{B}(\mathsf{H})$ is the complex algebra of operators $A : \mathsf{H} \to \mathsf{H}$. We remind that if $A \in \mathfrak{B}(\mathsf{H})$, H finite-dimensional, the *adjoint operator* $A^* \in \mathfrak{B}(\mathsf{H})$ is the unique linear operator satisfying

$$\langle A^*x|y\rangle = \langle x|Ay\rangle \quad \text{for all} x, y \in \mathsf{H}. \tag{1.2}$$

A is called *selfadjoint* when $A = A^*$. As a consequence,

$$\langle Ax|y\rangle = \langle x|Ay\rangle \quad \text{for all } x, y \in \mathsf{H}. \tag{1.3}$$

As $\langle\cdot|\cdot\rangle$ is linear in the second argument and anti-linear in the first, evidently all eigenvalues of a selfadjoint operator A must be real.

The mathematical axioms describing quantum systems are:

1. a quantum mechanical system S is associated with a (finite-dimensional, for now) complex vector space H endowed with a Hermitian scalar product $\langle\cdot|\cdot\rangle$;
2. observables are described by *selfadjoint* operators A on H;
3. states are equivalence classes of *unit* vectors $\psi \in \mathsf{H}$, with $\psi \sim \psi'$ iff $\psi = e^{ia}\psi'$ for some $a \in \mathbb{R}$.

Remark 1.2

(a) States are therefore in one-to-one correspondence to elements of the *complex projective space* $P\mathsf{H}$. The states we consider in this introduction are actually called *pure* states. A more general notion will be introduced later.
(b) H is a very simple instance of a complex Hilbert space: it is automatically complete in view of its finite-dimensionality.
(c) Since $\dim(\mathsf{H}) < +\infty$, every selfadjoint operator $A \in \mathfrak{B}(\mathsf{H})$ admits a spectral decomposition

$$A = \sum_{a\in\sigma(A)} a P_a^{(A)} , \tag{1.4}$$

where $\sigma(A)$ is the *finite* set of eigenvalues, which must be *real* as A is selfadjoint, and $P_a^{(A)}$ is the orthogonal projector onto the a-eigenspace. Note that $P_a P_{a'} = 0$ if $a \neq a'$, for eigenvectors with different eigenvalues are orthogonal. ■

Let us see how assumptions 1–3 allow to phrase the physical properties of quantum systems (1)–(3) in mathematically solid form.

(1) Randomness The eigenvalues of an observable A are interpreted physically as the possible values of the outcomes of a measurement of A.

Given a state, represented by the unit vector $\psi \in \mathsf{H}$, the probability to obtain $a \in \sigma(A)$ for A is

$$\mu_\psi^{(A)}(a) := ||P_a^{(A)}\psi||^2 .$$

Going along with this interpretation, the expectation value of A in state ψ is

$$\langle A\rangle_\psi := \sum_{a\in\sigma(A)} a\mu_\psi^{(A)}(a) = \langle\psi|A\psi\rangle .$$

Hence

$$\langle A\rangle_\psi = \langle\psi|A\psi\rangle . \tag{1.5}$$

Similarly, the standard deviation ΔA_ψ turns out to be

$$\Delta A_\psi^2 := \sum_{a\in\sigma(A)} (a - \langle A\rangle_\psi)^2\mu_\psi^{(A)}(a) = \langle\psi|A^2\psi\rangle - \langle\psi|A\psi\rangle^2 . \tag{1.6}$$

Remark 1.3

(a) We emphasize that the phase of a unit vector $\psi \in \mathsf{H}$ ($e^{ia}\psi$ and ψ represent the same quantum state for every $a \in \mathbb{R}$) is actually harmless.
(b) If A is an observable and $f : \mathbb{R} \to \mathbb{R}$ is a given map, $f(A)$ is interpreted as an observable whose values are $f(a)$ if $a \in \sigma(a)$: taking (1.4) into account,

$$f(A) := \sum_{a \in \sigma(A)} f(a) P_a^{(A)} . \tag{1.7}$$

For polynomials $f(x) = \sum_{k=0}^{n} a_k x^k$, we have $f(A) = \sum_{k=0}^{n} a_k A^k$, as expected. The selfadjoint operator A^2 can be interpreted in this way, as the natural observable whose values are a^2 when $a \in \sigma(A)$. Then the last term in (1.6) reads, by taking (1.5) into account,

$$\Delta A_\psi^2 = \langle A^2 \rangle_\psi - \langle A \rangle_\psi^2 = \langle (A - \langle A \rangle_\psi I)^2 \rangle_\psi = \langle \psi | (A - \langle A \rangle_\psi I)^2 \psi \rangle . \tag{1.8}$$

■

(3) Collapse of the State Let a be the outcome of the (idealized) measurement of A when the state is represented by ψ. The post-measurement state is given by the unit vector

$$\psi' := \frac{P_a^{(A)} \psi}{||P_a^{(A)} \psi||} . \tag{1.9}$$

Remark 1.4 The above formula is meaningless if $\mu_\psi^{(A)}(a) = 0$, as it should. Yet, the choice of phase in ψ does not cause trouble due to the linearity of $P_a^{(A)}$.

(2) Compatible and Incompatible Observables Two observables A and B are compatible—i.e. they can be measured simultaneously—if and only if the associated operators *commute*:

$$AB - BA = 0 .$$

Since H has finite dimension, A and B are compatible if and only if the associated spectral projectors commute as well (the proof is elementary):

$$P_a^{(A)} P_b^{(B)} = P_b^{(B)} P_a^{(A)} \quad a \in \sigma(A) , b \in \sigma(B) .$$

In particular,

$$||P_a^{(A)} P_b^{(B)} \psi||^2 = ||P_b^{(B)} P_a^{(A)} \psi||^2$$

has the natural interpretation of the probability to obtain outcomes a and b for a simultaneous measurement of A and B. If, conversely, A and B are incompatible, it may happen that

$$||P_a^{(A)} P_b^{(B)} \psi||^2 \neq ||P_b^{(B)} P_a^{(A)} \psi||^2 .$$

Furthermore, by exploiting (1.9) one can understand

$$||P_a^{(A)} P_b^{(B)} \psi||^2 = \left|\left| P_a^{(A)} \frac{P_b^{(B)} \psi}{||P_b^{(B)} \psi||} \right|\right|^2 ||P_b^{(B)} \psi||^2 \tag{1.10}$$

as *the probability of obtaining first b and then a in successive measurements of B and A.* ■

Remark 1.5

(a) In general the role of A and B in (1.10) cannot be swapped, because $P_a^{(A)} P_b^{(B)} \neq P_b^{(B)} P_a^{(A)}$ when A and B are incompatible. The measurement procedures "interfere with each other", as we saw earlier.
(b) The interpretation of (1.10) as probability of successive measurements is consistent also if A and B are compatible. In that case the probability of obtaining first b and then a in successive measurements of B and A is identical to the probability of measuring a and b simultaneously. In turn, it coincides with the probability of obtaining first a and then b in successive measurements of A and B.
(c) A is always compatible with itself. Moreover $P_a^{(A)} P_a^{(A)} = P_a^{(A)}$, by definition of projector. This fact has the immediate consequence that if we obtain a measuring A so that the state immediately after the measurement is represented by $\psi_a = ||P_a^{(A)} \psi||^{-1} \psi$, it will remain ψ_a even after other measurements of A, and the outcome will always be a. Versions of this phenomenon, especially in relationship to the decay of unstable particles, have been experimentally confirmed and go under the name of *quantum Zeno effect*. ■

Example 1.6 An electron admits a triple of internal observables S_x, S_y, S_z known as the three components of the *spin*. Very roughly speaking, we can think of the spin as the angular momentum of the particle in a moving frame always at rest with the centre of the particle and keeping its axes parallel to the ones of the reference frame of the laboratory where the electron moves. In view of its peculiar properties the spin cannot actually have a complete classical analogue, and this naive interpretation is eventually untenable. For instance, one cannot "stop" the spin of a particle or change the constant value of $S^2 = S_x^2 + S_y^2 + S_z^2$: this quantity is a characteristic property of the particle like the mass. The electron's spin is described by an *internal* Hilbert space H_s, which has dimension 2 so it can be identified with $\mathbb{C}^2$. Up to a constant factor involving $\hbar$ (depending on conventions), the spin observables

$$S_x = \frac{\hbar}{2}\sigma_x , \qquad S_y = \frac{\hbar}{2}\sigma_y , \qquad S_z = \frac{\hbar}{2}\sigma_z . \tag{1.11}$$

correspond to the well-known *Pauli matrices*

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} , \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} , \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} . \tag{1.12}$$

Observe that $[S_a, S_b] \neq 0$ if $a \neq b$, implying that the spin's components are incompatible observables. In fact, one has

$$[S_x, S_y] = i\hbar S_z$$

and the similar identities obtained by permuting cyclically the indices. These commutation relations are the same as for the observables L_x,L_y,L_z describing the *angular momentum* in the lab frame, which do possess classical analogues (we shall return to these in Example 7.44). In contrast to CM, the observables describing the angular momenta are incompatible and cannot be measured simultaneously. The failure of compatibility is related to the appearance of $\hbar$ in the right-hand side of

$$[L_x, L_y] = i\hbar L_z .$$

That number is extremely small when compared with macroscopic scales. This is the ultimate reason why the incompatibility of L_x and L_z is practically undetectable in macroscopic systems.

Direct inspection proves that $\sigma(S_a) = \{\pm\hbar/2\}$, and similarly $\sigma(L_a) = \{n\hbar \mid n \in \mathbb{Z}\}$. Therefore the components of the angular momentum take discrete values in QM, another difference with CM. Though since the gap between the two nearest values is extremely small if compared to typical angular momenta of macroscopic systems, in practice this discreteness becomes imperceptible and thus disappears. ■

1.2.1 Time Evolution

At this point a few words on time evolution are in order, while we reserve a broader discussion for later.

Among the class of observables of a quantum system described in a given inertial reference frame, the (quantum) *Hamiltonian* H plays a fundamental role. We are assuming that the system interacts with a stationary physical environment and everything refers to the rest space of an inertial system. The one-parameter group of unitary operators associated with H (see (1.7) for notation)

$$U_t := e^{-itH} := \sum_{h\in\sigma(H)} e^{-ith} P_h^{(H)} , \quad t \in \mathbb{R} \tag{1.13}$$

describes the *time evolution of quantum states*, as follows. Let the state at time $t = 0$ be represented by the unit vector $\psi \in \mathsf{H}$, so at time t the state is represented by

$$\psi_t = U_t \psi .$$

(The vector ψ_t has norm 1 since U_t is unitary and thus preserves norms.) Taking (1.13) into account, this identity is equivalent to

$$i\frac{d\psi_t}{dt} = H\psi_t . \tag{1.14}$$

Equation (1.14) is nothing but a form of the celebrated *Schrödinger equation*. If the environment is not stationary, a more complicated description can be given where H is replaced by a family of (selfadjoint) Hamiltonian operators $H(t)$ parametrised by time $t \in \mathbb{R}$. Time dependence accounts for the evolution in time of the external system interacting with our quantum system. In that case, it is simply assumed that the time evolution of states is again provided by the equation above where H is replaced by $H(t)$:

$$i\frac{d\psi_t}{dt} = H(t)\psi_t . \tag{1.15}$$

This equation permits one to define a two-parameter *groupoid* of unitary operators $U(t_2, t_1)$, where $t_2, t_1 \in \mathbb{R}$, such that

$$\psi_{t_2} = U(t_2, t_1)\psi_{t_1} , \quad t_2, t_1 \in \mathbb{R} .$$

The groupoid structure arises from the following identities: $U(t, t) = I$, $U(t_3, t_2)U(t_2, t_1) = U(t_3, t_2)$ and $U(t_2, t_1)^{-1} = U(t_2, t_1)^* = U(t_1, t_2)$.

In our elementary setup, where H is finite-dimensional, *Dyson's formula* holds

$$U(t_2, t_1) = \sum_{n=0}^{+\infty} \frac{(-i)^n}{n!} \int_{t_1}^{t_2} \cdots \int_{t_1}^{t_2} T[H(\tau_1)\cdots H(\tau_n)]\, d\tau_1 \cdots d\tau_n$$

with the simple hypothesis that the map $\mathbb{R} \ni t \mapsto H_t \in \mathfrak{B}(\mathsf{H})$ is continuous (adopting any topology compatible with the vector-space structure of $\mathfrak{B}(\mathsf{H})$) [Mor18]. In the above formula we set $T[H(\tau_1)\cdots H(\tau_n)] = H(\tau_{\pi(1)})\cdots H(\tau_\pi(n))$, where the bijective function $\pi : \{1, \ldots, n\} \to \{1, \ldots, n\}$ is a permutation with $\tau_{\pi(1)} \geq \cdots \geq \tau_{\pi(n)}$.

1.3 A First Look at the Infinite-Dimensional Case, CCRs and Quantization Procedures

All the formalism introduced, excluding certain technicalities we shall examine at a later stage, holds also for quantum systems whose complex vector space of states H is *infinite*-dimensional.

To extend the ideas of Sect. 1.2 to the setup where finite-dimensionality is relaxed, it only seems natural to assume that H is complete for the norm $\langle\cdot|\cdot\rangle$. Hence H becomes a *complex Hilbert space*. In particular, completeness ensures the existence of spectral decompositions generalizing (1.4), when referring to *compact* selfadjoint operators.

Notation 1.7 Henceforth $\mathscr{S}(\mathbb{R}^n)$ will denote the vector space of C^∞ complex-valued functions on $\mathbb{R}^n$ which, together with derivatives of all orders in any set of coordinates, decay faster than negative powers of $|x|$ as $|x| \to +\infty$.

From now on $C_c^\infty(\mathbb{R}^n)$ will indicate the vector space of C^∞ complex-valued maps on $\mathbb{R}^n$ with compact support. Finally, $d^n x$ will denote the Lebesgue measure on $\mathbb{R}^n$. ■

1.3.1 The $L^2(\mathbb{R}, dx)$ Model

The simplest example of a quantum system described in an infinite-dimensional Hilbert space is a quantum particle confined to the real line $\mathbb{R}$. In this case, the Hilbert space is $\mathsf{H} := L^2(\mathbb{R}, dx)$, dx denoting the standard Lebesgue measure on $\mathbb{R}$. States are still represented by elements of $P\mathsf{H}$, namely equivalence classes $[\psi]$ of measurable functions $\psi : \mathbb{R} \to \mathbb{C}$ with unit norm, $||[\psi]|| = \int_{\mathbb{R}} |\psi(x)|^2 dx = 1$.

Remark 1.8 Note how we have *two* distinct quotients: ψ and ψ' define the same element $[\psi]$ in $L^2(\mathbb{R}, dx)$ iff $\psi(x) - \psi'(x) \neq 0$ on a set of zero Lebesgue measure. Two unit vectors $[\psi]$ and $[\phi]$ define the same state if $[\psi] = e^{ia}[\phi]$ for some $a \in \mathbb{R}$. ■

Notation 1.9 In the sequel we shall adopt the standard convention of many functional analysis textbooks and denote by ψ, instead of $[\psi]$, the elements of spaces L^2. Tacitly we shall identify functions that differ at most on zero-measure sets. ■

The functions ψ defining states (up to zero-measure sets and phases) are called *wavefunctions*. There is a pair of fundamental observables describing our quantum particle moving in $\mathbb{R}$. One is the *position observable*. The corresponding selfadjoint operator X is the *position operator* defined by

$$(X\psi)(x) := x\psi(x)\,, \quad x \in \mathbb{R}\,, \quad \psi \in L^2(\mathbb{R}, dx)\,.$$

The other observable is the momentum P. Restoring $\hbar$ for the occasion, the *momentum operator* is

$$(P\psi)(x) := -i\hbar \frac{d\psi(x)}{dx}\,, \quad x \in \mathbb{R}\,, \quad \psi \in L^2(\mathbb{R}, dx)\,.$$

We are immediately confronted by a number of mathematical issues with these, actually quite naive, definitions. Let us begin with X. First of all, in general $X\psi \notin L^2(\mathbb{R}, dx)$ even if $\psi \in L^2(\mathbb{R}, dx)$. To fix the problem, one could simply restrict the domain of X to the linear subspace

$$D(X) := \left\{ \psi \in L^2(\mathbb{R}, dx) \;\middle|\; \int_{\mathbb{R}} |x\psi(x)|^2 dx < +\infty \right\}. \tag{1.16}$$

Even if

$$\langle X\psi|\phi\rangle = \langle\psi|X\phi\rangle \quad \text{for all } \psi, \phi \in D(X), \tag{1.17}$$

holds, we cannot argue that X is properly selfadjoint because we have *not yet* given the definition of adjoint to an operator defined on a non-maximal domain in an infinite-dimensional Hilbert space. Identity (1.2) in an infinite-dimensional Hilbert space does not define a (unique) operator X^* without further technical requirements. (Readers need not hold their breath, for X is truly selfadjoint on some domain (1.16) according to a general definition, see the next chapter.) From a very practical viewpoint however, (1.17) implies that all the eigenvalues of X, if any, must be real, which seems sufficient to adopt the standard interpretation of eigenvalues as outcomes of measurements of the observable X. Unfortunately life is not as easy: for every fixed $x_0 \in \mathbb{R}$ there is no $\psi \in L^2(\mathbb{R}, dx)$ with $X\psi = x_0\psi$ and $\psi \neq 0$. (A function ψ satisfying $X\psi = x_0\psi$ must also satisfy $\psi(x) = 0$ if $x \neq x_0$, due to the definition of X. Hence $\psi = 0$ in $L^2(\mathbb{R}, dx)$, simply because $\{x_0\}$ has zero Lebesgue measure!)

All this seems to prevent the existence of a spectral decomposition of X like (1.4), since X does not admit eigenvectors in $L^2(\mathbb{R}, dx)$ (and a fortiori in $D(X)$).

The definition of P appears to suffer from even worse problems. Its domain cannot be the whole $L^2(\mathbb{R}, dx)$ but should be a subset of differentiable functions with derivative in $L^2(\mathbb{R}, dx)$. The weakest notion of differentiability we can assume is *weak differentiability*, leading to this candidate for domain

$$D(P) := \left\{ \psi \in L^2(\mathbb{R}, dx) \;\middle|\; \exists\ \text{w-}\frac{d\psi(x)}{dx}\,, \int_{\mathbb{R}} \left|\text{w-}\frac{d\psi(x)}{dx}\right|^2 dx < +\infty \right\}. \tag{1.18}$$

Above w-$\frac{d\psi(x)}{dx}$ denotes the *weak derivative* of ψ.[1] As a matter of fact $D(P)$ coincides with the *Sobolev space* $H^1(\mathbb{R})$.

Again, without a precise definition of adjoint on an infinite-dimensional Hilbert space (with non-maximal domain) we cannot say anything more precise about the selfadjointness of P with that domain. (As before P will turn out to be selfadjoint under the general definition we shall give in the next chapter.)

Passing to the Fourier-Plancherel transform, one finds (some work is needed)

$$\langle P\psi|\phi\rangle = \langle\psi|P\phi\rangle \quad \text{for all } \psi, \phi \in D(P), \tag{1.19}$$

so that eigenvalues are real provided they exist. Exactly as we saw for X, neither P admits eigenvectors. The naive eigenvectors with eigenvalue $p \in \mathbb{R}$ are functions proportional to the map $\mathbb{R} \ni x \mapsto e^{ipx/\hbar}$, which does not belong to $L^2(\mathbb{R}, dx)$ nor $D(P)$. We will tackle these issues in the next chapter in a very general fashion.

Remark 1.10

(a) The space of *Schwartz functions* $\mathscr{S}(\mathbb{R})$ satisfies

$$\mathscr{S}(\mathbb{R}) \subset D(X) \cap D(P),$$

and furthermore $\mathscr{S}(\mathbb{R})$ is dense in $L^2(\mathbb{R}, dx)$ and *invariant* under X and P: $X(\mathscr{S}(\mathbb{R})) \subset \mathscr{S}(\mathbb{R})$ and $P(\mathscr{S}(\mathbb{R})) \subset \mathscr{S}(\mathbb{R})$. This observation has many technical consequences that will resurface elsewhere.

(b) Although we shall not pursue the following, we stress that X admits a set of eigenvectors if we enlarge the domain of X to the space $\mathscr{S}'(\mathbb{R})$ of *Schwartz distributions* in a standard way, taking (a) into account. If $T \in \mathscr{S}'(\mathbb{R})$,

$$\langle X(T), f\rangle := \langle T, X(f)\rangle \quad \text{for every } f \in \mathscr{S}(\mathbb{R}).$$

Thus the eigenvectors in $\mathscr{S}'(\mathbb{R})$ of X with eigenvalue $x_0 \in \mathbb{R}$ are the distributions $c\delta(x - x_0)$. This class of eigenvectors can be exploited to build a spectral decomposition of X similar to (1.4).

Using the same procedure P admits eigenvectors in $\mathscr{S}'(\mathbb{R})$, which are just the above exponential functions. As before, these eigenvectors allow to construct a spectral decomposition of P akin to (1.4). This procedure's core idea can be traced back to Dirac [Dir30], and in fact some 10 years later Schwartz established the *theory of distributions*. The modern construction of spectral decompositions of selfadjoint operators was developed by Gelfand using *rigged Hilbert spaces* [GeVi64]. ■

[1] $f : \mathbb{R} \to \mathbb{C}$, defined up to zero-measure sets, is the weak derivative of $g \in L^2(\mathbb{R}, dx)$ if $\int_{\mathbb{R}} g\frac{dh}{dx}dx = -\int_{\mathbb{R}} fhdx$ for every $h \in C_c^\infty(\mathbb{R})$. If g is differentiable, its standard derivative coincides with the weak one.

1.3.2 The $L^2(\mathbb{R}^n, d^n x)$ Model and Heisenberg's Inequalities

Consider a quantum particle moving in $\mathbb{R}^n$ with Hilbert space $L^2(\mathbb{R}^n, d^n x)$. Introduce observables X_k and P_k representing position and momentum with respect to the k-th axis, $k = 1, 2, \ldots, n$. These operators, which are defined in analogy to the case $n = 1$, have smaller domains than the full Hilbert space. We shall do not recall the domains' expressions (on which the operators turn out to be properly selfadjoint, see the definition in the next chapter). Let us just mention that all admit $\mathscr{S}(\mathbb{R}^n)$ as a common invariant subspace of their domains. On it

$$(X_k\psi)(x) = x_k\psi(x) , \qquad (P_k\psi)(x) = -i\hbar\frac{\partial\psi(x)}{\partial x_k} , \quad \psi \in \mathscr{S}(\mathbb{R}^n) \tag{1.20}$$

and so

$$\langle X_k\psi|\phi\rangle = \langle\psi|X_k\phi\rangle , \quad \langle P_k\psi|\phi\rangle = \langle\psi|P_k\phi\rangle \quad \text{for all } \psi, \phi \in \mathscr{S}(\mathbb{R}^n), \tag{1.21}$$

By direct inspection one easily proves that the *canonical commutation relations* (CCRs)

$$[X_h, P_k] = i\hbar\delta_{hk}I , \quad [X_h, X_k] = 0 , \quad [P_h, P_k] = 0 \tag{1.22}$$

hold provided the operators are restricted to $\mathscr{S}(\mathbb{R}^n)$. If A and B have different domains, the *commutator* $[A, B] := AB - BA$ is intended defined where both AB and BA make sense, $\mathscr{S}(\mathbb{R}^n)$ in the case of concern. Assuming that (1.5) and (1.8) are still valid for X_k and P_k and $\psi \in \mathscr{S}(\mathbb{R}^n)$, (1.22) easily leads to the *Heisenberg uncertainty relations*,

$$\Delta X_{k\psi}\Delta P_{k\psi} \geq \frac{\hbar}{2}, \quad \text{for } \psi \in \mathscr{S}(\mathbb{R}^n) , \quad ||\psi|| = 1 , \quad k = 1, 2, \ldots, n . \tag{1.23}$$

Exercise 1.11

(1) *Derive inequality (1.23) from (1.22), using (1.5) and (1.8).*

Solution Using (1.5), (1.8) and the Cauchy-Schwarz inequality, it is easy to show (we omit the index $_k$ for simplicity)

$$\Delta X_\psi \Delta P_\psi = ||X'\psi||||P'\psi|| \geq |\langle X'\psi|P'\psi\rangle|$$

where $X' := X - \langle X\rangle_\psi I$ and $P' := X - \langle X\rangle_\psi I$. Next notice that

$$|\langle X'\psi|P'\psi\rangle| \geq |Im\langle X'\psi|P'\psi\rangle| = \frac{1}{2}|\langle X'\psi|P'\psi\rangle - \langle P'\psi|X'\psi\rangle|.$$

Taking advantage of (1.21) and the definitions of X' and P', and exploiting (1.22), we obtain

$$|\langle X'\psi|P'\psi\rangle - \langle P'\psi|X'\psi\rangle| = |\langle\psi|(X'P' - P'X')\psi\rangle| = |\langle\psi|(XP - PX)\psi\rangle| = \hbar|\langle\psi|\psi\rangle|$$

Since $\langle\psi|\psi\rangle = ||\psi||^2 = 1$ by hypotheses, (1.23) is proved. Obviously we still have to justify the validity of (1.5) and (1.8) in the infinite-dimensional case. □

(2) *Prove that there exist no operators X_h, P_k, $h, k = 1, 2, \ldots, n$, on a finite-dimensional Hilbert space $\mathsf{H} \neq \{0\}$ satisfying (1.22).*

Solution Supposing such operators exist, we would have

$$i\delta_{hk}\dim(\mathsf{H}) = tr([X_h, P_k]) = tr(X_h P_k) - tr(P_k X_h) = tr(P_k X_h) - tr(P_k X_h) = 0,$$

and this is not possible for $h = k$ since $\dim(\mathsf{H}) > 0$. □

1.3.3 Failure of Dirac's Quantization and Deformation Quantization Procedure

A philosophically remarkable consequence of the CCRs (1.22) is that they resemble the *classical canonical commutation relations* of the Hamiltonian variables q^h, p_k for the standard *Poisson bracket* $\{\cdot,\cdot\}_P$,

$$\{q^h, p_k\}_P = \delta^h_k\,, \quad \{q^h, q^k\}_P = 0\,, \quad \{p_h, p_k\}_P = 0\,. \tag{1.24}$$

as soon as one identifies $(i\hbar)^{-1}[\cdot,\cdot]$ with $\{\cdot,\cdot\}_P$. This fact, initially noticed by Dirac [Dir30], leads to the idea of "quantization" of a classical Hamiltonian theory [Erc15, Lan17].

In modern language Dirac's procedure goes like this. Start from a classical system described on a symplectic manifold (Γ, ω), for instance $\Gamma := \mathbb{R}^{2n}$ and ω the canonical symplectic form. The (real) Lie algebra $\mathfrak{g} := (C^\infty(\Gamma, \mathbb{R}), \{\cdot,\cdot\}_P)$ with Lie bracket $\{f, g\}_P := \omega(df, dg)$ gives a *Poisson structure*. To "quantize" the system, one seeks a "quantization map" Q associating classical observables $f \in C^\infty(\Gamma, \mathbb{R})$ (or in a Lie subalgebra, e.g. a polynomial algebra if $\Gamma = \mathbb{R}^{2n}$) to quantum observables $Q(f)$, i.e. selfadjoint operators restricted[2] to a common invariant domain $\mathscr{S}$ in some Hilbert space H. The map $Q : f \mapsto Q(f)$ is expected

[2]The restriction should be defined so that it admits a unique selfadjoint extension. A sufficient requirement on $\mathscr{S}$ is that every $Q(f)$ is *essentially selfadjoint* on it, see the next chapter.

to satisfy certain conditions, including

1. injectivity;
2. $\mathbb{R}$-linearity;
3. $Q(1) = I|_{\mathscr{S}}$ (1 being the constant map 1 on Γ);
4. $[Q(f), Q(g)] = i\hbar Q(\{f, g\}_P)$
5. if (Γ, ω) is the standard $\mathbb{R}^{2n}$, then $Q(x_k) = X_k|_{\mathscr{S}}$ and $Q(p_k) = P_k|_{\mathscr{S}}$, $k = 1, 2, \dots, n$;
6. the image of Q is irreducible (the only operators commuting with all elements of $Q(\mathfrak{g})$ are multiples of I).

Requirements 1, 2 and 4 say that the map $Q : f \mapsto Q(f)$ is an injective Lie-algebra homomorphism transforming $\mathfrak{g}$ in a real Lie algebra of operators with Lie bracket proportional to $i[Q(f), Q(g)]$. This apparently natural set of requirements turns out to be *mathematically contradictory* in view of the various versions of the *Groenewold-van Hove theorem*. See [GGT96] for a reasoned survey on the subject. *Alas the problem persists if we only take a subset of the conditions, and replace* $C^\infty(\Gamma, \mathbb{R})$ *with a smaller subalgebra, for instance polynomials on* $\mathbb{R}^{2n}$. In summary, no quantization map exists if we insist it agree strictly with Dirac's original take. The problem can be overcome within the paradigm of *Deformation Quantization*, where requirement 4 is relaxed and one allows for additional higher powers of $\hbar$ in the right-hand side. Everything relies upon an associative but *non-commutative quantum product* $*_\hbar : C^\infty(\Gamma, \mathbb{R}) \times C^\infty(\Gamma, \mathbb{R}) \to C^\infty(\Gamma, \mathbb{R})$ encoding all quantum properties already on $C^\infty(\Gamma, \mathbb{R})$. Furthermore, the commutator associated with $*_\hbar$ is supposed to coincide with the commutator of operators under the quantization map. The latter does not add further quantum properties to the game, since everything is already included in $*_\hbar$; it just identifies elements of the quantum (non-commutative) structure $(C^\infty(\Gamma, \mathbb{R}), *_\hbar)$ with operators in a suitable (and in a sense unnecessary) Hilbert space:

$$[Q(f), Q(g)] = Q(f *_\hbar g - g *_\hbar f) .$$

Assuming that $*_\hbar$ can be expanded in powers of $\hbar$, the first-order approximation of the $*_\hbar$-commutator is requested to equal $\{\,,\,\}_P$, hence replacing requirement 4 above with:

$$[Q(f), Q(g)] = Q(f *_\hbar g - g *_\hbar f) = Q(i\hbar\{f, g\}_P + \mathcal{O}(\hbar^2)) = i\hbar Q(\{f, g\}_P) + \mathcal{O}(\hbar^2).$$

This modification proves to be feasible and fruitful. There are other remarkable procedures of "quantization" in the literature, but we shall not insist on them [Erc15, Lan17].

Example 1.12 Consider a spinless particle in $3D$ with mass $m > 0$, whose potential energy is a real function $U \in C^\infty(\mathbb{R}^3)$ with polynomial growth and bounded below. Classically, its Hamiltonian function reads

$$h := \sum_{k=1}^{3} \frac{p_k^2}{2m} + U(x) \, .$$

A brute-force quantization procedure in $L^2(\mathbb{R}^3, d^3x)$ would consist in replacing every classical object with operators. This may just about make sense when there are no ordering ambiguities when translating functions like $p^2 x$, since classically $p^2 x = pxp = xp^2$. But the new identities would be false at the quantum level. In our case these problems do not arise, so

$$H := \sum_{k=1}^{3} \frac{P_k^2}{2m} + U \, , \tag{1.25}$$

where $(U\psi)(x) := U(x)\psi(x)$, could be accepted as a first quantum model of the Hamiltonian function of our system. The operator is at least defined on $\mathscr{S}(\mathbb{R}^3)$, where $\langle H\psi|\phi\rangle = \langle\psi|H\phi\rangle$. The existence of selfadjoint extensions is a delicate issue (see [Mor18] and especially [Tes14]) that we shall not address. Taking (1.20) into account, one immediately finds that on $\mathscr{S}(\mathbb{R}^3)$

$$H := -\frac{\hbar^2}{2m}\Delta + U \, ,$$

where Δ is the standard Laplace operator on $\mathbb{R}^n$ ($n = 3$ at present)

$$\Delta = \sum_{k=1}^{n} \frac{\partial^2}{\partial x_k^2} \, . \tag{1.26}$$

If we assume that the equation describing the evolution of the quantum system is still[3] (1.14), we find the known form of Schrödinger's equation,

$$i\hbar \frac{d\psi_t}{dt} = -\frac{\hbar^2}{2m}\Delta\psi_t + U\psi_t \, ,$$

for $\psi_\tau \in \mathscr{S}(\mathbb{R}^3)$ and τ varying in a neighbourhood of t (this requirement may be relaxed). To be very accurate, the meaning of the derivative on the left should be specified. We shall only say that it is computed with respect to the natural topology of $L^2(\mathbb{R}^3, d^3x)$. ■

[3]The factor $\hbar$ has to be added in the left-hand side of (1.14) if our unit system has $\hbar \neq 1$.

Chapter 2
Hilbert Spaces and Classes of Operators

The main goal of this and the next chapter is to lay out the mathematics sufficient to extend to infinite dimensions the elementary formulation of QM of the first chapter. As we saw in Sect. 1.3, the main issue concerns the fact that in the infinite-dimensional case there exist operators representing observables, think X and P, which do not have proper eigenvalues and eigenvectors. So, naive expansions such as (1.4) cannot be extended verbatim. They, together with eigenvalues viewed as values of an observable associated with a selfadjoint operator, play a crucial role in the mathematical interpretation of the quantum phenomenology of Sect. 1.1 discussed in Sect. 1.2. In particular we need a precise definition of selfadjoint operator and something on spectral decompositions in infinite dimensions. These tools are basic elements of the *spectral theory of Hilbert spaces*, which von Neumann created in order to set up Quantum Mechanics rigorously and first saw the light in his famous book [Neu32]. It was successively developed by various scholars and has since branched out in many different directions in pure and applied mathematics. As a matter of fact the notion of Hilbert space itself, as we know it today, appeared in the second chapter of that book, and was born out of earlier constructions by Hilbert and Riesz. Reference textbooks include [Ped89, Rud91, Schm12, Tes14, Mor18].

2.1 Hilbert Spaces: A Round-Up

We shall assume the reader is well acquainted with the basic definitions of the theory of normed, Banach and Hilbert spaces, including in particular *orthogonality*, *Hilbert bases* (also called *complete orthonormal systems*), their properties and use [Rud91, Mor18]. We shall nevertheless summarize a few results especially concerning *orthogonal sets* and *Hilbert bases*.

V. Moretti, *Fundamental Mathematical Structures of Quantum Theory*,
https://doi.org/10.1007/978-3-030-18346-2_2

Remark 2.1 We shall only deal with *complex* Hilbert spaces, even if not mentioned explicitly. ■

2.1.1 Basic Properties

Definition 2.2 A **Hermitian inner product** on the complex vector space H is a map $\langle\cdot|\cdot\rangle : \mathsf{H} \times \mathsf{H} \to \mathbb{C}$ such that, for $a, b \in \mathbb{C}$ and $x, y, z \in \mathsf{H}$,

(i) $\langle x|y\rangle = \overline{\langle y|x\rangle}$,
(ii) $\langle x|ay + bz\rangle = a\langle x|y\rangle + b\langle x|z\rangle$,
(iii) $\langle x|x\rangle \geq 0$, and $x = 0$ if $\langle x|x\rangle = 0$.

The space H is a (complex) **Hilbert space** if it is complete for the norm $||x|| := \sqrt{\langle x|x\rangle}$, $x \in \mathsf{H}$. ■

Remark 2.3 A *closed* subspace H_0 in a Hilbert space H is a Hilbert space for the restriction of the inner product, since it contains the limit points of its Cauchy sequences. ■

The mere (semi-)positivity of the inner product, regardless of completeness, guarantees the **Cauchy-Schwartz inequality**

$$|\langle x|y\rangle| \leq ||x||\,||y||\,, \quad x, y \in \mathsf{H}\,.$$

Another easy, and purely algebraic observation is the **polarization identity** of the inner product (with H not necessarily complete)

$$4\langle x|y\rangle = ||x+y||^2 - ||x-y||^2 - i||x+iy||^2 + i||x-iy||^2 \quad \text{for of } x, y \in \mathsf{H}, \tag{2.1}$$

which immediately implies the following elementary fact.

Proposition 2.4 *If H is a complex vector space with Hermitian inner product $\langle\ |\ \rangle$, any linear isometry $L : \mathsf{H} \to \mathsf{H}$ ($||Lx|| = ||x||$ for all $x \in \mathsf{H}$) preserves the inner product: $\langle Lx|Ly\rangle = \langle x|y\rangle$ for $x, y \in \mathsf{H}$.*

The converse is obviously true. Similarly to the above identity, we have another useful formula for a linear map $A : \mathsf{H} \to \mathsf{H}$, namely:

$$4\langle x|Ay\rangle = \langle x+y|A(x+y)\rangle - \langle x-y|A(x-y)\rangle - i\langle x+iy|A(x+iy)\rangle$$
$$+ i\langle x-iy|A(x-iy)\rangle \quad \text{for of } x, y \in \mathsf{H}. \tag{2.2}$$

From it one deduces the next fact in an easy way.

Proposition 2.5 *Let $A : \mathsf{H} \to \mathsf{H}$ be a linear map on the complex vector space H with Hermitian inner product. If $\langle x|Ax\rangle = 0$ for all $x \in \mathsf{H}$, then $A = 0$.*

This is not always true if H is a real vector space with a symmetric real inner product.

Let us state another key result of the theory (e.g., see [Rud91, Mor18]):

Theorem 2.6 (Riesz's Lemma) *Let H be a Hilbert space. A functional $\phi : \mathsf{H} \to \mathbb{C}$ is linear and continuous if and only if it has the form $\phi = \langle x|\ \rangle$ for some $x \in \mathsf{H}$. The vector x is uniquely determined by ϕ.*

2.1.2 Orthogonality and Hilbert Bases

Notation 2.7 Given $M \subset \mathsf{H}$, the space $M^\perp := \{y \in \mathsf{H} \mid \langle y|x\rangle = 0 \quad \forall x \in M\}$ denotes the **orthogonal** (complement) to M. When $N \subset M^\perp$ (which is patently equivalent to $M \subset N^\perp$), we write $N \perp M$. ■

Evidently $M^\perp$ is a closed subspace of H because the inner product is continuous. The operation $^\perp$ enjoys several nice properties, all quite easy to prove (e.g., see [Rud91, Mor18]). In particular,

$$\overline{\text{span}M} = (M^\perp)^\perp \quad \text{and} \quad \mathsf{H} = \overline{\text{span}M} \oplus M^\perp \tag{2.3}$$

where span$M$ indicates the set of finite linear combinations of vectors in M, the overline denotes the topological closure and $\oplus$ is the *direct sum* of (orthogonal) subspaces. (We remind that a vector space $\mathcal{X}$ is the **direct** sum of subspaces $\mathcal{X}_1$, $\mathcal{X}_2$, written $\mathcal{X} = \mathcal{X}_1 \oplus \mathcal{X}_2$, if every $x \in \mathsf{H}$ can be decomposed as $x = x_1 + x_2$ for unique elements $x_1 \in \mathcal{X}_1$ and $x_2 \in \mathcal{X}_2$.)

Here is an elementary but important technical lemma [Mor18].

Lemma 2.8 *Let H be a Hilbert space. If $\{x_n\}_{n\in\mathbb{N}} \subset \mathsf{H}$ is a sequence such that $\langle x_k|x_h\rangle = 0$ for $h \neq k$, then the following facts are equivalent.*

(a) $\sum_{n=0}^{+\infty} x_n := \lim_{N\to+\infty} \sum_{n=0}^{N} x_n$ *exists in* H;
(b) $\sum_{n=0}^{+\infty} ||x_n||^2 < +\infty$.

If (a) and (b) hold, then

$$\sum_{n=0}^{+\infty} x_n = \sum_{n=0}^{+\infty} x_{f(n)} \in \mathsf{H}\,,$$

for every bijective map $f : \mathbb{N} \to \mathbb{N}$. In other words, the series in (a) can be rearranged arbitrarily and the sum does not change.

Definition 2.9 A Hilbert basis N of a Hilbert space H is a set of **orthonormal vectors** (i.e. $||u|| = 1$ and $\langle u|v\rangle = 0$ for $u, v \in N$ with $u \neq v$) such that if $s \in \mathsf{H}$ satisfies $\langle s|u\rangle = 0$ for every $u \in \mathsf{H}$, then $s = 0$. ■

Hilbert bases always exist as a consequence of Zorn's lemma. (An explicit example in $L^2(\mathbb{R}, dx)$ is constructed in Example 2.59 (4) below.) As a consequence of (2.3),

Proposition 2.10 *A set of orthonormal vectors $N \subset \mathsf{H}$ is a Hilbert basis for H if and only if $\overline{span\, N} = \mathsf{H}$.*

If $M \subset \mathsf{H}$ is an orthonormal set, **Bessel's inequality**

$$||x||^2 \geq \sum_{u \in M} |\langle u|x\rangle|^2 \quad \text{for every } x \in \mathsf{H}$$

can be proved in a straightforward way. Hilbert bases are exactly orthonormal sets saturating the inequality. In fact, a generalized version of *Pythagoras' theorem* holds.

Proposition 2.11 *A set of orthonormal vectors $N \subset \mathsf{H}$ is a Hilbert basis of H if and only if*

$$||x||^2 = \sum_{u \in N} |\langle u|x\rangle|^2 \quad \textit{for every } x \in \mathsf{H}.$$

The above sum is understood as the supremum *of $\sum_{u \in F} |\langle u|x\rangle|^2$ over finite sets $F \subset N$.*

Remark 2.12

(a) If N is a Hilbert basis and $x \in \mathsf{H}$, at most countably many elements $|\langle u|x\rangle|^2$, $u \in N$, are non-zero: only a finite number of values $|\langle u|x\rangle|^2$ can belong in $[1, +\infty)$ for otherwise the sum would diverge, and the same argument tells only a finite number can belong in $[1/2, 1)$, in $[1/3, 1/2)$ and so on. Since these sets form a countable partition of $[0, +\infty)$, the number of non-vanishing terms $|\langle u|x\rangle|^2$ is either finite or countable. The sum $||x||^2 = \sum_{u \in N} |\langle u|x\rangle|^2$ can therefore be interpreted as a standard series by summing over non-zero elements only. Furthermore, it may be rearranged without altering the sum because the series converges absolutely.

(b) All Hilbert bases of H have the same cardinality and H is **separable**, i.e. it admits a dense countable subset, if and only if H has a Hilbert basis that is either finite or countable. ■

As a consequence of Lemma 2.8 and remark (a) above, if $N \subset \mathsf{H}$ is a Hilbert basis, any $x \in \mathsf{H}$ may be written as a sum

$$x = \sum_{u \in N} \langle u|x\rangle u \,. \tag{2.4}$$

More precisely, since only finitely or countably many $\langle u_n|x\rangle$ do not vanish, the decomposition is either a finite sum or a series $\lim_{m\to+\infty}\sum_{n=0}^{m}\langle u_n|x\rangle u_n$, computed with respect to the norm of H, where the order of the u_n does not matter by Lemma 2.8. For this reason the terms are not labelled.

Decomposition (2.4) and the continuity of the inner product immediately imply, for every $x, y \in \mathsf{H}$,

$$\langle x|y\rangle = \sum_{u\in N}\langle x|u\rangle\langle u|y\rangle \tag{2.5}$$

The sum is absolutely convergent (by the Cauchy-Schwartz inequality), another reason for why it can be rearranged.

2.1.3 Two Notions of Hilbert Orthogonal Direct Sum

Hilbert structures can be built by *summing orthogonally* a given family of Hilbert spaces. There are two such constructions (see, e.g., [Mor18]).

(1) The first case is the *Hilbert (orthogonal direct) sum* of *closed* subspaces $\{\mathsf{H}_j\}_{j\in J}$ of a given Hilbert space H, with $\mathsf{H}_j \neq \{0\}$ for every $j \in J$. Here J is a set with arbitrary cardinality and we suppose $\mathsf{H}_r \perp \mathsf{H}_s$ when $r \neq s$. Let $\mathrm{span}\{\mathsf{H}_j\}_{j\in J}$ denote the set of finite linear combinations of vectors in the H_j, $j \in J$. The **Hilbert orthogonal direct sum** of the H_j is the closed subspace of H

$$\bigoplus_{j\in J}\mathsf{H}_j := \overline{\mathrm{span}\{\mathsf{H}_j\}_{j\in J}}\,.$$

By Proposition 2.10 if $N_j \subset \mathsf{H}_j$ is a Hilbert basis of H_j, then $\cup_{j\in J}N_j$ is a Hilbert basis of $\bigoplus_{j\in J}\mathsf{H}_j$. Decomposing $x \in \bigoplus_{j\in J}\mathsf{H}_j$ over every N_j, we have corresponding elements $x_j \in \mathsf{H}_j$ such that

$$\forall x \in \bigoplus_{j\in J}\mathsf{H}_j\,, \quad ||x||^2 = \sum_{j\in J}||x_j||^2\,.$$

Furthermore, by Lemma 2.8,

$$\forall x \in \bigoplus_{j\in J}\mathsf{H}_j\,, \quad x = \sum_{j\in J}x_j\,, \quad x_j \in \mathsf{H}_j \text{ for } j \in J$$

where the sum is a series, since at most countably many x_j do not vanish, and the sum can be rearranged. The sum is *direct* in the sense that every $x \in \bigoplus_{j\in J}\mathsf{H}_j$ can be decomposed *uniquely* as a sum of vectors $x_j \in \mathsf{H}_j$. If we take another decomposition, namely $x = \sum_{j\in J} x'_j$ with $x'_j \in \mathsf{H}_j$ for $j \in J$, then $0 = x - x = \sum_{j\in J}(x'_j - x_j)$. By computing the norm, and since for different j we have orthogonal vectors, $0 = \sum_{j\in J} ||x'_j - x_j||^2$ hence $x'_j = x_j$ for every $j \in J$.

(2) If $\{\mathsf{H}_j\}_{j\in J}$ is a family of *non-trivial* Hilbert spaces, we can define a second Hilbert space $\bigoplus_{j\in J} \mathsf{H}_j$, called **Hilbert (direct orthogonal) sum** of the $\{\mathsf{H}_j\}_{j\in J}$. To this end, consider the elements $x = \{x_j\}_{j\in J}$ of the standard direct sum of the complex vector spaces H_j whose norm $||x|| := \sqrt{\sum_{j\in J} ||x_j||_j^2}$ is finite. This defines a Hilbert-space structure for the inner product $\langle x|x'\rangle = \sum_{j\in J}\langle x_j|x'_j\rangle_j$, with obvious notation.

The two definitions are manifestly interrelated. Indeed, according to the *second* definition, (a) every H_j is a closed subspace of $\bigoplus_{j\in J} \mathsf{H}_j$, (b) $\mathsf{H}_j \perp \mathsf{H}_k$ if $j \neq k$ for the inner product $\langle\ |\ \rangle$, and (c) $\bigoplus_{j\in J} \mathsf{H}_j$ is also the Hilbert orthogonal direct sum according to the *first* definition.

2.1.4 Tensor Product of Hilbert Spaces

If $\{\mathsf{H}_j\}_{j=1,2,\ldots,N}$ is a *finite* family of Hilbert spaces (which are not necessarily subspaces of a larger Hilbert space), their *Hilbert tensor product* is constructed as follows. First consider the standard 'algebraic' tensor product $\mathsf{H}_1 \otimes_{alg} \cdots \otimes_{alg} \mathsf{H}_N$. We can endow this space with the inner product that extends

$$\langle x_1 \otimes \cdots \otimes x_N | y_1 \otimes \cdots \otimes y_N\rangle := \prod_{j=1}^{N} \langle x_j|y_j\rangle_j \quad \text{for} \quad x_j, y_j \in \mathsf{H}_j \;, j = 1, \ldots, N \tag{2.6}$$

(linearly in the first slot, anti-linearly in the second one). It is easy to prove [Mor18] that there exists only one such Hermitian inner product on $\mathsf{H}_1 \otimes_{alg} \cdots \otimes_{alg} \mathsf{H}_N$. The **Hilbert tensor product** $\mathsf{H}_1 \otimes \cdots \otimes \mathsf{H}_N$ of the family $\{\mathsf{H}_j\}_{j=1,2,\ldots,N}$ is the completion of $\mathsf{H}_1 \otimes_{alg} \cdots \otimes_{alg} \mathsf{H}_N$ with respect to the norm induced by the inner product extending (2.6).

As a consequence, given Hilbert bases $N_j \subset \mathsf{H}_j$, the orthonormal set

$$\{u_1 \otimes \cdots \otimes u_N \mid u_j \in N_j \;, j = 1, \ldots, N\}$$

is a Hilbert basis of $\mathsf{H}_1 \otimes \cdots \otimes \mathsf{H}_N$ [Mor18].

Remark 2.13 Consider the Hilbert spaces $L^2(X_j, \mu_j)$, $j = 1, \ldots, N$, where each μ_j is σ-finite. The Hilbert space $L^2(X_1 \times \cdots \times X_N, \mu_1 \otimes \cdots \otimes \mu_N)$ turns out to be naturally isomorphic to $L^2(X_1, \mu_1) \otimes \cdots \otimes L^2(X_N, \mu_N)$ [Mor18]. The Hilbert-space isomorphism is the unique continuous linear extension of

$$L^2(X_1,\mu_1)\otimes\cdots\otimes L^2(X_N,\mu_N)\ni f_1\otimes\cdots\otimes f_N \;\mapsto\; f_1\cdots f_N$$
$$\in L^2(X_1\times\cdots\times X_N,\mu_1\otimes\cdots\otimes\mu_N)\;,$$

where $f_1\cdots f_N$ is the pointwise product:

$$(f_1\cdots f_N)(s_1,\ldots,s_N):=f_1(s_1)\cdots f_n(s_N)\;,$$

if $(s_1,\ldots,s_n)\in X_1\times\cdots\times X_N$. ■

2.2 Classes of (Unbounded) Operators on Hilbert Spaces

Keeping in mind we are aiming for *spectral analysis* for its use in QM, we had better introduce a number of preparatory notions on operator algebras.

2.2.1 Operators and Abstract Algebras

From now on an **operator** will be a *linear* map $A : X \to Y$ from a complex linear space X to another linear space Y. In case $Y = \mathbb{C}$, we say that A is a **functional** on X.

As our interest lies in Hilbert spaces H, an **operator** A **on** H will implicitly mean a linear map $A : D(A) \to \mathsf{H}$, whose **domain** $D(A) \subset \mathsf{H}$ is a *subspace* of H. In particular

$$I : \mathsf{H}\ni x\mapsto x\in\mathsf{H}$$

denotes the **identity operator** defined on the *whole* space ($D(I) = \mathsf{H}$). If A is an operator on H, $Ran(A) := \{Ax \mid x \in D(A)\}$ is the **image** or **range** of A.

Notation 2.14 If A and B are operators on H

$$A\subset B \text{ means that } D(A)\subset D(B) \text{ and } B|_{D(A)}=A,$$

where $|_S$ indicates restriction to S. We also adopt the usual conventions regarding **standard domains** for combinations of A, B:

(i) $D(AB) := \{x \in D(B) \mid Bx \in D(A)\}$ is the domain of AB,
(ii) $D(A + B) := D(A) \cap D(B)$ is the domain of $A + B$,
(ii) $D(\alpha A) = D(A)$ for $\alpha \neq 0$ is the domain of αA. ■

With these definitions it is easy to prove that

(1) $(A + B) + C = A + (B + C)$,
(2) $A(BC) = (AB)C$,
(3) $A(B + C) = AB + BC$,
(4) $(B + C)A \supset BA + CA$,
(5) $A \subset B$ and $B \subset C$ imply $A \subset C$,
(6) $A \subset B$ and $B \subset A$ imply $A = B$,
(7) $AB \subset BA$ implies $A(D(B)) \subset D(B)$ if $D(A) = \mathsf{H}$,
(8) $AB = BA$ implies $D(B) = A^{-1}(D(B))$ if $D(A) = \mathsf{H}$ (so $A(D(B)) = D(B)$ if A is surjective).

In the next block we introduce abstract algebraic structures which describe spaces of operators on a Hilbert space.

Definition 2.15 Let $\mathfrak{A}$ be an associative algebra over $\mathbb{C}$.

(1) $\mathfrak{A}$ is a **Banach algebra** if it is a Banach space such that $||ab|| \leq ||a||\,||b||$ for $a, b \in \mathfrak{A}$. A **unital** Banach algebra is a Banach algebra with multiplicative unit $\mathbb{1}$ satisfying $||\mathbb{1}|| = 1$.
(2) $\mathfrak{A}$ is a (unital) ***-algebra** if it is an (unital) algebra equipped with an anti-linear map $\mathfrak{A} \ni a \mapsto a^* \in \mathfrak{A}$, called **involution**, such that $(a^*)^* = a$ and $(ab)^* = b^*a^*$ for $a, b \in \mathfrak{A}$. The *-algebra $\mathfrak{A}$ is said to be **positive** if $a^*a = 0$ implies $a = 0$.
(3) $\mathfrak{A}$ is a (unital) C^***-algebra** if it simultaneously is a (unital) Banach algebra and a *-algebra satisfying $||a^*a|| = ||a||^2$ for $a \in \mathfrak{A}$. (A C^*-algebra is automatically positive.)

A ***-homomorphism** $\mathcal{A} \to \mathfrak{B}$ of *-algebras is an algebra homomorphism preserving involutions and units if present. A bijective *-homomorphism is called ***-isomorphism**.

A (**unital** C)***-subalgebra** is a subset $\mathfrak{B}$ of a given (unital C)*-algebra $\mathfrak{A}$ that is a (unital C)*-algebra for the restricted (unital C)*-algebra operations of $\mathfrak{A}$, provided they are well defined. If present, the unit of $\mathfrak{B}$ is the unit of $\mathfrak{A}$. In case $\mathfrak{B}$ is a (unital) C^*-subalgebra, the two norms agree. ■

Exercise 2.16 Prove that $\mathbb{1}^* = \mathbb{1}$ in a unital *-algebra, and $||a^*|| = ||a||$ if $a \in \mathfrak{A}$ when $\mathfrak{A}$ is a C^*-algebra.

Solution From $\mathbb{1}a = a\mathbb{1} = a$ and the definition of *, we immediately have $a^*\mathbb{1}^* = \mathbb{1}^*a^* = a^*$. Since $(b^*)^* = b$, we have found that $b\mathbb{1}^* = \mathbb{1}^*b = b$ for every $b \in \mathfrak{A}$. The uniqueness of the unit implies $\mathbb{1}^* = \mathbb{1}$. Regarding the second property, $||a||^2 = ||a^*a|| \leq ||a^*||\,||a||$ so that $||a|| \leq ||a^*||$. Everywhere replacing a by a^* and using $(a^*)^*$, we also obtain $||a^*|| \leq ||a||$, so that $||a^*|| = ||a||$. □

We remind the reader that an operator $A : X \to Y$, where X and Y are *normed* complex vector spaces with respective norms $|| \cdot ||_X$ and $|| \cdot ||_Y$, is said to be

bounded if

$$||Ax||_Y \leq b||x||_X \quad \text{for some } b \in [0, +\infty) \text{ and all } x \in X. \tag{2.7}$$

As is well known [Rud91, Mor18],

Proposition 2.17 *An operator $A : X \to Y$ of normed spaces is continuous if and only if it is bounded.*

Proof It is evident that bounded implies continuous because, for $x, x' \in X$, $||Ax - Ax'||_Y \leq b||x - x'||_X$. Conversely, if A is continuous then it is continuous at $x = 0$, so $||Ax||_y \leq \epsilon$ for $\epsilon > 0$ if $||x||_X < \delta$ for $\delta > 0$ sufficiently small. If $||x|| = \delta/2$ we therefore have $||Ax||_Y < \epsilon$ and hence, dividing by $\delta/2$, we also find $||Ax'||_Y < 2\epsilon/\delta$, where $||x'||_X = 1$. Multiplying by $\lambda > 0$ gives $||A\lambda x'||_Y < 2\lambda\epsilon/\delta$, which can be rewritten $||Ax||_Y < 2\frac{\epsilon}{\delta}||x||$ for every $x \in X$, proving that A is bounded. □

For bounded operators it is possible to define the **operator norm**,

$$||A|| := \sup_{0 \neq x \in X} \frac{||Ax||_Y}{||x||_X} \qquad \left(= \sup_{x \in X,\, ||x||_X = 1} ||Ax||_Y \right) .$$

It is easy to prove that this is a norm on the complex vector space $\mathfrak{B}(X, Y)$ of bounded operators $T : X \to Y$, X, Y complex normed, with linear combinations $\alpha A + \beta B \in \mathfrak{B}(X, Y)$ for $\alpha, \beta \in \mathbb{C}$ and $A, B \in \mathfrak{B}(X, Y)$ defined by $(\alpha A + \beta B)x := \alpha Ax + \beta Bx$ for every $x \in X$.

An important, elementary technical result is stated in the following proposition.

Proposition 2.18 *Let $A : S \to Y$ be a bounded operator defined on the subspace $S \subset X$, where X, Y are normed spaces with Y complete. If S is dense in X, then A can be extended to a unique continuous, bounded operator $A_1 : X \to Y$. Moreover $||A_1|| = ||A||$.*

Proof Uniqueness is obvious from continuity: if $S \ni x_n \to x \in X$ and A_1, A'_1 are continuous extensions, $A_1x - A'_1x = \lim_{n\to+\infty} A_1x_n - A'_1x_n = \lim_{n\to+\infty} 0 = 0$. Let us construct a linear continuous extension. If $x \in X$, there exists a sequence $S \ni x_n \to x \in X$ since S is dense. But $\{Ax_n\}_{n\in\mathbb{N}}$ is Cauchy because $\{x_n\}_{n\in\mathbb{N}}$ is Cauchy and $||Ax_n - Ax_m||_Y \leq ||A||||x_n - x_m||_X$, so the limit $A_1x := \lim_{n\to+\infty} Ax_n$ exists because Y is complete. The limit does not depend on the sequence: if $S \ni x'_n \to x$, then $||Ax_n - Ax'_n|| \leq ||A||\,||x_n - x'_n|| \to 0$, so A_1 is well defined. It is immediate to prove that A_1 is linear from the linearity of A, hence A_1 is an operator which extends A to the whole X. By construction, $||A_1x||_Y = \lim_{n\to+\infty} ||Ax_n||_Y \leq \lim_{n\to+\infty} ||A||||x_n||_X \leq ||A||||x||_X$, so $||A_1|| \leq ||A||$, in particular A_1 is bounded. On the other hand

$$||A_1|| = \sup\{||A_1x||\,||x||^{-1} \mid x \in X \setminus \{0\}\} \geq \sup\{||A_1x||\,||x||^{-1} \mid x \in S \setminus \{0\}\}$$

$$= \sup\{||Ax||\,||x||^{-1} \mid x \in S \setminus \{0\}\} = ||A|| ,$$

so that $||A_1|| \geq ||A||$ as well, proving $||A_1|| = ||A||$. □

Notation 2.19 From now on, $\mathfrak{B}(\mathsf{H}) := \mathfrak{B}(\mathsf{H}, \mathsf{H})$ will denote the space of bounded operators $A : \mathsf{H} \to \mathsf{H}$ on the Hilbert space H. ■

$\mathfrak{B}(\mathsf{H})$ acquires the structure of a *unital Banach algebra*: the complex vector space structure is the standard one of operators, the algebra's associative product is the composition of operators with unit I, and the norm is the above operator norm,

$$||A|| := \sup_{0 \neq x \in \mathsf{H}} \frac{||Ax||}{||x||} .$$

This definition of $||A||$ holds also for bounded operators $A : D(A) \to \mathsf{H}$, if $D(A) \subset \mathsf{H}$ but $D(A) \neq \mathsf{H}$. It immediately follows

$$||Ax|| \leq ||A|| \, ||x|| \quad \text{if } x \in D(A).$$

As we already know, $|| \cdot ||$ is a norm on $\mathfrak{B}(\mathsf{H})$. Furthermore, it satisfies

$$||AB|| \leq ||A|| \, ||B|| \quad A, B \in \mathfrak{B}(\mathsf{H}) .$$

It is also evident that $||I|| = 1$. Actually $\mathfrak{B}(\mathsf{H})$ is a Banach space and hence *a unital Banach algebra*, due to the following fundamental result:

Theorem 2.20 *If* H *is a Hilbert space,* $\mathfrak{B}(\mathsf{H})$ *is a Banach space for the operator norm.*

Proof The only non-trivial property is the completeness of $\mathfrak{B}(\mathsf{H})$, so let us prove it. Consider a Cauchy sequence $\{T_n\}_{n\in\mathbb{N}} \subset \mathfrak{B}(\mathsf{H})$. We want to show that there exists $T \in \mathfrak{B}(\mathsf{H})$ which satisfies $||T - T_n|| \to 0$ as $n \to +\infty$. Define $Tx := \lim_{n\to+\infty} Tx$ for every $x \in \mathsf{H}$. The limit exists because $\{T_n x\}_{n\in\mathbb{N}}$ is Cauchy from $||T_n x - T_m x|| \leq ||T_n - T_m|| ||x||$. The linearity of T is easy to prove from the linearity of every T_n. Next observe that $||Tx - T_m x|| = || \lim_n T_n x - T_m x|| = \lim_n ||T_n x - T_m x|| \leq \epsilon ||x||$ if m is sufficiently large. Assuming that $T \in \mathfrak{B}(\mathsf{H})$, dividing by $||x||$ the inequality and taking the sup over $||x|| \neq 0$ proves that $||T - T_m|| \leq \epsilon$ and therefore $||T - T_m|| \to 0$ for $m \to +\infty$, as wanted. This ends the proof because $T \in \mathfrak{B}(\mathsf{H})$ since $||Tx|| \leq ||Tx - T_m x|| + ||T_m x|| \leq \epsilon ||x|| + ||T_m|| ||x||$, and thus $||T|| \leq (\epsilon + ||T_m||) < +\infty$. □

Remark 2.21 The same proof is valid for $\mathfrak{B}(X, Y)$, provided the normed space Y is $|| \cdot ||_Y$-complete. In particular the **topological dual** of the normed space X, denoted by $X^* = \mathfrak{B}(X, \mathbb{C})$, is complete since $\mathbb{C}$ is complete. ■

Exercise 2.22 Prove that on a Hilbert space $\mathsf{H} \neq \{0\}$ there are no operators $X_h, P_k \in \mathfrak{B}(\mathsf{H})$, $h, k = 1, 2, \ldots, n$ satisfying the CCRs (1.22).

Solution It is enough to consider $n = 1$. Suppose that $[X, P] = iI$ (where we set $\hbar = 1$ without loss of generality) for $X, P \in \mathfrak{B}(\mathsf{H})$. By induction $[X, P^k] =$

kiP^{k-1} if $k = 1, 2, \ldots$. Hence

$$k||P^{k-1}|| = ||[X, P^k]|| \leq 2||X||\,||P^k|| \leq 2||X||||P||||P^{k-1}||\,.$$

Dividing by $||P^{k-1}||$ (which cannot vanish, otherwise $P^{k-2} = 0$ from $[X, P^{k-1}] = (k-1)iP^{k-2}$, and then $P = 0$ by induction, which is forbidden since $[X, P] = iI \neq 0$), we have $k \leq 2||X||\,||P||$ for every $k = 1, 2, \ldots$. But this is impossible because $X, P \in \mathfrak{B}(\mathsf{H})$. □

2.2.2 Adjoint Operators

By introducing the notion of *adjoint* operator we can show $\mathfrak{B}(\mathsf{H})$ is a unital C^*-algebra. To this end, we may consider, more generally, unbounded operators defined on non-maximal domains.

Definition 2.23 Let A be a densely-defined operator on the Hilbert space H. Define the subspace of H

$$D(A^*) := \left\{ y \in \mathsf{H} \mid \exists z_y \in \mathsf{H} \text{ s.t. } \langle y|Ax\rangle = \langle z_y|x\rangle \; \forall x \in D(A) \right\} .$$

The linear map $A^* : D(A^*) \ni y \mapsto z_y$ is called the **adjoint** operator to A. ■

Let us explain why the definition is well posed. The element z_y is uniquely determined by y, since $D(A)$ is dense. If z_y, z'_y satisfy $\langle y|Ax\rangle = \langle z_y|x\rangle$ and $\langle y|Ax\rangle = \langle z'_y|x\rangle$, then $\langle z_y - z'_y|x\rangle = 0$ for every $x \in D(A)$. By taking a sequence $D(A) \ni x_n \to z_y - z'_y$ we conclude that $||z_y - z'_y|| = 0$. Therefore $z_y = z'_y$ and $A^* : D(A^*) \ni y \mapsto z_y$ is a well-defined function. Next, by definition of $D(A^*)$ we have that $az_y + bz_{y'}$ satisfies $\langle ay + by'|Ax\rangle = \langle az_y + bz_{y'}|x\rangle$ for $y, y' \in D(A^*)$ and $a, b \in \mathbb{C}$, by the inner product's (anti-)linearity, so eventually $A^* : D(A^*) \ni u \mapsto z_u$ is linear too.

Remark 2.24

(a) If $D(A)$ is not dense, A^* cannot be defined in general. As an example, consider a closed subspace $M \subsetneq \mathsf{H}$, so $M^\perp \neq \{0\}$. Define $A : D(A) = M \ni x \mapsto x \in \mathsf{H}$. If $0 \neq y \in M^\perp$ we have $\langle y|Ax\rangle = \langle y|x\rangle = 0$, and hence $y \in D(A^*)$ and $A^*y = y$. But this is inconsistent, for $\langle y|Ax\rangle = 0 = \langle 2y|x\rangle$ implies $A^*y = 2y$. In this context the alleged function A^* would necessarily be multi-valued.

(b) By construction, we immediately have that

$$\langle A^*y|x\rangle = \langle y|Ax\rangle \quad \text{for } x \in D(A) \text{ and } y \in D(A^*)\,.$$

■

Exercise 2.25 Prove that $D(A^*)$ can equivalently be defined as the set (subspace) of $y \in \mathsf{H}$ such that the functional $D(A) \ni x \mapsto \langle y|Ax\rangle$ is continuous.

Solution This is a simple application of the Riesz lemma, after extending $D(A) \ni x \mapsto \langle y|Ax\rangle$ to a continuous functional on $\overline{D(A)} = \mathsf{H}$ by continuity. □

Remark 2.26

(a) If both A and A^* are densely defined then $A \subset (A^*)^*$. The proof follows from the definition of adjoint operator.
(b) If A is densely defined and $A \subset B$ then $B^* \subset A^*$. The proof is immediate from the definition of adjoint.
(c) If $A \in \mathfrak{B}(\mathsf{H})$ then $A^* \in \mathfrak{B}(\mathsf{H})$ and $(A^*)^* = A$. Moreover

$$||A^*||^2 = ||A||^2 = ||A^*A|| = ||AA^*|| \,.$$

(See Exercise 2.28.)
(d) From the definition of adjoint one has, for densely defined operators A, B on H,

$$A^* + B^* \subset (A+B)^* \quad \text{and} \quad A^*B^* \subset (BA)^* \,.$$

Furthermore

$$A^* + B^* = (A+B)^* \quad \text{and} \quad A^*B^* = (BA)^* \,, \tag{2.8}$$

whenever $B \in \mathfrak{B}(\mathsf{H})$ and A is densely defined.
(e) By (c), and (2.8) in particular, it is clear that $\mathfrak{B}(\mathsf{H})$ is a unital C^*-algebra with involution $\mathfrak{B}(\mathsf{H}) \ni A \mapsto A^* \in \mathfrak{B}(\mathsf{H})$. ■

Definition 2.27 If $\mathfrak{A}$ is a (unital) *-algebra and H a Hilbert space, a **representation** of $\mathfrak{A}$ on H is a *-homomorphism $\pi : \mathfrak{A} \to \mathfrak{B}(\mathsf{H})$ for the natural (unital) *-algebra structure of $\mathfrak{B}(\mathsf{H})$. The representation π is called **faithful** if it is injective.

Two representations $\pi_1 : \mathfrak{A} \to \mathfrak{B}(\mathsf{H}_1)$ and $\pi_2 : \mathfrak{A} \to \mathfrak{B}(\mathsf{H}_2)$ are said to be **unitarily equivalent** if there exists a Hilbert space isomorphism $U : \mathsf{H}_1 \to \mathsf{H}_2$ such that

$$U\pi_1(a)U^{-1} = \pi_2(a) \quad \text{for all } a \in \mathfrak{A}.$$

■

Exercise 2.28 Prove that $A^* \in \mathfrak{B}(\mathsf{H})$ if $A \in \mathfrak{B}(\mathsf{H})$ and that, in this case, $(A^*)^* = A$, $||A|| = ||A^*||$ and $||A^*A|| = ||AA^*|| = ||A||^2$.

Solution If $A \in \mathfrak{B}(\mathsf{H})$, for every $y \in \mathsf{H}$ the linear map $\mathsf{H} \ni x \mapsto \langle y|Ax\rangle$ is continuous ($|\langle y|Ax\rangle| \leq ||y||||Ax|| \leq ||y||||A||||x||$), therefore Theorem 2.6 guarantees that there exists a unique $z_{y,A} \in \mathsf{H}$ with $\langle y|Ax\rangle = \langle z_{y,A}|x\rangle$ for all $x, y \in \mathsf{H}$. The map $\mathsf{H} \ni y \mapsto z_{y,A}$ is linear because $z_{y,A}$ is unique and the inner product is anti-linear on the left. The map $\mathsf{H} \ni y \mapsto z_{y,A}$ fits the definition of A^*, so it coincides with

A^* and $D(A^*) = \mathsf{H}$. Since $\langle A^*x|y\rangle = \langle x|Ay\rangle$ for $x, y \in \mathsf{H}$ implies (conjugating) $\langle y|A^*x\rangle = \langle Ay|x\rangle$ for $x, y \in \mathsf{H}$, we have $(A^*)^* = A$. To prove that A^* is bounded observe that $||A^*x||^2 = \langle A^*x|A^*x\rangle = \langle x|AA^*x\rangle \leq ||x||\,||A||\,||A^*x||$, so that $||A^*x|| \leq ||A||\,||x||$ and $||A^*|| \leq ||A||$. Using $(A^*)^* = A$, we have $||A^*|| = ||A||$. Regarding the last identity, it is evidently enough to prove that $||A^*A|| = ||A||^2$. First of all, $||A^*A|| \leq ||A^*||\,||A|| = ||A||^2$, so that $||A^*A|| \leq ||A||^2$. On the other hand $||A||^2 = (\sup_{||x||=1} ||Ax||)^2 = \sup_{||x||=1} ||Ax||^2 = \sup_{||x||=1}\langle Ax|Ax\rangle = \sup_{||x||=1}\langle x|A^*Ax\rangle \leq \sup_{||x||=1} ||x||||A^*Ax|| = \sup_{||x||=1} ||A^*Ax|| = ||A^*A||$. We have found that $||A^*A|| \leq ||A||^2 \leq ||A^*A||$, so $||A^*A|| = ||A||^2$. □

Exercise 2.29 Prove that if $A \in \mathfrak{B}(\mathsf{H})$, then A^* is bijective if and only if A is bijective. In this case $(A^{-1})^* = (A^*)^{-1}$.

Solution If $A \in \mathfrak{B}(\mathsf{H})$ is bijective we have $AA^{-1} = A^{-1}A = I$. Taking adjoints, $(A^{-1})^*A^* = A^*(A^{-1})^* = I^* = I$ from Remark 2.26 (d), which implies $(A^{-1})^* = (A^*)^{-1}$ by the uniqueness of inverses. If A^* is bijective, taking the adjoint of $(A^*)^{-1}A^* = A^*(A^*)^{-1} = I$ and using $(A^*)^* = A$ shows that A is bijective as well. ■

2.2.3 Closed and Closable Operators

Definition 2.30 Let A be an operator on the Hilbert space H.

(1) A is said to be **closed** if its **graph**

$$G(A) := \{(x, Ax) \subset \mathsf{H} \times \mathsf{H} \mid x \in D(A)\}$$

is closed in the product topology of $\mathsf{H} \times \mathsf{H}$.

(2) A is **closable** if it admits closed extensions. This is equivalent to saying that the closure of the graph of A is the graph of an operator, denoted by $\overline{A}$ and called the **closure** of A.

(3) If A is closable, a subspace $S \subset D(A)$ is called a **core** for A if $\overline{A|_S} = \overline{A}$. ■

Referring to (2), given an operator A we can always define the closure of the graph $\overline{G(A)}$ in $\mathsf{H} \times \mathsf{H}$. In general this closure will not be the graph of an operator, because there may exist sequences $D(A) \ni x_n \to x$ and $D(A) \ni x'_n \to x$ such that $Tx_n \to y$ and $Tx_n \to y'$ with $y \neq y'$. However, both pairs (x, y) and (x, y') belong to $\overline{G(A)}$. If this is not the case—this is precisely condition (a) below—$\overline{G(A)}$ is indeed the graph of an operator, written $\overline{A}$, that is closed by definition. Therefore A always admits closed extensions: at least there is $\overline{A}$. If, conversely, A admits extensions by closed operators, the intersection $\overline{G(A)}$ of the (closed) graphs of these extensions is still closed; furthermore, $\overline{G(A)}$ is the graph of an operator which must coincide with $\overline{A}$ by definition.

Remark 2.31

(a) Directly from the definition and using linearity, A is closable if and only if there are no sequences of elements $x_n \in D(A)$ such that $x_n \to 0$ and $Ax_n \to y \neq 0$ as $n \to +\infty$. Since $\overline{G(A)}$ is on one hand the union of $G(A)$ and its accumulation points in $\mathsf{H} \times \mathsf{H}$ and on the other, if A is closable, it is also the graph of the operator $\overline{A}$, we conclude that

   (i) $D(\overline{A})$ consists of the elements $x \in \mathsf{H}$ such that $x_n \to x$ and $Ax_n \to y_x$ for some sequence $\{x_n\}_{n\in\mathbb{N}} \subset D(A)$ and some $y_x \in D(A)$
   (ii) $\overline{A}x = y_x$.

(b) As a consequence of (a), if A is closable then $aA + bI$ is closable and $\overline{aA + bI} = a\overline{A} + bI$ for every $a, b \in \mathbb{C}$.
Caution: *this generally fails if we replace I with a closable operator B.*
(c) Directly by definition A is closed if and only if $D(A) \ni x_n \to x \in \mathsf{H}$ and $Ax_n \to y \in \mathsf{H}$ imply $x \in D(A)$ and $y = Ax$. ■

A useful proposition is the following.

Proposition 2.32 *Consider an operator $A : D(A) \to \mathsf{H}$, with $D(A)$ dense, on the Hilbert space H. The following facts hold.*

(a) *A^* is closed.*
(b) *A is closable if and only if $D(A^*)$ is dense, and in this case $\overline{A} = (A^*)^*$.*

Proof The Hermitian product $((x, y)|(x'y')) := \langle x|x'\rangle + \langle y|y'\rangle$ makes the standard direct sum $\mathsf{H} \oplus \mathsf{H}$ a Hilbert space. Now consider the operator

$$\tau : \mathsf{H} \oplus \mathsf{H} \ni (x, y) \mapsto (-y, x) \in \mathsf{H} \oplus \mathsf{H}\,. \tag{2.9}$$

It is easy to check that $\tau \in \mathfrak{B}(\mathsf{H} \oplus \mathsf{H})$ and

$$\tau^* = \tau^{-1} = -\tau \tag{2.10}$$

(adjoints in $\mathsf{H}\oplus\mathsf{H}$). By direct computation one sees that τ and $^\perp$ (on $\mathsf{H}\oplus\mathsf{H}$) commute

$$\tau(F^\perp) = (\tau(F))^\perp \quad \text{if } F \subset \mathsf{H} \oplus \mathsf{H}. \tag{2.11}$$

Let us prove (a). The following noteworthy relation is true for every operator $A : D(A) \to \mathsf{H}$ with $D(A)$ dense in H (so A^* exists)

$$G(A^*) = \tau(G(A))^\perp\,. \tag{2.12}$$

Since the right-hand side is closed (it is the orthogonal space to a set), the graph of A^* is closed and A^* is therefore closed by definition. To prove (2.12) observe that, by definition of τ, $\tau(G(A))^\perp = \{(y, z) \in \mathsf{H} \oplus \mathsf{H} \mid ((y, z)|(-Ax, x)) = 0\ , \forall x \in D(A)\}$, that is

$$\tau(G(A))^\perp = \{(y, z) \in \mathsf{H} \oplus \mathsf{H} \mid \langle y|Ax\rangle = \langle z|x\rangle\ , \forall x \in D(A)\}\ .$$

Since A^* exists, the pair $(y, z) \in \tau(G(A))^\perp$ can be written (y, A^*y) by definition of A^*. Hence $\tau(G(A))^\perp = G(A^*)$, proving (a).

(b) From the properties of $^\perp$ we immediately have $\overline{G(A)} = (G(A)^\perp)^\perp$. Since τ and $^\perp$ commute by (2.11), and $\tau\tau = -I$ (2.10),

$$\overline{G(A)} = -\tau \circ \tau((G(A)^\perp)^\perp) = -\tau(\tau(G(A))^\perp)^\perp = \tau(\tau(G(A))^\perp)^\perp = \tau(G(A^*))^\perp .$$

The minus sign disappeared since the subspace is closed under multiplication by scalars and by (2.12). Now suppose that $D(A^*)$ is dense, so that $(A^*)^*$ exists. Using (2.12) again, we have $\overline{G(A)} = G((A^*)^*)$. The right-hand side is the graph of an operator, so if $D(A^*)$ is dense, then A is closable. By definition of closure, $\overline{A} = (A^*)^*$.

Vice versa, suppose that A is closable, so that $\overline{A}$ exists and $G(\overline{A}) = \overline{G(A)}$. Then $\tau(G(A^*))^\perp = \overline{G(A)}$ is the graph of an operator and hence cannot contain pairs $(0, y)$ with $y \neq 0$, by linearity. In other words, if $(0, y) \in \tau(G(A^*))^\perp$, then $y = 0$. This is the same as saying that $((0, y)|(-A^*x, x)) = 0$ for all $x \in D(A^*)$ implies $y = 0$. Summing up, $\langle y|x\rangle = 0$ for all $x \in D(A^*)$ implies $y = 0$. As $\mathsf{H} = D(A^*)^\perp \oplus (D(A^*)^\perp)^\perp = D(A^*)^\perp \oplus \overline{D(A^*)}$, we conclude that $\overline{D(A^*)} = \mathsf{H}$, which proves the density. □

Corollary 2.33 *Let $A : D(A) \to \mathsf{H}$ an operator on the Hilbert space H. If both $D(A)$ and $D(A^*)$ are densely defined then*

$$A^* = \overline{A}^* = \overline{A^*} = (((A^*)^*)^*\ .$$

The Hilbert-space version of the *closed graph theorem* holds (e.g., see [Rud91, Mor18]).

Theorem 2.34 (Closed Graph Theorem) *Let $A : \mathsf{H} \to \mathsf{H}$ be an operator, H a Hilbert space. Then A is closed if and only if $A \in \mathfrak{B}(\mathsf{H})$.*

An important corollary is the Hilbert version of the *bounded inverse theorem of Banach* (e.g., see [Rud91, Mor18]).

Corollary 2.35 (Banach's Bounded Inverse Theorem) *Let $A : \mathsf{H} \to \mathsf{H}$ be an operator, H a Hilbert space. If A is bijective and bounded its inverse is bounded.*

Proof The graph of $A^{-1} : \mathsf{H} \to \mathsf{H}$ is closed because A is bounded and a fortiori closed, and its graph is the same as that of A^{-1}. Theorem 2.34 implies that A^{-1} is bounded. □

Exercise 2.36 Consider $B \in \mathfrak{B}(\mathsf{H})$ and a closed operator A on H such that $Ran(B) \subset D(A)$. Prove that $AB \in \mathfrak{B}(\mathsf{H})$.

Solution AB is well defined by hypothesis and $D(AB) = \mathsf{H}$. Exploiting Remark 2.31 (c) and the continuity of B, one easily sees that AB is closed as well. Theorem 2.34 eventually proves $AB \in \mathfrak{B}(\mathsf{H})$. □

2.2.4 Types of Operators Relevant in Quantum Theory

Definition 2.37 An operator A on a Hilbert space H is called

(0) **Hermitian** if $\langle Ax|y\rangle = \langle x|Ay\rangle$ for $x, y \in D(A)$,
(1) **symmetric** if it is densely defined and Hermitian, which is equivalent to say $A \subset A^*$.
(2) **selfadjoint** if it is symmetric and $A = A^*$,
(3) **essentially selfadjoint** if it is symmetric and $(A^*)^* = A^*$.
(4) **unitary** if $A^*A = AA^* = I$,
(5) **normal** if it is closed, densely defined and $AA^* = A^*A$. ■

Remark 2.38

(a) If A is unitary then $A, A^* \in \mathfrak{B}(\mathsf{H})$. Furthermore an operator $A : \mathsf{H} \to \mathsf{H}$ is unitary if and only if it is surjective and norm-preserving. (See Exercise 2.43). Unitary operators are the **automorphisms** of the Hilbert space. An **isomorphism** of Hilbert spaces H, H' is a surjective linear isometry $T : \mathsf{H} \to \mathsf{H}'$. Any such also preserves inner products by Proposition 2.1.2.
(b) A selfadjoint operator A does not admit proper symmetric extensions, and essentially selfadjoint operators admit only one selfadjoint extension. (See Proposition 2.39 below).
(c) A symmetric operator A is always closable because $A \subset A^*$ and A^* is closed (Proposition 2.32). In addition, by Proposition 2.32 and Corollary 2.33, the reader will have no difficulty in proving the following are equivalent for symmetric operators A:

    (i) $(A^*)^* = A^*$ (A is essentially selfadjoint),
    (ii) $\overline{A} = A^*$,
    (iii) $\overline{A} = (\overline{A})^*$.

(d) Unitary and selfadjoint operators are instances of normal operators. ■

The elementary results on (essentially) selfadjoint operators stated in (b) are worthy of a proof.

Proposition 2.39 *Let* $A : D(A) \to \mathsf{H}$ *be a densely-defined operator on the Hilbert space* H. *Then*

(a) *if A is selfadjoint, it does not admit proper symmetric extensions.*
(b) *If A is essentially selfadjoint, it admits a unique selfadjoint extension $A^* = \overline{A}$.*

Proof

(a) Let B be a symmetric extension of A. By Remark 2.26 (b) $A \subset B$ implies $B^* \subset A^*$. As $A = A^*$ we have $B^* \subset A \subset B$. Since $B \subset B^*$, we conclude that $A = B$.
(b) Let B be a selfadjoint extension of the essentially selfadjoint operator A, so that $A \subset B$. Therefore $A^* \supset B^* = B$ and $(A^*)^* \subset B^* = B$. Since A is essentially selfadjoint, we have $A^* \subset B$. Here A^* is selfadjoint and B is symmetric because selfadjoint, so (a) forces $A^* = B$. That is, every selfadjoint extension of A coincides with A^*. Finally, $A^* = \overline{A}$ by Remark 2.38 (c).

□

Here is an elementary yet important result that helps to understand why in QM observables are very often described by unbounded selfadjoint operators defined on proper subspaces.

Theorem 2.40 (Hellinger-Toeplitz Theorem) *A selfadjoint operator A on a Hilbert space H is bounded if and only if $D(A) = \mathsf{H}$ (and hence $A \in \mathfrak{B}(\mathsf{H})$).*

Proof Assume that $D(A) = \mathsf{H}$. As $A = A^*$, we have $D(A^*) = \mathsf{H}$. Since A^* is closed, Theorem 2.34 implies $A^*(= A)$ is bounded. Conversely, if $A = A^*$ is bounded, since $D(A)$ is dense, we can extend it with continuity to a bounded operator $A_1 : \mathsf{H} \to \mathsf{H}$. The extension, by continuity, trivially satisfies $\langle A_1 x | y \rangle = \langle x | A_1 y \rangle$ for all $x, y \in \mathsf{H}$, hence A_1 is symmetric. Since $A^* = A \subset A_1 \subset A_1^*$, Proposition 2.39 (a) implies $A = A_1$. □

Let us pass to unitary operators. The relevance of unitary operators is manifest from the fact that the nature of an operator does not change under Hermitian conjugation by a unitary operator.

Proposition 2.41 *Let $U : \mathsf{H} \to \mathsf{H}$ be a unitary operator on the complex Hilbert space H and A another operator on H. The operators UAU^* and U^*AU (defined on $U(D(A))$ and $U^*(D(A))$) are symmetric, selfadjoint, essentially selfadjoint, unitary or normal if A is respectively symmetric, selfadjoint, essentially selfadjoint, unitary or normal.*

Proof Since U^* is unitary when U is and $(U^*)^* = U$, it is enough to prove the claim for UAU^*. First of all notice that $D(UAU^*) = U(D(A))$ is dense if $D(A)$ is dense since U is bijective and isometric, and $U(D(A)) = \mathsf{H}$ if $D(A) = \mathsf{H}$ because U is bijective. By direct inspection, applying the definition of adjoint operator, one sees that $(UAU^*)^* = UA^*U^*$ and $D((UAU^*)^*) = U(D(A^*))$. Now, if A is symmetric $A \subset A^*$, then $UAU^* \subset UA^*U^* = (UAU^*)^*$, so that UAU^* is symmetric as well. If A is selfadjoint $A = A^*$, then $UAU^* = UA^*U^* = (UAU^*)^*$, so that UAU^* is selfadjoint as well. If A is essentially selfadjoint it is symmetric and $(A^*)^* = A^*$, so UAU^* is symmetric and $U(A^*)^*U^* = UA^*U^*$, that is $(UA^*U^*)^* = UA^*U^*$. This means $((UAU^*)^*)^* = (UAU^*)^*$, and UA^*U^* is essentially selfadjoint. If A is unitary, we have $A^*A = AA^* = I$ and hence $UA^*AU^* = UAA^*U^* = UU^*$. As $U^*U = I = UU^*$, the latter is equivalent to $UA^*U^*UAU^* = UAU^*UA^*U^* = U^*U = I$, that is $(UA^*U^*)UAU^* = (UAU^*)UA^*U^* = I$. Hence UAU^* is unitary as well. At last if A is normal, UAU^* is normal too, by the same argument of the unitary case.

□

Remark 2.42 The same proof goes through if $U : \mathsf{H} \to \mathsf{H}'$ is an isometric and surjective linear map. A minor change allows to adapt the proof to $U : \mathsf{H} \to \mathsf{H}'$ isometric, surjective but **anti-linear**, that is $U(\alpha x + \beta y) = \overline{\alpha}Ux + \overline{\beta}Uy$ if $\alpha, \beta \in \mathbb{C}$ and $x, y \in \mathsf{H}$. We leave to the reader these straightforward generalizations. ■

Exercise 2.43

(1) *Prove that* $A, A^* \in \mathfrak{B}(\mathsf{H})$ *if* A *is unitary.*

Solution Since $D(A) = D(A^*) = D(I) = \mathsf{H}$ and $||Ax||^2 = \langle Ax|Ax\rangle = \langle x|A^*Ax\rangle = ||x||^2$ if $x \in \mathsf{H}$, it follows that $||A|| = 1$. Due to Remark 2.26 (c), $A^* \in \mathfrak{B}(\mathsf{H})$. □

(2) *Prove that an operator* $A : \mathsf{H} \to \mathsf{H}$ *is unitary iff it is surjective and norm-preserving.*

Solution If A is unitary (Definition 2.37 (3)), it is manifestly bijective. As $D(A^*) = \mathsf{H}$, moreover, $||Ax||^2 = \langle Ax|Ax\rangle = \langle x|A^*Ax\rangle = \langle x|x\rangle = ||x||^2$, so A is also isometric. If $A : \mathsf{H} \to \mathsf{H}$ is isometric its norm is 1 and hence $A \in \mathfrak{B}(\mathsf{H})$. Therefore $A^* \in \mathfrak{B}(\mathsf{H})$. The condition $||Ax||^2 = ||x||^2$ can be rewritten as $\langle Ax|Ax\rangle = \langle x|A^*Ax\rangle = \langle x|x\rangle$, and so $\langle x|(A^*A - I)x\rangle = 0$ for $x \in \mathsf{H}$. Writing $x = y \pm z$ and $x = y \pm iz$, the previous identity implies $\langle z|(A^*A - I)y\rangle = 0$ for all $y, z \in \mathsf{H}$. By taking $z = (A^*A - I)y$ we finally have $||(A^*A - I)y|| = 0$ for all $y \in \mathsf{H}$ and thus $A^*A = I$. In particular, A is injective for it admits left inverse A^*. Since A is also surjective it is bijective, and its left inverse (A^*) is also a right inverse, that is $AA^* = I$.

(3) *Suppose* $A : \mathsf{H} \to \mathsf{H}$ *satisfies* $\langle x|Ax\rangle \in \mathbb{R}$ *for all* $x \in \mathsf{H}$ *(and in particular if* $A \geq 0$*, which means* $\langle x|Ax\rangle \geq 0$ *for all* $x \in \mathsf{H}$*). Show that* $A^* = A$ *and* $A \in \mathfrak{B}(\mathsf{H})$.

Solution We have $\langle x|Ax\rangle = \overline{\langle x|Ax\rangle} = \langle Ax|x\rangle = \langle x|A^*x\rangle$ where, as $D(A) = \mathsf{H}$, the adjoint A^* is well defined everywhere on H. Hence $\langle x|(A - A^*)x\rangle = 0$ for every $x \in \mathsf{H}$. Writing $x = y \pm z$ and $x = y \pm iz$ we obtain $\langle y|(A - A^*)z\rangle = 0$ for all $y, z \in \mathsf{H}$. We conclude that $A = A^*$ by choosing $y = (A - A^*)z$. Theorem 2.40 ends the proof. □

Example 2.44 Recall the **Fourier transform** $\mathscr{F} : \mathscr{S}(\mathbb{R}^n) \to \mathscr{S}(\mathbb{R}^n)$ of $f \in \mathscr{S}(\mathbb{R}^n)$ is defined as[1]

$$(\mathscr{F} f)(k) := \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-ik\cdot x} f(x) d^n x, \tag{2.13}$$

where $k\cdot x$ is the Euclidean inner product of k and x in $\mathbb{R}^n$, see, e.g. [Rud91, Mor18]). It is a linear bijection with inverse $\mathscr{F}_- : \mathscr{S}(\mathbb{R}^n) \to \mathscr{S}(\mathbb{R}^n)$,

$$(\mathscr{F}_- g)(x) := \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{ik\cdot x} g(k) d^n k\ , \tag{2.14}$$

so that

$$\mathscr{F} \circ \mathscr{F}_- = \mathscr{F}_- \circ \mathscr{F} = \iota_{\mathscr{S}(\mathbb{R}^n)}\ . \tag{2.15}$$

It is known (e.g., [Rud91, Mor18]) that $\mathscr{F}$ and $\mathscr{F}_-$ preserve the inner product

$$\langle \mathscr{F} f|\mathscr{F} g\rangle = \langle f|g\rangle\ , \quad \langle \mathscr{F}_- f|\mathscr{F}_- g\rangle = \langle f|g\rangle \quad \forall f, g \in \mathscr{S}(\mathbb{R}^n) \tag{2.16}$$

and therefore they also preserve the $L^2(\mathbb{R}^n, d^n x)$-norm. In particular, $||\mathscr{F}|| = ||\mathscr{F}_-|| = 1$. As a consequence of Proposition 2.18, the density of $\mathscr{S}(\mathbb{R}^n)$ in $L^2(\mathbb{R}^n, d^n x)$ [Rud91] implies that $\mathscr{F}$ and $\mathscr{F}_-$ extend to unique continuous bounded operators $\hat{\mathscr{F}} : L^2(\mathbb{R}^n, d^n x) \to L^2(\mathbb{R}^n, d^n k)$ and $\hat{\mathscr{F}}_- : L^2(\mathbb{R}^n, d^n k) \to L^2(\mathbb{R}^n, d^n x)$ such that $\hat{\mathscr{F}}^{-1} = \hat{\mathscr{F}}_-$, because also (2.15) trivially extends to $L^2(\mathbb{R}^n, d^n x)$ by continuity. Since the inner product is continuous, from (2.16) we finally obtain

$$\langle \hat{\mathscr{F}} f|\hat{\mathscr{F}} g\rangle = \langle f|g\rangle\ , \quad \langle \hat{\mathscr{F}}_- f|\hat{\mathscr{F}}_- g\rangle = \langle f|g\rangle \quad \forall f, g \in L^2(\mathbb{R}^n, d^n x)\ . \tag{2.17}$$

To summarize, $\hat{\mathscr{F}}$ is an isometric, surjective linear map from $L^2(\mathbb{R}^n, d^n x)$ to $L^2(\mathbb{R}^n, d^n x)$, and therefore a unitary operator. The same properties are enjoyed by the inverse $\hat{\mathscr{F}}_-$. The unitary map $\hat{\mathscr{F}}$ is the **Fourier-Plancherel operator**. ■

Remark 2.45 Let X be a topological space, and indicate the **space of continuous maps vanishing at infinity** by

$$C_0(X) := \{f : X \to \mathbb{C} \text{ continuous } \mid \forall \epsilon > 0\, \exists K_\epsilon \subset X \text{ compact with } |f(x)| < \epsilon \text{ if } x \notin K_\epsilon\}.$$

It is evident that the linear maps (2.13) and (2.14) are well defined if we allow $f \in L^1(\mathbb{R}^n, d^n x)$, $g \in L^1(\mathbb{R}^n, d^n k)$. The ranges of these extensions are not

[1] In QM, $k \cdot x$ has to be replaced by $\frac{k\cdot x}{\hbar}$ and $(2\pi)^{n/2}$ by $(2\pi\hbar)^{n/2}$ in unit systems where $\hbar \neq 1$.

subsets of L^1, however. They are called L^1**-Fourier transform** and **inverse** L^1**-Fourier transform** respectively, and satisfy the following properties (see, e.g., [Rud91, Mor18])

(a) $\mathscr{F}(L^1(\mathbb{R}^n, d^n x)) \subset C_0(\mathbb{R}^n)$, the latter being the Banach space of complex continuous maps on $\mathbb{R}^n$ vanishing at infinity with norm $||\cdot||_\infty$;
(b) $||\mathscr{F}(f)||_\infty \leq ||f||_1$, and hence $\mathscr{F} : L^1(\mathbb{R}^n, d^n x) \to C_0(\mathbb{R}^n)$ is continuous;
(c) $\mathscr{F} : L^1(\mathbb{R}^n, d^n x) \to C_0(\mathbb{R}^n)$ is *injective* and $\mathscr{F}_-(\mathscr{F}(f)) = f$ if $\mathscr{F}(f) \in L^1(\mathbb{R}, d^n k)$ for any $f \in L^1(\mathbb{R}, d^n x)$.

Analogous properties hold by swapping $\mathscr{F}$ and $\mathscr{F}_-$. It is worth pointing out that (a) implies the famed **Riemann-Lebesgue lemma**: $\mathscr{F}(f)(k) \to 0$ uniformly as $|k| \to +\infty$ provided $f \in L^1(\mathbb{R}^n, d^n x)$. ■

*2.2.5 The Interplay of Ker, Ran, *, and* $^\perp$

Pressing on, we establish two technical facts which will be useful several times in the sequel.

Proposition 2.46 *If* $A : D(A) \to \mathsf{H}$ *is a densely-defined operator on the Hilbert space* H*,*

$$Ker(A^*) = Ran(A)^\perp\,, \quad Ker(A) \subset Ran(A^*)^\perp\,. \tag{2.18}$$

The inclusion becomes an equality if $A \in \mathfrak{B}(\mathsf{H})$.

Proof By the definition of adjoint operator we know that

$$\langle A^* y|x\rangle = \langle y|Ax\rangle\,, \quad \forall x \in D(A)\,, \forall y \in D(A^*)\,. \tag{2.19}$$

If $y \in Ker(A^*)$, then $\langle y|Ax\rangle = 0$ for all $x \in D(A)$ due to (2.19), so that $y \in Ran(A)^\perp$. If, conversely, $y \in Ran(A)^\perp$, then $\langle y|Ax\rangle = 0$ for all $x \in D(A)$. This means that $y \in D(A^*)$, by definition of $D(A^*)$, and $A^* y = 0$. We have proved that $Ker(A^*) = Ran(A)^\perp$. Regarding the second inclusion, if $x \in Ker(A)$, we have from (2.19) that $\langle A^* y|x\rangle = 0$ for every $y \in D(A^*)$ and therefore $x \in Ran(A^*)^\perp$. Hence $Ker(A) \subset Ran(A^*)^\perp$. To conclude, observe that the requirement $x \in Ran(A^*)^\perp$ entails from (2.19) that $\langle y|Ax\rangle = 0$ for every $y \in D(A^*)$ *provided* $x \in D(A)$. If $A \in \mathfrak{B}(\mathsf{H})$, then $x \in \mathsf{H}$ belongs to $D(A) = \mathsf{H}$, and $\langle y|Ax\rangle = 0$ for every $y \in D(A^*) = \mathsf{H}$. Therefore $Ax = 0$, and so $Ker(A) \supset Ran(A^*)^\perp$. □

For densely-defined operators A the domain $D(A^*)$ is dense, and the first relation implies $Ker(A^{**}) = Ran(A^*)^\perp$. By Proposition 2.32 we can strengthen (2.18),

$$Ker(A^*) = Ran(A)^\perp\,, \quad Ker(\overline{A}) = Ran(A^*)^\perp\,. \tag{2.20}$$

Replacing A with $A - \lambda I$, $\lambda \in \mathbb{C}$ in (2.18) we find the following useful relations,

$$Ker(A^* - \overline{\lambda} I) = [Ran(A - \lambda I)]^\perp , \quad Ker(A - \lambda I) \subset [Ran(A^* - \overline{\lambda} I)]^\perp . \tag{2.21}$$

Once again, the inclusion becomes an equality if $A \in \mathfrak{B}(\mathsf{H})$, or if A is closable and A is replaced by $\overline{A}$.

2.2.6 *Criteria for (Essential) Selfadjointness*

Let us review common tools for studying the (essential) selfadjointness of symmetric operators, briefly. If A is a densely-defined symmetric operator on the Hilbert space H, define the **deficiency indices** [ReSi80, Rud91, Schm12, Tes14, Mor18]

$$n_\pm := \dim \mathsf{H}_\pm \quad \text{(cardinal numbers in general), where } \mathsf{H}_\pm := Ker(A^* \pm iI).$$

Proposition 2.47 *Let A be a symmetric operator on a Hilbert space H.*

(a) *The following are equivalent:*

  (i) *A is selfadjoint,*
  (ii) *$n_+ = n_- = 0$ and A is closed,*
  (iii) *$Ran(A \pm iI) = \mathsf{H}$.*

(b) *The following are equivalent as well:*

  (i) *A is essentially selfadjoint,*
  (ii) *$n_+ = n_- = 0$.*
  (iii) *$\overline{Ran(A \pm iI)} = \mathsf{H}$.*

Proof

(a) Assume (i) $A = A^*$. Then A is closed because A^* is closed. Furthermore, if $A^* x_\pm \pm ix = 0$ then $\langle x | A^* x \rangle = \pm i ||x_\pm||^2$. But $\langle x_\pm | A^* x_\pm \rangle = \langle x_\pm | A x_\pm \rangle$ is real, so the only possibility is $||x_\pm|| = 0$ and $n_\pm = 0$. We have proved that (i) implies (ii). Let us show that (ii) implies (iii). Suppose that A is symmetric, closed and $n_\pm = 0$. The latter condition explicitly reads $Ker(A^* \pm iI) = \{0\}$, which in turn means that $Ran(A \pm iI)$ is dense in H due to (2.21). Since $A \pm iI$ is closed because A is closed, we even have (iii) $Ran(A \pm iI) = \mathsf{H}$ because $Ran(A \pm iI)$ is closed as well. Indeed, suppose that $Ax_n + ix_n \to y$. As $A \subset A^*$ we get $||x_n||^2 \leq ||Ax_n||^2 + ||x_n||^2 = ||Ax_n + ix_n||^2$, and then $\{x_n\}_{n \in \mathbb{N}}$ is Cauchy, $x_n \to x \in \mathsf{H}$. Since $A + iI$ is closed, $x \in D(A + iI)$ and $y = (A + iI)x$ as we wanted. The case of $A - iI$ is identical. To conclude, let us prove that (iii) implies (i) $A^* = A$. Since A is symmetric it suffices to show $D(A^*) \subset D(A)$. Take $y \in D(A^*)$. Since $Ran(A \pm iI) = \mathsf{H}$, we must have $A^* y \pm iy = Ax_\pm \pm ix_\pm$

for some $x_+, x_- \in D(A)$. As $A^*\restriction_{D(A)} = A$, we have $(A^* \pm iI)(y - x_\pm) = 0$. But we know that $Ker(A^* \pm iI) = Ran(A \pm iI)^\perp = \{0\}$, so $y = x_\pm \in D(A)$, concluding the proof of (a).

(b) If (i) holds then A^* is selfadjoint: $A^{**} = A^*$, so (ii) holds by (ii) in part (a). Furthermore, (ii) is equivalent to (iii) by (2.21). To conclude, it is enough to demonstrate that (ii) forces the closure $\overline{A}$ to be selfadjoint ($\overline{A}$ exists because $A^* \supset A$). But this is equivalent to claim (i) by Remark 2.38 (c). As $\overline{A}$ is symmetric we can use (a). We know that $\overline{A}^* = A^*$ from Corollary 2.33. Since A^* satisfies (ii) by hypothesis, $\overline{A}^*$ satisfies (a)(ii) and $\overline{A}$ is closed, hence it is selfadjoint because (a)(ii) implies (a)(i).

□

When $A \subset A^*$ one has

$$D(A^*) = D(\overline{A}) \oplus_{A^*} \mathsf{H}_- \oplus_{A^*} \mathsf{H}_+ \,,$$

where the orthogonal sum is taken with respect to the inner product $\langle \psi|\phi\rangle_{A^*} := \langle \psi|\phi\rangle + \langle A^*\psi|A^*\phi\rangle$ and the three subspaces are closed in the induced norm topology. (This formula is proved in [ReSi75, p. 138], where A is also assumed closed. Here we exploit the fact that $\overline{A}^* = A^*$.) We are in a position to quote a celebrated theorem of von Neumann that relies on the above decomposition [ReSi75, Tes14, Mor18].

Theorem 2.48 *A symmetric operator $A : D(A) \to \mathsf{H}$ on a Hilbert space H admits selfadjoint extensions if and only if $n_+ = n_-$. These extensions A_U are restrictions of A^* and correspond one-to-one to surjective isometries $U : Ker(A^* - iI) \to Ker(A^* + iI)$. In fact,*

$$A_U(x + y + Uy) := \overline{A}x + A^*(y + Uy) = \overline{A}x + iy - iUy \,,$$

with $D(A_U) := \{x + y + Uy \mid x \in D(\overline{A}) \,,\, y \in \mathsf{H}_-\}$.

Remark 2.49

(a) It is easy to prove from the theorem that $A'_U : x + y + Uy \mapsto Ax + iy - iUy$, $x \in D(A)$, $y \in \mathsf{H}_-$, is symmetric, essentially selfadjoint and that A_U is its unique selfadjoint extension.

(b) The original version of Theorem 2.48 also assumed A closed. However, since: $\overline{A}$ is symmetric if A is symmetric; the deficiency indices of A and $\overline{A}$ are identical, as the reader easily proves; finally, A and $\overline{A}$ share the same selfadjoint extensions, then closedness can be dropped from the hypotheses [Mor18]. ■

In view of Theorem 2.48, there is a nice condition for symmetric operators to admit selfadjoint extensions due to von Neumann. Recall that by a **conjugation** we mean an isometric, surjective *anti-linear* map C with $CC = I$.

Proposition 2.50 *If $A : D(A) \to \mathsf{H}$ is a symmetric operator on a Hilbert space H and there is a conjugation $C : \mathsf{H} \to \mathsf{H}$ such that $CA \subset AC$, then A admits selfadjoint extensions.*

Proof Using the definition of A^* and $D(A^*)$ and observing that (from the polarization formula (2.1)) $\langle Cy|Cx\rangle = \overline{\langle y|x\rangle}$, the condition $AC \supset CA$ implies the condition $CA^* \subset A^*C$. Therefore, remembering $CC = I$, we have that $A^*x = \pm ix$ if and only if $A^*Cx = C(\pm ix) = \mp iCx$. Since C preserves orthogonality and norms, it transforms a Hilbert basis of H_+ into a Hilbert basis of H_- and vice versa. We conclude that $n_+ = n_-$. The claim then follows from Theorem 2.48. □

If we take C to be the standard conjugation of functions in $L^2(\mathbb{R}^n, d^n x)$, this result proves in particular that all operators in QM in *Schrödinger* form, such as (1.25), admit selfadjoint extensions when defined on dense domains.

Exercise 2.51 Relying on Proposition 2.47 and Theorem 2.48, prove that a symmetric operator that admits a unique selfadjoint extension is necessarily essentially selfadjoint.

Solution By Theorem 2.48, $n_+ = n_-$ if the operator admits selfadjoint extensions. Furthermore, if $n_\pm \neq 0$ there are many selfadjoint extension, again by Theorem 2.48. The only possibility to have uniqueness is $n_\pm = 0$. Proposition 2.47 implies A is essentially selfadjoint. □

Useful criteria to establish the essential selfadjointness of a symmetric operator are due to Nelson and Nussbaum. Both rely upon an important definition.

Definition 2.52 Let A be an operator on a Hilbert space H. A vector $\psi \in \cap_{n\in\mathbb{N}} D(A^n)$ such that

$$\sum_{n=0}^{+\infty} \frac{t^n}{n!}||A^n\psi|| < +\infty \quad \text{for some } t > 0, \quad \text{or} \quad \sum_{n=0}^{+\infty} \frac{t^n}{(2n)!}||A^n\psi|| < +\infty \quad \text{for some } t > 0,$$

is respectively called **analytic**, or **semi-analytic**, for A. ■

Let us then state the criteria of Nelson and Nussbaum [ReSi80, Mor18, Schm12].

Theorem 2.53 (Nelson's Criterion) *A symmetric operator A on a Hilbert space H is essentially selfadjoint if $D(A)$ contains a dense set of analytic vectors or, equivalently, a set of analytic vectors whose finite span is dense in H.*

The equivalence is due to the simple fact that a linear combination of analytic vectors is analytic. Recall that the (finite) span of a Hilbert basis is dense, and if $A\psi = a\psi$ then

$$\sum_{n=0}^{+\infty} \frac{t^n}{n!}||A^n\psi|| = \sum_{n=0}^{+\infty} \frac{a^n t^n}{n!}||\psi|| = e^{at}||\psi|| < +\infty \quad \text{for some } t \in \mathbb{R}.$$

Then

Corollary 2.54 *If A is a symmetric operator admitting a Hilbert basis of eigenvectors in $D(A)$, then A is essentially selfadjoint.*

Theorem 2.55 (Nussbaum's Criterion) *Let A be a symmetric operator on a Hilbert space H such that $\langle\psi|A\psi\rangle \geq c||\psi||^2$ for some constant $c \in \mathbb{R}$ and every $\psi \in D(A)$. Then A is essentially selfadjoint if $D(A)$ contains a dense set of semi-analytic vectors.*

Another useful criterion to establish the essential selfadjointness of a symmetric operator is due to Nussbaum and (independently) Masson and McClary. It relies upon an important definition.

Definition 2.56 Let A be an operator on a Hilbert space H. A vector $\psi \in \cap_{n\in\mathbb{N}} D(A^n)$ such that

$$\sum_{n=0}^{+\infty} ||A^n\psi||^{-\frac{1}{n}} = +\infty \quad \text{or} \quad \sum_{n=0}^{+\infty} ||A^n\psi||^{-\frac{1}{2n}} = +\infty$$

are respectively called **quasi-analytic**, or **Stieltjes**, for A. ■

Let us then state the criteria of Nussbaum and Masson-McClary [Sim71, ReSi80, Schm12].

Theorem 2.57 (Nussbaum-Masson-McClary Criterion) *Let A be a symmetric operator on a Hilbert space H such that $\langle\psi|A\psi\rangle \geq c||\psi||^2$ for some constant $c \in \mathbb{R}$ and every $\psi \in D(A)$. Then A is essentially selfadjoint if $D(A)$ contains a dense set of Stieltjes vectors.*

Remark 2.58 The following implications hold

- *analytic ⇒ quasi-analytic ⇒ Stieltjes*;
- *analytic ⇒ semi-analytic ⇒ Stieltjes.*

2.2.7 Position and Momentum Operators and Other Physical Examples

In this section we shall exhibit selfadjoint operators of great relevance in quantum physics.

Example 2.59

(1) Take $m \in \{1, 2, \ldots, n\}$ and define operators X'_m and X''_m in $L^2(\mathbb{R}^n, d^n x)$ with dense domains $D(X'_m) = C_c^\infty(\mathbb{R}^n)$, $D(X''_m) = \mathscr{S}(\mathbb{R}^n)$ by

$$(X'_m\psi)(x) := x_m\psi(x) \ , \quad (X''_m\phi)(x) := x_m\phi(x) \ ,$$

where x_m is the m-th component of $x \in \mathbb{R}^n$. Both are symmetric but not selfadjoint. They admit selfadjoint extensions because they commute with the standard complex conjugation of maps (see Proposition 2.50). It is possible to show that both are essentially selfadjoint, as we set out to do. First define the **k-axis position operator** X_m on $L^2(\mathbb{R}^n, d^n x)$ with domain

$$D(X_m) := \left\{ \psi \in L^2(\mathbb{R}^n, d^n x) \;\middle|\; \int_{\mathbb{R}^n} |x_m \psi(x)|^2 d^n x \right\}$$

and

$$(X_m \psi)(x) := x_m \psi(x) \,, \quad x \in \mathbb{R}^n \,. \tag{2.22}$$

Just by definition of adjoint $X_m^* = X_m$, so that X_m is selfadjoint [Mor18]. Similarly (see below) $X_m'^{\,*} = X_m''^{\,*} = X_m$, where we know the last is selfadjoint. Hence X_m' and X_m'' are essentially selfadjoint. By Proposition 2.39 (b), X_m' and X_m'' admit a unique selfadjoint extension which must coincide with X_m itself. We conclude that $C_c^\infty(\mathbb{R}^n)$ and $\mathscr{S}(\mathbb{R}^n)$ are *cores* (see Definition 2.30) for the m-axis position operator.

Let us prove that $X_m'^{\,*} = X_m$ (the proof for $X_m''^{\,*}$ is identical). By direct inspection one easily sees that $X_m'^{\,*} \subset X_m$. Let us prove the converse inclusion. As $\phi \in D(X_m'^{\,*})$ if and only if there exists $\eta_\phi \in L^2(\mathbb{R}^n, d^n x)$ such that $\int \overline{\phi(x)} x_m \psi(x) dx = \int \overline{\eta_\phi(x)} \psi(x) dx$, that is $\int \overline{(\phi(x) x_m - \eta_\phi(x))} \psi(x) dx = 0$, for every $\psi \in C_c^\infty(\mathbb{R}^n)$. Fix a compact set $K \subset \mathbb{R}^n$ of the form $[a, b]^n$. The function $K \ni x \mapsto \phi(x) x_m - \eta_\phi(x)$ clearly belongs in $L^2(K, dx)$ (the same would not hold if K were $\mathbb{R}^n$). Since we can $L^2(K)$-approximate that function with a sequence $\psi_n \in C_c^\infty(\mathbb{R}^n; \mathbb{C})$ such that $\mathrm{supp}(\psi_n) \subset K$, we conclude that $\int_K |\phi(x) x_m - \eta_\phi(x)|^2 dx = 0$, so that $K \ni x \mapsto \phi(x) x_m - \eta_\phi(x)$ is zero a.e. Since $K = [a, b]^n$ was arbitrary, we infer that $\mathbb{R}^n \ni x \mapsto \phi(x) x_m = \eta_\phi(x)$ a.e. In particular, both ϕ and $\mathbb{R}^n \ni x \mapsto x_m \phi(x)$ are in $L^2(\mathbb{R}^n, dx)$ (the latter because it coincides a.e. with $\eta_\phi \in L^2(\mathbb{R}^n, dx)$). Therefore $D(X_m'^{\,*}) \ni \phi$ implies $\phi \in D(X_m)$, and consequently $X_m'^{\,*} \subset X_m$ as required.

(2) For $m \in \{1, 2, \dots, n\}$, the **k-axis momentum operator** P_m is obtained from the position operator using the unitary Fourier-Plancherel operator $\hat{\mathscr{F}}$ introduced in Example 2.44. On

$$D(P_m) := \left\{ \psi \in L^2(\mathbb{R}^n, d^n x) \;\middle|\; \int_{\mathbb{R}^n} |k_m (\hat{\mathscr{F}} \psi)(k)|^2 d^n k \right\}$$

it is defined by

$$(P_m \psi)(x) := (\hat{\mathscr{F}}^{-1} K_m \hat{\mathscr{F}} \psi)(x) \,, \quad x \in \mathbb{R}^n \,. \tag{2.23}$$

Above, K_m is the m-axis *position operator* written for functions (in $L^2(\mathbb{R}^n, d^n k)$) whose variable, for pure convenience, is called k instead of

x. Indicating by $\widehat{\psi}$ these functions (as is customary in quantum physics' textbooks) we have

$$\left(K_m\widehat{\psi}\right)(k) := k_m\widehat{\psi}(k) \quad k \in \mathbb{R}^n . \tag{2.24}$$

Proposition 2.41, as a consequence of the fact that $\hat{\mathscr{F}}$ is unitary, guarantees that P_m is selfadjoint since K_m is. It is possible to describe P_m more explicitly if we restrict the domain. Taking $\psi \in C_c^\infty(\mathbb{R}^n) \subset \mathscr{S}(\mathbb{R}^n)$ or directly $\psi \in \mathscr{S}(\mathbb{R}^n)$, $\hat{\mathscr{F}}$ reduces to the standard integral Fourier transform (2.13) with inverse (2.14). Using these,

$$(P_m\psi)(x) = (\hat{\mathscr{F}}^{-1}K_m\hat{\mathscr{F}}\psi)(x) = -i\frac{\partial}{\partial x_m}\psi(x) \tag{2.25}$$

because in $\mathscr{S}(\mathbb{R}^n)$, which is invariant under the Fourier (and inverse Fourier) transformation,

$$\int_{\mathbb{R}^n} e^{ik\cdot x}k_m(\mathscr{F}\psi)(k)d^nk = -i\frac{\partial}{\partial x_m}\int_{\mathbb{R}^n} e^{ik\cdot x}(\mathscr{F}\psi)(k)d^nk .$$

Hence we are led to consider the operators P'_m and P''_m on $L^2(\mathbb{R}^n, d^nx)$ with

$$D(P'_m) = C_c^\infty(\mathbb{R}^n) , \quad D(P''_m) = \mathscr{S}(\mathbb{R}^n)$$

$$(P'_m\psi)(x) := -i\frac{\partial}{\partial x_m}\psi(x) , \quad (P''_m\phi)(x) := -i\frac{\partial}{\partial x_m}\phi(x)$$

for $x \in \mathbb{R}^n$ and ψ, ϕ in the respective domains. These two operators are symmetric as one can easily prove by integrating by parts, but not selfadjoint. They admit selfadjoint extensions because they commute with the conjugation $(C\psi)(x) = \overline{\psi(-x)}$ (see Proposition 2.50). It is further possible to prove that they are essentially selfadjoint using Proposition 2.47 [Mor18]. However we already know that P''_m is essentially selfadjoint for it coincides with the essentially selfadjoint operator $\hat{\mathscr{F}}^{-1}K''_m\hat{\mathscr{F}}$, because $\mathscr{S}(\mathbb{R}^n)$ is invariant under $\hat{\mathscr{F}}$. The unique selfadjoint extension of both operators turns out to be P_m. We conclude that $C_c^\infty(\mathbb{R}^n)$ and $\mathscr{S}(\mathbb{R}^n)$ are *cores* for the m-axis momentum operator.

$\mathscr{S}(\mathbb{R}^n)$ is an invariant domain for the selfadjoint operators X_k and P_k, on which the CCRs (1.22) hold.

As a final observation note that for $n = 1$ the domain $D(P)$ coincides with (1.18). On that domain P is $(-i)$ times the weak derivative.

(3) The simplest manifestation of Nelson's criterion occurs in $L^2([0, 1], dx)$. Consider $A = -\frac{d^2}{dx^2}$ with domain $D(A)$ given by the maps in $C^2([0, 1])$ such that $\psi(0) = \psi(1)$ and $\frac{d\psi}{dx}(0) = \frac{d\psi}{dx}(1)$. The operator A is symmetric (just

integrate by parts), in particular its domain is dense since it contains the Hilbert basis of exponential maps $e^{i2\pi nx}$, $n \in \mathbb{Z}$, which are eigenvectors of A. Therefore A is also essentially selfadjoint on $D(A)$.

(4) A more interesting case is the **Hamiltonian operator of the harmonic oscillator** H [SaTu94]. The classical Hamiltonian of a *one-dimensional harmonic oscillator* of mass $m > 0$ and angular frequency $\omega > 0$ is

$$h = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} \quad \text{where } (x, p) \in \mathbb{R}^2 .$$

In terms of the momentum and position operators defined on the common invariant domain $\mathscr{S}(\mathbb{R})$, one obtains the symmetric—but not selfadjoint—operator

$$H_0 = \frac{1}{2m} P^2\restriction_{\mathscr{S}(\mathbb{R})} + \frac{m\omega^2}{2} X^2\restriction_{\mathscr{S}(\mathbb{R})} = -\frac{1}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2}{2} x^2$$

where $P := P_1$ in the notation of Example (2), $D(H_0) := \mathscr{S}(\mathbb{R})$ (evidently), and both $\frac{d}{dx}$ and the multiplication by x^2 act on $\mathscr{S}(\mathbb{R})$.

We claim H_0 is essentially selfadjoint. It is convenient to define operators $A, A^\dagger, \mathcal{N} : \mathscr{S}(\mathbb{R}) \to L^2(\mathbb{R}, dx)$ by

$$A^\dagger := \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{\hbar}{m\omega}\frac{d}{dx}\right) , \quad A := \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{\hbar}{m\omega}\frac{d}{dx}\right) , \quad \mathcal{N} := A^\dagger A . \tag{2.26}$$

These operators have common domain $\mathscr{S}(\mathbb{R})$ which is also invariant:

$$A(\mathscr{S}(\mathbb{R})) \subset \mathscr{S}(\mathbb{R}) , \;\; A^\dagger(\mathscr{S}(\mathbb{R})) \subset \mathscr{S}(\mathbb{R}) , \;\; \mathcal{N}(\mathscr{S}(\mathbb{R})) \subset \mathscr{S}(\mathbb{R}) .$$

Applying Definition 2.23 to the first two objects in (2.26) and integrating by parts gives $A^\dagger \subsetneq A^*$ and $A \subsetneq (A^\dagger)^*$. The inclusion is strict because $D(A^*)$ and $D((A^\dagger)^*)$ also contain, for instance, C^1 maps with compact support which do not belong to $\mathscr{S}(\mathbb{R})$. The operator $\mathcal{N}$ is Hermitian and symmetric because $\mathscr{S}(\mathbb{R})$ is dense in $L^2(\mathbb{R}, dx)$. By direct computation

$$H_0 = \hbar\left(A^\dagger A + \frac{1}{2} I\right) = \hbar\left(\mathcal{N} + \frac{1}{2} I\right) .$$

We have the commutation relation

$$[A, A^\dagger] = I_{\mathscr{S}(\mathbb{R})} \tag{2.27}$$

(both sides are viewed as operators $\mathscr{S}(\mathbb{R}) \to \mathscr{S}(\mathbb{R})$). Let us suppose that there exists $\psi_0 \in \mathscr{S}(\mathbb{R})$ such that

$$||\psi_0|| = 1\,, \quad A\psi_0 = 0\,. \tag{2.28}$$

Starting from (2.27) and using an inductive procedure on the vectors

$$\psi_n := \frac{1}{\sqrt{n!}}(A^\dagger)^n \psi_0 \in \mathscr{S}(\mathbb{R})\,, \tag{2.29}$$

it is easy to prove that (e.g., see [SaTu94, Mor18] for elementary details)

$$A\psi_n = \sqrt{n}\psi_{n-1}\,, \quad A^\dagger\psi_n = \sqrt{n+1}\psi_{n+1}\,, \quad \langle\psi_n|\psi_m\rangle = \delta_{nm} \tag{2.30}$$

for $n, m = 0, 1, 2, \ldots$. Finally, the ψ_n are eigenvectors of H_0 (and $\mathcal{N}$) since

$$H_0\psi_n = \hbar\omega\left(A^\dagger A\psi_n + \frac{1}{2}\psi_n\right) = \hbar\omega\left(A^\dagger\sqrt{n}\psi_{n-1} + \frac{1}{2}\psi_n\right) = \hbar\omega\left(n + \frac{1}{2}\right)\psi_n\,. \tag{2.31}$$

As a consequence, if we can find ψ_0, $\{\psi_n\}_{n\in\mathbb{N}}$ is an orthonormal set. It actually is a *Hilbert basis* called the Hilbert basis of **Hermite functions**. To prove it, by Definition 2.10 it suffices to demonstrate that the span of the ψ_n has trivial orthogonal complement:

$$\text{if } f \in L^2(\mathbb{R}, dx), \quad \int_{\mathbb{R}} f(x)\psi_n(x)dx = 0 \quad \text{for every } n \in \mathbb{N} \text{ implies } f = 0.$$

To this end, observe that (2.28) admits a unique solution in $\mathscr{S}(\mathbb{R})$ up to constant unit factors, namely

$$\psi_0(x) = \frac{1}{\pi^{1/4}\sqrt{s}}e^{-\frac{x^2}{2s^2}}\,, \quad s := \sqrt{\frac{\hbar}{m\omega}}\,.$$

From (2.29), by rescaling the argument of ψ_n,

$$\psi_n(x) = \sqrt{s}H_n(x/s)\,, \quad H_n(x) := \frac{1}{\sqrt{2^n\pi^{1/2}n!}}\left(x - \frac{d}{dx}\right)^n e^{-x^2/2}\,, \quad n = 0, 1, \ldots\,.$$

In particular $\psi_n \in \mathscr{S}(\mathbb{R})$. Furthermore, since $H_n(x)e^{+\frac{x^2}{2}}$ is a polynomial of degree n, the condition $\int_{\mathbb{R}} f\psi_n dx = 0$ for every $n \in \mathbb{N}$ implies by induction

$$\int_{\mathbb{R}} f(x)x^n e^{-x^2/2}dx = 0 \quad \text{for every } n \in \mathbb{N}.$$

(Notice that the integrand is a product of L^2 functions, and hence is L^1). Hence, $\forall k \in \mathbb{R}$,

$$\int_{\mathbb{R}} e^{-ikx} f(x) e^{-\frac{x^2}{2}} dx = \int_{\mathbb{R}} \lim_{N\to+\infty} \sum_{n=0}^{N} \frac{(-ik)^n}{n!} x^n f(x) e^{-\frac{x^2}{2}} dx$$
$$= \lim_{N\to+\infty} \sum_{n=0}^{N} \frac{(-ik)^n}{n!} \int_{\mathbb{R}} f(x) x^n e^{-\frac{x^2}{2}} dx = 0 .$$

Integral and sum can be exchanged by dominated convergence, since

$$\left| \sum_{n=0}^{N} \frac{(-ik)^n}{n!} x^n f(x) e^{-\frac{x^2}{2}} \right| \le \sum_{n=0}^{N} \frac{|k|^n}{n!} |x|^n |f(x)| e^{-\frac{x^2}{2}}$$
$$= \sum_{n=0}^{+\infty} \frac{|k|^n}{n!} |x|^n |f(x)| e^{-\frac{x^2}{2}} = e^{|kx| - \frac{x^2}{2}} |f(x)|$$

and the function $\mathbb{R} \ni x \mapsto e^{|kx|-\frac{x^2}{2}} |f(x)|$ is L^1.

We have shown that the L^1-Fourier transform of $\mathbb{R} \ni x \mapsto f(x)e^{-x^2/2}$ vanishes everywhere. Since the L^1-Fourier transform is linear and injective (see Remark 2.45), $f(x)e^{-x^2/2} = 0$ a.e., and hence $f = 0$ in L^2 as we wanted. We have established that the set of eigenvectors $\{\psi_n\}_{n\in\mathbb{N}} \subset \mathscr{S}(\mathbb{R})$ of H_0 is a Hilbert basis of $L^2(\mathbb{R}, dx)$, as promised.

Using Nelson's criterion the symmetric operator H_0 is essentially selfadjoint in $D(H_0) = \mathscr{S}(\mathbb{R})$, because H_0 admits a Hilbert basis of eigenvectors with corresponding eigenvalues $\hbar\omega(n + \frac{1}{2})$. It is worth stressing that, physically speaking, the *Hamiltonian operator of the harmonic oscillator* is the selfadjoint operator $H := \overline{H_0} = H_0^*$. This is however completely determined by the non-selfadjoint operator H_0.

(5) Assume as usual $\hbar = 1$. The operator

$$P' := -i\frac{d}{dx} \quad \text{acting on} \quad f \in D(P') := \{f \in C^2([0,1]) \mid \text{supp}(f) \subset (0,1)\}$$

is sometimes called, improperly, *momentum operator in a box*. (Evidently at 0 and 1 only the right and the left derivatives are considered, and with little effort one may define it on $[a, b]$ instead of $[0, 1]$). $D(P')$ is dense in $L^2([0, 1], dx)$ and it is easy to prove that P' is symmetric using integration by parts. Moreover P' commutes with the conjugation $(C\psi)(x) := \overline{\psi\left(\frac{1}{2} - x\right)}$, so it admits selfadjoint extensions ($n_+ = n_-$) by Proposition 2.50. It is easy to see that $n_\pm \ge 1$ because $\chi_\pm(x) := e^{\pm x}$ satisfies $\langle \chi_\pm | P' f \rangle = \pm i \langle \chi_\pm | f \rangle$ for every $f \in D(P')$, which means $P'^* \chi_\pm = \pm i \chi_\pm$. Actually a closer scrutiny (exercise!) shows that $n_\pm = 1$. In any case, Proposition 2.47 tells P' is *not* essentially selfadjoint because $n_\pm > 0$. It is possible to find various selfadjoint extensions of P' (the only ones admitted, by Theorem 2.48) as we proceed to illustrate. For $\alpha \in \mathbb{R}$, extend P' to

$$P'_\alpha f := -i\frac{df}{dx} \quad \text{for} \quad f \in D(P'_\alpha) := \{f \in C^2([0,1]) \mid f(1) = e^{i\alpha} f(0)\} \tag{2.32}$$

and observe that $D(P'_\alpha) = D(P'_{\alpha'})$ if $\alpha' = \alpha + 2k\pi$, $k \in \mathbb{Z}$, so that we can restrict α to $[0, 2\pi)$. By direct inspection, it is also evident that $P'_\alpha \subset P'^*_\alpha$, i.e., P'_α is symmetric: boundary terms cancel out in the inner product and $\langle f|P'_\alpha g\rangle = \langle P'_\alpha f|g\rangle$ if $f, g \in D(P'_\alpha)$. Actually P'_α is essentially selfadjoint because it admits the Hilbert basis of eigenvectors

$$u_{\alpha,n}(x) := e^{i2\pi(\alpha+n)x}\,, \quad n \in \mathbb{Z}\,.$$

That is indeed a Hilbert basis because $u_{\alpha,n} = U_\alpha u_{0,n}$ where $(U_\alpha\psi)(x) := e^{i\alpha x}\psi(x)$, $\psi \in L^2([0,1], dx)$, defines a unitary operator, and $u_{0,n}(x) = e^{i2\pi nx}$, $n \in \mathbb{Z}$, is a well-known Hilbert basis of $L^2([0,1], dx)$. Thus we have found a family of selfadjoint extensions of P' labelled by $\alpha \in [0, 2\pi)$: $P_\alpha := \overline{P'_\alpha} = P'^*_\alpha$. If $\alpha, \alpha' \in [0, 2\pi)$ and $\alpha \neq \alpha'$, then $P_\alpha \neq P_{\alpha'}$ since the eigenvalues are different: $\alpha + 2n\pi$ and and $\alpha' + 2n\pi$ $(n \in \mathbb{Z})$ respectively. These selfadjoint extensions were constructed just by specializing the boundary conditions defining the domain of the original symmetric operator P' according to (2.32). Using Theorem 2.48 and Remark 2.49 (a) it is easy to prove that (exercise!) P' has no further selfadjoint extensions (i.e., other than the P_α, $\alpha \in [0, \pi)$) [ReSi80, Tes14, Mor18]. In contrast to what happens for the momentum operator defined on the entire $L^2(\mathbb{R}, dx)$, P_α does not leave invariant its core $D(P'_\alpha)$ (think of the core $\mathscr{S}(\mathbb{R})$, which is invariant under the action of the momentum operator on $L^2(\mathbb{R}, dx)$). Given these domain issues, P_α fails in particular the Heisenberg commutation relations relatively to the natural definition of the selfadjoint *position operator* X,

$$(Xf)(x) = xf(x) \quad \text{for} \quad f \in D(X) := \left\{ f \in L^2([0,1], dx) \;\middle|\; \int_0^1 |xf(x)|^2 dx < +\infty \right\},$$

restricted to the common core $D(P'_\alpha)$. In fact, this space is a core for X as well but, again, it is not invariant under it: in general $P_\alpha X f$ will not make sense if $f \in D(P'_\alpha)$, so $[X, P_\alpha]$ cannot be computed on $D(P_\alpha)$, in contrast to the position and momentum operators on $\mathbb{R}$ and referring to the common core $\mathscr{S}(\mathbb{R})$. ■

Chapter 3
Observables and States in General Hilbert Spaces: Spectral Theory

The overall goal of this chapter is to extend the elementary decomposition of a Hermitian operator (1.4) on a finite-dimensional Hilbert space seen in Chap. 1 to a formula valid in the infinite-dimensional case. We do this to make rigorous sense of the spectral decompositions of (generally unbounded) selfadjoint operators representing observables, such as *momentum* and *position*. What we need is called *Spectral Theory* on Hilbert spaces, which will be the subject of this chapter. After stating and proving the theory's major theorems, we shall apply them to the elementary presentation of quantum theory introduced in the first chapter to produce a mathematically sound formulation. The proofs to certain technical results are relegated to the last section. Reference books are [Ped89, Rud91, Schm12, Tes14, Mor18].

3.1 Basics on Spectral Theory

As we shall see in a short while, when we pass to infinite dimensions sums are replaced by integrals and $\sigma(A)$ must be enlarged to encompass more than just the eigenvalues of A. This is because, as already noticed in the first chapter, there exist operators playing crucial roles in QM that should be decomposed as prescribed by (1.4) yet do not have eigenvalues.

Notation 3.1 If $A : D(A) \to \mathsf{H}$ is injective, A^{-1} indicates its *inverse* when the codomain of A is restricted to $Ran(A)$. In other words, $A^{-1} : Ran(A) \to D(A)$. ■

3.1.1 Resolvent and Spectrum

The definition of *spectrum* of the operator $A : D(A) \to \mathsf{H}$ extends the notion eigenvalue. The eigenvalues of A are numbers $\lambda \in \mathbb{C}$ such that $(A - \lambda I)^{-1}$ is not

V. Moretti, *Fundamental Mathematical Structures of Quantum Theory*,
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defined. A naive generalization to infinite dimensions is not viable due to a number of topological issues. As a matter of fact, even if $(A - \lambda I)^{-1}$ does exist it may be bounded or unbounded, and its domain $Ran(A - \lambda I)$ may or not be dense. These features permit us to define a suitable extension of the notion of eigenvalue.

Definition 3.2 Let A be an operator on the Hilbert space H. The **resolvent set** of A is the subset of $\mathbb{C}$

$$\rho(A) := \{\lambda \in \mathbb{C} \,|\, (A-\lambda I) \text{ is injective, } \overline{Ran(A - \lambda I)} = \mathsf{H}, (A-\lambda I)^{-1} \text{is bounded}\}.$$

The **spectrum** of A is the complement $\sigma(A) := \mathbb{C} \setminus \rho(A)$ and consists of the union of the following pairwise-disjoint three parts:

(i) the **point spectrum**, $\sigma_p(A)$, for which $A - \lambda I$ is not injective (its elements are the **eigenvalues** of A),
(ii) the **continuous spectrum**, $\sigma_c(A)$, for which $A - \lambda I$ is injective, $\overline{Ran(A - \lambda I)} = \mathsf{H}$ and $(A - \lambda I)^{-1}$ is not bounded,
(iii) the **residual spectrum**, $\sigma_r(A)$, where $A - \lambda I$ is injective and $\overline{Ran(A - \lambda I)} \neq \mathsf{H}$.

If $\lambda \in \rho(A)$, the operator

$$R_\lambda(A) := (A - \lambda I)^{-1} : Ran(A - \lambda I) \to D(A)$$

is called the **resolvent operator** of A. ■

The following technically elementary fact defines *approximate eigenvector* an element of the *continuous spectrum*. Even if proper eigenvectors do not exist, they can be approximated arbitrarily well.

Proposition 3.3 *Let* $A : D(A) \to \mathsf{H}$ *be an operator on the Hilbert space* H *and take* $\lambda \in \sigma_c(A)$. *For every* $\epsilon > 0$ *there exists* $x_\epsilon \in D(A)$ *with* $||x_\epsilon|| = 1$ *such that* $||Ax_\epsilon - \lambda x_\epsilon|| < \epsilon$.

Proof Since $\lambda \in \sigma_c(A)$, we have that $(A - \lambda I)^{-1} : Ran(A - \lambda I) \to D(A)$ is not bounded. Therefore, for every $\epsilon > 0$ there is $y_\epsilon \in Ran(A - \lambda I)$ with $y_\epsilon \neq 0$ such that

$$||(A - \lambda I)^{-1} y_\epsilon|| > \epsilon^{-1} ||y_\epsilon|| \,.$$

By construction, we may write $y_\epsilon = (A - \lambda I)z_\epsilon$ for some $z_\epsilon \in D(A) \setminus \{0\}$, so that

$$||(A - \lambda I)^{-1}(A - \lambda I)z_\epsilon|| > \epsilon^{-1}||(A - \lambda I)z_\epsilon|| \,.$$

In other words, $\epsilon||z_\epsilon|| > ||Az_\epsilon - \lambda z_\epsilon||$. It is now evident that $x_\epsilon := ||z_\epsilon||^{-1} z_\epsilon$ fulfils the claim. □

The property is also valid (a) if $\lambda \in \sigma_p(A)$, simply by choosing x_ϵ as a λ-eigenvector irrespective of ϵ, and also (b) if $\lambda \in \sigma_r(A)$ in case $(A - \lambda I)^{-1}$ is not bounded. For this reason, it is sometimes convenient to decompose $\sigma(A)$ in a different way when we deal with operators *admitting residual spectrum* (this is not the case for normal operators, as we shall see shortly). The **approximate point spectrum** $\sigma_{ap}(A)$ consists of $\lambda \in \sigma(A)$ such that, for every $\epsilon > 0$, there exists $x_\epsilon \in D(A)$ with $||Ax_\epsilon - \lambda x_\epsilon|| < \epsilon$ and $||x_\epsilon|| = 1$ (including the case $Ker(A - \lambda I) = \{0\}$). The **residual pure spectrum** $\sigma_{rp}(A)$ is just $\sigma(A) \setminus \sigma_{ap}(A)$.

In Hilbert spaces the spectrum and the resolvent are invariant under unitary operators and, more generally, under isomorphisms or anti-isomorphisms. The following elementary result, proven by using basic properties of surjective linear isometries, confirms this.

Proposition 3.4 *If $U : \mathsf{H} \to \mathsf{H}'$ is an isometric surjective linear (or anti-linear) map between Hilbert spaces and A is any operator on H, then $\sigma(UAU^{-1}) = \sigma(A)$. In particular,*

$$\sigma_p(UAU^*) = \sigma_p(A) , \quad \sigma_c(UAU^{-1}) = \sigma_c(A) , \quad \sigma_r(UAU^{-1}) = \sigma_r(A) . \tag{3.1}$$

The next technically important proposition is concerned with resolvents and spectra of closed operators, where things simplify quite a lot.

Proposition 3.5 *Let $A : D(A) \to \mathsf{H}$ be a closed operator on the Hilbert space H (for instance $A \in \mathfrak{B}(\mathsf{H})$). Then $\lambda \in \rho(A)$ if and only if the inverse to $A - \lambda I$ exists and belongs in $\mathfrak{B}(\mathsf{H})$. In particular $Ran(A - \lambda I) = \mathsf{H}$.*

Proof If $(A - \lambda I)^{-1} \in \mathfrak{B}(\mathsf{H})$, then $\overline{Ran(A - \lambda I)} = Ran(A - \lambda I) = \mathsf{H}$ and $(A - \lambda I)^{-1}$ is bounded, so that $\lambda \in \rho(A)$ by definition. Let us prove the converse, and suppose that $\lambda \in \rho(A)$. We know that $(A - \lambda I)^{-1}$ is defined on the dense domain $Ran(A - \lambda I)$ and is bounded. To conclude, it is therefore enough to prove that $y \in \mathsf{H}$ implies $y \in Ran(A - \lambda I)$. To this end, notice that if $y \in \mathsf{H} = \overline{Ran(A - \lambda I)}$, then $y = \lim_{n\to+\infty}(A - \lambda I)x_n$ for some $x_n \in D(A - \lambda I)$. The sequence of elements x_n converges. Indeed, H is complete and $\{x_n\}_{n\in\mathbb{N}}$ is Cauchy because (1) $x_n = (A - \lambda I)^{-1}y_n$, (2) $||x_n - x_m|| \leq ||(A - \lambda I)^{-1}|| \, ||y_n - y_m||$, and (3) $y_n \to y$. To finish the proof, we observe that $A - \lambda I$ is closed since A is closed (Remark 2.31 (b)). Consequently (Remark 2.31 (c)) $x = \lim_{n\to+\infty} x_n \in D(A - \lambda I)$ and $y = (A - \lambda I)x \in Ran(A - \lambda I)$. □

Remark 3.6

(a) As a consequence of this result, if $A : D(A) \to \mathsf{H}$ is closed or $A \in \mathfrak{B}(\mathsf{H})$ the definition of resolvent simplifies:

$$\rho(A) := \{\lambda \in \mathbb{C} \mid \exists (A - \lambda I)^{-1} \in \mathfrak{B}(\mathsf{H})\} .$$

Some textbooks give this definition from the very beginning. In these cases, since the operators $(A - \lambda I)^{-1}$ have the same domain H when $\lambda \in \rho(A)$, $R_\mu(A) - R_\lambda(A)$ is defined everywhere.

(b) The conclusion of Proposition 3.5 can actually be stated in an even stronger form. Since A is closed, $A - \lambda I$ and its inverse $(A - \lambda I)^{-1}$ are closed as well (they have the same graph). So if A is defined everywhere on H, it is automatically bounded by the closed graph theorem. So we have an alternative version of Proposition 3.5. ■

Proposition 3.7 *Let $A : D(A) \to \mathsf{H}$ be a closed operator on the Hilbert space H (for example, $A \in \mathfrak{B}(\mathsf{H})$). Then $\lambda \in \rho(A)$ if and only if $A - \lambda I : D(A) \to \mathsf{H}$ is a bijection.*

The definitions of resolvent and spectrum can be extended as they stand to the case where H is replaced by a complex Banach space [Rud91, Mor18]. Even more generally, they adapt to abstract unital Banach algebras if we interpret operators as elements of the algebra.

Definition 3.8 If $\mathcal{A}$ is a unital Banach algebra, the **resolvent** of an element $a \in \mathfrak{A}$ is made of all $\lambda \in \mathbb{C}$ such that $a - \lambda \mathbb{1}$ admits inverse, written $R_\lambda(a)$, in $\mathfrak{A}$. The **spectrum** of $a \in \mathfrak{A}$ is $\sigma(a) := \mathbb{C} \setminus \rho(a)$. ■

No finer spectral decompositions are made in this context.

A closed operator A satisfies the *resolvent identity*, which is evidently valid also for unital Banach algebras (replacing $R_z(A)$ by $R_z(a)$).

Proposition 3.9 *Let $A : D(A) \to \mathsf{H}$ be a closed operator (or, more strongly, $A \in \mathfrak{B}(\mathsf{H})$) on the Hilbert space H and take $\mu, \lambda \in \rho(A)$. Then*

$$R_\mu(A) - R_\lambda(A) = (\mu - \lambda) R_\mu(A) R_\lambda(A) \,, \tag{3.2}$$

called the **resolvent identity**.

Proof First of all $R_\lambda(A)(A - \lambda I) = I \restriction_{D(A)}$ and $(A - \mu I)R_\mu(A) = I$. As a consequence, $R_\lambda(A)(A-\lambda I)R_\mu(A) = R_\mu(A)$ and $R_\lambda(A)(A-\mu I)R_\mu(A) = R_\lambda(A)$. Taking the difference produces (3.2). □

We shall prove that if $A \in \mathfrak{B}(\mathsf{H})$ then $\rho(A) \neq \varnothing$. The same applies to unital Banach algebras.

Proposition 3.10 *Let H be a Hilbert space and $A \in \mathfrak{B}(\mathsf{H})$. Then $\lambda \in \rho(A)$ if $|\lambda| > ||A||$, so $\sigma(A)$ is bounded by $||A||$.*

Proof The series $S_\lambda := -\sum_{n=0}^{+\infty} \lambda^{-(n+1)} A^n$ (where $A^0 := I$) converges in the operator norm of $\mathfrak{B}(\mathsf{H})$ when $|\lambda| > ||A||$ since it is dominated by the complex series $\sum_{n=0}^{+\infty} |\lambda|^{-(n+1)} ||A||^n$ and $\mathfrak{B}(\mathsf{H})$ is a Banach space. Furthermore

$$S_\lambda(A - \lambda I) = (A - \lambda I)S_\lambda = \sum_{n=0}^{+\infty} \left(-\lambda^{-(n+1)} A^{n+1} + \lambda^{-n} A^n \right) = I \,,$$

so $S_\lambda = R_\lambda(A)$ and $\lambda \in \rho(A)$. □

A few general properties of the spectrum and the resolvent set deserve special attention because they crop up in QM. The most important are encapsulated in the following proposition.

Proposition 3.11 *Let $A : D(A) \to \mathsf{H}$ be a closed operator on the Hilbert space H. Then*

(a) $\rho(A)$ *is* open, $\sigma(A)$ *is* closed *and* $\rho(A) \ni \lambda \mapsto \langle x|R_\lambda(A)y\rangle \in \mathbb{C}$ *is holomorphic for every* $x, y \in \mathsf{H}$ *if* $\rho(A) \neq \varnothing$.

(b) *If* $A \in \mathfrak{B}(\mathsf{H})$, *then*

   (i) $\sigma(A) \neq \varnothing$,

   (ii) $\rho(A) \neq \varnothing$.

   (iii) $\sigma(A)$ *is compact.*

If $\mathfrak{A}$ *is a unital Banach algebra and* $a \in \mathfrak{A}$, *then* $\rho(a)$ *is open,* $\sigma(a)$ *is closed and part (b) holds with* a *replacing* A.

Proof Let us start from (b). Statement (ii) has already been proved in Proposition 3.10, and this proves (iii) provided (i) holds. (i) is established by studying the function $\rho(A) \ni \lambda \mapsto f_{xy}(\lambda) := \langle y|(A-\lambda I)^{-1}x\rangle \in \mathbb{C}$ for every given $x, y \in \mathsf{H}$. Using the expansion in the proof of Proposition 3.10, we have $f_{xy}(\lambda) = -\sum_{n=0}^{+\infty} \lambda^{-(n+1)}\langle y|A^n x\rangle$. The series, for $|\lambda| > |\lambda_0|$, is dominated by the numerical series $\sum_{n=0}^{+\infty} \lambda_0^{-(n+1)}||A||^n||x||||y||$, which converges as $|\lambda_0| > ||A||$. Therefore the series of f_{xy} converges absolutely and uniformly on $\{\lambda \in \mathbb{C} \,|\, |\lambda| > |\lambda_0|\}$. Exploiting the dominated convergence theorem we conclude that $f_{xy}(\lambda) \to 0$ as $|\lambda| \to +\infty$. But f_{xy} is holomorphic because it is a uniform limit of holomorphic maps (use Morera's theorem). Now, if $\rho(A) = \mathbb{C}$ Liouville's theorem would imply that f_{xy} is constant for every $y, x \in \mathsf{H}$, so $f_{xy}(\lambda) = 0$ everywhere because of the limit we computed. It would follow $(A-\lambda I)^{-1} = 0$, a contradiction. We conclude that $\rho(A) \neq \mathbb{C}$, so $\sigma(A) \neq \varnothing$.

If we look at the Banach algebra picture and take $a \in \mathfrak{A}$, the function f_{xy} has to be replaced by $F(\lambda) = f((a-\lambda\mathbb{1})^{-1})$ for every element f of the topological dual $\mathfrak{A}^*$, but the proof proceeds similarly.

(a) Assume $\lambda_0 \in \rho(A)$ and consider $\lambda \in \mathbb{C}$ with $|\lambda - \lambda_0| < ||R_{\lambda_0}(A)||^{-1}$. We therefore have

$$A - \lambda I = [(\lambda_0 - \lambda)I + (A - \lambda_0 I)] = (A - \lambda_0 I)[(\lambda - \lambda_0)R_{\lambda_0}(A) + I]$$
$$= R_{\lambda_0}(A)^{-1}[(\lambda - \lambda_0)R_{\lambda_0}(A) + I]\,,$$

so that

$$(A - \lambda I)^{-1} = [(\lambda - \lambda_0)R_{\lambda_0}(A) + I]^{-1}R_{\lambda_0}(A)$$

provided $[(\lambda - \lambda_0 I)R_{\lambda_0}(A) + I]^{-1}$ exists. With the same argument used for Proposition 3.10, when $|\lambda - \lambda_0| < ||R_{\lambda_0}(A)||^{-1}$ we have

$$[(\lambda - \lambda_0)R_{\lambda_0}(A) + I]^{-1} = \sum_{n=0}^{+\infty} (\lambda_0 - \lambda)^n R_{\lambda_0}(A)^n \,. \tag{3.3}$$

We have demonstrated that every point $\lambda_0 \in \rho(A)$ admits an open neighbourhood where $R_\lambda(A)$ exists. We can therefore say that $\rho(A) \subset \mathbb{C}$ is open and its complement $\sigma(A)$ is closed. If $\rho(A) \neq \varnothing$ the map $\rho(A) \ni \lambda \mapsto \langle x|(A - \lambda I)^{-1} y\rangle$ admits Taylor expansion around every $\lambda \in \rho(A)$, constructed trivially out of (3.3). Hence the function is holomorphic.

The same proof works for unital Banach algebras $\mathfrak{A}$, by simply replacing $\langle x|R_\lambda(A)y\rangle$ with $f(R_\lambda(a))$, where $f \in \mathfrak{A}^*$.

□

Remark 3.12

(a) If $A \in \mathfrak{B}(\mathsf{H})$ is *normal*, the **spectral radius formula** holds

$$\sup\{|\lambda| \mid \lambda \in \sigma(A)\} = ||A|| \,. \tag{3.4}$$

The **spectral radius** of A is the expression on left. We shall derive this formula for selfadjoint operators as an immediate consequence of the spectral theorem. However, Proposition 3.80 provides a general version for normal operators whose proof is *independent* of the spectral theorem. This formula holds also in abstract unital C^*-algebras: replacing A is a normal element a: $a^*a = aa^*$.

(b) Item (i) in Proposition 3.11 (b) for unital Banach algebras implies the well-known **Gelfand–Mazur** theorem, whereby *a Banach algebra whose every non-zero element is invertible is isomorphic to* $\mathbb{C}$. Indeed $a - \lambda_a \mathbb{1}$ must be non-invertible for some $\lambda_a \in \sigma(a) \subset \mathbb{C}$, and hence $a = \lambda_a \mathbb{1}$. ■

3.1.2 Spectra of Special Operator Types

We are ready to state and prove general properties of the spectra of selfadjoint and unitary operators.

Proposition 3.13 *Let $A : D(A) \to \mathsf{H}$ be a densely-defined operator on the Hilbert space H. Then*

(a) *if A is selfadjoint, then $\sigma(A) \subset \mathbb{R}$.*
(b) *If A is unitary, then $\sigma(A) \subset \mathbb{T} := \{z \in \mathbb{C} \mid |z| = 1\}$.*
(c) *If A is normal, in particular selfadjoint or unitary, the following hold (where the bar denotes complex conjugation of the single elements):*

(i) $\sigma_r(A) = \sigma_r(A^*) = \varnothing$,
(ii) $\sigma_p(A) = \overline{\sigma_p(A^*)}$; *in particular if* $x \neq 0$, $Ax = \lambda x$ *if and only if* $A^*x = \overline{\lambda}x$,
(iii) $\sigma_c(A) = \overline{\sigma_c(A^*)}$.

(d) *If A is normal (in particular selfadjoint or unitary), then eigenvectors with distinct eigenvalues are orthogonal.*

Proof

(a) Suppose $\lambda = \mu + i\nu$ with $\nu \neq 0$ and let us prove $\lambda \in \rho(A)$. If $x \in D(A)$,

$$\langle (A-\lambda I)x|(A-\lambda I)x\rangle = \langle (A-\mu I)x|(A-\mu I)x\rangle + \nu^2\langle x|x\rangle + i\nu[\langle Ax|x\rangle - \langle x|Ax\rangle]\,.$$

The last summand vanishes as A is selfadjoint. Hence $||(A-\lambda I)x|| \geq |\nu|\,||x||$. With a similar argument we obtain $||(A-\overline{\lambda}I)x|| \geq |\nu|\,||x||$. The operators $A-\lambda I$ and $A-\overline{\lambda}I$ are injective, and $||(A-\lambda I)^{-1}|| \leq |\nu|^{-1}$, where $(A-\lambda I)^{-1} : Ran(A-\lambda I) \to D(A)$. Notice that, from (2.21),

$$\overline{Ran(A-\lambda I)}^{\perp} = [Ran(A-\lambda I)]^{\perp} = Ker(A^* - \overline{\lambda}I) = Ker(A-\overline{\lambda}I) = \{0\}\,,$$

where the last equality makes use of the injectivity of $A-\overline{\lambda}I$. Summarising: $A-\lambda I$ in injective, $(A-\lambda I)^{-1}$ bounded and $\overline{Ran(A-\lambda I)}^{\perp} = \{0\}$, i.e. $Ran(A-\lambda I)$ is dense in H; therefore $\lambda \in \rho(A)$, by definition of resolvent set.

(b) Suppose that $\lambda \in \mathbb{C}$ and $|\lambda| \neq 1$, and we want to prove $\lambda \in \rho(A)$. If $x \in \mathsf{H} = D(A)$ we have

$$\langle (A-\lambda I)x|(A-\lambda I)x\rangle = \langle Ax|Ax\rangle + |\lambda|^2\langle x|x\rangle - 2Re(\overline{\lambda}\langle Ax|x\rangle)\,.$$

In other words, using $\langle Ax|Ax\rangle = \langle x|x\rangle = ||x||^2$ and $|\langle Ax|x\rangle| \leq ||x||^2||A|| = ||x||^2$,

$$||(A-\lambda I)x||^2 \geq (1+|\lambda|^2)||x||^2 - 2|\lambda|||x||^2 = (1+|\lambda|^2 - 2|\lambda|)||x||^2\,.$$

Summing up, we have proved that $||(A-\lambda I)x||^2 \geq (1-|\lambda|)^2||x||^2$.

As in (a), since $(1-|\lambda|)^2 \neq 0$, the previous inequality implies that $Ker(A-\lambda I) = \{0\}$, that $||(A-\lambda I)^{-1}|| \leq (1-|\lambda|)^{-1}$, and that $Ran(A-\lambda I)$ is dense because $\overline{Ran(A-\lambda I)}^{\perp} = Ker(A^* - \overline{\lambda}I) = \{0\}$ (A^* is unitary as A is unitary and $|\overline{\lambda}| = |\lambda| \neq 1$, so the previous argument applies).

(c) First of all observe that A normal implies $Ker(A) = Ker(A^*)$. Indeed, if $x \in Ker(A)$, then $Ax = 0$ and hence $A^*Ax = A^*0 = 0$, so by definition of normal operator $AA^*x = A^*Ax = 0$. In particular $x \in D(A^*)$ and therefore $\langle x|AA^*x\rangle = 0$. As a consequence, $||A^*x||^2 = \langle A^*x|A^*x\rangle = \langle x|AA^*x\rangle = 0$ and then $x \in Ker(A^*)$. Suppose, conversely, that $x \in Ker(A^*)$. Then $A^*x = 0$ and $AA^*x = A0 = 0$. Using normality, $A^*Ax = AA^*x = 0$. In particular, since normal operators are closed by definition, $x \in D(A) = D(\overline{A}) =$

$D((A^*)^*)$ and therefore $\langle x|A^*Ax\rangle = 0$ means $\langle (A^*)^*x|Ax\rangle = \langle Ax|Ax\rangle = 0$, which is nothing but $||Ax||^2 = 0$, i.e. $x \in Ker(A)$.

Let us prove (i) $\sigma_r(A) = \varnothing$. Suppose $\lambda \in \sigma(A)$, but $\lambda \notin \sigma_p(A)$. Then $A - \lambda I$ must be injective, that is $Ker(A - \lambda I) = \{0\}$. Since $A - \lambda I$ is normal if A is normal (in particular closed Remark 2.31 (b)), we conclude that $Ker(A^* - \overline{\lambda} I) = Ker(A - \lambda I) = \{0\}$. Therefore $[Ran(A - \lambda I)]^\perp = Ker(A^* - \overline{\lambda} I) = \{0\}$ due to (2.21), and $\overline{Ran(A - \lambda I)} = \mathsf{H}$. Consequently $\lambda \in \sigma_c(A)$ and no complex number in $\sigma(A)$ is allowed to belong in $\sigma_r(A)$. Observing that A^* is normal if A is normal, we conclude that $\sigma_r(A^*) = \varnothing$ as well. Statement (ii) $\sigma_p(A) = \overline{\sigma_p(A^*)}$ immediately descends from $Ker(A - \lambda I) = Ker(A^* - \overline{\lambda} I)$, using (2.20) and noticing that the operators are closed. Let us apply the argument used above to show that $Ker(A) = Ker(A^*)$ on $A - \lambda I$ and $A^* - \overline{\lambda} I$: then $||(A - \lambda I)x|| = 0$ if and only if $||(A^* - \overline{\lambda} I)x|| = 0$, furnishing (ii). The proof of (iii) $\sigma_c(A) = \overline{\sigma_c(A^*)}$ is more involved. Suppose $\lambda \in \sigma_c(A)$, so $Ker(A - \lambda I)$ is trivial—also $Ker(A^* - \overline{\lambda} I)$ is trivial and $(A^* - \overline{\lambda} I)^{-1}$ exists—and the inverse $(A - \lambda I)^{-1}$ is an element of $\mathfrak{B}(\mathsf{H})$ due to Proposition 3.5 since normal operators are closed by definition. From $(A - \lambda I)^{-1}(A - \lambda I) = I|_{D(A)}$, using (2.8), we have $(A^* - \overline{\lambda} I)(A - \lambda I)^{-1*} = I|^*_{D(A)} = I$. In particular $(A^* - \overline{\lambda} I)(A - \lambda I)^{-1*}|_{Ran(A^* - \overline{\lambda} I)} = I|_{Ran(A^* - \overline{\lambda} I)}$. Since we know that $(A^* - \overline{\lambda} I)$ is a bijection from $D(A^*)$ to $Ran(A^* - \overline{\lambda} I)$, we conclude

$$(A - \lambda I)^{-1*}|_{Ran(A^* - \overline{\lambda} I)} = (A^* - \overline{\lambda} I)^{-1}$$

because inverses are unique. In particular, the right-hand side is bounded since the left-hand side is bounded. Hence $\lambda \in \sigma_c(A)$ implies $\overline{\lambda} \in \sigma_c(A^*)$. We may replicate the argument starting from A^* and observe that $(A^* - \overline{\lambda} I)^* = A - \lambda I$ to conclude that $\overline{\lambda} \in \sigma_c(A^*)$ implies $\lambda = \overline{\overline{\lambda}} \in \sigma_c(A)$. This ends the proof of (iii).

(d) If $\lambda \neq \mu$ and $Au = \lambda u$, $Av = \mu v$, then $\mu\langle u|v\rangle = \langle u|Av\rangle = \langle A^*u|v\rangle = \lambda\langle u|v\rangle$, so $(\mu - \lambda)\langle u|v\rangle = 0$. The latter is only possible for $\langle u|v\rangle = 0$ because $\mu - \lambda \neq 0$. □

Example 3.14 The m-axis position operator X_m on $L^2(\mathbb{R}^n, d^n x)$, introduced in Example 2.59 (1), satisfies

$$\sigma(X_m) = \sigma_c(X_m) = \mathbb{R} . \tag{3.5}$$

The arguments is as follows. First observe that $\sigma(X_m) \subset \mathbb{R}$ since the operator is selfadjoint (Proposition 3.13). However we saw in Sect. 1.3 that $\sigma_p(X_m) = \varnothing$, and $\sigma_r(X_m) = \varnothing$ again by selfadjointness (Proposition 3.13). Let us examine when a number $r \in \mathbb{R}$ belongs to $\rho(X_m)$. If no $r \in \mathbb{R}$ belongs to $\rho(X_m)$, we must conclude that $\sigma(X_m) = \sigma_c(X_m) = \mathbb{R}$.

Suppose that, for some $r \in \mathbb{R}$, $(X_m - rI)^{-1}$ exists and is bounded. If $\psi \in D(X_m - rI) = D(X_m)$ with $||\psi|| = 1$ then $||\psi|| = ||(X_m - rI)^{-1}(X_m - rI)\psi||$, and hence $||\psi|| \leq ||(X_m - rI)^{-1}|| \, ||(X_m - rI)\psi||$. Therefore $||(X_m - rI)^{-1}|| \geq ||(X_m - rI)\psi||^{-1}$. For every given $\epsilon > 0$, it is easy to manufacture $\psi \in D(X_m)$ with $||\psi|| = 1$ and $||(X_m - rI)\psi|| < \epsilon$. Assuming $m = 1$, it suffices to consider sets of the form $[r - 1/k, r + 1/k] \times \mathbb{R}^{n-1}$ and functions $\psi_k \in C_c^\infty(\mathbb{R}^n, \mathbb{C})$ such that $\text{supp}(\psi_k) \subset [r - 1/k, r + 1/k] \times \mathbb{R}^{n-1}$ and $\int_{\mathbb{R}^n} |\psi_k|^2 d^n x = 1$. As $k \to +\infty$

$$0 \leq ||(X_m - rI)\psi||^2 \leq \int_{\mathbb{R}^n} |x_1 - r|^2 |\psi(x)|^2 d^n x \leq \frac{4}{k^2} \int_{\mathbb{R}^n} |\psi(x)|^2 d^n x = \frac{4}{k^2} \to 0 .$$

Therefore $(X_m - rI)^{-1}$ cannot be bounded and $r \in \sigma(X_m)$. More precisely $r \in \sigma_c(X_m)$, since no other possibility is allowed.

By Proposition 3.4 we also conclude that

$$\sigma(P_m) = \sigma_c(P_m) = \mathbb{R} , \tag{3.6}$$

simply because the momentum operator P_m is related to the position operator by means of a unitary operator, namely the Fourier-Plancherel operator $\hat{\mathscr{F}}$ of Example 2.59 (2). ■

3.2 Integration of Projector-Valued Measures

We introduce in this section the most important technical tool in spectral theory, the notion of *projector-valued measure*, whose repercussions in the interpretation of quantum theories are paramount. Before we do it, let us prove a few important and elementary facts concerning *orthogonal projectors*.

3.2.1 Orthogonal Projectors

Definition 3.15 Let H be a Hilbert space. An operator $P \in \mathfrak{B}(\mathsf{H})$ is called an **orthogonal projector** when $PP = P$ and $P^* = P$. The set of orthogonal projectors of H is denoted by $\mathscr{L}(\mathsf{H})$. ■

A well-known relation exists between orthogonal projectors and closed subspaces.

Proposition 3.16 *Let* H *be a Hilbert space with orthogonal projectors* $\mathscr{L}(\mathsf{H})$. *Then*

(a) *if* $P \in \mathscr{L}(\mathsf{H})$, *then* $P(\mathsf{H})$ *is a closed subspace.*
(b) *If* $P \in \mathscr{L}(\mathsf{H})$, *then* $Q := I - P \in \mathscr{L}(\mathsf{H})$ *and* $Q(\mathsf{H}) = P(\mathsf{H})^\perp$.
(c) *There is an orthogonal sum* $\mathsf{H} = P(\mathsf{H}) \oplus Q(\mathsf{H})$, *so any* $z \in \mathsf{H}$ *decomposes uniquely as* $z = x + y$ *with* $x = P(z) \in P(\mathsf{H})$, $y = Q(z) \in Q(\mathsf{H})$.

(d) *If* $\mathsf{H}_0 \subset \mathsf{H}$ *is a closed subspace, there exists exactly one* $P \in \mathscr{L}(\mathsf{H})$ *that projects* H *onto* H_0*, i.e.* $P(\mathsf{H}) = \mathsf{H}_0$.

Proof

(a) It is clear that $P(\mathsf{H})$ is a subspace. It is also closed because, if $x = \lim_{n\to+\infty} Px_n$, then $x = Px$. Indeed, $Px = P\lim_{n\to+\infty} P(x_n) = \lim_{n\to+\infty} PPx_n = \lim_{n\to+\infty} Px_n = x$ since P is continuous.

(b) We have $(I-P)^* = I^* - P^* = I - P$ and $(I-P)(I-P) = I - 2P + PP = I - 2P + P = I - P$, so $Q := I - P \in \mathscr{L}(\mathsf{H})$. Let us prove that $Q(\mathsf{H}) = P(\mathsf{H})^\perp$. First of all, observe that $y \in Q(\mathsf{H})$ and $x \in P(\mathsf{H})$ yield $\langle y|x\rangle = \langle (I-P)y|Px\rangle = \langle y|(I-P)Px\rangle = \langle y|(P-PP)x\rangle = \langle y|(P-P)x\rangle = 0$. Therefore $Q(\mathsf{H}) \subset P(\mathsf{H})^\perp$. To conclude, we have to prove that $Q(\mathsf{H}) \supset P(\mathsf{H})^\perp$. If $y \in P(\mathsf{H})^\perp$ we have $\langle Py|u\rangle = \langle y|Pu\rangle = 0$ for $u \in \mathsf{H}$ and therefore $Py = 0$. As a consequence, if we define $z = y + x$ with $x \in P(\mathsf{H})$, we obtain $Qz = (I-P)y+(I-P)x = x+y-Py-Px = z-Py-Px = z-0-x = y$. In other words, if $y \in P(\mathsf{H})^\perp$, then $y \in Q(\mathsf{H})$, proving $Q(\mathsf{H}) \supset P(\mathsf{H})^\perp$.

(d) and (c). Consider a closed subspace H_0. It is a Hilbert space in its own right since it contains the limits of its Cauchy sequences (which converge in H since H is Hilbert). Therefore H_0 admits a Hilbert basis N. It is easy to prove that if N' is a Hilbert basis of $\mathsf{H}_0^\perp$, then $N \cup N'$ is a Hilbert basis of H. By taking $M = \mathsf{H}_0$, so that $\overline{\text{span } M} = \mathsf{H}_0$, in (2.3) we obtain the orthogonal sum $\mathsf{H} = \mathsf{H}_0 \oplus \mathsf{H}_0^\perp$. Consider the operator $Px := \sum_{z\in N}\langle z|x\rangle z$ for $x \in \mathsf{H}$. Using the Hilbert decomposition $u = \sum_{z\in N\cup N'}\langle z|u\rangle z$, one immediately proves that $||P|| \leq 1$, $PP = P$, $\langle Px|y\rangle = \langle x|Py\rangle$ and hence $P = P^*$, so $P \in \mathscr{L}(\mathsf{H})$. Finally, $P(\mathsf{H}) = \mathsf{H}_0$ since N is a Hilbert basis of H_0.

Let us demonstrate that the orthogonal projector P satisfying $P(\mathsf{H}) = \mathsf{H}_0$ is uniquely determined by H_0. The same proof also establishes (c). Since $P(\mathsf{H}) \cap Q(\mathsf{H}) = \{0\}$, because the subspaces are mutually orthogonal and $I = P+Q$, we conclude that $z \in \mathsf{H}$ can be decomposed *uniquely* as $z = x + y$ with $x \in P(\mathsf{H})$ and $y \in Q(\mathsf{H})$ and $x = Pz$, $y = Qz$. This fact proves that a P with $P(\mathsf{H}) = \mathsf{H}_0$ is unique: if $P'(\mathsf{H}) = \mathsf{H}_0$, we would have that $Q' := I - P'$ projects onto $\mathsf{H}_0^\perp$ and $z \in \mathsf{H}$ is uniquely decomposed as $z = x + y$ with $x \in \mathsf{H}_0$, $y \in \mathsf{H}_0^\perp$ where $x = Pz = P'z$ and $y = Qz = Q'z$. Hence $P'z = Pz$ for all $z \in \mathsf{H}$.

□

If $P \in \mathscr{L}(\mathsf{H})$, then P and $Q := I - P$ project onto mutually orthogonal subspaces, and $PQ = QP = 0$. This fact is rather general, according to the next elementary result.

Proposition 3.17 *Let* H *be a Hilbert space. Two projectors* $P, Q \in \mathscr{L}(\mathsf{H})$ *project onto orthogonal subspaces if and only if* $PQ = 0$. *In this case* $QP = 0$ *as well.*

Proof If $P(\mathsf{H}) \perp Q(\mathsf{H})$ then for every $x, y \in \mathsf{H}$ we have $0 = \langle Px|Qy\rangle = \langle x|PQy\rangle$. Therefore $PQ = 0$. Taking adjoints we obtain $QP = 0$. If conversely $PQ = 0$, from the identity above we have $\langle Px|Qy\rangle = 0$ for every $x, y \in \mathsf{H}$, so that $P(\mathsf{H}) \perp Q(\mathsf{H})$. □

Let us prove further properties of orthogonal projectors related with a natural order relation, which will play a crucial role in the next chapter.

Notation 3.18 Referring to Proposition 3.16, if $P, Q \in \mathscr{L}(\mathsf{H})$ we write $P \geq Q$ whenever $P(\mathsf{H}) \supset Q(\mathsf{H})$. ■

Proposition 3.19 *If* H *is a Hilbert space and* $P, Q \in \mathscr{L}(\mathsf{H})$,

(a) $P \geq Q$ *is equivalent to* $PQ = Q$. *In this case* $QP = Q$ *too.*
(b) $P \geq Q$ *is equivalent to* $\langle x|Px\rangle \geq \langle x|Qx\rangle$ *for every* $x \in \mathsf{H}$.

Proof

(a) If $P(\mathsf{H}) \supset Q(\mathsf{H})$, there exists a Hilbert basis $N_P = N_Q \cup N'_Q$ of $P(\mathsf{H})$ where N_Q, N'_Q are a Hilbert bases of $Q(\mathsf{H})$, $Q(\mathsf{H})^{\perp_P}$ (orthogonality referring to $P(\mathsf{H})$). From $Q = \sum_{z\in N_Q}\langle z|\cdot\rangle z$ and $P = Q + \sum_{z\in N'_Q}\langle z|\cdot\rangle z$ we have $PQ = Q$. The converse implication is obvious. Assume $PQ = Q$. If $x \in Q(\mathsf{H})$ then $Qx = x$. Therefore $Px = PQx = Qx = x$, hence $x \in P(\mathsf{H})$ and then $Q(\mathsf{H}) \subset P(\mathsf{H})$ as wanted. Finally, taking adjoints on $PQ = Q$ we obtain $QP = Q$ since P and Q are selfadjoint.
(b) Assume $P \geq Q$, i.e. $Q(\mathsf{H}) \subset P(\mathsf{H})$. If $x \in \mathsf{H}$, the vector $Px \in P(\mathsf{H})$ decomposes as $y + z$ where $y := QPx \in Q(\mathsf{H})$ and $z \in P(\mathsf{H})$ is orthogonal to y. Therefore $||Px||^2 = ||QPx||^2 + ||z||^2$. From (a), $||Px||^2 = ||Qx||^2 + ||z||^2$ which implies $||Px||^2 \geq ||Qx||^2$, namely $\langle x|Px\rangle \geq \langle x|Qx\rangle$ for every $x \in \mathsf{H}$. Conversely, if $\langle x|Px\rangle \geq \langle x|Qx\rangle$ for every $x \in \mathsf{H}$, then $||Px||^2 \geq ||Qx||^2$ for every $x \in \mathsf{H}$, so that $Px = 0$ implies $Qx = 0$ for every $x \in \mathsf{H}$. In other words $P(\mathsf{H})^\perp \subset Q(\mathsf{H})^\perp$. Applying $^\perp$ again, we eventually get $P(\mathsf{H}) \supset Q(\mathsf{H})$.

□

Proposition 3.20 *If* H *is a Hilbert space and* $\{P_n\}_{n\in\mathbb{N}} \in \mathscr{L}(\mathsf{H})$ *is a sequence such that either (i)* $P_n \leq P_{n+1}$ *for all* $n \in \mathbb{N}$ *or (ii)* $P_n \geq P_{n+1}$ *for all* $n \in \mathbb{N}$, *then* $P_n x \to Px$, *for every* $x \in \mathsf{H}$ *and some* $P \in \mathscr{L}(\mathsf{H})$, *as* $n \to +\infty$.

Proof Assume $P_n \leq P_{n+1}$ for all $n \in \mathbb{N}$. For any $x \in \mathsf{H}$, the sequence $\{P_n x\}_{n\in\mathbb{N}}$ is Cauchy. Indeed, for $n > m$ and using Proposition 3.19 (a) alongside the selfadjointness and idempotence of orthogonal projectors, $||P_n x - P_m x||^2$ equals

$$\langle x|(P_n - P_m)(P_n - P_m)x\rangle = \langle x|(P_n - P_m - P_m + P_m)x\rangle = ||P_n x||^2 - ||P_m x||^2\,.$$

Since the sequence of numbers $||P_n x||^2 = \langle x|P_n x\rangle$ is non-decreasing and bounded by $||x||^2$, it converges to some real number and hence it is a Cauchy sequence. This implies that $\{P_n x\}_{n\in\mathbb{N}}$ is Cauchy as well. The map $P : \mathsf{H} \ni x \mapsto \lim_{n\to+\infty} P_n x \in \mathsf{H}$ is linear by construction. Furthermore, $\langle Px|y\rangle = \langle x|Py\rangle$ for every $x, y \in \mathsf{H}$ by continuity of the inner product, so $P = P^*$. Finally, for every $x, y \in \mathsf{H}$ we also have $\langle Px|Py\rangle = \lim_{n\to+\infty}\langle P_n x|P_n y\rangle = \lim_{n\to+\infty}\langle x|P_n y\rangle = \langle x|Py\rangle$, so that $PP = P$ and therefore $P \in \mathscr{L}(\mathsf{H})$. The other case's proof is identical up to trivial changes.

□

3.2.2 Projector-Valued Measures (PVMs)

At this juncture we can state one of the most important definitions in spectral theory.

Definition 3.21 Let H be a Hilbert space and $\Sigma(X)$ a σ-algebra on X. A **projector-valued measure (PVM)** on X is a map $P : \Sigma(X) \ni E \mapsto P_E \in \mathscr{L}(\mathsf{H})$ such that

(i) $P_X = I$,
(ii) $P_E P_F = P_{E\cap F}$,
(iii) if $N \subset \mathbb{N}$ and $\{E_k\}_{k\in N} \subset \Sigma(X)$ satisfies $E_j \cap E_k = \varnothing$ for $k \neq j$, then

$$\sum_{j\in N} P_{E_j} x = P_{\cup_{j\in N} E_j} x \quad \text{for every } x \in \mathsf{H}.$$

We say that P is **concentrated** on $S \in \sigma(X)$ if $P_E = P_{E\cap S}$ for every $E \in \Sigma(X)$. ■

Remark 3.22

(a) Taking $N = \{1, 2\}$ in (i) and (iii) tells that $P_\varnothing = 0$, using $E_1 = X$ and $E_2 = \varnothing$. Property (ii) entails that $P_E P_F = 0$ if $E \cap F = \varnothing$ from Proposition 3.17. In particular, the vectors $P_{E_j} x$ in (iii) are orthogonal. Therefore a series (for $N = \mathbb{N}$)

$$\sum_{j\in\mathbb{N}} P_{E_j} x\ , \tag{3.7}$$

where $E_j \cap E_k = \varnothing$ for $k \neq j$, always converges. An alternative argument for convergence is to invoke Proposition 3.20, since the operators $\sum_{j=0}^{n} P_{E_j}$ are orthogonal projectors and $\sum_{j=0}^{n} P_{E_j} \leq \sum_{j=0}^{n+1} P_{E_j}$. (Series (3.7) can be rearranged because by Bessel's inequality (2.1.2) we have

$$\sum_{j\in\mathbb{N}} ||P_{E_j} x||^2 \leq \sum_{j\in N} \sum_{u\in M_j} |\langle u|x\rangle|^2 < +\infty,$$

where $M_j \subset P_{E_j}(\mathsf{H})$ is a Hilbert basis of $P_{E_j}(\mathsf{H})$. Now Lemma 2.8 guarantees (3.7) converges and can be rearranged.) Proving explicitly that the series converges is nonetheless a useful exercise. For a given $\epsilon > 0$, we use the inner product's continuity and the fact that $P_{E_j} x \perp P_{E_k} x$ if $j \neq k$, to compute, for $m > n > N_\epsilon$,

$$\left|\left|\sum_{j=0}^{m} P_{E_j} x - \sum_{j=0}^{n-1} P_{E_j} x\right|\right|^2 = \left|\left|\sum_{j=n}^{j=m} P_{E_j} x\right|\right|^2 = \left\langle \sum_{j=n}^{j=m} P_{E_j} x \middle| \sum_{k=n}^{k=m} P_{E_k} x \right\rangle$$
$$= \sum_{j=n}^{j=m} \left\langle P_{E_j} x \middle| \sum_{k=n}^{k=m} P_{E_k} x \right\rangle$$

$$= \sum_{j=n}^{j=m} \left\langle x \left| P_{E_j} \sum_{k=n}^{k=m} P_{E_k} x \right.\right\rangle = \sum_{j=n}^{j=m} \left\langle x \left| \sum_{k=n}^{k=m} P_{E_j} P_{E_k} x \right.\right\rangle = \sum_{j=n}^{j=m} \left\langle x \left| \sum_{k=n}^{k=m} \delta_{jk} P_{E_k} x \right.\right\rangle$$

$$= \sum_{j=n}^{j=m} \left\langle x \left| P_{E_j} x \right.\right\rangle = \sum_{j=n}^{j=m} \left\langle x \left| P_{E_j} P_{E_j} x \right.\right\rangle = \sum_{j=n}^{j=m} \left\langle P_{E_j} x \left| P_{E_j} x \right.\right\rangle = \sum_{j=n}^{j=m} ||P_{E_j} x||^2 < \epsilon.$$

Hence (3.7) converges, as truncated sums form a Cauchy sequence.

In summary, (iii) can be viewed as a condition on the value of the sum of the series and not an assumption about its convergence.

(b) If $x, y \in \mathsf{H}$, $\Sigma(X) \ni E \mapsto \langle x|P_E y\rangle =: \mu_{xy}^{(P)}(E)$ is a *complex measure* whose (finite) *total variation* [Rud91] will be denoted by $|\mu_{xy}^{(P)}|$. This follows from the definition of PVM, in particular the inner product's continuity implying σ-additivity: if the sets $E_n \subset \Sigma(X)$, $n \in N \subset \mathbb{N}$, are pairwise disjoint ($E_n \cap E_m = \varnothing$ for $n \neq m$),

$$\mu_{xy}^{(P)}\left(\cup_{n\in N} E_n\right) = \left\langle x \left| P_{\cup_{n\in N} E_n} y \right.\right\rangle = \left\langle x \left| \sum_{n\in N} P_{E_n} y \right.\right\rangle = \sum_{n\in N} \left\langle x \left| P_{E_n} y \right.\right\rangle = \sum_{n\in N} \mu_{xy}^{(P)}(E_n)\,.$$

The definition of μ_{xy} gives us immediately three important facts.

(i) $\mu_{xy}^{(P)}(X) = \langle x|y\rangle$.
(ii) $\mu_{xx}^{(P)}$ is always positive and finite, and $\mu_{xx}^{(P)}(X) = ||x||^2$.
(iii) Consider a *simple function* [Rud91] $s = \sum_{k=1}^{n} s_k \chi_{E_k}$, where $s_k \in \mathbb{C}$ and the sets $E_k \in \Sigma(X)$, $k = 1, \ldots, n$, are pairwise disjoint, and χ_E is the **characteristic function** of the set E, i.e. the map $\chi_E(x) = 0$ if $x \notin E$ and $\chi_E(x) = 1$ if $x \in E$. If h denotes the *Radon–Nikodym derivative* of μ_{xy} with respect to its total variation $|\mu_{xy}|$ (see, e.g., [Mor18]), we have

$$\int_X s d\mu_{xy} = \int_X s h d|\mu_{xy}| = \sum_{k=1}^{n} s_k \int_{E_k} h d|\mu_{xy}| = \sum_{k=1}^{n} s_k \mu_{xy}(E_k)$$
$$= \left\langle x \left| \sum_{k=1}^{n} s_k P_{E_k} y \right.\right\rangle .$$

If we *define*

$$\int_X s(\lambda) dP(\lambda) := \sum_{k=1}^{n} s_k P_{E_k}$$

we may then write

$$\int_X s d\mu_{xy} = \left\langle x \left| \int_X s(\lambda) dP(\lambda) \, y \right. \right\rangle . \tag{3.8}$$

The entire machinery of Spectral Theory and Measurable Functional Calculus is contingent on formula (3.8) (extended from simple functions s to general measurable functions f). ∎

Example 3.23

(1) The simplest example of a PVM arises from a Hilbert basis N in a Hilbert space H. Let $\Sigma(N)$ be the power set of N. For $E \in \Sigma(N)$ and $z \in \mathsf{H}$ we define

$$P_E z := \sum_{x \in E} \langle x|z\rangle x$$

and $P_\varnothing := 0$. It is easy to prove that the collection of P_E thus defined forms a PVM on N. (This definition works even if H is not separable and N is uncountable, since for every $y \in \mathsf{H}$ at most countably many elements $x \in E$ satisfy $\langle x|y\rangle \neq 0$). Observe that $P_N x = \sum_{u \in N} \langle u|x\rangle u = x$ for every $x \in \mathsf{H}$, so that $P_N = I$ as required.

In particular $\mu^{(P)}_{xy}(E) = \langle x|P_E y\rangle = \sum_{z \in E} \langle x|z\rangle\langle z|y\rangle$ and $\mu^{(P)}_{xx}(E) = \sum_{z \in E} |\langle x|z\rangle|^2$.

(2) A more sophisticated version of (1) is built out of the Hilbert sum of a family of non-trivial, pairwise-orthogonal closed subspaces $\{\mathsf{H}_j\}_{j \in J}$ of a Hilbert space $\mathsf{H} = \bigoplus_{j \in J} \mathsf{H}_j$. Defining once again $\Sigma(J)$ as the family of subsets of J, for $E \in \Sigma(J)$ and $z \in \mathsf{H}$ we set $P_\varnothing = 0$ and

$$P_E z := \sum_{j \in E} Q_j z ,$$

where Q_j is the orthogonal projector onto H_j. It is easy to prove that the P_E form a PVM on $\mathbb{N}$. Since $\bigoplus_{j \in J} \mathsf{H}_j = \mathsf{H}$ we have $\sum_{j \in J} Q_j x = x$ for every $x \in \mathsf{H}$, so $P_J = I$ as requested.

In particular $\mu^{(P)}_{xy}(E) = \langle x|P_E y\rangle = \sum_{j \in E} \langle x|Q_j y\rangle$ and $\mu^{(P)}_{xx}(E) = \sum_{j \in E} ||Q_j x||^2$.

The reader can prove without difficulty that

$$\int_J f(j) d\mu_{xx}(j) = \sum_{j \in J} f(j) ||Q_j x||^2 \tag{3.9}$$

if f is μ_{xx}-integrable. This formula is trivial for simple functions, and extends easily to general maps using dominated convergence.

(3) Here is a PVM of a completely different sort, this time on $L^2(\mathbb{R}^n, d^n x)$. To every E in the Borel σ-algebra $\mathscr{B}(\mathbb{R}^n)$ associate the orthonormal projector

$$(P_E\psi)(x) := \chi_E(x)\psi(x) \quad \forall \psi \in L^2(\mathbb{R}^n, d^n x) .$$

Note $P_\varnothing := 0$. It is easy to prove that the collection of P_E is a PVM. In particular $\mu^{(P)}_{fg}(E) = \langle f|P_E g\rangle = \int_E \overline{f(x)}g(x)d^n x$ and $\mu^{(P)}_{ff}(E) = \int_E |f(x)|^2 d^n x$.

The reader can easily check that

$$\int_{\mathbb{R}^n} f(x)d\mu_{gg}(x) = \int_{\mathbb{R}^n} f(x)|g(x)|^2 d^n x \tag{3.10}$$

if f is μ_{gg}-integrable. This is trivial for simple functions, and can be generalized easily to measurable functions using the theorem of dominated convergence. ■

The following pivotal result [Rud91, Mor18, Schm12] generalizes (3.8) from simple functions to measurable functions of a suitable type.

Theorem 3.24 *Let* H *be a Hilbert space,* $P : \Sigma(X) \to \mathscr{L}(\mathsf{H})$ *a PVM, and* $f : X \to \mathbb{C}$ *a measurable function. Define*

$$\Delta_f := \left\{ x \in \mathsf{H} \;\middle|\; \int_X |f(\lambda)|^2 \mu^{(P)}_{xx}(\lambda) < +\infty \right\} .$$

The following facts hold.

(a) Δ_f *is a dense subspace in* H *and there exists a unique operator*

$$\int_X f(\lambda)dP(\lambda) : \Delta_f \to \mathsf{H} \tag{3.11}$$

such that

$$\left\langle x \;\middle|\; \int_X f(\lambda)dP(\lambda)y \right\rangle = \int_X f(\lambda)d\mu^{(P)}_{xy}(\lambda) \quad \forall x \in \mathsf{H}\,, \forall y \in \Delta_f \,. \tag{3.12}$$

(b) *The operator in (3.11) is closed and normal.*
(c) *The adjoint operator to (3.11) satisfies*

$$\left(\int_X f(\lambda)\, dP(\lambda)\right)^* = \int_X \overline{f(\lambda)}\, dP(\lambda) . \tag{3.13}$$

(d) *The operator in (3.11) satisfies*

$$\left|\left|\int_X f(\lambda)\, dP(\lambda)x\right|\right|^2 = \int_X |f(\lambda)|^2 d\mu_{xx}^{(P)}(\lambda) \quad \forall x \in \Delta_f \,. \tag{3.14}$$

Proof (I. Existence and Uniqueness) We start by proving that if Δ_f is subspace of H, then there is a unique operator denoted by $\int_X f(\lambda) dP(\lambda)$ satisfying (3.12). The proof of this fact relies on this preliminary lemma.

Lemma 3.25 *If $f : X \to \mathbb{C}$ is measurable, then*

$$\int_X |f(\lambda)|\, d|\mu_{xy}^{(P)}|(\lambda) \le ||x|| \sqrt{\int_X |f(\lambda)|^2 d\mu_{yy}^{(P)}(\lambda)} \qquad \forall y \in \Delta_f \,, \forall x \in \mathsf{H} \,. \tag{3.15}$$

Proof We henceforth write μ_{xy} in place of $\mu_{xy}^{(P)}$ for the sake of shortness. The idea is initially to establish the inequality for simple functions and then pass to arbitrary functions. Take $x \in \mathsf{H}$ and $y \in \Delta_f$. Let $s : X \to \mathbb{C}$ be a simple function, $h : X \to \mathbb{C}$ the Radon–Nikodym derivative of μ_{xy} with respect to $|\mu_{xy}|$, so that $|h(x)| = 1$ and $\mu_{xy}(E) = \int_E hd|\mu_{xy}|$. For an increasing sequence of simple functions z_n such that $z_n \to h^{-1}$ pointwise, with $|z_n| \le |h^{-1}| = 1$, by the dominated convergence theorem we have

$$\int_X |s| d|\mu_{xy}| = \int_X |s| h^{-1} d\mu_{xy} = \lim_{n\to+\infty} \int_X |s| z_n d\mu_{xy} = \lim_{n\to+\infty} \left\langle x \left| \sum_{k=1}^{N_n} z_{n,k} P_{E_{n,k}}\, y \right.\right\rangle \,.$$

In the last step we used part (iii) in Remark 3.22 (b) for the simple function

$$|s| z_n = \sum_{k=1}^{N_n} z_{n,k} \chi_{E_{n,k}}$$

and we have supposed that, for fixed n, the sets $E_{n,k}$ are disjoint from one another. The Cauchy–Schwartz inequality immediately yields

$$\int_X |s| d|\mu_{xy}| \le ||x|| \lim_{n\to+\infty} \left|\left| \sum_{k=1}^{N_n} z_{n,k} P_{E_{n,k}} y \right|\right| = ||x|| \lim_{n\to+\infty} \sqrt{\int_X |s z_n|^2 d\mu_{yy}} \,,$$

where, in computing the norm, we used $P^*_{E_{n,k}} P_{E_{n,k'}} = P_{E_{n,k}} P_{E_{n,k'}} = \delta_{kk'} P_{E_{n,k}}$ since $E_{n,k} \cap E_{n,k'} = \varnothing$ for $k \ne k'$. Next observe that as $|s z_n|^2 \to |s h^{-1}|^2 = |s|^2$, dominated convergence yields

$$\int_X |s| d|\mu_{xy}| \leq ||x|| \sqrt{\int_X |s|^2 d\mu_{yy}} \,.$$

At last, replace s above by a sequence of simple functions $s_n \to f \in L^2(X, d\mu_{yy})$ pointwise, with $|s_n| \leq |s_{n+1}| \leq |f|$. The monotone convergence theorem and the dominated convergence theorem, applied respectively to the left- and right-hand side of the previous inequality, eventually produce (3.15). □

To proceed with the main proof we notice that inequality (3.15) also proves that $f \in L^2(X, d\mu^{(P)}_{yy})$ implies $f \in L^1(X, d|\mu^{(P)}_{xy}|)$ for $x \in \mathsf{H}$, hence the right-hand side of (3.12) makes sense. General measure theory guarantees that

$$\left| \int_X f(\lambda)\, d\mu^{(P)}_{xy}(\lambda) \right| \leq \int_X |f(\lambda)|\, d|\mu^{(P)}_{xy}|(\lambda) \,,$$

whence (3.15) implies that $\mathsf{H} \ni x \mapsto \int_X f(\lambda)\, d\mu^{(P)}_{xy}(\lambda)$ is continuous at $x = 0$. This map is also anti-linear if f is simple, as follows from the definition of μ_{xy} and the left anti-linearity of the inner product. Anti-linearity extends to measurable functions f via the usual approximation procedure of measurable functions by simple functions. We conclude that, for $y \in \Delta_f$, the map

$$\mathsf{H} \ni x \mapsto \overline{\int_X f(\lambda)\, d\mu^{(P)}_{xy}(\lambda)}$$

is linear and continuous. Riesz's Lemma guarantees the existence of a unique vector, indicated by $\int_X f(\lambda) dP(\lambda) y$, satisfying

$$\overline{\int_X f(\lambda)\, d\mu^{(P)}_{xy}(\lambda)} = \left\langle \int_X f(\lambda) dP(\lambda) y \middle| x \right\rangle .$$

Conjugating both sides we obtain (3.12). As we have assumed Δ_f is a subspace, the map

$$\Delta_f \ni y \mapsto \int_X f(\lambda)\, d\mu^{(P)}_{xy}(\lambda)$$

is linear when f is simple, as immediately follows from the definition of $\mu^{(P)}_{xy}$ and the right linearity of the inner product. As before, linearity extends to measurable functions f by approximating measurable functions with simple maps. As a consequence of (3.12)

$$\Delta_f \ni y \mapsto \int_X f(\lambda) dP(\lambda) y$$

is linear as well. The uniqueness of this operator is an immediate consequence of the uniqueness in Riesz's Lemma.

(II. Δ_f is a Dense Subspace) Let us show that Δ_f is a subspace first. It contains 0 so it is not empty. Moreover, directly by definition of Δ_f, it is clear that if $x \in \Delta_f$, then $ax \in \Delta_f$ for every $a \in \mathbb{C}$, because $\mu^{(P)}_{ax,ax}(E) = |a|^2 \mu^{(P)}_{xx}(E)$ independently of E and so

$$\int_X |f|^2 d\mu^{(P)}_{ax,ax} = |a|^2 \int_X |f|^2 d\mu^{(P)}_{x,x} < +\infty \,.$$

Next suppose that $x, y \in \Delta_f$. We therefore have $||P_E(x+y)||^2 \leq (||P_E x|| + ||P_E y||)^2 \leq 2||P_E x||^2 + 2||P_E y||^2$. As a consequence $\mu^{(P)}_{x+y,x+y}(E) = ||P_E(x+y)||^2 \leq 2\mu^{(P)}_{xx}(E) + 2\mu^{(P)}_{yy}(E)$. Therefore

$$\int_X |f|^2 d\mu^{(P)}_{x+y,x+y} \leq 2 \int_X |f|^2 d\mu^{(P)}_{xx} + \int_X |f|^2 d\mu^{(P)}_{yy} < +\infty \,,$$

and hence $x + y \in \Delta_f$. Let us pass to the density of Δ_f. Consider the countable partition of X made by measurable sets $F_n := \{\lambda \in X \mid n \leq |f(\lambda)|^2 < n+1\}$, for $n = 0, 1, 2, \ldots$. By the σ-additivity of P, if $z \in H$ then $z = P_X z = \sum_{n=0}^{+\infty} P_{F_n} z$. Therefore the span of the unions of closed subspaces $\mathsf{H}_n := P_{F_n}(\mathsf{H})$ is dense in H. If we prove that $\mathsf{H}_n \subset \Delta_f$ for every n, since Δ_f is a subspace, we immediately infer that it is dense. Let us prove it. If $x \in H_n$, then $x = P_{F_n} x$ and therefore $\mu^{(P)}_{xx}(E) = \langle P_{F_n} x | P_E P_{F_n} x \rangle = \langle x | P_{E \cap F_n} x \rangle = \mu^{(P)}_{xx}(E \cap F_n)$. Since

$$\int_X |f|^2 d\mu^{(P)}_{xx} = \int_{F_n} |f|^2 d\mu^{(P)}_{xx} \leq \int_{F_n} (n+1) d\mu^{(P)}_{xx} \leq (n+1)||x||^2 < +\infty$$

we have $x \in \Delta_f$, as wanted.

(III. Proof of Eq. (3.14)) For $x \in \Delta_f$, using (3.12), we obtain

$$\left|\left| \int_X f dPx \right|\right|^2 = \left\langle \int_X f dPx \middle| \int_X f dPx \right\rangle = \int_X f d\nu \tag{3.16}$$

where

$$\nu(E) = \mu^{(P)}_{\int_X f dPx, x}(E) = \left\langle \int_X f dPx \middle| P_E x \right\rangle = \overline{\int_X f d\mu^{(P)}_{P_E x, x}} \,.$$

Since $\mu^{(P)}_{P_E x, x}(F) = \langle P_E x | P_F x \rangle = \langle x | P_{E\cap F} x \rangle$, we have

$$\nu(E) = \int_E \overline{f} d\mu^{(P)}_{xx} .$$

Using the definition of integral (of a complex measure), it immediately follows

$$\int_X s d\nu = \int_X s \cdot \overline{f} d\mu^{(P)}_{xx}$$

for a simple function s. A standard argument based of dominated convergence (take a sequence of simple maps s_n tending to f pointwise, with $|s_n| \leq |f|$) allows to establish

$$\int_X f d\nu = \int_X |f|^2 d\mu^{(P)}_{xx}$$

as $|f|^2$ is μ_{xx}-integrable. Inserting this result in (3.16) we obtain (3.14), as claimed.

(IV. Proof of Eq. (3.13) and the Closure of $\int_X f dP$) Since the adjoint is always closed, Eq. (3.13) and $\int_X f dP = (\int_X \overline{f} dP)^*$ would imply $\int_X f dP$ is closed. So let us prove Eq. (3.13). From (3.12) it is easy to see that $\int_X \overline{f} dP \subset (\int_X \overline{f} dP)^*$: noticing that $\mu^{(P)}_{yx}(E) = \overline{\mu^{(P)}_{xy}(E)}$, namely, if $x, y \in \Delta_f$ then

$$\left\langle y \middle| \int_X f dP x \right\rangle = \int_X f d\mu^{(P)}_{yx} = \overline{\int_X \overline{f} d\mu^{(P)}_{xy}} = \overline{\left\langle x \middle| \int_X \overline{f} dP y \right\rangle} = \left\langle \int_X \overline{f} dP y \middle| x \right\rangle . \quad (3.17)$$

Therefore we only have to prove that $\int_X \overline{f} dP \supset (\int_X \overline{f} dP)^*$. This is equivalent to show that if $y \in D((\int_X \overline{f} dP)^*)$ then $y \in \Delta_{\overline{f}} = \Delta_f$. So let us prove this then, for which we need an intermediate result.

Lemma 3.26 *Under the assumptions of Theorem 3.24*

(i) $\int_X \chi_E dP = P_E$ *for every* $E \in \Sigma(X)$
(ii) $\int_X f dP P_E = \int_X f \cdot \chi_E dP$ *for every* $E \in \Sigma(X)$
(iii) if f *is bounded on* $E \in \Sigma(X)$ *then* $(\int_X f \cdot \chi_E dP)^* = \int_X \overline{f} \cdot \chi_E dP$.

Proof (i) is true since $\langle x | P_E y \rangle = \mu_{xy}(E) = \int_E 1 d\mu^{(P)}_{xy}$, and so (3.12) holds and uniquely determines $\int_X \chi_E dP$.

Concerning (ii), the domain of $\int_X f dP P_E$ consists of the $x \in \mathsf{H}$ such that $P_E x \in \Delta_f$, that is $\int_X |f|^2 d\mu^{(P)}_{P_E x, P_E x} < +\infty$. Since $\mu^{(P)}_{P_E x, P_E x}(F) = \langle P_E x | P_F P_E x \rangle = \langle x | P_{E\cap F} x \rangle = \mu^{(P)}_{xx}(E \cap F)$, the condition can be rephrased as $\int_X \chi_E \cdot |f|^2 d\mu^{(P)}_{xx} < +\infty$, or $\int_X |\chi_E \cdot f|^2 d\mu^{(P)}_{xx} < +\infty$. Therefore $\int_X f dP P_E$ and $\int_X \chi_E \cdot f dP$ have the same domain. If $x \in \mathsf{H}$ and $y \in \Delta_{\chi \cdot f}$, $\langle x | \int_X f dP P_E y \rangle = \int_X f d\mu^{(P)}_{x, P_E y} =$

$\int_X f d\mu^{(P)}_{P_E x, P_E y} = \int_E f d\mu^{(P)}_{x,y} = \int_E f \cdot \chi_E d\mu^{(P)}_{x,y}$, which implies $\int_X f dP P_E = \int_X f \cdot \chi_E dP$ again by (3.12).

(iii) is true because $\Delta_{f \cdot \chi_E} = \mathsf{H}$ and $\int_X \overline{f} \cdot \chi_E dP \in \mathfrak{B}(\mathsf{H})$ from (3.14). Hence replacing f with $f \cdot \chi_E$ in (3.17) ensures that $\int_X \overline{f \cdot \chi_E} dP = \int_X \overline{f} \cdot \chi_E dP$ is the adjoint of $\int_X f \cdot \chi_E dP$. □

To resume part IV of the main theorem, we claim (i), (ii), and (iii) imply $y \in \Delta_{\overline{f}}$ if $y \in D((\int_X \overline{f} dP)^*)$. We start by defining $E_n := \{\lambda \in X \mid |f(\lambda)| < n\}$. Then from (i)–(iii) we have

$$P_{E_n} \left(\int_X f dP \right)^* = P^*_{E_n} \left(\int_X f dP \right)^* \subset \left(\int_X f dP P_{E_n} \right)^* = \left(\int_X f \cdot \chi_{E_n} dP \right)^*$$
$$= \int_X \overline{f} \cdot \chi_{E_n} dP \, .$$

Hence if $y \in D((\int_X \overline{f} dP)^*)$ we infer

$$\int_X \overline{f} \cdot \chi_{E_n} dPy = P_{E_n} \left(\int_X f dP \right)^* y \, ,$$

and so

$$\left\| \int_X \overline{f} \cdot \chi_{E_n} dPy \right\|^2 = \left\| P_{E_n} \left(\int_X f dP \right)^* y \right\|^2 \leq \left\| \left(\int_X f dP \right)^* y \right\|^2 .$$

Using (3.14),

$$\int_X |\overline{f} \cdot \chi_{E_n}|^2 d\mu^{(P)}_{yy} \leq \left\| \left(\int_X f dP \right)^* y \right\|^2 .$$

Since $|\overline{f} \cdot \chi_{E_n}|^2 \leq |\overline{f} \cdot \chi_{E_{n+1}}|^2 \to |\overline{f}|^2$ as $n \to +\infty$, the monotone convergence theorem implies

$$\int_X |\overline{f}|^2 d\mu^{(P)}_{yy} \leq \left\| \left(\int_X f dP \right)^* y \right\|^2 < +\infty \, ,$$

that is to say $y \in \Delta_{\overline{f}}$, as wanted.

(V. Proof that $\int_X f dP$ is Normal) The same argument used in the previous lemma to establish (ii) gives $P_E \int_X f dPx = \int_X \chi_E \cdot f dPx$ if $x \in \Delta_f$. Consider the domain of $\int_X \overline{f} dP \int_X f dP$. It consists of vectors $x \in \Delta_f$ such that

$$\int_X |f|^2 d\mu^{(P)}_{\int_X f dPx, \int_X f dPx} < +\infty \, . \tag{3.18}$$

Let us write this condition in a simpler way. First observe that

$$\mu^{(P)}_{\int_X f dPx, \int_X f dPx}(E) = \left\langle \int_X f dPx \middle| P_E \int_X f dPx \right\rangle = \left\langle P_E \int_X f dPx \middle| P_E \int_X f dPx \right\rangle$$

$$= \left\langle \int_X \chi_E \cdot f dPx \middle| \int_X \chi_E \cdot f dPx \right\rangle = \int_E |f|^2 d\mu^{(P)}_{xx} .$$

Starting from simple functions and generalizing to measurable functions, it is therefore easy to prove that

$$\int_X g d\mu^{(P)}_{\int_X f dPx, \int_X f dPx} = \int_X |f|^2 g d\mu^{(P)}_{xx} .$$

In summary, (3.18) reads

$$D\left(\int_X \overline{f} dP \int_X f dP\right) = \Delta_{|f|^2} .$$

Now replace f by $|f|^2$ in the first statement of the theorem we are proving: that domain is dense and $D(\int_X \overline{f} dP \int_X f dP) = D(\int_X f dP \int_X \overline{f} dP)$. To finish the proof consider $x \in D(\int_X \overline{f} dP \int_X f dP) = D(\int_X f dP \int_X \overline{f} dP)$. We have

$$\left\langle x \middle| \int_X \overline{f} dP \int_X f dPx \right\rangle = \left\langle \int_X f dPx \middle| \int_X f dPx \right\rangle = \int_X |f|^2 d\mu^{(P)}_{xx} = \left\langle \int_X \overline{f} dPx \middle| \int_X \overline{f} dPx \right\rangle$$

$$= \left\langle x \middle| \int_X f dP \int_X \overline{f} dPx \right\rangle .$$

In other words

$$\left\langle x \middle| \left(\int_X f dP \int_X \overline{f} dP - \int_X \overline{f} dP \int_X f dP\right) x \right\rangle = 0 .$$

By polarization we finally obtain

$$\left\langle y \middle| \left(\int_X f dP \int_X \overline{f} dP - \int_X \overline{f} dP \int_X f dP\right) x \right\rangle = 0 ,$$

for every $x, y \in D(\int_X \overline{f} dP \int_X f dP) = D(\int_X f dP \int_X \overline{f} dP)$. Since this domain is dense, $\int_X f dP \int_X \overline{f} dP - \int_X \overline{f} dP \int_X f dP = 0$, and the proof ends.

□

The theorem just proved has technically important consequences, which we list in the following corollary and the subsequent proposition.

Corollary 3.27 *Under the hypotheses of Theorem 3.24, the following hold.*

(a) *If $f : X \to \mathbb{C}$ only assumes non-negative real values, then*

$$\left\langle x \left| \int_X f dPx \right.\right\rangle \geq 0 \quad \forall x \in \Delta_f \ .$$

(b) *If T is an operator on H with $D(T) = \Delta_f$ such that*

$$\langle x | Tx \rangle = \int_X f(\lambda)\, d\mu_{xx}^{(P)}(\lambda) \quad \forall x \in \Delta_f \ , \tag{3.19}$$

then

$$T = \int_X f(\lambda) dP(\lambda) \ .$$

Proof

(a) The proof is evident from (3.12), taking $y = x$ and noticing that $\mu_{xx}^{(P)}$ is positive.
(b) From the definition of μ_{xy} we easily have (for simplicity we omit the superscript $^{(P)}$)

$$4\mu_{xy}(E) = \mu_{x+y,x+y}(E) - \mu_{x-y,x-y}(E) - i\mu_{x+iy,x+iy}(E) + i\mu_{x-iy,x-iy}(E) \ .$$

This identity implies, by the definition of integral, that for a simple function

$$4\int_X s d\mu_{xy} = \int_X s d\mu_{x+y,x+y} - \int_X s d\mu_{x-y,x-y} - i\int_X s d\mu_{x+iy.x+iy} + i\int_X s d\mu_{x-iy,x-iy}$$

if $x, y \in \Delta_s$. The customary approximation of measurable functions f by simple functions (via dominated convergence) gives

$$4\int_X f d\mu_{xy} = \int_X f d\mu_{x+y,x+y} - \int_X f d\mu_{x-y,x-y} - i\int_X f d\mu_{x+iy.x+iy} + i\int_X f d\mu_{x-iy,x-iy}$$

for $x, y \in \Delta_f$. Similarly, by the elementary properties of the inner product

$$4\langle x|Ty\rangle = \langle x+y|T(x+y)\rangle - \langle x-y|T(x-y)\rangle - i\langle x+iy|T(x+iy)\rangle + i\langle x-iy|T(x-iy)\rangle$$

when $x, y \in D(T)$. Collecting everything, it is now obvious that (3.19) implies

$$\langle x | Ty \rangle = \int_X f(\lambda)\mu_{xy}^{(P)}(\lambda) \quad \forall x, y \in \Delta_f \ ,$$

so

$$\left\langle x \middle| \left(T - \int_X f(\lambda) dP(\lambda) \right) y \right\rangle = 0 \quad \forall x, y \in \Delta_f \,.$$

Since x varies in a dense set Δ_f, we have that $Ty - \int_X f(\lambda)dP(\lambda)y = 0$ for every $y \in \Delta_f$, which is the claim.

□

Example 3.28

(1) Consider the PVM of Example 3.23 (2). Using Corollary 3.27 (b) and (3.9) we have

$$\int_J f(\lambda)dP(\lambda)z = \sum_{n \in J} f(j) Q_j z$$

for every $f : J \to \mathbb{C}$ (which is necessarily measurable with our definition of $\Sigma(J)$). Correspondingly, the domain of $\int_J f(\lambda)dP(\lambda)$ is

$$\Delta_f := \left\{ z \in \mathsf{H} \;\middle|\; \sum_{j \in J} |f(j)|^2 ||Q_j z||^2 < +\infty \right\} .$$

According to Corollary 3.27 (b) in fact, from (3.10) we have

$$\left\langle z \middle| \int_J f(j) dP(j) z \right\rangle = \sum_{j \in J} f(j) ||Q_j z||^2 = \int_{\mathbb{R}} f(j) d\mu_{zz}$$

for every $z \in \Delta_f$.

(2) Now take to PVM in Example 3.23 (3). By Corollary 3.27 (b) and (3.10)

$$\left(\int_{\mathbb{R}^n} f(\lambda)dP(\lambda)\psi \right)(x) = f(x)\psi(x) \,, \quad x \in \mathbb{R}^n \,.$$

Correspondingly, the domain of $\int_{\mathbb{R}^n} f(\lambda)dP(\lambda)$ turns out to be

$$\Delta_f := \left\{ \psi \in L^2(\mathbb{R}^n, d^n x) \;\middle|\; \int_{\mathbb{R}^n} |f(x)|^2 |\psi(x)|^2 d^n x < +\infty \right\} .$$

In fact, for every $\psi \in \Delta_f$, Corollary 3.27 (b) and (3.10) give

$$\left\langle \psi \middle| \int_{\mathbb{R}^n} f(\lambda)dP(\lambda)\psi \right\rangle = \int_{\mathbb{R}^n} f(x)|\psi(x)|^2 d^n x = \int_{\mathbb{R}^n} f d\mu_{\psi\psi} \,.$$

■

3.2.3 PVM-Integration of Bounded Functions

We now state and prove a proposition about the most important properties of $\int_X f dP$ when $f : X \to \mathbb{C}$ is bounded or, more weakly, *P-essentially bounded*. Some of these have already been exploited in the proof of Theorem 3.24; however, they turn out to be so useful in the practice that they deserve a separate presentation.

If μ is a σ-additive positive measure on a σ-algebra $\Sigma(X)$,

$$||f||_\infty^{(\mu)} := \inf\{r \geq 0 \mid \mu(\{x \in X \mid |f(x)| > r\}) = 0\} \ .$$

Since the integral sees only non-zero measure sets in $\Sigma(X)$, for instance,

$$\int_X |f| d\mu \leq ||f||_\infty^{(\mu)} \int_X 1 d\mu \ .$$

The same definition can be extended to PVMs:

$$||f||_\infty^{(P)} := \inf\{r \geq 0 \mid P(\{x \in X \mid |f(x)| > r\}) = 0\}$$

and f is said to be ***P*-essentially bounded** if $||f||_\infty^{(P)} < +\infty$.

Note that if $P_E = 0$, then $\mu_{xy}^{(P)}(E) = 0$ for $E \in \Sigma(X)$. Therefore a P-essentially bounded map f is also $\mu_{xx}^{(P)}$-essentially bounded for every $x \in \Delta_f$. In particular, since zero-measure sets for P evidently have zero measure for $\mu_{xx}^{(P)}$ as well,

$$0 \leq ||f||_\infty^{(\mu_{xx}^{(P)})} \leq ||f||_\infty^{(P)} \leq ||f||_\infty \leq +\infty \ . \tag{3.20}$$

A **seminorm** $p : X \to \mathbb{R}$ on a complex vector space X by definition satisfies $p(x) \geq 0$, $p(ax) = |a|p(x)$ and $p(x + y) \leq p(x) + p(y)$ for all $x, y \in X$ and $a \in \mathbb{C}$.

It is easy to prove that $|| \ ||_\infty^{(P)}$ is a *seminorm* on the vector space of P-essentially bounded, measurable, complex-valued functions on X. Moreover, $|f| \leq |g|$ pointwise implies $||f||_\infty^{(P)} \leq ||g||_\infty^{(P)}$ and $||f \cdot g||_\infty^{(P)} \leq ||f||_\infty^{(P)} ||g||_\infty^{(P)}$, where $f \cdot g$ is the pointwise product $(f \cdot g)(x) = f(x)g(x)$ for $x \in X$.

Proposition 3.29 *Let* $P : \Sigma(X) \to \mathscr{L}(\mathsf{H})$ *be a PVM.*

(a) *A map f is P-essentially bounded if and only if*

$$\int_X f(\lambda) \, dP(\lambda) \in \mathfrak{B}(\mathsf{H}) \ .$$

In this case

$$\left|\left|\int_X f(\lambda) \, dP(\lambda)\right|\right| \leq ||f||_\infty^{(P)} \leq ||f||_\infty \ . \tag{3.21}$$

(b) *We have*

$$\int_X \chi_E \, dP = P_E \,, \quad \text{if } E \in \Sigma(X). \tag{3.22}$$

In particular,

$$\int_X 1 \, dP = I \,. \tag{3.23}$$

For a simple function $s = \sum_{k=1}^{n} s_k \chi_{E_k}$, *where* $s_k \in \mathbb{C}$ *and* $E_k \in \Sigma(X)$, $k = 1, \ldots, n$,

$$\int_X \sum_{k=1}^{n} s_k \chi_{E_k} dP = \sum_{k=1}^{n} s_k P_{E_k} \,. \tag{3.24}$$

(c) *Let* $f, f_n : X \to \mathbb{R}$ *be measurable functions such that* $||f||_\infty^{(P)}, ||f_n||_\infty^{(P)} \leq K < +\infty$ *for some* $K \in \mathbb{R}$ *and every* $n \in \mathbb{N}$. *If* $f_n \to f$ *pointwise as* $n \to +\infty$, *then*

$$\int_X f_n dPx \to \int_X f dPx \quad \text{as } n \to +\infty, \text{ for every } x \in \mathsf{H} \,. \tag{3.25}$$

(d) *If* $f, g : X \to \mathbb{C}$ *are* P*-essentially bounded and* $a, b \in \mathbb{C}$, *then*

$$\int_X (af + bg) \, dP = a \int_X f dP + b \int_X g dP \,, \tag{3.26}$$

$$\int_X f dP \int_X g dP = \int_X f \cdot g \, dP \,. \tag{3.27}$$

Proof

(a) Assume f is P-essentially bounded. Since $\mu_{xx}(X) = ||x||^2 < +\infty$ for every $x \in \mathsf{H}$,

$$\int_X |f(\lambda)|^2 d\mu_{xx}^{(P)}(\lambda) \leq (||f||_\infty^{(\mu_{xx}^{(P)})})^2 \int_X 1 d\mu_{xx}^{(P)} \leq (||f||_\infty^{(P)})^2 \int_X 1 d\mu_{xx}^{(P)} = ||x||^2 \, (|f||_\infty^{(P)})^2 \,,$$

so that $\Delta_f = \mathsf{H}$. Next, dividing by $||x||^2$ and taking the sup over the elements $x \neq 0$, (3.14) implies (3.21). If, instead, f is not P-essentially bounded, then for every $n \in \mathbb{N}$, there is $E_n \in \Sigma(X)$ with $P_{E_n} \neq 0$ and $|f(\lambda)| \geq n$ if $\lambda \in E_n$. Pick $x_n \in P_{E_n}(\mathsf{H})$ with $||x_n|| = 1$ for every $n \in \mathbb{N}$. If $x_n \notin \Delta_f$ for some n, then $\int_X f dP \notin \mathfrak{B}(\mathsf{H})$ because the domain of the operator is smaller than the entire H and the proof ends. If $x_n \in \Delta_f$ for every $n \in \mathbb{N}$, from Theorem 3.24 (d), we have $||\int_X f dPx_n||^2 = \int_X |f|^2 d\mu^{(P)}_{x_n x_n} = \int_{E_n} |f|^2 d\mu^{(P)}_{x_n x_n}$, where we have used that $\mu^{(P)}_{x_n x_n}(F) = \langle x_n | P_F x_n\rangle = \langle P_{E_n} x_n | P_F P_{E_n} x_n\rangle = \langle x_n | P_{F\cap E_n} x_n\rangle = \mu^{(P)}_{x_n x_n}(F \cap E_n)$. Therefore $||\int_X f dPx_n||^2 \geq \int_{E_n} n^2 d\mu^{(P)}_{x_n x_n} = n^2 \int_{E_n} 1 d\mu_{x_n x_n} = n^2 \int_X 1 d\mu^{(P)}_{x_n x_n} = n^2 ||x_n||^2 = n^2$. Hence $||\int_X f dP||$ cannot be finite and $\int_X f dP \notin \mathfrak{B}(\mathsf{H})$.

(b) By direct inspection

$$\langle y | P_E x\rangle = \mu^{(P)}_{yx}(E) = \int_E 1 d\mu^{(P)}_{yx}(\lambda) = \int_X \chi_E(\lambda) d\mu^{(P)}_{yx}(\lambda) \quad \forall x, y \in \Delta_{\chi_E} = \mathsf{H}\,.$$

This proves (3.22), which also implies (3.23) for $E = X$, since $P_X = I$. The proof of (3.24) is a trivial extension of this argument by linearity of the integral in $\mu^{(P)}_{yx}$ and linearity of the inner product.

(c) Under the given hypotheses,

$$\left|\left|\left(\int_X f dP - \int_X f_n dP\right)x\right|\right|^2 = \left|\left|\int_X f - f_n\, dPx\right|\right|^2 = \int_X |f - f_n|^2 d\mu^{(P)}_{xx}\,.$$

The first equality comes from (3.26), whose proof is independent of the present argument. Note that $|f - f_n|^2 \leq 4K^2$ almost everywhere with respect to P, and hence also with respect to $\mu^{(P)}_{xx}$. In addition, $\int |K^2| d\mu^{(P)}_{xx} = ||x||^2 K^2 < +\infty$, so the dominated convergence theorem implies $\int_X |f - f_n|^2 d\mu^{(P)}_{xx} \to 0$ as $n \to +\infty$, proving our assertion.

(d) (i) First observe that $\Delta_{af+bg}, \Delta_f, \Delta_g = \mathsf{H}$ because $f, g, af + bg$ are P-essentially bounded ($||af + bg||^{(P)}_\infty \leq |a| ||f||^{(P)}_\infty + |b| ||g||^{(P)}_\infty$), so both sides of (c)(i) are defined everywhere. Next, from standard properties of the integral, for every $x \in \mathsf{H}$

$$\int_X af + bg\, d\mu^{(P)}_{yx} = a \int_X f d\mu^{(P)}_{yx} + b \int_X g d\mu^{(P)}_{yx}\,.$$

Using (3.12) we find

$$\left\langle y \left| \int_X af + bg\, dPx \right.\right\rangle = a \left\langle y \left| \int_X f\, dPx \right.\right\rangle + b \left\langle y \left| \int_X g\, dPx \right.\right\rangle$$
$$= \left\langle y \left| \left(a \int_X f dP + b \int_X g\, dP\right) x \right.\right\rangle\,.$$

The proof ends since $x, y \in \mathsf{H}$ are arbitrary.

Let us prove (3.27). First consider a pair of simple functions $s = \sum_{k=1}^{n} s_k \chi_{E_k}$ and $t = \sum_{h=1}^{m} t_h \chi_{F_h}$. The pointwise product $s \cdot t$ is simple. Indeed,

$$s \cdot t = \sum_{k=1}^{n} s_k \chi_{E_k} \sum_{h=1}^{m} t_h \chi_{F_h} = \sum_{k,h} s_k t_h \chi_{E_k} \chi_{F_h} = \sum_{(k,h) \in I_n \times I_m} s_k t_h \chi_{E_k \cap F_h}$$

$$= \sum_{(k,h) \in I_n \times I_m} (s \cdot t)_{(k,h)} P_{G_{(k,h)}} ,$$

where $I_l := \{1, 2, \dots, l\}$ and $G_{(k,h)} := E_k \cap F_h$. Exploiting (3.24), we immediately find

$$\int_X s dP \int_X t dP = \sum_{k=1}^{n} s_k P_{E_k} \sum_{h=1}^{m} t_h P_{F_h} = \sum_{h,k} s_k t_h P_{E_k} P_{F_h}$$

$$= \sum_{(k,h) \in I_n \times I_m} s_k t_h P_{E_k \cap F_h} = \sum_{(k,h) \in I_n \times I_m} (s \cdot t)_{(k,h)} P_{G_{(k,h)}} = \int_X s \cdot t dP .$$

We have proved the claim for simple functions f, g. Taking arbitrary P-essentially bounded functions f, g, consider two sequences of simple maps $s_n \to f$ and $t_n \to g$ pointwise, such that $|s_n| \leq |s_{n+1}| \leq |f|$ and $|t_n| \leq |t_{n+1}| \leq |g|$ for all $n \in \mathbb{N}$. Evidently $s_n \cdot t_n \to f \cdot g$, $|s_n \cdot t_n| \leq |s_{n+1} \cdot t_{n+1}| \leq |f \cdot g|$ plus $||s_n||_\infty^{(P)} \leq ||f||_\infty^{(P)}$, $||t_n||_\infty^{(P)} \leq ||g||_\infty^{(P)}$ and $||s_n \cdot t_n||_\infty^{(P)} \leq ||f \cdot g||_\infty^{(P)} \leq ||f||_\infty^{(P)} ||g||_\infty^{(P)}$. We can apply (c) to obtain, for every $x, y \in \mathsf{H}$,

$$\left\langle \int_X \overline{s_n} dPx \middle| \int_X t_n dPy \right\rangle = \left\langle x \middle| \int_X s_n dP \int_X t_n dPy \right\rangle$$

$$= \left\langle x \middle| \int_X s_n \cdot t_n dPy \right\rangle \to \left\langle x \middle| \int_X f \cdot g dPy \right\rangle$$

as $n \to +\infty$. On the other hand, using (c) again and exploiting the inner product's continuity, we also have

$$\left\langle \int_X \overline{s_n} dPx \middle| \int_X t_n dPy \right\rangle \to \left\langle \int_X \overline{f} dPx \middle| \int_X g dPy \right\rangle$$

as $n \to +\infty$. Summarizing,

$$\left\langle \int_X \overline{f} dPx \middle| \int_X g dPy \right\rangle = \left\langle x \middle| \int_X f \cdot g dPy \right\rangle ,$$

which, from (3.13) and using that the domain of $\int_X f dP$ is H, implies

$$\left\langle x \left| \int_X f dP \int_X g dP y \right.\right\rangle = \left\langle x \left| \int_X f \cdot g \, dP y \right.\right\rangle .$$

Since $x, y \in \mathsf{H}$ are arbitrary, (3.27) indeed holds.

□

Remark 3.30

(a) Consider $f : X \to \mathbb{C}$ measurable and P-essentially bounded. We may redefine it so that it maps complex numbers $z \in \mathbb{C}$ with $|z| > ||f||_\infty^{(P)}$ to 0. We thus obtain a measurable function $f' \in M_b(X)$ such that $\int_X f' dP = \int_X f dP$. With regard to the integration of measurable functions in a PVM, therefore, bounded functions carry the same information as P-essentially bounded functions.

(b) The first inequality in Proposition 3.29 (a) is actually an equality [Rud91, Mor18],

$$\left|\left| \int_X f(\lambda) \, dP(\lambda) \right|\right| = ||f||_\infty^{(P)} . \tag{3.28}$$

See the solution of Exercise 3.35 for a proof.

(c) Consider a set X equipped with a σ-algebra $\Sigma(X)$. The set

$$M_b(X) := \{f : X \to \mathbb{C} \mid f \text{ is measurable and } ||f||_\infty < +\infty\}$$

is a *commutative C^*-algebra with unit*. The norm making $M_b(X)$ a complete vector space is $||\cdot||_\infty$, the involution the standard complex conjugation of functions $f^*(x) = \overline{f(x)}$ for $x \in X$, the algebra multiplication is the *commutative* pointwise product of maps $(f \cdot g)(x) = f(x)g(x)$, and the complex vector space structure is the standard one: $(af + bg)(x) := af(x) + bg(x)$ if $x \in X$, $a, b \in \mathbb{C}$, and $f, g \in M_b(X)$. The algebra's unit is the constant map $\mathbb{1}(x) = 1$ if $x \in X$. The C^*-property $||f^* \cdot f||^2 = ||f||^2$ is nothing but $|||f|^2||_\infty = ||f||_\infty^2$.

Suppose now a PVM $P : \Sigma(X) \to \mathscr{L}(\mathsf{H})$ is also given. The map

$$\pi_P : M_b(X) \ni f \mapsto \int_X f dP \in \mathfrak{B}(\mathsf{H})$$

preserves the structure of *-algebra and the unit, and hence is a *representation*. It is further *continuous* and *norm-decreasing* because of (3.21). This representation is neither injective nor isometric in general; however it enjoys a topological property unrelated to the continuity in the norms of $M_b(X)$ and $\mathfrak{B}(\mathsf{H})$. The feature descends immediately from (3.14), by using $\mu_{xx}^{(P)}(X) < +\infty$.

Proposition 3.31 *Retaining the above notation, if $M_b(X) \ni f_n \to f$ pointwise as $n \to +\infty$, and there is a constant $K \geq 0$ such that $|f_n| \leq K$, then $\pi_P(f_n)x \to \pi_P(f)x$ for every $x \in \mathsf{H}$.*

(d) Consider a topological space X and take its Borel σ-algebra $\mathscr{B}(X)$ as $\Sigma(X)$. Then the observation made in (c) holds provided we replace $M_b(X)$ with the commutative unital C^*-algebra $C_b(X) := \{f : X \to \mathbb{C} \mid f \text{ is continuous and } ||f||_\infty < +\infty\}$. Recall that if X is compact, then $C_b(X) = C(X) := \{f : X \to \mathbb{C} \mid f \text{ is continuous}\}$. An important result in the theory of C^*-algebras (see [Mor18]) establishes that

Theorem 3.32 (Commutative Gelfand–Najmark Theorem) *A commutative unital C^*-algebra is isometrically *-isomorphic to the unital C^*-algebra $C(X)$ for some compact Hausdorff space X.* ■

3.2.4 PVM-Integration of Unbounded Functions

To conclude, we state a proposition concerning the most important and general properties of the integral in a PVM of a measurable, possibly unbounded, function.

Proposition 3.33 *Consider a PVM $P : \Sigma(X) \to \mathsf{H}$, measurable functions $f, g : X \to \mathbb{C}$ and let af, $f \cdot g$, and $f + g$, with $a \in \mathbb{C}$, indicate the pointwise operations. Then*

(a) *For $a \in \mathbb{C}$*

$$a \int_X f dP = \int_X af dP \,.$$

(b) $D(\int_X f dP + \int_X g dP) = \Delta_f \cap \Delta_g$ *and*

$$\int_X f dP + \int_X g dP \subset \int_X (f + g) dP \,,$$

with equality if and only if $\Delta_{f+g} = \Delta_f \cap \Delta_g$.

(c) $D(\int_X f dP \int_X g dP) = \Delta_{f \cdot g} \cap \Delta_g$ *and*

$$\int_X f dP \int_X g dP \subset \int_X (f \cdot g) dP$$

with equality if and only if $\Delta_{f \cdot g} \subset \Delta_g$.

(d) $D\left((\int_X f dP)^* \int_X f dP\right) = D\left(\int_X f dP (\int_X f dP)^*\right) = \Delta_{|f|^2}$ *and*

$$\left(\int_X f dP\right)^* \int_X f dP = \int_X |f|^2 dP = \int_X f dP \left(\int_X f dP\right)^* \,.$$

(e) *If* $U : \mathsf{H} \to \mathsf{H}'$ *is a surjective linear (or anti-linear) isometry,* $\Sigma(X) \ni E \mapsto P'_E := U P_E U^{-1}$ *is a PVM on* H' *and*

$$U\left(\int_X f dP\right) U^{-1} = \int_X f dP' \,.$$

In particular, $D\left(\int_X f dP'\right) = UD(\int_X f dP) = U(\Delta_f)$.

(f) *If* $\phi : X \to X'$ *is measurable for the* σ*-algebras* $\Sigma(X)$, $\Sigma'(X')$ *and* $f : X' \to \mathbb{C}$ *is measurable, then*

(i) $\Sigma'(X') \ni E' \mapsto P'(E') := P(\phi^{-1}(E'))$ *is a PVM on* X'.
(ii) *we have*

$$\int_{X'} f \, dP' = \int_X f \circ \phi \, dP \,.$$

Furthermore

$$\Delta'_f = \Delta_{f \circ \phi} \,,$$

where Δ'_f *is the domain of* $\int_{X'} f \, dP'$.

Proof Items (a), (e), and (f) are proved straightforwardly by checking the definitions. (d) is a trivial consequence of (c) and Theorem 3.24 (b)–(c). Part (b) can be proved in $\Delta_f \cap \Delta_g$ with the same argument used for the first identity in Proposition 3.29 (d). Besides, $D(\int_X f dP + \int_X g dP) = \Delta_f \cap \Delta_g$ is the very definition of domain of a sum of operators $A + B$. By this relation the last statement is obvious. Similarly, (c) can be proved as the second identity in Proposition 3.29 (d), by working in $D(\int_X f dP \int_X g dP)$ and using $D(\int_X f dP \int_X g dP) = \Delta_{f \cdot g} \cap \Delta_g$. The latter is established as follows. $D(\int_X f dP \int_X g dP)$ is made of vectors $x \in \mathsf{H}$ such that both $x \in \Delta_g$ and

$$\int_X |f|^2 d\mu^{(P)}_{\int_X g dPx, \int_X g dPx} < +\infty \,.$$

By the definition of $\mu^{(P)}_{zz}$ it is easy to prove that

$$\int_X |f|^2 d\mu^{(P)}_{\int_X g dPx, \int_X g dPx} = \int_X |f|^2 |g|^2 d\mu^{(P)}_{xx} \,,$$

hence $D(\int_X f dP \int_X g dP) = \Delta_{f \cdot g} \cap \Delta_g$. With this the last statement is now obvious. □

Remark 3.34 It is moreover possible to prove [Mor18] that if $P : \Sigma(X) \to \mathsf{H}$ is a PVM and $f, g : X \to \mathbb{C}$ are measurable functions, then

$$\overline{\int_X f dP \int_X g dP} = \int_X (f \cdot g) dP \,,$$

and

$$\overline{\int_X f dP + \int_X g dP} = \int_X (f+g) dP \,,$$

the bar denoting the closure.

Exercise 3.35 Prove formula (3.28) when $f : X \to \mathbb{C}$ is measurable and P-essentially bounded.

Solution We already know that $||\int_X f dP|| \leq ||f||_\infty^{(P)}$. In particular if $||f||_\infty^{(P)} = 0$ the claim is obvious. Assume then $||f||_\infty^{(P)} > 0$. Exactly as in the proof of Proposition 3.29 (a), for $n > 0$ there exists $E_n \in \Sigma(X)$ such that $P_E \neq 0$ and $|f(\lambda)| \geq ||f||_\infty^{(P)} - 1/n > 0$ if $\lambda \in E_n$ and n is sufficiently large. Choosing $x_n \in P_{E_n}(\mathsf{H})$ with $||x_n|| = 1$, we have

$$\left|\left|\int_X f dP x_n\right|\right|^2 = \int_X |f|^2 d\mu^{(P)}_{x_n x_n} \geq \left(||f||_\infty^{(P)} - 1/n\right)^2 \int_{E_n} 1 d\mu^{(P)}_{x_n x_n} = \left(||f||_\infty^{(P)} - 1/n\right)^2 ,$$

that is

$$||f||_\infty^{(P)} \leq \left|\left|\int_X f dP x_n\right|\right| + 1/n \,.$$

Since we know that $||\int_X f dP x_n|| \leq ||f||_\infty^{(P)}$ (note $||x_n|| = 1$), this proves that there is a sequence of unit vectors x_n such that $||\int_X f dP x_n|| \to ||f||_\infty^{(P)}$ as $n \to +\infty$, demonstrating the assertion.

Exercise 3.36 Suppose $f_n \to f$ pointwise as $n \to +\infty$, where $f_n : X \to \mathbb{C}$ are measurable and $|f_n| \leq |f|$. Show that

$$\int_X f_n dP x \to \int_X f dP x \quad \text{if } n \to +\infty, \ \text{for every } x \in \Delta_f .$$

Solution Evidently $\Delta_{f_n} \subset \Delta_f$, so $x \in \Delta_{f_n}$ if $x \in \Delta_f$. Next, using Proposition 3.33 (b) and (3.14), dominated convergence implies directly $||\int_X f_n dP x - \int_X f \, dP x||^2 = \int_X |f - f_n|^2 d\mu^{(P)}_{xx} \to 0$ as $n \to +\infty$. □

3.3 Spectral Decomposition of Selfadjoint Operators

We are ready to state the fundamental result in the spectral theory of selfadjoint operators, which extends expansion (1.4) to an integral formula befitting infinite dimensions. The eigenvalue set is replaced by the full spectrum of the selfadjoint operator. After this we shall focus on some relevant consequences in quantum physics.

Notation 3.37 From now on $\mathscr{B}(T)$ will denote the Borel σ-algebra of the topological space T. ■

Definition 3.38 Given a PVM $P : \mathscr{B}(X) \to \mathscr{L}(\mathsf{H})$ on the Borel σ-algebra of a topological space X, the **support** $\text{supp}(P)$ of P is the complement in X of the union of all open sets $O \subset X$ with $P_O = 0$. ■

Remark 3.39 If X is second countable, P is necessarily **concentrated** on $\text{supp}(P)$, i.e.,

$$P_E = P_{E \cap supp(P)} \quad \text{if } E \subset X .$$

In fact, $D := X \setminus \text{supp}(P)$ is the union of a number of open sets O with $P_O = 0$. As the topology is second countable, we can extract a countable subcovering. By subadditivity of $\mu^{(P)}_{xx}$ we have $\mu^{(P)}_{xx}(D) = 0$ for every $x \in \mathsf{H}$. This can be rephrased as $||P_D x|| = 0$ for every $x \in \mathsf{H}$. Hence $P_D = 0$. If $E \in \mathscr{B}(X)$, we therefore have $P_E = P_{E \cap \text{supp}(P)} + P_{E \cap D} = P_{E \cap \text{supp}(P)}$. ■

3.3.1 Spectral Theorem for Selfadjoint, Possibly Unbounded, Operators

Prior to stating the theorem, note that (3.13) implies $\int f(\lambda) dP(\lambda)$ is selfadjoint when f is real. The idea of the theorem is that every selfadjoint operator looks like that for a certain map f and a PVM on $\mathbb{R}$ associated with the operator itself.

Theorem 3.40 (Spectral Theorem for Selfadjoint Operators) *Let A be a selfadjoint operator on the complex Hilbert space H.*

(a) *There exists a unique PVM $P^{(A)} : \mathscr{B}(\mathbb{R}) \to \mathscr{L}(\mathsf{H})$, called the **spectral measure** of A, such that*

$$A = \int_{\mathbb{R}} \lambda dP^{(A)}(\lambda) .$$

In particular $D(A) = \Delta_\iota$, where $\iota : \mathbb{R} \ni \lambda \mapsto \lambda$.

(b) *We have*

$$supp(P^{(A)}) = \sigma(A)$$

so that $P^{(A)}$ is concentrated on $\sigma(A)$ (as the standard $\mathbb{R}$ is second countable):

$$P^{(A)}(E) = P^{(A)}(E \cap \sigma(A)) , \quad \forall E \in \mathscr{B}(\mathbb{R}) . \tag{3.29}$$

(c) $\lambda \in \sigma_p(A)$ *if and only if* $P^{(A)}(\{\lambda\}) \neq 0$. *This happens in particular when* λ *is an isolated point of* $\sigma(A)$. *At last,* $P^{(A)}_{\{\lambda\}}$ *is the orthogonal projector onto the* λ*-eigenspace.*
(d) $\lambda \in \sigma_c(A)$ *if and only if* $P^{(A)}(\{\lambda\}) = 0$, *but* $P^{(A)}(E) \neq 0$ *if* $E \ni \lambda$ *is an open set in* $\mathbb{R}$.

Proof

(a) The existence part of the proof is involved and we postpone it to Sect. 3.6: Theorem 3.84 for the bounded case and Theorem 3.86 for the unbounded case (see also [Rud91, Mor18, Schm12]). Let us pass to the issue of uniqueness. Suppose there are two PVMs P_1 and P_2 on $\mathscr{B}(\mathbb{R})$ satisfying

$$A = \int_{\mathbb{R}} \lambda d P_k(\lambda) \quad k = 1, 2 \,.$$

Consider the bounded normal operators

$$T_k := \int_{\mathbb{R}} \frac{1}{r - i} d P_k(r) \,.$$

As we shall see below, either T_k coincides with the resolvent operator $R_i(A)$ of A for $\lambda = i$, so these operators are actually identical and we shall write simply T.

Using Proposition 3.33 (f) we define new PVMs on the image $\Gamma' \subset \mathbb{C}$ of the continuous, injective map $\phi : \mathbb{R} \ni r \mapsto \frac{1}{r-i} \in \Gamma$ (which turns out to be a homeomorphism on the image equipped with the topology induced by $\mathbb{C}$). We also assume $\Sigma(\Gamma') := \mathscr{B}(\Gamma)$ so that $\phi : \mathbb{R} \to \Gamma'$ is measurable. So we set

$$Q'_k(E) := P_k(\phi^{-1}(E)) \,, \quad E \in \mathscr{B}(\Gamma') \,, k = 1, 2 \,.$$

With this choices,

$$T = \int_{\Gamma'} z d Q'_k(z, \overline{z}) \,, \quad k = 1, 2 \,.$$

In Cartesian coordinates,

$$\Gamma = \left\{ x + iy \in \mathbb{C} \setminus \{0\} \;\middle|\; x^2 + \left(y - \frac{1}{2}\right)^2 = \frac{1}{4} \right\}$$

is a circle—centred at $i/2$ with radius $1/2$—without a point (the origin). If oriented in anti-clockwise manner, the ‘initial’ point 0^- formally corresponds to $r = -\infty$, and the ‘end’ point 0^+ is reached when $r = +\infty$.

It is certainly more practical to consider its compactification $\Gamma := \overline{\Gamma'} = \Gamma \cup \{0\}$, again assuming $\Sigma(\Gamma) = \mathscr{B}(\Gamma)$, and extend the PVMs in a trivial way

$$Q_k(F) := Q'_k(F \setminus \{0\}) \,, \quad F \in \mathscr{B}(\Gamma) \,, \quad k = 1, 2 \,.$$

The reader can easily prove that this extension does define well-behaved PVMs on $\mathscr{B}(\Gamma)$. In this way the added point satisfies $Q_k(\{0\}) = 0$, even if it belongs to the *supports* of the measures (defined as we did for $P^{(A)}$). For this reason we also have

$$T = \int_\Gamma z dQ_k(z, \overline{z}) \,, \quad k = 1, 2 \,.$$

It is also convenient to have at hand the adjoint of T,

$$T^* = \int_\Gamma \overline{z} dQ_k(z, \overline{z}) \,, \quad k = 1, 2 \,.$$

These operators are bounded and therefore we can apply Proposition 3.29 (d) to obtain that, for $p \in \mathbb{C}[z, \overline{z}]$,

$$p(T, T^*) = \int_\Gamma p(z, \overline{z}) dQ_k(z, \overline{z}) \,,$$

where the polynomial on the left is defined *thinking of the product of operators as their composition*. We also have, for $x, y \in \mathsf{H}$,

$$\int_\Gamma p(z, \overline{z}) d\mu_{xy}^{(Q_1)} = \langle x | p(T, T^*) y \rangle = \int_\Gamma p(z, \overline{z}) d\mu_{xy}^{(Q_2)} \,. \tag{3.30}$$

Since Γ is Hausdorff and compact, and $\mathbb{C}[z, \overline{z}]$ (i) contains the constant polynomial 1, (ii) is closed under complex conjugation and (iii) separates points in $\mathbb{C}$ and hence in Γ (i.e. if $\gamma \neq \gamma' \in \Gamma$ there exists a polynomial p with $p(\gamma) \neq p(\gamma')$), the *Stone–Weierstrass* theorem implies that these polynomials are $||\cdot||_\infty$-dense in the Banach space $C(\Gamma)$ of continuous complex-valued functions on Γ. Using a continuity argument coming from (3.21) and approximating continuous functions on Γ in terms of the above polynomials, Eq. (3.30) implies

$$\int_\Gamma f(z, \overline{z}) d\mu_{xx}^{(Q_1)} = \int_\Gamma f(z, \overline{z}) d\mu_{xx}^{(Q_2)} \quad \text{for every } f \in C(\Gamma).$$

Since in the locally compact Hausdorff space Γ an open set is a countable union of compact sets with finite $\mu_{xx}^{(Q_2)}$-measure, these Borel measures are *regular* [Rud86]. Hence, the uniqueness in Riesz's theorem for positive Borel measures [Rud86] implies that $\mu_{xx}^{(Q_1)}(E) = \mu_{xx}^{(Q_2)}(E)$ for every $E \in \mathscr{B}(\Gamma)$. In particular, for every $E \in \mathscr{B}(\Gamma)$ and every $x \in \mathsf{H}$,

$$\langle x|(Q_1(E) - Q_2(E))x\rangle = \int_\Gamma \chi_E d\mu_{xx}^{(Q_1)} - \int_\Gamma \chi_E d\mu_{xx}^{(Q_2)} = 0\,,$$

proving that $Q_1(E) = Q_2(E)$ for every $E \in \mathscr{B}(\Gamma)$. Let us return to the initial PVMs: noting that $\phi : \mathbb{R} \to \Gamma'$ is a homeomorphism, so $\phi^{-1} : \Gamma' \to \mathbb{R}$ is measurable and $\phi(F) \in \mathscr{B}(\Gamma')$ if $F \in \mathscr{B}(\mathbb{R})$, we have

$$P_1(F) = Q_1'(\phi(F)) = Q_1(\phi(F)) = Q_2(\phi(F)) = Q_2'(\phi(F)) = P_2(F)\,, \quad F \in \mathscr{B}(\mathbb{R})\,.$$

We have established that $P^{(A)}$ is uniquely determined by A.

(b) If $\lambda \notin \mathrm{supp}(P^{(A)})$, the map $\mathbb{C} \ni r \mapsto \frac{1}{r-\lambda} = g(r)$ is P-essentially bounded, so $\int_\mathbb{R} \frac{1}{r-\lambda} dP(r) \in \mathfrak{B}(\mathsf{H})$ and $\Delta_g = \mathsf{H}$. According to Proposition 3.33 (c),

$$(A - \lambda I)\int_\mathbb{R} \frac{1}{r-\lambda} dP(r) = \int_\mathbb{R} \frac{r-\lambda}{r-\lambda} dP^{(A)}(r) = \int_\mathbb{R} 1 dP^{(A)}(r) = I$$

and

$$\int_\mathbb{R} \frac{1}{r-\lambda} dP(r)(A-\lambda I)x = \int_\mathbb{R} \frac{r-\lambda}{r-\lambda} dP^{(A)}(r)x = \int_\mathbb{R} 1 dP^{(A)}x = x \quad \text{if } x \in D(A)\,.$$

We conclude that $\int_\mathbb{R} \frac{1}{r-\lambda} dP(r) = R_\lambda(A)$ and $\lambda \notin \sigma(A)$. Suppose conversely that $\lambda \notin \sigma(A)$, and so $R_\lambda(A) := (A - \lambda I)^{-1} \in \mathfrak{B}(\mathsf{H})$ exists. Then for $x \in D(A)$ we have $x = R_\lambda(A)(A - \lambda I)x$ and $||x|| \leq ||R_\lambda(A)||\,||(A-\lambda)x||$, so $||(A-\lambda)x||^2 \geq ||x||^2/||R_\lambda(A)||^2$. According to (3.14), taking $||x|| = 1$,

$$\int_\mathbb{R} |r-\lambda|^2 d\mu_{xx}^{(P^{(A)})}(r) \geq \frac{1}{||R_\lambda(A)||^2} > 0\,. \tag{3.31}$$

If $\lambda \in \mathrm{supp}(P^{(A)})$, we would have $P^{(A)}_{(\lambda-1/n,\lambda+1/n)} \neq 0$ and consequently we would be able to pick out a sequence $x_n \in P^{(A)}_{(\lambda-1/n,\lambda+1/n)}(\mathsf{H})$ with $||x_n|| = 1$, finding $\int_\mathbb{R} |r-\lambda|^2 d\mu_{xx}^{(P^{(A)})}(r) \leq 4||x_n||/n^2 = 4/n^2 \to 0$ as $n \to +\infty$. As (3.31) prevents this from happening, $\lambda \notin \mathrm{supp}(P^{(A)})$. This concludes the proof of (b).

(c) If $P^{(A)}_{\{\lambda\}} \neq 0$, let $0 \neq x \in P^{(A)}_{\{\lambda\}}(\mathsf{H})$. We have, from (3.22) and Proposition 3.33 (c),

$$Ax = AP^{(A)}_{\{\lambda\}}x = \int_\mathbb{R} r dP^{(A)}(r) \int_\mathbb{R} \chi_{\{\lambda\}}(r) dP(r)x = \int_\mathbb{R} r\chi_{\{\lambda\}}(r) dP^{(A)}x$$

$$= \int_\mathbb{R} \lambda\chi_{\{\lambda\}}(r) dP^{(A)}x = \lambda P^{(A)}_{\{\lambda\}}x = \lambda x\,.$$

Hence $\lambda \in \sigma_p(A)$. If conversely $\lambda \in \sigma_p(A)$, then $Ax = \lambda x$ for some eigenvector $x \in D(A)$ with $||x|| = 1$, so that $(A - iI)x = (1 - i)x$ and $(A - iI)^{-1}x = (\lambda - i)^{-1}x$. Similarly, $(A + iI)^{-1}x = (\lambda + i)^{-1}x$. Exploiting the same argument we used in proving the uniqueness of $P^{(A)}$, and writing Q in place of $Q_1 = Q_2$, the relations found read

$$Tx = \int_\Gamma z dQ(z, \overline{z})x = \frac{1}{\lambda - i}x \quad \text{and} \quad T^*x = \int_\Gamma \overline{z} dQ(z, \overline{z})x = \frac{1}{\lambda + i}x \,.$$

By considering polynomial compositions of the operators T and T^* these relations can be extended: for instance

$$\int_\Gamma (a\overline{z} + bzz) dQ(z, \overline{z})x = aT^* + bTTx = a\frac{1}{\lambda - i}x + b\frac{1}{\lambda + i}Tx$$
$$= \left[a\frac{1}{\lambda - i} + b\left(\frac{1}{\lambda + i}\right)^2\right]x \,,$$

and so on. In complete generality, defining $t := \frac{1}{\lambda - i}$, we have

$$\int_\Gamma p(z, \overline{z}) dQ(z, \overline{z})x = p(T, T^*)x = p(t, \overline{t})x$$

for every polynomial p in the variables z and $\overline{z}$. As before, we can extend to continuous functions $f : \Gamma \to \mathbb{C}$ via the Stone–Weierstrass theorem and uniformly approximating a continuous functions $f = f(z, \overline{z})$ on the compact set Γ by means of a sequence of polynomials $p_n = p_n(z, \overline{z})$ restricted to Γ. As $||f - p_n \restriction_\Gamma ||_\infty \to 0$ as $n \to +\infty$, (3.21) implies in particular

$$p_n(t, \overline{t})x = \int_\Gamma p_n(z, \overline{z}) dQ(z, \overline{z})x \to \int_\Gamma f(z, \overline{z}) dQ(z, \overline{z})x \quad \text{if } n \to +\infty \,.$$

Since $p_n(t, \overline{t}) \to f(t, \overline{t})$, we eventually obtain

$$\int_\Gamma f(z, \overline{z}) dQ(z, \overline{z})x = f(t, \overline{t})x \,. \tag{3.32}$$

Now it is not hard to construct a sequence of continuous maps on Γ such that $f_n \to \chi_{\{t\}}$ pointwise on Γ as $n \to +\infty$ and $|f_n(z, \overline{z})| < K < +\infty$ for some $K > 0$ and every $(z, \overline{z}) \in \Gamma$. (c) and (b) in Proposition 3.29 imply, from (3.32),

$$Q_{\{t\}}x = \int_\Gamma \chi_{\{t\}}(z, \overline{z}) dQ(z, \overline{z})x = \lim_{n \to +\infty} \int_\Gamma f_n(z, \overline{z}) dQ(z, \overline{z})x$$
$$= \lim_{n \to +\infty} f_n(t, \overline{t})x = \chi_{\{t\}}(t, \overline{t})x = x \,.$$

Since $t \in \Gamma'$ by construction, $Q_{\{t\}} = Q'_{\{t\}} = P^{(A)}_{\{\phi^{-1}(t)\}} = P^{(A)}_{\{\lambda\}}$. We have discovered that $P^{(A)}_{\{\lambda\}}x = x$. Since $x \neq 0$, we also have $P^{(A)}_{\{\lambda\}} \neq 0$, which concludes the proof.

It is clear that if $\lambda \in \sigma(A) = \text{supp}(P^{(A)})$ is isolated, so that there is an open set $O \ni \lambda$ such that $O \setminus \{\lambda\}$ is contained in $\mathbb{R} \setminus \text{supp}(P^{(A)})$, then $P^{(A)}_{\{\lambda\}} \neq 0$. For otherwise by additivity we would have $P^{(A)}_O = 0$ for some open set $O \ni \lambda$, forbidding $\lambda \in \text{supp}(P^{(A)})$. Let us prove the last statement in (c): $P^{(A)}_{\{\lambda\}}(\mathsf{H}) = \mathsf{H}_\lambda$, where H_λ is the eigenspace of $\lambda \in \sigma_p(A)$. We established that if $P^{(A)}_{\{\lambda\}} \neq 0$ (or equivalently, $\lambda \in \sigma_p(A)$), $x \in P^{(A)}_{\{\lambda\}}(\mathsf{H})$ satisfies $Ax = \lambda x$. Therefore $P^{(A)}_{\{\lambda\}}(\mathsf{H}) \subset \mathsf{H}_\lambda$. We have also proved that $x \in \mathsf{H}_\lambda$ implies $P^{(A)}_{\{\lambda\}}x = x$, that is $\mathsf{H}_\lambda \subset P^{(A)}_{\{\lambda\}}(\mathsf{H})$. In summary, $P^{(A)}_{\{\lambda\}}(\mathsf{H}) = \mathsf{H}_\lambda$.

(d) Assuming $\lambda \in \sigma_c(A)$, due to (c), necessarily $P^{(A)}_{\{\lambda\}} = 0$, because otherwise $\lambda \in \sigma_p(A)$, which is disjoint from $\sigma_c(A)$. On the other hand, since $\lambda \in \text{supp}(P^{(A)})$, for every open set O containing λ, $P^{(A)}_O \neq 0$. Suppose $P^{(A)}_O \neq 0$ for every open neighbourhood O of λ. This fact forces $\lambda \in \text{supp}(P^{(A)}) = \sigma(A)$, and the further requirement $P^{(A)}_{\{\lambda\}} = 0$ yields $\lambda \in \sigma_c(A)$ due to (c).

□

Remark 3.41

(a) If P is a PVM on $\mathbb{R}$ and $f : \mathbb{R} \to \mathbb{C}$ is measurable, we can always write

$$\int_{\mathbb{R}} f(\lambda) dP(\lambda) = f(A),$$

for the selfadjoint operator A obtained as

$$A = \int_{\mathbb{R}} \iota(\lambda) dP(\lambda)\ , \tag{3.33}$$

due to (3.13), where $\iota : \mathbb{R} \ni \lambda \to \lambda$. By virtue of the uniqueness statement in the spectral theorem $P^{(A)} = P$, which leads us to the conclusion that *on a Hilbert space* H, *projector-valued measures on* $\mathscr{B}(\mathbb{R})$ *correspond one-to-one to selfadjoint operators on* H.

(b) Theorem 3.40 is a particular case of a more general theorem (see [Rud91, Mor18] and especially [Schm12]) that is valid when A is a (densely-defined closed) normal operator. The statement is identical, with the proviso of replacing $\mathbb{R}$ with $\mathbb{C}$. A special case is that in which A is unitary. The spectral theorem for normal operators on $\mathfrak{B}(\mathsf{H})$ will show up in Sect. 3.6 disguised as Theorem 3.85.

■

Notation 3.42 Suppose $f : \sigma(A) \to \mathbb{C}$ is measurable for the σ-algebra obtained by restricting the elements of $\mathscr{B}(\mathbb{R})$ to $\sigma(A)$, *which coincides with* $\mathscr{B}(\sigma(A))$ *when* $\sigma(A)$ *has the induced topology*. In view of Theorem 3.40, part (b) in particular, we will indifferently use the notations

$$f(A) := \int_{\sigma(A)} f(\lambda) dP^{(A)}(\lambda) := \int_{\mathbb{R}} g(\lambda) dP^{(A)}(\lambda) =: g(A) . \quad (3.34)$$

where $g : \mathbb{R} \to \mathbb{C}$ is the extension of f to zero outside $\sigma(A)$, or any other measurable function equal to f on $\text{supp}(P^{(A)}) = \sigma(A)$. Obviously $g(A) = g'(A)$ if $g, g' : \mathbb{R} \to \mathbb{C}$ coincide on $\text{supp}(P^{(A)}) = \sigma(A)$. ■

Example 3.43

(1) Consider the m-axis position operator X_m on $L^2(\mathbb{R}^n, d^n x)$ introduced in Example 2.59 (1). We know that $\sigma(X_m) = \sigma_c(X_m) = \mathbb{R}$ from Example 3.14. We are interested in the PVM $P^{(X_m)}$ of X_m defined on $\mathbb{R} = \sigma(X_m)$. Let us fix $m = 1$, for the other cases are analogous. The PVM associated to X_1 is

$$(P_E^{(X_1)} \psi)(x) = \chi_{E \times \mathbb{R}^{n-1}}(x) \psi(x) \quad \psi \in L^2(\mathbb{R}^n, d^n x) , \quad (3.35)$$

where $E \in \mathscr{B}(\mathbb{R})$ is a subset of the first factor of $\mathbb{R} \times \mathbb{R}^{n-1} = \mathbb{R}^n$. Indeed, indicating by $P\psi$ the right-hand side of (3.35), one easily verifies that $\Delta_{x_1} = D(X_1)$. Furthermore, approximating the function $\mathbb{R}^n \ni x \mapsto x_1 \in \mathbb{R}$ with simple maps,[1]

$$\int_{\mathbb{R}^n} x_1 |\psi(x)|^2 d^n x = \int_{\mathbb{R}} x_1 \mu_{\psi,\psi}^{(P)}(x_1) = \int_{\mathbb{R}} \lambda \mu_{\psi,\psi}^{(P)}(\lambda) \quad \forall \psi \in D(X_1) = \Delta_{x_1}$$

where $\mu_{\psi,\psi}^{(P)}(E) = \langle \psi | P_E \psi \rangle = \int_{E \times \mathbb{R}^{n-1}} |\psi(x)|^2 d^n x$. Since the left-hand side is nothing but $\langle \psi | X_1 \psi \rangle$, Corollary 3.27 (b) confirms (3.35) holds.

(2) Take the m-axis momentum operator P_m on $L^2(\mathbb{R}^n, d^n x)$, introduced in Example 2.59(2). Taking (2.23) into account, where $\hat{\mathscr{F}}$ (and thus $\hat{\mathscr{F}}^*$) is unitary, by Proposition 3.60 (i) the PVM of P_m is

$$Q_E^{(P_m)} := \hat{\mathscr{F}}^* P_E^{(K_m)} \hat{\mathscr{F}} .$$

The operator K_m is X_m represented in $L^2(\mathbb{R}^n, d^n k)$, see Example 2.59 (1).

(3) By a similar argument the PVM of the operator $H = \overline{H_0}$ relative to the *harmonic oscillator* of Example (2.59) (4) is, for $E \in \mathscr{B}(\mathbb{R})$,

$$P_E = \sum_{\lambda \in E \cap \hbar\omega(\mathbb{N}+1/2)} \langle \psi_\lambda | \cdot \rangle \psi_\lambda$$

[1] More generally: $\int_{\mathbb{R}} \int_{\mathbb{R}^{n-1}} g(x_1) |\psi(x)|^2 dx d^{n-1} x = \int_{\mathbb{R}} g(x_1) d\mu_{\psi,\psi}^{(P)}(x_1)$ is patently valid for simple functions. It extends to arbitrary measurable functions, provided both sides make sense, in view of, for instance, Lebesgue's dominated convergence theorem for positive measures.

where

$$H = \sum_{\lambda \in \hbar\omega(\mathbb{N}+1/2)} \lambda \langle \psi_\lambda | \cdot \rangle \psi_\lambda = \sum_{n \in \mathbb{N}} \hbar\omega(n+1/2) \langle \psi_n | \cdot \rangle \psi_n \, . \tag{3.36}$$

has domain

$$D(H) = \left\{ \psi \in L^2(\mathbb{R}, dx) \;\middle|\; \sum_{n=0}^{+\infty} (n+1/2)^2 |\langle \psi_n | \psi \rangle|^2 < +\infty \right\} .$$

Indeed, since $\{\psi_n\}_{n\in\mathbb{N}}$ is a Hilbert basis of $L^2(\mathbb{R}, dx)$, the right-hand side of (3.36) is selfadjoint as integral of the (real) function $\iota : \mathbb{R} \ni \lambda \mapsto \lambda \in \mathbb{R}$ of the said PVM (notice that $D(H) = \Delta_\iota$). Therefore the right-hand side of (3.36) is a selfadjoint extension of the H_0 in Example (2.59) (4), which is essentially selfadjoint, so $H = \overline{H_0}$. We will show that the *spectrum of the Hamiltonian H of the harmonic oscillator* is

$$\sigma(H) = \sigma_p(H) = \{\hbar\omega(n+1/2) \mid n = 0, 1, \ldots\} .$$

Evidently $\sigma(H)$ contains the closed set of eigenvalues $\hbar\omega(n+1/2)$. We claim it cannot contain any point λ other than these numbers. Indeed, suppose that there is a further λ in $\sigma_p(H)$, so that $P^{(H)}_{\{\lambda\}} \neq 0$. If $x \in P^{(H)}_{\{\lambda\}}(\mathsf{H})$, we would have $\langle x|\psi_n\rangle = \langle P^{(H)}_{\{\lambda\}} x | P^{(H)}_{\{\hbar\omega(n+1/2)\}} \psi_n \rangle = \langle x | P^{(H)}_{\{\lambda\}\cap\{\hbar\omega(n+1/2)\}} \psi_n \rangle = \langle x | P^{(H)}_{\varnothing} \psi_n \rangle = 0$. Therefore x must vanish because it is orthogonal to a Hilbert basis, and $P^{(H)}_{\{\lambda\}} = 0$ contrarily to the hypothesis. There only remains the possibility that $\lambda \in \sigma_c(H)$. Since $\{\hbar\omega(n+1/2) \mid n = 0, 1, \ldots\}$ is closed and λ does not belong to that set, it cannot be an accumulation point. We can therefore find $\delta > 0$ such that $(\lambda - \delta, \lambda + \delta) \cap \{\hbar\omega(n+1/2) \mid n = 0, 1, \ldots\} = \varnothing$. With the same argument as before we can prove that $x \in P^{(H)}_{(\lambda-\delta,\lambda+\delta)}(\mathsf{H})$ forces $x = 0$, and thus $P^{(H)}_{(\lambda-\delta,\lambda+\delta)} = 0$. This violates Theorem 3.40 (d), so we conclude that $\sigma(H) = \sigma_p(H) = \{\hbar\omega(n+1/2) \mid n = 0, 1, \ldots\}$.

(4) An argument similar to that of (2) and (3) applies to the symmetric *momentum operator in a box P'*, introduced in Example (2.59) (5). The selfadjoint extensions P_α, $\alpha \in [0, 2\pi)$ of P' are

$$P_\alpha = \sum_{n\in\mathbb{Z}} (\alpha + 2n\pi) \langle u_{\alpha,n} | \cdot \rangle \, u_{\alpha,n} \; ,$$

so in particular

$$\sigma(P_\alpha) = \sigma_p(P_\alpha) = \{\alpha + 2\pi n \mid n \in \mathbb{Z}\} .$$

Replacing α with $\alpha + 2k\pi$, $k \in \mathbb{Z}$, leaves P_α invariant since it merely relabels the same eigenvectors coherently with their eigenvalues.

(5) In general it is *false* that if a selfadjoint operator A admits a Hilbert basis of eigenvectors then its spectrum only contains eigenvalues. Since $\sigma(A)$ is closed, but $\sigma_p(A)$ is not always closed, points of $\sigma_p(A)$ might accumulate in the continuous spectrum.

Using the Hilbert basis $\{\psi_n\}_{n\in\mathbb{N}}$ of the previous example, consider the selfadjoint bounded operator

$$A = \sum_{\lambda\in\mathbb{Q}\cap[0,1]} \lambda\langle\psi_{n_\lambda}|\cdot\rangle\psi_{n_\lambda} : L^2(\mathbb{R}, dx) \to L^2(\mathbb{R}, dx)$$

where $\mathbb{Q} \cap [0, 1] \ni q \mapsto n_q \in \mathbb{N}$ a bijection. We may define A equivalently as

$$A = \int_{\mathbb{R}} \lambda dP(\lambda)$$

where, for every $E \in \mathscr{B}(\mathbb{R})$,

$$P_E = \sum_{\lambda\in E\cap\mathbb{Q}\cap[0,1]} \lambda\langle\psi_{n_\lambda}|\cdot\rangle\psi_{n_\lambda} .$$

The operator A is evidently bounded and it is easy to prove that $||A|| = 1$. The domain of A is therefore the whole $L^2(\mathbb{R}, dx) = \Delta_\iota$. By the same argument of the previous example, $\mathbb{Q} \cap [0, 1] = \sigma_p(A)$ because $\{\psi_n\}_{n\in\mathbb{N}}$ is a Hilbert basis of $L^2(\mathbb{R}, dx)$. As $\sigma_p(A) \subset \sigma(A) = \overline{\sigma(A)}$, we have $\overline{\mathbb{Q} \cap [0, 1]} = [0, 1] = \overline{\sigma_p(A)} \subset \sigma(A)$. It is easy to prove from (3.37) that $\sigma(A) \subset [0, 1]$ because $||A|| = 1$. We conclude that $\sigma(A) = [0, 1]$ and $[0, 1] \setminus \mathbb{Q}$ must lie in $\sigma_c(A)$.

(6) More complicated situations exist. Consider an operator of *Schrödinger form*

$$H := \frac{1}{2m}\sum_{k=1}^{n} P_k^2 + U(x) = -\frac{1}{2m}\Delta + U(x)$$

where Δ is the Laplacian on $\mathbb{R}^n$, P_k is the momentum operator on $L^2(\mathbb{R}^k, d^kx)$ associated to the k-th coordinate, $m > 0$ is a constant and U is a real-valued function on $\mathbb{R}$ acting as multiplication operator. Suppose $U = U_1 + U_2$ where $U_1 \in L^2(\mathbb{R}^k, d^kx)$ and $U_2 \in L^\infty(\mathbb{R}^k, d^kx)$, $k = 1, 2, 3$, are real-valued and $D(H) = C^\infty(\mathbb{R})$. Then H turns out to be (trivially) symmetric but also essentially selfadjoint [ReSi80, Mor18] as a consequence of a well-known result (the *Kato–Rellich theorem*). The unique selfadjoint extension $\overline{H} = (H^*)^*$ of H physically represents the Hamiltonian operator of a quantum particle living in $\mathbb{R}^n$ with potential energy described by U. (This in particular applies to the Hamiltonian of an electron with attractive *Coulomb potential*: this is proportional to $-1/||x||$ in $\mathbb{R}^3$ and decomposes as a sum of functions exactly as above.) In general $\sigma(\overline{H})$ has both point and continuous parts. If P_λ denotes the orthogonal projector onto the λ-eigenspace of $\overline{H}$, then $\int_{\sigma_p(\overline{H})} \lambda dP^{(\overline{H})}(\lambda)$ takes this form

$$\int_{\sigma_p(\overline{H})} \lambda dP^{(\overline{H})}(\lambda) = \sum_{\lambda \in \sigma_p(\overline{H})} \lambda P_\lambda^{(\overline{H})} .$$

On the contrary, $\int_{\sigma_c(\overline{H})} \lambda dP^{(\overline{H})}(\lambda)$ has a much more complicated expression. Under a unitary transformation, $\int_{\sigma_c(\overline{H})} \lambda dP^{(\overline{H})}(\lambda)$ decomposes spectrally in analogy to the position operator X, which acts by multiplication on $L^2(\mathbb{R}, dx)$; the difference is that now several copies of L^2-spaces may appear. If $\mathsf{H}_p := P^{(\overline{H})}_{\sigma_p(\overline{H})}(\mathsf{H})$ is the closed subspace spanned by the eigenspaces of $\overline{H}$ and $\mathsf{H}_c := P^{(\overline{H})}_{\sigma_c(\overline{H})}(\mathsf{H})$, we have an *orthogonal* decomposition $\mathsf{H} = \mathsf{H}_c \oplus \mathsf{H}_p$. The operator $H_p := \int_{\sigma_p(\overline{H})} \lambda dP^{(\overline{H})}(\lambda)$ leaves invariant the subspace

$$D(H_p) := \left\{ \psi \in H_p \;\middle|\; \sum_{E \in \sigma_p(\overline{H})} E^2 ||P_E^{(\overline{H})} \psi||^2 < +\infty \right\} ,$$

whereas $H_c := \int_{\sigma_c(\overline{H})} \lambda dP^{(\overline{H})}(\lambda)$ fixes

$$D(H_c) := \left\{ \psi \in H_p \;\middle|\; \int_{\sigma_c(\overline{H})} E^2 d\mu_{\psi,\psi}^{P^{(\overline{H})}}(E) < +\infty \right\} .$$

In this sense, $\overline{H} = H_c \oplus H_p$. A possible situation (not the only one) is that H_c is isomorphic to a direct sum $\oplus_{n=1}^N L^2(\sigma_c(\overline{H}), dE)$, and $H_c : (\psi_1, \dots, \psi_N) \mapsto (\imath \cdot \psi_1, \dots, \imath \cdot \psi_N)$ acts as a multiple of the identity in each slot: $(\imath \cdot \psi_k)(E) := E\psi_k(E)$. ■

Definition 3.44 Selfadjoint operators admitting a Hilbert basis of eigenvectors are said to have a **pure point spectrum**. ■

Remark 3.45 Having a pure point spectrum does *not* automatically mean that $\sigma_p(A) = \sigma(A)$, as illustrated in example (4) above. However it implies that $\sigma_c(A)$ cannot have interior points (this is forbidden by Theorem 3.40 (d)). ■

3.3.2 Some Technically Relevant Consequences of the Spectral Theorem

The spectral theorem has repercussions pointing in several directions. We shall mention just a few which have a relevant impact on quantum theory. The first result concerns the positivity of selfadjoint operators.

Proposition 3.46 *If A is a selfadjoint operator on the Hilbert space H, A is positive, that is $\langle x|Ax\rangle \geq 0$ for every $x \in D(A)$ (also written $A \geq 0$) if and only if $\sigma(A) \subset [0, +\infty)$.*

Proof Suppose $\sigma(A) \subset [0, +\infty)$. If $x \in D(A)$ we have $\langle x|Ax\rangle = \int_{\sigma(A)} \lambda d\mu_{x,x} \geq 0$ by (3.12) (where μ stands for $\mu^{(P^{(A)})}$), since $\mu_{x,x}$ is a positive measure ad $\sigma(A) \in [0, +\infty)$.

Conversely, we shall prove that A is not positive if $\sigma(A)$ contains a $\lambda_0 < 0$. Using parts (c) and (d) of Theorem 3.40, one finds an interval $[a, b] \subset \sigma(A)$ with $[a, b] \subset (-\infty, 0)$ and $P^{(A)}_{[a,b]} \neq 0$ (possibly $a = b = \lambda_0$). If $x \in P^{(A)}_{[a,b]}(\mathsf{H})$ with $x \neq 0$, then $\mu_{xx}(E) = \langle x|P_E x\rangle = \langle x|P^*_{[a,b]} P_E x P_{[a,b]}\rangle = \langle x|P_{[a,b]} P_E P_{[a,b]} x\rangle = \langle x|P_{[a,b]\cap E} x\rangle = 0$ if $[a, b] \cap E = \varnothing$. Therefore, $\langle x|Ax\rangle = \int_{\sigma(A)} \lambda d\mu_{x,x} = \int_{[a,b]} \lambda d\mu_{x,x} \leq \int_{[a,b]} b\mu_{x,x} < b||x||^2 < 0$. □

Another remarkable result, about bounds on the extended spectrum, holds for normal operators as well, and is independent of the spectral theorem (it can be used to *prove* the spectral theorem, actually). We shall follow a much more elementary route in Proposition 3.80.

Proposition 3.47 *A selfadjoint operator is bounded (and its domain is the entire H) if and only if $\sigma(A)$ is bounded. In this case*

$$||A|| = \sup\{|\lambda| \mid \lambda \in \sigma(A)\} .$$

Proof From Proposition 3.10 we have that if $A \in \mathfrak{B}(\mathsf{H})$ then $||A|| \geq \sup\{|\lambda| \mid \lambda \in \sigma(A)\}$. If, conversely, $\sigma(A)$ is bounded and hence compact (it is closed), by restricting the integration domain to $X = \sigma(A)$ the continuous map $\iota : \sigma(A) \ni \lambda \to \lambda$ is bounded. Then (3.14) implies that $A = \int_{\sigma(A)} \iota dP^{(A)}$ is bounded and the following inequality holds

$$||Ax||^2 = \int_{\sigma(A)} |\lambda|^2 d\mu^{(P^{(A)})}_{xx}(\lambda) \leq (\sup\{|\lambda| \mid \lambda \in \sigma(A)\})^2 \int_{\sigma(A)} 1 d\mu^{(P^{(A)})}_{xx}(\lambda)$$

$$= (\sup\{|\lambda| \mid \lambda \in \sigma(A)\})^2 \, ||x||^2 .$$

Hence $||A|| \leq \sup\{|\lambda| \mid \lambda \in \sigma(A)\}$, so

$$||A|| = \sup\{|\lambda| \mid \lambda \in \sigma(A)\} . \tag{3.37}$$

In this case, furthermore, $D(A) = \Delta_\iota = \mathsf{H}$. □

Remark 3.48 Proposition 3.47 explains the reason why observables A in QM are very often represented by unbounded selfadjoint operators. The spectrum $\sigma(A)$ is the set of values of the observable A. When, as it frequently happens, an observable is allowed to take arbitrarily large values (think of X or P), it cannot be represented by a bounded selfadjoint operator simply because its spectrum is not bounded. ■

Concerning the covariance of a selfadjoint operator and its PVM under unitary transformations (or surjective linear isometries), another simple yet technically important result is the following.

Proposition 3.49 *Let $A : D(A) \to \mathsf{H}$ be a selfadjoint operator on the Hilbert space H and $U : \mathsf{H} \to \mathsf{H}'$ an isometric, surjective linear (or anti-linear) map. Then UAU^{-1}, with domain $D(UAU^{-1}) = U(D(A))$, is selfadjoint as well (Proposition 2.41 and the subsequent remark) and*

$$P_E^{(UAU^{-1})} = UP_E^{(A)}U^{-1} \quad \textit{for every } E \in \mathscr{B}(\mathbb{R}).$$

Proof If $x \in D(A)$,

$$\int_{\mathbb{R}} \iota \, d\mu_{xx}^{(P^{(A)})} = \langle x|Ax\rangle = \langle Ux|UAU^{-1}Ux\rangle = \int_{\mathbb{R}} \iota \, d\mu_{Ux,Ux}^{(P^{(UAU^{-1})})} = \int_{\mathbb{R}} \iota \, d\mu_{x,x}^{(U^{-1}P^{(UAU^{-1})}U)} .$$

In the last passage we used

$$\mu_{Ux,Ux}^{(P^{(UAU^{-1})})}(E) = \langle Ux|P_E^{(UAU^{-1})}Ux\rangle = \langle x|U^{-1}P_E^{(UAU^{-1})}Ux\rangle = \mu_{x,x}^{(U^{-1}P^{(UAU^{-1})}U)}(E) .$$

Applying Corollary 3.27 (b), we conclude that

$$A = \int_{\mathbb{R}} \iota \, d\, U^{-1}P^{(UAU^{-1})}U .$$

The uniqueness of the PVM of A implies

$$P_E^{(A)} = U^{-1}P_E^{(UAU^{-1})}U , \quad \text{if } E \in \mathscr{B}(\mathbb{R}),$$

which is the claim we wanted to prove. □

The notion of function of a selfadjoint operator (3.34) is just a generalization of the analogous (1.7) that was introduced for the finite-dimensional case, and may be used in QM applications. In finite dimensions the eigenvalue set of $f(A)$ is the image under f of the eigenvalue set of A: $\sigma(f(A)) = f(\sigma(A))$. But what about the infinite-dimensional case?

If $f : \mathbb{R} \to \mathbb{C}$ is Borel measurable (we could equivalently use an $f : \sigma(A) \to \mathbb{C}$ Borel measurable for $\mathscr{B}(\sigma(A))$) and $A : D(A) \to \mathsf{H}$ is selfadjoint, it is quite evident that

$$f(\sigma_p(A)) \subset \sigma_p(f(A)) \,. \tag{3.38}$$

In fact, if $\lambda \in \sigma_p(A)$ there is $x = P^{(A)}_{\{\lambda\}}x \neq 0$ by the spectral theorem. Therefore

$$\int_{\mathbb{R}} f dP^{(A)} x = \int_{\mathbb{R}} f dP^{(A)} P^{(A)}_{\{\lambda\}} x = \int_{\mathbb{R}} f dP^{(A)} \int_{\mathbb{R}} \chi_{\{\lambda\}} dP^{(A)} x = \int_{\mathbb{R}} f \cdot \chi_{\{\lambda\}} dP^{(A)} x$$

$$= \int_{\mathbb{R}} f(\lambda) \chi_{\{\lambda\}} dP^{(A)} x = f(\lambda) \int_{\mathbb{R}} \chi_{\{\lambda\}} dP^{(A)} x = f(\lambda) x \,,$$

hence $f(\lambda) \in \sigma_p(f(A))$. In the infinite-dimensional case there exist simple counterexamples disproving the converse inclusion $f(\sigma_p(A)) \supset \sigma_p(f(A))$. The simples instance is $\chi_E(A) = P^{(A)}_E$. This operator is an orthogonal projector and as such it only has point spectrum, given by a non-empty subset of $\{0, 1\}$, even in case $\sigma(A) = \sigma_c(A)$ so $\chi_E(\sigma_p(A)) = \varnothing$.

Pressing on, let us introduce a new notion to the purpose.

Definition 3.50 Let $P : \mathscr{B}(X) \to \mathscr{L}(\mathsf{H})$ be a PVM on a topological space X. If $f : X \to \mathbb{C}$ is measurable, we call P-**essential rank** the set

$$essrank(f) := \{z \in \mathbb{C} \mid P_{f^{-1}(O)} \neq 0 \quad \text{if } O \text{ is open and } O \ni z\} \,.$$

■

Since f is Borel measurable and O (open) belongs to $\mathscr{B}(\mathbb{C})$, $f^{-1}(O) \in \mathscr{B}(X)$ and therefore the essential rank is well defined. Here is an almost immediate consequence of the definition.

Proposition 3.51 *Let $P : \mathscr{B}(X) \to \mathscr{L}(\mathsf{H})$ be a PVM on a topological space X. If $f : X \to \mathbb{C}$ is measurable, then*

$$\sigma\left(\int_X f dP\right) = essrank(f) \,.$$

Proof If $z \notin essrank(f)$ there exists an open set $B \ni z$ in $\mathbb{C}$ with $P_{f^{-1}(B)} = 0$. If $B_r(z)$ is an open ball of radius r centred at z and contained in B, by additivity $P_{f^{-1}(B_r(z))} = 0$ (and $P_{f^{-1}(B \setminus B_r(z))} = 0$). The map $X \ni \lambda \mapsto g(\lambda) := \frac{1}{f(\lambda)-z}$ is therefore P-essentially bounded with $||g||^{(P)}_\infty \leq 1/r$, since $P_{\{\lambda \in X \,|\, |g(\lambda)| > 1/r\}} = 0$. Hence $\int_X \frac{1}{f(\lambda)-z} dP(\lambda) \in \mathfrak{B}(\mathsf{H})$ from Proposition 3.29 (a). In addition, by Propositions 3.33 (c) and 3.29 (a)

$$\int_X \frac{1}{f(\lambda)-z} dP(\lambda) \int_X (f(\lambda)-z) dP(\lambda) x = \int_X \frac{f(\lambda)-z}{f(\lambda)-z} dP(\lambda) x = x \quad \text{if } x \in D(\int_x f dP)$$

so that $z \in \rho\left(\int_X f dP\right)$, i.e. $z \notin \sigma\left(\int_X f dP\right)$.

If $z \in essrank(f)$, then $P_{f^{-1}(O)} \neq 0$ for every open set O containing z. This holds for every ball $B_{1/n}(z)$ of radius $1/n$, $n = 1, 2, \ldots$, centred at z. (In particular $f^{-1}(B_{1/2}(z)) \neq \varnothing$, otherwise $P_{f^{-1}(B_{1/2}(z))} = 0$.) We claim that if $R := (\int_X (f - zI) dP)^{-1}$ exists it cannot be bounded, and hence $z \in \sigma_c\left(\int_X f dP\right)$. Indeed, $||x|| = ||R \int_X (f - zI) dPx||$ would imply, taking $||x|| = 1$,

$$||R||^2 \geq \frac{1}{||\int_X (f - zI) dPx||^2} = \frac{1}{\int_X |f - zI|^2 d\mu^{(P)}_{xx}}$$
$$\geq \frac{1}{\sup_{f(\lambda) \in B_{1/n}(z)} |f(\lambda) - z|^2 \int_X 1 d\mu^{(P)}_{xx}} = n^2 ,$$

which is not bounded as $n = 1, 2, \ldots$. If $R := (\int_X (f - zI) dP)^{-1}$ is not defined, then $z \in \sigma_p\left(\int_X f dP\right)$. Since the residual spectrum is empty, as $\int_X (f - zI) dP$ is normal, we have established that $z \in essrank(f)$ implies $z \in \sigma\left(\int_X f dP\right)$, concluding the proof. □

Remark 3.52 A subtler argument [Rud91, Mor18] proves that $z \in essrank(f)$ belongs to $\sigma_p\left(\int_X f dP\right)$ if and only if $P_{f^{-1}(\{z\})} \neq 0$. ■

The relevant corollary of Proposition 3.51 and the spectral theorem is the following one.

Corollary 3.53 *Let A be a selfadjoint operator on the Hilbert space H and $f : \sigma(A) \to \mathbb{C}$ a continuous map. Then*

$$\sigma(f(A)) = \overline{f(\sigma(A))} . \tag{3.39}$$

The closure above is unnecessary if A is bounded.

Proof In view of Proposition 3.51 and Theorem 3.40, we just need to prove $essrank(f) = \overline{f(\text{supp}(P^{(A)}))}$. If $z = f(r)$ for some $r \in \text{supp}(P^{(A)})$ and $O \ni z$ is open, then $f^{-1}(O)$ is open since f is continuous and it contains r. Hence $P_{f^{-1}(O)} \neq 0$ by the very definition of support. This proves $essrank(f) \subset f(\text{supp}(P^{(A)}))$. As $essrank(f)$ is closed by definition (its complement is open), we have $essrank(f) = \overline{essrank(f)} \subset \overline{f(\text{supp}(P^{(A)}))}$. To conclude, suppose $z \in \overline{f(\text{supp}(P^{(A)}))}$. If $O \ni z$ is open, it must have non-empty intersection with $f(\text{supp}(P^{(A)})$. Hence $f^{-1}(O)$ is open, non-empty and $f^{-1}(O) \cap \text{supp}(P^{(A)}) \neq \varnothing$. From the definition of support, $P^{(A)}_{f^{-1}(O)} \neq 0$. By definition $z \in essrank(f)$. We established that $essrank(f) \supset \overline{f(\text{supp}(P^{(A)}))}$ and hence concluded the proof. Regarding the last statement, if A is bounded $\sigma(A)$ is compact by Proposition 3.11 (b). Since f is continuous, $f(\sigma(A))$ is compact, and closed because $\mathbb{C}$ is Hausdorff, so that $f(\sigma(A)) = \overline{f(\sigma(A))}$. □

Remark 3.54 It is fundamental to stress that in QM (3.39) permits us to adopt the standard operational approach to interpret the observable $f(A)$: it is the observable whose set of possible values is (the closure of) the set of real numbers $f(a)$ where a is a value of A. ■

A final result which will be useful later in many contexts is the following proposition.

Proposition 3.55 *If H is a Hilbert space and $B \in \mathfrak{B}(\mathsf{H})$, then B is a linear combination of unitary operators.*

Proof As we know, B can be written as complex linear combination of selfadjoint operators $B = \frac{1}{2}(B + B^*) + i\frac{1}{2i}(B - B^*)$, so it is sufficient to prove the claim for selfadjoint operators. Consider $A^* = A \in \mathfrak{B}(\mathsf{H})$. If $||A|| = 0$ the thesis is trivial, so we assume $||A|| > 0$. Then $A' := \frac{1}{||A||}A$ satisfies $||A'|| \leq 1$, so $\sigma(A') \subset [-1, 1]$ by Proposition 3.47. Moreover, $A'_\pm := A' \pm i\sqrt{I - A'^2} \in \mathfrak{B}(\mathsf{H})$ are well defined via spectral theory (integrating the corresponding functions on $\sigma(A')$). It is easy to prove that $A'_\pm$ are unitary, for Theorem 3.24 and Proposition 3.29 guarantee ${A'_\pm}^* A'_\pm = A'_\pm {A'_\pm}^* = I$. By construction, $A' = \frac{1}{2}A_+ + \frac{1}{2}A_-$. □

3.3.3 Joint Spectral Measures

The last spectral tool we need to introduce are *joint spectral measures* (see, e.g., [ReSi80, Mor18]). Everything is stated in the following theorem, whose proof is long and technical in most books. In Sect. 3.6 we shall present an original argument, which by character befits our presentation of the spectral machinery.

Theorem 3.56 (Joint Spectral Measure) *Let $\mathfrak{A} := \{A_1, A_2, \ldots, A_n\}$ be a set of selfadjoint operators on the Hilbert space H. Suppose that their spectral measures commute:*

$$P^{(A_k)}_{E_k} P^{(A_h)}_{E_h} = P^{(A_h)}_{E_h} P^{(A_k)}_{E_k} \quad \forall k, h \in \{1, \ldots, n\}, \forall E_k, E_h \in \mathscr{B}(\mathbb{R}) .$$

Then there exists a unique PVM $P^{(\mathfrak{A})}$ on $\mathbb{R}^n$ such that

$$P^{(\mathfrak{A})}_{E_1 \times \cdots \times E_n} = P^{(A_1)}_{E_1} \cdots P^{(A_n)}_{E_n} , \quad \forall E_1, \ldots, E_n \in \mathscr{B}(\mathbb{R}) .$$

For every $f : \mathbb{R} \to \mathbb{C}$ measurable,

$$\int_{\mathbb{R}^n} f(x_k) dP^{(\mathfrak{A})}(x) = f(A_k) , \quad k = 1, \ldots, n \tag{3.40}$$

where $x = (x_1, \ldots, x_k, \ldots, x_n)$ and $f(A_k) := \int_{\mathbb{R}} f(\lambda) dP^{(A_k)}$.

Finally, $B \in \mathfrak{B}(\mathsf{H})$ commutes with $P^{(\mathfrak{A})}$ if and only if it commutes with all $P^{(A_k)}$, $k = 1, 2, \ldots, n$.

Proof See Sect. 3.6. □

Definition 3.57 The PVM $P^{(\mathfrak{A})}$ in Theorem 3.56 is called the **joint spectral measure** of $A_1, A_2, \ldots, A_n$, and its support $\text{supp}(P^{(\mathfrak{A})})$, i.e. the complement in $\mathbb{R}^n$ of the largest open set O with $P_O^{(\mathfrak{A})} = 0$, is called the **joint spectrum** of $A_1, A_2, \ldots, A_n$. ■

Example 3.58 The simplest example is provided by considering the n position operators X_m on $L^2(\mathbb{R}^n, d^n x)$. It should be clear that the n spectral measures commute because the operator $P_E^{(X_k)}$, for $E \in \mathscr{B}(\mathbb{R})$, acts as multiplication by $\chi_{\mathbb{R}\times\cdots\times\mathbb{R}\times E\times\mathbb{R}\times\cdots\times\mathbb{R}}$, where E is in the k-th position. The joint spectrum of the n operators X_m coincides with $\mathbb{R}^n$ itself.

A completely analogous situation holds for the n momentum operators P_k, since they are related to the position operators by means of the unitary Fourier-Plancherel operator, as already seen several times. Again, the joint spectrum of the n operators P_m coincides with $\mathbb{R}^n$ itself. ■

Here is a useful fact proved by von Neumann (see [RiNa90] for a proof).

Theorem 3.59 *Let A, B be (possibly unbounded) selfadjoint operators on the Hilbert space H. If the spectral measures of A and B commute, then there is a third (possibly unbounded) selfadjoint operator C on H such that $A = f(C)$ and $B = g(C)$ for some Borel measurable functions $f, g : \mathbb{R} \to \mathbb{R}$.*

3.3.4 Measurable Functional Calculus

The following proposition provides useful features of $f(A)$, where A is selfadjoint and $f : \mathbb{R} \to \mathbb{C}$ is Borel measurable. These properties constitute the so-called *measurable functional calculus*. We suppose here that $A = A^*$, but statements can be reformulated for normal operators too [Mor18].

Proposition 3.60 *Let A be a selfadjoint operator on the complex Hilbert space H and let $f, g : \sigma(A) \to \mathbb{C}$ be measurable functions. Let af, $f \cdot g$, $f + g$ indicate the pointwise operations ($a \in \mathbb{C}$). The following facts hold.*

(a) *If $f(\lambda) = p_n(\lambda) := \sum_{k=0}^{n} a_k \lambda^k$ with $a_n \neq 0$, then*

$$p_n(A) = \sum_{k=0}^{n} a_k A^k \quad \text{with } D(p_n(A)) = \Delta_{p_n} = D(A^n),$$

where the right-hand side is defined on its standard domain, and $A^0 := I$, $A^1 := A$, $A^2 := AA$, and so forth.

(b) *If* $f = \chi_E$ *is the characteristic function of* $E \in \mathscr{B}(\sigma(A))$*, then*

$$f(A) = P^{(A)}(E) .$$

(c) *Using bar to denote complex conjugation,*

$$f(A)^* = \overline{f}(A) .$$

(d) *For* $a \in \mathbb{C}$*,*

$$af(A) = (af)(A) .$$

(e) $D(f(A) + g(A)) = \Delta_f \cap \Delta_g$ *and*

$$f(A) + g(A) \subset (f + g)(A) .$$

There is equality above if and only if $\Delta_{f+g} = \Delta_f \cap \Delta_g$*.*

(f) $D(f(A)g(A)) = \Delta_{f\cdot g} \cap \Delta_g$ *and*

$$f(A)g(A) \subset (f \cdot g)(A) ,$$

with equality if and only if $\Delta_{f\cdot g} \subset \Delta_g$*.*

(g) *We have* $D(f(A)^* f(A)) = \Delta_{|f|^2}$ *and*

$$f(A)^* f(A) = |f|^2(A) .$$

(h) *If* $f \geq 0$ *then*

$$\langle x|f(A)x\rangle \geq 0 \quad \textit{for } x \in \Delta_f .$$

(i) *If* $x \in \Delta_f$*,*

$$||f(A)x||^2 = \int_{\sigma(A)} |f(\lambda)|^2 d\mu_{xx}^{(P^{(A)})}(\lambda) .$$

In particular, if f *is bounded or* $P^{(A)}$*-essentially bounded on* $\sigma(A)$*,* $f(A) \in \mathfrak{B}(\mathsf{H})$ *and*

$$||f(A)|| \leq ||f||_\infty^{(P^{(A)})} \leq ||f||_\infty .$$

(j) *If* $U : \mathsf{H} \to \mathsf{H}'$ *is a linear (or anti-linear) surjective isometry, then*

$$Uf(A)U^{-1} = f(UAU^{-1})$$

and, in particular, $D(f(UAU^{-1})) = UD(f(A)) = U(\Delta_f)$.

(k) *If* $\phi : \mathbb{R} \to \mathbb{R}$ *is measurable, then* $\mathscr{B}(\mathbb{R}) \ni E \mapsto P'(E) := P^{(A)}(\phi^{-1}(E))$ *is a PVM on* $\mathbb{R}$. *Defining the selfadjoint operator*

$$A' = \int_{\mathbb{R}} \lambda' dP'(\lambda')$$

such that $P^{(A')} = P'$, *we have*

$$A' = \phi(A)$$

and

$$f(A') = (f \circ \phi)(A) \quad \textit{and} \quad \Delta'_f = \Delta_{f\circ\phi}$$

for every $f : \mathbb{R} \to \mathbb{C}$ *measurable.*

Proof Everything but (a), (b), (c) and (i) are trivial reformulations of the corresponding statements in Proposition 3.33. As a matter of fact, (b), (c), (h) and (i) are nothing but (3.22), (3.13), (a) in Corollary 3.27 and (3.14) respectively. Item (a) is easy to prove. Let us initially focus on the case $p_n(\lambda) = \lambda^n$. Observe that $A = \int_{\sigma(A)} \lambda dP^{(A)}\lambda = p_1(A)$. Let us prove claim for a given n knowing it is true for $n-1$: $A^n = AA^{n-1} = \int_{\mathbb{R}} \lambda dP^{(A)}(\lambda) \int_{\mathbb{R}} \lambda^{n-1} dP^{(A)}(\lambda) = \int_{\mathbb{R}} \lambda^n dP^{(A)}(\lambda) = p_n(A)$. In the penultimate equality we used Proposition 3.33 (c): the condition $\Delta_{f\cdot g} \subset \Delta_g$ is satisfied for $f = \iota$ and $g = \iota^{n-1}$ because the measure $\mu^{(P)}_{xx}$ is finite and hence $\int_{\mathbb{R}} |\lambda|^{2n} d\mu_{xx}(\lambda) < +\infty$ implies $\int_{\mathbb{R}} |\lambda|^{2(n-1)} d\mu_{xx}(\lambda) < +\infty$.

Let us pass to polynomials. For every polynomial $p_m(\lambda) = \sum_{k=0}^m a_k \lambda^k$ of degree m (i.e. $a_m \neq 0$) set $p_m(A) := \sum_{k=0}^m a_k A^k$. For $m = 0$ it is clear that $p_1(A) = \int a_0 dP^{(A)}(\lambda) = a_0 I$. Suppose inductively that $p_{n-1}(A) = \int_{\sigma(A)} p_{n-1}(\lambda) dP^{(A)}(\lambda)$. From Proposition 3.33 (b), if $a_n \neq 0$ then $a_n A^n + p_{n-1}(A) = \int_{\mathbb{R}} a_n \lambda^n + p_{n-1}(\lambda) dP^{(A)}(\lambda)$. This is because the condition $\Delta_{f+g} = \Delta_f \cap \Delta_g$ in Proposition 3.33 (b) is satisfied for $f = a_n \iota^n$ and $g = p_{n-1}$ since $\Delta_{a_n \iota^n + p_{n-1}} = \Delta_{\iota^n}$, again from the finiteness of $\mu^{(P)}_{xx}$. Putting everything together, we have $\sum_{k=0}^n a_k A^k = \int_{\sigma(A)} p(\lambda) d\lambda$ for every polynomial $p(\lambda) = \sum_{k=0}^n a_k \lambda^k$ of degree n. It is obvious that $D(p_n(A)) = D(A^n)$ (if $a_n \neq 0$) by the definition of standard domain. □

3.3.5 A First Glance at One-Parameter Groups of Unitary Operators

Let us start with an elementary result based on Proposition 3.60.

Proposition 3.61 *If $A : D(A) \to H$ is a selfadjoint operator on the Hilbert space* H*, then*

$$\mathbb{R} \ni t \mapsto U_t := e^{itA}$$

is a one-parameter group of unitary operators, i.e.

(i) U_t is unitary for $t \in \mathbb{R}$,
(ii) $U_0 = I$ and $U_t U_s = U_{t+s}$ for every $t, s \in \mathbb{R}$.

As a consequence of (i) and (ii), $U_t^* = (U_t)^{-1} = U_{-t}$ for $t \in \mathbb{R}$.

Proof $U_t = \int_{\mathbb{R}} e^{it\lambda} dP^{(A)}(\lambda)$ is an element of $\mathfrak{B}(\mathsf{H})$ because the function in the integral is bounded due to Proposition 3.60 (i). Then the conclusion follows immediately from (b), (c) and (f) in Proposition 3.60, since $e^{i0} = 1$, $e^{it\lambda}e^{is\lambda} = e^{i(t+s)\lambda}$ and $\overline{e^{it\lambda}} = e^{-it\lambda}$. □

We have a pair of important technical facts about the one-parameter group of unitary operators introduced above.

Proposition 3.62 *If $A : D(A) \to H$ is a selfadjoint operator on the Hilbert space* H*, the one-parameter group of unitary operators*

$$\mathbb{R} \ni t \mapsto U_t := e^{itA}$$

is **strongly continuous***, i.e. $U_t x \to U_s x$ if $t \to s$ for every fixed $x \in \mathsf{H}$. Furthermore*

$$U_t(D(A)) = D(A) \quad \textit{and} \quad U_t A = AU_t \quad \textit{for } t \in \mathbb{R}.$$

Proof Since U_u is isometric, $||U_t x - U_s x|| = ||U_s(U_{t-s}x - x)|| = ||U_{t-s}x - x||$. Therefore continuity at any $s \in \mathbb{R}$ is equivalent to continuity at 0. Next, Proposition 3.60 (i) entails that

$$||U_t x - x||^2 = \int_{\mathbb{R}} |e^{it\lambda} - 1|^2 d\mu_{xx}^{(P^{(A)})} \to 0 \quad \text{for } t \to 0,$$

where we used dominated convergence theorem and noticed that $\mu_{xx}^{(P^{(A)})}$ is finite and $|e^{it\lambda} - 1|^2 \leq 4$. Regarding the second statement, observe that

$$U_t P_E^{(A)} = \int_{\mathbb{R}} e^{it\lambda} dP^{(A)} \int_{\mathbb{R}} \chi_E dP^{(A)} = \int_{\mathbb{R}} \chi_E e^{it\lambda} dP^{(A)}$$
$$= \int_{\mathbb{R}} \chi_E dP^{(A)} \int_{\mathbb{R}} e^{it\lambda} dP^{(A)} = P_E^{(A)} U_t \ ,$$

by (i), (b) and (f) in Proposition 3.60. As a consequence, $\mu^{(P^{(A)})}_{U_t x, U_t x}(E) = ||P^{(A)}_E U_t x||^2 = ||U_t P^{(A)}_E x||^2 = ||P^{(A)}_E x||^2 = \mu^{(P^{(A)})}_{xx}(E)$. Therefore $\int_{\mathbb{R}} |\lambda|^2 d\mu^{(P^{(A)})}_{xx} = \int_{\mathbb{R}} |\lambda|^2 d\mu^{(P^{(A)})}_{U_t x, U_t x}$, meaning $U_t(D(A)) = D(A)$. Now Proposition 3.60 (f) proves that $U_t A = \int_{\mathbb{R}} e^{it\lambda} \lambda dP^{(A)} = AU_t$ if we write these operators in terms of integrals and observing that the condition on the domains necessary and sufficient to write $=$ in place of $\subset$ is here satisfied. □

Proposition 3.63 *If $A : D(A) \to H$ is a selfadjoint operator on the Hilbert space* H *and $x \in D(A)$, then*

$$-i \left.\frac{d}{dt}\right|_{t=s} e^{itA}x = e^{isA}Ax = Ae^{isA}x \,.$$

Proof Let us start with $s = 0$. Notice that if $x \in D(A)$, Proposition 3.60 (i) yields

$$\left|\left|\frac{1}{h}(e^{ihA}x - x) - iAx\right|\right|^2 = \int_{\mathbb{R}} \left|\frac{1}{h}(e^{ihr} - 1) - ir\right|^2 d\mu^{(P^{(A)})}_{xx}(r) \,. \quad (3.41)$$

The integrand tends to 0 pointwise as $h \to 0$. On the other hand the mean value theorem, applied to real and imaginary parts of the argument of the absolute value, says that

$$\left|\frac{1}{h}(e^{ihr} - 1) - ir\right|^2 = \left|-r\sin(h_0 r) + ir\cos(h'_0 r) - ir\right|^2$$
$$= \left|-\sin(h_0 r) + i\cos(h'_0 r) - i\right|^2 r^2 \leq 9r^2$$

for some $h_0, h'_0 \in [-|H|, |H|]$. The map $\mathbb{R} \ni r \mapsto r^2$ is $\mu^{(P^{(A)})}_{xx}$-integrable since $x \in D(A) = \Delta_{\iota^2}$. Finally, dominated convergence theorem proves that the limit of the left-hand side of (3.41) vanishes when $h \to 0$. This establishes the claim for $s = 0$. The case $s \neq 0$ can be proved by observing that

$$\left|\left|\frac{1}{h}(e^{i(s+h)A}x - e^{isA}x) - ie^{isA}Ax\right|\right|^2 = \left|\left|e^{isA}\left[\frac{1}{h}(e^{ihA}x - x) - iAx\right]\right|\right|^2$$
$$= \left|\left|\frac{1}{h}(e^{ihA}x - x) - iAx\right|\right|^2$$

and applying the previous proposition. □

Exercise 3.64 Prove that if $A \in \mathfrak{B}(H)$ is selfadjoint on the Hilbert space H, then

$$e^{itA} = \sum_{n=0}^{+\infty} \frac{(it)^n}{n!} A^n$$

for every $t \in \mathbb{R}$, where the series converges in operator norm.

Solution By Proposition 3.60 (i), using the fact that $e^{itA} - \sum_{n=0}^{N} \frac{(it)^n}{n!} A^n$ is bounded,

$$\left\| e^{itA} - \sum_{n=0}^{N} \frac{(it)^n}{n!} A^n \right\| = \left\| \int_{\sigma(A)} e^{itr} - \sum_{n=0}^{N} \frac{(it)^n}{n!} r^n \, dP^{(A)} \right\| \leq \sup_{r \in \sigma(A)} \left| e^{itr} - \sum_{n=0}^{N} \frac{(itr)^n}{n!} \right| .$$

For a fixed $t \in \mathbb{R}$, the limit as $N \to +\infty$ of the right-most term vanishes, proving the thesis. This is because the power series $e^z = \sum_{n=0}^{+\infty} \frac{z^n}{n!}$ has convergence radius $+\infty$, hence it converges uniformly in every closed disc centred at the origin with finite radius. Therefore the convergence is uniform on any compact set of $\mathbb{C}$. In particular on $\sigma(A)$, which is compact by Proposition 3.47) since A is bounded. □.

3.4 Elementary Quantum Formalism: A Rigorous Approach

We return to the discussion started in the introduction to show how, in practice, the physical hypotheses on quantum systems (1)–(3) must be interpreted mathematically on infinite-dimensional Hilbert spaces. (For convenience we reversed the order of (2) and (3).)

3.4.1 Elementary Formalism for the Infinite-Dimensional Case

Let us begin by listing the general assumptions for a mathematical description of quantum systems.

1. A quantum mechanical system S is always associated to a Hilbert space H, either finite- or infinite-dimensional;
2. observables are represented in terms of (generally unbounded) *selfadjoint* operators A on H,
3. states are equivalence classes

$$[\psi] = \{e^{i\alpha}\psi \mid \alpha \in \mathbb{R}\}$$

of *unit* vectors $\psi \in \mathsf{H}$ (the equivalence relation being $\psi \sim \psi'$ iff $\psi = e^{ia}\psi'$ for some $a \in \mathbb{R}$).

We set out to show how the above mathematical assumptions enable us to set the physical properties of quantum systems (1)–(3) of Sect. 1.1.2 in a mathematically nice form for infinite-dimensional Hilbert spaces H.

(1) Randomness The Borel subset $E \subset \sigma(A)$ represents the outcomes of measurement procedures of the observable associated with the selfadjoint operator A. (In case of continuous spectrum the outcome of a measurement is at least an interval in view of the experimental errors.) Given a state represented by the unit vector $\psi \in \mathsf{H}$, the probability to obtain outcome $E \subset \sigma(A)$ when measuring A is

$$\mu^{(P^{(A)})}_{\psi,\psi}(E) := ||P^{(A)}_E \psi||^2 , \tag{3.42}$$

where we have used the PVM $P^{(A)}$ of the operator A.

Pursuing this interpretation, the **expectation value** $\langle A\rangle_\psi$ of A, when the state is represented by the unit vector $\psi \in \mathsf{H}$, turns out to be

$$\langle A\rangle_\psi := \int_{\sigma(A)} \lambda \, d\mu^{(P^{(A)})}_{\psi,\psi}(\lambda) . \tag{3.43}$$

This relation makes sense provided $\iota : \sigma(A) \ni \lambda \to \lambda$ belongs to $L^1(\sigma(A), \mu^{(P^{(A)})}_{\psi,\psi})$ (which is equivalent to say that $\psi \in \Delta_{|\iota|^{1/2}}$ and, in turn, $\psi \in D(|A|^{1/2})$). Otherwise the expectation value is not defined. Since

$$L^2(\sigma(A), \mu^{(P^{(A)})}_{\psi,\psi}) \subset L^1(\sigma(A), \mu^{(P^{(A)})}_{\psi,\psi})$$

because $\mu^{(P^{(A)})}_{\psi,\psi}$ is finite, we have the popular formula, derived from (3.12):

$$\langle A\rangle_\psi = \langle\psi|A\psi\rangle \quad \text{if } \psi \in D(A) . \tag{3.44}$$

The associated **standard deviation** ΔA_ψ is

$$\Delta A_\psi := \sqrt{\int_{\sigma(A)} (\lambda - \langle A\rangle_\psi)^2 \, d\mu^{(P^{(A)})}_{\psi,\psi}(\lambda)} . \tag{3.45}$$

This definition makes sense provided $\iota \in L^2(\sigma(A), \mu^{(P^{(A)})}_{\psi,\psi})$ (i.e. $\psi \in \Delta_\iota$, or $\psi \in D(A)$).

As before, functional calculus permits us to write the other famed formula

$$\Delta A_\psi = \sqrt{\langle\psi|A^2\psi\rangle - \langle\psi|A\psi\rangle^2} \quad \text{if } \psi \in D(A^2) \subset D(A) . \tag{3.46}$$

We stress that the Heisenberg inequalities, established in Exercise 1.11(1), are now completely justified, as the reader can easily check.

(3) Collapse of the State If the Borel set $E \subset \sigma(A)$ is the outcome of an (idealized) measurement of A when the state is represented by the unit vector $\psi \in \mathsf{H}$, the new state immediately after the measurement is represented by the unit vector

$$\psi' := \frac{P^{(A)}_E \psi}{||P^{(A)}_E \psi||} . \tag{3.47}$$

Remark 3.65 Lo and behold this formula does not make sense if $\mu^{(P^{(A)})}_{\psi,\psi}(E) = 0$. Moreover the arbitrary phase affecting ψ does not really matter due to the linearity of $P^{(A)}_E$. ■

(2) Compatible and Incompatible Observables Two observables A, B are compatible—i.e. they can be measured simultaneously—if and only if their **spectral measures commute**, which means

$$P^{(A)}_E P^{(B)}_F = P^{(B)}_F P^{(A)}_E , \quad E \in \mathscr{B}(\sigma(A)) , \quad F \in \mathscr{B}(\sigma(B)) . \tag{3.48}$$

In this case

$$||P^{(A)}_E P^{(B)}_F \psi||^2 = ||P^{(B)}_F P^{(A)}_E \psi||^2 = ||P^{(A,B)}_{E\times F} \psi||^2 ,$$

where $P^{(A,B)}$ is the joint spectral measure of A and B, has the natural interpretation of the probability to obtain outcomes E and F for a simultaneous measurement of A and B. If instead A and B are incompatible, it may happen that

$$||P^{(A)}_E P^{(B)}_F \psi||^2 \neq ||P^{(B)}_F P^{(A)}_E \psi||^2 .$$

Sticking to A, B incompatible, (3.47) gives

$$||P^{(A)}_E P^{(B)}_F \psi||^2 = \left|\left| P^{(A)}_E \frac{P^{(B)}_F \psi}{||P^{(B)}_F \psi||} \right|\right|^2 ||P^{(B)}_F \psi||^2 . \tag{3.49}$$

The meaning is *the probability of obtaining first F and then E in subsequent measurements of B and A*.

Remark 3.66 It is worth stressing that the notion of probability we are using here cannot be the classical one, because of the presence of incompatible observables. The theory of conditional probability cannot follow the standard rules. The probability $\mathbb{P}_\psi(E_A|F_B)$, that (in a state defined by a unit vector ψ) a certain observable A takes value E_A when the observable B has value F_B, cannot be computed by the standard procedure

$$\mathbb{P}_\psi(E_A|F_B) = \frac{\mathbb{P}_\psi(E_A \text{ AND } F_B)}{\mathbb{P}_\psi(F_B)}$$

if A and B are incompatible: in general, there is nothing which can be interpreted as the event "E_A AND F_B" if $P^{(A)}_E$ and $P^{(B)}_F$ do not commute! The correct formula is

$$\mathbb{P}_\psi(E_A|F_B) = \frac{\langle\psi|P^{(B)}_F P^{(A)}_E P^{(B)}_F \psi\rangle}{||P^{(B)}_F \psi||^2} ,$$

which leads to well-known properties that depart from the classical theory, the so-called combination of "probability amplitudes" in particular. As a matter of fact, to the day we still do not have a clear notion of (quantum) probability. This issue will be clarified in the next chapter. ■

3.4.2 Commuting Spectral Measures

The reason to pass from operators to their spectral measures to define compatible observables is that, if A ad B are selfadjoint and defined on distinct domains, $AB = BA$ does not make sense in general. Moreover, there are counterexamples (due to Nelson) where the commutativity of selfadjoint operators A and B on a common dense invariant subspace, which is a core for A and B, does not imply that their spectral measures commute. Nevertheless, general results again due to Nelson give us the following nice result, which we shall prove later (see Exercise 7.43).

Proposition 3.67 *If selfadjoint operators A and B on a Hilbert space H commute on a common dense invariant domain D where $A^2 + B^2$ is essentially selfadjoint, then the spectral measures of A and B commute.*

Definition 3.68 When the spectral measures of two selfadjoint operators A, B commute, i.e., (3.48) holds, one says that A and B **commute strongly**. ■

In addition to the aforementioned direct result by Nelson, there are several other technical facts providing necessary and sufficient conditions for the commutativity of the spectral measures of pairs of selfadjoint operators. The most elementary and perhaps useful is the following one.

Proposition 3.69 *Let A, B be selfadjoint operators on the complex Hilbert space H. The following facts are equivalent:*

(i) A and B strongly commute,
(ii) $e^{itA}e^{isB} = e^{isB}e^{itA}$ for every $s, t \in \mathbb{R}$,
(iii) $e^{itA}P^{(B)}_E = P^{(B)}_E e^{itA}$ for every $t \in \mathbb{R}$ and $E \in \mathscr{B}(\mathbb{R})$,
(iv) $e^{itA}B \subset Be^{itA}$ for all $t \in \mathbb{R}$, or equivalently $e^{itA}B = Be^{itA}$ for all $t \in \mathbb{R}$.

Under any of the above statements: $e^{itA}(D(B)) = D(B)$ for all $t \in \mathbb{R}$.

Proof Evidently (i) implies (ii) since $\int_{\mathbb{R}} s\,dP^{(A)} \int_{\mathbb{R}} t\,dP^{(B)} = \int_{\mathbb{R}} t\,dP^{(B)} \int_{\mathbb{R}} s\,dP^{(A)}$ if s and t are complex simple functions, due to (3.24); the result extends to the exponentials by Proposition (3.29) (c) with suitable sequences of bounded simple functions tending to the exponential functions. Let us prove that (ii) implies (iii). From (ii) and for $x, y \in \mathsf{H}$, we have $\langle x|e^{-itA}e^{isB}e^{itA}y\rangle = \langle x|e^{isB}y\rangle$, which may be rephrased as

$$\int_{\mathbb{R}} e^{isr} d\mu^{(P^{(B)})}_{U_t x, U_t y}(r) = \int_{\mathbb{R}} e^{isr} d\mu^{(P^{(B)})}_{xy}(r) ,$$

where $U_t := e^{itA}$. If $f \in \mathscr{S}(\mathbb{R})$, since both $\mu^{(P^{(B)})}_{xy}$ and $\mu^{(P^{(B)})}_{U_t x, U_t y}$ are complex measures (so their absolute variations are finite measures) we have

$$\int_{\mathbb{R}} |f(s)| \int_{\mathbb{R}} |e^{isr}| d|\mu^{(P^{(B)})}_{U_t x, U_t y}|(r) ds < +\infty, \quad \int_{\mathbb{R}} |f(s)| \int_{\mathbb{R}} |e^{isr}| d|\mu^{(P^{(B)})}_{x,y}|(r) ds < +\infty.$$

The very definition of integral in a complex measure and the Fubini-Tonelli theorem imply that

$$\int_{\mathbb{R}} \left(\int_{\mathbb{R}} f(s) e^{isr} ds \right) d\mu^{(P^{(B)})}_{U_t x, U_t y}(r) = \int_{\mathbb{R}} \left(\int_{\mathbb{R}} f(s) e^{isr} e^{isr} ds \right) d\mu^{(P^{(B)})}_{xy}(r) .$$

Since the Fourier transform is a bijection from $\mathscr{S}(\mathbb{R})$ onto $\mathscr{S}(\mathbb{R})$, the previous relation reads

$$\int_{\mathbb{R}} g(r) d\mu^{(P^{(B)})}_{U_t x, U_t y}(r) = \int_{\mathbb{R}} g(r) d\mu^{(P^{(B)})}_{xy}(r) , \tag{3.50}$$

for every $g \in \mathscr{S}(\mathbb{R})$. Using the Stone–Weierstrass theorem and a smoothing procedure, it is possible to prove that if f is a complex, continuous map with compact support in $\mathbb{R}$, say $\text{supp}(f) \in [-a, a]$, there exists a sequence of smooth functions f_n with compact support contained in $[-2a, 2a]$ (obtained by approximating truncated polynomials outside $[-2a, 2a]$, and then smoothing), such that $||f - f_n||_\infty \to 0$ when $n \to +\infty$. Since the measures in (3.50) are finite, this fact immediately implies that (3.50) holds also when g is continuous and compactly supported. Both Borel measures are regular because, being finite, open sets are countable unions of compact sets with finite measure [Rud86]. Riesz's theorem for positive (regular) Borel measures [Rud86] implies that $\mu^{(P^{(B)})}_{xy}(E) = \mu^{(P^{(B)})}_{U_t x, U_t y}(E)$ for every Borel set $E \in \mathscr{B}(\mathbb{R})$. In other words $\langle x|(U_t^* P^{(B)}_E U_t - P^{(B)}_E)y\rangle = 0$ for every $x, y \in \mathsf{H}$, which in turn means $U_t P^{(B)}_E = P^{(B)}_E U_t$, namely (iii). In order to prove that (iii) implies the measures $P^{(A)}$, $P^{(B)}$ commute, we proceed as above. Begin by observing that for $x, y \in \mathsf{H}$ we have $\langle x|e^{itA} P^{(B)}_E y\rangle = \langle x|P^{(B)}_E e^{itA} y\rangle$. The argument used earlier leads to $\mu^{(A)}_{P^{(B)}_E x, y}(F) = \mu^{(A)}_{x, P^{(B)}_E y}(F)$, namely $\langle x|P^{(B)}_E P^{(A)}_F y\rangle = \langle x|P^{(A)}_F P^{(B)}_E y\rangle$ for all $x, y \in \mathsf{H}$ and $E, F \in \mathscr{B}(\mathbb{R})$. This is equivalent to (i).

Finally, assuming $e^{itA} B \subset B e^{itA}$ for all $t \in \mathbb{R}$, applying e^{-itA} to the right of both sides and using the fact that t is arbitrary, proves $B e^{itA} \subset e^{itA} B$ for all $t \in \mathbb{R}$, so $e^{itA}B = Be^{itA}$ $t \in \mathbb{R}$. This fact is equivalent to $e^{itA}Be^{-itA} = B$. In turn, the latter is the same as saying that (iii) holds, $e^{itA}P^{(B)}_E e^{-itA} = P^{(B)}_E$ for all $t \in \mathbb{R}$ and $E \in \mathscr{B}(\mathbb{R})$, in view of Proposition 3.49. The last statement is immediate from the second assertion in (iv), by the fact that e^{itA} is bijective. □

With similar arguments one can proved straightforwardly the following proposition regarding a special case $A \in \mathfrak{B}(\mathsf{H})$.

Proposition 3.70 *Let A, B be selfadjoint operators on the complex Hilbert space H. If $A \in \mathfrak{B}(\mathsf{H})$ the following facts are equivalent:*

(i) A and B strongly commute,
(ii) $AB \subset BA$ (with equality if, additionally, $B \in \mathfrak{B}(\mathsf{H})$),
(iii) $Af(B) \subset f(B)A$ if $f : \sigma(B) \to \mathbb{R}$ is Borel measurable,
(iv) $P^{(B)}_E A = AP^{(B)}_E$ if $E \in \mathscr{B}(\sigma(B))$.

Proof (i) implies (iv) just using the definition of integral in a PVM that integrates the function ι with respect to $P^{(A)}$. Integrating again f with respect to $P^{(B)}$ we obtain (iii) from (iv): observe that $\mu^{(P^{(B)})}_{Ax,Ax}(E) \leq ||A||^2\mu^{(P^{(B)})}_{x,x}(E)$ (since $P^{(B)}$ and A commute), so $Ax \in D(f(B))$ if $x \in D(f(B))$. The special choice $f = \iota$ produces (ii) from (iii). Finally (ii) implies $A^nB \subset BA^n$ and also, by Exercise 3.64 and because our B is closed as selfadjoint, we have $e^{itA}B \subset Be^{itA}$ for every $t \in \mathbb{R}$. Proposition 3.69 now gives (i). □

Another useful result directed toward the converse statement is the following.

Proposition 3.71 *Let A, B be selfadjoint operators on the complex Hilbert space H whose spectral measures commute. Then*

(a) $ABx = BAx$ *if* $x \in D(AB) \cap D(BA)$.
(b) $\langle Ax|By\rangle = \langle Bx|Ay\rangle$ *if* $x, y \in D(A) \cap D(B)$.

Proof

(a) Take $y \in D(B)$ and $x \in D(AB)$. Since $e^{itB}e^{isA} = e^{isA}e^{itB}$, we have $\langle e^{-itB}y|e^{isA}x\rangle = \langle y|e^{isA}e^{itB}x\rangle$. Computing the t-derivative at $t = 0$ with Proposition 3.63 and using the continuity of e^{isA}, we obtain $\langle By|e^{isA}x\rangle = \langle y|e^{isA}Bx\rangle$. By the definition of adjoint we have $e^{isA}x \in D(B^*) = D(B)$ and $e^{isA}Bx = B^*e^{isA}x = Be^{isA}x$. Assuming $x \in D(BA)$ and exploiting Proposition 3.63 once more, we can finally differentiate $e^{isA}Bx = Be^{isA}x$ in s and evaluate at $s = 0$, using the fact that B is closed. This produces $ABx = BAx$.
(b) It suffices to differentiate $\langle e^{-itB}y|e^{isA}x\rangle = \langle e^{-isA}y|e^{itB}x\rangle$ and use Proposition 3.63.

□

3.4.3 A First Look at the Time Evolution of Quantum States

We have already mentioned that for quantum systems in an inertial frame subject to *temporal homogeneity*, the *time evolution of states* is described in terms of a strongly continuous one-parameter group of unitary operators of the form $U_t := e^{-\frac{it}{\hbar}H}$, $t \in \mathbb{R}$, where the selfadjoint operator H is called the **Hamiltonian operator** of the quantum system (it depends on the reference frame). The observable H has the physical meaning of the *energy of the quantum system* in the frame of reference considered. If a quantum state is represented at time $t = 0$ by the unit vector $\psi \in \mathsf{H}$, where H is the Hilbert space of the system, the evolved state ψ_t at a generic time instant t is therefore

$$\psi_t = U_t\psi \; . \tag{3.51}$$

We shall not discuss here the motivations of this description of time evolution, but only make a few observations.

Remark 3.72

(a) If we represent the state ψ at $t = 0$ by another vector $\psi' := e^{i\alpha}\psi$, the evolved state is represented, coherently, by $\psi'_t = U_t\psi' = e^{i\alpha}U_t\psi$ in view of linearity of U_t. This ensures that the description of time evolution is phase-independent as expected: it preserves equivalence classes

$$[\psi] = \{e^{i\alpha}\psi \mid \alpha \in \mathbb{R}\}$$

of unit vectors, i.e. states. As a consequence, *we can define an action of time evolution on states unambiguously*: $U_t[\psi] := [U_t\psi]$.

(b) Since U_t is isometric, the unit normalization of ψ_t is preserved by time evolution, in agreement with the interpretation of the measures $\mu^{(P^{(A)})}_{\psi_t,\psi_t}$, whereby $\mu^{(P^{(A)})}_{\psi_t,\psi_t}(\mathbb{R}) = 1$ (they are probability measures). ■

According to Propositions 3.62 and 3.63, *if* $\psi \in D(H)$, from (3.51) we have

$$\frac{d}{dt}\psi_t = \frac{d}{dt}e^{-i\frac{t}{\hbar}H}\psi = -i\frac{1}{\hbar}He^{-i\frac{t}{\hbar}H}\psi = -i\frac{1}{\hbar}H\psi_t \; .$$

We have thus recovered the celebrated **Schrödinger equation**:

$$i\hbar\frac{d\psi_t}{dt} = H\psi_t \; . \tag{3.52}$$

It is worth stressing that the correct topology to calculate the derivative is the topology of the Hilbert space. In other words, the Schrödinger equation is *not* a standard PDE in the simplest situation in standard QM, namely $\mathsf{H} = L^2(\mathbb{R}^3, d^3x)$:

there

$$H := \overline{H_0} \quad \text{and} \quad H_0 = -\frac{\hbar^2}{2m}\Delta + V$$

for some real function $V : \mathbb{R}^n \to \mathbb{R}$, and H_0 is defined on a suitable dense linear domain $D(H_0) \subset \mathsf{H}$ of smooth functions, where furthermore it is essentially selfadjoint. Nevertheless, it is possible to prove that under suitable hypotheses jointly regular solutions $\psi : \mathbb{R} \times \mathbb{R}^3 \to \mathbb{C}$ of the PDE interpretation of (3.52),

$$i\hbar\frac{\partial\psi(t,x)}{\partial t} + \frac{\hbar^2}{2m}\Delta_x\psi(t,x) - V(x)\psi(t,x) = 0$$

define proper solutions of (3.52).

A very particular class of physically interesting solutions are the so-called **stationary states** of a given Hamiltonian operator H. They are defined when $\sigma_p(H) \neq \varnothing$. If $E \in \sigma_p(H)$ and $\psi_E \in D(H)$ is a corresponding eigenstate, so that $H\psi_E = E\psi_E$, its time evolution is trivial

$$e^{-i\frac{t}{\hbar}H}\psi_E = e^{-i\frac{t}{\hbar}E}\psi_E \ .$$

The quantum state $[\psi_E]$ associated to ψ_E is a *stationary state* with energy E. Notice that this state is *fixed* under time evolution, since states are (normalized) vectors *up to phase*, and $e^{-i\frac{t}{\hbar}E}$ is such.

Consider a non-relativistic spinless particle described on $\mathsf{H} = L^2(\mathbb{R}^3, d^3x)$, where the position operators along the Cartesian axes of the inertial reference frame are the multiplication operators X_j of Example 2.59. For a stationary state $\psi_E \in L^2(\mathbb{R}^3, dx)$ the probability density $|\psi_{Et}(x)|^2 = |\psi_E(x)|^2$ of finding the particle at $x \in \mathbb{R}^3$ is constant. For example, look at the electron in the hydrogen atom (with mass m and electrical charge e, and assuming the proton is located at the origin and generates the Coulomb force as a geometric point of the matter). Stationary states with energy levels corresponding to the spectrum of the Coulomb Hamiltonian $\overline{H_0}$, where

$$H_0 := -\frac{\hbar^2}{2m}\Delta - \frac{e^2}{||x||} : \mathscr{S}(\mathbb{R}^3) \to L^2(\mathbb{R}^3, d^3x) \ ,$$

define the *orbitals* of the atom.

Remark 3.73 Roughly speaking stationary states are stable states of matter, and all relatively stable structures of physical objects are described in terms of stationary quantum states of the Hamiltonian operator of the system. These states may cease to be stable when the Hamiltonian changes because of interactions with some external quantum system. For instance, the stationary states of the electron of the hydrogen atom are stationary as soon as the system is kept isolated. When interacting with other systems (especially photons), these states become non-stationary because they are not represented by eigenvectors of the complete Hamiltonian operator of the overall system. Even in an isolated hydrogen atom the proton should be treated quantistically, and the complete system is made of a pair of quantum particles described on an overall Hilbert space $L^2(\mathbb{R}^3_e \times \mathbb{R}^3_p, d^3x_e \otimes d^3x_p)$. Usually the motion of the proton is neglected and is treated classically. This is because its mass is around 2000 times that of the electron, and in many applications where one is essentially interested in the motion of the electron, it may as well be considered as a fixed classical particle. ■

Example 3.74 Let us consider a *free* spinless particle of mass $m > 0$. In orthonormal Cartesian coordinates of an inertial reference frame, its Hilbert space is $L^2(\mathbb{R}^3, d^3x)$. This explicit representation of the Hilbert space of a non-relativistic particle, where the position operators are multiplication operators, is called **position picture** (or position representation). The Hamiltonian operator H is the unique selfadjoint extension of the essentially selfadjoint operator

$$H_0 := \frac{1}{2m}\sum_{k=1}^{3} P_k^2 : \mathscr{S}(\mathbb{R}^3) \to L^2(\mathbb{R}^3, d^3x) .$$

It is evident that it includes only the *kinetic part* of the energy. In this sense the particle is *free*. Now, it is easier to represent the Hilbert space as an L^2 space where the momentum operators are described by multiplication operators. As we know from the content of Example 2.59 (2) (use Eq. (2.24) in particular), this realisation of the Hilbert space is related to the position representation by means of the Fourier-Plancherel operator

$$\hat{\mathscr{F}} : L^2(\mathbb{R}^3, d^3x) \ni \psi \mapsto \widehat{\psi} \in L^2(\mathbb{R}^3, d^3k) .$$

This Hilbert space isomorphism reduces to the standard integral Fourier transform on $\mathscr{S}(\mathbb{R}^3)$, and transforms this subspace into itself bijectively (changing the variable of the functions from x to k). The representation $L^2(\mathbb{R}^3, d^3k)$ of the Hilbert space, where momenta are multiplication operators, is popularly known as the **momentum picture** (or momentum representation). The corresponding Hamiltonian operator $H = \overline{H_0}$ is represented by the selfadjoint operator

$$H' := \hat{\mathscr{F}} H \hat{\mathscr{F}}^{-1} .$$

Since it is the square of the momentum operator up to the constant factor $(2m)^{-1}$, it must act as

$$\left(H'\widehat{\psi}\right)(k) = \frac{k^2}{2m}\widehat{\psi}(k) \tag{3.53}$$

where $k^2 := \sum_{j=1}^3 k_j^2$, and

$$D(H') := \left\{ \widehat{\psi} \in L^2(\mathbb{R}^3, d^3k) \;\middle|\; k^2\widehat{\psi} \in L^2(\mathbb{R}^3, d^3k) \right\} .$$

The spectrum of H is continuous and it is not difficult to prove that $\sigma(H) = \sigma_c(H) = [0, +\infty)$ as a byproduct of (3.53). This is expected from physical considerations, since the energy is purely kinetic.

Time evolution has a direct representation here:

$$\left(e^{-itH'}\widehat{\psi}\right)(k) := e^{-it\frac{k^2}{2m}}\widehat{\psi}(k) . \tag{3.54}$$

Notice that the right-hand side belongs to $\mathscr{S}(\mathbb{R}^3)$ at every time t if it does at $t = 0$.

Time evolution has a corresponding representation in the space $L^2(\mathbb{R}^3, d^3x)$, obtained through the action of the Fourier-Plancherel isomorphism

$$e^{-itH} = \hat{\mathscr{F}}^{-1} e^{-itH'} \hat{\mathscr{F}} .$$

If $\psi \in \mathscr{S}(\mathbb{R}^3)$, we can use the standard integral Fourier transform

$$\widehat{\psi}(k) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{-ikx}\psi(x)d^3x \quad \text{and} \quad \psi(x) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{ikx}\widehat{\psi}(k)d^3k . \tag{3.55}$$

Composing these transformations with (3.54) we find

$$\left(e^{-itH}\psi\right)(x) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{i(kx - \frac{k^2t}{2m})}\widehat{\psi}(k)d^3k \quad \text{for } \psi \in \mathscr{S}(\mathbb{R}^3) .$$

Note in particular that the time evolution leaves fixed the space $\mathscr{S}(\mathbb{R}^3)$. ■

3.4.4 A First Look at (Continuous) Symmetries and Conserved Quantities

As we shall discuss better later, physical operations changing the states of a given quantum system are pictured in terms of either *unitary* or *anti-unitary* transformations $U : \mathsf{H} \to \mathsf{H}$, called (quantum) symmetries.

Symmetries U transform vectors $\psi \mapsto \psi_U := U\psi$ but preserve norms (U is isometric by hypothesis) and *do not depend on the phase* ($e^{i\alpha}\psi$ maps to $e^{i\alpha}\psi_U$). We may therefore pass to the quotient, to the effect that *the action of a symmetry is well defined on equivalence classes of vectors, i.e., on pure states*: $U[\psi] := [U\psi]$.

A particular subclass of symmetries are **continuous symmetries**. These are strongly continuous one-parameter groups of *unitary* operators $\{e^{isA}\}_{s\in\mathbb{R}}$ generated by some selfadjoint operator $A : D(A) \to \mathsf{H}$. This A is interpreted as an observable somehow related to the continuous symmetry, and is called the **generator** of the symmetry.

When a continuous symmetry *commutes* with time evolution, i.e. (always assuming $\hbar = 1$)

$$e^{isB}e^{-itH} = e^{-itH}e^{isB} \quad \text{for all } t, s \in \mathbb{R}\,, \tag{3.56}$$

the symmetry is said to be a **dynamical symmetry**. This feature has a fundamental consequence. The generator B becomes a **constant of motion**, in the sense that all statistical properties of the outcomes of measurements of B on a given state $\psi \in \mathsf{H}$ turn out to be *independent of the time evolution* of ψ. Applying Proposition 3.69, if $E \in \mathscr{B}(\mathbb{R})$ the probability that the outcome of measuring B at time t belongs to E is

$$\mu^{P^{(B)}}_{U_t\psi,U_t\psi}(E) = ||P^{(B)}_E U_t\psi_t||^2 = ||U_t P^{(B)}_E \psi||^2 = ||P^{(B)}_E \psi||^2 = \mu^{P^{(B)}}_{\psi,\psi}(E)\,,$$

which coincides to the probability of obtaining E at time $t = 0$ when measuring B. The crucial passage above is the swap $P^{(B)}_E U_t = U_t P^{(B)}_E$, which is consequence of (3.56) and Proposition 3.69 for $A = H$.

Remark 3.75 If B is a constant of motion as defined above, the expectation value of B and its standard deviation are constant in time, just by definition of expectation value and standard deviation.

These two facts, albeit immediate from the definition of expectation value and standard deviation, are usually derived by physicists using Eqs. (3.44) and (3.45) (when the requirements on the domains are fulfilled) and Proposition 3.69:

$$\langle B\rangle_{\psi_t} = \langle U_t\psi|BU_t\psi\rangle = \langle\psi|U_t^*BU_t\psi\rangle = \langle\psi|BU_t^*U_t\psi\rangle = \langle\psi|B\psi\rangle = \langle B\rangle_\psi\,,$$

and

$$\Delta B_{\psi_t} = \langle U_t\psi|B^2U_t\psi\rangle - \langle B\rangle^2_{\psi_t} = \langle\psi|U_t^*B^2U_t\psi\rangle - \langle B\rangle^2_\psi = \langle\psi|B^2U_t^*U_t\psi\rangle - \langle B\rangle^2_\psi = \Delta B_\psi\,.$$

■

Example 3.76 Consider the momentum operator P_j along the j-th axis in $\mathbb{R}^3$. We want to examine the strongly continuous one-parameter group of unitary operators $V_a := e^{-iaP_j}$ with $a \in \mathbb{R}$. It is convenient to deal with the *momentum representation*. As we know, here P_j is nothing but the multiplication operator $\left(P'_j\widehat{\psi}\right)(k) = k_j\widehat{\psi}(k)$, for every $\psi \in L^2(\mathbb{R}^3, d^3k)$. As in Example 3.74, we adopt the notation $A' := \hat{\mathscr{F}}A\hat{\mathscr{F}}^{-1}$ to write down the momentum representation A' of operators given by A in position representation. It is easy to prove that

$$\left(V'_a\widehat{\psi}\right)(k) = e^{-ik_ja}\widehat{\psi} \quad \text{for every} \quad \psi \in L^2(\mathbb{R}^3, d^3k)\,.$$

Using (3.55), if $\psi \in \mathscr{S}(\mathbb{R}^3)$ then $\widehat{\psi} \in \mathscr{S}(\mathbb{R}^3)$ and *vice versa*, so

$$(V_a\psi)(x) = \frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3} e^{ikx}e^{-ik_ja}\widehat{\psi}(k)d^3k = \frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3} e^{ikx-k_ja}\widehat{\psi}(k)d^3k = \psi(x-ae_j)\,.$$

In other words, V_a shift wavefunctions in $\mathscr{S}(\mathbb{R}^3)$ along the coordinate unit vector e_j by the length a. Note that $\mathscr{S}(\mathbb{R}^3)$ is dense in $L^2(\mathbb{R}^3, d^3x)$ and V_a is continuous. Moreover, if $\mathscr{S}(\mathbb{R}^3) \ni \psi_n \to \psi \in L^2(\mathbb{R}^3, d^3x)$ as $n \to +\infty$, then $\mathscr{S}(\mathbb{R}^3) \ni \psi_n(\cdot - ae_j) \to \psi(\cdot - ae_j) \in L^2(\mathbb{R}^3, d^3x)$ as $n \to +\infty$ by the translational invariance of the Lebesgue measure d^3x. Summing up,

$$e^{-iaP_j}\psi = e^{-iaP_j}\lim_{n\to+\infty}\psi_n = \lim_{n\to+\infty}e^{-iaP_j}\psi_n = \lim_{n\to+\infty}\psi_n(\cdot - ae_j) = \psi(\cdot - ae_j)\,.$$

In other words,

$$\left(e^{-iaP_j}\psi\right)(x) = \psi(x-ae_j) \quad \text{for every} \quad \psi \in L^2(\mathbb{R}^3, d^3x)\,. \tag{3.57}$$

In the language of physicists, *the momentum along the j-th direction is the generator of physical spatial translations of the quantum system along the j-th axis*.

This is not the whole story if we also assume that the Hamiltonian of the particle is the free Hamiltonian (3.53) in momentum representation. If so, time evolution is represented by (3.54) again in momentum representation. It is therefore evident that

$$e^{-itH}e^{-iaP_j} = e^{-iaP_j}e^{-itH} \quad \text{for every } t, a \in \mathbb{R}.$$

We conclude that with the above free Hamiltonian *the momentum operator along the j-th direction is a constant of motion*. Therefore the statistical features of the measurements of P_j are invariant along the temporal evolution of the state of the system. ■

3.5 Round-Up of Operator Topologies

There are at least 7 to 9 relevant topologies [KaRi97, BrRo02] in Quantum Theory which enter the game when one discusses sequences of operators. We shall limit ourselves to illustrate quickly a few of the most important ones [Mor18]. We shall work in a Hilbert space H, even though some of our examples adapt to more general ambient spaces.

(a) The finest (strongest) topology of all is the **uniform operator topology** on $\mathfrak{B}(\mathsf{H})$. It is the Hausdorff topology induced by the operator norm $|| \; ||$ defined in (2.8).

As a consequence of the definition, a sequence of elements $A_n \in \mathfrak{B}(\mathsf{H})$ is said to converge **uniformly** to $A \in \mathfrak{B}(\mathsf{H})$ when $||A_n - A|| \to 0$ as $n \to +\infty$.

We already know that $\mathfrak{B}(\mathsf{H})$ is a Banach algebra for that norm, and a unital C^*-algebra too.

(b) Take a subspace $D \subset \mathsf{H}$ and the complex vector space $\mathfrak{L}(D; \mathsf{H})$ of operators $A : D \to \mathsf{H}$. The **strong operator topology** on $\mathfrak{L}(D; \mathsf{H})$ is the Hausdorff topology **induced by the seminorms** p_x where $x \in D$ and $p_x(A) := ||Ax||$ for $A \in \mathfrak{L}(D; \mathsf{H})$. By definition of *topology induced by a family of seminorms*, the open sets are the empty set and (arbitrary) unions of intersections of a finite number n of open balls $B^{(x_1,\ldots,x_n)}_{r_1,\ldots,r_n}(A_0)$ associated to the seminorms p_{x_i} with $x_i \in D$ distinct, of arbitrary finite radii $r_i > 0$ and common fixed centre $A_0 \in \mathfrak{L}(D; \mathsf{H})$:

$$B^{(x_1,\ldots,x_n)}_{r_1,\ldots,r_n}(A_0) := \{A \in \mathfrak{L}(D; \mathsf{H}) \mid p_{x_i}(A - A_0) \leq r_i \;, i = 1, \ldots, n\} \,.$$

Therefore a sequence of elements $A_n \in \mathfrak{L}(D; \mathsf{H})$ converges **strongly** to $A \in \mathfrak{L}(D; \mathsf{H})$ when $||(A_n - A)x|| \to 0$ as $n \to +\infty$ for every $x \in D$.

It should be evident that, if we restrict ourselves to work in $\mathfrak{B}(\mathsf{H})$, the uniform operator topology is finer (larger) than the strong operator topology.

(c) The **weak operator topology** on $\mathfrak{L}(D; \mathsf{H})$ is the Hausdorff topology induced by the seminorms $p_{x,y}$ with $x \in \mathsf{H}$, $y \in D$ and $p_{x,y}(A) := |\langle x|Ay\rangle|$ if $A \in \mathfrak{L}(D; \mathsf{H})$. In other words, its open sets are the empty set and (arbitrary) unions of intersections of a finite number n of open balls $B^{(x_1,y_1,\ldots,x_n,y_n)}_{r_1,\ldots,r_n}(A_0)$ associated to the seminorms p_{x_i,y_i} with $x_i \in \mathsf{H}$ and $y_i \in D$ distinct, of arbitrary finite radii $r_i > 0$ and a common fixed centre $A_0 \in \mathfrak{L}(D; \mathsf{H})$:

$$B^{(x_1,y_1,\ldots,x_n,y_n)}_{r_1,\ldots,r_n}(A_0) := \{A \in \mathfrak{L}(D; \mathsf{H}) \mid p_{x_i,y_i}(A - A_0) \leq r_i \;, i = 1, \ldots, n\} \,.$$

A sequence of elements $A_n \in \mathfrak{L}(D; \mathsf{H})$ is said to converge **weakly** to $A \in \mathfrak{L}(D; \mathsf{H})$ when $|\langle x|(A_n - A)y\rangle|| \to 0$ as $n \to +\infty$ for every $x \in \mathsf{H}$ and $y \in D$. The weak operator topology lies at the opposite end to the uniform operator topology, for it is the coarsest (smallest) of all.

We present two more intermediate topologies which depend on the space $\mathfrak{B}_1(\mathsf{H})$ of trace-class operators we will discuss later.

(d) The **ultrastrong topology** (also known as **σ-strong topology**) on $\mathfrak{B}(\mathsf{H})$ is the Hausdorff topology associated as above to seminorms p_T, with $T \in \mathfrak{B}_1(\mathsf{H})$ and $T \geq 0$, where $p_T(A) := \sqrt{tr(TA^*A)}$ if $A \in \mathfrak{B}(\mathsf{H})$. In spite of the name, it is weaker than the uniform operator topology.

(e) The **ultraweak topology** (or **σ-weak topology**) on $\mathfrak{B}(\mathsf{H})$ is the Hausdorff topology induced as above by seminorms q_T, $T \in \mathfrak{B}_1(\mathsf{H})$, defined as $q_T(A) := |\sqrt{tr(TA)}|$ if $A \in \mathfrak{B}(\mathsf{H})$. It is finer than the weak operator topology.

The topological dual of $\mathfrak{B}(\mathsf{H})$ possesses a special topology of its own.

(f) Any normed space $\mathfrak{B}(\mathsf{H})$ induces a significant weak topology on its **topological dual**

$$\mathfrak{B}(\mathsf{H})^* := \{f : \mathfrak{B}(\mathsf{H}) \to \mathbb{C} \mid f \text{ linear and continuous}\} .$$

The ***-weak topology** on $\mathfrak{B}(\mathsf{H})^*$ is associated as above to the family of seminorms $\{p_A\}_{A\in\mathfrak{B}(\mathsf{H})}$ defined as $p_A(f) := |f(A)|$ for every $f \in \mathfrak{B}(\mathsf{H})'$. The definition is general, and valid for normed spaces $\mathfrak{B}$ and their duals $\mathfrak{B}^*$ (replacing $\mathfrak{B}(\mathsf{H})$ and $\mathfrak{B}(\mathsf{H})^*$). The *Hahn–Banach theorem* says that the *-weak topology is Hausdorff because the functionals in $\mathfrak{B}'$ separate the elements of $\mathfrak{B}$. Notice that $\mathfrak{B}'$ is also a normed Banach space for the standard operator norm

$$||f|| = \sup_{0\neq A\in\mathfrak{B}} \frac{|f(A)|}{||A||_{\mathfrak{B}}} .$$

This topology is stronger than the *-weak one. The relevance of the *-weak topology is due in particular to the **Banach–Alaoglu theorem**, whereby the closed unit ball in $\mathfrak{B}(\mathsf{H})^*$ is compact in the *-weak topology.

Example 3.77

(1) If $f : \mathbb{R} \to \mathbb{C}$ is Borel measurable, and A a selfadjoint operator on H, consider the sets

$$R_n := \{r \in \mathbb{R} \mid |f(r)| < n\} \quad \text{for } n \in \mathbb{N} .$$

It is clear that $\chi_{R_n} f \to f$ pointwise as $n \to +\infty$ and $|\chi_{R_n} f|^2 \leq |f|^2$. As a consequence, if we restrict to Δ_f the operators appearing below on the left,

$$\left.\int_{\sigma(A)} \chi_{R_n} f dP^{(A)}\right|_{\Delta_f} \to f(A) \quad \text{strongly, as } n \to +\infty,$$

as an immediate consequence of Lebesgue's dominated convergence theorem and the first part of Proposition 3.60 (i). (See also exercise 3.36.)

(2) If in the previous example f is bounded on $\sigma(A)$, and $f_n \to f$ uniformly on $\sigma(A)$ (or $||f - f_n||_\infty^{(P^{(A)})} \to 0$ P-essentially uniformly), then

$$f_n(A) \to f(A) \quad \text{uniformly, as } n \to +\infty,$$

again by the second part of Proposition 3.60 (i). ■

Exercise 3.78 Prove that a selfadjoint operator A on the Hilbert H admits a dense set of analytic vectors in its domain.

Solution Consider the family of functions $f_n = \chi_{[-n,n]}$ where $n \in \mathbb{N}$. As in Example 3.77 (1), we have $\psi_n := f_n(A)\psi = \int_{[-n,n]} 1 dP^{(A)}\psi \to \int_{\mathbb{R}} 1 dP^{(A)}\psi = P^{(A)}_{\mathbb{R}}\psi = \psi$ when $n \to +\infty$. Therefore the set $D := \{\psi_n \mid \psi \in \mathsf{H}, n \in \mathbb{N}\}$ is dense in H. The elements of D are analytic vectors for A as we go on to prove. Clearly $\psi_n \in D(A^k)$ since $\mu^{(P^{(A)})}_{\psi_n,\psi_n}(E) = \mu^{(P^{(A)})}_{\psi,\psi}(E \cap [-n,n])$ by definition of $\mu^{(P^{(A)})}_{x,y}$. Therefore $\int_{\mathbb{R}} |\lambda^k|^2 d\mu^{(P^{(A)})}_{\psi_n,\psi_n}(\lambda) = \int_{[-n,n]} |\lambda|^{2k} d\mu^{(P^{(A)})}_{\psi,\psi}(\lambda) \leq \int_{[-n,n]} |n|^{2k} d\mu^{(P^{(A)})}_{\psi,\psi}(\lambda) \leq |n|^{2k} \int_{\mathbb{R}} d\mu^{(P^{(A)})}_{\psi,\psi}(\lambda) = |n|^{2k}||\psi||^2 < +\infty$. Similarly $||A^k\psi_n||^2 = \langle A^k\psi_n|A^k\psi_n\rangle = \langle \psi_n|A^{2k}\psi_n\rangle = \int_{\mathbb{R}} \lambda^{2k} d\mu^{(P^{(A)})}_{\psi_n,\psi_n}(\lambda) \leq |n|^{2k}||\psi||^2$. We conclude that $\sum_{k=0}^{+\infty} \frac{(it)^k}{k!}||A^k\psi_n||$ converges for every $t \in \mathbb{C}$ because it is dominated by $\sum_{k=0}^{+\infty} \frac{|t|^k}{k!}|n|^{2k}||\psi||^2 = e^{|t|\,|n|^2}||\psi||^2$. ■

3.6 Existence Theorems of Spectral Measures

This final section is devoted to proving the existence of a PVM $P^{(A)} : \mathscr{B}(\mathbb{R}) \to \mathscr{L}(\mathsf{H})$ for a selfadjoint operator $A : D(A) \to \mathsf{H}$ on a Hilbert space H, which was announced in Theorem 3.40 (a). The remaining statements of that theorem have been already established. As an intermediate result we shall demonstrate the spectral theorem for *normal operators* on $\mathfrak{B}(\mathsf{H})$. We will furnish a proof of Theorem 3.56 on joint spectral measures.

3.6.1 Continuous Functional Calculus

Let us start by establishing general properties of the spectral theory of bounded operators and unital C^*-algebras.

Proposition 3.79 *Take $A \in \mathfrak{B}(\mathsf{H})$ for some Hilbert space H and let $p : \mathbb{C} \to \mathbb{C}$ be a complex polynomial of fixed degree $n = 0, 1, \ldots$. Then*

$$\sigma(p(A)) = p(\sigma(A)) , \tag{3.58}$$

where $p(A)$ is understood as in Proposition 3.60 (a). Furthermore

$$\sigma(A^*) = \{\overline{\lambda} \mid \lambda \in \sigma(A)\} .$$

All this holds also if we replace $A \in \mathfrak{B}(\mathsf{H})$ by $a \in \mathfrak{A}$, where $\mathfrak{A}$ is any unital C^*-algebra.

Proof We use explicitly Proposition 3.7: *for any $A \in \mathfrak{B}(\mathsf{H})$, $\lambda \in \sigma(A)$ iff $A - \lambda I : \mathsf{H} \to \mathsf{H}$ is bijective.*

First of all we factor polynomials irreducibly with help of the fundamental theorem of algebra: $p(z) = c(z-\lambda_1)^{n_1}\cdots(z-\lambda_k)^{n_r}$, where the complex roots $\lambda_1,\ldots,\lambda_r$ have multiplicity $n_1,\ldots,n_r > 0$, $\sum_l n_k = n$ and $c \neq 0$. A corresponding decomposition holds for $p(A) = c(A-\lambda_1 I)^{n_1}\cdots(A-\lambda_k I)^{n_k}$. Define $\mu := p(\lambda)$. As the polynomial $\mathbb{C} \ni z \mapsto p'(z) := p(z)-\mu$ has a zero at $z=\lambda$, its factorization contains the term $(z-\lambda)$, whence $p(A)-\mu I$ has $(A-\lambda I)$ as a factor. If $\lambda \in \sigma(A)$, the operator $(A-\lambda I)$ is not bijective and therefore $p'(A) := p(A)-\mu I$ (factored as $(A-\lambda'_k I)^{n'_k}$) cannot be a bijection from H to H: indeed, if $(A-\lambda I)$ is not injective, we can swap it over to the end in the product $p'(A)$ (factors commute), whence $p'(A)$ cannot be injective. If $(A-\lambda I)$ is not surjective, we can move it in front of $p'(A)$ (as first factor), so $p'(A)$ cannot be surjective. All in all, $\lambda \in \sigma(A)$ implies $\mu = p(\lambda) \in \sigma(p(A))$, i.e. $p(\sigma(A)) \subset \sigma(p(A))$. Let us prove the opposite inclusion. Suppose $\mu \in \sigma(p(A))$. We know that $p(z)-\mu = c(z-\alpha_1)^{n'_1}\cdots(z-\alpha_{k'})^{n'_{r'}}$. If all $\alpha_{k'}$ belonged to $\rho(A)$, the operator $p(A) : \mathsf{H} \to \mathsf{H}$ would be bijective with left and right inverse $c^{-1}(A-\alpha_1 I)^{-n'_1}\cdots(A-\alpha_{k'} I)^{-n'_{r'}}$, an absurd. So at least one of the $\alpha_{k'}$ must belong to $\sigma(A)$, and $p(\alpha_{k'})-\mu = 0$. In other words $\mu \in p(\sigma(A))$, which proves $\sigma(p(A)) \subset p(\sigma(A))$.

The second statement is quite obvious by observing that if $T \in \mathfrak{B}(\mathsf{H})$, then T^* is bijective if and only if T is (Exercise 2.29). In this case $(T^*)^{-1} = (T^{-1})^*$. Applying this to $A-\lambda I$ proves the claim. With obvious modifications the argument still holds when $\mathfrak{B}(\mathsf{H})$ is replaced by a unital C^*-algebra $\mathfrak{A}$. □

We pass now to an important consequence, whose proof holds for any unital C^*-algebra in place of $\mathfrak{B}(\mathsf{H})$. The first assertion extends Proposition 3.47 and proves that it is actually independent of the spectral theorem.

Proposition 3.80 *If $A \in \mathfrak{B}(\mathsf{H})$ is normal ($A^*A = AA^*$) then*

$$\sup\{|\lambda| \mid \lambda \in \sigma(A)\} = ||A|| . \tag{3.59}$$

If $A = A^*$ and $p : \mathbb{R} \to \mathbb{C}$ is a polynomial, then

$$||p(A)|| = ||p\restriction_{\sigma(A)}||_\infty . \tag{3.60}$$

The results are valid also by replacing A with a in a unital C^*-algebra $\mathfrak{A}$.

Proof Let us prove (3.59). We need a preliminary, and quite interesting, lemma.

Lemma 3.81 (Gelfand's Formula for the Spectral Radius) *If $A \in \mathfrak{B}(\mathsf{H})$ for some Hilbert space H, then*

$$\sup\{|\lambda| \mid \lambda \in \sigma(A)\} = \lim_{n\to+\infty} ||A^n||^{1/n} . \tag{3.61}$$

The formula is valid for elements $a \in \mathfrak{A}$ in a unital C^*-algebra as well.

Proof Define $r_A := \sup\{|\lambda| \mid \lambda \in \sigma(A)\}$. If $|\lambda| > r_A$, then the resolvent $R_\lambda(A)$ is well defined. The Banach-space-valued map $\rho(A) \ni \lambda \mapsto R_\lambda(A)$ is holomorphic, and its Taylor expansion reads

$$R_\lambda(A) = -\sum_{n=0}^{+\infty} \zeta^{n+1} T^n$$

where $\zeta = 1/\lambda$. It converges at least for $|\zeta| < 1/||A||$ (Proposition 3.10). The renowned Hadamard theorem (very easily generalizable to holomorphic maps with values in Banach spaces) guarantees that the convergence radius is determined by the first singularity, which necessarily belongs to $\sigma(A)$. The series $-\sum_{n=0}^{+\infty} \zeta^{n+1} T^n$ therefore converges for $|\zeta| < 1/r_A$ and has convergence radius $R \geq 1/r_A$. Hadamard's formula for R then reads

$$1/R = \limsup_n ||T^n||^{1/n} \leq r_A \, .$$

On the other hand (3.58) implies $\sigma(A^n) = \{\mu^n \mid \mu \in \sigma(A)\}$, so by Proposition 3.10 we have

$$r_A^n = r_{A^n} \leq ||A^n||$$

and hence $r_A \leq \liminf_n ||A^n||^{1/n}$. In summary $r_A \leq \liminf_n ||A^n||^{1/n} \leq \limsup_n ||A^n||^{1/n} = r_A$, which is what we claimed. □

Let us take up the proof of Proposition 3.80 and suppose $A = A^*$. Then $||A^2|| = ||A^*A|| = ||A||^2$ and, similarly, $||(A^2)^2|| = ||A^2||^2 = ||A||^4$, $||(A^4)^2|| = ||A^4||^2 = ||A||^8$ and so on. In general $||A^{2^n}|| = ||A||^{2^n}$. Applying (3.61), we find

$$\sup\{|\lambda| \mid \lambda \in \sigma(A)\} = \lim_{n\to+\infty} ||A^n||^{1/n} = \lim_{n\to+\infty} ||A^{2^n}||^{1/2^n} = \lim_{n\to+\infty} ||A||^{2^n/2^n} = ||A|| \, .$$

Now consider $A \in \mathfrak{B}(\mathsf{H})$, so $||A^n|| = ||(A^n)^* A^n||^{1/2} = ||(A^*)^n A^n||^{1/2}$. If A is normal, all operators commute and $||A^n|| = ||(A^*A)^n||^{1/2}$. Since A^*A is selfadjoint, we can implement the result above:

$$\sup\{|\lambda| \mid \lambda \in \sigma(A)\} = \lim_{n\to+\infty} ||A^n||^{1/n} = \lim_{n\to+\infty} ||(A^*A)^n||^{1/(2n)} = \left(\lim_{n\to+\infty} ||(A^*A)^n||^{1/n}\right)^{1/2}$$

$$= ||A^*A||^{1/2} = ||A|| \, .$$

At last, let us prove (3.60). Since A is selfadjoint, $p(A)$ is normal. Therefore

$$||p(A)|| = \sup\{|\lambda| \mid \lambda \in \sigma(p(A))\} = \sup\{|\lambda| \mid \lambda \in p(\sigma(A))\} = ||p\restriction_\sigma (A)||_\infty \, ,$$

where we exploited (3.58) in the last passage. □

The utmost consequence of these propositions is the following theorem, which establishes the existence and continuity of the so-called *continuous functional calculus for bounded selfadjoint operators*. The theorem holds as it stands for unital C^*-algebras.

Theorem 3.82 *Let $A \in \mathfrak{B}(\mathsf{H})$ be a selfadjoint operator on the Hilbert space H. There exists a unique representation of unital *-algebras (Definition 2.27), called* **continuous functional calculus***,*

$$\Psi : C(\sigma(A)) \ni f \to f(A) \in \mathfrak{B}(\mathsf{H})$$

that is continuous (with respect to $||\cdot||_\infty$ on the domain and the operator norm on the codomain) and such that $\Psi(\iota) = A$ (where $\iota : \sigma(A) \ni x \mapsto x \in \mathbb{R}$). Furthermore

(a) *Ψ is isometric and hence injective,*
(b) *$B \in \mathfrak{B}(\mathsf{H})$ commutes with every $f(A)$ if B commutes with A.*

The theorem holds replacing $\mathfrak{B}(\mathsf{H})$ by a unital C^*-algebra $\mathfrak{A}$ and A by a selfadjoint element $a \in \mathfrak{A}$.

Proof If $f \in C(\sigma(A))$, there exist complex polynomials $p_n \to f$ uniformly on $\sigma(A)$ as $n \to +\infty$ by the Stone–Weierstrass theorem. Define $f(A) := \lim_{n\to+\infty} p_n(A)$. Due to (3.60), the sequence $p_n(A)$ is Cauchy. Hence there is a limit element in $\mathfrak{B}(\mathsf{H})$ because this space is complete (Theorem 2.20). It is evident that the limit point does not depend on the sequence, since a different sequence would satisfy $||p'_n(A) - p_n(A)|| = ||p'_n \restriction_{\sigma(A)} - p_n \restriction_{\sigma(A)} ||_\infty \to 0$. The map $f \mapsto f(A)$ is evidently isometric. Next observe that, if we only consider polynomials, $f \mapsto f(A)$ is linear, it preserves the product, and $\overline{f} \mapsto f(A)^*$. These features are preserved under the limiting process when $f \in C(\sigma(A))$ is a general map. By construction $f(1) = I$ and $f(\iota) = A$. If B commutes with A, it commutes with all polynomials $p(A)$. Hence

$$Bf(A) = B \lim_{n\to+\infty} p_n(A) = \lim_{n\to+\infty} Bp_n(A) = \lim_{n\to+\infty} p_n(A)B = f(A)B\,.$$

To conclude, we prove that a continuous representation of unital *-algebras $\Phi : C(\sigma(A)) \to \mathfrak{B}(\mathsf{H})$ coincides with Ψ if we impose $\Phi(\iota) = A$. In fact, $\Psi(\iota) = \Phi(\iota) = A$ and $\Psi(1) = \Phi(1) = I$, therefore $\Psi(p) = \Phi(p)$ for every polynomial p. By continuity, if $p_n \to f$ as $n \to +\infty$ in the norm $||\cdot||_\infty$ on $\sigma(A)$, we have $\Psi(f) = \Phi(f)$. All arguments carry through if we take a unital C^*-algebra $\mathfrak{A}$ instead of $\mathfrak{B}(\mathsf{H})$ and an element $a = a^* \in \mathfrak{A}$ instead of A.

□

3.6.2 Existence of Spectral Measures for Bounded Selfadjoint Operators

A cardinal consequence of Theorem 3.82 is the following proposition, which goes in the direction of the spectral theorem. Recall that $M_b(\sigma(A))$ indicates the unital C^*-algebra of complex, bounded and Borel-measurable functions on $\sigma(A)$, with norm $||\cdot||_\infty$. We point out that in order to formulate this result the Hilbert structure is essential, so no straightforward generalizations exist for abstract C^*-algebras.

Proposition 3.83 *Let $A \in \mathfrak{B}(\mathsf{H})$ be a bounded selfadjoint operator on the Hilbert space H. There exists a norm-decreasing (hence continuous) representation of unital *-algebras (Definition 2.27) $\Psi' : M_b(\sigma(A)) \to \mathfrak{B}(\mathsf{H})$ such that $\Psi'(\iota) = A$. The representation also satisfies:*

(a) $\Psi'\restriction_{C(\sigma(A))} = \Psi$,
(b) *$B \in \mathfrak{B}(\mathsf{H})$ commutes with $\Psi'(f)$ for every $f \in M_b(\sigma(A))$ if B commutes with A,*
(c) *Suppose $M_b(\sigma(A)) \ni f_n \to f$ pointwise as $n \to +\infty$ and $|f_n| \leq K$ for some $K \in [0, +\infty)$ and all n. Then*

$$\Psi'(f_n)x \to \Psi'(f)x \quad \textit{for every } x \in \mathsf{H}.$$

Proof Taking $x, y \in \mathsf{H}$, the linear map $C(\sigma(A)) \ni f \mapsto F_{x,y}(f) := \langle x|\Psi(A)y\rangle$ satisfies $|F_{x,y}(f)| \leq ||x||\,||y||\,||f||_\infty$. Riesz's theorem for complex measures [Rud91] implies that there exists a unique complex, regular Borel measure $\mu_{xy} : \mathscr{B}(\sigma(A)) \to \mathbb{C}$ such that

$$\langle x|\Psi(f)y\rangle = \int_{\sigma(A)} f d\mu_{xy} \quad \forall f \in C(\sigma(A))\,, \tag{3.62}$$

and also $||F_{xy}|| = |\mu_{xy}|(\sigma(A)) \leq ||x||\,||y||$. Actually, all complex Borel measures on $\mathscr{B}(\sigma(A))$ are regular since the open sets of $\sigma(A)$ are unions of countably many compact sets [Rud91]. Since $\Psi(\overline{f}) = \overline{\Psi(f)^*}$ and by standard inner product properties the complex measures $\mu_{xy}(E)$, $\overline{\mu_{yx}(E)}$ produce the same result when we integrate continuous functions. In view of uniqueness, therefore, $\mu_{xy}(E) = \overline{\mu_{yx}(E)}$. Using Riesz's Lemma, if $f \in M_b(\sigma(A))$ there exists a unique operator $\Psi'(f) \in \mathfrak{B}(\mathsf{H})$ such that

$$\langle x|\Psi'(f)y\rangle = \int_{\sigma(A)} f d\mu_{xy} \quad \forall x, y \in \mathsf{H}\,, \tag{3.63}$$

and $|\langle x|\Psi'(f)y\rangle| \leq ||f||_\infty|\mu_{xy}|(\sigma(A)) \leq ||f||_\infty||x||\,||y||$, so $||\Psi'(f)|| \leq ||f||_\infty$. By construction $\Psi'(1) = I$ and $\Psi'(\iota) = A$. Furthermore $M_b(\sigma(A)) \ni f \mapsto \Psi'(f)$ is linear and therefore it coincides with Ψ on polynomials. Continuity implies that it coincides with Ψ on $C(\sigma(A))$, proving (a). Ψ' satisfies $\Psi'(f)^* = \Psi'(\overline{f})$ as a consequence of (3.63), the fact that the inner product is Hermitian, and $\mu_{xy}(E) = \overline{\mu_{yx}(E)}$. To conclude the proof of the first statement it is enough to prove $\Psi'(f)\Psi'(g) = \Psi'(f \cdot g)$. Take $f, g \in C(\sigma(A))$. Since $\Psi(f \cdot g) = \Psi(f)\Psi(g)$ and Ψ' extends Ψ:

$$\int_{\sigma(A)} f \cdot g d\mu_{x,y} = \langle x|\Psi'(f \cdot g)y\rangle = \langle x|\Psi'(f)\Psi'(g)y\rangle = \int_{\sigma(A)} f d\mu_{x,\Psi'(g)y} .$$

Riesz's theorem implies that $\mu_{x,\Psi'(g)y}$ equals the complex, regular Borel measure λ such that

$$\lambda(E) = \int_{\sigma(A)} g d\mu_{xy} .$$

Therefore

$$\int_{\sigma(A)} f \cdot g d\mu_{xy} = \int_{\sigma(A)} f d\lambda = \int_{\sigma(A)} f d\mu_{x,\Psi'(g)y} \quad \text{if } f \in M_b(\sigma(A)) \text{ and } g \in C(\sigma(A)).$$

As a consequence

$$\int_{\sigma(A)} f \cdot g d\mu_{xy} = \int_{\sigma(A)} f d\mu_{x,\Psi'(g)y} = \langle x|\Psi'(f)\Psi'(g)y\rangle = \langle \Psi'(f)^* x|\Psi'(g)y\rangle$$
$$= \int_{\sigma(A)} g d\mu_{\Psi'(f)^* x,y}$$

for $x, y \in \mathsf{H}$, $f \in M_b(\sigma(A))$, $g \in C(\sigma(A))$. By a similar reasoning

$$\int_{\sigma(A)} f \cdot g d\mu_{xy} = \int_{\sigma(A)} g d\mu_{\Psi'(f)^* x,y}$$

must hold also if $g \in M_b(\sigma(A))$. Summing up, for $x, y \in \mathsf{H}$, $f, g \in M_b(\sigma(A))$, we have

$$\langle x|\Psi'(f \cdot g)y\rangle = \int_{\sigma(A)} f \cdot g \mu_{xy} = \int_{\sigma(A)} g \mu_{\Psi'(f)^* x,y} = \langle \Psi'(f)^* x|\Psi'(g)y\rangle$$
$$= \langle x|\Psi'(f)\Psi'(g)y\rangle$$

whence $\Psi'(f \cdot g) = \Psi'(f)\Psi'(g)$ as required.

The proof of (b) is analogous: if $B \in \mathfrak{B}(\mathsf{H})$ commutes with A, it also commutes with every polynomial $p(A)$ and hence with every $\Psi'(f)$ with $f \in C(\sigma(A))$ by continuity. Therefore, for every $f \in C(\sigma(A))$.

$$\int_{\sigma(A)} f d\mu_{x,By} = \langle x|\Psi'(f)By\rangle = \langle x|B\Psi'(f)y\rangle = \langle B^*x|\Psi'(f)y\rangle$$
$$= \int_{\sigma(A)} f d\mu_{B^*x,y} \,.$$

Riesz's theorem implies that $\mu_{x,By} = \mu_{Bx,y}$. The definition of Ψ' immediately entails that $\langle x|\Psi'(f)By\rangle = \langle B^*x|\Psi'(f)y\rangle = \langle x|B\Psi'(f)y\rangle$ for every $f \in M_b(\sigma(A))$. But this is the thesis, since $x, y \in \mathsf{H}$ are arbitrary.

Let us prove (c). Since Ψ' is a representation of unital *-algebras we immediately have

$$||\Psi'(f_n)x - \Psi'(f)x||^2 = ||\Psi'(f - f_n)x||^2 = \langle\Psi'(f - f_n)x|\Psi'(f - f_n)x\rangle = \langle x|\Psi'(|f - f_n|^2)x\rangle \,.$$

By (3.63)

$$||\Psi'(f_n)x - \Psi'(f)x||^2 = \int_{\sigma(A)} |f - f_n|^2 d\mu_{xy} \to 0$$

when $n \to +\infty$ by dominated convergence, since $|\mu_{xy}|$ is finite. □

We are ready to prove the existence claim in the Spectral Theorem (Theorem 3.40) for *bounded* selfadjoint operators.

Theorem 3.84 *If $A \in \mathfrak{B}(\mathsf{H})$ is selfadjoint on the Hilbert space H, there exists a PVM $P^{(A)} : \mathscr{B}(\mathbb{R}) \to \mathscr{L}(\mathsf{H})$ such that*

$$A := \int_{\mathbb{R}} \iota \, dP^{(A)} \,.$$

More generally, if $\Psi' : M_b(\sigma(A)) \to \mathfrak{B}(\mathsf{H})$ is defined as in Proposition 3.83,

$$\Psi'(f) = \int_{\sigma(A)} f \, dP^{(A)}$$

for every $f \in M_b(\sigma(A))$.

Proof Refer to Proposition 3.83. The required PVM is nothing but $P^{(A)}_E := \Psi'(\chi_{E\cap\sigma(A)})$ for every $E \in \mathscr{B}(\mathbb{R})$, $P^{(A)}_{\varnothing} := 0$. Indeed, suppose $P^{(A)}$ is a PVM. If $s = \sum_{j=1}^N s_j \chi_{E_j}$ is a simple function, the linearity of Ψ' immediately shows $\Psi'(s) = \sum_{j=1}^N s_j \Psi'(\chi_{E_j}) = \int_{\mathbb{R}} s \, dP^{(A)}$. Now consider a sequence of simple functions s_n such that $|s_n| \le |s_{n+1}| \le |\iota|$ on the compact set $\sigma(A)$, vanishing outside $\sigma(A)$, and converging pointwise to ι on $\sigma(A)$. As the PVM is concentrated on $\sigma(A)$ by construction, Propositions 3.83 (a)–(c) and 3.29

(c) imply

$$\int_{\mathbb{R}} \iota \, dP^{(A)}x = \int_{\sigma(A)} \iota \, dP^{(A)}x = \lim_{n\to+\infty} \int_{\sigma(A)} s_n \, dP^{(A)}x = \lim_{n\to+\infty} \Psi'(s_n) = \Psi'(\iota)x = Ax \, .$$

Since $x \in \mathsf{H}$ is arbitrary, we get $A = \int_{\mathbb{R}} \iota \, dP^{(A)}$, as we wanted. The same argument (using a sequence of simple functions s_n converging to $f \in M_b(\sigma(A))$ pointwise and such that $|s_n| \leq |s_{n+1}| \leq |f|$) returns the second claim.

To end the proof, there remains to prove that $P_E^{(A)} := \Psi'(\chi_{E\cap\sigma(A)})$ with $E \in \mathscr{B}(\mathbb{R})$ (and obviously $P_\varnothing^{(A)} := 0$) defines a PVM. But $P_{\mathbb{R}}^{(A)} = I$, $P_E^{(A)} P_F^{(A)} = P_{E\cap F}^{(A)}$, $(P_E^{(A)})^* = P_E^{(A)}$ (in particular $P_E^{(A)} \in \mathscr{L}(\mathsf{H})$) are immediate consequences of the fact that Ψ' is a representation of unital *-algebras, together with trivial properties of characteristic functions χ_E, plus $\Psi'(1) = \Psi'(\chi_{\sigma(A)}) = I$. Finally, σ-additivity follows from Proposition 3.83 (c): taking a countable collection of disjoint sets $E_k \in \mathscr{B}(\mathbb{R})$, we have

$$\sum_{k=1}^{N} \chi_{E_k \cap \sigma(A)} \to \chi_{\sigma(A)\cap\cup_{k=1}^{N} E_k} \quad \text{pointwise as } n \to +\infty$$

(all functions are bounded by the constant 1). □

3.6.3 Spectral Theorem for Normal Operators in $\mathfrak{B}(\mathsf{H})$

The functional calculus developed in the previous section permits us to prove the spectral theorem for *normal operators* on $\mathfrak{B}(\mathsf{H})$. In particular it handles selfadjoint operators on $\mathscr{B}(\mathsf{H})$ and unitary operators.

Theorem 3.85 (Spectral Theorem for Normal Operators on $\mathfrak{B}(\mathsf{H})$) *Let $T \in \mathfrak{B}(\mathsf{H})$ be a normal operator on the complex Hilbert space H.*

(a) *There exists a unique PVM $P^{(A)} : \mathscr{B}(\mathbb{C}) \to \mathscr{L}(\mathsf{H})$, called the* ***spectral measure*** *of T, such that*

$$T = \int_{\mathbb{C}} z dP^{(T)}(z, \overline{z}) \, .$$

In particular $D(T) = \Delta_\iota$, where $\iota : \mathbb{C} \ni z \mapsto z$.

(b) *We have*

$$supp(P^{(T)}) = \sigma(T).$$

As the standard topology of $\mathbb{C}$ is second-countable, $P^{(T)}$ is concentrated on $\sigma(T)$:

$$P^{(T)}(E) = P^{(T)}(E \cap \sigma(T)) , \quad \forall E \in \mathscr{B}(\mathbb{C}) . \tag{3.64}$$

(c) *$z \in \sigma_p(T)$ if and only if $P^{(T)}(\{z\}) \neq 0$; in particular this happens if z is an isolated point of $\sigma(T)$. Finally $P^{(T)}_{\{z\}}$ is the orthogonal projector onto the eigenspace of $z \in \sigma_p(A)$.*

(d) *$z \in \sigma_c(T)$ if and only if $P^{(T)}(\{\lambda\}) = 0$, but $P^{(T)}(E) \neq 0$ if $E \ni \lambda$ is an open set of $\mathbb{C}$.*

Proof (a) Let us prove that there exists a PVM on $\mathbb{C}$ with $T = \int_{\mathbb{C}} z dP^{(T)}(z)$. Decompose $T = A + iB$ where $A = \frac{1}{2}(T + T^*)$ and $A = \frac{1}{2i}(T - T^*)$ are selfadjoint, belong to $\mathfrak{B}(\mathsf{H})$, and commute because T and T^* commute by hypothesis. Notice that, as a consequence of Proposition 3.83 (b) the spectral measure $P^{(A)}$ of A, which exists by Theorem 3.84 and satisfies $P^{(A)}_E = \Psi'_A(\chi_E)$, commutes with B. By the same argument the spectral measure $P^{(B)}$ of B commutes with the spectral measure of A.

Next consider *step functions* on the compact set $K = [-||A||, ||A||] \times [-||B||, ||B||] \subset \mathbb{R}^2 \equiv \mathbb{C}$. A **step function** is a simple function of the form

$$s(x, y) = \sum_{i=1}^{N} \sum_{j=1}^{M} s_{ij} \chi_{I_i}(x) \chi_{J_j}(y) , \quad z = x + iy \in K \tag{3.65}$$

where $s_{ij} \in \mathbb{C}$ are fixed numbers, $I_1 := [-||A||, a_2]$, $J_1 := [-||B||, b_2]$, $I_i := (a_i, a_{i+1}]$, $J_j := (b_j, b_{j+1}]$ for $i, j > 1$, and $a_{N+1} = ||A||$, $b_{n+1} = ||B||$. The decomposition of $s \in S(K)$ in (3.65) is not unique, since every such expression can be refined by adding points a_i or b_j. It is easy to prove that the set $S(K)$ of step functions on K is closed under linear combinations and products. Since it evidently contains the constant function 1 and it is invariant under conjugation, $S(K)$ is a unital *-subalgebra of $M_b(K)$. Referring to (3.65), let us define $\Phi_0 : S(K) \to \mathfrak{B}(\mathsf{H})$ by

$$\Phi_0(s) := \sum_{i=1}^{N} \sum_{j=1}^{M} s_{ij} P^{(A)}_{I_i} P^{(B)}_{J_j} = \sum_{i=1}^{N} \sum_{j=1}^{M} s_{ij} P^{(B)}_{J_j} P^{(A)}_{I_i} . \tag{3.66}$$

The definition is well-posed irrespective of the various expansions (3.65) that s possesses. By direct inspection, one sees that Φ_0 is a homomorphism of unital *-algebras and also that

$$||\Phi_0(s)\psi||^2 = \sum_{i=1}^{N} \sum_{j=1}^{M} |s_{ij}|^2 ||P^{(A)}_{I_i} P^{(B)}_{J_j} \psi||^2 \leq \sup_{i,j} |s_{ij}|^2 \sum_{i=1}^{N} \sum_{j=1}^{M} ||P^{(A)}_{I_i} P^{(B)}_{J_j} \psi||^2$$
$$= \sup_{ij} |s_{ij}|^2 ||\psi||^2 ,$$

using that the sets $I_i \times J_j$ are pairwise disjoint and $\sum_{i,j} P^{(A)}_{I_i} P^{(B)}_{J_j} = I$ because $\cup_{i,j} I_i \times J_j = K$. As a consequence

$$||\Phi_0(s)|| \leq ||s||_\infty \quad \text{if } s \in S(K).$$

Since $S(K)$ is dense in $C(K)$ in norm $|| \cdot ||_\infty$ (a continuous function on a compact set is uniformly continuous), the same proof as for Theorem 3.82 ensures that the continuous unital *-homomorphism Φ_0 generates a norm-decreasing unital *-homomorphism $\Phi : C(K) \to \mathfrak{B}(\mathsf{H})$. Notice that Φ is *not* an extension of Φ_0, since its domain contains continuous maps only, whereas the domain of Φ_0 contains discontinuous functions as well. By definition $\Phi(1) = I$, and by setting $\imath_1 : K \ni (x, y) \mapsto x$ and $\imath_2 : K \ni (x, y) \mapsto y$ we have

$$\Phi(\imath_1) = A \quad \text{and} \quad \Phi(\imath_2) = B \, .$$

Indeed, let $s_n : [-||A||, ||A||] \times [-||B||, ||B||] \to \mathbb{R}$ be a sequence of step functions, constant in the variable $y \in [-||B||, ||B||]$ and converging uniformly to the map $\imath_1$. Applying (3.66) gives, with obvious notation,

$$\Phi_0(s_n) = \int_{\mathbb{R}} s_n dP^{(A)} \to \Phi(\imath_1) = \int_{\mathbb{R}} \imath_1 dP^{(A)} = A \, , \quad \text{in the uniform topology as } n \to +\infty,$$

where we exploited (3.21). The story for $\imath_2$ is identical.

As last step, and proceeding as in the proof of Proposition 3.83, we may extend Φ to a unital *-algebra homomorphism $\Phi' : M_b(K) \to \mathfrak{B}(\mathsf{H})$ completely determined by the requirement

$$\langle \psi | \Phi'(f) \phi \rangle = \int_K f d\nu_{\psi,\phi} \quad \psi, \phi \in \mathsf{H} \, , \, f \in M_b(K) \, ,$$

where $\nu_{\psi.\phi} : \mathscr{B}(K) \to \mathbb{C}$ is the unique complex regular Borel measure satisfying the above relation for $f \in C(K)$. An argument that essentially replicates Proposition 3.83 shows that the homomorphism of unital *-algebras $\Phi' : M_b(K) \to \mathfrak{B}(\mathsf{H})$ is norm-decreasing ($||\Phi'(f)|| \leq ||f||_\infty$), satisfies

$$\Phi'(\imath_1) = A \quad \text{and} \quad \Phi'(\imath_2) = B \, , \tag{3.67}$$

and finally

$$\Phi'(f_n)\psi \to \Phi'(f)\psi \quad \text{for every } \psi \in \mathsf{H}, \tag{3.68}$$

if $M_b(K) \ni f_n \to f$ pointwise as $n \to +\infty$ and $|f_n| \leq M$ for some $M \in [0, +\infty)$ and all n.

The last convergence property in particular implies, along the same lines of Theorem 3.84, that $P^{(T)}_E := \Phi'(\chi_{E \cap K})$ (with $P^{(T)}_\varnothing := 0$) is a PVM on $\mathbb{C} \equiv \mathbb{R}^2$

when E varies in $\mathscr{B}(\mathbb{C})$. By (3.67) moreover,

$$\int_{\mathbb{C}} \iota_1 dP^{(T)} = \Phi'(\iota_1) = A\;, \quad \int_{\mathbb{C}} \iota_2 dP^{(T)} = \Phi'(\iota_2) = B\;. \tag{3.69}$$

Since $T = A + iB$ and $T^* = A - iB$, these relations read

$$\int_{\mathbb{C}} z dP^{(T)}(z, \overline{z}) = T\;, \quad \int_{\mathbb{C}} \overline{z} dP^{(T)}(z, \overline{z}) = T^*\;. \tag{3.70}$$

Let us pass to the uniqueness issue. First of all observe that if $T = \int_{\mathbb{C}} z dP(z, \overline{z})$ then P must have bounded support: if not, for every $n \in \mathbb{N}$, we could find $E_n \in \mathscr{B}(\mathbb{C})$ outside the disc of radius n at the origin of $\mathbb{C}$ such that $P_{E_n} \neq 0$. Hence we could pick $x_n \in P_{E_n}(\mathsf{H})$ with $||x_n|| = 1$. As a consequence $||Tx_n||^2 \geq |n|^2 \int_{\mathbb{C}} 1 d\mu^{(P)}_{x_n x_n} = |n|^2 \to +\infty$ as $n \to +\infty$, contradicting $||T|| < +\infty$. We conclude that there exists a sufficiently large compact rectangle $K := [a, b] \times [c, d] \subset \mathbb{R}^2 \equiv \mathbb{C}$ (we can always assume it to be larger than $[-||A||, ||A||] \times [-||B||, ||B||]$), so that $\text{supp}(P) \subset K$. Hence it suffices to work in K. Taking adjoints of $\int_K z dP(z, \overline{z}) = T = \int_K z dP^{(T)}(z, \overline{z})$ produces $\int_K \overline{z} dP(z, \overline{z}) = T^* = \int_K \overline{z} dP^{(T)}(z, \overline{z})$. Using standard properties of bounded PVMs, we immediately have that $\int_K p(z, \overline{z}) dP(z, \overline{z}) = \int_K p(z, \overline{z}) dP^{(T)}(z, \overline{z})$ for every polynomial p defined on K. But polynomials are $||\cdot||_\infty$-dense in $C(K)$ (Stone–Weierstrass theorem), so (3.21) implies $\int_K f(z, \overline{z}) dP(z, \overline{z}) = \int_K f(z, \overline{z}) dP^{(T)}(z, \overline{z})$ for every $f \in C(K)$. Applying now the Riesz theorem for positive Borel measures to

$$\int_K f d\mu^{(P)}_{\psi\psi} = \left\langle \psi \left| \int_K f dP\; \psi \right.\right\rangle = \left\langle \psi \left| \int_K f dP^{(T)}\; \psi \right.\right\rangle = \int_K f d\mu^{(P^{(T)})}_{\psi\psi} \quad \forall f \in C(K)$$

we conclude $\mu^{(P^{(T)})}_{\psi\psi}(E) = \mu^{(P)}_{\psi\psi}(E)$ for every $E \in \mathscr{B}(K)$. Since the supports of the two measures stay in K, the relation we have found reads $\mu^{(P^{(T)})}_{\psi\psi}(E) = \mu^{(P)}_{\psi\psi}(E)$ for every $E \in \mathscr{B}(\mathbb{C})$, i.e. $\langle \psi | (P^{(T)}_E - P_E)\psi \rangle = 0$ for every $\psi \in \mathsf{H}$. This result immediately leads to the thesis, $P^{(T)}_E = P_E$ for every $E \in \mathscr{B}(\mathbb{C})$.

The proofs of (b), (c) and (d) are identical to those of the corresponding statements in Theorem 3.40, up to trivial changes ($\mathbb{R}$ becomes $\mathbb{C}$ and λ becomes z). □

3.6.4 Existence of Spectral Measures for Unbounded Selfadjoint Operators

At the end of this long detour, we are finally ready to justify the existence of PVMs for *unbounded* selfadjoint operators (the Spectral Theorem, 3.40).

Theorem 3.86 *If A is a (generally unbounded) selfadjoint operator on the Hilbert space H, there exists a PVM $P^{(A)} : \mathscr{B}(\mathbb{R}) \to \mathscr{L}(\mathsf{H})$ such that*

$$A := \int_{\mathbb{R}} \imath \, dP^{(A)} .$$

Proof First of all observe that, if A is normal, its resolvent satisfies $R_\lambda(A)^* = R_{\overline{\lambda}}(A^*)$. Indeed, we know that $\lambda \in \rho(A)$ iff $\overline{\lambda} \in \rho(A^*)$ by Proposition 3.13 (c). In this case $R_\lambda(A)(A - i\lambda I) = I\upharpoonright_{D(A)}$ implies $(A - i\lambda I)^* R_\lambda(A)^* = I\upharpoonright^*_{D(A)} = I$, namely $(A^* + i\lambda I)R_\lambda(A)^* = I$. Since we also have $(A^* + i\lambda I)R_{\overline{\lambda}}(A^*) = I$ and the inverse is unique, necessarily $R_\lambda(A)^* = R_{\overline{\lambda}}(A^*)$. This results is in particular true when $A = A^*$. Next, assuming $A = A^*$, consider the operator

$$U := I - 2i R_{-i}(A) ,$$

called the **Cayley transform** of A. By the resolvent identity (3.2) and $R_\lambda(A)^* = R_{\overline{\lambda}}(A)$, one immediately proves that $UU^* = U^*U = I$. Hence U is unitary and $\sigma(U)$ is a closed subset of $\mathbb{T} = \{z \in \mathbb{C} \mid |z| = 1\}$ in the topology induced by $\mathbb{C}$ due to Proposition 3.13. Finally,

$$U = \int_{\sigma(U)} z dP^{(U)}(z, \overline{z})$$

by Theorem 3.85. We claim that the statement's selfadjoint operator A coincides with the selfadjoint operator

$$A' := \int_{\sigma(U)} i \frac{1+z}{1-z} dP^{(U)}(z, \overline{z}) \tag{3.71}$$

(the integrand is real since $\overline{z} = 1/z$ as $z \in \mathbb{T}$). In fact, since $R_{-i}(A) = \frac{i}{2}(U - I)$ and taking Proposition 3.33 (c) into account,

$$(A' + iI)R_{-i}(A) = \int_{\sigma(U)} \left[i\frac{1+z}{1-z} + i \right] dP^{(U)}(z, \overline{z}) \int_{\sigma(U)} \frac{i}{2}(z-1) dP^{(U)}(z, \overline{z})$$

$$= \int_{\sigma(U)} \left[i\frac{1+z}{1-z} + i \right] \frac{i}{2}(z-1) dP^{(U)}(z, \overline{z}) = \int_{\sigma(U)} 1 dP^{(U)}(z, \overline{z}) = I .$$

We conclude that $A' + iI$ is defined on a domain that contains $Ran(R_{-i}A) = D(A)$, on which it coincides with the unique left inverse of $R_{-i}(A)$. In other words $A' + iI$ is an extension of $A + iI$, so $A' \supset A$. Since A' and A are selfadjoint, $A' = A$ by Proposition 2.39 (b). To conclude, we shall prove that (3.71) can be decomposed spectrally on $\mathbb{R}$. As

$$\phi : \mathbb{T} \ni z \mapsto i\frac{1+z}{1-z} \in \mathbb{R} \cup \{\infty\}$$

is a homeomorphism ($\mathbb{R} \cup \{\infty\}$ is the standard 1-point compactification), then

$$A = A' := \int_{\mathbb{T}} i\frac{1+z}{1-z} dP^{(U)}(z, \overline{z}) = \int_{\mathbb{R}\cup\{\infty\}} r dP(r) ,$$

where we have defined the PVM $P_E = P^{(T)}_{\phi^{-1}(E)}$ for $E \in \mathscr{B}(\mathbb{R} \cup \{+\infty\})$ following Proposition 3.33 (f). Let us explain why ∞ is reached by ϕ only for $z = 1$ and $P^{(U)}_{\{1\}} = 0$. If $P^{(U)}_{\{1\}} \neq 0$ we would have $Ux = x$ for some $x \in P^{(U)}_{\{1\}}(\mathsf{H}) \setminus \{0\}$. Since $U := I - 2iR_{-i}(A)$, then $R_{-i}(A)x = 0$, contradicting the fact that $R_{-i}(A)$ is invertible since A is selfadjoint and so $-i \in \rho(A)$. We can rewrite the equation as

$$A = \int_{\mathbb{T}\setminus\{1\}} i\frac{1+z}{1-z} dP^{(U)}(z, \overline{z}) = \int_{\mathbb{R}} r dP(r) .$$

It is easy to check that the restriction P' of P to $\mathscr{B}(\mathbb{R})$ is still a PVM on $\mathbb{R}$ and the integral above can be thought of as

$$A = \int_{\mathbb{R}} r dP'(r) .$$

The proof is over once we take $P^{(A)} := P'$. □

3.6.5 Existence of Joint Spectral Measures

We shall provide a proof for Theorem 3.56. The argument differs from that appearing in [Mor18] in view of the distinct presentation of the spectral technology we have chosen here. In particular, the current proof does not require that the Hilbert space be separable.

Theorem 3.56 (Joint Spectral Measure) *Let $\mathfrak{A} := \{A_1, A_2, \dots, A_n\}$ be a set of selfadjoint operators on the Hilbert space H with commuting spectral measures:*

$$P^{(A_k)}_{E_k} P^{(A_h)}_{E_h} = P^{(A_h)}_{E_h} P^{(A_k)}_{E_k} \quad \forall k, h \in \{1, \dots, n\} , \forall E_k, E_h \in \mathscr{B}(\mathbb{R}) .$$

Then there exists a unique PVM $P^{(\mathfrak{A})}$ on $\mathbb{R}^n$ such that

$$P^{(\mathfrak{A})}_{E_1\times\cdots\times E_n} = P^{(A_1)}_{E_1} \cdots P^{(A_n)}_{E_n} , \quad \forall E_1, \dots, E_n \in \mathscr{B}(\mathbb{R}) . \tag{3.72}$$

For every $f : \mathbb{R} \to \mathbb{C}$ measurable, furthermore,

$$\int_{\mathbb{R}^n} f(x_k) dP^{(\mathfrak{A})}(x) = f(A_k) , \quad k = 1, \dots, n \tag{3.73}$$

where $x = (x_1, \ldots, x_k, \ldots, x_n)$ *and* $f(A_k) := \int_{\mathbb{R}} f(\lambda) dP^{(A_k)}$.

Finally, $B \in \mathfrak{B}(\mathsf{H})$ *commutes with* $P^{(\mathfrak{A})}$ *if and only if it commutes with all* $P^{(A_k)}$, $k = 1, 2, \ldots, n$.

Proof (Existence) We start by assuming $A_k \in \mathfrak{B}(\mathsf{H})$ for $k = 1, \ldots, n$. Then we may replicate the initial part of the proof of Theorem 3.85, only replacing the two commuting selfadjoint operators in $A, B \in \mathfrak{B}(\mathsf{H})$ by n commuting selfadjoint operators $A_k \in \mathfrak{B}(\mathsf{H})$. In this way if $K := [-a, a]^n \subset \mathbb{R}^n$ is sufficiently large and $K \supset \times_{k=1}^n \sigma(A_k)$, there exists a map $\Phi' : M_b(K) \to \mathfrak{B}(\mathsf{H})$ with the following features. It is a norm-decreasing *-homomorphism of unital *-algebras, it satisfies

$$\Phi'(\iota_k) = A_k \quad \text{for } k = 1, \ldots, n \tag{3.74}$$

where $\iota_k : \mathbb{R}^n \ni (x_1, \ldots, x_n) \mapsto x_k \in \mathbb{R}$, and finally

$$\Phi'(f_n)\psi \to \Phi'(f)\psi \qquad \text{for every } \psi \in \mathsf{H}, \tag{3.75}$$

if $M_b(K) \ni f_n \to f$ pointwise as $n \to +\infty$ and $|f_n| \leq M$ for some $M \in [0, +\infty)$ and all n.

Invoking the proof of Theorem 3.84, the last convergence property implies that

$$P_E^{(\mathfrak{A})} := \Phi'(\chi_{E \cap K}) \tag{3.76}$$

(with $P_\varnothing^{(\mathfrak{A})} := 0$) defines a PVM on $\mathbb{R}^n$ when E varies in $\mathscr{B}(\mathbb{R}^n)$ and

$$\int_{\mathbb{R}^n} \iota_k dP^{(\mathfrak{A})} = \Phi'(\iota_k) = A_k\,, \quad k = 1, \ldots, n \tag{3.77}$$

by (3.74). Now observe that as $E \in \mathscr{B}(\mathbb{R})$ varies, the family of orthogonal projectors $P_E := P^{(\mathfrak{A})}_{E \times \mathbb{R}^{n-1}}$ defines a PVM on $\mathbb{R}$. Take a sequence of simple functions s_n on K, constant in the variables $x_2, \ldots, x_n$ and such that $s_n \to \iota_1$ pointwise with $|s_n| \leq |\iota_1|$ (which is bounded on K). Equation (3.75) and Proposition 3.29 (c) allow to rephrase (3.77) for $k = 1$ as

$$\int_{\mathbb{R}} \iota \, dP = A_1\,. \tag{3.78}$$

The uniqueness of the spectral measure of A_1 (Theorem 3.40) implies that

$$P^{(\mathfrak{A})}_{E \times \mathbb{R}^{n-1}} = P_E = P_E^{(A_1)} \quad \forall E \in \mathscr{B}(\mathbb{R})\,.$$

By the same argument,

$$P^{(\mathfrak{A})}_{\mathbb{R}^{k-1} \times E \times \mathbb{R}^{n-k}} = P_E^{(A_k)}\,, \quad E \in \mathscr{B}(\mathbb{R})\,,\ k = 1, 2, \ldots, n\,.$$

This relation implies, together with (3.76) and the fact that Φ' preserves products,

$$P^{(\mathfrak{A})}_{E_1\times\cdots\times E_n} = \Phi'(\chi_{E_1\times\mathbb{R}^{n-1}}\cdots\chi_{\mathbb{R}^{n-1}\times E_n}) = \Phi'(\chi_{E_1\times\mathbb{R}^{n-1}})\cdots\Phi'(\chi_{\mathbb{R}^{n-1}\times E_n})$$

$$= P^{(\mathfrak{A})}_{E_1\times\mathbb{R}^{n-1}}\cdots P^{(\mathfrak{A})}_{\mathbb{R}^{n-1}\times E_n} = P^{(A_1)}_{E_1}\cdots P^{(A_n)}_{E_n}\,.$$

Hence (3.72) is true. Let us pass to unbounded selfadjoint operators A_k. We shall reduce this to the case of bounded operators. To this end, define a family $\mathfrak{B} := \{B_1,\ldots,B_n\}$,

$$B_k := \int_{\mathbb{R}} \frac{x_k}{\sqrt{1+x_k^2}}dP^{(A_k)}(x_k)$$

for every $k = 1,2,\ldots,n$. It is clear that $B_k^* = B_k \in \mathfrak{B}(\mathsf{H})$ due to Theorem 3.24 (c) and Proposition 3.29 (a). Moreover, by Corollary 3.53 $\sigma(B_k) \subset [-1,1]$, but $\pm 1 \notin \sigma_p(B_k)$. By contradiction, in fact, if $\pm 1 \in \sigma_p(B_k)$ and $\psi_\pm \in \mathsf{H}$ were a corresponding eigenvector, then $(B_k \pm I)\psi_\pm = 0$, and so

$$0 = ||(B_k \pm I)^2\psi_\pm||^2 = \int_{\mathbb{R}}\left(\frac{x_k}{\sqrt{1+x_k^2}} \pm 1\right)^2 d\mu^{(P_k)}_{\psi_\pm\psi_\pm}\,.$$

Since the positive measure $\mu^{(P_k)}_{\psi_\pm\psi_\pm}$ does not vanish ($\psi_\pm \neq 0$ because it is an eigenvector), the integrand would be zero almost everywhere. This is not possible because

$$\left(\frac{x_k}{\sqrt{1+x_k^2}} \pm 1\right)^2 > 0 \quad \text{for every } x_k \in \mathbb{R}.$$

Let us now focus on the map

$$\phi : \overline{\mathbb{R}} \ni x \mapsto \frac{x}{\sqrt{1+x^2}} \in [-1,1]\,,$$

where $\overline{\mathbb{R}} = \mathbb{R}\cup\{\pm\infty\}$ is the compactification and $[-1,1]$ is standard. Note that $\phi(\mathbb{R}) = (-1,1)$ and $\phi(\pm\infty) = \pm 1$. It is easy to see that ϕ is an homeomorphism, so ϕ and ϕ^{-1} are Borel measurable.

In view of these properties of ϕ it is preferable to extend the spectral measures $P^{(A_k)}$ to new PVMs $\widetilde{P}^{(A_k)}$ defined on the Borel algebra $\mathscr{B}(\overline{R})$, by simply declaring that $\widetilde{P}^{(A_k)}_{+\infty} = \widetilde{P}^{(A_k)}_{-\infty} = 0$ and $\widetilde{P}^{(A_k)}_E = P^{(A_k)}_E$ when $E\cap\{+\infty\} = E\cap\{-\infty\} = \varnothing$

for $E \in \mathscr{B}(\overline{R})$. Now it is safe to write

$$B_k := \int_{\overline{\mathbb{R}}} \frac{x_k}{\sqrt{1+x_k^2}} d\widetilde{P}^{(A_k)}(x_k) .$$

Using the extension, Proposition 3.33 (f) tells

$$B_k = \int_{[-1,1]} y_k dP^{(B_k)}(y_k) ,$$

where

$$P^{(B_k)}(F) = \widetilde{P}^{(A_k)}(\phi^{-1}(F)) \quad \text{for } F \in \mathscr{B}([-1,1]) . \tag{3.79}$$

We could extend $P^{(B_k)}$ to the whole $\mathscr{B}(\mathbb{R})$ by setting $P_1^{(B_k)}(F) := P_1^{(B_k)}(F \cap [-1,1])$ for $F \in \mathscr{B}(\mathbb{R})$ trivially; we shall however stick to the first choice for the sake of simplicity, and allow ourselves to interpret the relevant PVM as their extensions where necessary.

Observe that the spectral measures $P^{(B_k)}$ commute with each other due to (3.79) and the fact that the PVMs $\widetilde{P}^{(A_k)}$ do (the added points $\pm\infty$ are harmless). We can therefore apply the previous proof, construct a PVM $P^{(\mathfrak{B})}$ on $\mathscr{B}(\mathbb{R}^n)$, with support in $[-1,1]^n$, which satisfies

$$P^{(\mathfrak{B})}_{F_1\times\cdots\times F_n} = P^{(B_1)}_{F_1}\cdots P^{(B_n)}_{F_n} \quad \text{if } F_k \in \mathscr{B}(\mathbb{R}) \text{ for } k=1,\ldots,n. \tag{3.80}$$

Let us go back to the unbounded operators A_k, define the homeomorphism

$$\Phi : \overline{\mathbb{R}}^n \ni (x_1,\ldots,x_n) \mapsto (\phi(x_1),\ldots,\phi(x_n)) \in [-1,1]^n$$

and the PVM on $\overline{\mathbb{R}}^n$

$$P_E := P^{(\mathfrak{B})}_{\Phi(E)} \quad E \in \mathscr{B}(\overline{\mathbb{R}}^n) .$$

This is allowed by Proposition 3.33 (f) ($\Phi = (\Phi^{-1})^{-1}$ and Φ^{-1} is Borel measurable since Φ is an homeomorphism). With this definition, (3.80) implies

$$P_{E_1\times\cdots\times E_n} = \widetilde{P}^{(A_1)}_{E_1}\cdots\widetilde{P}^{(A_n)}_{E_n} , \quad \forall E_1,\ldots,E_n \in \mathscr{B}(\overline{\mathbb{R}}) . \tag{3.81}$$

To conclude the proof of existence, it is enough to rid ourselves of the 'annoying' points $\pm\infty$. The boundary of $\overline{\mathbb{R}}^n$ is the union of the $2n$ sets

$$F_\pm^{(k)} := \overline{\mathbb{R}^{k-1}} \times \{\pm\infty\} \times \overline{\mathbb{R}^{n-k}} .$$

Every such set has zero P-measure: exploiting (3.81), in fact,

$$P_{F_+^{(1)}} = \widetilde{P}^{(A_1)}_{\{+\infty\}} \cdots \widetilde{P}^{(A_n)}_{\overline{\mathbb{R}}} = 0$$

because $\widetilde{P}^{(A_1)}_{\{+\infty\}} = P^{(B_1)}_{+1} = 0$ since $+1 \notin \sigma_p(B_1)$ and by Theorem 3.40 (c)–(d). Hence the boundary of $\overline{\mathbb{R}}^n$ has zero measure for P. This means that, restricting to the interior $\mathbb{R}^n$ of $\overline{\mathbb{R}}^n$, the map $P^{(\mathfrak{A})}_E := P_E$ with $E \in \mathscr{B}(\mathbb{R}^n)$, still defines a PVM, in particular $P^{(\mathfrak{A})}_{\mathbb{R}^n} = I$. By construction, $P^{(\mathfrak{A})}$ satisfies (3.73) since (3.80) holds, and that ends the existence part of the proof.

(Uniqueness) Let us show uniqueness. We have the following known result of general measure theory [Coh80, Corollary 1.6.3].

Lemma 3.57 *Let $\Sigma(X)$ be a σ-algebra on X and $\mathcal{P} \subset \Sigma(X)$ such that*

(i) $\mathcal{P}$ is closed under finite intersections;
(ii) the σ-algebra generated by P is $\Sigma(X)$ itself;
(iii) there is an increasing sequence $\{C_m\}_{m\in\mathbb{N}} \subset \mathcal{P}$ such that $\cup_{m\in\mathbb{N}} C_m = X$.

If μ and ν are positive σ-additive measures on $\Sigma(X)$ such that $\mu(C_m) = \nu(C_m) < +\infty$ for every $m \in \mathbb{N}$, then $\mu = \nu$.

Returning to our proof, define $\Sigma(X) := \mathscr{B}(\mathbb{R}^n)$ and let $\mathcal{P}$ be the collection of sets $E_1 \times \cdots \times E_n$ for $E_k \in \mathscr{B}(\mathbb{R})$. It it known that ($\mathbb{R}$ is a separable metric space) the σ-algebra generated by $\mathcal{P}$ is just $\mathscr{B}(\mathbb{R}^n)$. Now set $C_m = (-r, r)^m$ with $m \in \mathbb{N}$. Finally, fix $x \in \mathsf{H}$ and define $\mu(F) := \langle x|P_F x\rangle$ and $\nu(F) := \langle x|P'_F x\rangle$ for $F \in \mathscr{B}(\mathbb{R}^n)$, where both P and P' satisfy (3.72) in place of $P^{(\mathfrak{A})}$. These measures are finite, as $\mu(F) = \nu(F) = ||x||^2$ by definition of PVM, and satisfy $\mu(C_n) = \nu(C_n) < +\infty$ because of (3.72). Lemma 3.57 proves that $\langle x|P_F x\rangle = \langle x|P'_F x\rangle$, so that $\langle x|(P_F - P'_F)x\rangle = 0$. The arbitrariness of $x \in \mathsf{H}$ and the usual polarization formula imply $P_F = P'_F$ for every $F \in \mathscr{B}(\mathbb{R})$.

(Equation (3.73)) The proof is easy. Consider $k = 1$ for instance. There exists a sequence of simple functions s_m on $\mathbb{R}$ converging pointwise to the measurable function $f : \mathbb{R} \to \mathbb{C}$, as $m \to +\infty$, and such that $|s_m| \leq |s_{m+1}| \leq |f|$. Let us write $s_m(x_1) := \sum_{r=1}^N c_r \chi_{E_r}$ and define $s'_m(x_1, \ldots, x_n) := \sum_{r=1}^N c_r \chi_{E_r \times \mathbb{R}^{n-1}}(x_1, \ldots, x_n)$ (so that s'_m is constant in $x_1, \ldots, x_n$ and equals s_m in the remaining variable). If $\psi \in \Delta^{(A_1)}_f$, by Theorem 3.24 (d) and dominated convergence we have

$$f(A_1) = \int_{\mathbb{R}} f(x_1) dP^{(A_1)}\psi = \lim_{m\to+\infty} \int_{\mathbb{R}} s_m dP^{(A_1)}\psi$$

$$= \lim_{m\to+\infty} \int_{\mathbb{R}^n} s'_m dP^{(\mathfrak{A})}\psi = \int_{\mathbb{R}^n} f(x_1) dP^{(\mathfrak{A})}\psi \, , \qquad (3.82)$$

where the penultimate equality is justified by (3.72). The same argument, using monotone convergence and the identity $\int_{\mathbb{R}} |s_m|^2 d\mu^{(P^{(A_1)})}_{\psi\psi} = \int_{\mathbb{R}} |s'_m|^2 d\mu^{(P^{(\mathfrak{A})})}_{\psi\psi}$, also proves that $\psi \in \Delta^{(\mathfrak{A})}_f$ with obvious notation. Therefore $\int_{\mathbb{R}^n} f(x_1) dP^{(\mathfrak{A})}\psi$ is well defined.

(Last Statement) If $B \in \mathfrak{B}(\mathsf{H})$ commutes with $P^{(\mathfrak{A})}$ it evidently commutes with every $P^{(A_k)}$, $k = 1, 2, \ldots, n$ due to (3.72) by just taking all $E_k = \mathbb{R}$ but one. Suppose conversely that $U \in \mathfrak{B}(\mathsf{H})$ is unitary and commutes with every $P^{(A_k)}$. The PVM defined by the projectors $UP^{(\mathfrak{A})}_E U^{-1}$, for $E \in \mathscr{B}(\mathbb{R}^n)$, therefore coincides with $P^{(\mathfrak{A})}$ when $E = E_1 \times \cdots \times E_n$ with $E_k \in \mathscr{B}(\mathbb{R})$. By the established uniqueness property, we immediately have $UP^{(\mathfrak{A})}_E U^{-1} = P^{(\mathfrak{A})}_E$ for every $E \in \mathscr{B}(\mathbb{R}^n)$. In other words $UP^{(\mathfrak{A})}_E = P^{(\mathfrak{A})}_E U$ for every $E \in \mathscr{B}(\mathbb{R}^n)$. In order to pass from U to a general $B \in \mathfrak{B}(\mathsf{H})$, it suffices to invoke Proposition 3.55 (whose proof relies only upon the spectral theorem of selfadjoint operators), write $B = aU + bU'$ as complex linear combination of unitary operators, and finally use the composition's linearity in the relation above.

□

Chapter 4
Fundamental Quantum Structures on Hilbert Spaces

The question we want to address now is: *is there anything deeper behind the phenomenological facts (1), (2), and (3) discussed in the first chapter and the formalization of Sect. 3.4?*

An appealing attempt to answer that question and justify the formalism based on the spectral theory is due to von Neumann [Neu32] (and subsequently extended by Birkhoff and von Neumann). This chapter will review quickly the elementary content of those ideas, adding however several modern results (see also [Var07, Mor18] for a similar approach and [Red98] for an extensive technical account on quantum lattice theory and applications).

4.1 Lattices in Classical and Quantum Mechanics

This section introduces the mathematical notion of *lattice*, which will be used later to construct a bridge between classical and quantum systems.

4.1.1 A Different Viewpoint on Classical Mechanics

Let us start by analyzing Classical Mechanics (CM). Consider a classical Hamiltonian system described on a symplectic manifold (Γ, ω), where $\omega = \sum_{k=1}^{n} dq^k \wedge dp_k$ in any system of local symplectic coordinates $q^1, \ldots, q^n, p_1, \ldots, p_n$. The state of the system at time t is a point $s \in \Gamma$, in local coordinates $s \equiv (q^1, \ldots, q^n, p_1, \ldots, p_n)$, whose evolution $\mathbb{R} \ni t \mapsto s(t)$ solves the *Hamiltonian*

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equations of motion. Always in local symplectic coordinates, they read

$$\frac{dq^k}{dt} = \frac{\partial h(t,q,p)}{\partial p_k}\,, \quad \frac{dp_k}{dt} = -\frac{\partial h(t,q,p)}{\partial q^k}\,, \qquad k = 1,\dots,n\,,$$

h being the Hamiltonian function of the system, depending on the reference frame. Every physical *elementary property* E that the system may possess at a certain time t, i.e. which can be true or false at that time, can be identified with a subset $E \subset \Gamma$. The property is true if $s \in E$ and it is not if $s \notin E$. From this point of view, the standard set operations $\cap$, $\cup$, $\subset$, $\neg$ (where $\neg E := \Gamma \setminus E$ from now on is the **complementation**) have a logical interpretation:

(i) $E \cap F$ corresponds to the property "E AND F",
(ii) $E \cup F$ corresponds to the property "E OR F",
(iii) $\neg E$ corresponds to the property "NOT E",
(iv) $E \subset F$ means "E IMPLIES F".

In this context,

(v) Γ is the property which is always true
(vi) $\varnothing$ is the property which is always false.

This identification is possible because, as is well known, the logical connectives define the same algebraic structure as the set-theory operations.

As soon as we admit the possibility to construct statements including *countably many disjunctions or conjunctions*, we can move into abstract measure theory and interpret states as *probability Dirac measures* supported on a single point. To this end, we initially restrict the class of possible elementary properties to the Borel σ-algebra of Γ, $\mathscr{B}(\Gamma)$. For various reasons this class of sets seems to be sufficiently large to describe the physics (in particular $\mathscr{B}(\Gamma)$ contains the pre-images of measurable sets under continuous functions). A state at time t, $s \in \Gamma$, can be viewed as a Dirac measure, δ_s, supported on s itself. If $E \in \mathscr{B}(\Gamma)$, $\delta_s(E) = 0$ if $s \notin E$ or $\delta_s(E) = 1$ if $s \in E$.

If we do not have a perfect knowledge of the system, as for instance it happens in *statistical mechanics*, the state μ at time t is a proper probability measure on $\mathscr{B}(\Gamma)$, which now is allowed to attain all values in $[0, 1]$. If $E \in \mathscr{B}(\Gamma)$ is an elementary property of the physical system, $\mu(E)$ denotes the probability that the property E is true for the system at time t.

Remark 4.1 The evolution equation of μ, in statistical mechanics is given by the well-known *Liouville equation* associate with the Hamiltonian flow. In that case μ is proportional to the natural symplectic volume of Γ, $\Omega = \omega \wedge \cdots \wedge \omega$ (n-times, where $2n = dim(\Gamma)$). In fact we have $\mu = \rho\Omega$, where the non-negative function ρ is the so-called **Liouville density** satisfying the famous **Liouville equation**. In symplectic local coordinates that equation reads

$$\frac{\partial \rho(t,q,p)}{\partial t} + \sum_{k=1}^{n} \left(\frac{\partial \rho}{\partial q^k} \frac{\partial h}{\partial p_k} - \frac{\partial \rho}{\partial p_k} \frac{\partial h}{\partial q^k} \right) = 0 \, .$$

We shall not deal any further with this equation in this book. ■

More complicated classical quantities of the system can be described by *Borel measurable* functions $f : \Gamma \to \mathbb{R}$. Measurability is a good requirement as it permits one to perform physical operations like computing, for instance, the *expectation value* (at a given time) when the state is μ:

$$\langle f \rangle_\mu = \int_\Gamma f \, d\mu \, .$$

Also elementary properties can be described by measurable functions, in fact they are identified faithfully with Borel measurable functions $g : \Gamma \to \{0, 1\}$. The Borel set E_g associated to g is $g^{-1}(\{1\})$ and in fact $g = \chi_{E_g}$.

A generic physical quantity, a measurable function $f : \Gamma \to \mathbb{R}$, is completely determined by the class of Borel sets (elementary properties) $E_B^{(f)} := f^{-1}(B)$ where $B \in \mathscr{B}(\mathbb{R})$. The meaning of $E_B^{(f)}$ is

$$E_B^{(f)} = \text{“the value of } f \text{ belongs to } B\text{”} \tag{4.1}$$

It is possible to prove [Mor18] that the map $\mathscr{B}(\mathbb{R}) \ni B \mapsto E_B^{(f)}$ permits one to reconstruct the function f. The sets $E_B^{(f)} := f^{-1}(B)$ form a σ-algebra as well and the class of sets $E_B^{(f)}$ satisfies the following elementary properties when B ranges in $\mathscr{B}(\mathbb{R})$.

(Fi) $E_{\mathbb{R}}^{(f)} = \Gamma$,
(Fii) $E_B^{(f)} \cap E_C^{(f)} = E_{B\cap C}^{(f)}$,
(Fiii) If $N \subset \mathbb{N}$ and $\{B_k\}_{k\in N} \subset \mathscr{B}(\mathbb{R})$ satisfies $B_j \cap B_k = \varnothing$ for $k \neq j$, then

$$\cup_{j\in N} E_{B_j}^{(f)} = E_{\cup_{j\in N} B_j}^{(f)} \, .$$

These conditions just say that $\mathscr{B}(\mathbb{R}) \ni B \mapsto E_B^{(f)} \in \mathscr{B}(\Gamma)$ is a **homomorphism of σ-algebras**. Notice in particular that, keeping (Fi) and (Fiii), requirement (Fii) can be replaced by $E_{\mathbb{R}\setminus E}^{(f)} = \Gamma \setminus E_E^{(f)}$ as the reader immediately proves.

We observe that our model of *classical* elementary properties can be also viewed as another mathematical structure, when referring to the notion of *lattice* we go to introduce.

4.1.2 The Notion of Lattice

We remind the reader that in a *partially ordered set* $(X, \geq)$ (or poset), if $Y \subset X$, the symbol $\sup Y$ denotes, if it exists, the smallest element x of X such that $x \geq y$ for every $y \in Y$. Similarly, the symbol $\inf Y$ denotes, if it exists, the largest element x of X such that $y \geq x$ for every $y \in Y$.

Definition 4.2 A partially ordered set $(X, \geq)$ is a **lattice** when, for any $a, b \in X$,

(a) $\sup\{a, b\}$ exists in X, and is called **join** $a \vee b$;
(b) $\inf\{a, b\}$ exists in X, and is called **meet** $a \wedge b$.

(The poset is not required to be totally ordered.) ■

Remark 4.3

(a) In the concrete cases where $X = \mathscr{B}(\mathbb{R})$ or $X = \mathscr{B}(\Gamma)$, $\geq$ is nothing but $\supset$ and thus $\vee$ means $\cup$ and $\wedge$ has the meaning of $\cap$.
(b) In the general case $\vee$ and $\wedge$ turn out to be *associative*, so it makes sense to write $a_1 \vee \cdots \vee a_n$ and $a_1 \wedge \cdots \wedge a_n$ in a lattice. Moreover they are *commutative* so

$$a_1 \vee \cdots \vee a_n = a_{\pi(1)} \vee \cdots \vee a_{\pi(n)} \quad \text{and} \quad a_1 \wedge \cdots \wedge a_n = a_{\pi(1)} \wedge \cdots \wedge a_{\pi(n)}$$

for every permutation $\pi : \{1, \ldots, n\} \to \{1, \ldots, n\}$.
The **absorption laws** are moreover valid: $a \vee (a \wedge b) = a$ and $a \wedge (a \vee b) = a$.
(c) It is easy to prove that in a lattice $a \geq b$ iff $a \vee b = a$ (equivalently $a \wedge b = b$). ■

Definition 4.4 A lattice $(X, \geq)$ is said to be:

(a) **distributive** if $\vee$ and $\wedge$ distribute over one another: for any $a, b, c \in X$,

$$a \vee (b \wedge c) = (a \vee b) \wedge (a \vee c)\,, \quad a \wedge (b \vee c) = (a \wedge b) \vee (a \wedge c)\,;$$

(b) **bounded** if it admits a minimum $\mathbf{0}$ and a maximum $\mathbf{1}$, called **bottom** and **top**;
(c) **orthocomplemented** if bounded and equipped with a mapping $X \ni a \mapsto \neg a$, where $\neg a$ is the **orthocomplement** of a, such that:

 (i) $a \vee \neg a = \mathbf{1}$ for any $a \in X$,
 (ii) $a \wedge \neg a = \mathbf{0}$ for any $a \in X$,
 (iii) $\neg(\neg a) = a$ for any $a \in X$,
 (iv) $a \geq b$ implies $\neg b \geq \neg a$ for any $a, b \in X$;

(d) **complete** (resp. **σ-complete**), if every (countable) set $\{a_j\}_{j \in J} \subset X$ admits infimum $\vee_{j \in J} a_j$ and supremum $\wedge_{j \in J} a_j$.

A lattice with properties (a), (b) and (c) is called a **Boolean algebra**. A Boolean algebra satisfying (d) *with* $J = \mathbb{N}$ is a **Boolean σ-algebra**.

A **sublattice** is a subset $X_0 \subset X$ inheriting the lattice structure from X, in the following precise sense: the infimum and the supremum of any pair of elements of X must exist and coincide with the corresponding infimum and supremum in X. Referring to bounded sublattices and orthocomplemented sublattices, the top, the bottom and the orthocomplement of the substructure must coincide, by definition, with those in the larger structure. ■

It is easy to prove **De Morgan's laws** for an orthocomplemented lattice [Red98, Mor18] just applying the relevant definitions.

Proposition 4.5 *If* $(X, \geq, \mathbf{0}, \mathbf{1}, \neg)$ *is an orthocomplemented lattice and* $A \subset X$ *is finite then, with an obvious notation,*

$$\neg \vee_{a\in A}\, a = \wedge_{a\in A} \neg a \quad \textit{and} \quad \neg \wedge_{a\in A}\, a = \vee_{a\in A} \neg a \ .$$

If A *is infinite, the terms on either side exist or do not exist simultaneously. If they do, the formula holds.*

Definition 4.6 If X, Y are lattices, a map $h : X \to Y$ is a **lattice homomorphism** when

$$h(a \vee_X b) = h(a) \vee_Y h(b)\ , \quad h(a \wedge_X b) = h(a) \wedge_Y h(b)\ , \quad a, b \in X$$

(with the obvious notations.) If X and Y are bounded, a homomorphism h is further required to satisfy

$$h(\mathbf{0}_X) = \mathbf{0}_Y\ , \quad h(\mathbf{1}_X) = \mathbf{1}_Y\ .$$

If X and Y are orthocomplemented, in addition,

$$h(\neg_X a) = \neg_Y h(x)\ .$$

If X, Y are complete (σ-complete), h it is further required to satisfy (with $J = \mathbb{N}$)

$$h(\vee_{j\in J} a_j) = \vee_{j\in J} h(a_j)\ , \quad h(\wedge_{j\in J} a_j) = \wedge_{j\in J} h(a_j) \quad \text{if } \{a_j\}_{j\in J} \subset X\ .$$

In all cases (bounded, orthocomplemented, (σ-)complete lattices, Boolean (σ-) algebras) if h is bijective it is called **isomorphism**. ■

It is clear that, just because it is a concrete σ-algebra, the lattice of the elementary properties of a classical system is a lattice which is *distributive*, *bounded* (here $0 = \varnothing$ and $1 = \Gamma$), *orthocomplemented* (the orthocomplement being the set complement in Γ) and *σ-complete*. Moreover, as the reader can easily prove, the above map, $\mathscr{B}(\mathbb{R}) \ni B \mapsto E^{(f)}_B \in \mathscr{B}(\Gamma)$, is also a homomorphism of Boolean σ-algebras.

Remark 4.7 Given an abstract Boolean σ-algebra X, does there exist a concrete σ-algebra of sets that is isomorphic to it? The *Loomis-Sikorski theorem* [Sik48] gives an answer. This guarantees that every Boolean σ-algebra is isomorphic to a quotient Boolean σ-algebra $\Sigma/\mathcal{N}$, where Σ is a concrete σ-algebra of sets on a measurable space and $\mathcal{N} \subset \Sigma$ is closed under countable unions; moreover, $\varnothing \in \mathcal{N}$ and for any $A \in \Sigma$ with $A \subset N \in \mathcal{N}$, then $A \in \mathcal{N}$. The equivalence relation is $A \sim B$ iff $A \cup B \setminus (A \cap B) \in \mathcal{N}$, for any $A, B \in \Sigma$. It is easy to see the coset space $\Sigma/\mathcal{N}$ inherits the structure of Boolean σ-algebra from Σ with respect to the (well-defined) partial order $[A] \geq [B]$ if $A \supset B$, $A, B \in \Sigma$.

In the simpler case of an abstract Boolean algebra, the celebrated *Stone's representation theorem* [Sto36] proves that it is always isomorphic to a concrete algebra of sets. ■

4.2 The Non-Boolean Logic of QM

It is evident that the classical-like picture illustrated in Sect. 4.1 is untenable for quantum systems. The deep reason is that there are pairs of elementary properties E, F of quantum systems which are incompatible. Here, an elementary property is an observable which, if measured by means of a corresponding experimental apparatus, can only attain two values: 0 if it is false or 1 if it is true. For instance, $E =$ "the component S_x of the electron is $\hbar/2$" and $F =$ "the component S_y of the electron is $\hbar/2$". There is no physical instrument capable to establish if E AND F is true or false. We conclude that some of elementary observables of quantum systems cannot be combined the standard logical connectives. The model of Borel σ-algebra seems not to be appropriate for quantum systems. However one could try to use some form of lattice structure different form the classical one.

4.2.1 The Lattice of Quantum Elementary Observables

The fundamental ideas of von Neumann were the following two.

(N1) Given a quantum system, there is a complex separable Hilbert space H such that the **elementary observables**—the ones which only assume values in $\{0, 1\}$—are represented faithfully by elements of $\mathscr{L}(\mathsf{H})$, the orthogonal projectors in $\mathfrak{B}(\mathsf{H})$.

(N2) Two elementary observables P, Q are compatible if and only if they commute as projectors.

Remark 4.8

(a) As we shall see later, (N1) has to be modified for quantum systems admitting *superselection rules*. For the moment we stick to the above version of (N1).

(b) Separability will play a crucial role in several technical constructions. This technical requirement could actually be omitted, and proved to hold later for specific quantum systems (e.g., elementary particles) as a consequence of specific physical requirements. However we shall assume it from the beginning. ■

Let us analyse the reasons for von Neumann's postulates. First of all we observe that $\mathscr{L}(\mathsf{H})$ is in fact a lattice if one remembers the relation between orthogonal projectors and closed subspaces stated in Proposition 3.16 and equipping the set of closed subspaces with the natural ordering relation given by set-theoretic inclusion relation.

Referring to Notation 3.18, if $P, Q \in \mathscr{L}(\mathsf{H})$, we write $P \geq Q$ if and only if $P(\mathsf{H}) \supset Q(\mathsf{H})$. As announced, it turns out that $(\mathscr{L}(\mathsf{H}), \geq)$ is a lattice and, in particular, it enjoys the following properties.

Proposition 4.9 *Let* H *be a complex (not necessarily separable) Hilbert space. For every* $P \in \mathscr{L}(\mathsf{H})$*, define* $\neg P := I - P$ *(the orthogonal projector onto* $P(\mathsf{H})^\perp$ *according to Proposition 3.16). Then* $(\mathscr{L}(\mathsf{H}), \geq, 0, I, \neg)$ *is a bounded, orthocomplemented, complete (so also* σ*-complete) lattice which is not distributive if* $dim(\mathsf{H}) \geq 2$.

More precisely,

(i) $P \vee Q$ *is the orthogonal projector onto* $\overline{P(\mathsf{H}) + Q(\mathsf{H})}$.
The analogue holds for a set $\{P_j\}_{j\in J} \subset \mathscr{L}(\mathsf{H})$*, namely* $\vee_{j\in J} P_j$ *is the orthogonal projector onto* $\overline{span\{P_j(\mathsf{H})\}_{j\in J}}$.

(ii) $P \wedge Q$ *is the orthogonal projector on* $P(\mathsf{H}) \cap Q(\mathsf{H})$.
The analogue holds for a set $\{P_j\}_{j\in J} \subset \mathscr{L}(\mathsf{H})$*, namely* $\wedge_{j\in J} P_j$ *is the orthogonal projector onto* $\cap_{j\in J} P_j(\mathsf{H})$.

(iii) *The bottom and top elements are respectively* 0 *and* I.

(iv) *Referring to (i) and (ii), if* $J = \mathbb{N}$

$$\vee_{n\in\mathbb{N}} P_n = s\text{-}\lim_{k\to+\infty} \vee_{n\leq k} P_n \quad \textit{and} \quad \wedge_{n\in\mathbb{N}} P_n = s\text{-}\lim_{k\to+\infty} \wedge_{n\leq k} P_n \tag{4.2}$$

where "s-" indicates that the limits are computed in the strong operator topology.

Proof The fact that $\mathscr{L}(\mathsf{H})$ is a lattice is evident when we interpret it as a poset of closed subspaces. It is clear that $\sup\{P(\mathsf{H}), Q(\mathsf{H})\} = \overline{P(H) + Q(H)}$ if $P, Q \in \mathscr{L}(\mathsf{H})$, since $\sup\{P(\mathsf{H}), Q(\mathsf{H})\}$ contains both $P(\mathsf{H})$ and $Q(\mathsf{H})$ and every closed subspace containing these subspaces must also contain $\overline{P(H) + Q(H)}$ by linearity and definition of closure. It is clear that $\inf\{P(\mathsf{H}), Q(\mathsf{H})\} = P(H) \cap Q(H)$ if $P, Q \in \mathscr{L}(\mathsf{H})$, since the closed subspace $P(\mathsf{H}) \cap Q(\mathsf{H})$ is contained in both $P(\mathsf{H})$ and $Q(\mathsf{H})$ and every closed subspaces that is part of both $P(\mathsf{H})$ and $Q(\mathsf{H})$ must be contained in these subspaces must be contain in the closed subspace $P(\mathsf{H}) \cap Q(\mathsf{H})$. A trivial extension of the same arguments proves (i) and (ii). It is evident that $\mathscr{L}(\mathsf{H})$ is bounded with said top and bottom. The fact that $\neg P := I - P$ (that is the orthogonal projector onto $P(\mathsf{H})^\perp$ as established in Proposition 3.16 (b)) is an orthocomplement can be immediately proved by direct inspection using properties of $^\perp$ presented in Sect. 2.1.2 and in Proposition 3.16. Failure of distributivity for $\dim(\mathsf{H}) \geq 2$ immediately arises form the analog for $\mathsf{H} = \mathbb{C}^2$ we go to prove. Let $\{e_1, e_2\}$ be the standard basis of $\mathbb{C}^2$ and define the subspaces $\mathsf{H}_1 := \text{span}\{e_1\}$, $\mathsf{H}_2 := \text{span}\{e_2\}$, $\mathsf{H}_3 := \text{span}\{e_1 + e_2\}$. Finally P_1, P_2, P_3 respectively denote the orthogonal projectors onto these spaces. By direct inspection one sees that $P_1 \wedge (P_2 \vee P_3) = P_1 \wedge I = P_1$ and $(P_1 \wedge P_2) \vee (P_1 \wedge P_3) = 0 \vee 0 = 0$, so that $P_1 \wedge (P_2 \vee P_3) \neq (P_1 \wedge P_2) \vee (P_1 \wedge P_3)$. To end the proof, let us prove (4.2). Consider the former limit. $P := \text{s-}\lim_{k\to+\infty} \vee_{n\leq k} P_n$ exists in $\mathscr{L}(\mathsf{H})$ in view of Proposition 3.20 since $\vee_{n\leq k} P_n$ projects onto larger and larger subspaces as n increases. We want to prove that the limit P coincides to the projector onto $\overline{\text{span}\{P_j(\mathsf{H})\}_{j\in J}}$ denoted by $\vee_{n\in\mathbb{N}} P_n$ in (i). It is clear that $\vee_{n\leq k} P_n \leq P$ by definition of P as it holds that

$$\langle x| \vee_{n\leq k} P_n x\rangle \leq \sup_{k\in\mathbb{N}} \langle x| \vee_{n\leq k} P_n x\rangle = \lim_{k\to+\infty} \langle x| \vee_{n\leq k} P_n x\rangle = \langle x|Px\rangle ,$$

so $P(\mathsf{H})$ contains all subspaces $\vee_{n\leq k} P_n$ and also each single $P_n(\mathsf{H})$. So $P(\mathsf{H})$ contains their finite span, by linearity, and also the closure of the span, because $P(\mathsf{H})$ is closed. Hence $P(\mathsf{H}) \supset \overline{\text{span}\{P_n(\mathsf{H})\}_{n\in\mathbb{N}}}$. On the other hand, if $x \in P(\mathsf{H})$, then $x = \lim_{k\to+\infty} \vee_{n\leq k} P_n x \in \overline{\text{span}\{P_n(\mathsf{H})\}_{n\in\mathbb{N}}}$, hence $P(\mathsf{H}) \subset \overline{\text{span}\{P_n(\mathsf{H})\}_{n\in\mathbb{N}}}$. We conclude that $P(\mathsf{H}) = \overline{\text{span}\{P_n(\mathsf{H})\}_{n\in\mathbb{N}}}$. For (i), this is the same as saying $P = \vee_{n\in\mathbb{N}} P_n$. The proof of the second formula in (4.2) is identical barring trivial changes. □

4.2.2 Part of Classical Mechanics is Hidden in QM

To go on, the crucial observation is that $(\mathscr{L}(\mathsf{H}), \geq, 0, I, \neg)$ contains lots of Boolean σ-algebras, and precisely the maximal sets of pairwise compatible projectors. These σ-algebras in the quantum context could be interpreted as made of classical observables at least concerning mutual relations.

Proposition 4.10 *Let* H *be a complex separable Hilbert space and consider the lattice of orthogonal projectors* $(\mathscr{L}(\mathsf{H}), \geq, 0, I, \neg)$.

Assume that $\mathscr{L}_0 \subset \mathscr{L}(\mathsf{H})$ *is a maximal subset of pairwise commuting elements (i.e. if* $Q \in \mathscr{L}(\mathsf{H})$ *commutes with every* $P \in \mathscr{L}_0$ *then* $Q \in \mathscr{L}_0$*). Then* $\mathscr{L}_0$ *contains* 0, I*, it is* $\neg$*-closed. Furthermore, when equipped with the restriction of the lattice structure of* $(\mathscr{L}(\mathsf{H}), \geq, 0, I, \neg)$*, it becomes a Boolean* σ*-algebra (in particular the supremum and the infimum of sequences of elements computed in* $\mathscr{L}_0$ *coincide with the corresponding inf and sup in the whole* $\mathscr{L}(\mathsf{H})$*). Finally, if* $P, Q \in \mathscr{L}_0$,

(i) $P \vee Q = P + Q - PQ$,
(ii) $P \wedge Q = PQ$.

Proof $\mathscr{L}_0$ contains both 0 and I because $\mathscr{L}_0$ is maximally commutative and is $\neg$ closed: $\neg P = I - P$ commutes with every element of $\mathscr{L}_0$ if $P \in \mathscr{L}_0$, so $\neg P \in \mathscr{L}_0$ due to the maximality condition. Taking advantage of the associativity of $\vee$ and $\wedge$, and using (iv) in Proposition 4.9, the sup and inf of a sequence of projectors $\{P_n\}_{n\in\mathbb{N}} \subset \mathscr{L}_0$ commute with the elements of $\mathscr{L}_0$ since every element $\vee_{n\leq k} P_n$ and $\wedge_{n\leq k} P_n$ does by direct application of (i) and (ii). Maximality implies that these limit projectors belong to $\mathscr{L}_0$. Finally (i) and (ii) prove by direct inspection that $\vee$ and $\wedge$ are mutually distributive. Let us prove (ii) and (i) to conclude. If $PQ = QP$, PQ is an orthogonal projector and $PQ(\mathsf{H}) = QP(\mathsf{H}) \subset P(\mathsf{H}) \cap Q(\mathsf{H})$. On the other hand, if $x \in P(\mathsf{H}) \cap Q(\mathsf{H})$ then $Px = x$ and $x = Qx$ so that $PQx = x$ and thus $P(\mathsf{H}) \cap Q(\mathsf{H}) \subset PQ(\mathsf{H})$ and (ii) holds. To prove (i) observe that $\overline{P(\mathsf{H}) + Q(\mathsf{H})}^{\perp} = (P(\mathsf{H}) + Q(\mathsf{H}))^{\perp}$. By linearity, $(P(\mathsf{H}) + Q(\mathsf{H}))^{\perp} = P(\mathsf{H})^{\perp} \cap Q(\mathsf{H})^{\perp}$. Therefore $\overline{P(\mathsf{H}) + Q(\mathsf{H})} = (\overline{P(\mathsf{H}) + Q(\mathsf{H})}^{\perp})^{\perp} = (P(\mathsf{H})^{\perp} \cap Q(\mathsf{H})^{\perp})^{\perp}$. Using (ii), and the fact that $I - R$ is the orthogonal projector onto $R(\mathsf{H})^{\perp}$, this can be rephrased as $P \vee Q = I - (I - P)(I - Q) = I - (I - P - Q + PQ) = P + Q - PQ$. □

Remark 4.11

(a) Every set of pairwise commuting orthogonal projectors can be completed to a maximal set as an elementary application of Zorn's lemma. However, since the commutativity property is *not* transitive, there are many possible maximal subsets of pairwise commuting elements in $\mathscr{L}(\mathsf{H})$ with non-empty intersection.
(b) As a consequence of the proposition, the symbols $\vee$, $\wedge$ and $\neg$ have the same properties in $\mathscr{L}_0$ as the connectives of classical logic OR, AND and NOT. Moreover $P \geq Q$ can be interpreted as "Q IMPLIES P". ■

There have been and still are many attempts to interpret $\vee$ and $\wedge$ as connectives of a new non-distributive logic when dealing with the whole $\mathscr{L}(\mathsf{H})$: a *quantum logic*. The first noticeable proposal was due to Birkhoff and von Neumann [BivN36]. Nowadays there are lots of quantum logics [BeCa81, Red98, EGL09], all regarded with suspicion by physicists. Indeed, the most difficult issue is the physical operational interpretation of these connectives is to take in account the fact that they put together incompatible propositions, which cannot be measured simultaneously. An interesting interpretative attempt, due to Jauch, relies up an identity discovered by von Neumann. For the proof we will use the machinery of spectral theory and produce an original proof. More elementary proofs appear in [Red98] and [Mor18], based on technical propositions we did not discuss in these lectures.

Proposition 4.12 *In a Hilbert space* H, *for every* $P, Q \in \mathscr{L}(\mathsf{H})$ *and* $x \in \mathsf{H}$,

$$(P \wedge Q)x = \lim_{n\to+\infty} (PQ)^n x \tag{4.3}$$

Proof Fix $x \in \mathsf{H}$ and (uniquely) decompose it as

$$x = x_0 + y\,, \text{ where } x_0 \in (P \wedge Q)(\mathsf{H}) = P(\mathsf{H}) \cap Q(\mathsf{H}) \text{ and } y \in (P(\mathsf{H}) \cap Q(\mathsf{H}))^{\perp}. \tag{4.4}$$

Consider the sequence of operators $A_1 := P,\ A_n := QP,\ A_3 := PQP,\ A_4 := QPQP, \cdots$ We want to prove that

$$A_n y \to 0\,. \tag{4.5}$$

This would conclude the proof because $A_n x_0 = x_0$ since $x_0 \in P(\mathsf{H})$ and $x_0 \in Q(\mathsf{H})$, so that $Px_0 = Qx_0 = x_0$ and $A_n x \to x_0 + 0 = x_0$; finally, the sequence $\{(PQ)^n x\}_{n\in\mathbb{N}}$ is a subsequence of $\{A_n x\}_{n\in\mathbb{N}}$ and thus it converges to the same limit x_0, proving (4.3).

To prove (4.5), observe that the sequence of operators applied to y, $\{A_n y\}_{n\in\mathbb{N}}$, satisfies

$$||A_{n+1}y|| \leq ||A_n y||\,,$$

since either $A_{n+1} = PA_n$ or $A_{n+1} = QA_n$ and $||P||, ||Q|| \leq 1$. The non-increasing sequence $\{||A_n y||\}_{n\in\mathbb{N}}$ must therefore admit a limit in view of elementary results of calculus. If we found a *subsequence* of $\{A_n y\}_{n\in\mathbb{N}}$ converging to 0 we would prove that also $||A_n y|| \to 0$ as $n \to +\infty$ which, in turn, would entail (4.5). The following lemma concludes the proof.

Lemma 4.13 *The subsequence* $\{A_{2n+1}y\}_{n\in\mathbb{N}}$ *tends to* 0 *as* $n \to +\infty$.

Proof Consider the subsequence of operators $\{A_{2n+1}\}_{n\in\mathbb{N}}$. Remembering that $PP = P$, we have

$$A_3 = PQP =: B,\ A_5 = PQPQP = (PQP)^2 = B^2,\ A_7 = PQPQPQP = (PQP)^3 = B^3, \cdots$$

$$\cdots, A_{2n+1} = B^n, \cdots$$

Notice that

(1) $B^* = (PQP)^* = P^*Q^*P^* = PQP = B \in \mathfrak{B}(\mathsf{H})$,
(2) $||B|| \leq ||P||||Q||||P|| \leq 1$,
(3) $\sigma(B) \subset [-||B||, ||B||]$ (Proposition 3.47),
(4) $\sigma(B) \in [0, +\infty)$ (Proposition 3.46) as $\langle z|Bz\rangle = \langle Pz|QPz\rangle = \langle Pz|QQPz\rangle = ||QPz||^2 \geq 0$.

Collecting these results, we have from the spectral theory

$$B^n z = \int_{[0,1]} \lambda^n dP^{(B)}(\lambda) z \quad \text{if } z \in \mathsf{H}\,.$$

Since $\lambda^n \to \chi_{\{1\}}(\lambda)$ pointwise for $\lambda \in [0,1]$ if $n \to +\infty$, exploiting Proposition 3.29 (b), we conclude that

$$B^n z \to Ez := P^{(B)}_{\{1\}} z \quad \text{as } n \to +\infty \text{ and } z \in \mathsf{H}. \tag{4.6}$$

With the same argument we can also prove that

$$C^n z \to Fz := P^{(C)}_{\{1\}} z \quad \text{as } n \to +\infty \text{ and } z \in \mathsf{H}, \tag{4.7}$$

where we have defined the other sequence of operators (which is not a subsequence of $\{A_n\}_{n\in\mathbb{N}}$)

$$C := QPQ,\ C^2 = (QPQ)^2 = QPQPQ,\ B^3 = (QPQ)^3 = QPQPQPQ, \cdots .$$

We now prove that the formula of orthogonal projectors holds $E = F$. To this end, notice that

$$(PQP)^n (QPQ)^m (PQP)^l z = (PQP)^{n+m+l+1} z\,,$$

which implies $EFE = E$. (To prove it, take first the limit as $m \to +\infty$ using the continuity of $(PQP)^n$, next the limit as $l \to +\infty$ using the continuity of $(PQP)^n F$ and eventually the limit as $n \to +\infty$.) Swapping the role of P and Q we also have $FEF = F$. From $EFE = E$ we obtain

$$0 = \langle z|(E - EFE - EFE + EFE)z\rangle = \langle z|(E^2 - EFE - EFE + EFE)z\rangle = \langle z|(E - EF)(E - FE)z\rangle$$

$$= \langle z|(E - FE)^*(E - FE)z\rangle = ||(E - FE)z||^2 \text{ for } z \in \mathsf{H}.$$

Hence $E = FE$. Starting from $FEF = F$, with the same argument, we find $F = EF$. Putting together the found results, we find $F = E$ as wanted, since $F = F^* = (EF)^* = FE = E$.

To go on, observe that, by construction of E and F, $PE = E$ and $QF = F$, so that

$$E(\mathsf{H}) = F(\mathsf{H}) \subset P(\mathsf{H}) \cap Q(\mathsf{H})\,.$$

If we apply the result to the sequence $B^n y$ in (4.6) with y in (4.4), we obtain

$$A_{2n+1} y = B^n y \to Ey \in P(\mathsf{H}) \cap Q(\mathsf{H})\,. \tag{4.8}$$

However we also have that

$$A_{2n+1} y = B^n y \to Ey \in (P(\mathsf{H}) \cap Q(\mathsf{H}))^\perp \tag{4.9}$$

because $(P(\mathsf{H}) \cap Q(\mathsf{H}))^\perp$ is closed and every $A_{2n+1}y$ belongs to $(P(\mathsf{H}) \cap Q(\mathsf{H}))^\perp$ since, if $s \in P(\mathsf{H}) \cap Q(\mathsf{H})$ then $\langle s|A_{2n+1}y\rangle = \langle s|(QP \cdots QP)y\rangle = \langle (PQ \cdots PQ)s|y\rangle = \langle s|y\rangle = 0$ because $y \in (P(\mathsf{H}) \cap Q(\mathsf{H}))^\perp$ by (4.4).

The only possibility permitted by (4.8) and (4.9) is $A_{2n+1}y \to 0$. □

As said above, the lemma ends the proof. □

Remark 4.14

(a) The proof actually proves the stronger fact:

$$Px,\ QPx,\ PQPx,\ QPQPx,\ PQPQPQPx,\ \cdots \to (P \wedge Q)x \quad \forall x \in \mathsf{H}.$$

We also have

$$Qx,\ PQx,\ QPQx,\ PQPQx,\ QPQPQPQx,\ \cdots \to (P \wedge Q)x \quad \forall x \in \mathsf{H},$$

since $P \wedge Q = Q \wedge P$

(b) Notice that the result holds in particular if P and Q do not commute, so they are incompatible elementary observables. The right-hand side of the formula above can be interpreted as the consecutive and alternated measurement of an infinite sequence of elementary observables P and Q. As

$$||(P \wedge Q)x||^2 = \lim_{n\to+\infty} ||(PQ)^n x||^2 \quad \text{for every } P, Q \in \mathscr{L}(\mathsf{H}) \text{ and } x \in \mathsf{H},$$

the probability that $P \wedge Q$ is true for a state represented by the unit vector $x \in \mathsf{H}$ is the probability that the infinite sequence of consecutive alternated measurements of P and Q produce is true at each step. ■

Exercise 4.15 Prove that, if $P, Q \in \mathscr{L}(\mathsf{H})$, then $P + Q \in \mathscr{L}(\mathsf{H})$ if and only if P and Q project onto orthogonal subspaces.

Solution If P and Q project onto orthogonal subspaces then $PQ = QP = 0$ (Proposition 3.17), so that $\mathscr{L}(\mathsf{H}) \ni P \vee Q = P + Q - PQ = P + Q$ due to Proposition 4.10. Suppose conversely that $P + Q \in \mathscr{L}(\mathsf{H})$. Therefore $(P + Q)^2 = P+Q$. In other words, $P^2+Q^2+PQ+QP = P+Q$, namely $P+Q+PQ+QP = P + Q$ so that we end up with $PQ = -QP$. Applying P on the right, we obtain $PQP = -QP$ and applying P on the left we produce $PQP = -PQP$. Hence $PQP = 0$. From $PQP = -QP$, we also have $QP = 0$ and also $PQ = 0$ if taking the adjoint. Proposition 3.17 implies that P and Q project onto orthogonal subspaces. □

4.2.3 A Reason Why Observables Are Selfadjoint Operators

We are in a position to clarify why, in this context, observables are PVMs on $\mathscr{B}(\mathbb{R})$ and therefore they are also selfadjoint operators in view of the spectral integration and disintegration procedure, since $PVMs$ on $\mathscr{B}(\mathbb{R})$ are one-to-one with selfadjoint operators. Exactly as in CM, an observable A can be viewed as collection of elementary YES-NO observables $\{P_E\}_{E\in\mathscr{B}(\mathbb{R})}$ labeled on the Borel sets E of $\mathbb{R}$. Exactly as for classical quantities, (4.1) we can say that the meaning of P_E is

$$P_E = \text{“the value of the observable belongs to } E\text{''} . \tag{4.10}$$

Assuming, as is obvious, that all those elementary observables are pairwise compatible, we can complete $\{P_E\}_{E\in\mathscr{B}(\mathbb{R})}$ to a maximal set of compatible elementary observables $\mathscr{L}_0$ and we can work in there forgetting Quantum Theory. We therefore expect that they also satisfy the same properties (Fi)-(Fiii) of the classical quantities. Notice that (Fi)-(Fiii) immediately translate into

(i)' $P_{\mathbb{R}} = I$,
(ii)' $P_E \wedge P_F = P_{E\cap F}$,
(iii)' If $N \subset \mathbb{N}$ and $\{E_k\}_{k\in N} \subset \mathscr{B}(\mathbb{R})$ satisfies $E_j \cap E_k = \varnothing$ for $k \neq j$, then

$$\vee_{j\in N} P_{E_j} = P_{\cup_{j\in N} E_j} \; .$$

Next, taking Proposition 4.10 into account (in particular Propositions 4.9 (iv) and 4.10 (iv), for (iii) below), these properties become

(i) $P_{\mathbb{R}} = I$,
(ii) $P_E P_F = P_{E\cap F}$,
(iii) If $N \subset \mathbb{N}$ and $\{E_k\}_{k\in N} \subset \mathscr{B}(\mathbb{R})$ satisfies $E_j \cap E_k = \varnothing$ for $k \neq j$, then

$$\sum_{j\in N} P_{E_j} x = P_{\cup_{j\in N} E_j} x \quad \text{for every } x \in \mathsf{H}.$$

(The presence of x is due to the fact that the convergence of the series if N is infinite is in the strong operator topology as declared in the last statement of Proposition 4.9.)

In other words we have just found Definition 3.21, specialized to a PVM on $\mathbb{R}$: observables in QM (viewed as collections of elementary propositions labelled over the Borel sets of $\mathbb{R}$) are PVMs on $\mathbb{R}$. We also know that PVMs on $\mathbb{R}$ are associated in a 1-1 way to selfadjoint operators, in view of the results presented in the previous chapter. Indeed, integrating the function $\iota : \mathbb{R} \ni r \mapsto r \in \mathbb{R}$ with respect to P we have the normal operator

$$A_P = \int_{\mathbb{R}} r \, dP(r)$$

according to Theorem 3.24. This operator is selfadjoint because the integrand function is real-valued (Theorem 3.24 (c)). Finally, Theorem 3.40 proves that P is the unique PVM associated to the operator A_P and the support of P is $\sigma(A_P)$. The operator A_P encapsulates all information of the PVM $\{P_E\}_{E\in\mathscr{B}(\mathbb{R})}$, i.e. of the associated observable A as a collection of elementary propositions labelled over the Borel sets of $\mathbb{R}$.

We conclude that, adopting von Neumann's framework, in QM observables are naturally described by selfadjoint operators, whose spectra coincide with the set of values attained by the observables.

4.3 Recovering the Hilbert Space Structure: The "Coordinatization" Problem

A reasonable question to ask is whether there are better reasons for choosing to describe quantum systems via a lattice of orthogonal projectors, other than the kill-off argument "it works". To tackle the problem we start by listing special properties of the lattice of orthogonal projectors, whose proofs are elementary. The notion of **orthomodularity** shows up below. It is a weaker version of distributivity of the $\vee$ with respect to $\wedge$, that we know to be untenable on $\mathscr{L}(\mathsf{H})$. A second notion is that of *atom*. (See [Red98] for a concise discussion on these properties and a list of alternative and equivalent reformulations of orthomodularity condition.)

Definition 4.16 If $(\mathscr{L}, \geq, \mathbf{0}, \mathbf{1})$ is a bounded lattice, $a \in \mathscr{L} \setminus \{\mathbf{0}\}$ is called **atom** if $p \leq a$ implies $p = \mathbf{0}$ or $p = a$. ■

The following theorem collects all relevant properties of the special lattice $\mathscr{L}(\mathsf{H})$, simultaneously defining them. These definitions may actually apply to a generic orthocomplemented lattice.

Theorem 4.17 *In the bounded, orthocomplemented, σ-complete lattice $\mathscr{L}(\mathsf{H})$ of Propositions 4.9 and 4.10, the orthogonal projectors onto one-dimensional spaces are the only atoms of $\mathscr{L}(\mathsf{H})$. Moreover $\mathscr{L}(\mathsf{H})$ satisfies these additional properties:*

(i) ***separability*** *(for H separable): if $\{P_a\}_{a\in A} \subset \mathscr{L}(\mathsf{H}) \setminus \{0\}$ satisfies $P_i \leq \neg P_j$, $i \neq j$, then A is at most countable;*
(ii1) ***atomicity***: *for any $P \in \mathscr{L}(\mathsf{H}) \setminus \{0\}$ there exists an atom A with $A \leq P$;*
(ii2) ***atomisticity***: *for every $P \in \mathscr{L}(\mathsf{H}) \setminus \{0\}$, then $P = \vee\{A \leq P \mid A$ is an atom of $\mathscr{L}(\mathsf{H})\}$;*
(iii) ***orthomodularity***: *$P \leq Q$ implies $Q = P \vee ((\neg P) \wedge Q)$;*
(iv) ***covering property***: *if $A, P \in \mathscr{L}(\mathsf{H})$, with A an atom, satisfy $A \wedge P = 0$, then*

  (1) *$P \leq A \vee P$ with $P \neq A \vee P$, and*
  (2) *$P \leq Q \leq A \vee P$ implies $Q = P$ or $Q = A \vee P$;*

(v) ***irreducibility***: *only 0 and I commute with every element of $\mathscr{L}(\mathsf{H})$.*

Proof Everything has an immediate elementary proof. The only pair of properties which are not completely trivial are orthomodularity and irreducibility. The former immediately arises form the observation that $P \leq Q$ is equivalent to $PQ = QP = Q$ (Proposition 3.17) so that, in particular P and Q commute. Embedding them in a maximal set of pairwise commuting projectors, we can use Proposition 4.10:

$$P \vee ((\neg P) \wedge Q) = P \vee ((I - P)Q) = P \vee (Q - P) = P + (Q - P) - P(Q - P)$$
$$= P + Q - P - P + P = Q\,.$$

Irreducibility can easily be proved observing that if $P \in \mathscr{L}(\mathsf{H})$ commutes with all projectors onto one-dimensional subspaces, $Px = \lambda_x x$ for every $x \in \mathsf{H}$. Thus $P(x + y) = \lambda_{x+y}(x + y)$ but also $Px + Py = \lambda_x x + \lambda_y y$ and thus $(\lambda_x - \lambda_{x+y})x = (\lambda_{x+y} - \lambda_y)y$, which entails $\lambda_x = \lambda_y$ if $x \perp y$. If $N \subset \mathsf{H}$ is a Hilbert basis, $Pz = \sum_{x \in N} \langle x|z\rangle \lambda x = \lambda z$ for some fixed $\lambda \in \mathbb{C}$. Since $P = P^* = PP$, we conclude that either $\lambda = 0$ or $\lambda = 1$, i.e. either $P = 0$ or $P = I$, as wanted. □

Actually, each of the listed properties admits a physical operational interpretation (e.g. see [BeCa81]). So, based on the experimental evidence of quantum systems, we could try to prove, in the absence of any Hilbert space, that elementary propositions with experimental outcome in $\{0, 1\}$ form a poset. More precisely, we could attempt to find a bounded, orthocomplemented σ-complete lattice that verifies conditions (i)–(v) above, and then try to prove this lattice is described by the orthogonal projectors of a Hilbert space. This is known as the *coordinatization problem* [BeCa81], which can be traced back to von Neumann's first works on the subject.

The partial order relation of elementary propositions can be defined in various ways. But it will always correspond to the logical implication, in some way or another. Starting from [Mac63] a number of approaches (either of essentially physical nature, or of formal character) have been developed to this end: in particular, those making use of the notion of (quantum) *state*, which we will see in a short while for the concrete case of propositions represented by orthogonal projectors. The object of the theory is now [Mac63] the pair $(\mathcal{O}, \mathscr{S})$, where $\mathcal{O}$ is the class of observables and $\mathscr{S}$ the one of states. The elementary propositions form a subclass $\mathscr{L}$ of $\mathcal{O}$ equipped with a natural poset structure $(\mathscr{L}, \geq)$ (also satisfying a weaker version of some of the conditions (i)–(v)). A state $s \in \mathscr{S}$, in particular, defines the probability $m_s(P)$ that P is true for every $P \in \mathscr{L}$ [Mac63]. As a matter of fact, if $P, Q \in \mathscr{L}$, $P \geq Q$ means by definition that the probability $m_s(P) \geq m_s(Q)$ for every state $s \in \mathscr{S}$. More difficult is to justify that the poset thus obtained is a lattice, i.e. that it admits a greatest lower bound $P \vee Q$ and a least upper bound $P \wedge Q$ for every P, Q. There are several proposals, very different in nature, to introduce this lattice structure (see [BeCa81] and [EGL09] for a general treatise) and make the physical meaning explicit in terms of measurement outcome. See Aerts in [EGL09] for an abstract but operational viewpoint and [BeCa81, §21.1] for a summary on several possible ways to introduce the lattice structure on the partially ordered sets.

If we accept the lattice structure on elementary propositions of a quantum system, then we may define the operation of orthocomplementation by the familiar logical/physical negation. An apparent problem is the abstract definition of the notion of *compatible propositions*, since this notion makes explicit use of the structure of $\mathscr{L}(\mathsf{H})$ as set of operators. Actually also this notion is general and can be defined for generic orthocomplemented lattices.

Definition 4.18 Let $(\mathscr{L}, \geq, \mathbf{0}, \mathbf{1}, \neg)$ be an orthocomplemented lattice and consider two elements $a, b \in \mathscr{L}$.

(a) They are said to be **orthogonal** written $a \perp b$, if $\neg a \geq b$ (or equivalently $\neg b \geq a$).
(b) They are said to be **commuting**, if $a = c_1 \vee c_3$ and $b = c_2 \vee c_3$ with $c_i \perp c_j$ if $i \neq j$.

■

Remark 4.19

(a) These notions of orthogonality and compatibility make sense because, a posteriori, they turn out to be the usual ones when propositions are interpreted via projectors.

Proposition 4.20 *If* H *Let* H *a Hilbert space and think of* $\mathscr{L}(\mathsf{H})$ *as an orthocomplemented lattice. Two elements* $P, Q \in \mathscr{L}(\mathsf{H})$

(i) *are orthogonal in the sense of Definition 4.18 if and only if they project onto mutually orthogonal subspaces, which it is equivalent to saying* $PQ = QP = 0$*;*
(ii) *commute in accordance with Definition 4.18 if and only if* $PQ = QP$.

Proof

(i) $\neg P \geq Q$ is equivalent to $Q(\mathsf{H}) \subset P(\mathsf{H})^\perp$; in turn, this is the same as $PQ = QP = 0$ for Proposition 3.17.
(ii) Assume that $P = P_1 \vee P_3$ and $Q = P_1 \vee P_2$ where $P_i P_j = 0$ if $i \neq j$ so that, in particular, P_i and P_j commute. Therefore, embedding the P_j in a maximal set of commuting projectors $\mathscr{L}_0$, in view of Proposition 4.10 we have $P = P_1 + P_2 - P_1P_2 = P_1 + P_2$ and $Q = P_1 + P_3 - P_1P_3 = P_1 + P_3$ and also $PQ = QP$ since P_i and P_j commute. If conversely, $PQ = QP$, the required decomposition comes from choosing $P_3 := PQ$, $P_1 := P(I - Q)$, $P_2 := Q(I - P)$. □

(b) It is not difficult to prove [BeCa81, Mor18] that, in an orthocomplemented lattice $\mathscr{L}$, p, q commute if and only if the intersection of all orthocomplemented sublattices containing both p and q (an orthocomplemented sublattice in its own right) is Boolean. ■

Now, fully fledged with an orthocomplemented lattice and the notion of compatible propositions, we can attach a physical meaning (an interpretation backed by experimental evidence) to the requests that the lattice be orthocomplemented, complete, atomistic, irreducible and that it have the covering property [BeCa81]. Under these hypotheses and assuming there exist at least four pairwise-orthogonal atoms, Piron ([Pir64, JaPi69],[BeCa81, §21], Aerts in [EGL09]) used projective geometry techniques to show that the lattice of quantum propositions can be canonically identified with the closed (in a generalized sense) subsets of a Hilbert space of sorts. In the latter:

(a) the field is replaced by a division ring (typically not commutative) equipped with an involution, and
(b) there exists a certain non-singular Hermitian form associated with the involution.

It has been conjectured by many people (see [BeCa81]) that if the lattice is also orthomodular and separable, the division ring can only be picked among $\mathbb{R}$, $\mathbb{C}$ or $\mathbb{H}$ (quaternion algebra).

More recently Solèr [Sol95] first and then Holland [Hol95] and Aerts–van Steirteghem [AeSt00] have found sufficient hypotheses, in terms of the existence of infinite orthogonal systems, for this to happen. These results are usually quoted as *Solèr's theorem*. Under these hypotheses, if the ring is $\mathbb{R}$ or $\mathbb{C}$, we obtain precisely the lattice of orthogonal projectors of the separable Hilbert space. In the case of $\mathbb{H}$, one gets a similar generalized structure (see, e.g., [GMP13, GMP17]).

In all these arguments irreducibility is not really crucial: if property (v) fails, the lattice can be split into irreducible sublattices [Jau78, BeCa81]. Physically speaking this situation is natural in the presence of *superselection rules*, of which more later.

An evident issue arises here: *why do physicists do not know quantum systems described on real or quaternionic Hilbert spaces?*

This is a longstanding problem which was recently solved, at least for the physical description of elementary relativistic systems [MoOp17, MoOp19]. It seems that the complex structure is just a sort of accident imposed by relativistic symmetry.

Remark 4.21 It is worth stressing that the *covering property* in Theorem 4.17 is crucial. Indeed there are other lattice structures relevant in physics verifying all the remaining properties in the aforementioned theorem. Remarkably the family of so-called *causally closed sets* in a general spacetime satisfies all said properties but the covering law (see, e.g. [Cas02]). This obstruction prevents one from endowing a spacetime with a natural (generalized) Hilbert structure, while it suggests ideas towards a formulation of quantum gravity. ■

4.4 Quantum States as Probability Measures and Gleason's Theorem

As commented in Remark 3.66, the probabilistic interpretation of quantum states is not well defined because there is no true probability measure in view of the fact that there are incompatible observables. The idea is to redefine the notion of probability in the bounded, orthocomplemented, σ-complete lattice like $\mathscr{L}(\mathsf{H})$ instead of on a σ-algebra. The study of these generalized measures is the final goal of this section.

4.4.1 Probability Measures on $\mathscr{L}(\mathsf{H})$

Exactly as in CM, where the generic states are probability measures on Boolean lattice $\mathscr{B}(\Gamma)$ of the elementary properties of the system (Sect. 4.1), we can think of states of a quantum system as σ-additive probability measures on the non-Boolean lattice of the elementary observables $\mathscr{L}(\mathsf{H})$. A state is therefore a map $\rho : \mathscr{L}(\mathsf{H}) \ni P \mapsto \rho(P) \in [0, 1]$ that satisfies $\rho(I) = 1$ and a σ-additive requirement

$$\rho\left(\vee_{n\in\mathbb{N}} P_n\right) = \sum_{n\in\mathbb{N}} \rho(P_n) \ ,$$

where the sequence $\{P_n\}_{n\in\mathbb{N}} \subset \mathscr{L}(\mathsf{H})$ is made of **mutually exclusive** elementary propositions, i.e., simultaneously *compatible* ($P_i P_j = P_j P_i$) and *independent* ($P_i \wedge P_j = 0$ if $i \neq j$). In other words, since $P_i \wedge P_j = P_i P_j$ when the projectors commute, the said condition can be equivalently stated by requiring that $P_i P_j = P_j P_i = 0$ for $i \neq j$, also written $P_i \perp P_j$ if $i \neq j$. Making use of associativity of $\vee$ and Proposition 4.10 (i), we have

$$\vee_{n\leq k} P_n = \sum_{n=0}^{k} P_n \ .$$

Next, exploiting Proposition 4.9 (iv), we can write the projector $\vee_{n\in\mathbb{N}} P_n$ into a more effective way:

$$\vee_{n\in\mathbb{N}} P_n = \text{s-}\lim_{k\to+\infty} \vee_{n\leq k} P_n = \text{s-}\lim_{k\to+\infty} \sum_{n=0}^{k} P_n = \text{s-}\sum_{n\in\mathbb{N}} P_n \ .$$

(As usual "s-" denotes the limit in the strong operator topology.) The σ-additivity requirement can be rephrased as

$$\rho\left(\text{s-}\sum_{n\in\mathbb{N}} P_n\right) = \sum_{n\in\mathbb{N}} \rho(P_n) \qquad (4.11)$$

where the sequence $\{P_n\}_{n\in\mathbb{N}} \subset \mathscr{L}(\mathsf{H})$ satisfies $P_n P_m = 0$ for $n \neq m$. Notice that simple additivity is subsumed just assuming that $P_n = 0$ for all n excluding a finite subset of $\mathbb{N}$.

Remark 4.22

(a) The class $\{P_n\}_{n\in\mathbb{N}}$ can always be embedded in a maximal set of commuting elementary observables $\mathscr{L}_0$ that has the structure of a Boolean σ-algebra. A quantum state ρ restricted to $\mathscr{L}_0$ is a standard Kolmogorov probability measure. Its quantum nature relies on the peculiarity that it acts also on projectors which are not contained in a common Boolean σ-algebra, namely incompatible elementary observables.

(b) This is the most general notion of quantum state. The issue remains open about the existence of *sharp states* associating either 0 or 1 *and not intermediate values* to every elementary proposition, as the non-probabilistic states in phase space do. If they exist, they must be a special case of these probability measures. We shall see that actually sharp states do *not* exist in quantum theories, in the Hilbert space formulation, differently from classical theories. In this sense quantum theory is *intrinsically probabilistic*. ■

We address now two fundamental questions.

(1) *Do quantum states as above exist?*

The answer is positive: if $\psi \in \mathsf{H}$ and $||\psi|| = 1$, the map $\rho_\psi : \mathscr{L}(\mathsf{H}) \ni P \mapsto \langle\psi|P\psi\rangle \in [0, 1]$ satisfies the requirement as the reader immediately proves: $\rho_\psi(I) = \langle\psi|\psi\rangle = 1$ and (4.11) is valid simply because the inner product is continuous. It is worth stressing that, as expected form elementary formulations, ρ_ψ depends on ψ up to a phase. In fact, $\rho_{a\psi} = \rho_\psi$ if $a \in \mathbb{C}$ with $|a| = 1$.

(2) *Are unit vectors, up to phase, the unique quantum states?*

The answer is negative and quite articulate. The rest of this section is mainly devoted to answer this question properly. To do it, we need to focus on a particular class of operators called *trace-class operators* because they play a central role in a celebrated characterization due to Gleason of the aforementioned measures. To define trace-class operators we need two ingredients, the *polar decomposition theorem* and the class of *compact operators*.

4.4.2 Polar Decomposition

Complex numbers $z \neq 0$ can be decomposed in a product $z = u|z|$ of a positive number, the absolute value $|z|$, and the phase u, with $|u| = 1$. Bounded (actually closed) operators $A \neq 0$ can be analogously decomposed as composition $A = U|A|$ of their absolute value $|A|$, which is positive, and a "partial isometry" U with $||U|| = 1$. To explain how this decomposition works we needs a preliminary result.

Proposition 4.23 *Let* H *be a Hilbert space and* $A : \mathsf{H} \to \mathsf{H}$ *a* ***positive operator****:* $\langle x|Ax\rangle \geq 0$ *for every* $x \in \mathsf{H}$*. There exists a unique positive operator* $B : \mathsf{H} \to \mathsf{H}$ *such that* $A = B^2$*. This operator is bounded and commutes with every operator in* $\mathfrak{B}(\mathsf{H})$ *commuting with* A*.*

It is called the ***square root*** *of* A *and is denoted by* $\sqrt{A}$*.*

Proof We remind the reader that a positive operator $T : \mathsf{H} \to \mathsf{H}$ is necessarily in $\mathfrak{B}(\mathsf{H})$ and selfadjoint in view of (3) Exercise 2.43. As $A \in \mathfrak{B}(\mathsf{H})$ is selfadjoint, $A = \int_{\sigma(A)} \lambda dP^{(A)}(\lambda)$ by Theorem 3.40. Moreover $\sigma(A) \in [0, +\infty)$ as proved in Proposition 3.46. So $B := \int_{\sigma(A)} \sqrt{\lambda} dP^{(A)}(\lambda)$ is selfadjoint positive (using the same proof as for Proposition 3.46) and

$$BB = \int_{\sigma(A)} \sqrt{\lambda} dP^{(A)}(\lambda) \int_{\sigma(A)} \sqrt{\lambda} dP^{(A)}(\lambda) = \int_{\sigma(A)} \lambda dP^{(A)}(\lambda) = A\,,$$

by Proposition 3.29 (d) as all operators are in $\mathfrak{B}(\mathsf{H})$. If $B' \in \mathfrak{B}(\mathsf{H})$ is positive and $B'B' = A$ we have $\int_{[0+\infty)} r^2 dP^{(B')}(r) = A = \int_{[0,+\infty)} r^2 dP^{(B)}(r)$, that is $\int_{[0+\infty)} s dQ'(s) = A = \int_{[0,+\infty)} s dQ(s)$ where we have defined $Q_E := P^{(B')}_{\phi^{-1}(E)}$ and $Q_E := P^{(B)}_{\phi^{-1}(E)}$ and the homeomorphism $\phi : [0, +\infty) \ni r \mapsto r^2 \in [0, +\infty)$ according to Proposition 3.33 (f). The uniqueness of the spectral measure of a selfadjoint operator (extending Q and Q' on $\mathscr{B}(\mathbb{R})$ in the simplest way, i.e. $Q_{1E} := Q_{E\cap[0,+\infty)}$) implies that $Q = Q' = P^{(A)}$ so that $P^{(B)}_E = Q_{\phi(E)} = Q'_{\phi(E)} = P^{(B')}_E$. Hence $B = B'$.

To conclude, observe that if $D^* = D \in \mathfrak{B}(\mathsf{H})$ commutes with A, then D commutes with A^n and hence with e^{itA} for every $t \in \mathbb{R}$ as a consequence of Exercise 3.64. Proposition 3.69 entails that D commutes with the spectral measure of A and thus with every operator $s(A) = \int_{\sigma(A)} s dP^{(A)}$, where s is a simple function. Approximating essentially bounded functions f with simple functions according to Proposition 3.29 (c), we extend the result to operators $f(A)$. In particular D commutes with $\sqrt{A}$ (which is bounded on $\sigma(A)$ since compact). If $D \in \mathfrak{B}(\mathsf{H})$ is not selfadjoint, the previous argument holds true for the selfadjoint operators $\frac{1}{2}(D+D^*)$ and $\frac{1}{2i}(D - D^*)$. Hence, it holds for their sum D. □

Definition 4.24 If $A \in \mathfrak{B}(\mathsf{H})$ for a Hilbert space H, the **absolute value** of A is the operator $|A| := \sqrt{A^*A}$. ■

We are ready for the *polar decomposition theorem*. An extensive discussion, also applied to closed unbounded operators, appears in [Mor18].

Theorem 4.25 (Polar Decomposition) *Let* $A \in \mathfrak{B}(\mathsf{H})$ *for a Hilbert space* H*. There is a unique pair* $P \in \mathfrak{B}(\mathsf{H})$*,* $U \in \mathfrak{B}(\mathsf{H})$ *such that*

(a) $A = UP$ *(called* ***polar decomposition of*** A*),*
(b) P *is positive,*
(c) U *vanishes on* $Ker(A)$ *and is isometric on* $Ran(P)$*.*

Moreover, $P = |A|$ *and* $Ker(U) = Ker(A) = Ker(P)$*.*

Proof Let us start by observing that A and $|A|$ have the same kernel, since we have $|||A|x||^2 = \langle |A|x||A|x\rangle = \langle x||A|^2x\rangle = \langle x|A^*Ax\rangle = \langle Ax|Ax\rangle = ||Ax||^2$ Hence, on $Ker(A)^{\perp} = Ker(|A|)^{\perp} = \overline{Ran(|A|^*)} = \overline{Ran(|A|)}$ they are injective. So define $U : Ran(|A|) \to \mathsf{H}$ by means of $Uy := A|A|^{-1}y$ if $y \in Ran(|A|)$. With this definition, we have $A = U|A|$ no matter how we extend U outside $Ran(|A|)$. Now notice that $||Ax||^2 = ||U|A|x||^2 = |||A|x||^2$ as established above. This formula proves that U is isometric on $Ran(|A|)$ and, with the standard argument based on polarization formula, we also have that $\langle Uu|Uv\rangle = \langle u|v\rangle$ provided $u, v \in Ran(|A|)$. The operator U is in particular continuous and can be extended on $\overline{Ran(|A|)}$ by continuity, remaining isometric there. Since $\mathsf{H} = Ker(A) \oplus Ker(A)^{\perp} = Ker(A) \oplus Ker(|A|)^{\perp} = Ker(A) \oplus \overline{Ran(|A|^*)} = Ker(A) \oplus \overline{Ran(|A|)}$, if we define $U = 0$ on $Ker(A)$, we have constructed an operator $U \in \mathfrak{B}(\mathsf{H})$ such that, together with $P := |A|$, all requirements (a),(b) and (c) are valid and also $Ker(U) = Ker(A) = Ker(P)$. In particular $Ker(U)$ cannot contain non-vanishing vectors orthogonal to $Ker(A)$, i.e. in $\overline{Ran(|A|)}$, since U is isometric thereon. Suppose conversely that there exist $U', P' \in \mathfrak{B}(\mathsf{H})$ satisfying (a),(b) and (c). From $A = U'P'$, we have $A^* = P'^*U'^* = P'$ and thus $A^*A = P'U'^*U'P' = P'P' = P'^2$ (where we have used the fact that, since U' is isometric on $Ran(P')$, for every $x, y \in \mathsf{H}$, we have $\langle x|P'P'y\rangle = \langle P'x|P'y\rangle = \langle U'P'x|U'P'y\rangle = \langle x|P'U'^*U'P'y\rangle$, so that $P'P' = P'U'^*U'P'$). Since P' is positive, we have $P' = \sqrt{A^*A} = |A|$ by uniqueness of the square root. As A is injective on $Ran(|A|)$, the formula $A = U'|A|$ implies $Uy := A|A|^{-1}y = Uy$ if $y \in Ran(|A|)$. As before, since U' is bounded, $U' = U$ on $\overline{Ran(|A|)}$ by continuity. Finally $U = U'$ also on $\overline{Ran(|A|)}^{\perp} = Ker(|A|)$ since both vanish by hypothesis there. Summing up, $U = U'$. □

Remark 4.26 Observe that if $A \neq 0$, U cannot vanish. Since $||Ux|| \leq ||x||$ by construction and $||Ux|| = ||x||$ on a non-trivial subspace ($Ran(P) \neq \{0\}$ if $A \neq 0$), we conclude that $||U|| = 1$. ■

Another related technically useful notion is that of *partial isometry*.

Definition 4.27 If H is an Hilbert space, an operator $U \in \mathfrak{B}(\mathsf{H})$ that restricts to an isometry on $K_1 := Ker(U)^{\perp}$ is called a **partial isometry** with **initial space** K_1 and **final space** $K_2 := Ran(U)$. ■

Evidently the U in the polar decomposition $A = UP$ is a partial isometry with initial space $Ker(A)^{\perp}$.

Exercise 4.28 Prove that if $U \in \mathfrak{B}(\mathsf{H})$ is a partial isometry with initial space K_1 and final space K_2, then K_2 is closed.

Solution First of all, if $y \in \overline{Ran(U)} = \overline{K_2}$, there is a sequence of vectors $x_n \in \mathsf{H}$ with $Ux_n \to y$. Decomposing $x_n = x'_n + x''_n$ with respect to the standard decomposition $Ker(U)^{\perp} \oplus Ker(U)$, we can omit the part $x''_n \in Ker(U)$ since $Ux''_n = 0$, and we are allowed to assume $Ux'_n \to y$. Since U acts isometrically on x'_n, and the sequence of Ux'_ns is Cauchy, the sequence of the x'_ns must be

Cauchy as well. By continuity of U, $y = U(\lim_{n\to+\infty} x'_n) \in Ran(U)$. Therefore $\overline{Ran(U)} = Ran(U)$, namely K_2 is closed. □

Exercise 4.29 Prove that $U \in \mathfrak{B}(\mathsf{H})$ is a partial isometry with initial space K_1 if and only if U^*U is the orthogonal projector onto K_1.

Solution If U is a partial isometry with initial space $K_1 = Ker(U)^\perp$, then $\langle Ux|Uy\rangle = \langle x|y\rangle$ for $x, y \in K_1$. However, since $\mathsf{H} = K_1 \oplus Ker(U)$, we can extend by linearity this formula to $\langle Ux|Uy\rangle = \langle x|y\rangle$ for $x \in K_1$ and $y \in \mathsf{H}$. This is equivalent to $\langle U^*Ux|y\rangle = \langle x|y\rangle$ for $x \in K_1$ and $y \in \mathsf{H}$, namely $U^*Ux = x$ if $x \in K_1$. On the other hand, $U^*Ux = 0$ if $x \in Ker(U) = K_1^\perp$. In other words, $U^*U : K_1 \oplus K_1^\perp \ni x + y \mapsto x + 0 \in K_1 \oplus K_1^\perp$, so that it coincides with the orthogonal projector onto K_1. If, conversely $U \in \mathfrak{B}(\mathsf{H})$ is such that U^*U is the orthogonal projector onto the closed subspace K_1, we have that $\langle Ux|Uy\rangle = \langle U^*Ux|y\rangle = \langle x|y\rangle$ for $x, y \in K_1$, so that U is an isometry on it. Furthermore $Ux = 0$ is equivalent to $||Ux||^2 = 0$, that is $\langle x|U^*Ux\rangle = 0$. Since U^*U is idempotent and selfadjoint, this is equivalent to $\langle U^*Ux|U^*Ux\rangle = 0$, namely $||U^*Ux|| = 0$. We have proved that $Ker(U) = U^*U(\mathsf{H})^\perp = K_1^\perp$. In other words, $K_1 = Ker(U)^\perp$. In summary, U is a partial isometry with initial space K_1. □

Exercise 4.30 Prove that if $U \in \mathfrak{B}(\mathsf{H})$ is a partial isometry with initial space K_1 and final space K_2, then U^* is a partial isometry with initial space K_2 and final space K_1. Consequently, UU^* is the orthogonal projector onto K_2.

Solution From the previous exercise, $U^*(Ux) = x$ if $x \in K_1$, so $Ux \in K_2$. Since $||Ux|| = ||x||$, we have obtained that U^* is isometric on $K_2 = Ran(U) = Ker(U^*)^\perp$. We furthermore have $Ker(U^*) = \overline{Ran(U)} = K_1$. The last statement immediately follows form the previous exercise noticing that $(U^*)^* = U$. □

4.4.3 *The Two-Sided *-Ideal of Compact Operators*

We give here the definition of *compact operator* on a Hilbert space. However the definition is much more general and can be given for operators $A \in \mathfrak{B}(X, Y)$ with X, Y normed spaces, preserving many properties of these types of bounded operators (see, e.g., [Mor18]).

Definition 4.31 Let H be a Hilbert space. An operator $A \in \mathfrak{B}(\mathsf{H})$ is said to be **compact** if $\{Ax_n\}_{n\in\mathbb{N}}$ admits a convergent subsequence if $\{x_n\}_{n\in\mathbb{N}} \subset \mathsf{H}$ is bounded. The class of compact operators on H is indicated by $\mathfrak{B}_\infty(\mathsf{H})$. ■

Example 4.32

(1) As an example, every operator $A \in \mathfrak{B}(\mathsf{H})$ such that $Ran(A)$ is a finite-dimensional subspace of H is necessarily compact. In fact, let us identify $Ran(A)$ with $\mathbb{C}^n$ for n given by the (finite) dimension of $Ran(A)$ by fixing

a Hilbert basis of $Ran(A)$ (which coincides with $\overline{Ran(A)}$, since all finite-dimensional subspaces are closed, the proof being elementary). If $\{x_n\}_{n\in\mathbb{N}} \subset \mathsf{H}$ is bounded, i.e. $||x_n|| \leq C$ for all $n \in \mathbb{N}$ and some (finite) constant $C > 0$, then $||Ax_n|| \leq ||A||C$ for $n \in \mathbb{N}$. The vectors Ax_n are therefore contained in the closed ball in $\mathbb{C}^n$ of radius $||A||C$ and centred at the origin, which is necessarily compact. Hence $\{Ax_n\}_{n\in\mathbb{N}}$ admits a convergent subsequence. An example of such type of compact operator is a finite linear combination of operators $A_{x,y} : \mathsf{H} \ni z \mapsto \langle x|z\rangle y$, for $x, y \in \mathsf{H}$ fixed.

(2) If $A \in \mathfrak{B}(\mathsf{H})$ and $P \in \mathscr{L}(\mathsf{H})$ is an orthogonal projector onto a finite-dimensional subspace, then $AP \in \mathfrak{B}_\infty(\mathsf{H})$. In fact, if $e_1, \ldots, e_n$ is an orthonormal basis of $P(\mathsf{H})$, we have

$$Ran(AP) = \left\{ \sum_{j=1}^{n} c_j f_j \;\middle|\; c_j \in \mathbb{C}\,,\; j = 1, \ldots, n \right\} ,$$

where $f_j := Ae_j$ for $j = 1, \ldots, n$. Therefore $Ran(AP)$ has dimension $\leq n$ and AP is compact due to (1). ∎

We summarize below the most important properties of compact operators on Hilbert spaces.

Theorem 4.33 *Let H be a Hilbert space and focus on the set of compact operators $\mathfrak{B}_\infty(\mathsf{H})$. $A \in \mathfrak{B}(\mathsf{H})$ is compact if and only if $|A|$ is compact.*

Furthermore $\mathfrak{B}_\infty(\mathsf{H})$ is:

(a) *a linear subspace of $\mathfrak{B}(\mathsf{H})$;*

(b) *a two-sided *-ideal of $\mathfrak{B}(\mathsf{H})$, i.e,*

  (i) *$AB, BA \in \mathfrak{B}_\infty(\mathsf{H})$ if $B \in \mathfrak{B}(\mathsf{H})$ and $A \in \mathfrak{B}_\infty(\mathsf{H})$,*

  (ii) *$A^* \in \mathfrak{B}_\infty(\mathsf{H})$ if $A \in \mathfrak{B}_\infty(\mathsf{H})$.*

(c) *a C^*-algebra (without unit if H is not finite-dimensional) with respect to the structure induced by $\mathfrak{B}(\mathsf{H})$. In particular $\mathfrak{B}_\infty(\mathsf{H})$ is a closed subspace of $\mathfrak{B}(\mathsf{H})$.*

Proof The first statement immediately arises from the definition of compact operator and formula $|||A|x||^2 = \langle |A|x||A|x\rangle = \langle x||A|^2x\rangle = \langle x|A^*Ax\rangle = \langle Ax|Ax\rangle = ||Ax||^2$, that implies that $\{|A|x_n\}_{n\in\mathbb{N}}$ is Cauchy if and only if $\{Ax_n\}_{n\in\mathbb{N}}$ is Cauchy.

(a) Fix $a, b \in \mathbb{C}$, $A, B \in \mathfrak{B}_\infty(\mathsf{H})$, and a bounded sequence $\{x_n\}_{n\in\mathbb{N}}$. Extract a subsequence $\{x_{n_k}\}_{k\in\mathbb{N}}$ such that $Ax_{n_k} \to y$ as $k \to +\infty$. $\{x_{n_k}\}_{k\in\mathbb{N}}$ is bounded, so that there is a subsequence $\{x_{n_{k_h}}\}_{h\in\mathbb{N}}$ such that $Bx_{n_{k_h}} \to z$ as $h \to +\infty$. By construction $(aA + bB)x_{n_{k_h}} \to ay + bz$ as $h \to +\infty$. Hence, $aA + bB$ is compact.

(b) The fact that AB and BA are compact if $A \in \mathfrak{B}_\infty(\mathsf{H})$ and $B \in \mathfrak{B}(\mathsf{H})$ are immediate consequences of the fact that B is bounded and the definition of compact operator. The fact that A^* is compact if A is compact now immediately follows from the first statement and the polar decomposition (Theorem 4.25).

In fact, from $A = U|A|$ we have $A^* = |A|U^*$, since $|A|$ is compact and $U^* \in \mathfrak{B}(\mathsf{H})$, A^* is compact as well.

(c) Let us prove that $\mathfrak{B}_\infty(\mathsf{H})$ is a Banach space with respect to the operator norm, since the remaining requirements for defining a C^*-algebra are valid because of (a) and (b). Let $\mathfrak{B}(\mathsf{H}) \ni A = \lim_{i\to+\infty} A_i$ with $A_i \in \mathfrak{B}_\infty(\mathsf{H})$. Take a bounded sequence $\{x_n\}_{n\in\mathbb{N}}$ in H: $||x_n|| \le C$ for any n. We want to prove the existence of a convergent subsequence of $\{Ax_n\}$. Using a hopefully clear notation, we build recursively a family of subsequences:

$$\{x_n\} \supset \{x_n^{(1)}\} \supset \{x_n^{(2)}\} \supset \cdots \tag{4.12}$$

such that, for any $i = 1, 2, \ldots$, $\{x_n^{(i+1)}\}$ is a subsequence of $\{x_n^{(i)}\}$ with $\{A_{i+1}x_n^{(i+1)}\}$ convergent. This is always possible, because any $\{x_n^{(i)}\}$ is bounded by C, being a subsequence of $\{x_n\}$, and A_{i+1} is compact by assumption. We claim that $\{Ax_i^{(i)}\}$ is the subsequence of $\{Ax_n\}$ that will converge. From the triangle inequality

$$||Ax_i^{(i)} - Ax_k^{(k)}|| \le ||Ax_i^{(i)} - A_nx_i^{(i)}|| + ||A_nx_i^{(i)} - A_nx_k^{(k)}|| + ||A_nx_k^{(k)} - Ax_k^{(k)}|| .$$

With this estimate,

$$||Ax_i^{(i)} - Ax_k^{(k)}|| \le ||A - A_n||(||x_i^{(i)}|| + ||x_k^{(k)}||) + ||A_nx_i^{(i)} - A_nx_k^{(k)}||$$

$$\le 2C||A - A_n|| + ||A_nx_i^{(i)} - A_nx_k^{(k)}|| .$$

Given $\epsilon > 0$, if n is large enough then $2C||A-A_n|| \le \epsilon/2$, since $A_n \to A$. Fix n and take $r \ge n$. Then $\{A_n(x_p^{(r)})\}_p$ is a subsequence of the convergent sequence $\{A_n(x_p^{(n)})\}_p$. Consider the sequence $\{A_n(x_p^{(p)})\}_p$, for $p \ge n$: it picks up the "diagonal" terms of all those subsequences, *each of which is a subsequence of the preceding one by (4.12)*; moreover, it is still a subsequence of the convergent sequence $\{A_n(x_p^{(n)})\}_p$, so it, too, converges (to the same limit). We conclude that if $i, k \ge n$ are large enough, then $||A_nx_i^{(i)} - A_nx_k^{(k)}|| \le \epsilon/2$. Hence if i, k are large enough then $||Ax_i^{(i)} - Ax_k^{(k)}|| \le \epsilon/2 + \epsilon/2 = \epsilon$. This finishes the proof, for we have produced a Cauchy subsequence in the Banach space H, which must converge in the space.

To end the proof of (c), we notice that, evidently, I cannot be compact if H is infinite-dimensional, since every orthonormal sequence $\{u_n\}_{n\in\mathbb{N}}$ cannot admit a convergent subsequence because $||u_n - u_m||^2 = 2$ for $n \neq m$. □

To conclude this essential summary of properties of compact operators on Hilbert spaces, we state and prove the version of spectral theorem for selfadjoint compact operators due to Hilbert and Schmidt. (An alternate proof of this classical theorem can be found in [Mor18].)

Theorem 4.34 (Hilbert-Schmidt Decomposition) *Let* H *be a Hilbert space and consider* $T^* = T \in \mathfrak{B}(\mathsf{H})$ *a compact operator with* $T \neq 0$. *The following facts hold.*

(a) $\sigma(T) \setminus \{0\} = \sigma_p(T) \setminus \{0\}$, *so that, if* $0 \in \sigma(T)$, *either* $0 \in \sigma_p(T)$ *or* 0 *is the unique element of* $\sigma_c(T)$.
(b) $\sigma(T)$ *is finite or countable. In the latter case* 0 *is unique accumulation point of* $\sigma_p(T)$.
(c) *There exists* $\lambda \in \sigma_p(T)$ *with* $||T|| = |\lambda|$.
(d) *If* $\lambda \in \sigma_p(T) \setminus \{0\}$, *the* λ*-eigenspace has dimension* $d_\lambda < +\infty$.
(e) *The spectral decomposition*

$$Tx = \sum_{n \in N} \lambda_n \langle u_n | x \rangle u_n \quad \forall x \in \mathsf{H} \tag{4.13}$$

holds (the ordering is irrelevant), for a finite ($N \subsetneq \mathbb{N}$) *or countable* ($N = \mathbb{N}$) *Hilbert basis of eigenvectors* $\{u_n\}_{n \in N}$ *of* $\overline{Ran(T)}$, *where* $\lambda_n \in \sigma_p(T)$ *is the eigenvalue of* u_n.
(f) *If* $N = \mathbb{N}$ *and the ordering of the* u_n *is such that* $|\lambda_n| \geq |\lambda_{n+1}|$, *then*

$$T = \sum_{n=0}^{+\infty} \lambda_n \langle u_n | \; \rangle u_n \;, \tag{4.14}$$

in the uniform operator topology.

Proof

(a) Take $\lambda \in \sigma_c(T) \setminus \{0\}$ assuming that it exists. Due to Proposition 3.3, for every natural number $n > 0$ there is $x_n \in \mathsf{H}$ with $||x_n|| = 1$ and $||Tx_n - \lambda x_n|| < \frac{2}{n}$. In particular, if $P^{(T)}$ is the PVM of T, we can always fix x_n in the closed subspace $P_{[\lambda-1/n, \lambda+1/n]}(\mathsf{H})$. This subspace is not trivial because of (d) Theorem 3.40, as it contains the non-trivial subspace $P_{(\lambda-1/n,\lambda+1/n)}(\mathsf{H})$. Consequently,

$$||x_n - x_m|| = |\lambda|^{-1} \, ||\lambda x_n - \lambda x_m|| \leq |\lambda|^{-1} \, ||\lambda x_n - Tx_n - \lambda x_m + Tx_m|| + |\lambda|^{-1} \, ||Tx_n - Tx_m|| \,.$$

Hence

$$||x_n - x_m|| \leq \frac{4}{|\lambda| n} + \frac{1}{|\lambda|} ||Tx_n - Tx_m|| \,,$$

so that

$$||Tx_n - Tx_m|| \geq |\lambda| ||x_n - x_m|| - \frac{4}{n} \,. \tag{4.15}$$

Moreover, since $\lambda \in \sigma_c(T)$ and invoking Proposition 3.29 (c), we have as $m \to +\infty$

$$P^{(T)}_{[\lambda-1/m,\lambda+1/m]}x_n = \int_{\mathbb{R}} \chi_{[\lambda-1/m,\lambda+1/m]}dP^{(T)}x_n \to \int_{\mathbb{R}} \chi_{\{\lambda\}}dP^{(T)}x_n$$
$$= P^{(T)}_{\{\lambda\}}x_n = 0x_n = 0\,.$$

This fact has the implication that, if n is fixed, then $\langle x_n|x_m\rangle \to 0$ if $m \to +\infty$, because $\langle x_n|x_m\rangle = \langle x_n|P^{(T)}_{[\lambda-1/m,\lambda+1/m]}x_m\rangle = \langle P^{(T)}_{[\lambda-1/m,\lambda+1/m]}x_n|x_m\rangle \to 0$. Hence, we also have that $||x_n - x_m||^2 = 2 - 2Re\langle x_n|x_m\rangle \to 2$ as $m \to +\infty$. In summary, looking at (4.15), if n is sufficiently large such that

$$\frac{4}{n} < \frac{|\lambda|\sqrt{2}}{4}\,,$$

we can always take m so large that $||x_n - x_m|| \geq \frac{\sqrt{2}}{2}$, obtaining

$$||Tx_n - Tx_m|| \geq |\lambda|\frac{\sqrt{2}}{2} - |\lambda|\frac{\sqrt{2}}{4} = |\lambda|\frac{\sqrt{2}}{4}\,.$$

Even if the sequence $\{x_n\}_{n\in\mathbb{N}}$ is bounded (because $||x_n|| = 1$ for every $n \in \mathbb{N}$), its image $\{Tx_n\}_{n\in\mathbb{N}}$ cannot contain Cauchy subsequences since $||Tx_n - Tx_m|| \geq |\lambda|\frac{\sqrt{2}}{4}$ if n and m are sufficiently large. This is impossible because T is compact. The only possibility is $\lambda = 0$ concluding the proof of (a).

(b) Suppose that for some sequence of elements $\sigma_p(T) \ni \lambda_n \to a \neq 0$ as $n \to +\infty$. Consider eigenvectors x_n with $Tx_n = \lambda_n x_n$ for $||x_n|| = 1$. Since $x_n \perp x_m$ if $n \neq m$ (Proposition 3.13 (d)) and $\lambda_n \to a$ as $n \to +\infty$, we have

$$||Tx_n - Tx_m||^2 = ||\lambda_n x_n - \lambda_m x_m||^2 = |\lambda_n|^2 + |\lambda_m|^2 \geq 2|a|^2 - \epsilon$$

for $n, m > N_\epsilon$. If $|a| > 0$, taking $\epsilon = |a|^2$, we conclude that the sequence $\{Tx_n\}_{n\in\mathbb{N}}$ cannot admit Cauchy subsequences, since $||Tx_n - Tx_m||^2 \geq |a|^2 > 0$ for sufficiently large n, m as it instead should, since T is compact and $\{x_n\}_{n\in\mathbb{N}}$ is bounded. In summary, the accumulation point $a \neq 0$ does not exist. Now remember that $\sigma(T)$, and hence $\sigma_p(T)$, are contained in $[-||T||, ||T||]$ (Proposition 3.47). In every compact set $[-||T||, -1/n] \cup [1/n, ||T||]$ for $n \in \mathbb{N}$ with $1/n < ||T||$, the there are finitely many (possibly none) elements of $\sigma_p(T)$, otherwise there would be an accumulation point and this is forbidden since the set does not contain 0. We have found that $\sigma_p(T)$ is either finite or countable and, in this case, 0 is the only accumulation point.

(c) Since $\sup\{|\lambda|\,|\lambda \in \sigma(T)\} = \sup\{|\lambda|\,|\lambda \in \sigma_p(T)\} = ||T||$ (Proposition 3.47), and $||T|| \neq 0$ cannot be an accumulation point of $\sigma_p(T)$, there must be $\lambda \in \sigma_p(T)$ with $|\lambda| = ||T||$.

(d) If $\lambda \in \sigma_p(T) \neq \{0\}$, define H_λ as the corresponding eigenspace of T and let $\{x_j\}_{j\in J}$ be a Hilbert basis of H_λ. As a consequence $||Tx_j - Tx_k||^2 = |\lambda|^2||x_j - x_k||^2 = |\lambda|^2 2$ if $j \neq k$. So $\{Tx_j\}_{j\in J}$ cannot admit a Cauchy subsequence when J is not finite in spite of $\{x_j\}_{j\in J}$ being bounded and T compact. We conclude that J is finite, namely $\dim(\mathsf{H}_\lambda) < +\infty$.

(e) We assume $N = \mathbb{N}$ since the finite case is trivial. Consider a collection of sets $E_n \subset \sigma_p(T)$ with $n \in \mathbb{N}$ such that every set E_n is finite, $E_{n+1} \supset E_n$ and $\cup_{n\in\mathbb{N}} E_n = \sigma_p(T)$. Notice that $\sigma_p(T) = \sigma(T)$, possibly up to the point $0 \in \sigma_c(T)$, that however does not play any role in the following because $P^{(T)}_{\{\lambda\}} = 0$ if $\lambda \in \sigma_c(T)$ as we know by Theorem 3.40. The sequence of functions $\chi_{E_n}\iota$ tends pointwise to $\chi_{\sigma_p(T)}\iota$ and is bounded by the constant $||T||$ since $\sigma(T) \subset [-||T||, ||T||]$. Applying Proposition 3.29 (c), we have since $P^{(T)}$ is concentrated on the eigenvalues,

$$Tx = \int_{\mathbb{R}} \iota \, dP^{(T)}x = \lim_{n\to+\infty} \int_{\mathbb{R}} \chi_{E_n}\iota \, dP^{(T)}x = \lim_{n\to+\infty} \sum_{\lambda\in E_n} \lambda P^{(T)}_{\{\lambda\}}x = \sum_{\lambda\in\sigma_p(T)} \lambda P^{(T)}_{\{\lambda\}}x \,,$$

where in the final formula the procedure we adopt to enumerate the eigenvalues does not matter because the sets E_n are chosen arbitrarily. If we fix an orthonormal basis $N_\lambda = \{u^{(\lambda)}_j\}_{j=1,\ldots,d_\lambda}$ in every eigenspace $P_\lambda(\mathsf{H})$ with $\lambda \neq 0$ (if $\lambda = 0$ is an eigenvalue it does not give contribution to the total sum defining Tx), so that $P^{(T)}_{\{\lambda\}} = \sum_{j=1}^{d_\lambda} \langle u^{(\lambda)}_j| \ \rangle u^{(\lambda)}_j$, we can rearrange the formula as

$$Tx = \sum_{\lambda\in\sigma_p(T)} \sum_{j=1}^{d_\lambda} \lambda \langle u^{(\lambda)}_j|x\rangle u^{(\lambda)}_j \,.$$

According to Lemma 2.8, since the vectors in the sum are pairwise orthogonal, the sum can be rearranged arbitrarily and written into the form where the pairwise-orthogonal u_n are the vectors in the union of bases $\cup_{\lambda\in\sigma_p(T)\setminus\{0\}} N_\lambda$,

$$Tx = \sum_{n\in\mathbb{N}} \lambda_n \langle u_n|x\rangle u_n \quad \forall x \in \mathsf{H} \,,$$

with $Tu_n = \lambda_n u_n$. Observe that, from the formula above, the set of orthonormal vectors u_n spans the whole range of T and also its closure, so that they form a Hilbert basis of $\overline{Ran(T)}$. The proof of (e) is over.

(f) Suppose again that $N = \mathbb{N}$, otherwise everything becomes trivial. In this case 0 must be the unique limit point of the λ_n in view of (b). Assuming to order the eigenvectors so that $|\lambda_{n+1}| \leq |\lambda_n|$, consider the operators

$T_N := \sum_{n=0}^{N-1} \lambda_n \langle u_n | \;\rangle u_n$. Then

$$||(T - T_N)x||^2 = \left|\left|\sum_{n=N}^{+\infty} \lambda_n \langle u_n|x\rangle u_n\right|\right|^2 = \sum_{n=N}^{+\infty} |\lambda_n|^2 |\langle u_n|x\rangle|^2$$

$$\leq |\lambda_N|^2 \sum_{n=N}^{+\infty} |\langle u_n|x\rangle|^2 \leq |\lambda_N|^2 ||x||^2 ,$$

Hence, dividing by $||x||$ and taking the sup over the vectors x with $||x|| \neq 0$,

$$||T - T_N|| \leq |\lambda_N| \to 0 \quad \text{if } N \to +\infty.$$

We have proved that (4.14) is valid in the uniform operator topology, completing the proof.

□

Example 4.35 Let us come back to the Hamiltonian operator H of the harmonic oscillator discussed in (3) Example 3.43. It turns out that $H^{-1} \in \mathfrak{B}_\infty(\mathsf{H})$. Since $0 \notin \sigma(H)$, necessarily $H^{-1} = R_0(H)$ (the resolvent operator for $\lambda = 0$), hence $H^{-1} \in \mathfrak{B}(\mathsf{H})$. Moreover applying Corollary 3.53,

$$\sigma(H^{-1}) = \overline{\left\{ \frac{1}{\hbar\omega(n + 1/2)} \middle| n = 0, 1, 2, \dots \right\}} = \{0\} \cup \left\{ \frac{1}{\hbar\omega(n + 1/2)} \middle| n = 0, 1, 2, \dots \right\} ,$$

where the points $\frac{1}{\hbar\omega(n+1/2)}$ are in the point spectrum as they are isolated (Theorem 3.40). Using the same proof as for proving (f) of Theorem 4.33, we have that

$$H^{-1} = \lim_{N\to+\infty} \sum_{n=0}^{N} \frac{1}{\hbar\omega(n + 1/2)} \langle \psi_n|\cdot\rangle \psi_n$$

where the ψ_n are the eigenvectors of H, according to (3) Example 3.43, and the limit is in the uniform operator topology. Since the operators after the limit symbol are of finite rank and thus compact, applying Theorem 4.33 (c), we have that also H^{-1} is compact. The same result actually holds true for $H^{-\alpha}$ with $\alpha > 0$.

4.4.4 Trace-Class Operators

Let us finally introduce an important family of compact operators of *trace class*. As a matter of fact, these operators $A : \mathsf{H} \to \mathsf{H}$ are those which admit a well-defined *trace*

$$tr(A) = \sum_{u \in N} \langle u|Au\rangle ,$$

where $N \subset \mathsf{H}$ is a Hilbert basis and $tr(A)$ does not depend on the choice of the Hilbert basis. This notion of trace is evidently the direct generalization of the analogous notion in finite-dimensional vectors spaces. This family of compact operators will play a decisive role in characterization of the class of quantum states.

The traditional procedure to introduce them (see, e.g., [Mor18]) passes through *Hilbert-Schmidt operators*, or even *Schatten-class* operators. However, since these types are not of great relevance in our concise presentation, we shall follow a much more direct route.

We start with a definition which becomes illuminating if we think of the trace as an integration procedure: we should deal with absolutely integrable functions to make effective the notion of integral. The same happens for the trace.

Definition 4.36 If H is a Hilbert space, $\mathfrak{B}_1(\mathsf{H}) \subset \mathfrak{B}(\mathsf{H})$ denotes the set of **trace-class** or **nuclear** operators, i.e. the operators $T \in \mathfrak{B}(\mathsf{H})$ satisfying

$$\sum_{z\in M} \langle z||T|z\rangle < +\infty \tag{4.16}$$

for some Hilbert basis $M \subset \mathsf{H}$. ■

A technical proposition is in order after an important remark concerning alternative definitions of $\mathfrak{B}_1(\mathsf{H})$.

Remark 4.37 A weaker version of condition (b) below, namely,

$$\sum_{u\in N} |\langle u|Tu\rangle| < +\infty \quad \text{for every Hilbert basis } N,$$

is *equivalent* to $T \in \mathfrak{B}_1(\mathsf{H})$ in complex Hilbert spaces [Mor18] (but *not* in real Hilbert spaces). This condition is sometimes adopted as an alternative definition of $\mathfrak{B}_1(\mathsf{H})$ in complex Hilbert spaces. ■

Proposition 4.38 *Let H be a complex Hilbert space. Then for every $T \in \mathfrak{B}_1(\mathsf{H})$*

(a) *for every Hilbert basis $N \subset \mathsf{H}$,*

$$||T||_1 := \sum_{u\in N} \langle u||T|u\rangle < +\infty$$

and $||T||_1$ does not depend on N.

(b) *For every Hilbert basis $N \subset \mathsf{H}$,*

$$\sum_{u\in N} |\langle u|Tu\rangle| \leq ||T||_1 < +\infty\,.$$

(c) *T, $|T|$ and $\sqrt{|T|}$ belong to $\mathfrak{B}_\infty(\mathsf{H})$.*

Proof

(a) From Definition 4.36,

$$+\infty > \sum_{z\in M}\langle z||T|z\rangle = \sum_{z\in M}\left\langle \sqrt{|T|}z \left| \sqrt{|T|}\, z\right.\right\rangle = \sum_{z\in M}\left|\left|\sqrt{|T|}z\right|\right|^2 = \sum_{z\in M}\sum_{u\in N}\left|\left\langle u \left| \sqrt{|T|}\, z\right.\right\rangle\right|^2$$

$$= \sum_{z\in M}\sum_{u\in N}\left|\left\langle \sqrt{|T|}u \right| z\right\rangle\right|^2 = \sum_{u\in N}\sum_{z\in M}\left|\left\langle \sqrt{|T|}u \right| z\right\rangle\right|^2 = \sum_{u\in N}\left|\left|\sqrt{|T|}u\right|\right|^2 = \sum_{u\in N}\langle u||T|u\rangle\ .$$

The crucial passage is swapping the sums $\sum_{z\in M}\sum_{u\in N} \to \sum_{u\in N}\sum_{z\in M}$. This exchange is allowed by interpreting the sum as a product integration of a pair of counting measures on a product space $N \times M$ and using the Fubini-Tonelli theorem. Observe that only countably many terms $|\langle u|\sqrt{|T|}z\rangle|^2$ of the Cartesian product $N \times M$ do not vanish, so the spaces are σ-finite and their product can be defined.

(b) Making use of the polar decomposition of T (Theorem 4.25), we have

$$\sum_{u\in N}|\langle u|Tu\rangle| = \sum_{u\in N}|\langle u|U|T|u\rangle| = \sum_{u\in N}\left|\left\langle u \left| U\sqrt{|T|}\sqrt{|T|}u\right.\right\rangle\right| = \sum_{u\in N}\left|\left\langle \sqrt{|T|}U^*u \left| \sqrt{|T|}u\right.\right\rangle\right|$$

$$\leq \sum_{u\in N}\left|\left|\sqrt{|T|}U^*u\right|\right|\,\left|\left|\sqrt{|T|}u\right|\right| \leq \sqrt{\sum_{u\in N}\left|\left|\sqrt{|T|}U^*u\right|\right|^2}\sqrt{\sum_{u\in N}\left|\left|\sqrt{|T|}u\right|\right|^2} \leq C\sqrt{||T||_1}\ , \tag{4.17}$$

where

$$C := \sqrt{\sum_{u\in N}\left|\left|\sqrt{|T|}U^*u\right|\right|^2} = \sqrt{\sum_{u\in N}\langle u|U|T|U^*u\rangle}\ .$$

Let us study the value of C, proving that it is finite. We start by noticing that $U|T|U^*$ is positive and thus coincides with $|U|T|U^*|$. On the other hand, $U|T|U^* \in \mathfrak{B}_1(\mathsf{H})$ since it satisfies (4.16) for a Hilbert basis M we go to construct. First observe that U^* is a partial isometry according to Exercise 4.30, so that it is an isometry on a closed subspace $K = Ker(U^*)^\perp$. If L is a Hilbert basis of K, the vectors U^*v for $v \in L$ are an orthonormal system in $\overline{Ran(U^*)}$ and this system can always be completed to a Hilbert basis M of H. In summary,

$$+\infty > ||T||_1 = \sum_{z\in M}\langle z||T|z\rangle = \sum_{v\in L}\langle U^*v||T|U^*v\rangle + \sum_{v\in M\setminus L}\langle z||T|z\rangle \geq \sum_{v\in L}\langle v|U|T|U^*|v\rangle$$

$$= \sum_{v\in N'}\langle v|U|T|U^*|v\rangle = ||U|T|U^*||_1\ ,$$

where, in the last line, we have completed the basis L of K with a Hilbert basis L' of $K^{\perp} = Ker(U^*)$, obtaining a Hilbert basis $N' = L \cup L'$ of H, so that $\langle v|U|T|U^*v\rangle = \langle U^*v||T|U^*v\rangle = 0$ when $v \in L'$. Since we have in this way established that $U|T|U^* \in \mathfrak{B}_1(\mathsf{H})$, the value of $||U|T|U^*||_1 \leq ||T||_1$ must be independent of the used basis and we can conclude that

$$C = \sqrt{\sum_{u\in N}\langle u|U|T|U^*|u\rangle} \leq \sqrt{||T||_1}\,.$$

Inserting in (4.17), we finish the proof of (b), $\sum_{u\in N}|\langle u|Tu\rangle| \leq \sqrt{||T||_1}\sqrt{||T||_1} = ||T||_1 < +\infty$.

(c) Consider a Hilbert basis $M \subset \mathsf{H}$. If $T \in \mathfrak{B}_1(\mathsf{H})$, we have $||T_1|| = \sum_{u\in M}\left|\left|\sqrt{|T|}u\right|\right|^2 < +\infty$. As a consequence, the elements $u \in M$ such that $\left|\left|\sqrt{|T|}u\right|\right| \neq 0$ form a finite or countable subset $\{u_n\}_{n\in N}$. We henceforth assume $N = \mathbb{N}$, the finite case being trivial. Consider the compact operator $\sqrt{|T|}P_N$ (see (2) Example 4.32), where $P_N = \sum_{n=0}^{N-1}\langle u_n|\ \rangle u_n$. We have

$$\left|\left|\left(\sqrt{|T|} - \sqrt{|T|}P_N\right)x\right|\right| = \left|\left|\sum_{n=N}^{+\infty}\langle u_n|x\rangle\sqrt{|T|}u_n\right|\right| \leq \sum_{n=N}^{+\infty}|\langle u_n|x\rangle|\left|\left|\sqrt{|T|}u_n\right|\right|$$

$$\leq \sqrt{\sum_{n=N}^{+\infty}|\langle u_n|x\rangle|^2}\sqrt{\sum_{n=N}^{+\infty}\left|\left|\sqrt{|T|}u_n\right|\right|^2} \leq ||x||\sqrt{\sum_{n=N}^{+\infty}\left|\left|\sqrt{|T|}u_n\right|\right|^2}\,.$$

Hence

$$\left|\left|\sqrt{|T|} - \sqrt{|T|}P_N\right|\right| \leq \sqrt{\sum_{n=N}^{+\infty}\left|\left|\sqrt{|T|}u_n\right|\right|^2}\,.$$

The right-hand side vanishes as $N \to +\infty$ because the series $\sum_{n=1}^{+\infty}\left|\left|\sqrt{|T|}u_n\right|\right|^2$ converges to $||T||_1 < +\infty$. Since $\sqrt{|T|}P_N \in \mathfrak{B}_\infty(\mathsf{H})$ and this space is closed in the uniform topology, it being a C^*-algebra in $\mathfrak{B}(\mathsf{H})$ (Theorem 4.33), we have $\sqrt{|T|} \in \mathfrak{B}_\infty(\mathsf{H})$. Since $\mathfrak{B}_\infty(\mathsf{H})$ is a two-sided ideal (Theorem 4.33 again) we have both that $|T| = \sqrt{|T|}\sqrt{|T|} \in \mathfrak{B}_\infty(\mathsf{H})$, and $T = U|T| \in \mathfrak{B}_\infty(\mathsf{H})$, where we have used the polar decomposition of T, so that $U \in \mathfrak{B}(\mathsf{H})$.

□

The general properties of $\mathfrak{B}_1(\mathsf{H})$ are listed in the next proposition.

Proposition 4.39 *Let* H *a Hilbert space. Then* $\mathfrak{B}_1(\mathsf{H})$ *satisfies the following properties.*

(a) $\mathfrak{B}_1(\mathsf{H})$ *is a subspace of* $\mathfrak{B}(\mathsf{H})$ *and a two-sided* **-ideal, namely*

  (i) $AT, TA \in \mathfrak{B}_1(\mathsf{H})$ *if* $T \in \mathfrak{B}_1(\mathsf{H})$ *and* $A \in \mathfrak{B}(\mathsf{H})$,
  (ii) $T^* \in \mathfrak{B}_1(\mathsf{H})$ *if and only if* $T \in \mathfrak{B}_1(\mathsf{H})$.

(b) $|| \ ||_1$ *is a norm making* $\mathfrak{B}_1(\mathsf{H})$ *a Banach space and satisfying*

  (i) $||TA||_1 \leq ||A||\,||T||_1$ *and* $||AT||_1 \leq ||A||\,||T||_1$ *if* $T \in \mathfrak{B}_1(\mathsf{H})$ *and* $A \in \mathfrak{B}(\mathsf{H})$,
  (ii) $||T||_1 = ||T^*||_1$ *if* $T \in \mathfrak{B}_1(\mathsf{H})$.

Proof

(a) (We closely follow the proof of [ReSi80].) First of all, observe that $|aA| = |a||A|$ for $a \in \mathbb{C}$ so that, to prove that $\mathfrak{B}_1(\mathsf{H})$ is a vector space it suffices to check that $A + B \in \mathfrak{B}_1(\mathsf{H})$ for $A, B \in \mathfrak{B}_1(\mathsf{H})$. Let U, V, and W the partial isometries arising from polar decompositions of $A + B$, A, and B: $A + B = U|A + B|\,, \quad A = V|A|\,, \quad B = W|B|$. As a consequence, if N is a Hilbert basis of H,

$$\sum_{u\in N}\langle u||A+B|u\rangle = \sum_{u\in N}\langle u|U^*(A+B)u\rangle \leq \sum_{u\in N}|\langle u|U^*V|A|u\rangle| + \sum_{u\in N}|\langle u|U^*W|B|u\rangle|.$$

However,

$$\sum_{u\in N}|\langle u|U^*VAu\rangle| \leq \sum_{u\in N}||\sqrt{|A|}V^*Uu||\,||\sqrt{|A|}u|| \leq \sqrt{\sum_{u\in N}||\sqrt{|A|}V^*Uu||^2}\sqrt{\sum_{u\in N}||\sqrt{|A|}u||^2}.$$

The same argument is valid for B. Hence, if we can prove that

$$\sum_{u\in N}||\sqrt{|A|}V^*Uu||^2 \leq tr(|A|)\,, \tag{4.18}$$

we can conclude that

$$\sum_{u\in N}\langle u||A+B|u\rangle \leq tr(|A|) + tr(|B|) < +\infty\,,$$

establishing that $A + B \in \mathfrak{B}_1(\mathsf{H})$ as wanted. To show (4.18) we need only to prove that

$$tr(U^*V|A|V^*U) \leq tr(|A|)\,.$$

Referring to a Hilbert basis $N \ni u$ whose elements satisfy either $u \in Ker(U)$ or $u \in Ker(U)^\perp$, we see that

$$tr(U^*V|A|V^*U) \leq tr(V|A|V^*) .$$

Iterating the procedure for $tr(V|A|V^*)$, using a Hilbert basis $N \ni u$ whose elements satisfy either $u \in Ker(V)$ or $u \in Ker(V)^\perp$, we also conclude that

$$tr(V|A|V^*) \leq tr(|A|) ,$$

proving our assertion.

(a)(i) Since Proposition 3.55 is valid, exploiting the fact that $\mathfrak{B}_1(\mathsf{H})$ is a linear space, we have only to prove that $UT, TU \in \mathfrak{B}_1(\mathsf{H})$ if $T \in \mathfrak{B}_1(\mathsf{H})$ and $U \in \mathfrak{B}(\mathsf{H})$ is unitary. Observe that $|UT|^2 = T^*U^*UT = |T|^2$ so $|UT| = |T|$ and thus $tr(|UT|) = tr(|T|) < +\infty$ proving that $UT \in \mathfrak{B}_1(\mathsf{H})$. Similarly $|TU|^2 = U^*T^*TU = U^*|T|^2U$, so that $|TU| = U^*|T|U$ (because this operator is positive and its square is $U^*|T|^2U$). Therefore we have $tr(|TU|) = tr(U^*|T|U) = \sum_{u\in N}\langle Uu||T|Uu\rangle = tr(|T|) < +\infty$ (because $\{Uu\}_{u\in N}$ is a Hilbert basis if N is since U is unitary) and so $TU \in \mathfrak{B}_1(\mathsf{H})$.

(a)(ii) Let $T = U|T|$ the polar decomposition of T. Therefore $T^* = |T|U^*$ and $|T^*|^2 = TT^* = U|T|^2U^*$. Since $U|T|U^*\, U|T|U^* = U|T|^2U^*$ because U^*U is the orthogonal projector onto $Ran(|A|)$ (Theorem 4.25 and Exercise 4.29), we conclude that $|T^*| = U|T|U^*$. Now (i) implies that $T^* \in \mathfrak{B}_1(\mathsf{H})$ if $T \in \mathfrak{B}_1(\mathsf{H})$. Since $(T^*)^* = T$ we have also that $T^* \in \mathfrak{B}_1(\mathsf{H})$ entails $T \in \mathfrak{B}_1(\mathsf{H})$.

(b) If $a \in \mathbb{C}$ and $A \in \mathfrak{B}_1(\mathsf{H})$, we find

$$||aA||_1 = \sum_{u\in N}\langle u||aA|u\rangle = \sum_{u\in N}\langle u||a||A|u\rangle = |a|\sum_{u\in N}\langle u||A|u\rangle = |a|||A||_1 .$$

Proving (a), we have established that $||A + B||_1 \leq ||A||_1 + ||B||_1$ for $A, B \in \mathfrak{B}_1(\mathsf{H})$, so that $||\ \ ||_1 : \mathfrak{B}_1(\mathsf{H}) \to \mathbb{C}$ is a seminorm. On the other hand, if $||A||_1 = 0$ it means that $\sum_{u\in N}\langle u||A|u\rangle = 0$ for every Hilbert basis N. Since every unit vector $x \in \mathsf{H}$ can be completed to a basis, this implies in particular that $||\sqrt{|A|}x||^2 = \langle x||A|x\rangle = 0$ and thus $|A|x = \sqrt{|A|}^2x = 0$ for every $x \in \mathsf{H}$, so that $||Ax||^2 = \langle Ax|Ax\rangle = |||A|^2x|| = 0$ for every $x \in \mathsf{H}$ meaning that $A = 0$. Hence $||\ ||_1 : \mathfrak{B}_1(\mathsf{H}) \to \mathbb{C}$ is a norm. The proof of the fact that the norm makes $\mathfrak{B}_1(\mathsf{H})$ a Banach space can be found in [Scha60].

(b)(i) It is sufficient to check that $||AT||_1 \leq ||A||||T||_1$. Indeed, assuming it, from (ii) whose proof is independent form the present one, we have $||TA||_1 = ||A^*T^*||_1 \leq ||T^*||||A^*||_1 = ||T||||A||_1$. Let us prove $||AT||_1 \leq ||A||||T||_1$. Consider the polar decomposition $T = U|T|$ and also $|AT| =$

$W|AT|$, so that $|AT| = W^*(AT) = W^*AU|T|$. Putting $S = W^*AU$, we have, exploiting the usual Hilbert basis N of eigenvectors of the selfadjoint positive compact operator $|T|$

$$||AT||_1 = tr(|AT|) = tr(S|T|) = \sum_{u\in N}\langle u|S|T|u\rangle = \sum_{u\in N}\lambda_u\langle u|Su\rangle \leq \sum_{u\in N}|\lambda_u\langle u|Su\rangle|$$

$$\leq \sum_{u\in N}\lambda_u|\langle u|Su\rangle| \leq \sum_{u\in N}\lambda_u||S|| = ||S||||T||_1 \,.$$

Since W^* and U are partial isometries, $||S|| \leq ||A||$, proving that $||AT||_1 \leq ||A||||T||_1$.

(b)(ii) The proof of (a)(ii) established that $|T^*| = U|T|U^*$. Making use of a Hilbert basis N whose elements belong either to $Ker(U^*)$ or $Ker(U^*)^\perp$, we immediately have $||T^*||_1 = \sum_{u\in N}\langle U^*u||T|Uu\rangle = ||T||_1$.

□

We are now in a position to introduce the central mathematical tool of this section, i.e. the notion of *trace* of a trace-class operator, listing and proving its main properties with direct interest to quantum physics.

Proposition 4.40 *Let* H *be a Hilbert space and focus on the space of operators* $\mathfrak{B}_1(\mathsf{H})$. *If* $N \subset \mathsf{H}$ *is a Hilbert basis, the map*

$$\mathfrak{B}_1(\mathsf{H}) \ni T \mapsto tr(T) := \sum_{u\in N}\langle u|Tu\rangle \,, \tag{4.19}$$

is well defined, the sum can be rearranged and does not depend on the choice of N.

The complex number $tr(T)$ *is called the* ***trace*** *of* T *and satisfies the following further properties.*

(a) $tr(aA + bB) = a\,tr(A) + b\,tr(B)$ *for every* $a, b \in \mathbb{C}$ *and* $A, B \in \mathfrak{B}_1(\mathsf{H})$.
(b) $tr(A^*) = \overline{tr(A)}$ *for every* $A \in \mathfrak{B}_1(\mathsf{H})$.
(c) $tr(AB) = tr(BA)$ *if* $A \in \mathfrak{B}_1(\mathsf{H})$ *and* $B \in \mathfrak{B}(\mathsf{H})$.
(d) *For every* $A \in \mathfrak{B}_1(\mathsf{H})$,
   (i) $|tr(A)| \leq tr(|A|) = ||A||_1$,
   (ii) $||A|| \leq tr(|A|) = ||A||_1$.
(e) *If* $A^* = A \in \mathfrak{B}_1(\mathsf{H})$ *then*

$$tr(A) = \sum_{\lambda\in\sigma_p(A)} d_\lambda\lambda$$

   where d_λ *is the dimension of the* λ*-eigenspace and we assume* $+\infty\cdot 0 = 0$.
(f) *If* $U \in \mathfrak{B}(\mathsf{H})$ *is a bijective operator (in particular unitary), then* $tr(UAU^{-1}) = tr(A)$ *for every* $A \in \mathfrak{B}_1(\mathsf{H})$.
(g) *If* $A \geq 0$ *and* $A \in \mathfrak{B}_1(\mathsf{H})$, *then* $tr(A) \geq 0$.

Proof First of all we notice that $\sum_{u\in N}\langle u|Tu\rangle$ converges absolutely due to Proposition 4.38 (b), so that it can be rearranged. Let us prove that the sum is even independent of the basis N. Since $T = A + iB$ with $A = \frac{1}{2}(T + T^*)$ and $B = \frac{1}{2i}(T - T^*)$, where A and B are selfadjoint and belong to $\mathfrak{B}_1(\mathsf{H})$ because of Proposition 4.39 (a), it would be enough demonstrating the assertion for the case $T = T^*$, simply exploiting the linearity of the trace ((a) below, whose proof does not depend on the present argument). If $T^* = T \in \mathfrak{B}(\mathsf{H})$, we can decompose it as $T = T_+ - T_-$ where $T_+ := \int_{[0,+\infty)} \imath dP^{(T)} = TP^{(T)}_{[0,+\infty)}$ and $T_- := -\int_{(-\infty,0)} \imath dP^{(T)} = -TP^{(T)}_{(-\infty,0)}$. Since $T \in \mathfrak{B}_1(\mathsf{H})$, also $T_\pm \in \mathfrak{B}_1(\mathsf{H})$ due to (a) Proposition 4.39. Since $T_\pm \geq 0$, exploiting again the linearity of the trace, to complete the proof it is sufficient to establish it in the case $T^* = T \in \mathfrak{B}_1(\mathsf{H})$ with $T \geq 0$. In this case however $T = |T|$ and therefore Proposition 4.38 (a) proves that $tr(T) = \sum_{u\in N}\langle u|Tu\rangle = \sum_{u\in N}\langle u||T|u\rangle$ does not depend on N, concluding the proof.

(a) and (b) Observing that $aA + bB,\ A^* \in \mathfrak{B}_1(\mathsf{H})$ if $A, B \in \mathfrak{B}_1(\mathsf{H})$ due to Proposition 4.40 (a), the proofs of statements (a) and (b) immediately arise from elementary properties of inner products, using the fact that $\langle u|(aA + bB)u\rangle = a\langle u|Au\rangle + b\langle u|Au\rangle$ and $\langle u|Au\rangle = \overline{\langle u|A^*u\rangle}$.

(c) It is sufficient to prove the statement with $A^* = A \in \mathfrak{B}_1(\mathsf{H})$ and $B \in \mathfrak{B}(\mathsf{H})$, since we can always decompose a generic $A \in \mathfrak{B}_1(\mathsf{H})$ into a linear combination of a pair of selfadjoint trace-class operators $\frac{1}{2}(A + A^*)$ and $\frac{1}{2i}(A - A^*)$ taking advantage of Proposition 4.39 (a) and finally exploiting the linearity of the trace map. So let us stick to $A^* = A \in \mathfrak{B}_1(\mathsf{H})$ and $B \in \mathfrak{B}(\mathsf{H})$. We know that $AB, BA \in \mathfrak{B}_1(\mathsf{H})$ by Proposition 4.39 (a). Moreover, we compute the traces with respect to a Hilbert basis obtained by completing the Hilbert basis of $\overline{Ran(A)}$ made of eigenvectors of A according to Theorem 4.34 (e), noticing that $A \in \mathfrak{B}_\infty(\mathsf{H})$ from Proposition 4.38 (c). Notice that the elements added to the initial basis do not give contribution to the trace as they belong to $Ker(A) = Ker(A^*)$, so we can ignore them in the sums below.

$$tr(AB) = \sum_{n\in N}\langle u_n|ABu_n\rangle = \sum_{n\in N}\langle Au_n|Bu_n\rangle = \sum_{n\in N}\overline{\lambda_n}\langle u_n|Bu_n\rangle = \sum_{n\in N}\lambda_n\langle u_n|Bu_n\rangle\,,$$

where we have used $\sigma(A) \subset \mathbb{R}$ since $A = A^*$. Similarly

$$tr(BA) = \sum_{n\in N}\langle u_n|BAu_n\rangle = \sum_{n\in N}\langle u_n|Bu_n\rangle\lambda_n = \sum_{n\in N}\lambda_n\langle u_n|Bu_n\rangle = tr(AB)\,.$$

(d) First of all take advantage of the polar decomposition $A = U|A|$. Here $|A|$ is compact due to Proposition 4.38 (c). Since $|A|$ is selfadjoint it being positive (so it is selfadjoint in view of (3) in Exercise 2.43)), there is a Hilbert basis N of eigenvectors of $|A|$ obtained by completing that in Theorem 4.34 (e). We have

$$|tr(A)| = \left|\sum_{u\in N}\langle u|U|A|u\rangle\right| = \left|\sum_{u\in N}\langle u|Uu\rangle\lambda_u\right| \leq \sum_{u\in N}|\lambda_u|\,|\langle u|Uu\rangle|\,.$$

Next observe that $|\lambda_u| = \lambda_u$ because $|A| \geq 0$ and $|\langle u|Uu\rangle| \leq ||u||\,||Uu|| \leq 1||Uu|| \leq ||u|| = 1$ ($||U|| \leq 1$ since it is a partial isometry). Hence

$$|tr(A)| \leq \sum_{u \in N} \lambda_u = \sum_{u \in N} \langle u||A|u\rangle = tr|A| = ||A||_1 \,.$$

The second statement is obvious. Since $A \in \mathfrak{B}_\infty(\mathsf{H})$ (Proposition 4.38 (c)), there is $\lambda \in \sigma_p(A)$ such that $|\lambda| = ||A||$ because of Theorem 4.34 (c). On the other hand from (e), whose proof is independent of this argument, $||A||_1 \geq |\lambda| = ||A||$.
(e) Since $A^* = A \in \mathfrak{B}_\infty(\mathsf{H})$, there is a Hilbert basis of eigenvectors of A obtained by completing that in Theorem 4.34 (e). Computing the trace using this basis, taking Theorem 4.34 (d) into account, we immediately have the thesis.
(f) Exploiting (c), we immediately have $tr(UAU^{-1}) = tr((UA)U^{-1}) = tr(U^{-1}UA) = tr(A)$.
(g) The proof is evident form the definition of trace.

□

Remark 4.41 It is easy to prove that (c) can be generalized to

$$tr(T_1 \cdots T_n) = tr(T_{\pi(1)} \cdots T_{\pi(n)})$$

if at least one of the T_k belongs to $\mathfrak{B}_1(\mathsf{H})$, the remaining ones are in $\mathfrak{B}(\mathsf{H})$, and

$$\pi : \{1, \ldots, n\} \to \{1, \ldots, n\}$$

is a *cyclic* permutation. The elementary proof arises by decomposing π in a product of 2-*cycles* and finally using (c) recursively, redefining A and B appearing in (c) at every action of the elementary cyclic permutations. The formula is recalled by saying that **the trace is cyclic**. ■

Example 4.42 Consider the Hamiltonian operator H of the harmonic oscillator discussed in (3) Example 3.43, where $H^{-2} \in \mathfrak{B}_1(\mathsf{H})$. The proof is easy: since $0 \notin \sigma(H)$, it must be $H^{-2} = R_0(H^2)$ (the resolvent operator for $\lambda = 0$), hence $H^{-2} \in \mathfrak{B}(\mathsf{H})$. Moreover $H^{-2} \geq 0$ because its spectrum is positive

$$\sigma(H^{-2}) = \overline{\left\{ \frac{1}{\hbar^2\omega^2(n+1/2)^2} \,\middle|\, n = 0, 1, 2, \ldots \right\}} \,.$$

Finally, computing $||H^{-2}||_1$ using the Hilbert basis of eigenvectors of H, we have

$$||H^{-2}||_1 = \sum_{n=0}^{+\infty} \frac{1}{\hbar^2\omega^2(n+1/2)^2} < +\infty \,.$$

The same result actually holds true for $H^{-\alpha}$ with $\alpha > 1$.

4.4.5 *The Mathematical Notion of Quantum State and Gleason's Theorem*

We have constructed all the mathematical machinery to pursue the description of quantum states in terms of probability measures of $\mathscr{L}(\mathsf{H})$ as discussed in Sect. 4.4.1. According to the discussion in that section, we can give the following general definition.

Definition 4.43 Let H be a Hilbert space. A **quantum probability measure** on H is a map $\rho : \mathscr{L}(\mathsf{H}) \to [0, 1]$ such that the following requirements are satisfied.

(1) $\rho(I) = 1$.
(2) If $\{P_n\}_{n\in\mathbb{N}} \subset \mathscr{L}(\mathsf{H})$ satisfies $P_k P_h = 0$ when $h \neq k$ for $h, k \in \mathbb{N}$, then

$$\rho\left(\text{s-}\sum_{n\in\mathbb{N}} P_n\right) = \sum_{n\in\mathbb{N}} \rho(P_n) . \tag{4.20}$$

The convex set of quantum probability measures in H will be denoted by $\mathscr{M}(\mathsf{H})$. ■

The last statement refers to the evident fact that $\lambda\rho_1 + (1-\lambda)\rho_2 \in \mathscr{M}(\mathsf{H})$ if $\lambda \in [0, 1]$ and $\rho_1, \rho_2 \in \mathscr{M}(\mathsf{H})$. This result extends trivially to a *finite convex combination*

$$\rho = \sum_{k=1}^{n} p_k \rho_k \ ,$$

where $p_k \in [0, 1]$ and $\sum_{k=1}^{n} p_k = 1$, which defines an element of $\mathscr{M}(\mathsf{H})$ if all $\rho_k \in \mathscr{M}(\mathsf{H})$.

Remark 4.44 We stress that in these notes the term *quantum state* corresponds to the mathematical notion of *quantum probability measure*. We prefer to explicitly use the latter in mathematical statements because the former is used ambiguously in physics, where *quantum states* are confused with *quantum state operators*, that we will introduce shortly. This confusion is usually harmless, but becomes significant when dealing with superselection rules, see later. ■

As already observed in Sect. 4.4.1, unit vectors $\psi \in \mathsf{H}$ define, up to phase, quantum probability measures by $\rho_\psi(P) := \langle\psi|P\psi\rangle$ for every $P \in \mathscr{L}(\mathsf{H})$. This is not the only case, since finite convex combinations of quantum probability measures are quantum probability measures as well, as just said. Suppose in particular that $\langle\psi_k|\psi_h\rangle = \delta_{hk}$ and consider the finite convex combination

$$\rho = \sum_{k=1}^{n} p_k \rho_{\psi_k} \ ,$$

where $p_k \in [0, 1]$ and $\sum_{k=1}^{n} p_k = 1$. By direct inspection, completing the finite orthonormal system $\{\psi_k\}_{k=1,\dots,n}$ to a full Hilbert basis of H, one quickly proves that, defining

$$T = \sum_{k=1}^{n} p_k \langle \psi_k | \ \rangle \psi_k \ , \tag{4.21}$$

$\rho(P)$ can be computed as

$$\rho(P) = tr(TP) \ , \quad P \in \mathscr{L}(\mathsf{H}) \ ,$$

In particular, it turns out that T is in $\mathfrak{B}_1(\mathsf{H})$, it satisfies $T \geq 0$ (so it is selfadjoint due to (3) in Exercise 2.43) and $tr(T) = 1$. As a matter of fact, (4.21) is just the spectral decomposition of T, whose spectrum is $\{p_k\}_{k=1,\dots,n}$. This result is general.

Proposition 4.45 *Let* H *be a Hilbert space and define the convex subset of* $\mathfrak{B}_1(\mathsf{H})$ *of* ***quantum state operators***

$$\mathscr{S}(\mathsf{H}) := \{T \in \mathfrak{B}_1(\mathsf{H}) \mid T \geq 0 \, , tr(T) = 1\} \ .$$

If $T \in \mathscr{S}(\mathsf{H})$*, the map*

$$\rho_T : \mathscr{L}(\mathsf{H}) \ni P \mapsto tr(TP) = tr(PT)$$

is well defined and $\rho_T \in \mathscr{M}(\mathsf{H})$.

Proof Observe that $tr(TP) = tr(PT)$ is valid in view of Proposition 4.40 (c). The trace-class operator T is positive, hence selfadjoint, so the eigenvalues λ belong to $[0, +\infty)$. Furthermore, according to Proposition 4.40 (e), $1 = tr(T) = \sum_{\lambda \in \sigma_p(A)} d_\lambda \lambda$ and thus $\lambda \in [0, 1]$. Exploiting in particular Proposition 4.34 (e), since $T \in \mathfrak{B}_\infty(\mathsf{H})$ by Proposition 4.38,

$$tr(TP) = \sum_{n \in M} \langle u_n | TPu_n \rangle = \sum_{n \in M} \lambda_n \langle u_n | Pu_n \rangle \leq \sum_{n \in M} \lambda_n ||u_n|| ||Pu_n|| \leq \sum_{n \in M} \lambda_n = 1 \ ,$$

where $M \subset \mathbb{N}$ and $\{u_n\}_{n \in M}$ is a Hilbert basis of $\overline{Ran(T)}$ which can be completed to a Hilbert basis of $Ker(T) = Ran(T)^\perp$, however these added vectors do not give contribution to traces as the reader immediately proves. On the other hand, since $T \geq 0$,

$$0 \leq \sum_{n \in M} \langle Pu_n | TPu_n \rangle = tr(PTP) = tr(TPP) = tr(TP)$$

and, trivially, $tr(IT) = tr(T) = 1$. Let us prove that the map $\mathscr{L}(\mathsf{H}) \ni P \mapsto tr(PT)$ is σ-additive to conclude that it fulfils Definition 4.43. If $\{P_n\}_{n \in \mathbb{N}} \subset \mathscr{L}(\mathsf{H})$

satisfies $P_n P_m = 0$ for $n \neq 0$, taking advantage of a Hilbert basis of H completing the Hilbert basis of $\overline{Ran(T)}$ made of eigenvectors of T as said in Proposition 4.34 (e),

$$tr\left(T\text{s-}\sum_{n\in\mathbb{N}} P_n\right) = \sum_{l\in M}\left\langle u_l \left| T\sum_{n\in\mathbb{N}} P_n u_l \right.\right\rangle = \sum_{l\in M}\sum_{n\in\mathbb{N}} \langle u_l\, | T P_n u_l\,\rangle = \sum_{l\in M}\sum_{n\in\mathbb{N}} \lambda_l\, \langle u_l\, | P_n u_l\,\rangle\ .$$

In other words, since $\langle u_l|P_n u_l\rangle = \langle u_l|P_n P_n u_l\rangle = \langle P_n u_l|P_n u_l\rangle$,

$$tr\left(T\text{s-}\sum_{n\in\mathbb{N}} P_n\right) = \sum_{l\in N}\sum_{n\in\mathbb{N}} \lambda_n ||P_n u_l||^2\ .$$

Applying the Fubini-Tonelli theorem, since $\lambda_n ||P_n u_l||^2 \geq 0$, the sums can be exchanged:

$$tr\left(T\text{s-}\sum_{n\in\mathbb{N}} P_n\right) = \sum_{n\in\mathbb{N}}\sum_{l\in N} \lambda_n ||P_n u_l||^2 = \sum_{n\in\mathbb{N}} tr(T P_n)\ ,$$

proving σ-additivity. □

Remark 4.46 Actually, with a little change, remembering that $\mathscr{L}(\mathsf{H})$ is complete and not only σ-complete and that the notion of trace does not need the Hilbert space's separability, the proof can be extended to prove that $\mathscr{L}(\mathsf{H}) \ni P \mapsto tr(TP)$ is **completely additive**. In other words, if $\{P_k\}_{k\in K} \subset \mathscr{L}(\mathsf{H})$ is such that $P_k P_h = 0$ if $k \neq h$ and K has *any cardinality* (when H is not separable), then

$$tr\ (T(\vee_{k\in k} P_k)) = \sum_{k\in K} tr(T P_k)\ ,$$

where the sum is understood as the supremum of the sums over finite subsets $K_0 \subset K$.

The very remarkable fact is that these operators exhaust $\mathscr{S}(\mathsf{H})$ if H is *separable* with *dimension* $\neq 2$, as established by Gleason in 1957; his celebrated theorem [Gle57] will be adapted to these lectures (see [Ham03] and [Dvu92] for general treatises on the subject).

Theorem 4.47 (Gleason's Theorem) *Let* H *be a Hilbert space of finite dimension* $\neq 2$*, or infinite-dimensional and separable. The set of quantum probability measures* $\rho \in \mathscr{M}(\mathsf{H})$ *is in one-to-one correspondence with the set of quantum-state operators* $T \in \mathscr{S}(\mathsf{H})$*. The bijection is such that*

$$tr(TP) = \rho(P) \quad \textit{for every } P \in \mathscr{L}(\mathsf{H}),$$

and preserves the convex structures of the two sets. Finally, quantum probability measures separate elements in $\mathscr{L}(\mathsf{H})$ *because quantum-state operators do so.*

Comments on the Proof The only very hard part of Gleason's theorem is the existence claim, and we will not try to address it here (see [Dvu92, Ham03]). The remaining statements are quite easy. It is evident by the trace's linearity that the complex structures are preserved. The T associated to ρ is unique for the following elementary reason. Any other T' of trace class such that $\rho(P) = tr(T'P)$ for any $P \in \mathscr{L}(\mathsf{H})$ must also satisfy $\langle x|(T - T')x\rangle = 0$ for any $x \in \mathsf{H}$. If $x = 0$ this is clear, while if $x \neq 0$ we may complete the vector $x/||x||$ to a basis, in which $tr((T - T')P_x) = 0$ reads $||x||^{-2}\langle x|(T - T')x\rangle = 0$, where P_x is the projector onto span$\{x\}$. By (3) in Exercise 2.43, we obtain $T - T' = 0$.[1] The fact that quantum-state operators separe the elements of $\mathscr{L}(\mathsf{H})$ is quite obvious since, if $tr(TP) = tr(TP')$ for all $T \in \mathscr{S}(\mathsf{H})$, we have in particular $\langle x|Px\rangle = \langle x|P'x\rangle$, where we have chosen $T = \langle x|\cdot\rangle x$ for every $x \in \mathsf{H}$ with $||x|| = 1$. As before, this implies that $P = P'$. □

Remark 4.48

(a) Imposing $\dim \mathsf{H} \neq 2$ is mandatory, due to a well-known counterexample. Identifying H to $\mathbb{C}^2$, one-dimensional projectors $P_{\mathbf{n}}$ correspond one-to-one with unit vectors $\mathbf{n} = (n_1, n_2, n_3)^t \in \mathbb{R}^3$ by means of $P_{\mathbf{n}} = \frac{1}{2}\left(I + \sum_{j=1}^3 n_j\sigma_j\right)$, where σ_j are the standard *Pauli matrices*. Observe that we have $P_{\mathbf{n}} \perp P_{\mathbf{n}'}$ if and only if $\mathbf{n} = -\mathbf{n}'$. If $\mathbf{m} \in \mathbb{R}^3$ is a fixed unit vector, the map $\rho(P_{\mathbf{n}}) := \frac{1}{2}\left(1 + \sum_{j=1}^3 (n_j m_j)^3\right)$ uniquely extends to a quantum probability measure on $\mathscr{L}(\mathbb{C}^2)$ by additivity, as the reader immediately proves. However, there is no T as in Gleason's theorem such that $\rho(TP_{\mathbf{n}}) = \rho(P_{\mathbf{n}})$ for every one-dimensional orthogonal projector $P_{\mathbf{n}}$. This is because, imposing this formula leads to $\sum_{j=1}^3 n_j T_j = \sum_{j=1}^3 n_j^3 m_j^3$ for a fixed unit vector $\mathbf{m} := (m_1, m_2, m_3)^t$ and all unit vectors $\mathbf{n}$. It is easy to prove that this is impossible for every choice of the constants $T_j = tr(T\sigma_j)$.

(b) Particles with spin 1/2, like electrons, admit a Hilbert space – in which the observable spin is defined – of dimension 2. The same occurs to the Hilbert space on which the polarisation of light is described (cf. helicity of photons). When these systems are described in full, however, for instance when including degrees of freedom relative to position or momentum, they are representable on a separable Hilbert space of infinite dimension.

(c) Gleason's theorem extends to real and quaternionic Hilbert spaces in accordance to *Solér's theorem*, to formulate quantum theories. However this extension is technically complicated especially in the second case, and it involves subtle

[1] In a real Hilbert space $\langle x|Ax\rangle = 0$ for all x does not imply $A = 0$. Think of real skew-symmetric matrices in $\mathbb{R}^n$ equipped with the standard inner product. Gleason's theorem is valid in real and quaternionic Hilbert spaces: in the former case uniqueness is valid if we require explicitly that $T = T^*$.

problems related with the notion of trace. These have been fixed [MoOp18] only recently. ■

Gleason's characterization of quantum states has an important consequence discussed explicitly by Bell in 1966 [Bel66] (but already known to Specker in 1960). It proves that there are no sharp states in QM, i.e. probability measures assigning 1 to some elementary observables and 0 to the remaining ones, differently to what happens in CM. In a sense, QM is intrinsically probabilistic since it does not admit sharp measures, as happens in CM. We state Bell's theorem below and prove it through a different—but mathematically equivalent—procedure from Bell's original argument.

Theorem 4.49 (Bell's Theorem) *Let* H *be a Hilbert space of finite dimension* > 2*, or infinite-dimensional and separable. There is no quantum probability measure* $\rho : \mathscr{L}(\mathsf{H}) \to [0, 1]$*, in the sense of Definition 4.43, such that* $\rho(\mathscr{L}(\mathsf{H})) = \{0, 1\}$*.*

Proof Define $\mathbb{S} := \{x \in \mathsf{H} \mid ||x|| = 1\}$ endowed with the topology induced by H, and let $T \in \mathfrak{B}_1(\mathsf{H})$ be the representative of ρ using Gleason's theorem. The map $f_\rho : \mathbb{S} \ni x \mapsto \langle x|Tx\rangle = \rho(\langle x|\ \ \rangle x) \in \mathbb{C}$ is continuous because T is bounded. We have $f_\rho(\mathbb{S}) \subset \{0, 1\}$, where $\{0, 1\}$ is equipped with the topology induced by $\mathbb{C}$. Since $\mathbb{S}$ is connected (because path-connected, as the reader can prove easily) its image must be connected, too. So either $f_\rho(\mathbb{S}) = \{0\}$ or $f_\rho(\mathbb{S}) = \{1\}$. In the first case $T = 0$ which is impossible because $tr(T) = 1$, in the second case $tr(T) > 2$ which is similarly impossible. □

This negative result can be strengthened physically, or so it seems, by the *Kochen-Specker theorem* (Theorem 5.5) we shall discuss shortly. It produces no-go theorems within certain attempts to explain QM in terms of CM based on so-called *hidden variables*. Actually Theorem 4.49 has the same physical content of the Kochen-Specker theorem and can be applied to more general situations. We will also prove an alternative form in Theorem 5.2 below.

Remark 4.50 In view of Proposition 4.45 and Theorem 4.47, when dealing with Hilbert spaces with physical meaning, we could assume that H has finite dimension or is separable so that we automatically identify the set of σ-additive quantum probability measures $\mathscr{M}(\mathsf{H})$ with the set of quantum states $\mathscr{S}(\mathsf{H})$. (We can simply disregard the quantum measures in a two-dimensional H which are not represented by elements of $\mathscr{S}(\mathsf{H})$, especially taking (b) Remark 4.48 into account.) However, as most of the subsequent propositions are valid for the elements of $\mathscr{S}(\mathsf{H})$ even if H does not fulfil Gleason's hypotheses, we will always deal with the class of quantum-state operators $\mathscr{S}(\mathsf{H})$ *without restrictions on* H. When H is not separable, the elements of $\mathscr{S}(\mathsf{H})$ define *completely additive* (see Remark 4.46) probability measures on $\mathscr{L}(\mathsf{H})$ which satisfy a stronger requirement than σ-additivity, and define a *proper* subset of $\mathscr{M}(\mathsf{H})$ [Dvu92, Ham03]. (If H is separable, the two notions of additivity coincide.) It is possible to reformulate Gleason's theorem for Hilbert spaces of dimension $\neq 2$ (separable or not), proving that completely additive probability measures correspond one-to-one with unit-trace, positive trace-class operators [Dvu92, Ham03]. ■

We are in a position to state some definitions of interest to physicists, especially the distinction between *pure* and *mixed* states, so we proceed to analyze the structure of the space of the quantum-state operators. We remind the reader that, if C is a convex set in a vector space, $e \in C$ is called **extremal** if it cannot be written as $e = \lambda x + (1-\lambda)y$, with $\lambda \in (0,1)$, $x, y \in C \setminus \{e\}$. We have the following simple result.

Proposition 4.51 *Let* H *be a Hilbert space. Then*

(a) *The extremal points of the convex set* $\mathscr{S}(\mathsf{H})$ *are those of the form:* $\rho_\psi := \langle\psi|\ \rangle\psi$ *for every vector* $\psi \in \mathsf{H}$ *with* $||\psi|| = 1$. *(This sets up a bijection between extremal-state operators and elements of the complex projective space* $P\mathsf{H}$.*)* *Under the hypotheses of Gleason's theorem, the extremal points of* $\mathscr{S}(\mathsf{H})$ *are in one-to-one correspondence with the extremal points of* $\mathscr{M}(\mathsf{H})$.
(b) *Any quantum state operator* $T \in \mathscr{S}(\mathsf{H})$ *is a linear combination of extremal quantum-state operators, including infinite combinations in the strong operator topology. In particular there is always a decomposition*

$$T = \sum_{u\in M} p_u \langle u|\ \rangle u \ ,$$

where M *is a Hilbert basis of* T*-eigenvectors of* H, $p_u \in [0,1]$ *for any* $u \in M$, *and*

$$\sum_{u\in M} p_u = 1 \ .$$

Proof We start by proving (b). The expansion is a trivial consequence of Theorem 4.34 (e), since trace-class operators are compact because of (c) Proposition 4.38. Next observe that T is positive, hence selfadjoint, so that its eigenvalues p_u belong to $[0,+\infty)$. M is obtained by completing the Hilbert basis of $\overline{Ran(T)}$ by adding a Hilbert space of $Ker(T)$. Furthermore, according to Proposition 4.40 (e), $1 = tr(T) = \sum_{u\in M} p_u$ and and also $p_u \in [0,1]$.

(a) Consider $T \in \mathfrak{B}_1(\mathsf{H})$ and refer to the expansion used in the proof of (b), $T = \sum_{u\in N} p_u \langle u|\ \rangle u$. If T is not a one-dimensional orthogonal projector there are at least two different u_1 and u_2 with $p_{u_1} > 0$ and $1 - p_{u_1} \geq p_{u_2} > 0$. As a consequence, T decomposes as a convex combination $T = p_{u_1}T_1 + (1-p_{u_1})T_2$ for

$$T_1 = \langle u_1|\ \rangle u_1 \quad \text{and} \quad T_2 := \sum_{u\neq u_1} \frac{p_u}{1-p_{u_1}} \langle u|\ \rangle u \ .$$

Notice that (i) $T_1 \neq T_2$, (ii) $T_1, T_2 \neq 0$, (iii) $T_1, T_2 \in \mathfrak{B}_1(\mathsf{H})$ by construction, (iv) they are selfadjoint, (v) $T_1, T_2 \geq 0$ and (vi) $tr(T_1) = tr(T_2) = 1$, so T_1 and T_2

belong to $\mathscr{S}(\mathsf{H})$. We conclude that T cannot be extremal. To complete the proof, let us prove that $P = \langle\psi|\ \rangle\psi$, with $||\psi|| = 1$, does not admit non-trivial convex decompositions. Suppose that

$$P = \lambda T_1 + (1-\lambda)T_2 \quad \text{for } \lambda \in (0,1) \text{ and } T_1, T_2 \in \mathfrak{B}_1(\mathsf{H}).$$

We want to prove that $T_1 = T_2 = P$. As a consequence of the hypothesis, if $P^\perp = I - P$,

$$0 = P^\perp P = \lambda P^\perp T_1 + (1-\lambda)P^\perp T_2\,,$$

so that

$$0 = \lambda tr(P^\perp T_1) + (1-\lambda)tr(P^\perp T_2) = \lambda tr(P^\perp T_1 P^\perp) + (1-\lambda)tr(P^\perp T_2 P^\perp)\,.$$

Since λ, $(1-\lambda) > 0$ and both $P^\perp T_j P^\perp \geq 0$ for $j = 1, 2$, it must be $tr(P^\perp T_1 P^\perp) = tr(P^\perp T_2 P^\perp) = 0$. Since $T_j \geq 0$, if N is a Hilbert basis of $P^\perp(\mathsf{H}) = P(\mathsf{H})^\perp$, the said conditions can be rephrased as $\sum_{u\in N} ||\sqrt{T_j}u||^2 = 0$, so that $T_j P^\perp = 0$ and, taking the adjoint, $P^\perp T_j = 0$ because $T_j = T_j^*$. Decomposing $T_j = PT_jP + P^\perp T_j P + PT_j P^\perp + P^\perp T_j P^\perp$, we conclude that

$$T_j = PT_jP = t_j\langle\psi|\ \rangle\psi$$

for some $t_j \in \mathbb{C}$ and $j = 1, 2$. The condition $tr(T_j) = 1$ fixes $t_j = 1$. □

Exercise 4.52 Consider $T \in \mathscr{S}(\mathsf{H})$. Prove that

(i) $T^2 \leq T$ (i.e. $\langle x|T^2x\rangle \leq \langle x|Tx\rangle$ for all $x \in \mathsf{H}$);
(ii) T is extremal if and only if $T^2 = T$.

Solution By decomposition of T along the Hilbert basis of eigenvectors of $T \in \mathscr{S}(\mathsf{H})$, we have $T^2 = \sum_{u\in N} p_u^2\langle u|\ \rangle u$. Since $p_u \in [0,1]$, it follows that $0 \leq p_u^2 \leq p_u$ so that $\langle x|T^2x\rangle \leq \langle x|Tx\rangle$ for all $x \in \mathsf{H}$. Since $tr(T^2) = \sum_{u\in N} p_u^2$, if $T^2 = T$ is valid so that $\sum_{u\in N} p_u^2 - p_u = 0$, and $p_u^2 - p \leq 0$, we conclude that $p_u = p_u^2$ for all u, so that $p_u = 0$ or $p_u = 1$. Since $\sum_{u\in N} p_n = 1$, this is possible only if all p_u vanish but one, which takes the value 1. In other words $T = \langle u|\ \rangle u$. Conversely, if $T = \langle u|\ \rangle u$, evidently $T^2 = T$. □.

Exercise 4.53 Prove that the quantum probability measure $\rho : \mathscr{L}(\mathsf{H}) \to [0,1]$ associated to $T \in \mathscr{S}(\mathsf{H})$ according to Proposition 4.45 satisfies the so-called *Jauch-Piron property*: if $\rho(P) = \rho(Q) = 0$ is true for $P, Q \in \mathscr{L}(\mathsf{H})$, then $\rho(P \vee Q) = 0$.

Solution $tr(TP) = 0$ can be rewritten as $\sum_{u\in N} ||\sqrt{T}Pu||^2 = 0$ for every Hilbert basis $N \subset \mathsf{H}$. Fix N and complete to a Hilbert basis of $P(\mathsf{H})$: the formula entails $\sqrt{T}x = 0$ if x belongs to that basis and also for $x \in P(\mathsf{H})$ in view of the continuity of $\sqrt{T}$. As a consequence $Tx = \sqrt{T}\sqrt{T}x = 0$ for $x \in P(\mathsf{H})$. The same result is true when replacing P by Q. Every vector in $P \vee Q(\mathsf{H})$ is the limit of linear combinations of vectors in $P(\mathsf{H})$ and $Q(\mathsf{H})$. Hence $Tx = 0$ if $x \in P \vee Q(\mathsf{H})$ by the linearity and continuity of T. Computing $tr(TP \vee Q)$ using a Hilbert basis which completes a Hilbert basis of $P \vee Q(\mathsf{H})$ by adding a Hilbert basis of $(P \vee Q(\mathsf{H}))^{\perp}$, we immediately find $tr(TP \vee Q) = 0$, namely $\rho(P \vee Q) = 0$. □

4.4.6 Physical Interpretation

The proposition allows us to introduce some notions and terminology relevant in physics.

(a) First of all, extremal elements in $\mathscr{S}(\mathsf{H})$ are usually said to describe **pure states** by physicists. We shall denote their set by $\mathscr{S}_p(\mathsf{H})$.
(b) Non-extremal quantum state operators are called **statistical operators** or also **density matrices**. They are said to describe **mixed states**, **mixtures** or **non-pure states**.
(c) If

$$\psi = \sum_{i \in I} a_i \phi_i \ ,$$

with I finite or countable (and the series converges in the topology of H in the second case), where the vectors $\phi_i \in \mathsf{H}$ are all non-null and $0 \neq a_i \in \mathbb{C}$, physicists call the state operator $\langle \psi | \ \rangle \psi$ a **coherent superposition** of the state operators $\langle \phi_i | \ \rangle \phi_i / ||\phi_i||^2$.
(d) The possibility of creating pure states by non-trivial combinations of vectors associated to other pure states is called, in the jargon of QM, **superposition principle of (pure) states**.
(e) There is however another type of superposition of states. If $T \in \mathscr{S}(\mathsf{H})$ satisfies:

$$T = \sum_{i \in I} p_i T_i$$

with I finite, $T_i \in \mathscr{S}(\mathsf{H})$, $0 \neq p_i \in [0, 1]$ for any $i \in I$, and $\sum_i p_i = 1$, the state operator T is said to describe an **incoherent superposition** of the states described by the operators T_i (possibly pure).
(f) If $\psi, \phi \in \mathsf{H}$ satisfy $||\psi|| = ||\phi|| = 1$ the following terminology is very popular: the complex number $\langle \psi | \phi \rangle$ is the **transition amplitude** or **probability amplitude** of the state operator $\langle \phi | \ \rangle \phi$ on the state operator $\langle \psi | \ \rangle \psi$. Moreover the non-negative real number $|\langle \psi | \phi \rangle|^2$ is the **transition probability** of the state operator $\langle \phi | \ \rangle \phi$ on the state operator $\langle \psi | \ \rangle \psi$.

We make some comments about these notions. Consider the extremal state operator $T_\psi \in \mathscr{S}_p(\mathsf{H})$, written $T_\psi = \langle \psi | \ \rangle \psi$ for some $\psi \in \mathsf{H}$ with $||\psi|| = 1$. What we want to emphasise is that this extremal state operator is also an orthogonal projector $P_\psi := \langle\psi|\ \rangle\psi$, so it must correspond to an elementary observable of the system (an *atom* using the terminology of Theorem 4.17). The naive and natural interpretation[2] of that observable is this: *"the system's state is the pure state given by the vector ψ"*. We can therefore interpret the square modulus of the transition amplitude $\langle\phi|\psi\rangle$ as follows. If $||\phi|| = ||\psi|| = 1$, as the definition of transition amplitude imposes, $tr(T_\psi P_\phi) = |\langle\phi|\psi\rangle|^2$, where $T_\psi := \langle\psi|\ \rangle\psi$ and $P_\phi = \langle\phi|\ \rangle\phi$. Using (4) we conclude:

$|\langle\phi|\psi\rangle|^2$ *is the probability that the state, given (at time t) by the vector ψ, following a measurement (at time t) on the system becomes determined by ϕ.*

Notice $|\langle\phi|\psi\rangle|^2 = |\langle\psi|\phi\rangle|^2$, so the probability transition of the state determined by ψ on the state determined by ϕ coincides with the analogous probability where the vectors are swapped. This fact is, *a priori*, highly non-evident in physics.

4.4.7 Post-measurement States: The Meaning of the Lüders-von Neumann Postulate

Since we have introduced a new notion of state, the axiom concerning the collapse of the state (Sect. 3.4) must be upgraded to encompass all state operators of $\mathscr{S}(\mathsf{H})$. The standard formulation of QM assumes the following axiom (introduced by von Neumann and generalized by Lüders) about what occurs to the physical system, in a state described by the operator $T \in \mathscr{S}(\mathsf{H})$ at time t, when subjected to the measurement of an elementary observable $P \in \mathscr{L}(\mathsf{H})$, if the latter is true (so in particular $tr(TP) > 0$, prior to the measurement). We are referring to *non-destructive* testing, also known as *indirect measurement* or *first-kind measurement*, where the physical system examined (typically a particle) is not absorbed/annihilated by the instrument. It is an idealised version of the actual processes used in labs, and only in part they can be modelled in such a way.

Collapse of the State: General Formulation If the quantum system is in the state described by $T \in \mathscr{S}(\mathsf{H})$ at time t and proposition $P \in \mathscr{L}(\mathsf{H})$ is true after a measurement at time t, the system's state immediately afterwards is described by

$$T_P := \frac{PTP}{tr(TP)}\,. \tag{4.22}$$

[2] We cannot but notice how this interpretation muddles the semantic and syntactic levels. Although this could be problematic in a formulation within formal logic, the use physicists make of the interpretation eschews the issue.

In particular, if T is pure and determined by the unit vector ψ, the state immediately after measurement is still pure, and determined by:

$$\psi_P = \frac{P\psi}{||P\psi||} . \tag{4.23}$$

(Obviously, in either case T_P and ψ_P define states. In the former, in fact, T_P is positive of trace class, with unit trace, while in the latter $||\psi_P|| = 1$.)

The postulate has an important characterization. Suppose that the initial state is described by $T \in \mathscr{S}(\mathsf{H})$, we measure $P \in \mathscr{L}(\mathsf{H})$ and we want to know the probability to measure $Q \in \mathscr{L}(\mathsf{H})$. This is a problem of *conditional probability*. In general, if Q is not compatible with P, i.e. if P and Q do not commute, the rules to handle conditional probability are different from the classical ones, as physicists know very well. However, if we deal with compatible elementary observables, we expect that the quantum rules and the classical ones coincide, by including these observables in a maximal set of commuting elementary observables as we already did elsewhere. In particular, let us assume $Q \leq P$. In this case $P \wedge Q = PQ = QP = Q$ (Proposition 3.19), so the classical rule of conditional probability is expected to hold with an obvious meaning of the symbols,

$$\mathbb{P}_T(Q|P) = \frac{\mathbb{P}_T(P \wedge Q)}{\mathbb{P}_T(P)} = \frac{\mathbb{P}_T(Q)}{\mathbb{P}_T(P)} .$$

This requirement, if assumed, completely characterizes the post-measurement state and implies that the Lüders-von Neumann postulate holds, as established in the following proposition.

Proposition 4.54 *Let $T \in \mathscr{S}(\mathsf{H})$ be a quantum state operator for a Hilbert space H and suppose that, for $P \in \mathscr{L}(\mathsf{H})$, $tr(TP) > 0$. There exists exactly one other quantum state operator $T' \in \mathscr{S}(\mathsf{H})$ such that*

$$tr(T'Q) = \frac{tr(TQ)}{tr(TP)} \quad \textit{for every } Q \in \mathscr{L}(\mathsf{H}) \textit{ with } Q \leq P. \tag{4.24}$$

Moreover,

$$T' = \frac{PTP}{tr(TP)} .$$

Proof One immediately proves that T' satisfies the condition. Let us prove the converse statement. If $x \in \mathsf{H}_0 := P(\mathsf{H})$ has unit norm, consider the orthogonal projector $Q_x := \langle x| \ \rangle x$. Since $Q \leq P$, condition (4.24) reads $tr(T'Q_x) = tr(TP)^{-1}tr(TQ_x)$. Computing traces by completing x to a basis of H, we have $\langle x|T'x\rangle - tr(TP)^{-1}\langle x|Tx\rangle = 0$ and, since $x = Px$, it can be rearranged to $\langle x|T'x\rangle - tr(TP)^{-1}\langle Px|TPx\rangle = 0$, so that

$$\langle x|(T' - tr(TP)^{-1}PTP)x\rangle = 0 \quad \text{for every } x \in \mathsf{H}_0 . \tag{4.25}$$

Now observe that condition (4.24) for $Q = P$ leads to $tr(T'P) = 1$. Taking also advantage of the cyclic property of the trace and $PP = P$, we have $tr(T'P) = tr(PT'P) = 1$. On the other hand, using the decomposition $T' = PTP + P^\perp TP^\perp + P^\perp TP + PTP^\perp$, (where$P^\perp := I - P$), the normalization condition $tr(T') = 1$ implies $1 = tr(PT'P) + tr(P^\perp T'P^\perp)$. Comparing the results obtained, we conclude that $tr(P^\perp T'P^\perp) = 0$, namely $tr(P^\perp \sqrt{T}\sqrt{T}P^\perp) = \sum_{u\in N} ||\sqrt{T}u||^2 = 0$, where N is a Hilbert basis of $P^\perp(\mathsf{H})$. We have found that $T'P^\perp = 0$ and also, taking the adjoint $P^\perp T' = 0$. Coming back to the decomposition $T' = PT'P + P^\perp T'P^\perp + P^\perp T'P = PT'P^\perp$, we realize that $T' = PT'P$. In view of the analogous $\frac{PTP}{tr(TP)}$, we can restrict our analysis to the Hilbert space $\mathsf{H}_0 := P(\mathsf{H})$, since both operators vanish on the orthogonal of H_0 and their images are contained in H_0 viewed as a Hilbert space. To this regard, Proposition 2.5 implies that (4.25) is therefore equivalent to $(T' - tr(TP)^{-1}PTP)z = 0$ when $z \in \mathsf{H}_0$. Since, as we said, both operators vanish on the orthogonal of H_0, we have that $T'y = tr(TP)^{-1}PTPy$ for every $y \in \mathsf{H}$ proving our assertion. □

Conditional probability is an articulated part of quantum logic (quantum conditional and quantum conditional probability) with profound differences between the classical counterparts and open issues. See [Red98] for a technical account.

Remark 4.55

(a) Measuring a property of a physical quantity goes through the interaction between the system and an instrument (supposed to be macroscopic and obeying the laws of classical physics). Quantum Mechanics, in its standard formulation, does not establish what a measuring instrument is, it only says they exist; nor is it capable of describing the interaction of instrument and quantum system set out in the Lüders-von Neumann postulate discussed above. Several viewpoints and conjectures exist on how to complete the physical description of the measuring process; these are called, in the slang of QM, **collapse/reduction of the state** or **of the wavefunction**, and are also described in terms of *decoherence* (see [BLPY16, Lan17] for complete discussions and references).

(b) Measuring instruments are commonly employed to *prepare a system in a certain pure state*. Theoretically speaking the preparation of a *pure* state is carried out like this. A finite collection of *compatible* propositions $P_1, \ldots, P_n$ is chosen so that the projection subspace of $P_1 \wedge \cdots \wedge P_n = P_1 \cdots P_n$ is *one-dimensional*. In other words $P_1 \cdots P_n = \langle\psi|\ \rangle\psi$ for some vector with $||\psi|| = 1$. The existence of such propositions is seen in practically all quantum systems used in experiments. (From a theoretical point of view these are *atomic* propositions.) Then the P_i are simultaneously measured on several identical copies of the physical system of concern (e.g., electrons), whose initial states, though, are unknown. If for one system the measurements of all propositions are successful, the post-measurement state is determined by the vector ψ, and the system was **prepared** in that particular pure state.

Normally each projector P_i belongs to the PVM $P^{(A)}$ of an observable A_i whose spectrum is made of isolated points (thus a pure point spectrum according to Definition 3.44) and $P_i = P^{(A)}_{\{\lambda_i\}}$ with $\lambda_i \in \sigma_p(A_i)$. We will come back to this issue in Sect. 6.2.2.

(c) Let us finally explain how to obtain non-pure states from pure ones practically. Consider q_1 identical copies of system S prepared in the pure state associated to ψ_1, q_2 copies of S prepared in the pure state associated to ψ_2 and so on, up to ψ_n. If we mix these states each one will be in the non-pure state: $T = \sum_{i=1}^n p_i \langle \psi_i | \ \rangle \psi_i$, where $p_i := q_i / \sum_{i=1}^n q_i$. In general, $\langle \psi_i | \psi_j \rangle$ is not zero if $i \neq j$, so the above expression for T is not the decomposition with respect to an eigenvector basis for T. This procedure may seem to suggest the existence of two different types of probability, one intrinsic and due to the quantum nature of the state associated to ψ_i; the other epistemic, and encoded in the probability p_i. But this is not true: once a non-pure state has been created, as above, there is no way, within QM, to distinguish the states forming the mixture. For example, the same state operator T could have been obtained mixing pure states other than those determined by the ψ_i. In particular, one could have used those in the eigenvector decomposition of T. For physics, no kind of measurement would distinguish the two mixtures. ■

To conclude this quick discussion about measurements in Quantum Theories, it is fundamental to stress that the Lüders-von Neumann postulate refers to an extremely idealized notion of measurement. Similarly, the notion of observable viewed as the integral of a PVM, albeit representing a fundamental theoretical notion, appears to be a rigid idealization of concrete measurement instruments. Realistic quantum instruments are nowadays described through a mature and sophisticated mathematical theory based on the notion of *POVMs* (positive-operator valued measures) generalising our familiar PVM, and *completely positive maps*. We suggest [BLPY16] as a modern review on the subject.

4.4.8 Composite Systems in Elementary QM: The Use of Tensor Products

If a quantum system S described on the Hilbert space H contains two *independent* parts, S_1 and S_2, respectively described on the Hilbert spaces H_1 and H_2, we are committed to assume this triple of requirements at least.

(A) The elementary propositions P_i of each subsystem, the elements of $\mathscr{L}(\mathsf{H}_i)$ for $i = 1, 2$, must be (1-1) identified with corresponding elementary propositions P'_i on the full system, i.e., elements of $\mathscr{L}(\mathsf{H})$.
(B) Any pair of elementary propositions, one for each *independent* subsystem, viewed as elements of $\mathscr{L}(\mathsf{H})$ must be *compatible*.
(C) For every couple of states $T_1 \in \mathscr{S}(\mathsf{H}_1)$, $T_2 \in \mathscr{S}(\mathsf{H}_2)$, there is a state $T \in \mathscr{S}(\mathsf{H})$ such that $tr(T P'_1) = tr(T_1 P_1)$ and $tr(T P'_2) = tr(T_1 P_2)$ for every $P_1 \in \mathscr{L}(\mathsf{H}_i)$ and $P_2 \in \mathscr{L}(\mathsf{H}_2)$.

(C) says that we can fix states on S_1 and S_2 *independently*: for every choice of two independent states on the two parts of the system, there is a state of the overall system which embodies those choices.

A natural way to implement these requirements in elementary QM is assuming that the whole system is described on the *Hilbert tensor product* $\mathsf{H} = \mathsf{H}_1 \otimes \mathsf{H}_2$ (with further factors in case S_1 and S_2 do not exhaust the total system S, but further independent parts S_3 etc. are present) so that, in particular, the space of states is $\mathscr{S}(\mathsf{H}) = \mathscr{S}(\mathsf{H}_1 \otimes \mathsf{H}_2)$.

We quote here some basic technical facts [Mor18] regarding the tensor product of Hilbert spaces, useful when dealing with composite systems and leading to the assumption made above.

(1) (From Sect. 2.1.4.) The Hermitian inner product $\langle \cdot|\cdot \rangle$ on $\mathsf{H}_1 \otimes \mathsf{H}_2$ is the unique Hermitian inner product such that, with obvious notation,

$$\langle \psi_1 \otimes \psi_2 | \phi_1 \otimes \phi_2 \rangle = \langle \psi_1 | \phi_1 \rangle_1 \langle \psi_2 | \phi_2 \rangle_2 \quad \text{for every } \phi_i, \psi_i \in \mathsf{H}_i \text{ and } i = 1, 2. \tag{4.26}$$

(2) (From Proposition 10.32 in [Mor18]) If $A_i \in \mathfrak{B}(\mathsf{H}_i)$ $i = 1, 2$, there is a unique operator $A_1 \otimes A_2 \in \mathfrak{B}(\mathsf{H}_1 \otimes \mathsf{H}_2)$ called the **tensor product** of A_1 and A_2 such that

$$A_1 \otimes A_2(\psi_1 \otimes \psi_2) = (A_1\psi_1) \otimes (A_2\psi_2) \quad \text{for every } \psi_i \in \mathsf{H}_i \text{ and } i = 1, 2 \tag{4.27}$$

and it turns out that

$$||A_1 \otimes A_2|| = ||A_1||_1 \, ||A_2||_2 \, . \tag{4.28}$$

Moreover, $A_i \geq 0$ imply $A_1 \otimes A_2 \geq 0$.

(3) It is easy to prove that if furthermore $A_i \in \mathfrak{B}_1(\mathsf{H}_i)$ then $A_1 \otimes A_2 \in \mathfrak{B}_1(\mathsf{H}_1 \otimes \mathsf{H}_2)$ and $tr(A_1 \otimes A_2) = tr(A_1)tr(A_2)$.

The stated facts lead straightforwardly to the following proposition.

Proposition 4.56 *If* $\mathsf{H}_1, \mathsf{H}_2$ *are Hilbert spaces, the following results are valid.*

(a) *The map*

$$\mathfrak{B}(\mathsf{H}_1) \ni A_1 \mapsto A_1 \otimes I_2 \in \mathfrak{B}(\mathsf{H}_1 \otimes \mathsf{H}_2) \tag{4.29}$$

is an injective and norm-preserving unital *-algebra homomorphism. *Furthermore,*

$$\sigma(A_1 \otimes I_2) = \sigma(A_1)\,, \quad \sigma_p(A_1 \otimes I_2) = \sigma_p(A_1)\,, \quad \sigma_c(A_1 \otimes I_2) = \sigma_c(A_1)\,,$$
$$\sigma_r(A_1 \otimes I_2) = \sigma_r(A_1)\,.$$

A similar statement holds replacing 1 *with* 2.

(b) *The map*

$$\mathscr{L}(\mathsf{H}_1) \ni P_1 \mapsto P_1 \otimes I_2 \in \mathscr{L}(\mathsf{H}_1 \otimes \mathsf{H}_2) \tag{4.30}$$

is well defined and is an injective homomorphism of orthocomplemented lattices. *A similar statement holds when replacing* 1 *by* 2.

(c) *The map*

$$\mathscr{S}(\mathsf{H}_1) \times \mathscr{S}(\mathsf{H}_2) \ni (T_1, T_2) \mapsto T_1 \otimes T_2 \in \mathscr{S}(\mathsf{H}_1 \otimes \mathsf{H}_2) \tag{4.31}$$

is well defined and $T := T_1 \otimes T_2$ *satisfies*

$$tr(T A_1 \otimes A_2) = tr(T_1 A_1) tr(T_2 A_2)\,, \quad \textit{for} \quad A_i \in \mathfrak{B}(\mathsf{H}_i)\,, i = 1, 2\,.$$

In particular,

$$tr(T(P_1 \otimes I_2)) = tr(T_1 P_1) \quad \textit{and} \quad tr(T(I_1 \otimes P_2)) = tr(T_2 P_2)$$
$$\textit{for} \quad P_i \in \mathscr{L}(\mathsf{H}_i)\,, i = 1, 2\,.$$

Sketch of Proof (a) is consequence of (2) and (1). In particular, $(A_1 \otimes I_2)^* = A_1^* \otimes I_2$ arises from $\langle \psi \otimes \phi | A_1 \otimes I_2(\psi' \otimes \phi')\rangle = \langle A_1^* \otimes I_2(\psi \otimes \phi) | A_1 \otimes I_2 \psi' \otimes \phi'\rangle$ which is valid due to (1),(2) and from the fact that linear combinations of elements $\psi \otimes \phi$ are dense in $\mathsf{H}_1 \otimes \mathsf{H}_2$, also using the boundedness of the operators involved. The identities between the various parts of the spectrum easily arise from (2), the linearity of operators, and the direct application of the relevant definitions. (b) is consequence of the relevant definitions, the continuity of the operators and in particular Proposition 4.12. (c) Is consequence of (3) and the comment before the remark in Sect. 2.1.4. □

Items (b) and (c) show that the tensor product yields a practical implementation of the requirements (A)–(C). In fact, (A) the elementary propositions of a subsystem are viewed as elementary propositions on the full system under the injective homomorphism (4.30). Moreover, (B) elementary propositions of two independent subsystems are always *compatible* because

$$(P_1 \otimes I_2)(I_1 \otimes P_2) = P_1 \otimes P_2 = (I_1 \otimes P_2)(P_1 \otimes I_2) \quad \text{for } P_i \in \mathscr{L}(\mathsf{H}_i) \text{ and } i = 1, 2\,.$$

There are natural extensions of these results to the case A_1, A_2 densely defined and selfadjoint, but we shall not enter the details here [Mor18]. The fact that (C) is valid is now trivial. All these results generalize to the case of a finite, and to some extent, countable number of subsystems.

Remark 4.57 The use of the tensor product of Hilbert spaces to formalize the notion of independent subsystems is a possibility usually exploited in elementary QM. However, this is not the only possibility and sometimes it is impossible to adopt that description. We will come back on this issue in Sect. 6.4. ■

Example 4.58

(1) An electron possesses an *electric charge* in addition to the spin. That is another *internal* quantum observable Q with two values $\pm e$, where $e \approx -1.6 \times 10^{-19}$ C is the value elementary electrical charge. So there are two types of electrons. *Proper electrons*, whose internal state of charge is an eigenvector of Q with eigenvalue $-e$ and *positrons*, whose internal state of charge is a eigenvector of Q with eigenvalue e. The simplest version of the internal Hilbert space of the electrical charge is therefore H_c which,[3] again, is isomorphic to $\mathbb{C}^2$. With this representation $Q = e\sigma_3$. The full Hilbert space of an electron must therefore contain a factor $\mathsf{H}_s \otimes \mathsf{H}_c$. Obviously this is by no means sufficient to describe an electron, since we must include the observables describing at least the position of the electron. The three observables describing the Cartesian coordinates of the positions of an electron in the rest space $\mathbb{R}^3$ of an inertial reference space are represented in $L^2(\mathbb{R}^3, d^3x)$ as we already know. The final space is therefore $L^2(\mathbb{R}^3, d^3x) \otimes \mathsf{H}_s \otimes \mathsf{H}_c$. Alternatively, the non-internal part of the state of the electron can be represented in the L^2 space associated with the momentum operators, the *momentum picture* introduced in Example 3.74. With this choice the total Hilbert space of an electron is $L^2(\mathbb{R}^3, d^3k) \otimes \mathsf{H}_s \otimes \mathsf{H}_c$ where the momentum operator is a multiplication. These two descriptions are unitarily equivalent (under the Fourier-Plancherel transform) and choosing one or another is just matter of convenience.

(2) Composite systems are in particular systems made of many (either identical or not) particles. If we have a pair of particles respectively described on the Hilbert space H_1 and H_2, the full system is described on $\mathsf{H}_1 \otimes \mathsf{H}_2$. Notice that, in the finite-dimensional case, the dimension of the final space is the *product* of the components' dimensions. In CM the system would instead be described on a phase space which is the Cartesian product of the two phase spaces. In that case the dimension would be the *sum*, rather than the product, of the dimensions of the component spaces. ■

4.5 General Interplay of Quantum Observables and Quantum States

This section is devoted to focus on the interplay of general observables and states and to prove that formulas familiar to physicists are well motivated by the rigorous formalism.

[3] As we shall say later, in view of a *superselection rule* not all normalized vectors of H_c represent (pure) states.

4.5.1 Observables, Expectation Values, Standard Deviations

When dealing with mixed states, Definitions (3.43) and (3.45) for the expectation value $\langle A\rangle_\psi$ and the standard deviation ΔA_ψ of an observable A referred to the pure state defined by $\langle\psi|\ \rangle\psi$ with $||\psi|| = 1$, are no longer valid. Extended natural definitions can be stated referring to the probability measure associated to both the mixed state defined by $T \in \mathscr{S}(\mathsf{H})$ and the observable A, more precisely its PVM $P^{(A)}$. In practice, we can define

$$\mu_T^{(A)} : \mathscr{B}(\sigma(A)) \ni E \mapsto tr(P_E^{(A)} T) \in [0, 1] \tag{4.32}$$

with the meaning of *the probability to obtain E after a measurement of A in the quantum state represented by $T \in \mathscr{S}(\mathsf{H})$*.

In particular, if T is *pure*, so that $T = \psi\langle\psi|\cdot\rangle$ for some unit vector $\psi \in \mathsf{H}$, we find again the probability already seen in (3.42),

$$\mu_T^{(A)}(E) = ||P_E^{(A)}\psi||^2 = \mu_{\psi,\psi}^{(A)}(E)\ .$$

The proof is trivial: just complete $\{\psi\}$ to a Hilbert basis of H and compute the trace. Adopting the definition of $\mu_T^{(A)}$ introduced in (4.32),

(a) the **expectation value** of A with respect to the state described by T is defined as

$$\langle A\rangle_T := \int_{\sigma(A)} \lambda\, d\mu_T^{(A)}(\lambda)\ , \tag{4.33}$$

provided the function $\sigma(A) \ni \lambda \to \lambda \in \mathbb{R}$ is in $L^1(\sigma(A), \mu_T^{(A)})$;

(b) the **standard deviation** is defined as

$$\Delta A_T := \sqrt{\int_{\sigma(A)} (\lambda - \langle A\rangle_T)^2\, d\mu_T^{(A)}(\lambda)} = \sqrt{\int_{\sigma(A)} \lambda^2\, d\mu_T^{(A)}(\lambda) - \langle A\rangle_T^2}\ , \tag{4.34}$$

provided $\sigma(A) \ni \lambda \to \lambda \in \mathbb{R}$ is in $L^2(\sigma(A), \mu_T^{(A)})$. (Notice $L^2(\sigma(A), \mu_T^{(A)}) \subset L^1(\sigma(A), \mu_T^{(A)})$ since the measure is finite.)

4.5.2 Relation with the Formalism Used in Physics

The next proposition establishes that the usual formal results handled by physicists (see formulas in (b)-(d) below) are valid under suitable conditions on the domains.[4] With reference to the domain issues in (b) and (c) below we observe that $D(A^2) = \Delta_{\iota^2} \subset \Delta_\iota = D(A) = D(|A|)$.

Proposition 4.59 *Let* H *be a Hilbert space,* $T \in \mathscr{S}(\mathsf{H})$ *a quantum state operator and* $A : D(A) \to \mathsf{H}$*, densely defined, an observable (i.e.* $A = A^*$*). The following facts hold.*

(1) $\mu_T^{(A)}$ *as in (4.32) is a well-defined probability measure on* $\mathscr{B}(\sigma(A))$.
(2) *If* $Ran(T) \subset D(A)$ *and* $|A|T \in \mathfrak{B}_1(\mathsf{H})$ *(always valid if* $A \in \mathfrak{B}(\mathsf{H})$*), then*

  (a) $\langle A\rangle_T$ *is well defined,*
  (b) $\langle A\rangle_T = tr(AT)$.

(3) *If* $Ran(T) \subset D(A^2)$ *and* $|A|T, A^2T \in \mathfrak{B}_1(\mathsf{H})$ *(always valid if* $A \in \mathfrak{B}(\mathsf{H})$*), then*

  (a) ΔA_T *is well defined,*
  (b) $\Delta A_T = \sqrt{tr(A^2T) - (tr(AT))^2}$.

(4) *Assume that* $T = \psi\langle\psi|\ \rangle$ *with* $||\psi|| = 1$

  (a) *If* $\psi \in D(A)$ *then the hypotheses in 2 are valid and* $\langle A\rangle_T = \langle\psi|A\psi\rangle$,
  (b) *If* $\psi \in D(A^2)$ *then the hypotheses in 3 are valid and* $\Delta A_T = \sqrt{\langle\psi|A^2\psi\rangle - \langle\psi|A\psi\rangle^2}$.

Proof

(1) Taking the definition PVM into account, the proof is a trivial adaptation of the proof of Proposition 4.45.

(2)(a) Let us assume $Ran(T) \subset D(A)$ and $|A|T \in \mathfrak{B}_1(\mathsf{H})$ that are automatically true if $A \in \mathfrak{B}(\mathsf{H})$. As already stressed, $D(|A|) = D(A)$ so $Ran(T) \subset D(A) = D(|A|)$ is true and both AT, $|A|T$ are well defined under said hypotheses. Next, the polar decomposition theorem for (unbounded) selfadjoint operators $A = U|A|$ (immediately obtained from the spectral decomposition in the three cases with $|A|$ and $U := \mathrm{sign}(A) \in \mathfrak{B}(\mathsf{H})$ defined spectrally) implies $AT = U|A|T \in \mathfrak{B}_1(\mathsf{H})$, because $U \in \mathfrak{B}(\mathsf{H})$ and $\mathfrak{B}_1(\mathsf{H})$ is two-sided ideal. Now, referring to the Borel σ-algebra on $\sigma(A) \subset \mathbb{R}$, we can construct a sequence of real simple functions

$$s_n = \sum_{i_n \in \mathfrak{I}_n} c_{i_n}^{(n)} \chi_{E_{i_n}^{(n)}} : \sigma(A) \to \mathbb{R} \quad \text{with } c_{i_n}^{(n)} \in \mathbb{R}, \text{ and } \mathfrak{I}_n \text{ finite}$$

[4] Weaker necessary and sufficient conditions assuring that these formulas are valid can be found in [Mor18] with reference to Hilbert-Schmidt operators, which we do not consider here.

which satisfies

$$0 \le |s_n| \le |s_{n+1}| \le |\imath| , \quad s_n \to \imath \quad \text{pointwise as } n \to +\infty, \tag{4.35}$$

where $\imath : \sigma(A) \ni \lambda \mapsto \lambda \in \mathbb{R}$. By direct application of the given definitions, if

$$A_n := \int_{\sigma(A)} s_n dP^{(A)} = \sum_{i_n \in \mathfrak{I}_n} c^{(n)}_{i_n} P^{(A)}_{E^{(n)}_{i_n}} \in \mathfrak{B}(\mathsf{H}) ,$$

exploiting Proposition 3.29 (c), monotone convergence and Lebesgue's dominated convergence, we have both

$$\langle\psi|A_n\psi\rangle \to \langle\psi|A\psi\rangle , \quad \langle\psi||A_n|\psi\rangle \to \langle\psi||A|\psi\rangle \quad \forall\psi \in D(A) \quad \text{as } n \to +\infty \tag{4.36}$$

and also

$$|\langle\psi|A_n\psi\rangle| \le \langle\psi||A_n|\psi\rangle \le \langle\psi||A|\psi\rangle . \tag{4.37}$$

On the other hand, if M is a Hilbert basis of H obtained by completing a Hilbert basis N of $Ker(T)^\perp$ made of eigenvectors of T according to Theorem 4.34 (e) and taking advantage of the cyclic property of the trace, we have both

$$tr(A_nT) = tr\left(\sum_{i_n \in \mathfrak{I}_n} c^{(n)}_{i_n} P^{(A)}_{E^{(n)}_{i_n}} T\right) = \sum_{i_n \in \mathfrak{I}_n} c^{(n)}_{i_n} tr(P^{(A)}_{E^{(n)}_{i_n}} T) = \sum_{i_n \in \mathfrak{I}_n} c^{(n)}_{i_n} tr(T P^{(A)}_{E^{(n)}_{i_n}}) =$$
$$= \sum_{i_n \in \mathfrak{I}_n} c^{(n)}_{i_n} \mu_T(E^{(n)}_{i_n}) = \int_{\sigma(A)} s_n d\mu^{(A)}_T \tag{4.38}$$

and similarly

$$tr(|A_n|T) = \int_{\sigma(A)} |s_n| \, d\mu^{(A)}_T . \tag{4.39}$$

Looking at the formula (4.39), by the monotone convergence theorem

$$tr(|A_n|T) = \int_{\sigma(A)} |s_n|(\lambda) \, d\mu^{(A)}_T(\lambda) \to \int_{\sigma(A)} |\lambda| \, d\mu^{(A)}_T(\lambda)$$

as $n \to +\infty$, and simultaneously

$$tr(|A_n|T) = \sum_{u \in N} s(u)\langle u||A_n|u\rangle \to \sum_{u \in N} s(u)\langle u|Au\rangle = tr(|A|T) ,$$

where $s(u) \geq 0$ are the eigenvalues of T, again by monotone convergence and (4.36). Putting all together, we find

$$tr(|A|T) = \int_{\sigma(A)} |\lambda| \, d\mu_T^{(A)}(\lambda) \, .$$

We have in particular established that the integral in the right-hand side is finite (because the left-hand side exists by hypothesis) and thus $\langle A \rangle_T$ is well defined.

(2)(b) Let us look at the formula in (4.38). From dominated convergence, taking (4.35) into account, we obtain as $n \to \infty$

$$tr(A_n T) = \int_{\sigma(A)} s_n(\lambda) \, d\mu_T^{(A)} \to \int_{\sigma(A)} \lambda \, d\mu_T^{(A)} \, .$$

On the other hand,

$$tr(A_n T) = \sum_{u \in N} \langle u | A_n u \rangle s(u) \to \sum_{u \in N} \langle u | A u \rangle s(u) = tr(AT) \, ,$$

where we have once again applied the dominated convergence theorem allowed by (4.37). Putting everything together we get

$$tr(AT) = \int_{\sigma(A)} \lambda \, d\mu_T^{(A)}(\lambda) =: \langle A \rangle_T \, ,$$

concluding the proof of 2.(b).

(3) The proof is strictly analogous to that of (2) by noticing that the hypotheses of (3) imply those of (2) and that $L^2(\sigma(A), \mu_T^{(A)}) \subset L^1(\sigma(A), \mu_T^{(A)})$ because $\mu_T^{(A)}$ is finite.

(4) The claim reduces to trivial subcases of (2) and (3), in particular by completing $\{\psi\}$ to a Hilbert basis of H to compute the various traces.

□

Example 4.60 Let us consider a quantum spinless particle of mass $m > 0$, living on the real line, whose Hamiltonian operator

$$H = \text{s-}\sum_{n=0}^{+\infty} \hbar\omega(n + 1/2) \langle \psi_n | \ \rangle \psi_n$$

is that of a harmonic oscillator (see (3) Example 3.43). In this case $\mathsf{H} = L^2(\mathbb{R}, dx)$. If the system is in contact with a *heat bath* at (absolute) temperature $(k_B \beta)^{-1} > 0$ (k_B being *Boltzmann's constant*), its state is mixed and is described by the *statistical operator*

$$T_\beta = Z_\beta^{-1} e^{-\beta H} \, ,$$

where expanding the trace in the Hilbert basis of eigenvectors ψ_n of H gives

$$Z_\beta = tr(e^{-\beta H}) = \sum_{n=0}^{+\infty} e^{-\beta\hbar\omega(n+1/2)} = \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}}\,, \tag{4.40}$$

the so-called *canonical partition function*. In other words

$$T_\beta = \text{s-}\sum_{n=0}^{+\infty} \frac{e^{-\beta\hbar\omega(n+1/2)}}{Z_\beta} \langle\psi_n|\ \rangle\psi_n\,.$$

It is easy to check that $T_\beta \in \mathscr{S}(\mathsf{H})$. Furthermore the elements of $Ran(T_\beta)$ have the form

$$\sum_{n=0}^{+\infty} e^{-\beta\hbar\omega(n+1/2)} c_n\psi_n \quad \text{with} \quad \sum_{n=0}^{+\infty} |c_n|^2 < +\infty.$$

It is therefore evident that $Ran(T_\beta) \subset D(H^m)$ for $m = 1, 2, \ldots$ and that $|H|T_\beta = H_\beta T_\beta$ and $H^2 T_\beta \in \mathfrak{B}_1(\mathsf{H})$. For instance

$$H^m T_\beta = \text{s-}\sum_{n=0}^{+\infty} \frac{(\hbar\omega)^m e^{-\beta\hbar\omega(n+1/2)}(n+1/2)^m}{Z_\beta} \langle\psi_n|\ \rangle\psi_n\,,$$

so that $H^m T_\beta \in \mathfrak{B}_1(\mathsf{H})$ with

$$||H^m T_\beta|| = \sup_{n\in\mathbb{N}} \frac{(\hbar\omega)^2 e^{-\beta\hbar\omega(n+1/2)}(n+1/2)^m}{Z_\beta} = \frac{(\hbar\omega)^m e^{-\beta\hbar\omega/2}}{2^m Z_\beta}\,,$$

$$||H^m T_\beta||_1 = \sum_{n=0}^{+\infty} \frac{(\hbar\omega)^m e^{-\beta\hbar\omega(n+1/2)}(n+1/2)^m}{Z_\beta} < +\infty\,.$$

Therefore we can apply Proposition 4.59. For instance

$$\langle H\rangle_{T_\beta} = tr(HT_\beta) = \frac{\hbar\omega}{Z_\beta}\sum_{n=0}^{+\infty} e^{-\beta\hbar\omega(n+1/2)}(n+1/2) = -\frac{1}{Z_\beta}\frac{d}{d\beta}Z_\beta = -\frac{d}{d\beta}\ln Z_\beta,$$

where in the penultimate passage we have moved the derivative in β inside the sum, as allowed by standard elementary theorems of calculus, since the series converges and the derivatives' series converges uniformly. ∎

Chapter 5
Realism, Non-Contextuality, Local Causality, Entanglement

We have accumulated enough theoretical material to tackle some aspects of an important and intriguing issue regarding the theoretical interpretation of the quantum realm.

5.1 Hidden Variables and no-go Results

There exist approaches to quantum phenomenology, called *hidden-variable formulations* (see, e.g.,[BeCa81, Ghi07, Lan17, BeZe17, SEP], and [Red98] for the viewpoint of QFT), that compete with the standard interpretation of the formalism also known as *Copenhagen interpretation*, which is the one adopted in this book.

The most important exemplar of these alternative formulations is certainly the well-known *Bohmian mechanics* [DüTe09], a quite articulate and healthy theory. Also known as *pilot-wave theory* or *de Broglie–Bohm theory*, Bohmian mechanics posits that a quantum particle has a definite position at every time (in this sense it is a partially classic system and the position is the hidden variable) and moves according to an equation of motion subsuming a "quantum" interaction due to a wavefunction that evolves under the usual Schrödinger equation. Randomness arises from the fact that we do not know which trajectory the particle actually follows among the plethora permitted by the evolution law. Bohmian mechanics is named after David Bohm, who was the first physicist to frame (in 1952) into a definite form this alternate description, which had already been proposed in similar yet vague forms by other scientists like de Broglie, thus enabling it to make correct predictions. A thorough examination would deserve more than an entire chapter, so we shall not discuss it here (see also [Tum17] for a recent review).

Another classical subject concerns the celebrated *Bell theorem* apropos the *BCHSH inequality* and the role of *locality* (or *local causality*) in QM, in relationship to the phenomenology of *entangled states*. The reader may profitably consult

V. Moretti, *Fundamental Mathematical Structures of Quantum Theory*,
https://doi.org/10.1007/978-3-030-18346-2_5

[BeZe17] for a recent review on Bell's achievements and the developments of his ideas on locality and entanglement in quantum theory—with regard to other topics discussed in the rest of this chapter—also including recent experimental achievements.

Although we will introduce two versions of Bell's analysis on the interplay between *entanglement*, *realism*, and *locality* in two sections of this chapter, we are also interested in discussing a different theoretical milestone about hidden-variable theories, known as the *Kochen–Specker theorem*, and the related notions of *realism* and *non-contextuality*. The last section tackles the interaction between entanglement and non-contextuality by addressing the *BCHSH inequality* from a different point of view.

5.1.1 Realistic Hidden-Variable Theories

The pivotal idea at the heart of hidden-variable formulations is that a quantum system is actually *partially* classic (quantum phenomenology and the constant $\hbar$ must however enter the theory, eventually) and the observed randomness of measurement outcomes is due to an *incomplete* knowledge of the system. There are in particular *hidden variables*, cumulatively denoted by $\lambda \in \Lambda$ usually, whose knowledge would completely fix a classical-like state of the system. For this school of thought it is implicit that *all observables always have definite values* when λ is given, even if we do not know them. *Measurements are thus simple observations of values which already exist.* This hypothesis goes under the name of *realism* after the celebrated analysis by Einstein et al. [EPR35] (though this notion of realism specifically refers to a theoretical context only, and should not be taken literally as a general philosophical assumption!). As we said above, due to reasons specified in concrete models, when we observe the quantum behaviour of our physical system, the knowledge of hidden variables is limited in a way similar to what happens in statistical mechanics. As a matter of fact, we only have access to a probability distribution of λ over Λ, which we shall denote by μ. The quantum fluctuations of the outcomes of a measurement are explained as *statistical fluctuations* related to μ. In this view, quantum randomness is merely *epistemic* rather than *ontic*, as in the Copenhagen interpretation.

5.1.2 The Bell and Kochen–Specker no-go Theorems

Let us get started with a non-existence theorem in the standard formulation of QM.

Under the hypotheses of Gleason's theorem, quantum-state operators and quantum probability measures correspond one-to-one, so the notion of *expectation value* and *standard deviation* of an observable can be ascribed to quantum probability measures $\rho \in \mathscr{M}(\mathsf{H})$. In particular $\langle A \rangle_\rho$ and ΔA_ρ can be defined when A is bounded simply by replacing ρ with the corresponding state T and using the already known definitions (4.33) and (4.34).

Definition 5.1 If H is a Hilbert space, a quantum probability measure $\rho \in \mathscr{M}(\mathsf{H})$ is called **dispersion-free** if $\Delta A_\rho = 0$ for every observable $A \in \mathfrak{B}(\mathsf{H})$. ■

Theorem 4.49 is the important consequence of Gleason's theorem discovered by Bell [Bel66] in 1966 (already known to von Neumann in 1932, however). Now we may rephrase it as a non-existence result for dispersion-free quantum probability measures.

Theorem 5.2 (Bell's Theorem (Alternative Statement)) *Let* H *be a Hilbert space, either of finite dimension* $\dim(\mathsf{H}) > 2$ *or infinite-dimensional and separable. There exist no dispersion-free quantum probability measures in* $\mathscr{M}(\mathsf{H})$.

Proof Suppose that such a $\rho \in \mathscr{M}(\mathsf{H})$ exists and let $T \in \mathscr{S}(\mathsf{H})$ be the associated quantum-state operator according to Gleason's theorem. Assuming $A = P \in \mathscr{L}(\mathsf{H})$, it follows $0 = (\Delta P_T)^2 = tr(TPP) - tr(TP)^2 = tr(TP) - tr(TP)^2$. As a consequence, either $tr(TP) = 0$ or $tr(TP) = 1$ for every $P \in \mathscr{L}(\mathsf{H})$. This is impossible by Theorem 4.49. □

Remark 5.3 The only technical difference with Theorem 4.49 is that now general bounded observables are considered, and not only elementary propositions. Notice that Theorem 5.2 easily implies Theorem 4.49 when we look at elementary observables. But is also uses Theorem 4.49 in its proof, so the two versions are indeed equivalent. ■

If we specialise to the finite-dimensional case, we can recast the theorem in a form that has several implications for the hidden-variable theory. Improving on an earlier non-existence result due to von Neumann (1932), the famous 1967 *Kochen–Specker theorem* [KoSp67] is actually an elementary corollary of Gleason's theorem, as Bell realized, even though the original proof was direct and completely different (see, e.g., [Lan17, SEP]). We state and prove the theorem below, and then discuss the relevant theoretical consequences.

Notation 5.4 For a given Hilbert space H, $\mathfrak{B}(\mathsf{H})_{sa}$ indicates the real linear space of selfadjoint elements of $\mathfrak{B}(\mathsf{H})$. ■

Theorem 5.5 (Kochen–Specker Theorem) *Let* H *be a finite-dimensional Hilbert space with* $\dim(\mathsf{H}) > 2$. *For any non-zero map* $v : \mathfrak{B}(\mathsf{H})_{sa} \to \mathbb{R}$, *the requirements*

(i) $v(A + B) = v(A) + v(B)$ *if* $A, B \in \mathfrak{B}(\mathsf{H})_{sa}$ *commute,*
(ii) $v(AB) = v(A)v(B)$ *if* $A, B \in \mathfrak{B}(\mathsf{H})_{sa}$ *commute,*

are incompatible.

Proof Every orthogonal projector $P \in \mathscr{L}(\mathsf{H})$ belongs to $\mathfrak{B}(\mathsf{H})_{sa}$. If a map v exists as in the hypotheses, then $v(P) = v(PP) = v(P)^2$ due to (ii), hence $v(P) \in \{0, 1\}$. In particular $v(I) = 1$, otherwise $v(A) = v(IA) = v(I)v(A) = 0$, which is not permitted ($v \not\equiv 0$). Observing that $P_i P_j = 0$ implies $P_i P_j = P_j P_i$ for $P_i, P_j \in \mathscr{L}(\mathsf{H})$, it is easy to check that the map $\rho : \mathscr{L}(\mathsf{H}) \ni P \mapsto v(P)$ defines a quantum probability measure by (i) and $v(I) = 1$. Note that (i) implies the additivity of this map on $\mathscr{L}(\mathsf{H})$. In turn, additivity implies σ-additivity because H is finite-dimensional and hence only finite sequences of non-vanishing orthogonal projectors onto pairwise orthogonal subspaces exist, and also $v(0) = 0$ from $v(I) = 1$ and (i). Such ρ is not allowed by Theorem 4.49, since $\rho(\mathscr{L}(\mathsf{H})) \subset \{0, 1\}$ and $\dim \mathsf{H} > 2$. Consequently v cannot exist. □

Remark 5.6 If H is infinite-dimensional but is separable, the thesis of Theorem 5.5 is still valid if we add the requirement that (iii) v is continuous in the *strong operator topology*. In fact, according to the above proof of Theorem 5.5, the only extra fact to be proved is that $\rho : \mathscr{L}(\mathsf{H}) \ni P \mapsto v(P)$ is σ-additive. If P is the strong limit of $\sum_{k=1}^{N} P_k$ as $N \to +\infty$, where $P_k P_h = 0$ if $k \neq h$, the additivity of v together with its strong continuity force the σ-additivity of ρ. ■

We will use quite often in the rest of the chapter a technical lemma related to the hypotheses of the Kochen–Specker theorem.

Lemma 5.7 *Let* H *be a Hilbert space of any dimension, and* $A \in \mathfrak{B}(\mathsf{H})_{sa}$. *Take a non-zero real-valued map* v *defined on the unital Abelian algebra of real polynomials of* A. *If* v *fulfils the Kochen–Specker requirements (i) and (ii), then it also satisfies* $v(I) = 1$ *and* $v(aA) = av(A)$ *for* $a \in \mathbb{R}$.

Proof The first relation was shown during the proof of Theorem 5.5 (without using $\dim \mathsf{H} < +\infty$). To prove the other one, recall a known analysis result whereby the only *non-zero* additive and multiplicative map $f : \mathbb{R} \to \mathbb{R}$ ($f(a+b) = f(a)+f(b)$ and $f(ab) = f(a)f(b)$ for every $a, b \in \mathbb{R}$) is the identity $f(a) = a$. The function $f(a) := v(aI)$ satisfies the conditions above (in particular $f(1) = v(I) = 1 \neq 0$). Hence, $v(aA) = v(aI)v(A) = av(A)$ for $a \in \mathbb{R}$ and $A \in \mathfrak{B}(\mathsf{H})_{sa}$. □

Let us start discussing the physical repercussions of the Kochen–Specker no-go result. Theorem 5.5 imposes strong limitations on any *theory of hidden variables* which assumes the *realism* hypothesis, when taking the quantum phenomenology into account.

As already said, within these approaches it is supposed that a quantum system S is actually partially classic and the observed randomness of measurement outcomes is due to an incomplete knowledge of the system making quantum randomness merely epistemic. There exist *hidden variables* $\lambda \in \Lambda$ that completely fix a classical-like state of the system and the values of every observable, that are *always defined* (*realism* hypothesis). If we knew λ, we would know also the precise value $v_\lambda(A) \in \sigma(A)$ every observable A has. Here the quantum observables A are seen as classical quantities that attain real values, the same permitted by the quantum theory, depending on the value of the hidden variable.

However, it is by no means evident how the assignment $A \mapsto v_\lambda(A) \in \sigma(A)$ should encompass *functional relations* between observables when these relations exist at quantum level. For instance, if $C = A + B$, we cannot in general assume that $v_\lambda(C) = v_\lambda(B) + v_\lambda(B)$, because it is not obvious how to interpret classically $C = A + B$ when the selfadjoint operators A and B do not commute, in other terms when these observables, in the quantum interpretation, cannot be measured simultaneously. (In this case also the relationship between the spectra of A, B, C is generally complicated and unexpected: think of $H = X^2 + P^2$ on $L^2(\mathbb{R}, dx)$.) Yet, there remains to explain how to interpret "A and B cannot be measured simultaneously" in a realistic hidden-variable theory, where we assume from the very beginning that every observable is always defined. In some sense, the values assumed to exist simultaneously for A and B in the hidden-variable theory cannot be measured (do they fluctuate wildly?).

The spirit of the Kochen–Specker theorem is just to *avoid* these difficult and subtle questions and concentrate on what we can reasonably assume. The eventual no-go result is independent of such nuanced details. Indeed, in the special case where *all the involved observables are pairwise compatible*, we expect that they can be treated as classical quantities measured on the system and thus, at least in this case, some functional relations may be preserved by the assignment v_λ. Observe in particular that, if H has finite dimension,

$$\sigma(A + B) \subset \{\nu + \mu \mid \nu \in \sigma(A)\,,\ \mu \in \sigma(B)\} \quad \text{when } A, B \in \mathfrak{B}(\mathsf{H})_{sa} \text{ commute,}$$

so maps $v_\lambda : \mathfrak{B}(\mathsf{H})_{sa} \to \mathbb{R}$ satisfying (i) $v_\lambda(C) = v_\lambda(B) + v_\lambda(B)$ are in principle conceivable. Condition (ii) can be similarly fulfilled, on the whole, since

$$\sigma(AB) \subset \{\nu\mu \mid \nu \in \sigma(A)\,,\ \mu \in \sigma(B)\} \quad \text{when } A, B \in \mathfrak{B}(\mathsf{H})_{sa} \text{ commute.}$$

The hypotheses of Theorem 5.5 concern the preservation of some very mild functional relations by the assignment of classical-like values $A \mapsto v_\lambda(A)$ fixed by the hidden variable λ when dealing with compatible observables. Even with such a minimal requirement, there can be no such map $\mathfrak{B}(\mathsf{H})_{sa} \ni A \mapsto v_\lambda(A) \in \sigma(A) \subset \mathbb{R}$. This is the powerfulness of the Kochen–Specker result.

The premises of the analogue 1932 no-go theorem by von Neumann can be phrased, in our setup, by making requirement (i) hold *also for incompatible observables* A, B—where v more generally represents an expectation value over a distribution of possible λ (including the assignment of a precise value, as before)—and weakening (ii) to $v(aA) = av(A)$, $a \in \mathbb{R}$. In 1966 Bell [Bel66] found a simple example showing that these stronger conditions cannot be fulfilled *regardless of the rest of von Neumann's argument*, thus proving the inadequacy of von Neumann's hypotheses. All that gave rise to an animated discussion to which the Kochen–Specker theorem put an end in 1967 [KoSp67] (see [Lan17] for a critical and historical discussion on the subject).

5.1.3 An Alternative Version of the Kochen–Specker Theorem

We present here an alternative version of the Kochen–Specker theorem which deals with the elementary observables, instead of insisting on functional identities of general observables. This is a formulation essentially analogous to Theorems 4.49 and 5.2 in the finite-dimensional case. Mild probabilistic requirements are assumed on a possible "probability distribution" p defined on a subset $\mathcal{P}$ (not necessarily the whole $\mathscr{L}(\mathsf{H})$) of elementary observables and only attaining sharp values 0 or 1. Such a distribution p cannot exist if $\mathcal{P}$ is sufficiently large, i.e. large enough to contain pairs of incompatible elementary observables. Assuming the standard interpretation of the quantum formalism regarding the notion of observable and its decomposition in elementary observables, this reformulation of the Kochen–Specker result is however equivalent to statement 5.5, as we prove below.

Theorem 5.8 (Kochen–Specker Theorem (Alternative Version)) *Let* H *be a Hilbert space with* $2 < \dim(\mathsf{H}) < +\infty$. *There exists a set of elementary observables* $\mathcal{P} \subset \mathscr{L}(\mathsf{H})$ *for which there is no map* $p : \mathcal{P} \to \{0, 1\}$ *satisfying the following requirements:*

- *(i')* $p(P)p(P') = 0$ *if* $P, P' \in \mathcal{P}$ *define compatible and mutually exclusive elementary observables (i.e.* $PP' = 0$*),*
- *(ii')* $\sum_{j\in J} p(P_j) = 1$ *for every subset* $\{P_j\}_{j\in J} \subset \mathcal{P}$ *made of compatible, pairwise exclusive elementary observables such that* $\vee_{j\in J} P_j = I$.

Proof Let us prove that Theorem 5.8 is a consequence of Theorem 5.5. Since the latter is true, this concludes the proof. Assume that Theorem 5.8 is false. Fix $\mathcal{P} := \mathscr{L}(\mathsf{H})$. There must exist a map $p : \mathcal{P} \to \{0, 1\}$ satisfying (i') and (ii'). Define the map $v : \mathfrak{B}(\mathsf{H})_{sa} \to \mathbb{R}$ such that $v(A) := \sum_{a\in\sigma(A)} ap(P_a^{(A)})$, where $A \in \mathfrak{B}(\mathsf{H})_{sa}$ and $P^{(A)}$ is the PVM of A. Notice that the map does not vanish because $v(I) = p(I) = 1$ by (ii'), with $\{P_j\}_{j\in J} := \{I\}$, and furthermore only one element of $\{p(P_a^{(A)})\}_{a\in\sigma(A)}$ does not vanish because the projectors $P_a^{(A)}$ are pairwise compatible and mutually exclusive and (i'), (ii') are assumed. Observe that, with this definition of v, $v(f(A)) = f(v(A))$ is satisfied for every $f : \mathbb{R} \to \mathbb{R}$ in view of the finite-dimensional version of the functional calculus, the uniqueness of the PVM of a selfadjoint operator, and the fact every $p(P_a^{(A)})$ vanishes but one. If $A, B \in \mathfrak{B}(\mathsf{H})_{sa}$ commute, using their spectral decompositions and the fact that $\dim(\mathsf{H}) < +\infty$, it is easy to prove that there exists $C \in \mathfrak{B}(\mathsf{H})_{sa}$ such that $A = f_A(C)$ and $B = f_B(C)$ for suitable functions $f_A, f_B : \mathbb{R} \to \mathbb{R}$. Indeed, the real number c is a discrete parameter which faithfully labels the finitely many $(a, b) \in \sigma(A) \times \sigma(B)$ and $P_c^{(C)} := P_{a_c}^{(A)} P_{b_c}^{(B)}$, $f_A(c) := a_c$, $f_B(c) := b_c$. The map v satisfies (i),(ii) of Theorem 5.5. In fact, $v(A + B) = v(f_A(C) + f_B(C)) = v((f_A + f_B)(C)) = (f_A + f_B)(v(C)) = f_A(v(C)) + f_B(v(C)) = v(A) + v(B)$ and a similar argument is valid for (ii). Hence Theorem 5.5 is false and this is not possible. □

Proposition 5.9 *The statement of Theorem 5.8 is equivalent to the statement of Theorem 5.5.*

Proof It is sufficient to prove that Theorem 5.8 implies Theorem 5.5 since the converse is part of the proof of Theorem 5.8. Assume that Theorem 5.5 is false and let $v : \mathfrak{B}(\mathsf{H})_{sa} \to \mathbb{R}$ be a non-vanishing map which satisfies (i) and (ii). Since $\mathscr{L}(\mathsf{H}) \subset \mathfrak{B}(\mathsf{H})_{sa}$, we have in particular that $v(P) = v(PP) = v(P)v(P)$, so that (a) $v(P) \in \{0, 1\}$ for $P \in \mathscr{L}(\mathsf{H})$ and also $v(I) = 1$, otherwise $v(A) = v(AI) = v(A)0 = 0$ for every $A \in \mathfrak{B}(\mathsf{H})_{sa}$ which is not permitted. Iterating (ii), noticing that J must be finite ($\leq \dim \mathsf{H}$), we find (b) $\sum_{j \in J} v(P_j) = v(I) = 1$ for any set $\{P_j\}_{j \in J} \subset \mathscr{L}(\mathsf{H})$ such that $\sum_j P_j = I$ and $P_j P_h = 0$ when $j \neq h$ (notice that $P_j P_h = P_h P_j$ in this case). It is now easy to prove that the map $p := v|_{\mathcal{P}}$ satisfies (i') and (ii') of Theorem 5.8, for every $\mathcal{P} \subset \mathscr{L}(\mathsf{H})$ such that (i') and (ii') are eligible, invalidating Theorem 5.8. In fact, if $P, P' \in \mathcal{P} \subset \mathscr{L}(\mathsf{H})$ satisfies $PP' = 0$, we can augment the sequence to $P, P', Q_1, \ldots, Q_n$, where the operators project onto pairwise-orthogonal subspaces and their sum is I. This implies, from (b), that $v(P) + v(P') + \sum_k v(Q_k) = 1$. Since $v(P), v(P'), v(Q_k) \in \{0, 1\}$ by (a), then $p(P)p(P') = v(P)v(P') = 0$ and (i') is satisfied. Similarly, if $\{P_j\}_{j \in J} \subset \mathcal{P}$, with $P_j P_h = 0$ when $j \neq h$, satisfy $\sum_j P_j = I$, then $\sum_j p(P_j) = \sum_j v(P_j) = 1$ from (b), proving (ii'). □

Remark 5.10 For every dimension $\dim \mathsf{H} \geq 3$, there is numerical evidence that the set $\mathcal{P}$ violating (i') and (ii') is a *proper, finite* subset of $\mathscr{L}(\mathsf{H})$. As a matter of fact, the original proof in [KoSp67] for $\dim(\mathsf{H}) = 3$ establishes that there exists a subset $\mathcal{P} \subset \mathfrak{B}(\mathsf{H})_{sa}$ of cardinality 117, whose elements project onto one-dimensional subspaces, satisfying the thesis of Theorem 5.8. See [Cab06] for a discussion about the minimal cardinality of $\mathcal{P}$, and [AHANBSC13] for an interesting discussion of the experimental tests on version 5.8 of the Kochen–Specker theorem. ■

Remark 5.11 In the rest of this chapter, the theorem quoted as 'Kochen–Specker theorem' will refer to Theorem 5.5, unless otherwise declared. ■

5.2 Realistic (Non-)Contextual Theories

The simplest way out of the no-go result by Kochen and Specker, if one insists on a hidden-variable formulation, is to just reject the *realism* assumption and accept that *not all observables are simultaneously defined, even if we fix the hidden state* λ.

Another possibility is to assume that all observables are always and simultaneously defined, and is contingent on the idea of *contextuality*. It must be said that the same proposal was addressed by Bell in 1966 in his second celebrated paper [Bel66] in a more general context and with reference to the consequences of Gleason's theorem for the theories of hidden variables.

5.2.1 An Impervious Way Out: The Notion of Contextuality

First of all, observe that $\mathfrak{B}(\mathsf{H})_{sa}$ contains a profusion of *real* unital Abelian algebras S of mutually compatible observables (whose unit and structure are inherited from the complex algebra $\mathfrak{B}(\mathsf{H})$). From a practical point of view S represents observables we may measure simultaneously. Among the different choices for S many will be inequivalent. The observation playing a crucial role in the following discussion is that a generic $A \in \mathfrak{B}(\mathsf{H})_{sa}$ will belong to *different* algebras S, since compatibility is not a transitive relation.[1] Notice furthermore that the Kochen–Specker constraints (i) and (ii) concern only compatible observables, so they may be imposed on the elements of a given real unital Abelian algebra. To fulfil them without running into the negative result of Theorem 5.5, we could try the following: drop the main hypothesis of the Kochen–Specker theorem, thus foregoing the *unique* assignment of values v_λ on $\mathfrak{B}(\mathsf{H})_{sa}$, and allow instead for distinct values $v_\lambda(A|S)$ of the observable A, for every real unital Abelian algebra S containing A.

Remark 5.12

(a) $S \ni A$ can be taken to be the space of real polynomials $p(A)$ of A (where $A^0 := I$). This choice of S means in practice that we are measuring A alone. In this case, measuring only A automatically permits us to know also the values of the remaining observables in S: the values of the polynomials $p(A)$ satisfy $v_\lambda(p(A)) = p(v_\lambda(A))$ by virtue of (i), (ii) in Kochen–Specker's theorem and the relations of Lemma 5.7.
(b) $S \ni A$ may be defined by means of several substantially distinct observables $A_1, \ldots, A_n$ that we measure together with A. In this case, S coincides with the family of real polynomials $p(A, A_1, \ldots, A_n)$. The values of $p(A, A_1, \ldots, A_n)$ are known from the values of the generators $A_1, \ldots, A_n$, again by (i) and (ii) and Lemma 5.7.
(c) In any case, to know the values of all the observables of a generic unital Abelian algebra S it suffices to measure a linear basis $A_1, \ldots, A_m$ of S. Since the elements of S are linear functions of these, once more by (i), (ii) in the Kochen–Specker theorem and Lemma 5.7 we have $v_\lambda(\sum_{j=1}^m c_j A_j) = \sum_{j=1}^m v_\lambda(A_j)$. Such a basis always exists, see Remark 5.14 below. ■

Let us now prove that it is possible to prescribe the values of any fixed A depending on the chosen $S \ni A$ satisfying (i) and (ii) in Kochen–Specker's theorem. The paradoxical aspect is that we are about to use the mathematical structure of quantum theory to corroborate the idea that a certain competitor theory is not mathematically contradictory!

[1] These sets of observables S represent the most classical structures one may extract form the whole set of observables of a quantum system. The fact that these structures are distinct and physically incompatible is one manifestation of *Bohr's complementarity principle*.

Proposition 5.13 *Assume* $\dim \mathsf{H} < +\infty$ *and let us denote by* $\mathfrak{C}$ *the family of real unital Abelian algebras* $S \subset \mathfrak{B}(\mathsf{H})_{sa}$. *For every given* $S \in \mathfrak{C}$, *there exists a non-zero map*

$$S \ni A \mapsto v(A|S) \in \sigma(A)$$

satisfying (i) and (ii) of the Kochen–Specker theorem and also

$$v(I|S) = 1 \quad \textit{and} \quad v(aA|S) = av(A|S) \quad \textit{for } A \in S \textit{ and } a \in \mathbb{R}.$$

Proof Since the selfadjoint operators in S commute with one another and $\dim \mathsf{H} = n < +\infty$, it is easy to prove that there exists a collection $\{P_k\}_{k=1,\ldots,m} \subset \mathscr{L}(\mathsf{H})$, $m \leq n$, of non-zero orthogonal projectors, with $\sum_{k=1}^{m} P_k = I$ and $P_r P_h = 0$ if $r \neq h$, such for every $A \in S$,

$$A = \sum_{k=1}^{m} a_k^{(A)} P_k \quad \text{for some } a_1^{(A)} \leq a_2^{(A)} \leq \cdots \leq a_m^{(A)} \in \mathbb{R}. \tag{5.1}$$

Notice that it may happen that $a_k^{(A)} = a_{k+1}^{(A)}$. By construction, $\{a_k^{(A)} \mid k = 1,\ldots,m\} = \sigma(A)$. Furthermore, every orthogonal projector $p_x = \langle x|\cdot\rangle x$, for $x \in P_k(\mathsf{H})$ of unit norm, satisfies $p_x A = A p_x$ for every $A \in S$. If $x \in \mathsf{H}$ is as above, define

$$S \ni A \mapsto v(A|S) := \langle x|Ax\rangle \, .$$

By construction $\langle x|Ax\rangle = a_k^{(A)} \in \sigma(A)$ for some $k = 1, 2, \ldots, m$, because x is a unit-norm eigenvector of A with eigenvalue $a_k^{(A)}$. Since this is valid for every $A \in S$, properties (i) and (ii) of Theorem 5.5 are immediate. Finally, $v(aA|S) = av(A|S)$ is due to linearity of the inner product, and $v(I|S) = 1$ because $\langle x|x\rangle = 1$. □

Remark 5.14 The m orthogonal projectors P_k appearing in the proof above are linearly independent because $P_k P_h = \delta_{hk} P_k$. Therefore (5.1) guarantees that $\{A_k\}_{k=1,\ldots,m}$ with $A_k := P_k$ is a linear basis of observables of the real unital Abelian algebra S. ■

In this abstract context, a hidden variable can be defined as the choice of $\lambda = \{x_S\}_{S\in\mathfrak{C}}$, where $x_S \in \mathsf{H}$ is a common eigenvector of all the observables $A \in S$ picked out as prescribed above. Hence for every λ and every S, the maps

$$S \ni A \mapsto v_\lambda(A|S) := \langle x_S|Ax_S\rangle \in \sigma(A)$$

possess the desired properties. The price to pay when adopting this new framework—*circumventing the Kochen–Specker no-go result*—is that the value $v_\lambda(A|S) \in \sigma(A)$ of an observable $A \in S$ is determined not only by the hidden variable λ, but also by (finitely many) mutually compatible other observables that we want to measure together with A (and that generate the chosen Abelian algebra S). This peculiar property a hidden-variable theory satisfies is called *contextuality*. Together with the *realism* assumption, the Kochen–Specker theorem only admits *realistic contextual* hidden-variable theories and denies *realistic non-contextual* ones.

Remark 5.15

(a) The existence of a finite linear basis of $S \in \mathfrak{C}$ is guaranteed if the Hilbert space is finite-dimensional and every element of $\mathfrak{B}(\mathsf{H})_{sa}$ represents an observable, whereas it is not warranted automatically if we relax these hypotheses.
(b) It has been argued that the standard formulation of QM is non-contextual, though this adjective is more often used do distinguish between theories of hidden variables alternative to the standard formulation. This means nothing but, when we fix the quantum state $T \in \mathscr{S}(\mathsf{H})$ of the system so that an observable A attains a definite value in that state ($\Delta A_T = 0$), this value does *not* depend on other possible observables we can measure simultaneously with A. The problem, so to speak, lies with the realism postulate: necessarily there exist other observables, different from A, that do not admit precise values for the quantum state T, as a consequence of Theorem 5.2.
(c) It is important to warn the reader that the notion of (non-)contextuality has acquired a wealth of different meanings originating in the debate on hidden variables. The rather cumbersome version discussed in this section is strictly pertaining to hidden variable theories in the framework of the Kochen–Specker theorem. The contextuality of Bohmian mechanics and the version dealing with Bell's inequality and entanglement have slightly different meanings. In all cases contextuality means that the value of one observable depends on the other observables (and their values) measured simultaneously; the specificities of this dependence may vary according to the notion of (non-)contextuality one adopts. ■

5.2.2 *The Peres–Mermin Magic Square*

The Kochen–Specker theorem, in the form of Theorem 5.5, assumes that the set of observables considered is the whole $\mathfrak{B}(\mathsf{H})_{sa}$. However, in the spirit of the reformulation of Theorem 5.8, the no-go result can be obtained also by restricting the family of observables to a smaller set made of orthogonal projectors. After [KoSp67] many explicit proofs of that kind were produced. There are alternative, but theoretically equivalent formulations of the Kochen–Specker no-go result where the attention is placed on a minimal number of observables (not necessarily orthogonal projectors) violating some statement concerning the possibility to assign values to them in accordance with realism and non-contextuality. A popular and direct argument for $\dim(\mathsf{H}) = 4$ is provided by the well-known *Peres–Mermin magic square* [Per90, Mer90]. It refers to a system of two particles of spin $1/2$, and focuses just on the spin part of the Hilbert space, $\mathsf{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$. One considers the 9 observables assembled in a square

$$\begin{array}{|c|c|c|}\hline A_{11} & A_{12} & A_{13} \\ \hline A_{21} & A_{22} & A_{23} \\ \hline A_{31} & A_{32} & A_{33} \\ \hline \end{array} \quad = \quad \begin{array}{|c|c|c|}\hline \sigma_x \otimes I & I \otimes \sigma_x & \sigma_x \otimes \sigma_x \\ \hline I \otimes \sigma_y & \sigma_y \otimes I & \sigma_y \otimes \sigma_y \\ \hline \sigma_x \otimes \sigma_y & \sigma_y \otimes \sigma_x & \sigma_z \otimes \sigma_z \\ \hline \end{array} \tag{5.2}$$

The standard Hermitian *Pauli matrices* σ_k (see (1.12)) have eigenvalues ± 1 and satisfy the equations

$$\sigma_x \sigma_y = i\sigma_z \ , \quad [\sigma_x, \sigma_y] = 2i\sigma_z \quad \text{for all cyclic permutations of } x, y, z.$$

It is easy to prove that the three operators on each row or column are linearly independent and pairwise commuting.[2] Furthermore, the row and column of any given element contain a pair of incompatible elements (if we choose $\sigma_x \otimes I$ for example, $I \otimes \sigma_x$ and $I \otimes \sigma_y$ are incompatible).

For this special case, we will prove a Kochen–Specker-type theorem on $\mathfrak{B}(\mathbb{C}^2 \otimes \mathbb{C}^2)_{sa}$ with the further hypothesis that $v(A) \in \sigma(A)$.

Proposition 5.16 *Let* $\mathsf{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$ *and* $A_{ij} \in \mathfrak{B}(\mathsf{H})_{sa}$ *be defined as in (5.2). There exists no assignment of real values* $A_{ij} \mapsto v(A_{ij}) \in \sigma(A_{ij})$, *for* $i, j = 1, 2, 3$, *satisfying (ii) of the Kochen–Specker theorem and* $v(\pm I) = \pm 1$.

Proof The product of the values in all rows $\prod_{i=1}^3 \prod_{j=1}^3 v(A_{ij})$ equals the product of the values in all columns $\prod_{j=1}^3 \prod_{i=1}^3 v(A_{ij})$, so their product is 1. On the other hand, requirement (ii) implies that $\prod_{i=1}^3 \prod_{j=1}^3 v(A_{ij}) = \prod_{i=1}^3 v(\prod_{j=1}^3 A_{ij})$ and $\prod_{j=1}^3 \prod_{i=1}^3 v(A_{ij}) = \prod_{j=1}^3 v(\prod_{i=1}^3 A_{ij})$ since row elements are pairwise compatible, and column elements too. Therefore $\prod_{j=1}^3 A_{ij} = I$ for $i = 1, 2, 3$ and $\prod_{i=1}^3 A_{ij} = I$ for $j = 1, 2$, but $\prod_{i=1}^3 A_{i3} = -I$. In summary, using $v(-I) = -1$, we find

$$1 = \left[\prod_{j=1}^3 \prod_{i=1}^3 v(A_{ij})\right] \prod_{i=1}^3 \prod_{j=1}^3 v(A_{ij}) = \left[\prod_{j=1}^3 v\left(\prod_{i=1}^3 A_{ij}\right)\right] \prod_{1=1}^3 v\left(\prod_{j=1}^3 A_{ij}\right)$$
$$= v(I)^3 v(I)^2 v(-I) = -1 \ ,$$

which is impossible. □

Remark 5.17 Proposition 5.16 automatically implies the thesis of the Kochen–Specker theorem *on the whole* $\mathfrak{B}(\mathbb{C}^2 \otimes \mathbb{C}^2)_{sa}$ (assuming also that $v(A_{ij}) \in$

[2]For instance, if $a\sigma_x \otimes I + bI \otimes \sigma_x + c\sigma_x \otimes \sigma_x = 0$, multiplying by $\sigma_a \otimes I$ or $I \otimes \sigma_a$ and computing the *partial trace* gives $a = b = c = 0$ easily, because $tr(\sigma_a) = 0$, $tr(\sigma_a \sigma_b) = 2\delta_{ab}$.

$\sigma(A_{ij})$), just because the restriction to the observables A_{ij} of the map v posited by the Kochen–Specker's theorem satisfies Proposition 5.16. However, here we are considering a smaller set of observables $A_{ij} \in \mathfrak{B}(\mathsf{H})_{sa}$ and we cannot say a priori that no assignment $v_\lambda(A_{ij}) \in \{\pm 1\}$ satisfies (some of the) requirements (i) and (ii) of Kochen–Specker and also Lemma 5.7. This is the relevance of the above proposition. ■

5.2.3 A State-Independent Test on Realistic Non-Contextuality

The Peres–Mermin square can be used as experimental test for the no-go assertion of the Kochen–Specker theorem restricted to the only observables of a quantum physical system described on $\mathsf{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$, interpreting the observables as classical quantities satisfying the *realism* and *non-contextuality* assumptions in a hidden-variable theory.

Consider a concrete physical system with Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^2$, and suppose we are able to give a definite interpretation to all observables A_{ij} in the Peres–Mermin square. If we measure the observables $A \in \mathfrak{B}(\mathbb{C}^2 \otimes \mathbb{C}^2)_{sa}$ repeatedly when the quantum state of the system $T \in \mathscr{S}(\mathsf{H})$ is fixed, the values will in general fluctuate. If we adopt a realistic non-contextual hidden-variable description, we are committed to assume that the fluctuation of the values $v_\lambda(A)$ is caused by a fluctuation of the state $\lambda \in \Lambda$, which is known only statistically and is described by a probability measure μ on a σ-algebra Σ of subsets of Λ (Σ obviously contains the singletons $\{\lambda\}$ as measurable sets). Quantum expectation values $tr(TA)$ must be interpreted as classical standard expectation values

$$\mathbb{E}_\mu(A) = \int_\Lambda v_\lambda(A) d\mu(\lambda) .$$

Suppose that the map $v_\lambda : \mathfrak{B}(\mathbb{C}^2 \otimes \mathbb{C}^2)_{sa} \to \mathbb{R}$ satisfies the very mild conditions of the Kochen–Specker theorem. There exists a quantity allowing, in principle, to choose between non-contextual hidden-variable models and a quantum description on the grounds of the experimental data. (Actually we already know that Proposition 5.16 rules out these assignments, but we will ignore this fact since we are interested in constructing an elementary experimental example.)

Consider the observable

$$\chi := A_{11}A_{12}A_{13} + A_{21}A_{22}A_{23} + A_{31}A_{32}A_{33} + A_{11}A_{21}A_{31} + A_{12}A_{22}A_{32} - A_{13}A_{23}A_{33}. \tag{5.3}$$

This is a selfadjoint operator because the selfadjoint operators in the products pairwise commute.

Remark 5.18 Notice that every observable A_{ij} appears in two different sets of pairwise compatible observables, yet these sets are not compatible to each other. E.g., A_{11}, A_{12}, A_{13} and A_{11}, A_{21}, A_{31} contain A_{11}, but $[A_{12}, A_{21}] \neq 0$. ■

Now consider the experimental expectation value $\langle\chi\rangle$ obtained by collecting many measurement outcomes. There are two main possibilities:

1. fluctuations have a quantum nature, so that $\langle\chi\rangle = tr(T\chi)$,
2. fluctuations have a hidden-variable nature, hence $\langle\chi\rangle = \mathbb{E}_\mu(\chi)$.

In case (1), since $\chi = 2I \otimes I + 2I \otimes I + 2I \otimes I$, we should obtain

$$\langle\chi\rangle = 6\,,$$

independently of the quantum state $T \in \mathscr{S}(\mathsf{H})$. In case (2), if we also assume the two Kochen–Specker hypotheses restricted to our observables—notice that the summands in (5.3) pairwise commute (each equals $\pm I \otimes I$!) so we may assume both (i) and (ii) in Kochen–Specker theorem—we have that

$$v_\lambda\left(\prod_{i=1}^{3} A_{ij}\right) = \prod_{i=1}^{3} v_\lambda\left(A_{ij}\right) \quad \text{and} \quad v_\lambda\left(\prod_{j=1}^{3} A_{ij}\right) = \prod_{j=1}^{3} v_\lambda\left(A_{ij}\right)\,.$$

Hence using Lemma 5.7 on the polynomials of $A_{13}A_{23}A_{33}$,

$$v_\lambda(\chi) := v_\lambda(A_{11})v_\lambda(A_{12})v_\lambda(A_{13}) + v_\lambda(A_{21})v_\lambda(A_{22})v_\lambda(A_{23}) + v_\lambda(A_{31})v_\lambda(A_{32})v_\lambda(A_{33})$$
$$+ v_\lambda(A_{11})v_\lambda(A_{21})v_\lambda(A_{31}) + v_\lambda(A_{12})v_\lambda(A_{22})v_\lambda(A_{32}) - v_\lambda(A_{13})v_\lambda(A_{23})v_\lambda(A_{33})\,.$$

Remark 5.19 It is very important to stress that we have explicitly made use of *non-contextuality* since each observable A_{ij} appears simultaneously in two sets that contain incompatible observables. Nonetheless, we have given A_{ij} a *unique* value $v_\lambda(A_{ij})$ independently of the set to which it belongs. ■

Each value $v_\lambda\left(A_{ij}\right) \in \{-1, +1\}$ is completely determined by λ, in some unknown way. It is however possible to prove that, in all cases, $-4 \leq v_\lambda(\chi) \leq 4$, so that the integration with respect to the probability measure μ gives

$$-4 \leq \langle\chi\rangle \leq 4\,.$$

This is consequence of the following more general proposition.

Proposition 5.20 *Let $M(3,\mathbb{R})$ denote the algebra of real 3×3 matrices and define the map $f : M(3,\mathbb{R}) \ni X \to f(X) \in \mathbb{R}$ by*

$$f(X) := X_{11}X_{12}X_{13} + X_{21}X_{22}X_{23} + X_{31}X_{32}X_{33} + X_{11}X_{21}X_{31} + X_{12}X_{22}X_{32} - X_{13}X_{23}X_{33}. \tag{5.4}$$

Then $|f(X)| \leq 4$ if $X \in [-1,1]^9$, where we have identified $M(3,\mathbb{R})$ with $\mathbb{R}^9$.

Proof The map f is continuous on $[-1,1]^9$ and $\Delta f = 0$ on $(-1,1)^9$. As a consequence of the maximum principle, $f\restriction_{[-1,1]^9}$ attains its extremal values on the boundary of $[-1,1]^9$. The boundary is the union of the 18 sets $Q^{\pm}_{ij} := \{X \in [-1,1]^9 \mid X_{ij} = \pm 1\}$. It is evident that the restriction of f to $Q^{\pm}_{ij}$ is continuous and harmonic in the interior of $Q^{\pm}_{ij} \subset \mathbb{R}^8$. The argument can be iterated, and eventually the extreme values of f belong in the discrete set $D = \{X \in [-1,1]^9 \mid X_{ab} = \pm 1 \text{ for } a,b = 1,2,3\}$. Therefore it is sufficient to prove that $|f(X)| \leq 4$ if $X_{ij} \in \{-1,1\}$. First of all, if $X_{ij} = 1$ then $f(X) = 4$. Let us prove that a larger value is impossible to achieve when $X_{ij} \in \{-1,1\}$. From the expression of f it immediately follows the only possible value greater than 4 which f could attain if all $X_{ij} \in \{-1,1\}$ is 6. This value would be reached iff the first 5 summands in (5.4) had value 1 and the last one ($X_{13}X_{23}X_{33}$) were -1. In turn this would mean that: (1) in each of first 5 addends an even number of factors X_{ij} (or none) take value -1; (2) in the last term an odd number take value -1. In summary, f attains value > 4 iff an *odd* number of factors X_{ij} in (5.4) take the value -1. This is impossible because every X_{ij} occurs twice with the same value. We conclude that $f(X) \leq 4$ in $[-1,1]^9$. Since $f(-X) = -f(X)$ and $[-1,1]^9$ is invariant under $X \mapsto -X$, we also have $-4 \leq f(X)$ in $[-1,1]^9$. □

To recap:

1. quantum mechanics implies $\langle \chi \rangle = 6$, independently of the quantum state;
2. realistic non-contextual hidden-variable models (assuming (i) and (ii) of the KS theorem) imply $-4 \leq \langle \chi \rangle \leq 4$, independently of the hidden-variable distribution μ.

It is evident that quantum theory is incompatible with realistic non-contextual hidden-variable models, and $\langle \chi \rangle$ could be exploited to test the difference experimentally.

Real experiments have been performed to test the Kochen–Specker theorem on concrete physical systems (photons [MWZ00, HLZPG03], neutrons [HLBBR06, BKSSCRH09] and trapped ions [KZGKGCBR09]) using observables similar to χ and possibly dealing with suitably prepared quantum states. State-independent tests have been studied in [AHANBSC13].

5.3 Entanglement and the BCHSH Inequality

According to Sect. 4.4.8, if a quantum system is made of two subsystems, the overall Hilbert space has the form $\mathsf{H}_1 \otimes \mathsf{H}_2$, where H_1 and H_2 are the Hilbert spaces of the two subsystems. $\mathscr{S}(\mathsf{H}_1 \otimes \mathsf{H}_2)$ contains the so-called (pure) **entangled states**: by definition these are represented by unit vectors that are *not* factorized as $\psi_1 \otimes \psi_2$, but rather *linear combinations* of such vectors

$$\Psi = \sum_{k=1}^{n} c_k \psi_{1k} \otimes \psi_{2k} ,$$

where at least two c_k do not vanish. As first observed by Einstein, Podolski and Rosen in a celebrated 1935 paper [EPR35], this sort of state gives rise to very peculiar phenomena—often mentioned as the *EPR paradox*—as soon as one assumes the postulate of collapse of the state after a measurement (see Sect. 4.4.7) with post-measurement state (4.23). Suppose the whole state is represented by the entangled vector

$$\Psi = \frac{1}{\sqrt{2}} \left(\psi_a \otimes \phi + \psi_{a'} \otimes \phi' \right) ,$$

where $\psi_a, \psi_{a'} \in \mathsf{H}_1$ and $\phi, \phi' \in \mathsf{H}_2$ are of unit norm. We also assume that $A_1\psi_a = a\psi_a$ and $A_1\psi_{a'} = a'\psi_{a'}$ for a certain observable $A_1 \in \mathfrak{B}(\mathsf{H}_1)_{sa}$ belonging to part S_1 of the total system and such that $a, a' \in \sigma_p(A_1)$. Due to the collapse of the state, when performing a measurement of A_1 on S_1 we actually act on the whole state, hence *also* on the part describing S_2. As a matter of fact,

(i) if the outcome of the measurement of $A_1 \otimes I$ is a, then the state of the full system after the measurement will be described by $\psi_a \otimes \phi$;
(ii) if the outcome of the measurement of $A_1 \otimes I$ is a' then the state of the full system after the measurement will be described by $\psi_{a'} \otimes \phi'$.

Therefore as we act on S_1 by measuring A_1, we "instantaneously" produce a change of S_2 which, in principle, can be observed by performing measurements on it. All of this happens even if the measuring apparatus of S_2 is very far from the instrument measuring S_1. It is further possible to realize a more subtle version of the experiment where we can measure different observables on each side of the experiment, and the (possibly random) choice of these observables and the associated measurement are made in such a short lapse of time that any non-superluminal exchange of information between the two sides is prevented (see [BeZe17] for up-to-date theoretical and experimental discussions). This seems to stand in flat contradiction to the *locality* postulate of Relativity (whereby a maximal speed exists, the speed of light, for propagating physical information) in connection with the *realism assumption* that the values of the observables pre-exist the measurements and can be changed only through sub-luminal interactions.

5.3.1 BCHSH Inequality from Realism and Locality

We shall give an outline of Bell's 1964 analysis [Bel64] of an improved version of the EPR phenomenon proposed by Aharonov and Bohm, for a physical system consisting of a pair of spin $1/2$ particles, so that

$$\mathsf{H} = \mathsf{H}_{\text{orbital}} \otimes \mathsf{H}_{1,\text{spin}} \otimes \mathsf{H}_{2,\text{spin}}$$

where $\mathsf{H}_{\text{orbital}} = L^2(\mathbb{R}^3, dx_1) \otimes L^2(\mathbb{R}^3, dx_2) \simeq L^2(\mathbb{R}^3 \times \mathbb{R}^3, dx_1 \otimes dx_2)$ and $\mathsf{H}_{i,\text{spin}} \simeq \mathbb{C}^2$ for $i = 1, 2$, and the entanglement takes place in the space of spins,

$$\Psi = \phi_1 \otimes \phi_2 \otimes \frac{1}{\sqrt{2}} \left(\psi_1 \otimes \psi_2 + \psi_1' \otimes \psi_2'\right) \quad \text{with} \quad \phi_i \in L^2(\mathbb{R}^3, dx_i) \quad \psi_i, \psi_i' \in \mathsf{H}_{i,\text{spin}}.$$

Once created into sharply separated wavepackets, the particles ϕ_1, ϕ_2 move along opposite directions towards the detectors where the spin observables are eventually measured.[3]

Bell's analysis considered the possibility of explaining the phenomenology of entanglement in terms of a hidden-variable theory and, most importantly, he proposed an experiment capable of checking if local realism is satisfied.

As in the previous sections, it is supposed that there exists a hidden variable $\lambda \in \Lambda$ which completely fixes the state of the couple of particles *when they are spacelike separated.* As before, we do not have direct access to λ but we do know its probability distribution μ over Λ, and this statistical description should be in agreement with (actually it should explain it!) the stochastic behaviour of measurement outcomes of QM. To be precise, λ generally indicates a *set* of hidden variables, and the state of S_1 only depends on a subset of these parameters while the state of S_2 depends on another subset. In a complete theory, one could also assume that hidden variables have a deterministic dynamical evolution. If so, our λ would represent the initial values of that evolution.

We are in particular interested in the value $A(\mathbf{a}|\lambda) \in \{\pm 1\}$ of the spin along the direction $\mathbf{a} \in \mathbb{S}^2$ (the unit sphere in $\mathbb{R}^3$) detected on particle S_1, and in the value $B(\mathbf{b}|\lambda) \in \{\pm 1\}$ of the spin along the direction $\mathbf{b} \in \mathbb{S}^2$ detected on particle S_2. (Actually the true spin values amount to $\hbar A(\mathbf{a}|\lambda)/2$ and $\hbar B(\mathbf{b}|\lambda)/2$ but we shall henceforth ignore the factor $\hbar/2$.)

Remark 5.21 As opposed to previous sections, we are *not* directly assuming that the spin is a *quantum observable*, i.e. a selfadjoint operator on a Hilbert space. It

[3] A more complete model would include the state's skew-symmetry (the electrons may be swapped), but we shall disregard details such as this one. When dealing with photons the spin must be replaced by the *polarization*, which is still described on $\mathbb{C}^2$, and the positions x_i by the momenta k_i; in this case the state must be symmetric when swapping the photons.

is just a quantity, taking values in $\{\pm 1\}$, that we can measure on both sides of the system depending on the choice of direction. ■

Let us make explicit two assumptions involved in Bell's picture.

1. *Realism*. The values of A and B exist at every time and for every choice of the directions $\mathbf{a}, \mathbf{b} \in \mathbb{S}^2$, independently of their explicit observation.
2. *Locality*. When measurements are performed on S_1 and S_2 by devices placed in causally separated regions of spacetime, the choice of $\mathbf{a} \in \mathbb{S}^2$ cannot have any influence on the outcome $B(\mathbf{b}|\lambda)$, and the choice of $\mathbf{b} \in \mathbb{S}^2$ cannot have any influence on the outcome $A(\mathbf{a}|\lambda)$; moreover, these outcomes are (pre-)determined by the hidden variable λ. (This is the reason why we write $A(\mathbf{a}|\lambda)$ but not, say, $A(\mathbf{a}|\lambda, \mathbf{b})$.)

Let us consider the quantity, obtained by measurements,

$$\chi(\mathbf{a}, \mathbf{a}', \mathbf{b}, \mathbf{b}'|\lambda) := A(\mathbf{a}|\lambda)B(\mathbf{b}|\lambda) + A(\mathbf{a}'|\lambda)B(\mathbf{b}|\lambda) + A(\mathbf{a}'|\lambda)B(\mathbf{b}'|\lambda) - A(\mathbf{a}|\lambda)B(\mathbf{b}'|\lambda)$$

which depends on four choices of directions $\mathbf{a}, \mathbf{a}'$ for S_1 and $\mathbf{b}, \mathbf{b}'$ for S_2. Since

$$\chi(\mathbf{a}, \mathbf{a}', \mathbf{b}, \mathbf{b}'|\lambda) = A(\mathbf{a}|\lambda)\left[B(\mathbf{b}|\lambda) - B(\mathbf{b}'|\lambda)\right] + A(\mathbf{a}'|\lambda)\left[B(\mathbf{b}|\lambda) + B(\mathbf{b}'|\lambda)\right] ,$$

and $B(\mathbf{b}|\lambda), B(\mathbf{b}'|\lambda) \in \{\pm 1\}$, only one summand survives. As $A(\mathbf{a}|\lambda), A(\mathbf{a}'|\lambda) \in \{\pm 1\}$, we conclude that

$$-2 \leq \chi(\mathbf{a}, \mathbf{a}', \mathbf{b}, \mathbf{b}'|\lambda) \leq 2 . \tag{5.5}$$

If we take the expectation value of $\chi(\mathbf{a}, \mathbf{a}', \mathbf{b}, \mathbf{b}'|\lambda)$ when λ varies in Λ according with its probability distribution μ,

$$\mathbb{E}_\mu(\chi) := \int_\Lambda \chi(\mathbf{a}, \mathbf{a}', \mathbf{b}, \mathbf{b}'|\lambda) d\mu(\lambda) ,$$

we find $-2 \leq \mathbb{E}_\mu(\chi) \leq 2$ since the measure is positive and the total integral is 1. Defining

$$E_\mu(\mathbf{a}, \mathbf{b}) := \int_\Lambda A(\mathbf{a}|\lambda)B(\mathbf{b}|\lambda) d\mu(\lambda) \quad \mathbf{a}, \mathbf{b} \in \mathbb{S}^2 ,$$

we obtain the famous **BCHSH inequality**, after J. Bell, J. Clauser, M. Horne, A. Shimony, and R. Holt[4]:

$$-2 \leq E_\mu(\mathbf{a}, \mathbf{b}) + E_\mu(\mathbf{a}', \mathbf{b}) + E_\mu(\mathbf{a}', \mathbf{b}') - E_\mu(\mathbf{a}, \mathbf{b}') \leq 2 \quad \text{for every } \mathbf{a}, \mathbf{a}', \mathbf{b}, \mathbf{b}' \in \mathbb{S}^2. \tag{5.6}$$

[4]The original paper of Bell [Bel64] presented a slightly less general inequality.

The BCHSH inequality—regarding correlations of measurements of spin components of pair of particles—must be satisfied by every realistic local theory.

What is the quantum prevision instead? First of all, the *spin observable along* $\mathbf{a} \in \mathbb{S}^2$ must be defined as the selfadjoint operator in $\mathfrak{B}(\mathbb{C}^2)_{sa}$

$$\mathbf{a} \cdot \sigma := \sum_{k=x,y,z} a_k \sigma_k \ . \tag{5.7}$$

In this context, we have to interpret $E_\mu(\mathbf{a}, \mathbf{b})$ as an expectation value with respect to a quantum state $T \in \mathscr{S}(\mathbb{C}^2 \otimes \mathbb{C}^2)$ (neglecting the state's orbital part, which plays no role at present):

$$E_T(\mathbf{a}, \mathbf{b}) = tr\left[T(\mathbf{a} \cdot \sigma \otimes \mathbf{b} \cdot \sigma)\right] \ . \tag{5.8}$$

We restrict the choice of state to *entangled* pure states $T_\pm = \langle \Psi_\pm | \cdot \rangle \Psi_\pm$ of a particular type, called **Bell states**,

$$\Psi_+ := \frac{1}{\sqrt{2}}(\psi_+ \otimes \psi_+ + \psi_- \otimes \psi_-) \ , \quad \Psi_- := \frac{1}{\sqrt{2}}(\psi_+ \otimes \psi_- - \psi_- \otimes \psi_+) \ , \tag{5.9}$$

where $\psi_\pm \in \mathbb{C}^2$ are ± 1-eigenvectors of σ_z: $\sigma_z \psi_\pm = \pm \psi_\pm$. If $\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z \in \mathbb{S}^2$ are the unit vectors along three orthogonal axes of the physical rest space of the laboratory, we choose

$$\mathbf{a} = \mathbf{e}_x \ , \quad \mathbf{a}' = \mathbf{e}_z \ , \quad \mathbf{b} = \frac{\mathbf{e}_x + \mathbf{e}_z}{\sqrt{2}} \ , \quad \mathbf{b}' = \frac{\mathbf{e}_z - \mathbf{e}_x}{\sqrt{2}} \tag{5.10}$$

An elementary but lengthy computation based on (1.12) yields

$$E_{T_\pm}(\mathbf{a}, \mathbf{b}) + E_{T_\pm}(\mathbf{a}', \mathbf{b}) + E_{T_\pm}(\mathbf{a}', \mathbf{b}') - E_{T_\pm}(\mathbf{a}, \mathbf{b}') = \pm 2\sqrt{2} \ . \tag{5.11}$$

Since $2\sqrt{2} > 2$, we conclude that *the result predicted by Quantum Theory, with said choices of directions and entangled states, is incompatible with realism and locality*.

The strong empirical evidence is that *local realism* is rejected by experimental data accumulated, over the years, in several very delicate experiments performed to test the BCHSH inequality on couples of particles in entangles states. See [GaCh08] for a review on the various experiments and [Han15] for a recent important experimental achievement on the subject. The non-locality of QM—with the above specific meaning due to Bell [BeZe17]—is nowadays widely accepted as a real and fundamental feature of Nature [Ghi07, SEP, Lan17].

Remark 5.22

(a) We stress, without entering in details, that the quantum violation of locality together with the stochastic nature of measurement outcomes do not permit superluminal propagation of physical information [Bell75, Ghi07].
(b) Incidentally, $2\sqrt{2}$ is the maximum value attainable for a quantum state $T \in \mathscr{S}(\mathsf{H})$ violating the BCHSH inequality [Tsi80], and is known as *Tsirelson's bound*. ■

5.3.2 BCHSH Inequality and Factorized States

Let us examine what happens to the BCHSH inequality if $T = \langle\Psi|\ \rangle\Psi$ is not entangled, i.e., if

$$\Psi := \psi_1 \otimes \psi_2 \tag{5.12}$$

is a product of unit vectors ψ_i. We need at technical proposition.

Proposition 5.23 *Let* $f : \mathbb{R}^4 \to \mathbb{R}$ *be the map* $f(x_1, x_2, x_3, x_4) = x_1x_3 + x_2x_3 + x_2x_4 - x_1x_4$. *Then* $|f(x_1, x_2, x_3, x_4)| \leq 2$ *if* $(x_1, x_2, x_3, x_4) \in [-1, 1]^4$.

Proof The map f is continuous on $[-1, 1]^4$ and satisfies $\Delta f = 0$ on the interior of $[-1, 1]^4$, so the maximum principle implies it is extremized on the boundary. The latter is the union of the eight sets $Q_i^\pm := \{(x_1, x_2, x_3, x_4) \in [-1, 1]^4 \mid x_i = \pm 1\}$. It is evident that the restriction of f to each $Q_i^\pm$ is still continuous and harmonic on the interior of $Q_i^\pm \subset \mathbb{R}^3$. Iterating the argument we eventually find that the extreme values of f are achieved on $D := \{(x_1, x_2, x_3, x_4) \in [-1, 1]^4 \mid x_i = \pm 1, i = 1, 2, 3, 4\}$. Since $f(x_1, x_2, x_3, x_4) = x_1(x_3 - x_4) + x_2(x_3 + x_4)$, when $x_3, x_4 = \pm 1$ only one of the summands is non-zero. Further imposing $x_1, x_2 = \pm 1$ tells $f(x_1, x_2, x_3, x_4) = \pm 2$ for every $(x_1, x_2, x_3, x_4) \in D$. Since $\max\{|f(z_1, z_2, z_3, z_4)| \mid (z_1, z_2, z_3, z_4) \in [-1, 1]^4\} = |f(x_1, x_2, x_3, x_4)|$ for some $(x_1, x_2, x_3, x_4) \in D$, the claim is proved. □

Given Ψ as in (5.12) and $T = \langle\Psi|\ \rangle\Psi$, a trivial computation proves that

$$\begin{aligned} &E_T(\mathbf{a}, \mathbf{b}) + E_T(\mathbf{a}', \mathbf{b}) + E_T(\mathbf{a}', \mathbf{b}') - E_T(\mathbf{a}, \mathbf{b}') \\ &\quad = \langle\psi_1|\mathbf{a}\cdot\sigma\psi_1\rangle\langle\psi_2|\mathbf{b}\cdot\sigma\psi_2\rangle + \langle\psi_1|\mathbf{a}'\cdot\sigma\psi_1\rangle\langle\psi_2|\mathbf{b}\cdot\sigma\psi_2\rangle \\ &\qquad + \langle\psi_1|\mathbf{a}'\cdot\sigma\psi_1\rangle\langle\psi_2|\mathbf{b}'\cdot\sigma\psi_2\rangle - \langle\psi_1|\mathbf{a}\cdot\sigma\psi_1\rangle\langle\psi_2|\mathbf{b}'\cdot\sigma\psi_2\rangle\,. \end{aligned} \tag{5.13}$$

But $||\mathbf{a}\cdot\sigma|| = \sup\{|\nu| \mid \nu \in \sigma(\mathbf{a}\cdot\sigma)\} = 1$, so $|\langle\psi_1|\mathbf{a}\cdot\sigma\psi_1\rangle| \leq ||\mathbf{a}\cdot\sigma||\,||\psi_1||^2 = 1$, and then $\langle\psi_1|\mathbf{a}\cdot\sigma\psi_1\rangle, \langle\psi_1|\mathbf{a}'\cdot\sigma\psi_1\rangle, \langle\psi_2|\mathbf{b}\cdot\sigma\psi_2\rangle, \langle\psi_2|\mathbf{b}'\cdot\sigma\psi_2\rangle \in [-1, 1]$. In summary, in view of Proposition 5.23, the absolute value of the right-hand side of (5.13) is bounded by 2. Therefore

$$-2 \leq E_T(\mathbf{a},\mathbf{b}) + E_T(\mathbf{a}',\mathbf{b}) + E_T(\mathbf{a}',\mathbf{b}') - E_T(\mathbf{a},\mathbf{b}') \leq 2 \quad \text{for every } \mathbf{a},\mathbf{a}',\mathbf{b},\mathbf{b}' \in \mathbb{S}^2.$$

Hence, factorized pure states satisfy the BCHSH inequality. An incoherent superposition of factorized pure states gives rise to the same result by construction. The lesson this story teaches us is:

Factorized pure states, and incoherent superpositions of them, do not violate the BCHSH inequality.

In a sense, they are more classical than entangled states.

Remark 5.24

(a) The natural question arising from our discovery is whether or not there exist pure *entangled* states satisfying the BCHSH inequality. As a matter of fact they do exist, and there also exist pure entangled states which violate the BCHSH inequality without reaching the maximum value $2\sqrt{2}$ [GaCh08, BeZe17].
(b) As a byproduct, the violation of the BCHSH inequality can be used to *detect entanglement*, paying attention that it only gives sufficient but not necessary conditions. ■

5.3.3 BCHSH Inequality from Relativistic Local Causality and Realism

In order to derive the BCHSH inequality, Bell presented [Bell75] the very general approach[5] we set out to introduce now (see also [Jar84] and [Shi90]).

We remind the reader that in a *time-oriented* spacetime M, such as Minkowski's spacetime, the **causal past** $J^-(O)$ (resp. **causal future** $J^+(O)$) of $O \subset M$ is the set of points $p \in M$ which admit a curve from p to O whose tangent vector is either timelike or lightlike, and future-directed (resp. past-directed). Since these curves represent causal interactions (at the macroscopic level at least), O cannot be influenced by anything that happens outside $J^-(O)$. Two subsets $O, O' \subset M$ are **causally separated** if $J^\pm(O) \cap O' = \varnothing$ (which is equivalent to $J^\pm(O') \cap O = \varnothing$): no causal relation can exist between them.

In Bell's view, a general relativistic physical system is described in terms of physical quantities, named **beables** by Bell in opposition to *observables*. These objects are supposed to always exist independently of our measurements, they ought to have objective properties and satisfy locality, *local causality* to be precise, in the

[5]The author is grateful to S.Mazzucchi for many clarifications and discussions on subtleties related to the content of this section.

sense we shall discuss below. Every physical description ought to be based on them. This is the strongest form of *realism* and *locality*.

In a typically stochastic description of a physical system S, a beable is a *random variable* $X : \Omega \to R_X$ defined on a probability measure space $(\Omega, \Sigma(\Omega), \mathbb{P})$ common to all beables, where R_X is any measurable space characteristic of X, typically a subset of some $\mathbb{R}^n$. The overall stochastic state of the system is represented by the probability measure $\mathbb{P}$ over Ω.

Remark 5.25

(a) Included in this are deterministic descriptions where (some) beables have definite values, simply by assuming that $\mathbb{P}$ is such that the physically relevant random variable attains the chosen value with probability 1.
(b) It is clear that this description is completely classic, as it relies on Kolmogorov's notion of probability and not on the quantum notion used in Gleason's theorem. ■

Beables are also *localized in spacetime regions* (Fig. 5.1) where they satisfy *causal locality* requirements, as we proceed to explain. We are interested in systems made of two parts S_1 and S_2, whose beables are localized in two *causally separated* regions O_1, O_2 of spacetime. In the following $P := J^-(O_1) \cap J^-(O_2)$ denotes the **common causal past** of the regions. As in the specific case of the EPR

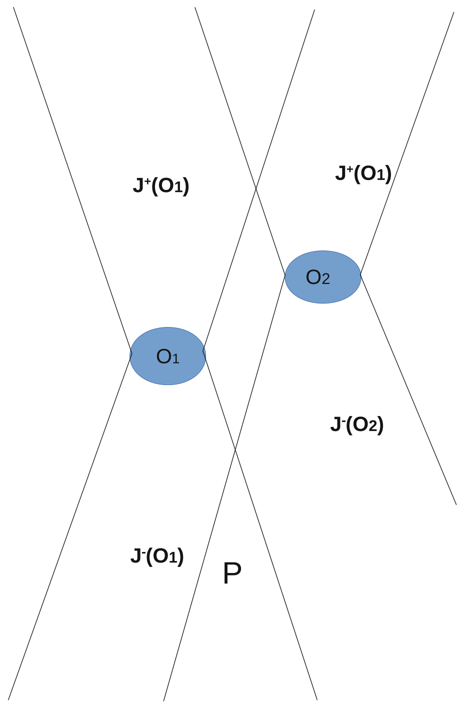

Fig. 5.1 Causally separated regions O_1 and O_2

phenomenology, where S consists of two entangled particles S_1 and S_2 localized in causally separated regions O_1 and O_2, we assume that beables are of three types:

(a) s_1 is a random variable localized at O_1 and taking values in V_1, and s_2 is a random variables localized at O_2 and taking values in V_2. We also assume that V_1 and V_2 are discrete subsets of $[-1, 1]$;
(b) $\mathbf{n}_1$ is a random variable localized at $J^-(O_1) \setminus P$ taking values in N_1, and $\mathbf{n}_2$ is a random variable localized at $J^-(O_2) \setminus P$ taking values in N_2;
(c) λ is a random variable localized in the common causal past P taking values in some measurable space Λ.

The physical interpretation (not the only one) goes as follows:

1. s_1 is the (normalized) value of the component of the spin of S_1 along the direction $\mathbf{n}_1$, s_2 is the (normalized) value of the spin of S_2 along the direction $\mathbf{n}_2$. The value of s_1 cannot have any influence on the value of s_2, for O_1 and O_2 are causally separated.
2. The random variables $\mathbf{n}_1$ and $\mathbf{n}_2$ represent the choice we made of the components of the spin we intend to measure on S_1 in O_1 and on S_2 in O_2. The possible directions of the spins are taken in subsets N_1, N_2 of $\mathbb{S}^2$.

   These choices are made in the causal past of O_1 and O_2 respectively. We also assumed that the choice of $\mathbf{n}_1$ cannot have any influence on what happens in O_2 and *vice versa*, since both beables are localized outside P.

   (The $\mathbf{n}_i$ appear here as stochastic variables—in real measurements of EPR correlations the components of the spin to be measured are actually chosen randomly—but non-random choices are subsumed by assuming that the probability of a certain choice is 1, see Remark 5.25.)
3. The role of the beable λ as a *hidden variable* is less precise than in the previous section: it lives in the common causal past P and represents a potential *common cause* responsible for possible *correlations* of the beables localized at O_1 and O_2, since no direct causal relations are permitted between them as O_1 and O_2 are causally separated. The measure μ introduced in the previous sections, which betrays our ignorance about the precise value of λ, can be defined here as $\mu(L) := \mathbb{P}(\lambda^{-1}(L))$, where $L \subset \Lambda$ is any measurable set.

Remark 5.26 Let us emphasize that we are not assuming that the particles have spin 1/2, and the following reasoning would go through, with trivial adjustments, even if s_2 and s_2 were continuous on $[-1, 1]$. The rest of the argument is actually valid provided (a), (b), (c) are true regardless of the particle-spin interpretation when assuming the statistical interpretation of local causality (5.15)–(5.17) below. ■

By assuming (a), (b) and (c) the discussion goes on in terms of *conditional probabilities*. We want to prove an inequality about the *expectation value*

$$E(\lambda_0, \mathbf{a}, \mathbf{b}) := \mathbb{E}(s_1 s_2 | \lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a}, \mathbf{n}_2 = \mathbf{b})$$

of the product $s_1 \cdot s_2$ under the conditions $\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a}, \mathbf{n}_2 = \mathbf{b}$, where

$$\begin{aligned}&\mathbb{E}(s_1 s_2|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a}, \mathbf{n}_2 = \mathbf{b}) \\ &\quad := \sum_{\alpha \in V_1\,,\, \beta \in V_2} \alpha\beta\, \mathbb{P}(s_1 = \alpha, s_2 = \beta|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a}, \mathbf{n}_2 = \mathbf{b})\,. \qquad (5.14)\end{aligned}$$

We start from the observation that, in a *locally causal* theory as the one presented above, the following relations declaring statistical independence of the two subsystems must be true:

$$\mathbb{P}(s_1 = \alpha|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a}, \mathbf{n}_2 = \mathbf{b}, s_2 = \beta) = \mathbb{P}(s_1 = \alpha|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a})\,, \quad (5.15)$$

$$\mathbb{P}(s_1 = \alpha|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a}, \mathbf{n}_2 = \mathbf{b}) = \mathbb{P}(s_1 = \alpha|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a})\,, \quad (5.16)$$

$$\mathbb{P}(s_1 = \alpha|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a}, s_2 = \beta) = \mathbb{P}(s_1 = \alpha|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a})\,. \quad (5.17)$$

This is because the values of $\mathbf{n}_2$ and s_2 cannot have any influence on what happens in O_1, see (1) and (2) above. The same holds if we swap the beables of S_1 and S_2. Let us therefore consider the joint conditional probability

$$\begin{aligned}&\mathbb{P}(s_1 = \alpha, s_2 = \beta|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a}, \mathbf{n}_2 = \mathbf{b}) \\ &= \mathbb{P}(s_1 = \alpha|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a}, \mathbf{n}_2 = \mathbf{b}, s_2 = \beta)\mathbb{P}(s_2 = \beta|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a}, \mathbf{n}_2 = \mathbf{b})\,.\end{aligned}$$

Using (5.15)–(5.17) and the analogous formulas with subsystems interchanged, we finally have

$$\begin{aligned}&\mathbb{P}(s_1 = \alpha, s_2 = \beta|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a}, \mathbf{n}_2 = \mathbf{b}) \\ &\quad = \mathbb{P}(s_1 = \alpha|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a})\mathbb{P}(s_2 = \beta|\lambda = \lambda_0, \mathbf{n}_2 = \mathbf{b})\,.\end{aligned}$$

Inserting the result in (5.14) gives

$$E(\lambda_0, \mathbf{a}, \mathbf{b}) = \mathbb{E}(s_1|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a})\mathbb{E}(s_2|\lambda = \lambda_0, \mathbf{n}_2 = \mathbf{b})\,. \qquad (5.18)$$

Since the values of s_1 and s_2 are bounded by 1 in absolute value, we also have

$$-1 \le \mathbb{E}(s_1|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a}) \le 1 \quad \text{and} \quad -1 \le \mathbb{E}(s_2|\lambda = \lambda_0, \mathbf{n}_2 = \mathbf{b}) \le 1\,. \quad (5.19)$$

As a consequence, using Proposition 5.23, we conclude that no matter how we fix $\mathbf{a}, \mathbf{a}' \in N_1$ and $\mathbf{b}, \mathbf{b}' \in N_2$, the absolute value of

$$\begin{aligned}&\mathbb{E}(s_1|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a})\mathbb{E}(s_2|\lambda = \lambda_0, \mathbf{n}_2 = \mathbf{b}) + \mathbb{E}(s_1|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a})\mathbb{E}(s_2|\lambda = \lambda_0, \mathbf{n}_2 = \mathbf{b}') \\ &+\mathbb{E}(s_1|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a}')\mathbb{E}(s_2|\lambda = \lambda_0, \mathbf{n}_2 = \mathbf{b}) - \mathbb{E}(s_1|\lambda = \lambda_0, \mathbf{n}_1 = \mathbf{a}')\mathbb{E}(s_2|\lambda = \lambda_0, \mathbf{n}_2 = \mathbf{b}')\end{aligned}$$

is bounded by 2. In other words, from (5.18),

$$-2 \leq E(\lambda_0, \mathbf{a}, \mathbf{b}) + E(\lambda_0, \mathbf{a}, \mathbf{b}') + E(\lambda_0, \mathbf{a}', \mathbf{b}) - E(\lambda_0, \mathbf{a}', \mathbf{b}') \leq 2 \,. \quad (5.20)$$

We can get rid of $\lambda_0 \in \Lambda$ by taking the expectation value with respect to the probability measure μ over Λ introduced in (3) above:

$$E(\mathbf{a}, \mathbf{b}) := \int_\Lambda E(\lambda, \mathbf{a}, \mathbf{b}) d\mu(\lambda) \,.$$

Using this definition in (5.20), the linearity of the integral and the fact that the total integral is 1, we eventually obtain the BCHSH inequality:

$$-2 \leq E(\mathbf{a}, \mathbf{b}) + E(\mathbf{a}, \mathbf{b}') + E(\mathbf{a}', \mathbf{b}) - E(\mathbf{a}', \mathbf{b}') \leq 2$$

under the hypotheses (a), (b), (c) and the natural interpretation of local causality (5.15)–(5.17).

5.3.4 BCHSH Inequality from Realism and Non-Contextuality

We do not wish to insist again on the interplay between entanglement, realism and locality, so we switch to the relationship between entanglement, realism, and *non-contextuality* instead.

Let us consider again a *quantum* system S made of two *independent* parts S_1 and S_2 which are not necessarily spatially separated. A physical example of such a system is a spin-$1/2$ massive particle, or a photon, where the polarization's two degrees of freedom are exploited in place of the two degrees of freedom of the spin. In principle, according to Sect. 4.4.8, the Hilbert space of this system is the Hilbert tensor product $L^2(\mathbb{R}^3, d^3k) \otimes \mathbb{C}^2$ (momentum picture). However, we can restrict the possibilities in the momentum space $L^2(\mathbb{R}^3, d^3k)$ to a 2-dimensional subspace. In practice, through a suitable experimental filter only the span of two states labelled by two momenta $k_1, k_2 \in \mathbb{R}^3$ is accessible to the system. These two pure states are defined by a pair of unit-norm vectors ψ_{k_1} and ψ_{k_1}. In terms of L^2 functions, these vectors are wavefunctions typically living in $\mathscr{S}(\mathbb{R}^3)$, whose support in momentum space is strictly concentrated around k_1 and k_2 respectively. Since $k_1 \neq k_2$, it is reasonable to assume $\langle \psi_{k_1} | \psi_{k_1} \rangle = 0$. In this way the span of the vectors is isomorphic to $\mathbb{C}^2$, the effective Hilbert space of the system is

$$\mathsf{H} = \mathbb{C}^2_{\text{momentum}} \otimes \mathbb{C}^2_{\text{polarization/spin}} \,,$$

and observables corresponding to real linear combinations of $\sigma_1, \sigma_2, \sigma_3$ can be introduced also on the first factor. From the experimental point of view all these observables correspond to devices like *beam-splitters*, *mirrors*, *polarization* *analyzers* and so on. A typical apparatus dealing with photons whose momentum states are confined to the $\mathbb{C}^2$ space is the *Mach–Zehnder interferometer* [GaCh08].

In contrast to Bell's analysis, we know a priori that the observables of S_1 are compatible with the observables of S_2, and *this fact has nothing to do with locality*.

We want to show that, in this context, the BCHSH inequality can be used to distinguish between the hidden-variable descriptions assuming realism and non-contextuality and the ones that *do not*. The difference with the similar discussion of Sect. 5.2.3 is that here we will obtain distinct results depending on the states used. In particular, entangled states will play a crucial role even if locality does not enter the game.

Referring again to notation (5.7), we define spin-like observables for each side of the system (whose meaning is not that of spin components in general):

$$A(\mathbf{a}) := \mathbf{a} \cdot \sigma \in \mathfrak{B}(\mathsf{H}_1)_{sa} \quad \text{and} \quad B(\mathbf{b}) := \mathbf{b} \cdot \sigma \in \mathfrak{B}(\mathsf{H}_2)_{sa}$$

so that $\sigma(A(\mathbf{a})) = \sigma(B(\mathbf{b})) = \{\pm 1\}$ in particular.

Let us now suppose that a quantum state $T \in \mathscr{S}(\mathsf{H})$ is given. If we believe in a realistic non-contextual hidden-variable theory, exactly as in Sect. 5.2.3, we must first assume that this state corresponds to a probability measure μ over the space Λ of hidden variables $\lambda \in \Lambda$. Realism and non-contextuality act as follows.

1. *Realism* prescribes that all observables $A(\mathbf{a})$, $B(\mathbf{b})$, for every $\mathbf{a}, \mathbf{b} \in \mathbb{S}^2$, attain a definite value $v_\lambda(A(\mathbf{a})) \in \{\pm 1\}$ and $v_\lambda(B(\mathbf{b})) \in \{\pm 1\}$, for $\lambda \in \Lambda$.
2. *Non-contextuality* demands that the value $v_\lambda(A(\mathbf{a}))$ does not depend on the choice of observables $B(\mathbf{b})$ and $B(\mathbf{b}')$ which can be measured simultaneously with $A(\mathbf{a})$, when $\mathbf{b}' \neq \mathbf{b}$ are such that $B(\mathbf{b})$ and $B(\mathbf{b}')$ are not compatible.

In the previous discussion, when we were considering a pair of *entangled particles*, this independence was due to locality; here, instead, locality cannot be imposed any longer.

As in Bell's analysis of entangled particles, it is convenient to introduce the quantity

$$\chi(\mathbf{a}, \mathbf{a}', \mathbf{b}, \mathbf{b}'|\lambda) = v_\lambda(A(\mathbf{a}))v_\lambda(B(\mathbf{b})) + v_\lambda(A(\mathbf{a}'))v_\lambda(B(\mathbf{b})) + v_\lambda(A(\mathbf{a}'))v_\lambda(B(\mathbf{b}')) - v_\lambda(A(\mathbf{a}))v_\lambda(B(\mathbf{b}')) \ . \tag{5.21}$$

If we take the expectation value of $\chi(\mathbf{a}, \mathbf{a}', \mathbf{b}, \mathbf{b}'|\lambda)$ when λ varies in Λ according with its probability distribution μ,

$$\mathbb{E}_\mu(\chi) := \int_\Lambda \chi(\mathbf{a}, \mathbf{a}', \mathbf{b}, \mathbf{b}'|\lambda) d\mu(\lambda) \ ,$$

with the same reasoning as in the previous section we find again $-2 \leq \mathbb{E}_\mu(\chi) \leq 2$. Defining

$$E_\mu(\mathbf{a}, \mathbf{b}) := \int_\Lambda v_\lambda(A(\mathbf{a}))v_\lambda(B(\mathbf{b}))d\mu(\lambda) \quad \mathbf{a}, \mathbf{b} \in \mathbb{S}^2 ,$$

produces the *BCHSH inequality*

$$-2 \leq E_\mu(\mathbf{a}, \mathbf{b}) + E_\mu(\mathbf{a}, \mathbf{b}') + E_\mu(\mathbf{a}', \mathbf{b}') - E_\mu(\mathbf{a}, \mathbf{b}') \leq 2 \qquad \text{for every } \mathbf{a}, \mathbf{a}', \mathbf{b}, \mathbf{b}' \in \mathbb{S}^2. \quad (5.22)$$

This inequality regarding correlations of measurements of the spin-like components of a bipartite system must be satisfied by every realistic non-contextual theory.

Passing to the quantum side, we can proceed exactly as in the previous section: restrict to *entangled* pure *Bell states* (5.9), take $T_\pm = \langle \Psi_\pm | \cdot \rangle \Psi_\pm$ and fix axes $\mathbf{a}, \mathbf{a}', \mathbf{b}, \mathbf{b}'$ as in (5.10). Then we find (5.11) again:

$$E_{T_\pm}(\mathbf{a}, \mathbf{b}) + E_{T_\pm}(\mathbf{a}, \mathbf{b}') + E_{T_\pm}(\mathbf{a}', \mathbf{b}') - E_{T_\pm}(\mathbf{a}, \mathbf{b}') = \pm 2\sqrt{2}\,.$$

Remark 5.27 The type of entanglement we are considering here is called **intra-particle entanglement**, as it is built with a unique particle entangling the orbital degrees of freedom described on $\mathbb{C}_{\text{orbital}}$ and the spin/polarization freedom degrees described on $\mathbb{C}^2_{\text{polarization/spin}}$. ■

Since $2\sqrt{2} > 2$, we conclude that *the result predicted by Quantum Theory, with the given choices of observables and Bell's intraparticle entangled states, is incompatible with non-contextual realism.*

Chapter 6
von Neumann Algebras of Observables and Superselection Rules

The aim of this chapter is to examine the observables of a quantum system, described on the Hilbert space H, by means of elementary results from the theory of *von Neumann algebras*. von Neumann algebras will be used as a tool to formalize *superselection rules*.

6.1 Introduction to von Neumann Algebras

Up to now, we have tacitly supposed that *all* selfadjoint operators on H represent observables, *all* orthogonal projectors represent elementary observables, *all* normalized vectors represent pure states. This is not the case in physics, due to the presence of the so-called *superselection rules* introduced by Wigner (and developed together with Wick and Wightman around 1952), and also by the possible appearance of a *(non-Abelian) gauge group*, alongside several other theoretical and experimental facts. Within the Hilbert space approach, the appropriate instrument to deal with these notions is a known mathematical structure: *von Neumann algebras*. The idea of restricting the algebra of observables made its appearance in Quantum Mechanics quite early. Around 1936 von Neumann tried to justify the intrinsic stochasticity of quantum systems "a priori", with a physically sound notion of quantum probability (see [Red98] for a historical account). Barring *finite-dimensional* Hilbert spaces, von Neumann's ideas were valid only for a special type of von Neumann algebras called *type-*II_1 *factors*, which satisfy a stronger version of orthomodularity known as *modularity*. Although nowadays the ideas of von Neumann about a priori quantum probability are considered physically untenable, the general theory of von Neumann algebras has become an important area of pure mathematics [KaRi97], and overlaps with disciplines other than functional analysis: non-commutative geometry for instance, and quantum theory in particular. The idea of restricting the algebra of observables survived von Neumann's approach to quantum probability and turned

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out to be far-reaching, as attested by the strong physical support received from the experimental evidence of Wigner's idea of superselection rules, the formulation of non-Abelian gauge theories, and from Quantum Field Theory—also formulated in terms of fermionic fields (which are not observables) [Emc72, Haa96, Ara09, Lan17].

For all these reasons, we will spend the initial part of this chapter, of pure mathematical flavour, to discuss the elegant notion of a von Neumann algebra.

6.1.1 The Mathematical Notion of von Neumann Algebra

Before we introduce von Neumann algebras, let us define first the *commutant* of a subset of $\mathfrak{B}(\mathsf{H})$ and state an important preliminary theorem.

Definition 6.1 Consider a Hilbert space H. If $\mathfrak{M} \subset \mathfrak{B}(\mathsf{H})$, the set of operators

$$\mathfrak{M}' := \{T \in \mathfrak{B}(\mathsf{H}) \mid TA - AT = 0 \quad \text{for any } A \in \mathfrak{M}\} \tag{6.1}$$

is called the **commutant** of $\mathfrak{M}$. ■

Remark 6.2 It is evident from the definition that, if $\mathfrak{M}_1, \mathfrak{M}_2, \mathfrak{N} \subset \mathfrak{B}(\mathsf{H})$, then

(1) $\mathfrak{M}_1 \subset \mathfrak{M}_2$ implies $\mathfrak{M}_2' \subset \mathfrak{M}_1'$
(2) $\mathfrak{N} \subset (\mathfrak{N}')'$.

■

Further properties of the commutant are stated below.

Proposition 6.3 *Let H be a Hilbert space and $\mathfrak{M} \subset \mathfrak{B}(\mathsf{H})$. The commutant $\mathfrak{M}'$ enjoys the following properties.*

(a) $\mathfrak{M}'$ *is a unital C^*-subalgebra in $\mathfrak{B}(\mathsf{H})$ if $\mathfrak{M}$ is *-closed (i.e. $A^* \in \mathfrak{M}$ if $A \in \mathfrak{M}$).*
(b) $\mathfrak{M}'$ *is both strongly and weakly closed.*
(c) $\mathfrak{M}' = ((\mathfrak{M}')')'$. *Hence there is nothing new beyond the second commutant.*

Proof

(a) $I \in \mathfrak{M}'$ in any of the cases. Furthermore, if $A \in \mathfrak{B}(\mathsf{H})$ satisfies $AB - BA = 0$ for every $B \in \mathfrak{M}$, then $B^*A^* - A^*B^* = 0$ for every $B \in \mathfrak{M}$. If $C \in \mathfrak{M}$, then $C^* \in \mathfrak{M}$ by hypothesis and $C = (C^*)^*$. Hence $CA^* - A^*C = 0$ for every $C \in \mathfrak{M}$ and thus $A^* \in \mathfrak{M}'$ if $A \in \mathfrak{M}'$. To conclude the proof of (a) it is enough to prove that $\mathfrak{M}'$ is closed in the uniform operator topology. If $A_nB = BA_n$ and $A_n \to A$ uniformly, where $A, A_n \in \mathfrak{B}(\mathsf{H})$ and $B \in \mathfrak{M}$, then $A \in \mathfrak{M}'$ because

$$||AB - BA|| = ||\lim_{n\to+\infty} A_nB - B\lim_{n\to+\infty} A_n|| = ||\lim_{n\to+\infty} A_nB - \lim_{n\to+\infty} BA_n|| = 0$$

$$= \lim_{n\to+\infty} ||A_nB - BA_n|| = \lim_{n\to+\infty} 0 = 0\,.$$

(b) Strong closure follows from weak closure, but we shall give an explicit and independent proof as an exercise. $A_n \to A$ strongly means that $A_n x \to Ax$ for every $x \in \mathsf{H}$. Assuming $A_n B - BA_n = 0$ where $A \in \mathfrak{B}(\mathsf{H})$, $A_n \in \mathfrak{M}'$ and $B \in \mathfrak{M}$, we have that $A \in \mathfrak{M}'$ since, for every $x \in \mathsf{H}$,

$$ABx - BAx = \lim_{n\to+\infty} A_n(Bx) - B \lim_{n\to+\infty} A_n x$$
$$= \lim_{n\to+\infty} (A_n Bx - BA_n x) = \lim_{n\to+\infty} 0 = 0 \,.$$

The case of the weak operator topology is treated similarly. $A_n \to A$ weakly means that $\langle y|A_n x\rangle \to \langle y|Ax\rangle$ for every $x, y \in \mathsf{H}$. Assuming $A_n B - BA_n = 0$ where $A \in \mathfrak{B}(\mathsf{H})$, $A_n \in \mathfrak{M}'$ and $B \in \mathfrak{M}$, we have $\langle y|ABx\rangle - \langle y|BAx\rangle = \lim_{n\to+\infty}\langle y|A_n(Bx)\rangle - \lim_{n\to+\infty}\langle B^* y|A_n x\rangle = \lim_{n\to+\infty}\langle y|(A_n B - BA_n)x\rangle = \lim_{n\to+\infty} 0 = 0$, so that $\langle y|(AB - BA)x\rangle = 0$ for every $x, y \in \mathsf{H}$, which implies $A \in \mathfrak{M}'$.

(c) If $\mathfrak{N} = \mathfrak{M}'$, Remark 6.2 (2) implies $\mathfrak{M}' \subset ((\mathfrak{M}')')'$. On the other hand $\mathfrak{M} \subset (\mathfrak{M}')'$ implies, via Remark 6.2 (1), $((\mathfrak{M}')')' \subset \mathfrak{M}'$. Summing up, $\mathfrak{M}' = ((\mathfrak{M}')')'$.

□

In the sequel we shall adopt the standard convention used for von Neumann algebras and write $\mathfrak{M}''$ in place of $(\mathfrak{M}')'$ etc. The next crucial classical result is due to von Neumann. It remarkably connects algebraic properties to topological ones.

Theorem 6.4 (von Neumann's Double Commutant Theorem) *If* H *is a Hilbert space and* $\mathfrak{A}$ *a unital* **-subalgebra in* $\mathfrak{B}(\mathsf{H})$*, the following statements are equivalent:*

(a) $\mathfrak{A} = \mathfrak{A}''$*;*
(b) $\mathfrak{A}$ *is weakly closed;*
(c) $\mathfrak{A}$ *is strongly closed.*

Proof (a) implies (b) because $\mathfrak{A} = (\mathfrak{A}')'$ and Proposition 6.3 (c)holds; moreover (b) implies (c) immediately, since the strong operator topology is finer than the weak operator topology. To conclude, we will prove that (c) implies (a). Since $\mathfrak{A}'' = (\mathfrak{A}')'$ is strongly closed (Proposition 6.3 (c)), the claim is true if we establish that $\mathfrak{A}$ is strongly dense in $\mathfrak{A}''$. Following definitions (b) presented in Sect. 3.5, assume that $Y \in \mathfrak{A}''$ and the set $\{x_i\}_{i\in I} \subset \mathsf{H}$, with I finite, are given. Then, for every choice of $\epsilon_i > 0$, $i \in I$, we claim there must exist $X \in \mathfrak{A}$ with $||(X - Y)x_i|| < \epsilon_i$ for $i \in I$. To prove this assertion, first consider the case $I = \{1\}$ and define $x := x_1$. Let us focus on the closed subspace $\mathsf{K} := \overline{\{Xx \mid X \in \mathfrak{A}\}}$, and note that $x \in \mathsf{K}$ because $I \in \mathfrak{A}$ by hypothesis. Let $P \in \mathscr{L}(\mathsf{H})$ be the orthogonal projector onto K. Evidently $Z(\mathsf{K}) \subset \mathsf{K}$ if $Z \in \mathfrak{A}$, since products of elements in $\mathfrak{A}$ are in $\mathfrak{A}$ (it is an algebra) and elements of $\mathfrak{A}$ are continuous. Saying $Z(\mathsf{K}) \subset \mathsf{K}$ is the same as $ZP = PZP$, for every $Z \in \mathfrak{A}$. Taking adjoints we also have $PZ = PZP$ for every $Z \in \mathfrak{A}$ (since $\mathfrak{A}$ is *-closed by hypothesis) and, comparing relations, we conclude that $PZ = ZP$ for $Z \in \mathfrak{A}$. We have found that $P \in \mathfrak{A}' = (\mathfrak{A}'')'$, and in particular $PY = YP$ since $Y \in \mathfrak{A}''$. In turn, this proves that $Y(\mathsf{K}) \subset \mathsf{K}$ so, in particular, $Yx \in \mathsf{K}$. In other words, Yx belongs to the closure of $\{Xx \mid X \in \mathfrak{A}\}$. Hence $||Xx - Yx|| < \epsilon$ if $X \in \mathfrak{A}$ is chosen suitably.

The result generalizes to finite $I \supset \{1\}$, by defining the direct sum $\mathsf{H}_I := \bigoplus_{i \in I} \mathsf{H}$ and the inner product $\langle \oplus_{i\in I} x_i | \oplus_{i \in I} y_i \rangle_I := \sum_{i \in I} \langle x_i | y_i \rangle$ making H_I a Hilbert space. The set of operators $\mathfrak{A}_I := \{X_I \mid X \in \mathfrak{A}(\mathsf{H})\} \subset \mathfrak{B}(\mathsf{H}_I)$, where

$$X_I(\oplus_{i\in I} x_i) := \oplus_{i \in I} X x_i \quad \forall \oplus_{i \in I} x_i \in \bigoplus_{i \in I} \mathsf{H}\,, \tag{6.2}$$

is a unital *-subalgebra of $\mathfrak{B}(\mathsf{H}_I)$. Now, for $Y \in \mathfrak{A}''$, define $Y_I \in \mathfrak{B}(\mathsf{H}_I)$ according to (6.2), giving $Y_I \in \mathfrak{A}''_I$. By a trivial extension of the above reasoning we may prove that if $\epsilon > 0$, there is $X_I \in \mathfrak{A}_I$ with $||X_I \oplus_{i\in I} x_i - Y_I \oplus_{i \in I} x_i||_I < \epsilon$. Therefore $||(X-Y)x_i||^2 \leq \sum_{j \in I} ||(X-Y)x_j||^2 \leq \epsilon^2$ for every $i \in I$. Taking $\epsilon = \min\{\epsilon_i\}_{i \in I}$ proves the claim. □

At this juncture we are ready to define von Neumann algebras.

Definition 6.5 Let H be a Hilbert space. A **von Neumann algebra** $\mathfrak{A}$ on H is a unital *-subalgebra of $\mathfrak{B}(\mathsf{H})$ that satisfies any of the equivalent properties appearing in von Neumann's Theorem 6.4. The **centre** of $\mathfrak{A}$ is the set $\mathfrak{A} \cap \mathfrak{A}'$. ■

von Neumann algebras are also known as **concrete W^*-algebras** (see also Example 8.3).

Remark 6.6

(a) Theorem 6.4 holds also if one replaces the strong topology with the *ultrastrong topology*, the weak topology with the *ultraweak topology* (see, e.g., [BrRo02].)
(b) If $\mathfrak{M}$ is a *-closed subset of $\mathfrak{B}(\mathsf{H})$, since $(\mathfrak{M}')'' = \mathfrak{M}'$ (Proposition 6.3 (c)), then $\mathfrak{M}'$ is a von Neumann algebra. In turn, $\mathfrak{M}'' = (\mathfrak{M}')'$ is a von Neumann algebra as well. As an elementary consequence, the centre of a von Neumann algebra is a *commutative* von Neumann algebra.
(c) A von Neumann algebra $\mathfrak{R}$ in $\mathfrak{B}(\mathsf{H})$ is a special instance of C^*-algebra with unit, or better, a unital C^*-subalgebra of $\mathfrak{B}(\mathsf{H})$. This comes from Proposition 6.3 (a), because $\mathfrak{R} = (\mathfrak{R}')'$.
(d) The intersection of a family (with arbitrary cardinality) of von Neumann algebras $\{\mathfrak{R}_j\}_{j \in J}$ on a Hilbert space H is a von Neumann algebra on H. (In fact, it is easy to see that $\bigcap_{j \in J} \mathfrak{R}_j$ is a unital *-subalgebra of $\mathfrak{B}(\mathsf{H})$. Furthermore, if $\bigcap_{j\in J} \mathfrak{R}_j \ni A_n \to A \in \mathfrak{B}(\mathsf{H})$ strongly, then $\mathfrak{R}_j \ni A_n \to A$ strongly for every fixed $j \in J$, so that $A \in \mathfrak{R}_j$ since $\mathfrak{R}_j$ is von Neumann. Therefore $A \in \bigcap_{j \in J} \mathfrak{R}_j$. This proves that $\bigcap_{j \in J} \mathfrak{R}_j$ is strongly closed and hence a von Neumann algebra.) ■

If $\mathfrak{M} \subset \mathfrak{B}(\mathsf{H})$ is *-closed, the smallest (set-theoretically) von Neumann algebra containing $\mathfrak{M}$ as a subset—the intersection of all von Neumann algebras containing $\mathfrak{M}$—has a very precise form. If $\mathfrak{U} \supset \mathfrak{M}$ is any von Neumann algebra, taking the commutant twice, we have $\mathfrak{U}' \subset \mathfrak{M}'$ and $\mathfrak{M}'' \subset \mathfrak{U}'' = \mathfrak{U}$, so $\mathfrak{M}'' \subset \mathfrak{U}$. As a consequence $\mathfrak{M}''$ is the intersection of all von Neumann algebras containing $\mathfrak{M}$. All this leads to the following definition.

Definition 6.7 Let H be a Hilbert space and consider a *-closed set $\mathfrak{M} \subset \mathfrak{B}(\mathsf{H})$. The double commutant $\mathfrak{M}''$ is also called the **von Neumann algebra generated** by $\mathfrak{M}$. ■

A topological characterization of $\mathfrak{M}''$ appears in Exercise 6.13 when $\mathfrak{M}$ is a unital *-subalgebra of $\mathfrak{B}(\mathsf{H})$.

If $\mathfrak{A}_1$ and $\mathfrak{A}_2$ are von Neumann algebras on H_1 and H_2, it is possible to define the **tensor product of von Neumann algebras** $\mathfrak{A}_1$ and $\mathfrak{A}_2$ as the von Neumann algebra on $\mathsf{H}_1 \otimes \mathsf{H}_2$

$$\mathfrak{A}_1 \overline{\otimes} \mathfrak{A}_2 := (\mathfrak{A}_1 \otimes \mathfrak{A}_2)''. \tag{6.3}$$

With reference to (4.27), we have exploited the notion of **algebraic tensor product** of *-subalgebras $\mathfrak{A}_i \subset \mathfrak{B}(\mathsf{H}_i)$

$$\mathfrak{A}_1 \otimes \mathfrak{A}_2 := \left\{ \sum_{j=1}^{N} c_j A_j \otimes B_j \;\middle|\; c_j \in \mathbb{C}\,,\, A_j \in \mathfrak{A}_1\,,\, B_j \in \mathfrak{A}_2\,,\, N \in \mathbb{N} \right\} . \tag{6.4}$$

It turns out that [KaRi97, BrRo02, Tak10]

$$(\mathfrak{A}_1 \overline{\otimes} \mathfrak{A}_2)' = \mathfrak{A}_1' \overline{\otimes} \mathfrak{A}_2'. \tag{6.5}$$

The notion of tensor product of von Neumann algebras *of observables* plays a relevant role in the description of independent subsystems of a quantum system, as discussed in Sect. 6.4.

Definition 6.8 A pair of concrete (i.e. subsets of some $\mathfrak{B}(\mathsf{H})$) unital *-algebras $\mathfrak{R}_1 \subset \mathfrak{B}(\mathsf{H}_1)$ and $\mathfrak{R}_2 \subset \mathfrak{B}(\mathsf{H}_2)$ on respective Hilbert spaces H_1 and H_2 are said

(a) **isomorphic** (or **quasi equivalent**) if there exists a unital *-algebra isomorphism $\phi : \mathfrak{R}_1 \to \mathfrak{R}_2$;
(b) **completely isomorphic** if the unital *-algebra isomorphism ϕ in (a) is also a homeomorphism for the weak and strong topologies;
(c) **spatially isomorphic** if there is a surjective linear isometry $V : \mathsf{H}_1 \to \mathsf{H}_2$ such and $\mathfrak{R}_1 \ni A \mapsto VAV^{-1} \in \mathfrak{R}_2$ is surjective, and hence a complete isomorphism. ■

Actually, cases (a) and (b) coincide in view of the following result [BrRo02], which proves an even stronger property.

Proposition 6.9 *A unital *-algebra isomorphism between two von Neumann algebras is a norm-preserving complete isomorphism. In particular isomorphic von Neumann algebras are also isometrically *-isomorphic as unital C^*-algebras.*

6.1.2 Unbounded Selfadjoint Operators Affiliated to a von Neumann Algebra

Handling unbounded selfadjoint operators is quite standard in Quantum Theory, so the definition of commutant and von Neumann algebra generated by a set should be extended to encompass unbounded selfadjoint operators (a further extension may concern closed operators, see, e.g., [Mor18]).

Definition 6.10 Let $\mathfrak{N}$ be a set of (typically unbounded) selfadjoint operators on the Hilbert space H.

(a) The **commutant** $\mathfrak{N}'$ of $\mathfrak{N}$ is defined as the commutant, in the sense of Definition 6.1, of the set of spectral measures $P^{(A)}$ of every $A \in \mathfrak{N}$.
(b) The von Neumann algebra $\mathfrak{N}''$ **generated by** $\mathfrak{N}$ is $(\mathfrak{N}')'$, where the outer dash is the commutant of Definition 6.1.

If $\mathfrak{M}$ is a von Neumann algebra on H, a selfadjoint operator $A : D(A) \to \mathsf{H}$ with $D(A) \subset \mathsf{H}$ is said to be **affiliated** to $\mathfrak{M}$ if its PVM $P^{(A)}$ belongs in $\mathfrak{M}$. ∎

Remark 6.11

(a) When $\mathfrak{N} \subset \mathfrak{B}(\mathsf{H})$ the commutant $\mathfrak{N}'$, computed as in (a), coincides with the standard commutant of Definition 6.1, as a consequence of Proposition 3.70 (ii) and (iv).
(b) If $A^* = A \in \mathfrak{N}$, then A is automatically affiliated to $(\mathfrak{N}')'$ because $P^{(A)}$ commutes with all selfadjoint operators in $\mathfrak{B}(\mathsf{H})$ commuting with A (Proposition 3.70) and, in particular, with every operator in $\mathfrak{B}(\mathsf{H})$ commuting with A, because these operators are linear combinations of similar selfadjoint operators. Therefore $P^{(A)} \subset (\mathfrak{N}')'$. In this sense "affiliation" is a weaker form of "belonging". ∎

Let us discuss how *unbounded* selfadjoint operators affiliated to a von Neumann algebra are strong limit points of the algebra *on the domain of the operator*. We have the following elementary result.

Proposition 6.12 *If $A : D(A) \to \mathsf{H}$ is a selfadjoint operator on the Hilbert space H and A is affiliated to the von Neumann algebra $\mathfrak{R}$, then A is the strong limit over $D(A)$ of a sequence of selfadjoint operators in $\mathfrak{R}$. Furthermore $A \in \mathfrak{R}$ if $D(A) = \mathsf{H}$.*

Proof Let us start by observing that, if A is an unbounded selfadjoint operator, for every $x \in D(A)$ we have

$$Ax = \lim_{n\to+\infty} \int_{[-n,n]\cap\sigma(A)} \lambda dP^{(A)}(\lambda)x \quad n \in \mathbb{N}$$

as a consequence of Proposition 3.24 (d) and dominated convergence. In other words, A is the strong limit *on* $D(A)$ of the sequence of operators $A_n \in \mathfrak{B}(\mathsf{H})$

defined by

$$A_n := \int_{[-n,n]\cap\sigma(A)} \lambda dP^{(A)}(\lambda) .$$

These operators are in $\mathfrak{B}(\mathsf{H})$ by Proposition 3.29, since the map $\iota : \mathbb{R} \ni \lambda \to \lambda \in \mathbb{R}$ is bounded on $[-n, n]$, so $||A_n|| \leq ||\iota \upharpoonright_{[-n,n]} ||_\infty$. Moreover, if A is affiliated to a von Neumann algebra $\mathfrak{R}$, then we claim $A_n \in \mathfrak{R}$. First notice that A_n is the strong limit, on the whole H, of integrals of simple functions $s_n \to \iota$ pointwise on $[-n, n]$ and such that $|s_n| \leq |\iota|$, using again Proposition 3.24 (d) and dominated convergence. The integrals $\int_{[-n,n]} s_n dP^{(A)}$ are linear combinations of projectors $P_E^{(A)} \in \mathfrak{R}$ by hypothesis, so $\int_{[-n,n]} s_n dP^{(A)} \in \mathfrak{R}$. Hence $A_n \in \mathfrak{R}$, it being the strong limit of elements of $\mathfrak{R}$ which is strongly closed. Suppose $D(A) = \mathsf{H}$, so $A \in \mathfrak{B}(\mathsf{H})$ (Theorem 2.40) is the strong limit of elements of $\mathfrak{R}$ everywhere on H. Then $A \in \mathfrak{R}$ since $\mathfrak{R}$ is strongly closed. □

Exercise 6.13

(1) If H is a Hilbert space, let $\mathfrak{A} \subset \mathfrak{B}(\mathsf{H})$ be a unital *-algebra. Prove that the von Neumann algebra generated by $\mathfrak{A}$ satisfies

$$\mathfrak{A}'' = \overline{\mathfrak{A}}^{\text{strong}} = \overline{\mathfrak{A}}^{\text{weak}} ,$$

with the obvious closure symbols.

Solution Evidently $\overline{\mathfrak{A}}^{\text{strong}} \subset \overline{\mathfrak{A}}^{\text{weak}}$. Next observe that, as $\mathfrak{A}''$ is a von Neumann algebra, it is weakly closed due to Theorem 6.4. Since it contains $\mathfrak{A}$, we have $\mathfrak{A} \subset \overline{\mathfrak{A}}^{\text{strong}} \subset \overline{\mathfrak{A}}^{\text{weak}} \subset \mathfrak{A}''$. It is enough to prove that $\mathfrak{A}'' \subset \overline{\mathfrak{A}}^{\text{strong}}$ to conclude. This fact was established in the proof of Theorem 6.4 when we proved that $\mathfrak{A}$ is dense in $\mathfrak{A}''$ in the strong topology: $\overline{\mathfrak{A}}^{\text{strong}} \supset \mathfrak{A}''$. □.

(2) If $\mathfrak{M}$ is a von Neumann algebra on the Hilbert space H and $A : D(A) \to \mathsf{H}$ is a selfadjoint operator with $D(A) \subset \mathsf{H}$, prove that the following facts are equivalent.

(a) A is affiliated to $\mathfrak{M}$.
(b) $UA \subset AU$ for every unitary operator $U \in \mathfrak{M}'$.
(c) $UAU^{-1} = A$ for every unitary operator $U \in \mathfrak{M}'$.

Solution Assume (a) is valid and consider a sequence of simple functions $s_n \to \iota$ pointwise such that $|s_n| \leq |\iota|$. With these hypotheses, if $x \in D(A)$, then $\int_{\mathbb{R}} s_n dP^{(A)}x \to Ax$ (using Proposition 3.24 (d), dominated convergence and Theorem 3.40). On the other hand, since $UP_E^{(A)} = P_E^{(A)}U$ (because $U \in \mathfrak{M}'$ and $P_E^{(A)} \in \mathfrak{M}$), (b) immediately follows, because $\mu_{xx}^{(P^{(A)})}(E) = ||P_E^{(A)}x||^2 = ||UP_E^{(A)}x||^2 = ||P_E^{(A)}Ux||^2 = \mu_{Ux,Ux}^{(P^{(A)})}(E)$ since U is unitary, so that $U(D(A)) = U(\Delta_\iota) \subset \Delta_\iota = D(A)$. Next suppose that (b) is valid, so

$UA \subset AU$ for every unitary operator $U \in \mathfrak{M}$. As a consequence, $UAU^{-1} \subset A$ for every unitary operator $U \in \mathfrak{M}$. Since $U^{-1} = U^* \in \mathfrak{M}$ if $U \in \mathfrak{M}$, we also have $U^{-1}AU \subset A$, which implies $A \subset UAU^{-1}$. Putting all together $UAU^{-1} \subset A \subset UAU^{-1}$, hence (c) holds. To conclude we shall prove that (c) implies (a). From Proposition 3.49 we have that, under (c), $P^{(A)}$ commutes with all unitary operators in $\mathfrak{M}'$. As a consequence of Proposition 3.55, $B \in \mathfrak{M}'$ can be written as linear combination of unitary operators U. The latter are obtained as spectral functions of the selfadjoint operators $B + B^* \in \mathfrak{M}'$ and $i(B - B^*) \in \mathfrak{M}'$. So the operators U can be constructed as strong limits of linear combinations of elements in the PVMs of $B + B^*$ and $i(B - B^*)$. These PVM belong to $\mathfrak{M}'$ as we shall prove at the very end of the argument. Since $\mathfrak{M}'$ is a von Neumann algebra and hence strongly closed, we conclude that $U \in \mathfrak{M}'$. Summing up, $P^{(A)}$ commutes with every element of $\mathfrak{M}'$, since an element of $\mathfrak{M}'$ is a linear combination of unitary elements in $\mathfrak{M}'$ and $P^{(A)}$ commutes with these operators. We have found that $P^{(A)} \subset \mathfrak{M}'' = \mathfrak{M}$ as wanted. To finish we only need to demonstrate that, if $B^* = B \in \mathfrak{M}'$, then $P^{(B)} \subset \mathfrak{M}'$ as well. By Proposition 3.70 we can assert that $P^{(B)}$ commutes with all operators in $\mathfrak{B}(\mathsf{H})$ commuting with B. In other words, $P^{(B)} \subset (\mathfrak{M}')'' = \mathfrak{M}'$, as required. □

(3) Let $\mathfrak{A}, \mathfrak{B} \subset \mathfrak{B}(\mathsf{H})$ be *-closed and define $\mathfrak{A} \vee \mathfrak{B} := (\mathfrak{A} \cup \mathfrak{B})''$ and $\mathfrak{A} \wedge \mathfrak{B} := \mathfrak{A} \cap \mathfrak{B}$. Prove the following statements.

(a) $(\mathfrak{A} \vee \mathfrak{B})' = \mathfrak{A}' \wedge \mathfrak{B}'$,
(b) $(\mathfrak{A} \wedge \mathfrak{B})' \supset \mathfrak{A}' \vee \mathfrak{B}'$,
(c) $(\mathfrak{A} \wedge \mathfrak{B})' = \mathfrak{A}' \vee \mathfrak{B}'$ if, additionally, $\mathfrak{A}, \mathfrak{B}$ are von Neumann algebras.
(d) The family of von Neumann algebras $\mathfrak{R} \subset \mathfrak{B}(\mathsf{H})$, partially ordered by inclusion, defines a complete orthocomplemented lattice with $\mathbf{0} = \{cI\}_{c\in\mathbb{C}}$, $\mathbf{1} = \mathfrak{B}(\mathsf{H})$ and $\neg\mathfrak{R} = \mathfrak{R}'$.

Solution Direct inspection and $\mathfrak{M}''' = \mathfrak{M}'$ prove (a) and (b). (c) follows from (a) replacing $\mathfrak{A}$ with $\mathfrak{A}'$, $\mathfrak{B}$ with $\mathfrak{B}'$ and using $\mathfrak{A} = \mathfrak{A}''$, $\mathfrak{B} = \mathfrak{B}''$, $(\mathfrak{A}' \vee \mathfrak{B}')'' = \mathfrak{A}' \vee \mathfrak{B}'$. (d) follows from the definitions. □

6.1.3 Lattices of Orthogonal Projectors of von Neumann Algebras and Factors

To conclude this quick mathematical survey of von Neumann algebras, we should say a few words about the *lattices of orthogonal projectors* associated to them, since these play a pivotal role in the physical formalization. The related notion of *factor* will be introduced too.

Let $\mathfrak{R}$ be a von Neumann algebra on the Hilbert space H. The intersection $\mathfrak{R} \cap \mathscr{L}(\mathsf{H})$ inherits $\vee$, $\wedge$ and $\neg$ from $\mathscr{L}(\mathsf{H})$.

(1) We see from (4.3) that, if $P, Q \in \mathfrak{R} \cap \mathscr{L}(\mathsf{H})$ then $P \wedge Q \in \mathscr{L}(\mathsf{H})$ must also belong to $\mathfrak{R}$ since $\mathfrak{R}$ is strongly closed (it is a von Neumann algebra). Formula (4.3) just says that $P \wedge Q$ is the strong limit of the sequence of elements $(PQ)^n$ which, in turn, belong to $\mathfrak{R}$ since it is closed under products. Also notice that $\inf_{\mathscr{L}(\mathsf{H})}\{P, Q\} =: P \wedge Q \in \mathfrak{R}$, so that $\inf_{\mathfrak{R}\cap\mathscr{L}(\mathsf{H})}\{P, Q\}$ exists and satisfies $\inf_{\mathfrak{R}\cap\mathscr{L}(\mathsf{H})}\{P, Q\} = \inf_{\mathscr{L}(\mathsf{H})}\{P, Q\} = P \wedge Q$.
(2) Similarly, one proves that $P \vee Q \in \mathfrak{R}\cap\mathscr{L}(\mathsf{H})$ if $P, Q \in \mathfrak{R}\cap\mathscr{L}(\mathsf{H})$, concluding as before that $\sup_{\mathfrak{R}\cap\mathscr{L}(\mathsf{H})}\{P, Q\} = \sup_{\mathscr{L}(\mathsf{H})}\{P, Q\} = P \vee Q$. To this end use of (4.3) and Proposition 4.5, obtaining

$$P \vee Q = \neg((\neg P) \wedge (\neg Q)) = I - \left(\text{s-}\lim_{n\to+\infty}[(I - P)(I - Q)]^n\right) .$$

Since evidently $0, I \in \mathscr{L}(\mathsf{H}) \cap \mathfrak{R}$ and $\neg P := I - P \in \mathscr{L}(\mathsf{H}) \cap \mathfrak{R}$ for $P \in \mathscr{L}(\mathsf{H}) \cap \mathfrak{R}$, the conclusion is that $\mathfrak{R} \cap \mathscr{L}(\mathsf{H})$ contains the supremum of any P, Q in it, and this supremum coincides with $P \vee Q$, as wanted.
(3) As a byproduct we also have that $(\mathscr{L}(\mathsf{H}) \cap \mathfrak{R}, \geq, 0, I, \neg)$ is a bounded and orthocomplemented lattice, with structure induced by $\mathscr{L}(\mathsf{H})$.
(4) $\mathscr{L}(\mathsf{H}) \cap \mathfrak{R}$ is σ-complete because σ-completeness involves only the strong topology by Proposition 4.9 (iv), and $\mathfrak{R}$ is strongly closed by Theorem 6.4 (it is actually even possible to prove that $\mathscr{L}(\mathsf{H}) \cap \mathfrak{R}$ is *complete* [Red98, Mor18]).
(5) $\mathscr{L}(\mathsf{H}) \cap \mathfrak{R}$ is orthomodular and (if H is separable) also separable. The proofs are trivial since these properties descend from $\mathscr{L}(\mathsf{H})$.
(6) Subtler properties like irreducibility, atomicity, atomisticity and the covering law are not always guaranteed, and should be considered on a case-by-case basis.

Properties (1)–(5) above permit to restate most of the quantum interpretations that we developed in the previous chapters, by thinking the elements of $\mathscr{L}(\mathsf{H}) \cap \mathfrak{R}$ as elementary observables of a quantum system, as we will do later.

On the mathematical side, it is interesting to remark that $\mathscr{L}(\mathsf{H}) \cap \mathfrak{R}$ retains all the information about $\mathfrak{R}$, since the following result holds.

Proposition 6.14 *Let $\mathfrak{R}$ be a von Neumann algebra on the Hilbert space H and define the lattice $\mathscr{L}_{\mathfrak{R}}(\mathsf{H}) := \mathfrak{R} \cap \mathscr{L}(\mathsf{H})$. Then $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})'' = \mathfrak{R}$.*

Proof Since $\mathscr{L}_{\mathfrak{R}}(\mathsf{H}) \subset \mathfrak{R}$, we have $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})' \supset \mathfrak{R}'$ and $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})'' \subset \mathfrak{R}'' = \mathfrak{R}$. Let us prove the other inclusion. $A \in \mathfrak{R}$ can always be decomposed as linear combination of two selfadjoint operators of $\mathfrak{R}$, $A + A^*$ and $i(A - A^*)$. Since $\mathfrak{R}$ is a complex vector space, we can restrict to the case of $A^* = A \in \mathfrak{R}$, proving that $A \in \mathscr{L}_{\mathfrak{R}}(\mathsf{H})''$ if $A \in \mathfrak{R}$. The PVM of A belongs to $\mathfrak{R}$ because of Proposition 3.70 (ii) and (iv): $P^{(A)}$ commutes with every bounded selfadjoint operator B which commutes with A. By the same argument as above, writing a generic element of $\mathfrak{B}(\mathsf{H})$ as linear combination of selfadjoint operators, $P^{(A)}$ commutes with every $B \in \mathfrak{B}(\mathsf{H})$ commuting with A. So $P^{(A)}$ commutes, in particular, with the elements of $\mathfrak{R}'$ because $\mathfrak{R} \ni A$. We conclude that $P_E^{(A)} \in \mathfrak{R}'' = \mathfrak{R}$, namely $P^{(A)} \subset \mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ if $A \in \mathfrak{R}$. Finally, as we know, there exists a sequence of simple functions s_n converging to ι uniformly on a compact interval $[-a, a] \supset \sigma(A)$. By construction $\int_{\sigma(A)} s_n dP^{(A)} \in \mathscr{L}_{\mathfrak{R}}(\mathsf{H})''$ because it is a linear combination of elements of $P^{(A)}$ and $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})''$ is a linear space. Finally $\int_{\sigma(A)} s_n dP^{(A)} \to A$ uniformly as $n \to +\infty$, and hence strongly, as seen in Example 3.77 (2). Since $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})''$ is strongly closed, we must have $A \in \mathscr{L}_{\mathfrak{R}}(\mathsf{H})''$, proving that $\mathscr{L}_{\mathfrak{R}}(\mathsf{H}) \supset \mathfrak{R}$ as wanted. □

A natural question is whether $\mathfrak{R}$ is *-isomorphic to $\mathfrak{B}(\mathsf{H}_1)$ for some suitable Hilbert space H_1 (in general different from the original H!). If yes, it would automatically imply that also the remaining properties of $\mathscr{L}(\mathsf{H}_1)$ are true for $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$. In particular there would exist atomic elements in $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$, and the covering property and irreducibility would hold. A *necessary* (but by no means *sufficient*) condition for that to happen, exactly as for $\mathfrak{B}(\mathsf{H}_1)$, is that $\mathfrak{R} \cap \mathfrak{R}'$ be trivial, since $\mathfrak{B}(\mathsf{H}_1) \cap \mathfrak{B}(\mathsf{H}_1)' = \mathfrak{B}(\mathsf{H}_1)' = \{cI\}_{c \in \mathbb{C}}$.

Definition 6.15 A **factor** in $\mathfrak{B}(\mathsf{H})$ is a von Neumann algebra $\mathfrak{R} \subset \mathfrak{B}(\mathsf{H})$ with trivial centre[1]:

$$\mathfrak{R} \cap \mathfrak{R}' = \mathbb{C}I \,,$$

where we set $\mathbb{C}I := \{cI\}_{c \in \mathbb{C}}$ from now on. ■

Centres, commutants and factors enter both the mathematical and the physical theory in several crucial places. First of all, they are related to the irreducibility of the lattice underlying a von Neumann algebra.

Proposition 6.16 *A von Neumann algebra $\mathfrak{R}$ on the Hilbert space H is a factor if and only if the associated lattice $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ is irreducible.*

Proof First observe that if $P \in \mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ commutes with every $Q \in \mathscr{L}_{\mathfrak{R}}(\mathsf{H})$, then it commutes also with the selfadjoint operators constructed out of the PVMs in $\mathfrak{R}$—as they are strong limits of linear combinations of these PVMs (Proposition 6.14)—and more generally with every operator in $\mathfrak{R}$, by writing it as linear combinations of selfadjoint operators. So if $P \in \mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ commutes with every $Q \in \mathscr{L}_{\mathfrak{R}}(\mathsf{H})$, it belongs to the centre of $\mathfrak{R}$. If $\mathfrak{R}$ is a factor, the only orthogonal projectors in $\mathfrak{R} \cap \mathfrak{R}'$ are 0 and I (obvious) and $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ is irreducible. Suppose conversely that $\mathfrak{R}$ is not a factor, so there exists $A \neq cI$ in $\mathfrak{R} \cap \mathfrak{R}'$. Therefore at least one of $A + A^*$, $i(A - A^*)$ must be different from cI for any $c \in \mathbb{C}$. In other words there is a non-trivial selfadjoint operator $S \in \mathfrak{R}$ commuting with all operators in $\mathfrak{R}$. As we know from the proof of Proposition 6.14, its PVM belongs to $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ and it commutes with all operators commuting with S, and in particular with all elements of $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$.

[1] According to (3)(d) Exercise 6.13, this is equivalent to requiring $\mathfrak{R} \vee \mathfrak{R}' = \mathfrak{B}(\mathsf{H})$.

The PVMs of S cannot reduce to only 0 and I, otherwise S would be of the form cI. Hence $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ contains a non-trivial projector commuting with all projectors in $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$, whence it cannot be irreducible by definition. □

6.1.4 A Few Words on the Classification of Factors and von Neumann Algebras

It is possible to prove that, on separable Hilbert spaces, a von Neumann algebra is always a direct sum or a direct integral of factors, a clear indication that factors play a distinguished role. The classification of factors, started by von Neumann and Murray and based on the properties of the elements of $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$, is one of the key chapters in the theory of operator algebras, and has enormous consequences in the local algebraic formulation of the theory of quantum fields. It is actually valid also for non-separable Hilbert spaces. *Type-I* factors are defined by requiring that they contain minimal projectors (atoms). *It turns out that a factor* $\mathfrak{R}$*is of type I if and only if it is isomorphic to* $\mathfrak{B}(\mathsf{H}_1)$ *as a unital* **-algebra, for some Hilbert space* H_1 (see also Proposition 6.46). Consequently they are atomic, atomistic and fulfil the covering property. The separability of $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ is equivalent to the separability of H_1. There exists a finer classification of factors of *type* I_n where n is a cardinal number (finite or infinite): the dimension of H_1. There also exist factors of type II and III, which do not admit atoms in $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ and are not important in elementary QM. A *type-*III factor $\mathfrak{R}$ is by definition a factor such that, if $P \in \mathscr{L}_{\mathfrak{R}}(\mathsf{H}) \setminus \{0\}$, then $P = VV^*$ for some $V \in \mathfrak{R}$ with $V^*V = I$. A minute analysis of type III was produced by Connes using the *Tomita-Takesaki modular theory* (see [KaRi97, BrRo02, Tak10] and also [HaMü06] for a recent review). Type-III factors play a crucial role in the description of extended (quantum) thermodynamical systems and also in algebraic relativistic quantum field theory [Yng05]. Under standard hypotheses, every von Neumann algebra of observables localized in a sufficiently regular, open and bounded region of Minkowski spacetime is isomorphic to the unique *hyperfinite* factor of type III_1. Moreover, by virtue of the so-called *split property* (valid in particular for the free theory), that we shall discuss again later, every such factor is contained in a type-I factor which, in turn, is contained in another local algebra associated with a slightly larger spacetime region.

von Neumann algebras are analogously divided in different *types*, and in separable Hilbert spaces the classification is such that a von Neumann algebra of a given *type* is the direct sum or the direct integral of factors of the same *type*. Generic von Neumann algebras can be decomposed uniquely in direct sums of definite-type von Neumann algebras even if the Hilbert space is not separable. See [Mor18] for a brief account, [Red98] for an extended discussion with many technical details and historical remarks, and [KaRi97, BrRo02] for complete treatises on the subject. Several physical implications are discussed in [Haa96, Ara09] especially for QFT, and in [BrRo02] concerning statistical mechanics.

6.1.5 Schur's Lemma

Let us talk about an elementary yet crucial technical result and at the same time important mathematical tool, but after the following general definition. The *-closed set $\mathfrak{M}$ below may be a von Neumann algebra, or for instance the image $\{U_g\}_{g\in G}$ of a *unitary representation* of a group $G \ni g \mapsto U_g$ (Definition 7.9). One may as well take the unitary representatives of a *unitary-projective representation* (Definition 7.10) of a group, as we shall discuss later (phases should be rearranged in order to produce a *-closed set and apply Theorem 6.19). Finally, $\mathfrak{M}$ could even be the image of a *-representation of a *-algebra. This goes to show that the concepts below encompass a variety of situations.

Definition 6.17 Let $\mathsf{H} \neq \{0\}$ be a Hilbert space and $\mathfrak{M} \subset \mathfrak{B}(\mathsf{H})$ a collection of operators.

(a) A closed subspace $\mathsf{H}_0 \subset \mathsf{H}$ is said to be **invariant** under $\mathfrak{M}$ (or **$\mathfrak{M}$-invariant**), if $A(\mathsf{H}_0) \subset \mathsf{H}_0$ for every $A \in \mathfrak{M}$.
(b) $\mathfrak{M}$ is called **topologically irreducible** if the only $\mathfrak{M}$-invariant *closed* subspaces are $\mathsf{H}_0 = \{0\}$ and $\mathsf{H}_0 = \mathsf{H}$. ■

Remark 6.18 The word "topologically" refers to the invariant spaces being *closed*, and we shall henceforth omit it for the sake of brevity: *irreducible* will mean *topologically irreducible* from now on. ■

Let us state and prove the simplest, and classical, version of *Schur's lemma* on (complex) Hilbert spaces, using the language of von Neumann algebras.

Theorem 6.19 (Schur's Lemma) *Consider a Hilbert space $\mathsf{H} \neq \{0\}$ and suppose the set $\mathfrak{M} \subset \mathfrak{B}(\mathsf{H})$ is *-closed.*

The following facts are equivalent.

(a) *$\mathfrak{M}$ is irreducible.*
(b) *$\mathfrak{M}' = \mathbb{C}I$.*
(c) *$\mathfrak{M}'' = \mathfrak{B}(\mathsf{H})$.*

Proof Assume that (a) is valid and let us we prove (b). If $A \in \mathfrak{M}'$ (so $A^* \in \mathfrak{M}'$ as well), we can write it as $A = B + iB'$ where $B := \frac{1}{2}(A + A^*) \in \mathfrak{M}'$, $B' := \frac{1}{2i}(A - A^*) \in \mathfrak{M}'$ are selfadjoint. The spectral measures of B and B' commute with all operators commuting with B and B' respectively, by Proposition 3.70. In turn, these PVMs commute with all the operators commuting with A and A^*, so that the PVMs belong to $\mathfrak{M}'$ as well. Let P be an orthogonal projector of $P^{(B)}$ or $P^{(B')}$. Since $PC = CP$ for every $C \in \mathfrak{M}$, the closed subspace $\mathsf{H}_0 := P(\mathsf{H})$ satisfies $C(\mathsf{H}_0) \subset \mathsf{H}_0$ and thus, by (a), either $\mathsf{H}_0 = \{0\}$, namely $P = 0$, or $\mathsf{H}_0 = \mathsf{H}$, namely $P = I$. Integrating these PVMs, whose projectors are either 0 or I, we find $B = bI$ and $B' = b'I$ for some $b, b' \in \mathbb{R}$, so $A = cI$ for some $c \in \mathbb{C}$. This is (b). We next prove that (b) implies (c). If (b) is true, $\mathfrak{M}'' = \mathbb{C}I' = \mathfrak{B}(\mathsf{H})$, so (c) is true as well. To conclude, we show (c) implies (a). If H_0 is a closed subspace invariant under every operator in $\mathfrak{M}$, the orthogonal projector P onto H_0 commutes with every

$A \in \mathfrak{M}$. Indeed $A(\mathsf{H}_0) \subset \mathsf{H}_0$ implies $AP = PAP$. Taking adjoints, $PA^* = PA^*P$. Since $\mathfrak{M}$ is *-closed and $A = (A^*)^*$, we can rewrite that relation as $PA = PAP$. Comparing with $AP = PAP$, we have $AP = PA$. Hence $P \in \mathfrak{M}' = \mathfrak{M}'''$, which means $P \in \mathfrak{B}(\mathsf{H})'$ when assuming (c). In particular, P must commute with every $Q \in \mathscr{L}(\mathsf{H})$. Since $\mathscr{L}(\mathsf{H})$ is irreducible (Theorem 4.17), either $P = 0$, namely $\mathsf{H}_0 = \{0\}$, or $P = I$, namely $\mathsf{H}_0 = \mathsf{H}$. Hence (a) is valid and the proof ends. □

Corollary 6.20 *Let $\pi : G \to \mathfrak{B}(\mathsf{H})$ (respectively, $\pi : \mathfrak{A} \to \mathfrak{B}(\mathsf{H})$) be a unitary representation of the group G (of the unital *-algebra $\mathfrak{A}$) on the Hilbert space $\mathsf{H} \neq \{0\}$. If G (resp. $\mathfrak{A}$) is Abelian, the image of π is irreducible if and only if* $\dim(\mathsf{H}) = 1$.

Proof Assume the representation is irreducible. Then $\mathfrak{M} := \pi(G)$, respectively $\mathfrak{M} := \pi(\mathfrak{A})$, is *-closed and every $\pi(A)$ with $A \in G$ (resp. $A \in \mathfrak{A}$) is a complex number by Schur's Lemma, since $\pi(A)$ commutes with $\mathfrak{M}$. Take $\psi \in \mathsf{H}$ with $||\psi|| = 1$, then the closure of the set of finite combinations of the $\pi(a)\psi$ is a closed $\mathfrak{M}$-invariant subspace, so it must coincide with H if the image of π is irreducible. In other words $\{\psi\}$ is a Hilbert basis of H, so $\dim(\mathsf{H}) = 1$. The converse implication is obvious. □

6.1.6 The von Neumann Algebra Associated to a PVM

The last mathematical feature of von Neumann algebras we discuss concerns the interplay with PVMs. We have the following important technical result.

Proposition 6.21 *Let $P : \Sigma(X) \to \mathscr{L}(\mathsf{H})$ be a PVM on the measurable space $(X, \Sigma(X))$ taking values in the lattice of orthogonal projectors on the Hilbert space H. If H is separable, then*

$$\{P_E \mid E \in \Sigma(X)\}'' = \left\{ \int_X f\, dP \;\middle|\; f \in M_b(X) \right\} .$$

If H is not separable, the above statement holds if $\supset$ replaces $=$.

Proof First of all, observe that the von Neumann algebra generated by the *-closed set $\{P_E | E \in \Sigma(X)\}$ coincides with the von Neumann algebra generated by the unital *-algebra $\mathfrak{A}_P$ of finite combinations of $\{P_E | E \in \Sigma(X)\}$. According to Exercise 6.13 (1), $\{P_E \mid E \in \Sigma(X)\}''$ is therefore nothing but the strong closure of $\mathfrak{A}_P$. Since $\int_X f\, dP \in \mathfrak{B}(\mathsf{H})$ if $f \in M_b(X)$, the integral can be computed as strong limit of elements in $\mathfrak{A}_P$, according to Proposition 3.29 (c), by approximating f with a bounded sequence of simple functions converging to f pointwise. Summing up, we necessarily have $\left\{ \int_X f\, dP \;\middle|\; f \in M_b(X) \right\} \subset \{P_E \mid E \in \Sigma(X)\}'' = \mathfrak{A}_P''$. Now we have to establish the converse inclusion. More precisely, we have to prove that if $\int_X s_n\, dP\psi \to A\psi$ as $n \to +\infty$ for every $\psi \in \mathsf{H}$, some $A \in \mathsf{H}$, and for a given sequence of simple functions $s_n \in M_b(X)$, then $A = \int_X f\, dP$ for some $f \in M_b(X)$. A lemma is useful to this end. □

Lemma 6.22 *Let $P : \Sigma(X) \to \mathscr{L}(\mathsf{H})$ be a PVM on the measurable space $(X, \Sigma(X))$ taking values in the lattice of orthogonal projectors on the Hilbert space H. There exist*

(i) a set of orthonormal vectors $\{\psi_n\}_{n\in N}$ with N of any cardinality and, in particular, finite or countable when H is separable;
(ii) a corresponding set $\{\mathsf{H}_n\}_{n\in N}$ of mutually orthogonal closed subspaces of H, such that $\mathsf{H} = \bigoplus_{n\in N} \mathsf{H}_n$ (Hilbert sum), and $P_E(\mathsf{H}_n) \subset \mathsf{H}_n$ for every $n \in N$ and every $E \in \Sigma(X)$;
(iii) a corresponding set of isometric surjective operators $U_n : \mathsf{H}_n \to L^2(X, \mu^{(P)}_{\psi_n\psi_n})$.

Proof Take a unit vector $\psi_1 \in \mathsf{H}$ and consider the map $V_1 : L^2(X, \mu^{(P)}_{\psi_1\psi_1}) \to \mathsf{H}$ defined as $V_1 f := \int_X f dP\psi_1$ for $f \in L^2(X, \mu^{(P)}_{\psi_1\psi_1})$. According to Proposition 3.33 (a) and (b), this map is linear and isometric (hence injective) by Theorem 3.24 (d). Therefore it also preserves the inner product as a consequence of the polarization formula. Its image is evidently the subspace $\mathsf{H}_1 := \{\int_X f dP\psi_1 | f \in L^2(X, \mu^{(P)}_{\psi_1\psi_1})\} \subset \mathsf{H}$. This subspace is closed. Indeed, if $H_1 \ni V(f_n) \to \phi \in \mathsf{H}$ as $n \to +\infty$, the sequence of the f_n must be Cauchy because $\{V_1(f_n)\}_{n\in\mathbb{N}}$ converges and V_1 is isometric. Therefore f_n converges to some $f \in L^2(X, \mu^{(P)}_{\psi_1\psi_1})$, because $L^2(X, \mu^{(P)}_{\psi_1\psi_1})$ is complete. Since V_1 is continuous being isometric, $V_1(f) = \phi$ and then $\phi \in H_1$, so H_1 is closed. The map $U_1 := V_1^{-1}$ (restricting the codomain of V_1 to its image) is exactly the map we argued existed in (ii), for $n = 1$. Finally observe that $P_E(\mathsf{H}_1) \subset \mathsf{H}_1$ by Propositions 3.29 (b) and 3.33 (c): $P_E \int_X f dP\psi_1 = \int_X f\chi_E dP\psi_1 \in \mathsf{H}_1$ noticing that, obviously, $f\chi_E \in L^2(X, \mu^{(P)}_{\psi_1\psi_1})$ if $f \in L^2(X, \mu^{(P)}_{\psi_1\psi_1})$. If $\mathsf{H}_1 \subsetneq \mathsf{H}$ we can fix $\psi_2 \in \mathsf{H}_1^\perp$ with $||\psi_2|| = 1$ and repeat the procedure, finding a corresponding isometric surjective map $U_2 : \mathsf{H}_2 \to L^2(X, \mu^{(P)}_{\psi_2\psi_2})$, with $\mathsf{H}_2 \subset \mathsf{H}$ a closed subspace satisfying $\mathsf{H}_2 \perp \mathsf{H}_1$ and $P_E(\mathsf{H}_2) \subset \mathsf{H}_2$ for every $E \in \Sigma(X)$. Then we iterate, taking $\psi_3 \in (\mathsf{H}_1 \cup \mathsf{H}_2)^\perp$ and so forth. A standard application of Zorn's lemma proves the thesis. In case H is separable, N must be finite or countable, because the number of orthonormal vectors $\{\psi_n\}_{n\in N}$ cannot exceed the cardinality of a Hilbert basis, since $\{\psi_n\}_{n\in N}$ is (or can be completed to) a Hilbert basis. □

Let us go back to the main proof. We may assume $N = \mathbb{N}$ since H is separable by hypothesis, and the case N finite is a trivial subcase. So, suppose that $\int_X s_k dP\psi \to A\psi$ as $k \to +\infty$ for every $\psi \in \mathsf{H}$, some $A \in \mathsf{H}$, and for a given sequence of simple functions $s_k \in M_b(X)$. Consequently $\{\int_X s_k dP\psi\}_{k\in\mathbb{N}}$ is Cauchy in H, so $\{s_k\}_{k\in\mathbb{N}}$ is Cauchy in $L^2(X, d\mu^{(P)}_{\psi\psi})$ because of Theorem 3.24 (d). In particular, the above must be true for $\psi = \sum_{n\in\mathbb{N}} \frac{1}{\sqrt{2^n}}\psi_n$, which belongs to H as the series converges

($\sum_{n\in\mathbb{N}} \frac{1}{2^n} = 2$ and the orthonormal vectors ψ_n form or can be completed to a Hilbert basis of H). From part (ii) of the Lemma $P_E(\mathsf{H}_n) \subset \mathsf{H}_n$, whence

$$0 \le \mu^{(P)}_{\psi\psi}(F) = \left\langle \sum_{n\in\mathbb{N}} \frac{1}{\sqrt{2^n}}\psi_n \,\middle|\, P_F \sum_{m\in\mathbb{N}} \frac{1}{\sqrt{2^m}}\psi_n \right\rangle = \sum_{n\in\mathbb{N}} \frac{1}{2^n}\langle\psi_n|P_F\psi_n\rangle$$
$$= \sum_{n\in\mathbb{N}} \frac{1}{2^n}\mu^{(P)}_{\psi_n\psi_n}(F) \le 2\,,$$

where we have used $\mu^{(P)}_{\psi_n\psi_n}(X) = ||\psi_n||^2 = 1$. Since $\{s_k\}_{k\in\mathbb{N}}$ is Cauchy in $L^2(X, d\mu^{(P)}_{\psi\psi})$, there exists a function $f \in L^2(X, d\mu^{(P)}_{\psi\psi})$ such that $s_k \to f$ as $k \to +\infty$ in $L^2(X, d\mu^{(P)}_{\psi\psi})$. Furthermore [Rud86], there is a subsequence, which we indicate with the same symbol $\{s_k\}_{k\in\mathbb{N}}$ for the sake of simplicity, that converges $\mu^{(P)}_{\psi\psi}$to f a.e. Since $\mu^{(P)}_{\psi_n\psi_n}(F) \le 2^n\mu^{(P)}_{\psi\psi}(F)$, the sequence s_k converges to f simultaneously in L^2 sense and a.e. for each of the measures $\mu^{(P)}_{\psi_n\psi_n}$. In particular $f \in L^2(X, d\mu^{(P)}_{\psi_n\psi_n})$. Now it is only natural to compare A and $\int_X f dP$, since both are limits of the $\int_X s_n dP$. Let us focus on one space H_n as from the Lemma above. Since $M_b(X)$ is dense in $L^2(X, d\mu^{(P)}_{\psi_n\psi_n})$, we conclude that $M_n := U_n^{-1}(M_b(X))$ is dense in H_n. However $M_n \subset D(\int_X f dP)$ because $D(\int_X f dP) = \{\phi \in \mathsf{H} \mid \int_X |f|^2 d\mu^{(P)}_{\phi\phi} < +\infty\}$. Indeed, if $\phi = \int_X g dP\psi_n$ for $g \in M_b(X)$, we have $\mu^{(P)}_{\phi\phi}(F) = \langle\int_X g dP\psi_n|P_F \int_X g dP\psi_n\rangle = \int_F |g|^2 d\mu^{(P)}_{\psi_n\psi_n}$. Then $\int_X |f|^2 d\mu^{(P)}_{\phi\phi} = \int_X |f|^2|g|^2 d\mu^{(P)}_{\psi_n\psi_n} \le ||g||_\infty \int_X |f|^2 d\mu^{(P)}_{\psi_n\psi_n} < +\infty$ and hence $\phi \in D(\int_X f dP)$, as said. This is not the end of the story, since we also have $\int_X f dP\phi = A\phi$ for $\phi \in M_n$. In fact we have $\int_X s_k dP\phi \to \int_X f dP\phi$ because (Theorem 3.24 (d))

$$\left|\left|\int_X (s_k - f)dP\phi\right|\right|^2 = \int_X |s_k - f|^2 d\mu^{(P)}_{\phi\phi} = \int_X |s_k - f|^2|g|^2 d\mu^{(P)}_{\psi_n\psi_n}$$
$$\le ||g||^2_\infty \int_X |s_k - f|^2 d\mu^{(P)}_{\psi_n\psi_n} \to 0$$

as $k \to +\infty$, and also $\int_X s_k dP\phi \to A\phi$ by hypothesis. Consider the formula just established: $\int_X f dP\phi = A\phi\,,\quad \forall\phi \in M_n$. As M_n is dense in H_n, the operator $\int_X f dP$ is closed (Theorem 3.24 (b)) and A is continuous, it follows that the formula is valid for every $\phi \in \mathsf{H}_n$. In particular, $\mathsf{H}_n \subset D(\int_X f dP)$. By linearity, the formula is true also when ϕ is a finite combination of elements in $\bigoplus_{n\in\mathbb{N}} \mathsf{H}_n$. Since these combinations are dense in H, the same argument used above proves that $\int_X f dP\phi = A\phi\,,\quad \forall\phi \in \mathsf{H}$. In particular $\int_X f dP = A \in \mathfrak{B}(\mathsf{H})$, making f P-essentially bounded (Proposition 3.29 (a)). By definition of $||\ ||^{(P)}_\infty$, we can modify

f on a set of P-zero measure, obtaining a function $f_1 \in M_b(X)$ producing the same integral $\int_X f_1 dP = \int_X f dP = A$. To sum up, every $A \in \{P_E \mid E \in \Sigma(X)\}''$ can be written as $A = \int_X f_1 dP$ for some $f_1 \in M_b(X)$, eventually ending the proof. □

6.2 von Neumann Algebras of Observables

Let us switch to physics and apply the previous notions and results to the formulation of quantum physics in Hilbert spaces.

6.2.1 The von Neumann Algebra of a Quantum System

If one relaxes the hypothesis that all selfadjoint operators on the Hilbert space H associated to a quantum system represent observables, there are many reasons to assume that observables are represented (in the sense we are going to illustrate) by the selfadjoint elements of a von Neumann algebra, called the **von Neumann algebra of observables** and hereafter indicated by $\mathfrak{R}$ (though only the selfadjoint elements are observables). In a sense (cf. Proposition 6.14) $\mathfrak{R}$ is the maximal set of operators we can manufacture out of the lattice of elementary propositions viewed as orthogonal projectors (which is smaller than $\mathscr{L}(\mathsf{H})$). The construction involves the algebra operations, adjoints and the strong operator topology (the most relevant one in spectral theory): all are necessary for motivating physically the relationship between PVM (elementary observables) and selfadjoint operators (observables).

A few important physical comments are in order.

(1) Including non-selfadjoint elements $B \in \mathfrak{R}$ is harmless, as they can be decomposed uniquely as sums of selfadjoint elements

$$B = B_1 + iB_2 = \frac{1}{2}(B + B^*) + i\frac{1}{2i}(B - B^*) .$$

These elements are mere complex linear combinations of bounded observables.

(2) Requiring that all the elements of $\mathfrak{R}$ are bounded, and thus ruling out unbounded observables, does not seem to be problem in physics. If $A = A^*$ is unbounded, the associated *collection* of bounded selfadjoint operators $\{A_n\}_{n\in\mathbb{N}}$, where

$$A_n := \int_{[-n,n]\cap\sigma(A)} \lambda dP^{(A)}(\lambda) ,$$

retains the same information as A. The operator A_n is bounded due to Proposition 3.47 because the support of its spectral measures is contained in $[-n, n]$. Physically speaking, we can say that A_n is nothing but the observable A when it is measured by an instrument unable to produce outcomes larger than $[-n, n]$. All real measuring devices are similarly limited. We can safely assume that every A_n belongs to $\mathfrak{R}$. Mathematically speaking, the (unbounded) observable A is recovered as a strong limit on $D(A)$:

$$Ax = \lim_{n\to+\infty} A_n x \quad \text{if } x \in D(A),$$

as we saw in Proposition 6.12. Finally, the spectral measure of A belongs to $\mathfrak{R}$ (A is affiliated to $\mathfrak{R}$) by Exercise 6.13 (2) and the limit above.

(3) In a sense, a more precise physical picture would arise by restricting to the only real vector space of bounded selfadjoint operators of $\mathfrak{R}$, equipped with the natural **Jordan product**

$$A \circ B = \frac{1}{2}(AB + BA)$$

(where A and B are bounded selfadjoint operators). The mathematical structure thus defined, disregarding topological features, is called a **Jordan algebra**. Though physically appealing, it features a number of mathematical complications in comparison to a *-algebra. In particular, *the Jordan product is not associative*. In [Emc72] Jordan algebras are intensively used to describe physical systems (see [Mor18] for further comments).

We stress again that, within the framework of von Neumann algebras of observables, the orthogonal projectors $P \in \mathfrak{R}$ represent all the elementary observables of the system. The lattice of these projectors, $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$, retains the amount of information about observables established by Proposition 6.14. As explained above, $\mathscr{L}_{\mathfrak{R}}(\mathsf{H}) \subset \mathfrak{R}$ is bounded, orthocomplemented, σ-complete, orthomodular and separable exactly like the larger $\mathscr{L}(\mathsf{H})$ (assuming H separable). That said, though, there is no guarantee the other properties listed in Theorem 4.17 will hold.

6.2.2 Complete Sets of Compatible Observables and Preparation of Vector States

A technically important result concerning both the spectral theory and von Neumann algebras is the following one.

Proposition 6.23 *Let $\mathfrak{A} = \{A_1, \ldots, A_n\}$ be a finite collection of selfadjoint operators on the separable Hilbert space H whose spectral measures commute in pairs. The von Neumann algebra $\mathfrak{A}''$ generated by $\mathfrak{A}$ satisfies*

$$\mathfrak{A}'' = \left\{ f(A_1, \ldots, A_n) \mid f \in M_b(\mathbb{R}^n) \right\} \quad \textit{with} \quad f(A_1, \ldots, A_n) := \int_{\mathbb{R}^n} f(x_1, \ldots, x_n) dP^{(\mathfrak{A})},$$

where $P^{(\mathfrak{A})}$ is the joint spectral measure (Theorem 3.56) of $\mathfrak{A} = \{A_1, \ldots, A_n\}$.

Proof The claim immediately follows from Proposition 6.21 by taking $P = P^{(\mathfrak{A})}$. Observe that if the A_k belong to $\mathfrak{B}(\mathsf{H})$, then the von Neumann algebra they generate is the same as the algebra generated by their spectral measures (see Remark 6.11 (a)). □

The aforementioned result authorizes us to introduce *maximal sets of compatible observables*, a common object in quantum systems.

Definition 6.24 Let $\mathfrak{R}$ be a von Neumann algebra of observables on the Hilbert space H and $\mathfrak{A} = \{A_1, \dots, A_n\}$ a finite set of pairwise compatible observables—that is, typically unbounded selfadjoint operators affiliated to $\mathfrak{R}$ whose PVMs commute. We call $\mathfrak{A}$ a **complete set of compatible (or commuting) observables** if every selfadjoint operator $B \in \mathfrak{B}(\mathsf{H})$ commuting with all the PVMs of $\mathfrak{A}$ is a *function* (in accordance with to Theorem 3.56) of them:

$$B = f(A_1, \dots, A_n) := \int_{\mathbb{R}^n} f(x_1, \dots, x_n) dP^{(\mathfrak{A})} ,$$

for some (real-valued) function $f \in M_b(\mathbb{R}^n)$. ■

Remark 6.25

(a) Completing the proof of Proposition 5.13, one easily proves that, if $\dim \mathsf{H} = n < \infty$, there always exist many complete sets of compatible observables of cardinality n. By Zorn's lemma, take a maximal set of pairwise commuting observables S. It is easy to prove that S is a real unital subalgebra of $\mathfrak{B}(\mathsf{H})$. Hence the proof of Proposition 5.13 provides a linear basis of S made of $m \leq n$ orthogonal projectors $\{P_k\}_{k=1,\dots,m}$ such that $P_k P_h = 0$ when $k \neq h$ and $\sum_{k=1}^m P_k = I$. If $x \in P_k(\mathsf{H})$ and $||x|| = 1$, the orthogonal projector p_x onto span(x) satisfies $p_x P_h = P_h p_x$ for $h = 1, \dots, m$. Therefore $p_x \in S'$. Since S is maximal, we have $p_x \in S$ and hence S is linearly generated by the projectors $P_1, \dots, P_m$. However, as $p_x P_k = p_x$ and $p_x P_h = 0$ if $h \neq k$, we conclude that $p_x = P_k$. Since every P_k projects onto a one-dimensional subspace and $\sum_{k=1}^m P_k = I$, necessarily$m = n$. By construction, every A commuting with all P_k belongs to their linear span, and is therefore a (linear) function of them. In other words, $\{P_k\}_{k=1,\dots,n}$ is a complete set of commuting observables.

(b) A complete set of compatible observables $\mathfrak{A}$ satisfies $\mathfrak{A}' \subset \mathfrak{A}''$ due to Proposition 6.23. The converse inclusion $\mathfrak{A}'' \subset \mathfrak{A}'$ is instead automatic since the PVM $P^{(\mathfrak{A})}$ commutes with every single PVM $P^{(A_k)}$ as the latter is part of $P^{(\mathfrak{A})}$ itself (e.g., $P^{(A_1)}_E = P^{(\mathfrak{A})}_{E\times\mathbb{R}\times\cdots\times\mathbb{R}}$). Hence $\mathfrak{A}' = \mathfrak{A}''$. In particular, a bounded selfadjoint operator B commuting with the PVMs of $\mathfrak{A}$ must belong to $\mathfrak{A}' = \mathfrak{A}'' \subset \mathfrak{R}'' = \mathfrak{R}$, and therefore B is an observable as well. ■

An important physical consequence of the previous notion is related to Remark 6.25 (a), and it is valid in the infinite-dimensional case as well. Suppose that the observables A_k, $k = 1, \dots, n$ forming a complete set of compatible observables have *pure point spectrum* (Definition 3.44). It easy to check that the spectral measure on $\mathbb{R}^n$ defined by

$$P_E := \text{s-}\sum_{(a_1,\ldots,a_n)\in E\cap\times_{k=1}^n \sigma_p(A_k)} P^{(A_1)}_{\{a_1\}}\cdots P^{(A_n)}_{\{a_n\}}\,, \quad E \in \mathscr{B}(\mathbb{R}^n) \tag{6.6}$$

satisfies the condition in Theorem 3.56 for the joint measure of $\mathfrak{A} = \{A_1, \ldots, A_n\}$, and therefore it is that joint measure. Let $\mathsf{H}_{\alpha_1,\ldots,\alpha_n}$ be a common eigenspace of the eigenvalues $\alpha_k \in \sigma(A_k)$. We argue that $\dim(\mathsf{H}_{\alpha_1,\ldots,\alpha_n}) = 1$. Indeed, if $\mathsf{H}_{\alpha_1,\ldots,\alpha_n}$ contained a pair of non-vanishing orthogonal vectors x_1, x_2, the orthogonal projector $P := \langle x_1|\ \ \rangle x_1$ would commute with every $P^{(A_k)}$ because $PP^{(A_k)}_{\{\alpha_k\}} = P^{(A_k)}_{\{\alpha_k\}}P = P$ and $PP^{(A_k)}_{\{a_k\}} = 0$ for $a_k \neq \alpha_k$. By Definition 6.24 the selfadjoint operator $P \in \mathfrak{B}(\mathsf{H})$ should be a function of $A_1, \ldots, A_n$. Yet it *cannot* be, because by (6.6) a function of $A_1, \ldots, A_n$ has the form

$$f(A_1, \ldots, A_n) = \text{s-}\sum_{a_1\in\sigma_1(A_1),\ldots,a_n\in\sigma_1(A_n)} f(a_1, \ldots, a_n) P^{(A_1)}_{\{a_1\}}\cdots P^{(A_n)}_{\{a_n\}}\,.$$

Therefore $f(A_1, \ldots, A_n)x = f(\alpha_1, \ldots, \alpha_n)x$ for *every* $x \in \mathsf{H}_{\alpha_1,\ldots,\alpha_n} = P^{(A_1)}_{\{\alpha_1\}}\cdots P^{(A_n)}_{\{\alpha_n\}}(\mathsf{H})$ and in particular $f(A_1, \ldots, A_n)x_1 = f(A_1, \ldots, A_n)x_2$. Conversely $Px_1 = x_1$ and $Px_2 = 0$, in spite of $x_j \in \mathsf{H}_{\alpha_1,\ldots,\alpha_n}$. We conclude that every common eigenspace $\mathsf{H}_{\alpha_1,\ldots,\alpha_n}$ must be one-dimensional.

The above argument has an important practical consequence when "preparing quantum states", because a quantum state can be prepared just by measuring $A_1, \ldots, A_n$. *After a simultaneous measurement of* $A_1, \ldots, A_n$*, the post-measurement state is necessarily represented by a unique unit vector (up to phase) contained in the one-dimensional space* $\mathsf{H}_{\alpha_1,\ldots,\alpha_n}$*, where* $\alpha_1, \ldots, \alpha_n$ *are the outcomes of the measurements*. In fact, if $T \in \mathscr{S}(\mathsf{H})$ is the *unknown* initial state, according to the Lüders-von Neumann postulate after we measure α_1 for A_1, α_2 for A_2, etc., the outcome state is always

$$T' = \frac{P^{(A_1)}_{\{\alpha_1\}}\cdots P^{(A_n)}_{\{\alpha_n\}} T P^{(A_1)}_{\{\alpha_1\}}\cdots P^{(A_n)}_{\{\alpha_n\}}}{tr\left(P^{(A_1)}_{\{\alpha_1\}}\cdots P^{(A_n)}_{\{\alpha_n\}} T\right)} = \langle \psi_{\alpha_1,\ldots,\alpha_n}| \qquad \rangle \psi_{\alpha_1,\ldots,\alpha_n}$$

where, up to phase, $\psi_{\alpha_1,\ldots,\alpha_n} \in \mathsf{H}_{\alpha_1,\ldots,\alpha_n}$ is the only unit vector.

Another physically relevant consequence is explained in the following proposition and the remark below it.

Proposition 6.26 *If a quantum physical system admits a complete set of compatible observables* $\mathfrak{A}$*, the commutant* $\mathfrak{R}'$ *of the von Neumann algebra of observables* $\mathfrak{R}$ *is Abelian, because it coincides with the centre of* $\mathfrak{R}$.

Proof As the spectral measure of each $A \in \mathfrak{A}$ belongs to $\mathfrak{R}$, necessarily (i) $\mathfrak{A}'' \subset \mathfrak{R}$. Since $\mathfrak{A}' = \mathfrak{A}''$, (i) yields $\mathfrak{A}' \subset \mathfrak{R}$ and so, taking the commutant, (ii) $\mathfrak{A}'' \supset \mathfrak{R}'$. Comparing (i) and (ii) we have $\mathfrak{R}' \subset \mathfrak{R}$. In other words $\mathfrak{R}' = \mathfrak{R}' \cap \mathfrak{R}$. In particular,

$\mathfrak{R}'$ must be Abelian because every element of $\mathfrak{R}'$ must commute with all elements of $\mathfrak{R}'$ itself since $\mathfrak{R}' \subset \mathfrak{R}$. □

Remark 6.27

(a) Observe that $\mathfrak{R}'$ is Abelian if and only if it coincides with the centre. One implication was proved above, the other is similarly obvious: if $\mathfrak{R}'$ is Abelian, then $\mathfrak{R}' \subset \mathfrak{R}'' = \mathfrak{R}$, so $\mathfrak{R}' = \mathfrak{R} \cap \mathfrak{R}'$ once more.
(b) As soon as $\mathfrak{R}'$ is *not* Abelian, as for the so-called *non-Abelian gauge theories*, there exist no complete sets of compatible observables and it is impossible to prepare vector states by measuring a complete set of compatible observables with pure point spectra, simply because they do not exist. ■

Example 6.28

(1) In $L^2(\mathbb{R}, dx)$, the Hamiltonian operator H of the harmonic oscillator alone is a complete set of commuting observables with pure point spectrum. The proof is easy following Example 3.43 (3):

$$H = \text{s-}\sum_{n\in\mathbb{N}} \hbar\omega \left(n + \frac{1}{2}\right) P_n$$

where we have defined the one-dimensional orthogonal projectors $P_n := \langle\psi_n|\ \rangle\psi_n$. If $B^* = B \in \mathfrak{B}(\mathsf{H})$ commutes with H, according to Proposition 3.70 it commutes with the spectral measure of H. Since $x = \sum_{n\in\mathbb{N}} P_n x$ for every $x \in \mathsf{H}$ and $P_n P_m = 0$ if $n \neq m$,

$$B\psi = \sum_{n\in\mathbb{N}} P_n B\psi = \sum_{n\in\mathbb{N}} P_n P_n B\psi = \sum_{n\in\mathbb{N}} P_n B P_n \psi\ .$$

But P_n projects onto a one-dimensional subspace, so the selfadjoint operator $P_n B P_n$ takes necessarily the form $b_n P_n$ for some $b_n \in \mathbb{R}$. We have so far obtained

$$B = \text{s-}\sum_{n\in\mathbb{N}} b_n P_n\ ,$$

which means that $B = f(H)$ if we set $f : \sigma(H) \to \mathbb{R}$, $f(\hbar\omega(n+1/2)) := b_n$. Note f must be bounded, for otherwise B would be unbounded against our hypothesis, since

$$\left|\left|\text{s-}\sum_{n\in\mathbb{N}} b_n P_n\right|\right| = \sup_{n\in\mathbb{N}} |b_n|\ .$$

(2) Consider a quantum particle without spin and refer to the rest space $\mathbb{R}^3$ of an inertial reference frame, so $\mathsf{H} = L^2(\mathbb{R}^3, d^3x)$. The three *position operators*

$\mathfrak{A}_1 = \{X_1, X_2, X_3\}$ form a complete set of compatible observables, as do the *momentum operators* $\mathfrak{A}_2 = \{P_1, P_2, P_3\}$, since the two are related by the unitary Fourier-Plancherel transform (Example 2.59 (2)). The fact that $\{X_1, X_2, X_3\}$ is a complete set of compatible observables can be proved as follows. If $A \in \mathfrak{B}(\mathsf{H})$ commutes with the joint spectral measure $P^{(\mathfrak{A}_1)}$ of X_1, X_2, X_3, it turns out that $A(\chi_E) = f_E$ for every bounded set $E \in \mathscr{B}(\mathbb{R}^3)$, where $f_E \in L^2(\mathbb{R}^3, d^3x)$ vanishes a.e. outside E. (This is because $P_E^{(\mathfrak{A}_1)}$ is the multiplication by χ_E, but $\chi_E \in P_E^{(\mathfrak{A}_1)}(L^2(\mathbb{R}^3, d^3x))$, so $A(\chi_E)$ must belong to the same subspace $P_E^{(\mathfrak{A}_1)}(L^2(\mathbb{R}^3, d^3x))$ since A commutes with $P_E^{(\mathfrak{A}_1)}$. Hence $A(\chi_E)$ is a function f_E that vanishes a.e. outside E.) Using the linearity of A, if $F \cap E \neq \varnothing$ then $f_F\restriction_{E\cap F}= f_E\restriction_{E\cap F}$ a.e.. In this way, a unique measurable function $f^{(A)}$ gets defined on the entire $\mathbb{R}^3$ by a partition made of bounded Borel sets such that $A(\chi_E) = f^{(A)} \cdot \chi_E$. Finally, using a sequence of simple functions suitably converging to $\psi \in L^2(\mathbb{R}^3, d^3x)$, and taking the continuity of A into account, we obtain $A\psi = f^{(A)} \cdot \psi$ a.e.. Since A is bounded, $f^{(A)}$ is $P^{(\mathfrak{A}_1)}$-essentially bounded, so it can be rendered bounded by redefining it on a zero-measure set. Saying $A\psi = f^{(A)} \cdot \psi$ for every $\psi \in L^2(\mathbb{R}^3, d^3x)$ is the same as stating $A = f^{(A)}(X_1, X_2, X_3)$.

(3) Referring to a quantum particle without spin, the full algebra of observables $\mathfrak{R}$ must contain $\mathfrak{A}_1 \cup \mathfrak{A}_2$, where $\mathfrak{A}_1 = \{X_1, X_2, X_3\}$ and $\mathfrak{A}_2 = \{P_1, P_2, P_3\}$ as before. It is possible to prove that the commutant of $(\mathfrak{A}_1 \cup \mathfrak{A}_2)'' = (\mathfrak{A}_1 \cup \mathfrak{A}_2)'$ is trivial $(\mathfrak{A}_1 \cup \mathfrak{A}_2)' = \mathbb{C}I$ (it contains a unitary irreducible representation of the Weyl-Heisenberg group). Therefore $\mathfrak{R} = \mathfrak{R}'' \supset \mathbb{C}I''' = \mathbb{C}I' = \mathfrak{B}(L^2(\mathbb{R}^3, d^3x)$, and $\mathfrak{R} = \mathfrak{B}(\mathsf{H})$ for a spinless, non-relativistic particle. As a consequence $\mathscr{L}_{\mathfrak{R}}(\mathsf{H}) = \mathscr{L}(L^2(\mathbb{R}^3, d^3x))$.

(4) If we incorporate the spin space (for instance when we study an electron "without charge"), $\mathsf{H} = L^2(\mathbb{R}^3, d^3x) \otimes \mathbb{C}^2$. Referring to (1.11), examples of complete sets of compatible observables are $\mathfrak{A}_1 = \{X_1 \otimes I, X_2 \otimes I, X_3 \otimes I, I \otimes S_z\}$ or $\mathfrak{A}_2 = \{P_1 \otimes I, P_2 \otimes I, P_3 \otimes I, I \otimes S_x\}$. As before $(\mathfrak{A}_1 \cup \mathfrak{A}_2)''$ is the von Neumann algebra of observables of the system (changing the component of the spin in passing from $\mathfrak{A}_1$ to $\mathfrak{A}_2$ is crucial for this result). In this case too, it turns out that the commutant of the von Neumann algebra of observables is trivial, yielding $\mathfrak{R} = \mathfrak{B}(\mathsf{H})$.

(5) It is possible to construct complete set of commuting observables with pure point spectra also in $L^2(\mathbb{R}^3, d^3x) \otimes \mathbb{C}^{2s+1}$ or in closed subspaces of it. A typical example for an electron ($s = 1/2$) is the quadruple made by the Hamiltonian operator of the hydrogen atom H, the total angular momentum squared L^2, the component L_z of the angular momentum, and the component S_z of the spin. If we restrict to the closed subspace defined by non-positive energy, the quadruple is a complete set of commuting observables with pure point spectra. ■

6.3 Superselection Rules and Other Structures of the Algebra of Observables

We have accumulated enough material to examine profitably the structure of the Hilbert space and the algebra of observables when not all selfadjoint operators represent observables and not all orthogonal projectors are interpreted as elementary observables. Readapting Wightman's approach [Wig95] to our framework, we start by making some assumptions describing so-called *Abelian discrete superselection rules* for QM formulated in a *separable* Hilbert space, where $\mathfrak{R}$ is the von Neumann algebra of observables. After, we will consider non-Abelian superselection rules by introducing *Gauge groups* [JaMi61, Haa96]. Finally, we shall discuss the concept of *independent subsystems*.

6.3.1 Abelian Superselection Rules and Coherent Sectors

We want to study the situation where a finite set of pairwise compatible observables exists which commute with all of the observables of the system, so that they belong to the centre $\mathfrak{R} \cap \mathfrak{R}'$ of the algebra of observables. The most recognized example is perhaps the *electric charge*. It is known that for all quantum systems carrying electrical charge, this observables commutes with all other observables of the system. It is evident that, assuming this constraint, not every selfadjoint operator of the Hilbert space can represent an observable: operators which do not commute with the electrical charge are ruled out.

We tackle the general case, and also consider the coexistence of distinct observables commuting with $\mathfrak{R}$, for example the mass and the electrical charge in non-relativistic systems. The shall assume that this set of preferred observables is exhaustive.

(a) These special central observables have *pure point spectra*, see Definition 3.44 (so their spectra essentially consist of their point spectra, in the sense that the possible elements of the continuous spectra are just limit points of the eigenvectors, and the continuous part of the spectrum has no internal points).
(b) These observables exhaust the centre $\mathfrak{R} \cap \mathfrak{R}'$, more precisely the centre is *generated* by them.
(c) The centre coincides with the commutant $\mathfrak{R}' = \mathfrak{R} \cap \mathfrak{R}'$.

The last requirement may be justified in the light of Proposition 6.26: we shall in fact stick to the quite frequent physical situation where there is a *complete set of commuting observables in* $\mathfrak{R}$.

Definition 6.29 (Abelian Discrete Superselection Rules) Given a quantum system described on the separable Hilbert space H with von Neumann algebra of observables $\mathfrak{R}$, we say that **Abelian (discrete) superselection rules occur** if the following conditions hold.

(S1) The centre of the algebra of observables coincides with the commutant $\mathfrak{R}' = \mathfrak{R}' \cap \mathfrak{R}$.
(S2) $\mathfrak{R}' \cap \mathfrak{R}$ contains a finite set of observables $\mathfrak{Q} = \{Q_1, \ldots, Q_n\}$ such that

(i) their spectra are pure point spectra,
(ii) they generate the centre: $\mathfrak{Q}'' = \mathfrak{R}' \cap \mathfrak{R}$.

(If some of the Q_k are unbounded they are supposed to be affiliated to $\mathfrak{R}' \cap \mathfrak{R}$.)

The Q_k are called **superselection charges**. ■

Remark 6.30 A mathematically equivalent, but physically less explanatory, way to state (S1) and (S2) consists in postulating that on the separable Hilbert space H,

(S1)′ $\mathfrak{R} = \{Q_1, \ldots, Q_n\}'$,
(S2)′ $Q_1, \ldots, Q_n$ are selfadjoint operators with commuting PVMs and pure point spectra.

Indeed, (S1) and (S2) imply (S1)′ and (S2)′. Conversely, starting from (S1)′ and (S2)′ we infer $\{Q_1, \ldots, Q_n\} \subset \mathfrak{R}$. Then (S1)′ implies $\mathfrak{R}' = \{Q_1, \ldots, Q_n\}'' \subset \mathfrak{R}'' = \mathfrak{R}$, so $\mathfrak{R}' \subset \mathfrak{R}$ and hence (S1) and (S2) are valid. ■

We have the following remarkable result, where we occasionally adopt the notation $\mathbf{q} := (q_1, \ldots, q_n)$ and $\sigma(\mathfrak{Q}) := \times_{k=1}^n \sigma_p(Q_k)$.

Proposition 6.31 *Let H be a complex separable Hilbert and suppose that the von Neumann algebra $\mathfrak{R}$ in H satisfies (S1) and (S2). The following facts hold.*

(a) *H admits the following Hilbert orthogonal decomposition into closed subspaces, called* **superselection sectors** *or* **coherent sectors**,

$$\mathsf{H} = \bigoplus_{\mathbf{q} \in \sigma(\mathfrak{Q})} \mathsf{H}_{\mathbf{q}} \quad \textit{where} \quad \mathsf{H}_{\mathbf{q}} := P_{\mathbf{q}}^{(\mathfrak{Q})}(\mathsf{H}), \tag{6.7}$$

and each $\mathsf{H}_{\mathbf{q}}$ is

(i) invariant under $\mathfrak{R}$, i.e. $A(\mathsf{H}_{\mathbf{q}}) \subset \mathsf{H}_{\mathbf{q}}$ if $A \in \mathfrak{R}$;
(ii) irreducible under $\mathfrak{R}$, i.e. there is no proper, non-trivial $\mathfrak{R}$-invariant subspace of $\mathsf{H}_{\mathbf{q}}$.

(b) *Correspondingly $\mathfrak{R}$ splits as a direct sum:*

$$\mathfrak{R} = \bigoplus_{\mathbf{q} \in \sigma(\mathfrak{Q})} \mathfrak{R}_{\mathbf{q}}, \quad \textit{where} \quad \mathfrak{R}_{\mathbf{q}} := \left\{ A\restriction_{\mathsf{H}_{\mathbf{q}}} : \mathsf{H}_{\mathbf{q}} \to \mathsf{H}_{\mathbf{q}} \;\middle|\; A \in \mathfrak{R} \right\} \tag{6.8}$$

is a von Neumann algebra on the Hilbert space $\mathsf{H}_{\mathbf{q}}$. *Finally,*

$$\mathfrak{R}_{\mathbf{q}} = \mathfrak{B}(\mathsf{H}_{\mathbf{q}}).$$

(c) *The algebras* $\mathfrak{R}_{\mathbf{q}}$ *enjoy the following properties.*

(i) Each map

$$\mathfrak{R} \ni A \mapsto A\restriction_{\mathsf{H}_{\mathbf{q}}} \in \mathfrak{R}_{\mathbf{q}}$$

is a non-faithful (i.e. non-injective) representation of unital **-algebras of* $\mathfrak{R}$ *(Definition 2.27) which is both strongly and weakly continuous.*

(ii) Representations associated with distinct values $\mathbf{q}$ *are unitarily inequivalent: there is no isometric surjective linear map* $U : \mathsf{H}_{\mathbf{q}} \to \mathsf{H}_{\mathbf{q}'}$ *such that*

$$UA\restriction_{\mathsf{H}_{\mathbf{q}}} U^{-1} = A\restriction_{\mathsf{H}_{\mathbf{q}'}} \quad \textit{when } \mathbf{q} \neq \mathbf{q}'.$$

Proof As the reader can easily prove, since the charges Q_k have pure point spectra and hence each admits a Hilbert basis of eigenvectors, the joint spectral measure $P^{(\mathfrak{Q})}$ on $\mathbb{R}^n$ has support given by the closure of $\times_{k=1}^n \sigma_p(Q_k)$ and, if $E \subset \mathbb{R}^n$,

$$P_E^{(\mathfrak{Q})} = \text{s-}\sum_{(q_1,\ldots,q_n)\in\times_{k=1}^n \sigma_p(Q_k)\cap E} P_{\{q_1\}}^{(Q_1)} \cdots P_{\{q_n\}}^{(Q_n)}\,, \tag{6.9}$$

where the spectral projector $P_{\{q_k\}}^{(Q_k)}$, according to Theorem 3.40, is nothing but the orthogonal projector onto the q_k-eigenspace of Q_k. Notice that every $P_E^{(\mathfrak{Q})}$ is an observable as it belongs to $\mathfrak{R}$. In fact, using Proposition 3.70, $P_E^{(\mathfrak{Q})}$ commutes with all bounded operators commuting with the PVMs of the Q_k which, by definition, belong to $\mathfrak{R}'$, so that $P_E^{(\mathfrak{Q})} \in (\mathfrak{R}')' = \mathfrak{R}$. Not only that: as the Q_k commute with the whole $\mathfrak{R}$, we also have $P_E^{(\mathfrak{Q})} \in \mathfrak{R}'$. In summary $P_E^{(\mathfrak{Q})} \in \mathfrak{R} \cap \mathfrak{R}'$.

(a) Since $P_{\mathbf{q}}^{(\mathfrak{Q})} P_{\mathbf{s}}^{(\mathfrak{Q})} = 0$ if $\mathbf{q} \neq \mathbf{s}$ and $\sum_{\mathbf{q}\in\sigma_p(\mathfrak{Q})} P_{\mathbf{q}}^{(\mathfrak{Q})} = I$, H decomposes as in (6.7). Since $P_{\mathbf{q}}^{(\mathfrak{Q})} \in \mathfrak{R}'$, the subspaces of the decomposition are invariant under the action of each element of $\mathfrak{R}$ because $AP_{\mathbf{q}}^{(\mathfrak{Q})} = P_{\mathbf{q}}^{(\mathfrak{Q})}A$ for every $A \in \mathfrak{R}$, so $A(\mathsf{H}_{\mathbf{q}}) = A(P_{\mathbf{q}}^{(\mathfrak{Q})}(\mathsf{H}_{\mathbf{q}})) = P_{\mathbf{q}}^{(\mathfrak{Q})}(A(\mathsf{H}_{\mathbf{q}})) \subset \mathsf{H}_{\mathbf{q}}$. Let us pass to irreducibility. Suppose $P \in \mathfrak{R}' \cap \mathfrak{R}$ is an orthogonal projector. Then it must be a function of the Q_k since $\mathfrak{Q}'' = \mathfrak{R}' \cap \mathfrak{R}$ by hypothesis and Proposition 6.23 (H is separable). Therefore

$$P = \text{s-}\sum_{(q_1,\ldots,q_n)\in\times_{k=1}^n \sigma_p(Q_k)\cap E} f(q_1,\ldots,q_n) P_{\{q_1\}}^{(Q_1)} \cdots P_{\{q_n\}}^{(Q_n)}$$

since $P = PP \geq 0$ and $P = P^*$. Exploiting measurable functional calculus, we easily find that $f(\mathbf{q}) = \chi_E(\mathbf{q})$ for some $E \subset \times_{k=1}^n \sigma_p(Q_k)$. In other words P is an element of the joint PVM of $\mathfrak{Q}$: that PVM exhausts all orthogonal projectors in $\mathfrak{R}' \cap \mathfrak{R}$. Now, if $\{0\} \neq \mathsf{K} \subset \mathsf{H}_\mathbf{s}$ is an $\mathfrak{R}$-invariant closed subspace, its orthogonal projector P_K must commute with every $A \in \mathfrak{R}$. In fact $P_\mathsf{K} A P_\mathsf{K} = A P_\mathsf{K}$, and taking the adjoint $P_\mathsf{K} A^* P_\mathsf{K} = P_\mathsf{K} A^*$. But since $\mathfrak{R}$ is *-closed, that reads $P_\mathsf{K} A P_\mathsf{K} = P_\mathsf{K} A$, for every $A \in \mathfrak{R}$. Comparing the relations found we have $A P_\mathsf{K} = P_\mathsf{K} A$. Therefore $P_\mathsf{K} \in \mathfrak{R}' = \mathfrak{R} \cap \mathfrak{R}'$ and hence P_K is an element of the PVM $P^{(\mathfrak{Q})}$. Furthermore $P_\mathsf{K} \leq P_\mathbf{s}^{(\mathfrak{Q})}$ because $\mathsf{K} \subset \mathsf{H}_\mathbf{s}$. But there are no projectors smaller than $P_\mathbf{s}^{(\mathfrak{Q})}$ in the PVM of $\mathfrak{Q}$. So $P_\mathsf{K} = P_\mathbf{s}^{(\mathfrak{Q})}$ and $\mathsf{K} = \mathsf{H}_\mathbf{s}$.

(b) $\mathfrak{R}_\mathbf{q} := \left\{ A\restriction_{\mathsf{H}_\mathbf{q}} \,\middle|\, A \in \mathfrak{R} \right\}$ is a von Neumann algebra on $\mathsf{H}_\mathbf{q}$ considered as a Hilbert space in its own right, because this is a strongly closed unital *-subalgebra of $\mathfrak{B}(\mathsf{H}_\mathbf{q})$. (Observe that $A_\mathbf{q} := P_\mathbf{q}^{(\mathfrak{Q})} A P_\mathbf{q}^{(\mathfrak{Q})} \in \mathfrak{R}$, and saying $A_n|_{\mathsf{H}_\mathbf{q}}\psi \to B\psi$ for all $\psi \in \mathsf{H}_\mathbf{q}$ and some $B \in \mathfrak{B}(\mathsf{H}_\mathbf{q})$ is equivalent to $A_{n\mathbf{q}}\phi \to B'\phi$ for every $\phi \in \mathsf{H}$, where B' extends B by zero on $\mathsf{H}_\mathbf{q}^\perp$ and therefore defines an element of $\mathfrak{B}(\mathsf{H})$. Since $\mathfrak{R}$ is a von Neumann algebra, $B' \in \mathfrak{R}$ and $B \in \mathfrak{R}_\mathbf{q}$.) Formula (6.8) holds by definition. Since $\mathsf{H}_\mathbf{q}$ is $\mathfrak{R}$-irreducible it is evidently irreducible also under $\mathfrak{R}_\mathbf{q}$ by construction. *Schur's lemma* (Theorem 6.19) implies that $\mathfrak{R}_\mathbf{q}'' = \mathfrak{B}(\mathsf{H}_\mathbf{q})$. As $\mathfrak{R}_\mathbf{q}'' = \mathfrak{R}_\mathbf{q}$ since we are dealing with a von Neumann algebra, necessarily $\mathfrak{R}_\mathbf{q} = \mathfrak{B}(\mathsf{H}_\mathbf{q})$.

(c) Each map $\mathfrak{R} \ni A \mapsto A\restriction_{\mathsf{H}_\mathbf{q}} \in \mathfrak{R}_\mathbf{q}$ is a strongly and weakly continuous representation of unital *-algebras, as we can check directly. This representation cannot be faithful, because for instance $P_\mathbf{q}^{(\mathfrak{Q})} \in \mathfrak{R}$ is represented by the zero operator on $\mathsf{H}_{\mathbf{q}'}$ if $\mathbf{q}' \neq \mathbf{q}$. Furthermore, if $\mathbf{q} \neq \mathbf{q}'$—say $q_1 \neq q_1'$—there is no isometric surjective linear map $U : \mathsf{H}_\mathbf{q} \to \mathsf{H}_{\mathbf{q}'}$ such that $UA\restriction_{\mathsf{H}_\mathbf{q}} U^{-1} = A\restriction_{\mathsf{H}_{\mathbf{q}'}}$. If such an operator existed one would have $q_1 I_{\mathsf{H}_{\mathbf{q}'}} = UQ_1|_{\mathsf{H}_\mathbf{q}} U^{-1} = Q_1|_{\mathsf{H}_{\mathbf{q}'}} = q_1' I_{\mathsf{H}_{\mathbf{q}'}}$ so that $q_1 = q_1'$. (If Q_1 is unbounded it suffices to consider the central bounded operator $Q_{1n} = \int_{[-n,n]} r\,dP^{(Q_1)}(r)$ with $[-n, n] \ni q_1, q_2$.)

□

We have found that in presence of superselection charges the Hilbert space decomposes into pairwise orthogonal subspaces which are invariant and irreducible under the algebra of observables, thus giving rise to inequivalent representations of the algebra itself. There exist several superselection structures in physics beside the one we pointed out. The three most renowned ones are very different in nature (see Examples 6.32 and 7.19):

- the superselection structure of the *electric charge*,
- the superselection structure of *integer/semi-integer angular momenta*,
- the superselection rule of the mass in non-relativistic physics, i.e. *Bargmann's superselection rule*.

These superselection rules take place simultaneously and can be described by pairwise compatible superselection charges so that the picture above is valid. Notice that, in each superselection sector, the physical description is essentially identical to the naive one where every selfadjoint operator is an observable (namely $\mathfrak{R} = \mathfrak{B}(\mathsf{H})$) and the superselection charges appear just in terms of fixed parameters.

Example 6.32 The electric charge is the typical example of a superselection charge. For instance, referring to an electron the Hilbert space is $L^2(\mathbb{R}^3, d^3x) \otimes \mathsf{H}_s \otimes \mathsf{H}_e$. The space of the electric charge is $\mathsf{H}_e = \mathbb{C}^2$, on which $Q = e\sigma_z$ (see (1.12)). In principle several other observables could exist on H_e, but the electric charge's superselection rule imposes that the only possible observables commute with Q and are functions of σ_3. The centre of the algebra of observables is $I \otimes I \otimes f(\sigma_3)$ for every function $f : \sigma(\sigma_3) = \{-1, 1\} \to \mathbb{C}$. We have the decomposition into coherent sectors

$$\mathsf{H} = (L^2(\mathbb{R}^3, d^3x) \otimes \mathsf{H}_s \otimes \mathsf{H}_+) \bigoplus (L^2(\mathbb{R}^3, d^3x) \otimes \mathsf{H}_s \otimes \mathsf{H}_-) ,$$

where $\mathsf{H}_\pm$ are the eigenspaces of Q relative to eigenvalues $\pm e$, respectively. ■

Remark 6.33 A fundamental requirement is that the superselection charges have pure point spectra. If instead $\mathfrak{R} \cap \mathfrak{R}'$ contains an operator A having a continuous part in its spectrum with non-empty interior (A may also be the strong limit on $D(A)$ of a sequence of elements in $\mathfrak{R} \cap \mathfrak{R}'$), the proposition does not hold, and H cannot be decomposed in a direct sum of closed subspaces. In this case it decomposes as a *direct integral*: this produces a much more complicated structure, whose physical meaning seems dubious. ■

6.3.2 Global Gauge Group Formulation and Non-Abelian Superselection

There are quantum physical systems with von Neumann algebra of observables $\mathfrak{R}$ for which $\mathfrak{R}'$ is not Abelian (think of chromodynamics, where $\mathfrak{R}'$ contains a faithful representation of $SU(3)$). In that case the centre of $\mathfrak{R}$ does not retain the full information about $\mathfrak{R}'$. A primary notion is here the group of unitary operators called the **commutant group** of $\mathfrak{R}$ (introduced in [JaMi61] and called *gauge group* there):

$$\mathfrak{G}_{\mathfrak{R}} := \{V \in \mathfrak{R}' \mid V \text{ is unitary}\} .$$

It holds all the information about $\mathfrak{R}$ and $\mathfrak{R}'$ because (making use of $\mathfrak{R}'' = \mathfrak{R}$ and Proposition 3.55)

$$\mathfrak{G}'_{\mathfrak{R}} = \mathfrak{R} \quad \text{and} \quad \mathfrak{G}''_{\mathfrak{R}} = \mathfrak{R}' . \tag{6.10}$$

In the presence of *Abelian* superselection rules, $\mathfrak{G}_{\mathfrak{R}}$ is Abelian ($\mathfrak{G}_{\mathfrak{R}} \subset \mathfrak{R}' = \mathfrak{R} \cap \mathfrak{R}'$). Similarly to (6.10), $\mathfrak{R}$ can be extracted from $\mathfrak{B}(\mathsf{H})$: one employs the former in (6.10) and uses a *subgroup* of $\mathfrak{G}_{\mathfrak{R}}$ constructed out of a set of physically meaningful superselection charges $Q_1, \ldots, Q_n$. $A \in \mathfrak{R}$ if and only if A commutes with the PVMs of $Q_1, \ldots, Q_n$. Decomposing $A = \frac{1}{2}(A + A^*) + i\frac{1}{2i}(A - A^*)$ and exploiting Proposition 3.70, this is equivalent to saying

$$U_{\mathbf{s}}A = AU_{\mathbf{s}} , \quad U_{\mathbf{s}} := e^{is_1 Q_1} \cdots e^{is_n Q_n} \quad \text{for } \mathbf{s} := (s_1, \ldots, s_n) \in \mathbb{R}^n \quad (6.11)$$

where $U : \mathbb{R}^n \ni \mathbf{s} \mapsto U_{\mathbf{s}}$ is a strongly-continuous unitary representation of the Abelian topological group $\mathbb{R}^n$ taking values in $\mathfrak{G}_{\mathfrak{R}}$. Looking at Remark 6.30, the occurrence of Abelian discrete superselection rules can be condensed in three facts: (a) H is separable, (b) $Q_1, \ldots, Q_n$ have pure point spectra, and (c)

$$\mathfrak{R} = U(\mathbb{R}^n)' . \quad (6.12)$$

Observe that $U(\mathbb{R}^n)$ is considerably smaller than $\mathfrak{G}_{\mathfrak{R}}$, since other choices for the charges Q_k and also for their number are possible. These would produce other subgroups of $\mathfrak{G}_{\mathfrak{R}}$ still satisfying (6.12): it is sufficient that the joint PVM of these charges is made of the same projectors $P_{\mathbf{q}}$ onto the sectors determined by the initial charges. We can do better if we use the separability of H: namely, out of the PVMs of the n charges Q_k we can construct the unique charge

$$Q := s\text{-}\sum_{\mathbf{q}\in\sigma(\mathfrak{Q})} m_{\mathbf{q}} P_{\mathbf{q}} ,$$

for some injective map $\mathbf{q} \mapsto m_{\mathbf{q}} \in \mathbb{Z}$, which must exist because there are at most countably many PVMs $P_{\mathbf{q}}$, since H is separable. Now, by Remark 6.30 and Proposition 3.70, the representation U of $\mathbb{R}^n$ in (6.12) can be replaced by a faithful and strongly-continuous representation of the *compact* Abelian group $U(1)$,

$$U : U(1) \ni e^{is} \mapsto e^{isQ} \in \mathfrak{G}_{\mathfrak{R}} . \quad (6.13)$$

We stress that (6.13) is well defined and is a representation of $U(1)$, not only of $\mathbb{R}$, simply because $\sigma(Q) \subset \mathbb{Z}$. (The charge Q has, however, no direct physical meaning in general, except perhaps for $n = 1$ with $Q = e^{-1}Q_1$, where Q_1 is the *electric charge* and e the *elementary electric charge*.) The splittings (6.7)–(6.8) hold and every $\mathfrak{R}$-invariant and $\mathfrak{R}$-irreducible closed subspace $\mathsf{H}_{\mathbf{q}}$ is U-invariant too, since $U\restriction_{\mathsf{H}_{\mathbf{q}}}$ is a pure phase (however U-irreducibility fails unless $\dim(\mathsf{H}_{\mathbf{q}}) = 1$).

In the *non-Abelian* case, decompositions similar to (6.7)–(6.8) are expected to hold with reference to a strongly-continuous faithful representation $U : G \ni g \mapsto U_g \in \mathfrak{G}_{\mathfrak{R}}$ of some (compact) group G, called the **global gauge group**, such that $U' = \mathfrak{G}'_{\mathfrak{R}} = \mathfrak{R}$ (here, and occasionally henceforth, $U' := U(G)'$):

$$\mathsf{H} = \bigoplus_{\chi\in K} \mathsf{H}_\chi , \quad \mathfrak{R} = \bigoplus_{\chi\in K} \mathfrak{R}_\chi , \quad U_g = \bigoplus_{\chi\in K} U_g^{(\chi)} . \quad (6.14)$$

Above, H_χ is a non-trivial closed subspace that is both $\mathfrak{R}$-invariant and U-invariant, determining corresponding (non-faithful, strongly and weakly continuous) representations

$$\mathfrak{R}_\chi : \mathfrak{R} \ni A \mapsto A\restriction_{\mathsf{H}_\chi} : \mathsf{H}_\chi \to \mathsf{H}_\chi\ , \quad U^{(\chi)} : G \ni g \mapsto U_g\restriction_{\mathsf{H}_\chi} : \mathsf{H}_\chi \to \mathsf{H}_\chi \ \text{ with } \quad \mathfrak{R}_\chi = (U^{(\chi)})' \tag{6.15}$$

where *the commutant refers to* $\mathfrak{B}(\mathsf{H}_\chi)$.

The fundamental difference with the Abelian case is that now $\mathfrak{R}_\chi$ is only a *factor* in $\mathfrak{B}(\mathsf{H}_\chi)$ rather than the entire $\mathfrak{B}(\mathsf{H}_\chi)$:

$$\mathfrak{R}_\chi \cap \mathfrak{R}'_\chi = \mathbb{C}I_\chi = (U^{(\chi)})' \cap (U^{(\chi)})'' \quad \text{for every } \chi \in K\ . \tag{6.16}$$

If everything we stated holds, the orthogonal projectors P_χ onto every subspace H_χ must commute with U and $\mathfrak{R}$, so they belong to the centre $\mathfrak{R} \cap \mathfrak{R}' = U' \cap U''$. Using the projectors P_χ we can still construct *superselection charges* whose joint PVM determines the *generalized* superselection sectors H_χ.

We have in fact the following general result where separability is not necessary.

Proposition 6.34 *Let $\mathfrak{R}$ be a von Neumann algebra on the Hilbert space $\mathsf{H} \neq \{0\}$. Suppose there exists a faithful, strongly-continuous unitary representation $U : G \ni g \mapsto U_g \in \mathfrak{G}_\mathfrak{R}$ of the compact Hausdorff group G such that $U(G)' = \mathfrak{R}$. Then*

(a) *(6.14)–(6.16) hold, where K is a set of equivalence classes of irreducible strongly-continuous and unitarily-equivalent representations of G,*
(b) *$\mathfrak{R}_\chi$ and $\mathfrak{R}_{\chi'}$ are unitarily inequivalent if $\chi \neq \chi'$.*

Proof (a) Let us start by proving (6.14). If G is Hausdorff and compact, as $G \ni g \mapsto U_g$ is strongly continuous, the *Peter-Weyl Theorem* (Theorem 7.35) gives an orthogonal Hilbert decomposition $\mathsf{H} = \bigoplus_{\chi \in K} \mathsf{H}_\chi$ where each H_χ is non-trivial, closed and U-invariant. K labels equivalence classes of irreducible strongly-continuous unitarily-equivalent representations of G. In particular we have a finer Hilbert orthogonal decomposition: $\mathsf{H}_\chi = \bigoplus_{\lambda \in \Lambda_\chi} \mathsf{H}_\chi^{(\lambda)}$, where every closed subspace $\mathsf{H}_\chi^{(\lambda)}$ is U-invariant, every restriction $U^{(\chi\lambda)} := U\restriction_{\mathsf{H}_\chi^{(\lambda)}} : \mathsf{H}_\chi^{(\lambda)} \to \mathsf{H}_\chi^{(\lambda)}$ is finite-dimensional and irreducible, and the $U^{(\chi\lambda)}$ are unitarily equivalent as $\lambda \in \Lambda_\chi$ varies, for every fixed χ. By direct inspection, using the irreducibility and unitary equivalence of the $U^{(\chi\lambda)}$ for fixed χ, one finds $(U^{(\chi)})'' \cap (U^{(\chi)})' = \mathbb{C}I$, where the commutant is referred to H_χ. On the other hand, since the $U^{(\chi)}$ with different χ are unitarily inequivalent and $U' = \mathfrak{G}'_\mathfrak{R} = \mathfrak{R}$, every H_χ is $\mathfrak{R}$-invariant and the subrepresentation $\mathfrak{R}_\chi$ obtained by restriction satisfies $\mathfrak{R}_\chi = (U^{(\chi)})'$ where the commutant is referred to H_χ. In particular $\mathfrak{R}_\chi$ is a von Neumann algebra on H_χ. Hence $(U^{(\chi)})' \cap (U^{(\chi)})'' = \mathbb{C}I$ can be translated into $\mathfrak{R}_\chi \cap \mathfrak{R}'_\chi = \mathbb{C}I$, and every $\mathfrak{R}_\chi$ is a factor, proving (6.16). (b) Let $P_\chi, P_{\chi'} \in \mathfrak{R} \cap \mathfrak{R}'$ be the orthogonal projectors onto H_χ and $\mathsf{H}_{\chi'}$ respectively, with $\chi \neq \chi'$. We claim $\mathfrak{R}_\chi$, $\mathfrak{R}_{\chi'}$ are unitarily inequivalent. If there were an isometric surjective map $V : \mathsf{H}_\chi \to \mathsf{H}_{\chi'}$

with $VA\restriction_{\mathsf{H}_\chi} V^{-1} = A\restriction_{\mathsf{H}_{\chi'}}$, we would find $\mathbb{1}_{\chi'} = -\mathbb{1}_{\chi'}$ when representing the operator $A = P_\chi - P_{\chi'} \in \mathfrak{R}$. □

For Abelian discrete superselection rules, the existence of a *global compact gauge group* G as in the theorem is guaranteed by the separability of H, as we established above for $G = U(1)$. In this case, decomposition (6.14) coincides with (6.7)–(6.8); additionally, we know that $\mathfrak{R}_\chi = \mathfrak{B}(\mathsf{H}_\chi)$ and $U^{(\chi)}$ is a pure phase. If $\mathfrak{G}_\mathfrak{R}$ is not Abelian the issue of whether such a G exists has to be examined case by case. In all physically interesting cases, G is a compact Lie group (hence a matrix group) and $U(G)$ is considerably smaller than $\mathfrak{G}_\mathfrak{R}$.

The approach to superselection rules based on the notion of a *global compact gauge group of internal symmetries* G turns out to be powerful and deep if used in addition to the request of spacetime *locality* in *algebraic quantum field theory* in Minkowski spacetime formulated in terms of von Neumann algebras. These remarkable results are due to several authors and rely on the so-called *Doplicher-Haag-Roberts (DHR) analysis* and the *Buchholz-Fredenhagen (BF) analysis* of superselection sectors [Haa96] describing theories with *short-range* interactions and without *topological charges* in BF sense. A rather complete technical review including fundamental references is [HaMü06].

6.3.3 Quantum States in the Presence of Abelian Superselection Rules

Let us come to the problem of characterizing states when an Abelian superselection structure is turned on a complex *separable* Hilbert space H, in accordance with (S1) and (S2). In principle, we can extend Definition 4.43 given for $\mathfrak{R}$ with trivial centre. As usual $\mathscr{L}_\mathfrak{R}(\mathsf{H})$ indicates the lattice of orthogonal projectors on $\mathfrak{R}$, which we know to be bounded by 0 and I, orthocomplemented, σ-complete, orthomodular and separable. It is not atomic and it does not satisfy the covering property in general. The atoms are one-dimensional projectors, exactly as pure states when $\mathfrak{R} = \mathfrak{B}(\mathsf{H})$, so we should expect some differences when $\mathfrak{R} \neq \mathfrak{B}(\mathsf{H})$. We start from the following general definition, valid also if H is not separable.

Definition 6.35 Let H be a complex Hilbert space. A **quantum probability measure** relative to the von Neumann algebra $\mathfrak{R} \subset \mathfrak{B}(\mathsf{H})$, is a map $\rho : \mathscr{L}_\mathfrak{R}(\mathsf{H}) \to [0, 1]$ satisfying the following requirements:

(1) $\rho(I) = 1$.

(2) If $\{Q_n\}_{n\in N} \subset \mathscr{L}_\mathfrak{R}(\mathsf{H})$, N at most countable, satisfies $Q_k \perp Q_h = 0$ when $h, k \in N$, then

$$\rho(\vee_{k\in N} Q_k) = \sum_{k\in N} \rho(Q_k) . \tag{6.17}$$

The set of the quantum probability measures relative to $\mathfrak{R}$ will be denoted by $\mathscr{M}_{\mathfrak{R}}(\mathsf{H})$. ■

Remark 6.36 Provided N is at most countable, $\vee_{k\in N} Q_k \in \mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ if every $Q_k \in \mathscr{L}_{\mathfrak{R}}(\mathsf{H})$, because this lattice is σ-complete (even if H is not separable). Without this fact the definition above would be meaningless. ■

Recall that a von Neumann algebra $\mathfrak{R}$ is strongly closed, and the strong topology is the one used to manipulate operators spectrally. Moreover $A = A^*$ is affiliated or belongs to $\mathfrak{R}$ if and only if its PVM belongs to $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$. Because of all this the definitions of Sect. 4.5.1 can be given also in the presence of Abelian superselection rules, and they give a meaning to notions like the *expectation value* and *standard deviation* of an observable for a given quantum state viewed as a probability measure on $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$.

The *procedures* presented in Sect. 4.5.1 to compute those statistical objects in terms of *traces* make sense when the quantum probability measures are represented by trace-class operators. This is possible also when we have superselection rules, as we shall prove, even if the picture is more complicated.

Assuming H separable, if there is an Abelian superselection structure, we can write simpler-looking decompositions:

$$\mathsf{H} = \bigoplus_{k\in K} \mathsf{H}_k \ , \quad \mathfrak{R} = \bigoplus_{k\in K} \mathfrak{R}_k \ , \quad \mathfrak{R}_k = \mathfrak{B}(\mathsf{H}_k) \ , \ k \in K \tag{6.18}$$

where K is some finite or countable set. The lattice $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$, as a consequence of (6.17), splits as (the notation should be obvious)

$$\mathscr{L}_{\mathfrak{R}}(\mathsf{H}) = \bigoplus_{k\in K} \mathscr{L}_{\mathfrak{R}_k}(\mathsf{H}_k) = \bigoplus_{k\in K} \mathscr{L}(\mathsf{H}_k) \tag{6.19}$$

where $\mathscr{L}_{\mathfrak{R}_k}(\mathsf{H}_k) \cap \mathscr{L}_{\mathfrak{R}_h}(\mathsf{H}_h) = \{0\} \quad \text{if } k \neq h$.

In other words $Q \in \mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ can be written uniquely as $Q = \oplus_{k\in K} Q_k$ where $Q_k \in \mathscr{L}(\mathfrak{B}(\mathsf{H}_k))$. In fact $Q_k = P_k Q$, where P_k is the orthogonal projector onto H_k.

Let us focus on the problem of characterizing quantum probability measures in terms of trace-class operators and unit vectors up to phase.

Remark 6.37 We shall avoid using already introduced terms like *mixed states* and *pure states* which correspond, in the absence of superselection rules, to *quantum-state operators* (positive trace-class operators of unit trace) and *unit vectors modulo phase*, respectively. We shall explain in a short while that these mathematical objects do not (yet) correspond one-to-one with extremal quantum probability measures and generic quantum probability measures. Physically, speaking, the safest approach is to assume that quantum states are nothing but quantum probability measures. ■

It is possible to adapt Gleason's result simply by observing that $\rho \in \mathscr{M}_{\mathfrak{R}}(\mathsf{H})$ defines an analogous quantum probability measure ρ_k on $\mathscr{L}_{\mathfrak{R}_k}(\mathsf{H}_k) = \mathscr{L}(\mathsf{H}_k)$ by

$$\rho_k(P) := \frac{1}{\rho(P_k)}\rho(P) , \quad P \in \mathscr{L}(\mathsf{H}_k) ,$$

provided $\rho(P_k) \neq 0$. If $\dim(\mathsf{H}_k) \neq 2$ we can exploit Gleason's theorem. According to Proposition 4.45, the set $\mathscr{S}(\mathsf{H})$ of *quantum-state operators* on H contains all operators $T \in \mathfrak{B}_1(\mathsf{H})$ satisfying $T \geq 0$ and $tr(T) = 1$.

Theorem 6.38 *Let* H *be a complex separable Hilbert space, and assume that the von Neumann algebra* $\mathfrak{R}$ *on* H *satisfies (S1) and (S2). In the ensuing coherent decomposition (6.18) we suppose* $\dim \mathsf{H}_k \neq 2$ *for every* $k \in K$. *Then the following facts hold.*

(a) *If* $T \in \mathscr{S}(\mathsf{H})$, *then* $\rho_T \in \mathscr{M}_{\mathfrak{R}}(\mathsf{H})$ *if*

$$\rho_T : \mathscr{L}_{\mathfrak{R}}(\mathsf{H}) \ni P \mapsto tr(TP) .$$

(b) *For* $\rho \in \mathscr{M}_{\mathfrak{R}}(\mathsf{H})$ *there exists* $T \in \mathscr{S}(\mathsf{H})$ *such that* $\rho = \rho_T$.
(c) *If* $T_1, T_2 \in \mathscr{S}(\mathsf{H})$, *then* $\rho_{T_1} = \rho_{T_2}$ *if and only if* $P_k T_1 P_k = P_k T_2 P_k$ *for all* $k \in K$, P_k *being the orthogonal projector onto* H_k.
(d) *A unit vector* $\psi \in \mathsf{H}$ *defines an extremal measure if and only if it belongs to a coherent sector. More precisely, a measure* $\rho \in \mathscr{M}_{\mathfrak{R}}(\mathsf{H})$ *is extremal if and only if there exist* $k_0 \in K$ *and a unit vector* $\psi \in \mathsf{H}_{k_0}$ *such that*

$$\rho(P) = 0 \quad \text{if } P \in \mathscr{L}(\mathsf{H}_k), k \neq k_0 \quad \text{and} \quad \rho(P) = \langle\psi|P\psi\rangle \text{ if } P \in \mathscr{L}(\mathsf{H}_{k_0})$$

Proof (a) is obvious from Proposition 4.45, as the restriction to $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ of a quantum probability measure ρ on $\mathscr{L}(\mathsf{H})$ is a similar measure. Let us prove (b). Evidently, every $\rho|_{\mathscr{L}(\mathsf{H}_k)}$ is a positive measure with $0 \leq \rho(P_k) \leq 1$. We can apply Gleason's theorem to find a positive $T_k \in \mathfrak{B}(\mathsf{H}_k)$ with $tr(T_k) = \rho(P_k)$ such that $\rho(Q) = tr(T_k Q)$ if $Q \in \mathscr{L}(\mathsf{H}_k)$. Notice also that $||T_k|| \leq \rho(P_k)$ because

$$||T_k|| = \sup_{\lambda \in \sigma_p(T_k)} |\lambda| = \sup_{\lambda \in \sigma_p(T_k)} \lambda \leq \sum_{\lambda \in \sigma_p(T_k)} d_\lambda \lambda = tr(T_k) = \rho(P_k) .$$

If $Q \in \mathscr{L}_{\mathfrak{R}}(\mathsf{H})$, $Q = \sum_k Q_k$, where $Q_k := P_k Q \in \mathscr{L}(\mathsf{H}_k)$, $Q_k Q_h = 0$ if $k \neq h$. Therefore by σ-additivity

$$\rho(Q) = \sum_k \rho(Q_k) = \sum_k tr(T_k Q_k)$$

since $\mathsf{H}_k \perp \mathsf{H}_h$, which can be written $\rho(Q) = tr(TQ)$ for $T := \oplus_k T_k \in \mathfrak{B}_1(\mathsf{H})$. It is clear that $T \in \mathfrak{B}(\mathsf{H})$ because, if $x = \sum_k x_k$, $x_k \in \mathsf{H}_k$, is a unit vector, then $||Tx|| \leq \sum_k ||T_k||\,||x_k|| \leq \sum_k ||T_k||1 \leq \sum_k \rho(P_k) = 1$. In particular $||T|| \leq 1$.

$T \geq 0$ because each $T_k \geq 0$. Hence $|T| = \sqrt{T^*T} = \sqrt{TT} = T$ via functional calculus, and also $|T_k| = T_k$. Moreover, using the spectral decomposition of T, whose PVM commutes with each P_k, one easily has $|T| = \oplus_k |T_k| = \oplus_k T_k$. The condition

$$1 = \rho(I) = \sum_k \rho(P_k) = \sum_k tr(T_k P_k) = \sum_k tr(|T_k| P_k)$$

is equivalent to saying $tr\ |T| = 1$, using a Hilbert basis of H made of the union of bases in each H_k. We have obtained, as we wanted, that $T \in \mathfrak{B}_1(\mathsf{H})$, $T \geq 0$, $tr(T) = 1$ and $\rho(Q) = tr(TQ)$ for all $Q \in \mathscr{L}_{\mathfrak{R}}(\mathsf{H})$.

(c) The proof is straightforward from $\mathscr{L}_{\mathfrak{R}_k}(\mathsf{H}_k) = \mathscr{L}(\mathfrak{B}(\mathsf{H}_k))$, because $\mathfrak{R}_k = \mathfrak{B}(\mathsf{H}_k)$ and, evidently, $\rho_{T_1} = \rho_{T_2}$ if and only if $\rho_{T_1} \upharpoonright_{\mathscr{L}(\mathsf{H}_k)} = \rho_{T_2} \upharpoonright_{\mathscr{L}(\mathsf{H}_k)}$ for all $k \in K$.

(d) It is clear that if ρ has more than one component, $\rho|_{\mathscr{L}(\mathsf{H}_k)} \neq 0$ cannot be extremal because it is, by construction, a convex combination of other states which vanish on some of the coherent subspaces. Therefore only states such that only one restriction $\rho \upharpoonright_{\mathscr{L}(\mathsf{H}_{k_0})}$ does not vanish may be extremal. Now Proposition 4.51 (a) implies that among these states the extremal ones are precisely those of the form claimed in (d). □

Remark 6.39

(a) Take $\psi = \sum_{k \in K} c_k \psi_k$ where the $\psi_k \in \mathsf{H}_k$ are unit vectors, and suppose $||\psi||^2 = \sum_k |c_k|^2 = 1$. This vector induces a state ρ_ψ on $\mathfrak{R}$ by means of the standard procedure (which is merely a trace with respect to $T_\psi := \langle \psi | \ \rangle \psi$)

$$\rho_\psi(P) = \langle \psi | P \psi \rangle \quad P \in \mathscr{L}_{\mathfrak{R}}(\mathsf{H}) .$$

In this case however, since $PP_k = P_k P$ and $\psi_k = P_k \psi_k$, we have

$$\begin{aligned}
\rho_\psi(P) = \langle \psi | P \psi \rangle &= \sum_k \sum_h \overline{c_k} c_h \langle \psi_k | P \psi_k \rangle \\
&= \sum_k \sum_h \overline{c_k} c_h \langle P_k \psi_k | P P_h \psi_k \rangle = \sum_k \sum_h \overline{c_k} c_h \langle \psi_k | P_k P P_h \psi_h \rangle \\
&= \sum_k \sum_h \overline{c_k} c_h \langle \psi_k | P P_k P_h \psi_k \rangle = \sum_k \sum_h \overline{c_k} c_h \langle \psi | P P_k \psi \rangle \delta_{kh} \\
&= \sum_k |c_k|^2 \langle \psi_k | P \psi_k \rangle = tr(T'_\psi P)
\end{aligned}$$

where

$$T'_\psi = \sum_{k \in K} |c_k|^2 \langle \psi_k | \ \rangle \psi_k \ .$$

We conclude that the apparent *pure state* described by the vector ψ and the apparent *mixed state* described by the operator T'_ψ cannot be distinguished, simply because the algebra $\mathfrak{R}$ is too small to distinguish between them. Actually they define the same probability measure, i.e. the same *quantum state*, and this is an elementary case of (c) in the above theorem, with $T_1 = \langle \psi | \ \rangle \psi$ and $T_2 = T'_\psi$. This fact is often stated as follows in the argot of physicists:

no coherent superpositions $\psi = \sum_{k \in K} c_k \psi_k$ *of pure states* $\psi_k \in \mathsf{H}_k$ *from different coherent sectors are possible; only incoherent superpositions* $\sum_{k \in K} |c_k|^2 \langle \psi_k | \ \rangle \psi_k$ *are allowed.*

(b) It should be clear that the one-to-one correspondence between extremal quantum measures and atomic elementary observables (one-dimensional projectors) here does not work. Consequently, notions like the *probability amplitude* must be handled with great care. In general, however, everything pans out—correspondence included—if one stays in a fixed superselection sector H_k.

(c) We leave to the reader the easy proof of the fact that the *Lüders-von Neumann postulate on post-measurement states* (see Sect. 4.4.7) can be stated as it stands also in the presence of superselection rules, no matter which $T \in \mathscr{S}(\mathsf{H})$ we use to describe a quantum probability measure ρ: the post-measurement probability measure ρ' does not depend on the chosen representation of ρ by operators. Besides, it is worth stressing that since the PVM of an observable in $\mathfrak{R}$ (or affiliated to $\mathfrak{R}$) commutes with the central projectors P_k defining the superselection sectors H_k, if an extremal quantum state is initially represented by a vector belonging to a sector H_k, there is no chance to leave that sector by means of a subsequent measurement of any observable in $\mathfrak{R}$. ■

Example 6.40 Going back to Example 6.32, states (probability measures on $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$) where Q takes the value $-e$ with probability 1 are said states of **electrons**. When Q takes the value $+e$ with probability 1 one talks about states of **positrons**, to be absolutely thorough. However, as soon as we measure Q, its value cannot later change due to measurements of other observables, since all physically meaningful observables commute with Q and the postulate of collapse leaves the state in the initial eigenspace of Q. This means that once the charge has been observed and the particle is baptized an electron or a positron, from that moment on it is impossible to put the system in a state where the value of Q is not defined and the particle is in an electron-positron superposition. In principle it could still be possible to put the system into a similar superposed state in view of time evolution. This is not the case however, since the conservation law of the electrical charge stipulates that the observable Q is a *constant of motion*. ■

6.3.4 The General Case $\mathfrak{R} \subset \mathfrak{B}(\mathsf{H})$: Quantum Probability Measures, Normal and Algebraic States

Let us finally focus on the various notions of quantum state one can adopt in the completely general setup $\mathfrak{R} \subset \mathfrak{B}(\mathsf{H})$, where H is not necessarily separable, and introduce the relevant terminology. In principle, amongst other possibilities, one can always define states in terms of quantum probability measures on $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$, so that they form the convex body $\mathscr{M}_{\mathfrak{R}}(\mathsf{H})$. In particular, due to Proposition 4.45, quantum state operators $T \in \mathscr{S}(\mathsf{H})$ still represent (certain) *quantum probability measures* in the sense of Definition 6.35, namely σ-additive probability measures in $\mathscr{M}_{\mathfrak{R}}(\mathsf{H})$. Obviously T and $T' := VTV^{-1}$, where $V \in \mathfrak{G}_{\mathfrak{R}}$, define the same measure if the global gauge group $\mathfrak{G}_{\mathfrak{R}}$ is not trivial (represented by pure phases), because

$$tr(AVTV^{-1}) = tr(V^{-1}AVT) = tr(AV^{-1}VT) = tr(AT)\,, \quad \text{if } A \in \mathfrak{R}.$$

So there are many ways to describe the same state in terms of quantum-state operators, and a meaningful definition of *pure quantum states* is again provided by extremal elements of $\mathscr{M}_{\mathfrak{R}}(\mathsf{H})$, if any, rather than unit vectors.

Let us pass to the converse problem: *can all σ-additive probability measures in $\mathscr{M}_{\mathfrak{R}}(\mathsf{H})$be written in terms of quantum-state operators, i.e., positive trace-class operators of trace one in the generic case $\mathfrak{R} \subset \mathfrak{B}(\mathsf{H})$?* The answer is only partially positive [Dvu92, Ham03].

(1) *If H is separable*, and assuming that the type decomposition of $\mathfrak{R}$ does not include type-I_2 summands, Gleason's theorem still holds: positive trace-class operators of unit trace represent all σ-additive probability measures on $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$, with the *caveat* that several distinct operators may represent the same measure if $\mathfrak{R} \subsetneq \mathfrak{B}(\mathsf{H})$.

(2) *If H is not separable*, and again dispensing with type-I_2 factors in $\mathfrak{R}$, then positive trace-class operators of trace one represent all *completely additive* probability measures on $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ but only them. The latter's set is denoted by $\mathscr{M}_{\mathfrak{R}}(\mathsf{H})_{ca}$, cf. Remark 4.46. Again the *proviso* holds that many operators may represent the same measure if $\mathfrak{R} \subsetneq \mathfrak{B}(\mathsf{H})$.

Notice that $\mathscr{M}_{\mathfrak{R}}(\mathsf{H})_{ca} \subset \mathscr{M}_{\mathfrak{R}}(\mathsf{H})$, with equality if and only if H is separable, for otherwise $\mathscr{M}_{\mathfrak{R}}(\mathsf{H})_{ca}$ is properly included in $\mathscr{M}_{\mathfrak{R}}(\mathsf{H})$. So, if we want to work with von Neumann algebras on non-separable Hilbert spaces with the intent to describe quantum states in terms of probability measures, it might be convenient to redefine quantum probability measures by restricting to the completely-additive ones if we also wish that these measures are represented by quantum-state operators. A far-reaching discussion on the structure of additive measures on von Neumann algebras in terms of operators can be found in [Ham03].

There is an alternative definition of quantum states on $\mathfrak{R}$ that does not identify them to (σ/completely-additive) probability measures on $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$, but still captures all probability measures (σ/completely-additive) induced by quantum-state operators: these are the *algebraic states*. We will discuss the concept further in the last chapter, motivating its necessity in a more general context.

Definition 6.41 Let $\mathfrak{R}$ be a von Neumann algebra on H.

(1) An **algebraic state** on $\mathfrak{R}$ is a linear map $\omega : \mathfrak{R} \to \mathbb{C}$ such that $\omega(I) = 1$ and $\omega(A^*A) \geq 0$ if $A \in \mathfrak{R}$
(2) The algebraic states ω_T induced by quantum-state operators $T \in \mathscr{S}(\mathsf{H})$:

$$\omega_T(A) := tr(TA) \quad \text{for } A \in \mathfrak{R},$$

are called **normal (algebraic) states of** $\mathfrak{R}$, and their set is the **folium** of $\mathfrak{R}$. A **pure normal state** is an extremal element of the convex body of normal states on $\mathfrak{R}$. ■

Remark 6.42

(a) We stress that the map associating $T \in \mathscr{S}(\mathsf{H})$ to the algebraic state $\omega_T : \mathfrak{R} \to \mathbb{C}$ is very far from being injective in general (it depends on how big $\mathfrak{R}$ is).
(b) If $\mathfrak{R} = \mathfrak{B}(\mathsf{H})$ (also with H non-separable), as we already know, the set of pure normal states coincides with the set of vector states $T = \langle\psi|\cdot\rangle\psi$ for unit vectors $\psi \in \mathsf{H}$. For smaller von Neumann algebras this fact is usually false.
(c) From the standpoint of the measure theory on $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$, algebraic states define *additive, but not necessarily σ-additive or completely additive* probability measures. The set of additive measures on $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ is denoted by $\mathscr{M}_{\mathfrak{R}}(\mathsf{H})_a$. Evidently $\mathscr{M}_{\mathfrak{R}}(\mathsf{H})_a \supset \mathscr{M}_{\mathfrak{R}}(\mathsf{H}) \supset \mathscr{M}_{\mathfrak{R}}(\mathsf{H})_{ca}$.
(d) Normal states are defined even if $\mathfrak{R}$ does contain type-I_2 summands. In this case, however, they are not able to capture all completely-additive probability measures on $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$.
(e) Suppose $\rho \in \mathscr{M}_{\mathfrak{R}}(\mathsf{H})_a$ and $\mathfrak{R}$ is free of type-I_2 summands. If there exists $P \in \mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ such that $\rho(Q) = 0$ for $Q \in \mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ iff $PQ = QP = 0$, then P is called the **support** of ρ. It turns out that $\rho \in \mathscr{M}_{\mathfrak{R}}(\mathsf{H})$ is induced by a normal state, i.e., $\rho \in \mathscr{M}(\mathsf{H})_{ca}$ if and only if it admits a support [Ham03]. ■

Remark 6.43 If the Hilbert space is finite-dimensional, the various definitions of quantum state based on additive, σ-additive, completely-additive probability measures, rather than normal states or algebraic states all coincide. In view of the assorted inequivalent possibilities in the general case, in the rest of the book we shall always specify which notion of quantum state we are adopting in that specific situation. At any rate algebraic states will not show up until the last chapter. ■

6.4 Composite Systems and von Neumann Algebras: Independent Subsystems

When departing from elementary QM, the notion of *independent subsystems* is much more delicate than the picture presented in Sect. 4.4.8 and has to be discussed carefully. We refer the reader to [Tak10] for general technical results, to [Sum90, Ham03] for a discussion on the various notions of independence of subsystems in Quantum Theory and their interplay, and to [Sum90, Haa96, Red98] for Quantum Field Theory.

6.4.1 *W*-Independence and Statistical Independence*

It is customary to work with von Neumann algebras of observables instead of lattices of orthogonal projectors, and the overall perspective of Sect. 4.4.8 to define independent subsystems is reversed: one starts from the overall system and defines the subsystems inside it. As a matter of fact, one demands that

(A)′ there exist a von Neumann algebra of observables $\mathfrak{A}$ on H associated to the *overall system*, and two (or more) von Neumann algebras $\mathfrak{A}_1, \mathfrak{A}_2 \subset \mathfrak{A}$ describing *subsystems*;

(B)′ the subsystems are *compatible*, in the sense that the algebras $\mathfrak{A}_1$ and $\mathfrak{A}_2$ *commute*: $A_1 A_2 = A_2 A_1$ for each pair of (selfadjoint) elements $A_1 \in \mathfrak{A}_1$, $A_2 \in \mathfrak{A}_2$;

(C)′ every pair of normal states on $\mathfrak{A}_1$ and $\mathfrak{A}_2$, respectively described by quantum-state operators $T_1 \in \mathfrak{B}_1(\mathsf{H})$, $T_2 \in \mathfrak{B}_1(\mathsf{H})$, admits a common extension on $(\mathfrak{A}_1 \cup \mathfrak{A}_2)''$ given by a quantum-state operator $T \in \mathfrak{B}_1(\mathsf{H})$, satisfying $tr(TA_1) = tr(T_1 A_1)$ and $tr(TA_2) = tr(T_2 A_2)$ for $A_1 \in \mathfrak{A}_1$ and $A_2 \in \mathfrak{A}_2$.

Property (C)′ goes under the name of W^***-independence**[2] of $\mathfrak{A}_1$ and $\mathfrak{A}_2$ [Sum90, Ham03]. What it means is we can fix states on $\mathfrak{A}_1$ and $\mathfrak{A}_2$ *independently*: for every choice of two independent states on the two parts of the system, there is a state of the overall system which encapsulates those choices.

If, in (C)′, for every given T_1, T_2 we can choose T so that $tr(TA_1A_2) = tr(T_1A_1)tr(T_2A_2)$ for every $A_1 \in \mathfrak{A}_1$ and $A_2 \in \mathfrak{A}_2$, then $\mathfrak{A}_1$ and $\mathfrak{A}_2$ are said to be **statistically independent**. In this case, T defines a normal **product state** of T_1 and T_2. **Algebraic independence** is a necessary condition for statistical independence [Sum90, Red98, Ham03]: if $A_1A_2 = 0$ then either $A_1 = 0$ or $A_2 = 0$.

From [Ham03, Proposition 11.2.16] and the picture representing the various implications on p. 364 of that book, we have the following general result.

[2]Considering *algebraic* states instead of *normal* states defines C^***-independence**, a notion eligible for generic C^*-algebras as well.

Proposition 6.44 *Under hypotheses (A)′,(B)′, (C)′, the unital* **-algebra in* $\mathfrak{A}$ *consisting of finite linear combinations of finite products of elements in* $\mathfrak{A}_1, \mathfrak{A}_2$ *is naturally isomorphic to the* algebraic *tensor product* $\mathfrak{A}_1 \otimes \mathfrak{A}_2$ *(6.4) as a unital* **-algebra. The isomorphism* ϕ *is the unique linear extension of* $A_1A_2 \mapsto A_1 \otimes A_2$*, for* $A_1 \in \mathfrak{A}_1$ *and* $A_2 \in \mathfrak{A}_2$*.*

The result can be strengthened when $\mathfrak{A}_1, \mathfrak{A}_2, \mathfrak{A}$ are *factors*, in accordance with [Tak10, vol. I, p. 228, Exercise 1].

Proposition 6.45 *Assume (A)′, (B)′ and suppose that (C)′ holds true at least for one triple* (T_1, T_2, T)*, where* T *is a product state of* T_1, T_2*. If* $\mathfrak{A}_1, \mathfrak{A}_2, \mathfrak{A}$ *are* factors*, the von Neumann algebra* $(\mathfrak{A}_1 \cup \mathfrak{A}_2)'' \subset \mathfrak{A}$ generated *by* $\mathfrak{A}_1, \mathfrak{A}_2$ *is isomorphic to* $\mathfrak{A}_1 \overline{\otimes} \mathfrak{A}_2$ *as unital* **-algebra. Hence it is also* completely *and* isometrically isomorphic *to it as a von Neumann algebra (Proposition 6.9). The isomorphism* Φ *of unital* **-algebras is a weakly-continuous extension of* ϕ*.*

The most evident difference with the elementary case is that, in general, the isomorphisms ϕ and Φ do not force a *tensor factorization* of the Hilbert space itself. However there is an important situation discovered by von Neumann and Murray where this special decomposition takes place. See, e.g., the discussion in [Tak10, vol. I, p. 229, Notes].

Proposition 6.46 *Assume that* $\mathfrak{A}_1 \subset \mathfrak{B}(\mathsf{H})$ *is a* type-I factor*, and* $\mathfrak{A}_2 = \mathfrak{A}_1'$*. Then* H *is isometrically isomorphic to* $\mathsf{H}_1 \otimes \mathsf{H}_2$ *for a suitable couple of Hilbert spaces* $\mathsf{H}_1, \mathsf{H}_2$ *and a Hilbert space isomorphism* $U : \mathsf{H} \to \mathsf{H}_1 \otimes \mathsf{H}_2$ *such that* $U\mathfrak{A}_1U^{-1} = \mathfrak{B}(\mathsf{H}_1)\overline{\otimes}\, \mathbb{C}I_2$ *and* $U\mathfrak{A}_2U^{-1} = \mathbb{C}I_1\overline{\otimes}\, \mathfrak{B}(\mathsf{H}_2)$*. (In particular,* $\mathfrak{A}_2$ *is a type-I factor too,* **-isomorphic to* $\mathfrak{B}(\mathsf{H}_2)$*.)*

It is easy to prove that the two maps arising from U, $\pi_1 : \mathfrak{A}_1 \ni A_1 \mapsto A_1' \in \mathfrak{B}(\mathsf{H}_1)$, where $UA_1U^{-1} = A_1' \otimes I_2$, and the analogous π_2 are unital *-isomorphisms identifying the von Neumann algebras $\mathfrak{A}_i$ and $\mathfrak{B}(\mathsf{H}_i)$. These *-isomorphisms are actually isometric, weakly and strongly continuous due to Proposition 6.9. The claim of Proposition 6.46 can be rephrased by saying that the map $A_1A_2 \mapsto \pi_1(A_1) \otimes \pi_2(A_2)$, with $A_1 \in \mathfrak{A}_1$ and $A_2 \in \mathfrak{A}_2$, extends to a spatial isomorphism of the von Neumann algebras $\mathfrak{B}(\mathsf{H}) = (\mathfrak{A}_1 \cup \mathfrak{A}_2)''$ and $\pi_1(\mathfrak{A}_1)\overline{\otimes}\, \pi_2(\mathfrak{A}_2)$.

Remark 6.47 Under the hypotheses (and consequent thesis) of Proposition 6.46 with $\mathfrak{A} := \mathfrak{B}(\mathsf{H})$, (A)′ and (B)′ are evidently true, while (C)′ holds in its stronger version of *statistical independence*. In fact, if $T_1 \in \mathfrak{B}_1(\mathsf{H})$ represents a normal state on $\mathfrak{A}_1$, then $T_1' = U^{-1}T_1U \in \mathfrak{B}_1(\mathsf{H}_1 \otimes \mathsf{H}_2)$ represents a normal state on $\pi_1(\mathfrak{A}) \otimes \mathbb{C}I_2 = U^{-1}\mathfrak{A}_1U$ with $tr(T_1A_1) = tr(T_1'\pi_1(A_1) \otimes I_2)$ for every $A_1 \in \mathfrak{A}_1$. There is however (exercise) another positive unit-trace operator $T_1'' \in \mathfrak{B}_1(\mathsf{H}_1)$ such that $tr(T_1'\pi_1(A_1) \otimes I_2) = tr(T_1''\pi_1(A_1))$ for every $A_1 \in \mathfrak{A}_1$. Similarly for T_2 and a corresponding pair T_2', T_2''. Eventually, $T := U(T_1'' \otimes T_2'')U^{-1}$ satisfies $tr(TA_1A_2) = tr(T_1A_1)tr(T_2A_2)$ due to the first formula in Proposition 4.56 (c). ■

Example 6.48 As elementary example of "hidden" independent subsystems, consider a quantum system with Hilbert space $\mathsf{H} := \mathbb{C}^4$ (e.g., a physical system whose Hamiltonian has four eigenvalues and one-dimensional eigenspaces) and define the algebras of observables of two subsystems as (I henceforth denotes the identity operator on $\mathfrak{B}(\mathbb{C}^2)$)

$$\mathfrak{A}_1 := \left\{ \begin{bmatrix} A & 0 \\ 0 & A \end{bmatrix} \middle| A \in \mathfrak{B}(\mathbb{C}^2) \right\}, \quad \text{so that} \quad \mathfrak{A}_2 := \mathfrak{A}_1' = \left\{ \begin{bmatrix} \alpha I & \beta I \\ \gamma I & \delta I \end{bmatrix} \middle| \begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix} \in \mathfrak{B}(\mathbb{C}^2) \right\}.$$

$\mathfrak{A}_1$ is a factor as one immediately proves using that $\mathfrak{B}(\mathbb{C}^2)$ is irreducible. It is necessarily of type I (in fact, type I_2), since the overall space is finite-dimensional. Proposition 6.46 and Remark 6.47 imply that the two subalgebras represent independent subsystems (satisfying (A)′,(B)′,(C)′) which are *statistically independent*. As the reader can check, the unitary operator U of Proposition 6.46 is the unique linear map $U : \mathbb{C}^4 \to \mathbb{C}^2 \otimes \mathbb{C}^2$ such that $U(1,0,0,0)^t = (1,0)^t \otimes (1,0)^t$, $U(0,1,0,0)^t = (0,1)^t \otimes (1,0)^t$, $U(0,0,1,0)^t = (1,0)^t \otimes (0,1)^t$, and $U(0,0,0,1)^t = (0,1)^t \otimes (0,1)^t$. With these definitions,

$$U \begin{bmatrix} A & 0 \\ 0 & A \end{bmatrix} U^{-1} = A \otimes I \quad \text{and} \quad U \begin{bmatrix} \alpha I & \beta I \\ \gamma I & \delta I \end{bmatrix} U^{-1} = I \otimes \begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix},$$

and the maps

$$\pi_1 : \mathfrak{A}_1 \ni \begin{bmatrix} A & 0 \\ 0 & A \end{bmatrix} \mapsto A \in \mathfrak{B}(\mathbb{C}^2) \quad \text{and} \quad \pi_2 : \mathfrak{A}_2 \ni \begin{bmatrix} \alpha I & \beta I \\ \gamma I & \delta I \end{bmatrix} \mapsto \begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix} \in \mathfrak{B}(\mathbb{C}^2)$$

are injective unital *-homomorphisms. Throughout, $\mathsf{H}_1 := \mathbb{C}^4$ and $\mathsf{H}_2 := \mathbb{C}^2$ are the standard Hermitian inner product spaces, and $\mathbb{C}^2 \otimes \mathbb{C}^2$ comes equipped with the standard Hermitian inner product of Hilbert tensor products. It is worth stressing that, with the chosen subsystems, the unit vector $\Psi_+ = 2^{-1/2}(1,0,0,1)^t \in \mathsf{H}$ is actually an entangled state for the subsystems: it is a *Bell state* (5.9) producing the maximum possible violation of the BCHSH inequality. This fact can be tested if we are able to give a physical meaning to the selfadjoint operators of the two subalgebras in terms of observables, and concoct the experimental procedure to evaluate them. ■

In elementary QM, statistical independence is natural. By reversing the construction of Sect. 4.4.8, the algebras of observables of the subsystems S_i are assumed to be the full $\mathfrak{B}(\mathsf{H}_i)$ (here coinciding with $\pi_i(\mathfrak{A}_i)$), hence type I factors, and the Hilbert space of the compound is supposed to be $\mathsf{H}_1 \otimes \mathsf{H}_2$ (here $U(\mathsf{H})$). The first formula in Proposition 4.56 (c) is just stating statistical independence.

It should be evident from this analysis that every definition of *entangled state* on a system described by the von Neumann algebra $\mathfrak{A} = \mathfrak{A}(\mathsf{H})$, which can be given in this general context, depends heavily on the choice of the possible independent subsystems $\mathfrak{A}_1$ (here a factor of type I) and $\mathfrak{A}_2 = \mathfrak{A}'_1$ in the decomposition of $\mathfrak{A}$. *A given normal state on* $\mathfrak{A}$ *may be entangled for a certain choice of subsystems and not entangled for another*. Actually, the entire discussion of Chap. 5 on the BCHSH inequality and its quantum failure can be lifted to this more abstract and general level, also for independent subalgebras which are not type-I factors [Sum90, Red98, Ham03].

6.4.2 The Split Property

If we keep all the assumptions of Proposition 6.46 except the request that the factor $\mathfrak{A}_1$ be of type I the pair $\mathfrak{A}_1, \mathfrak{A}_2$ turn out to be W^*-independent, but statistical independence *necessarily fails* [Ham03]. So, with reference to a composite quantum system as in Proposition 6.46, *statistical independence holds only for type-I factors*, and this fact separates general quantum theory and elementary QM rather starkly. As already pointed out, in Local Quantum Field Theory in Minkowski spacetime, the von Neumann algebras of observables associated to relevant regions of spacetime are not of type I, but rather type III [Sum90, Haa96, Ara09, Yng05]. Therefore, using *Hilbert tensor products* to describe independent subsystems associated to causally separated regions and supposing statistical independence may be *mathematically and physically inappropriate*, unless very peculiar technical conditions are in place. One such is the so-called *split property* [Sum90, Haa96, Ara09, Yng05, Ham03], which generalizes the hypotheses of Proposition 6.46.

Definition 6.49 Two commuting von Neumann algebras $\mathfrak{A}_1, \mathfrak{A}_2$ satisfy the **split property** if there exists a type-I factor $\mathfrak{N}$ with $\mathfrak{A}_1 \subset \mathfrak{N}$ and $\mathfrak{A}_2 \subset \mathfrak{N}'$. ■

There is a technical result [Ham03] relating the split property to the tensor product. Let $\mathfrak{N}$ be a von Neumann algebra on a Hilbert space K (different from H in general). A homomorphism of unital *-algebras $\pi : \mathfrak{N} \to \mathfrak{B}(\mathsf{H})$ is said to be **normal** if for every unit vector $x \in \mathsf{H}$ there exists a positive unit-trace operator $T_x \in \mathfrak{B}(\mathsf{K})$ such that $\langle x|\pi(A)x\rangle = tr(T_x A)$ if $A \in \mathfrak{N}$. In this case $\pi(\mathfrak{N}) \subset \mathfrak{B}(\mathsf{H})$ is a von Neumann algebra as well [Ham03, p. 64]. We have the following result [Ham03, Sum90].

Proposition 6.50 *A pair of commuting von Neumann algebras* $\mathfrak{A}_1, \mathfrak{A}_2$ *on a common Hilbert space* H *satisfies the split property if and only if there exist Hilbert spaces* H_i *and normal, injective and unital* **-homomorphisms* $\pi_i : \mathfrak{A}_i \to \mathfrak{B}(\mathsf{H}_i)$, $i = 1, 2$, *such that the map* $A_1 A_2 \mapsto \pi_1(A_1) \otimes \pi_2(A_2)$, *with* $A_1 \in \mathfrak{A}_1$, $A_2 \in \mathfrak{A}_2$, *extends to a spatial isomorphism of the von Neumann algebras* $(\mathfrak{A}_1 \cup \mathfrak{A}_2)''$ *and* $\pi_1(\mathfrak{A}_1)\overline{\otimes}\,\pi_2(\mathfrak{A}_2)$.

Overlooking these issues is sometimes a source of misunderstandings when we deal with technically delicate subjects: for instance, the thermal properties of Minkowski vacuum restricted to the two causally separated Rindler wedges. Similar caution is recommended when one tries to construct quantum gravity theories within quantum information approaches based on finite-dimensional Hilbert spaces, where the tensor product of the subsystems' Hilbert spaces is a natural tool.

Generally speaking, when one handles a composite quantum system, the overall system's algebra of observables is always *isomorphic* to a tensor product, *of some sort or other*, of the algebras of observables of the subsystems. Which sort depends strictly on the kind of algebra one uses (*-algebra, C^*-algebra, von Neumann algebra) and the type of state (normal, algebraic) under requirements akin to (A)$'$, (B)$'$, (C)$'$. If the algebra of observables is defined in terms of unital C^*-algebras, as will happen in the last chapter, the notion of tensor product is even more delicate: for there exist many possibilities to define such an object, none physically more meaningful than the others [KaRi97, Tak10, BrRo02].

Chapter 7
Quantum Symmetries

The notion of *symmetry* in Quantum Theory is quite abstract. There are at least three distinct ideas, respectively due to Wigner, Kadison and Segal [Sim76]. We shall focus on the first two only, plus a fourth type which crops up naturally from our formulation of the quantum theory. The exhaustive discussion of [Lan17] introduces six different definitions of quantum symmetry and discusses their equivalence.

7.1 Quantum Symmetries According to Kadison and Wigner

Generally speaking, symmetries are supposed to describe mathematically certain concrete transformations acting either on the physical system or on the instruments used to analyze the system. From a very general standing a *symmetry* is an *active* transformation of either the quantum system or, by duality, the observables representing physical instruments. It is further required that

(1) the transformation is *bijective*, in the sense that

   (a) every state of the system or observable representing devices (according to the notion employed) can be reached by transforming the initial state or observable;
   (b) every symmetry admits an inverse;

(2) the transformation should *preserve some mathematical structure* of the space of the states or the space of observables. This is what distinguishes between the various notions of symmetry.

Alas, there exists in the literature an intrinsically different notion of *gauge symmetry*. A gauge symmetry is **not** a symmetry in the above sense. A symmetry acts on the physical system by explicitly changing its state or the (observables representing the) instruments, whereas a *gauge symmetry* is a mathematical transformation that

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does not change anything that is directly related to measurements, hence it does not affect the system's states nor the instruments. An example for a system with algebra of observables $\mathfrak{R}$ is the action of elements U of *commutant group* $\mathfrak{G}_{\mathfrak{R}}$ (the group of unitary operators in $\mathfrak{R}'$) on quantum probability measures on $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ describing the states of a quantum system, see Sect. 6.3.2. Quantum states associated to two measures ρ and $\rho(U \cdot U^{-1})$ cannot be distinguished by acting on $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ because $UPU^{-1} = P$ for every $P \in \mathscr{L}_{\mathfrak{R}}(\mathsf{H})$, as we observed in Sect. 6.3.4 from a slightly different perspective.

Nevertheless the idea of gauge symmetry is technically very useful. In some fundamental theories the initial relevant algebra of operators $\mathfrak{F}$ is larger (in the von Neumann algebra framework it is $\mathfrak{B}(\mathsf{H})$ itself) than the algebra of observables $\mathfrak{R}$. The latter is defined as the von Neumann algebra made of the operators in $\mathfrak{F}$ commuting with a suitable faithful and strongly-continuous representation U of a certain compact group G named the *global gauge group of internal symmetries*: $\mathfrak{R} = U'$. (As a consequence $U \subset \mathfrak{G}_{\mathfrak{R}}$ and $U' = \mathfrak{G}'_{\mathfrak{R}} = \mathfrak{R}$.) We have already seen this procedure at work in the first part of Sect. 6.3.2. When we deal with *spinor fields*, for instance, there are operators, in particular *spinor field operators*, that cannot be interpreted as observables (or complex combinations of observables) because they violate some fundamental physical requisite (typically *causality relations*) ascribed to meaningful observables. However, other operators constructed out of spinor field operators (typically *currents*) are observables. One way to select the observables inside the larger algebra $\mathfrak{F}$, thus defining the von Neumann algebra $\mathfrak{R}$, is to require that operators representing (linear combinations of) observables are fixed under the action of a suitable compact group G—in this case the Abelian group $U(1)$—of unitary operators belonging in the commutant $\mathfrak{G}_{\mathfrak{R}}$ of $\mathfrak{R}$, as in Sect. 6.3.2. Then $\mathfrak{R}$ turns out to be a sum of irreducible von Neumann algebras $\mathfrak{R}_k = \mathfrak{B}(\mathsf{H}_k)$ on an orthogonal sum of sectors H_k decomposing H. The procedure is general and works also when the commutant is non-Abelian, as in chromodynamics where $G = SU(3)$ (*colour*). Our $\mathfrak{R}$ is a sum of *factors* $\mathfrak{R}_k$ defined on an orthogonal sum of G-invariant sectors H_k. In this sense *internal symmetries* (distinct from those of the spacetime's geometry) are *not* symmetries at all, since they do not act on observables (see [Haa96] for further discussions related to locality and the so-called *DHR analysis* of superselection rules in the algebraic formulation).

7.1.1 Wigner Symmetries, Kadison Symmetries and Ortho-Automorphisms

We henceforth consider a quantum system described on the Hilbert space H. We assume that H is either the whole Hilbert space in the absence of superselection charges, or it denotes a single coherent sector when Abelian superselection rules are on. Let $\mathscr{S}(\mathsf{H})$ indicate the convex body of *quantum-state operators* on $\mathfrak{B}(\mathsf{H})$: these are positive trace-class operators of trace one representing *normal states* on $\mathfrak{B}(\mathsf{H})$

(see Sect. 6.3.4), and call $\mathscr{S}_p(\mathsf{H})$ the subset of operators representing *pure normal states* (orthogonal projectors onto one-dimensional subspaces). Everything refers to one sector if need be.

Two notions of symmetry can be defined when we look at the space of normal states. Since on separable Hilbert spaces states are actually better described in terms of σ-additive probability measures on $\mathscr{L}(\mathsf{H})$, the definitions above make totally sense in physics when the aforementioned measures are faithfully described by quantum-state operators under Gleason's theorem. This is the case when H is separable with dimension $\neq 2$. (As we said, separability can be dropped, but then normal states correspond to the smaller subset of *completely-additive* probability measures.)

Definition 7.1 If H is a Hilbert space, we have the following types of symmetries.

(a) A **Wigner symmetry** is a bijective map

$$s_W : \mathscr{S}_p(\mathsf{H}) \ni \langle\psi|\ \rangle\psi \to \langle\psi'|\ \rangle\psi' \in \mathscr{S}_p(\mathsf{H})$$

that preserves transition probabilities:

$$|\langle\psi_1|\psi_2\rangle|^2 = |\langle\psi'_1|\psi'_2\rangle|^2 \quad \text{if} \quad \psi_1\,,\,\psi_2 \in \mathsf{H} \ \ \text{with}\ \ ||\psi_1|| = ||\psi_2|| = 1\,.$$

(b) A **Kadison symmetry** is a bijection

$$s_K : \mathscr{S}(\mathsf{H}) \ni T \to T' \in \mathscr{S}(\mathsf{H})$$

that preserves linear convexity in the space of the states:

$$(pT_1 + qT_2)' = pT'_1 + qT'_2 \quad \text{if} \quad T_1, T_2 \in \mathscr{S}(\mathsf{H}) \quad \text{and} \quad p, q \geq 0 \text{ with } p + q = 1.$$

■

Remark 7.2 Wigner symmetries are well defined even if unit vectors define pure states just up to phase, as the reader can immediately prove, because transition probabilities are not affected by the phase ambiguity. ■

There is an apparently different approach to define symmetries that focuses on elementary observables in $\mathscr{L}(\mathsf{H})$ instead of normal states in $\mathscr{S}(\mathsf{H})$. Symmetries are viewed as active transformations preserving the lattice structure of elementary observables. From a practical viewpoint, these symmetries are interpreted as some sort of reversible active transformations on the measuring instruments. These transformations must preserve the *logical connectives* between elementary propositions.

Definition 7.3 If H is a Hilbert space, a **symmetry of elementary observables** is a map $h : \mathscr{L}(\mathsf{H}) \to \mathscr{L}(\mathsf{H})$ such that

(i) h is bijective,
(ii) $h(P) \geq h(Q)$ if $P, Q \in \mathscr{L}(\mathsf{H})$ and $P \geq Q$,
(iii) $h(I - P) = I - h(P)$ if $P \in \mathscr{L}(\mathsf{H})$.

Another name is **ortho-automorphism** of $\mathscr{L}(\mathsf{H})$. ■

Remark 7.4

(a) It is easy to prove that an ortho-automorphism $h : \mathscr{L}(\mathsf{H}) \to \mathscr{L}(\mathsf{H})$ preserves the entire complete orthocomplemented lattice structure. In particular

  (i) $h(0) = 0$ and $h(I) = I$,
  (ii) $h(\vee_{j\in J} P_j) = \vee_{j\in J} h(P_j)$, $h(\wedge_{j\in J} P_j) = \wedge_{j\in J} h(P_j)$ for every family $\{P_j\}_{j\in J} \subset \mathscr{L}(\mathsf{H})$.

  Furthermore, $h^{-1} : \mathscr{L}(\mathsf{H}) \to \mathscr{L}(\mathsf{H})$ is evidently an ortho-automorphism.

(b) As the reader can straightforwardly prove, a symmetry of elementary observables induces a Kadison symmetry by duality, *if we assume Gleason's theorem 4.47 holds*. In fact, if $T \in \mathscr{S}(\mathsf{H})$ and h is an ortho-automorphism, then

$$\rho_{T,h} : \mathscr{L}(\mathsf{H}) \ni P \mapsto tr(Th(P)) \in [0, 1]$$

  is a probability measure on $\mathscr{L}(\mathsf{H})$. The proof is trivial and relies on the fact that h preserves the lattice structures. Therefore there exists exactly one $T'_h \in \mathscr{S}(\mathsf{H})$ such that

$$\rho_{T,h}(P) = tr(T'_h P) \quad \text{for every } P \in \mathscr{L}(\mathsf{H}).$$

  By construction, $s_K^{(h)} : T \mapsto T'_h$ preserves the convex structure of $\mathscr{S}(\mathsf{H})$. Indeed,

$$\left(s_K^{(h)}(pT_1 + qT_2)\right)(P) = tr\left((pT_1 + qT_2)h(P)\right) = \left(ps_K^{(h)}(pT_1) + qs_K^{(h)}(T_2)\right)(P)\,.$$

  Since $P \in \mathscr{L}(\mathsf{H})$ is arbitrary,

$$s_K^{(h)}(pT_1 + qT_2) = ps_K^{(h)}(pT_1) + qs_K^{(h)}(T_2)\,,$$

  so $\left(s_K^{(h)}\right)^{-1} = s_K^{(h^{-1})}$.

(c) Symmetries of all three types do exist. If $U : \mathsf{H} \to \mathsf{H}$ is a unitary operator, the maps

$$s_W^{(U)} : \mathscr{S}_p(\mathsf{H}) \ni \langle\psi|\ \rangle\psi \mapsto \langle U\psi|\ \rangle U\psi \in \mathscr{S}_p(\mathsf{H})\,,$$

$$s_K^{(U)} : \mathscr{S}(\mathsf{H}) \ni T \to UTU^{-1} \in \mathscr{S}(\mathsf{H})$$

  and

$$h^{(U)} : \mathscr{L}(\mathsf{H}) \ni P \mapsto U^{-1}PU \in \mathscr{L}(\mathsf{H})$$

are respectively a Wigner symmetry, a Kadison symmetry and an ortho-automorphism of $\mathscr{L}(\mathsf{H})$. If Gleason's theorem holds, furthermore, $s_K^{(U)}$ is induced by $h^{(U)}$ by Remark (b).

(d) When Abelian superselection rules occur, a more general notion of symmetry exist that is defined between different superselection sectors. An example would be a bijection from $\mathscr{L}(\mathsf{H}_k)$ to $\mathscr{L}(\mathsf{H}_h)$, $k \neq h$, preserving the orthocomplemented lattice structure, or similar maps between normal states $\mathscr{S}(\mathsf{H}_k)$ and $\mathscr{S}(\mathsf{H}_h)$ that preserve the convex structure. Or even a bijective map between $\mathscr{S}_p(\mathsf{H}_k)$ and $\mathscr{S}_p(\mathsf{H}_h)$ preserving transition probabilities. A typical example of symmetry that swaps superselection sectors is the *charge conjugation*. We shall not discuss this sort of symmetries (see [Mor18]), but the reader can easily extend the theory developed below to these cases. ■

7.1.2 The Theorems of Wigner, Kadison and Dye

Although the previous three definitions are evidently different in nature, characterizations are in place (Theorem 7.6) to guarantee they lead to the same mathematical object. We need a preliminary definition first.

Definition 7.5 Let H, H' be Hilbert spaces. A map $U : \mathsf{H} \to \mathsf{H}'$ is called an **anti-unitary operator** if it is surjective, isometric and

$$U(ax + by) = \overline{a}Ux + \overline{b}Uy$$

when $x, y \in \mathsf{H}$ and $a, b \in \mathbb{C}$. ■

If $U : \mathsf{H} \to \mathsf{H}'$ is anti-unitary, then $\langle Ux|Uy\rangle = \overline{\langle x|y\rangle'}$ for $x, y \in \mathsf{H}$, by polarization.

We come to the announced theorem.

Theorem 7.6 *Let* $\mathsf{H} \neq \{0\}$ *be a Hilbert space.*

(a) **[Wigner's theorem]** *For every Wigner symmetry* s_W *there exists an operator* $U : \mathsf{H} \to \mathsf{H}$ *such that*

$$s_W : \langle\psi|\ \rangle\psi \mapsto \langle U\psi|\ \rangle U\psi\ , \quad \forall \langle\psi|\ \rangle\psi \in \mathscr{S}_p(\mathsf{H})\ . \tag{7.1}$$

U can be unitary or anti-unitary, but when $\dim(\mathsf{H}) \neq 1$ *the choice is fixed by* s_W.

If $\dim \mathsf{H} > 1$*, U and U' are associated to the same s_W if and only if $U' = e^{ia}U$ for $a \in \mathbb{R}$.*

(b) **[Kadison's Theorem]** *For every Kadison symmetry* s_K *there exists an operator* $U : \mathsf{H} \to \mathsf{H}$ *such that*

$$s_K : T \mapsto UTU^{-1}\ , \quad \forall T \in \mathscr{S}(\mathsf{H})\ . \tag{7.2}$$

U can be unitary or anti-unitary, but when $\dim(\mathsf{H}) \neq 1$ *the choice is fixed by* s_K.

If $\dim \mathsf{H} > 1$*, U and U' are associated to the same s_K if and only if* $U' = e^{ia}U$ *for* $a \in \mathbb{R}$.

(c) **[Dye's Theorem (Simplest Version)]** *If* H *is separable and* $\dim(\mathsf{H}) \neq 2$*, for every ortho-automorphism* $h : \mathscr{L}(\mathsf{H}) \to \mathscr{L}(\mathsf{H})$ *there exists an operator* $U : \mathsf{H} \to \mathsf{H}$ *such that*

$$h : P \mapsto U^{-1}PU \,, \quad \forall P \in \mathscr{L}(\mathsf{H}) \,. \tag{7.3}$$

U is unitary or anti-unitary, but for $\dim(\mathsf{H}) \neq 1$ *the choice is fixed by h.*

For $\dim \mathsf{H} > 1$*, U and U' are associated to the same h if and only if* $U' = e^{ia}U$ *for* $a \in \mathbb{R}$.

(d) *Conversely, a unitary or anti-unitary map* $U : \mathsf{H} \to \mathsf{H}$ *simultaneously defines a Wigner symmetry (the same one defined by* $e^{ia}U$ *for any* $a \in \mathbb{R}$*), a Kadison symmetry and an ortho-automorphism by recipes (7.1)–(7.3), respectively.*

Proof Statement (d) is trivial. The existence of U in (a) is difficult and can be found, e.g., in [Sim76, Var07, Lan17, Mor18]. The existence in case (b) comes from (a) and can be read in [Sim76, Lan17, Mor18]. As for (c) it is an immediate consequence of case (b) and Remark 7.4 (b).

Let us address the issue of uniqueness. If $\dim \mathsf{H} = 1$, the U map corresponding to a given symmetry can be taken unitary or anti-unitary as one pleases. The proof is direct and can be obtained by identifying H with $\mathbb{C}$. The fact that, for $\dim \mathsf{H} > 1$, U is fixed up to phase goes as follows. Suppose U and V are both unitary or both anti-unitary and define the same symmetry (any kind). Then $UPU^{-1} = VPV^{-1}$, for some orthogonal projector $P = \langle\psi|\ \rangle\psi$ onto a one-dimensional subspace. This P can be viewed simultaneously as an element of $\mathscr{S}_p(\mathsf{H})$, $\mathscr{S}(\mathsf{H})$, and $\mathscr{L}(\mathsf{H})$. As $V^{-1}UP = PV^{-1}U$, then $V^{-1}U\psi = a_\psi\psi$ for some complex vector $a_\psi \in \mathsf{H}$. If $\dim \mathsf{H} > 1$, we consider two orthogonal elements $\psi, \psi' \in \mathsf{H}$ with unit norm. Hence

$$\frac{a_\psi\psi + a_{\psi'}\psi}{\sqrt{2}} = V^{-1}U\frac{\psi+\psi'}{\sqrt{2}} = a_{\frac{\psi+\psi'}{\sqrt{2}}}\frac{\psi+\psi'}{\sqrt{2}} \,.$$

Consequently $\left(a_{\frac{\psi+\psi'}{\sqrt{2}}} - a_{\psi'}\right)\psi' = -\left(a_{\frac{\psi+\psi'}{\sqrt{2}}} - a_\psi\right)\psi$. Since the vectors are orthonormal, the only possibility is that the coefficients vanish. In particular $a_{\psi'} = a_\psi$. If $N \subset \mathsf{H}$ is a Hilbert basis, we therefore have $V^{-1}U\psi u = au$ for every $u \in N$ and for a unique constant $a \in \mathbb{C}$. Therefore

$$V^{-1}U\phi = V^{-1}U\sum_{u\in N}\langle u|\phi\rangle u = \sum_{u\in N}\langle u|\phi\rangle au = a\phi \quad \forall\phi \in \mathsf{H} \,.$$

But $V^{-1}U$ is unitary so $|a| = 1$ and $U = aV$.

An analogous argument proves that, for $\dim \mathsf{H} > 1$, U and V must be both unitary or both anti-unitary. In fact, if that were not the case, the above reasoning would prove that the anti-unitary operator $V^{-1}U$, for every Hilbert basis N, acted as $V^{-1}Uu = a_N u$ with $u \in N$ and $a_N \in \mathbb{C}$. Define a new Hilbert basis N' whose elements are those of N plus an extra element $u'_0 := iu_0$. Then the contradiction ensues: if $u \neq u_0$ we would have $a_{N'}u = V^{-1}Uu = a_N u$, but also $ia_{N'}u_0 = a_{N'}u'_0 = V^{-1}Uu'_0 = V^{-1}Uiu_0 = -iV^{-1}Uu_0 = -ia_N u_0$. Hence $a_{N'} = a_N = -a_N$ implying $a_N = 0$ and therefore that $V^{-1}U$ is the zero operator. This is not possible because $V^{-1}U$ is isometric by hypothesis and $\mathsf{H} \neq \{0\}$. □

Remark 7.7 If Abelian superselection rules are present, quantum symmetries are similarly described using unitary or anti-unitary operators either acting on a single coherent sector or swapping different sectors [Mor18]. ■

7.1.3 *Action of Symmetries on Observables and Physical Interpretation*

If a unitary or anti-unitary operator V represents a (Kadison or Wigner) symmetry s, it defines an action on observables, too. If A is an observable (a selfadjoint operator on H), we define the **transformed observable** under the action of s as

$$s^*(A) := V^{-1}AV \,. \tag{7.4}$$

Obviously $D(s^*(A)) = V(D(A))$. This is the **dual action** on an observable of a Kadison/Wigner symmetry. There is another similar action, the **inverse dual action**

$$s^{*-1}(A) := VAV^{-1} \,. \tag{7.5}$$

Again $D(s^{*-1}(A)) = V(D(A))$. It is evident that these definitions are not affected by the phase ambiguity in the choice of V when s is given. Moreover, by Proposition 3.60 (j), the spectral measure of $s^*(A)$ is

$$P_E^{(s^*(A))} = V^{-1}P_E^{(A)}V = s^*(P_E^{(A)}),$$

as expected, and this is nothing but the ortho-automorphism induced by the unitary operator U (s^{*-1} is the inverse ortho-automorphism.) The punchline is that *a symmetry's action on an observable A is completely equivalent to the same action on the elementary observables of the PVM $P^{(A)}$*. This fact is in perfect agreement with the physical idea, mathematically supported by the spectral theorem, that an observable (a selfadjoint operator) contains the same physical information as its PVM.

The meaning of the *inverse dual action* s^{*-1} on observables should be evident. The probability that the observable $s^{*-1}(A)$ produces outcome E when the state is

$s(T)$ $\left(\text{namely } tr\left(P_E^{(s^{*-1}(A))}s(T)\right)\right)$ equals the probability that the observable A produces outcome E when the normal state is $T \in \mathscr{S}(\mathsf{H})$ (that is $tr(P_E^{(A)}T)$). In other words, changing observables and states simultaneously and coherently does not alter a thing. Indeed

$$tr\left(P_E^{(s^{*-1}(A))}s(T)\right) = tr\left(VP_E^{(A)}V^{-1}VTV^{-1}\right) = tr\left(VP_E^{(A)}TV^{-1}\right)$$
$$= tr\left(P_E^{(A)}TV^{-1}V\right) = tr\left(P_E^{(A)}T\right) .$$

So, the inverse dual action of a Kadison/Wigner symmetry on observables is the transformation that reverses the symmetry's action on states. As an example think of an isolated quantum system in an inertial frame: a translation along the z-axis can be annulled by a z-translation of the origin.

The meaning of the *dual action* s^* on observables is similarly clear. *This operation on observables (whilst keeping states fixed) produces the same result as the action of* s *on states (keeping observables fixed).*

$$tr\left(P_E^{(s^*(A))}T\right) = tr\left(V^{-1}P_E^{(A)}VT\right) = tr\left(P_E^{(A)}VTV^{-1}\right) = tr\left(P_E^{(A)}s(T)\right) .$$

Again on an isolated quantum system in an inertial frame: as far as measurements of the position are concerned, translating along the z-axis is equivalent to displacing the origin in the opposite direction.

Example 7.8

(1) Fixing an inertial reference frame, the pure state of a quantum particle is defined, up to phase, as a unit element ψ of $L^2(\mathbb{R}^3, d^3x)$, where $\mathbb{R}^3$ stands for the rest three-space of the reference frame. The *group of isometries* $IO(3)$ of the standard (Euclidean) $\mathbb{R}^3$ acts on states by Wigner and Kadison symmetries. If

$$(R, t) : \mathbb{R}^3 \ni x \mapsto Rx + t \in \mathbb{R}^3$$

indicates the action of the generic element $(R, t) \in IO(3)$ on $x \in \mathbb{R}^3$, where $R \in O(3)$ and $t \in \mathbb{R}^3$, the associated quantum (Wigner) symmetry $s_{(R,t)}(\langle\psi|\ \rangle\psi) = \langle U_{(R,t)}\psi|\ \rangle U_{(R,t)}\psi$ is completely determined by the unitary operators

$$(U_{(R,t)}\psi)(x) := \psi((R,t)^{-1}x)$$
$$= \psi(R^{-1}(x-t)) , \quad x \in \mathbb{R}^3 , \psi \in L^2(\mathbb{R}^3, d^3x) , \quad ||\psi|| = 1 .$$

As the Lebesgue measure is $IO(3)$-invariant, $U_{(R,t)}$ is isometric and also unitary because it is surjective, as it admits $U_{(R,t)^{-1}}$ as right inverse.

It is furthermore easy to prove that

$$U_{(I,0)} = I \,, \quad U_{(R,t)}U_{(R',t')} = U_{(R,t)\circ(R',t')} \,, \quad \forall (R,t), (R',t') \in IO(3) \,. \tag{7.6}$$

(2) The transformation called *time reversal* corresponds classically to inverting the sign of all the velocities of the physical system. It is possible to prove [Mor18] (see also Exercise 7.33 (4) below) that in QM and systems whose energy is bounded below but not above, the time-reversal symmetry cannot be represented by unitary transformations, only anti-unitary ones. In the simplest situation, such as (1), time reversal is defined (up to phase) by the anti-unitary operator

$$(T\psi)(x) := \overline{\psi(x)} \,, \quad x \in \mathbb{R}^3 \,, \psi \in L^2(\mathbb{R}^3, d^3x) \,, \quad ||\psi|| = 1 \,.$$

(3) In relationship to example (1), let us focus on the group of displacements along x_1. These elements $\mathbb{R}^3 \ni x \mapsto x + u\mathbf{e}_1$ of $IO(3)$ are parametrised by $u \in \mathbb{R}$, where $\mathbf{e}_1$ denotes the unit vector in $\mathbb{R}^3$ along x_1. For every value of the parameter u, let s_u indicate the (Wigner) quantum symmetry $s_u(\langle\psi|\ \rangle\psi) = \langle U_u\psi|\ \rangle U_u\psi$ with

$$(U_u\psi)(x) = \psi(x - u\mathbf{e_1}) \,, \quad u \in \mathbb{R} \,.$$

The inverse dual action of this symmetry on the observable X_k turns out to be

$$s_u^{*-1}(X_k) = U_u X_k U_u^{-1} = X_k - u\delta_{k1} I \,, \quad u \in \mathbb{R} \,.$$

■

7.2 Groups of Quantum Symmetries

As in example (1) above, in physics one deals very often with *groups of symmetries*. In other words, there is a certain group G, with neutral element e and product $\cdot$, and one associates to each element $g \in G$ a symmetry s_g (whether Kadison or Wigner is immaterial here, in view of Theorem 7.6). In turn, s_g is related to an operator U_g, unitary or anti-unitary. This correspondence however is ambiguous, because we are free to modify operators by arbitrary phases. This section is devoted to the study of this sort of representations.

7.2.1 Unitary(-Projective) Representations of Groups of Quantum Symmetries

Let G be a group, which is supposed to represent a group of symmetries of a quantum system described on the Hilbert space H, with $\dim \mathsf{H} > 1$. The action is in practice implemented by unitary operators $U_g \in \mathfrak{B}(\mathsf{H})$, which gives us a map $G \ni g \mapsto U_g$. We know that multiplying U_g by a phase preserves the symmetry associated to it. It would be nice to fix U_g, though still allowing for arbitrary phase changes, in such a way that the map $G \ni g \mapsto U_g$ became a *unitary representation* of G on H.

Definition 7.9 A homomorphism $G \ni g \mapsto U_g$ from a group G to the group of unitary operators on the Hilbert space H is called a **unitary representation** of G on H.

Equivalently, a unitary representation $G \ni g \mapsto U_g$ is a map satisfying

$$U_e = I\ , \quad U_g U_{g'} = U_{g\cdot g'}\ , \quad U_g^{-1} = U_g^*\ , \quad \forall g, g' \in G\ . \tag{7.7}$$

■

Formulas (7.6) from Example 7.8 (1) show that unitary representations of group of symmetries do exist. Generally speaking, however, requirement (7.7) does not hold. If G is a group of quantum symmetries the only thing guaranteed in physics is that every U_g is unitary (or anti-unitary, but here we shall stick to the former only) and that $U_{g\cdot g'}$ equals $U_g U_{g'}$ only *up to phase*:

$$U_g U_{g'} U_{g\cdot g'}^{-1} = \omega(g, g') I \quad \text{with } \omega(g, g') \in \mathbb{T} \text{ for all } g, g' \in G. \tag{7.8}$$

(As usual, $\mathbb{T} := \{z \in \mathbb{C} \mid |z| = 1\}$.) For $g = g' = e$ this gives in particular

$$U_e = \omega(e, e) I\ . \tag{7.9}$$

The numbers $\omega(g, g')$ are called **multipliers**. They cannot be completely arbitrary, since associativity $((U_{g_1} U_{g_2}) U_{g_3} = U_{g_1}(U_{g_2} U_{g_3}))$ yields

$$\omega(g_1, g_2)\omega(g_1 \cdot g_2, g_3) = \omega(g_1, g_2 \cdot g_3)\omega(g_2, g_3)\ , \quad \forall g_1, g_2, g_3 \in G\ , \tag{7.10}$$

which also implies, for suitable choices of g_1, g_2, g_3 (the reader should prove it),

$$\omega(g, e) = \omega(e, g) = \omega(g', e)\ , \quad \omega(g, g^{-1}) = \omega(g^{-1}, g)\ , \quad \forall g, g' \in G\ . \tag{7.11}$$

All that leads us to the following important definition.

Definition 7.10 If G is a group, a map $G \ni g \mapsto U_g$—where the U_g are unitary operators on the Hilbert space H—is called a **unitary-projective representation** of

G on H if (7.8) holds for some function $\omega : G \times G \to \mathbb{T}$ satisfying (7.9) and (7.10). Moreover,

(i) two unitary-projective representation $G \ni g \mapsto U_g \in \mathfrak{B}(\mathsf{H})$ and $G \ni g \mapsto U'_g \in \mathfrak{B}(\mathsf{H})$ are said **equivalent** if $U'_g = \chi_g U_g$, where $\chi_g \in U(1)$ for every $g \in G$. This is the same as requiring that there exist numbers $\chi_g \in U(1)$ such that

$$\omega'(g, g') = \frac{\chi_{g \cdot g'}}{\chi_g \chi_{g'}} \omega(g, g') \quad \forall g, g' \in G , \tag{7.12}$$

where $\omega(g, g')I = U_g U_{g'} U^{-1}_{g \cdot g'}$ and $\omega'(g, g')I = U'_g U'_{g'} U'^{-1}_{g \cdot g'}$;

(ii) a unitary-projective representation with $\omega(e, e) = \omega(g, e) = \omega(e, g) = 1$ for every $g \in G$ is said to be **normalized**.

■

A unitary-projective representation $G \ni g \mapsto U_g \in \mathfrak{B}(\mathsf{H})$ acts both on normal states (quantum-state operators) $T \in \mathscr{S}(\mathsf{H})$ and on elementary observables $P \in \mathscr{L}(\mathsf{H})$ (and also on observables, as already discussed). The action on states reads

$$\mathscr{S}(\mathsf{H}) \ni T \mapsto U_g T U_g^{-1} \in \mathscr{S}(\mathsf{H}) \quad \text{for every } g \in G . \tag{7.13}$$

We have two possible actions on elementary observables: the *dual action*

$$\mathscr{S}(\mathsf{H}) \ni P \mapsto h'_g(P) := U_g^{-1} P U_g \in \mathscr{L}(\mathsf{H}) \quad \text{for every } g \in G , \tag{7.14}$$

or the *inverse dual action*

$$\mathscr{S}(\mathsf{H}) \ni P \mapsto h_g(P) := U_g P U_g^{-1} \in \mathscr{L}(\mathsf{H}) \quad \text{for every } g \in G . \tag{7.15}$$

Note that changing the phase of U_g does not affect the action on states and observables. Hence these actions are invariant under equivalences of unitary-projective representations. Both actions on elementary observables have a physical meaning, as discussed in Sect. 7.1.3, and the choice between dual or inverse dual depends on physical convenience. However, from a pure mathematical viewpoint, the maps $G \ni g \mapsto h_g$ and $G \ni g \mapsto h'_g$ have different properties. As the reader can prove, the following facts hold.

(1) The *inverse dual action* $G \ni g \mapsto h_g$ is a **representation of G by ortho-automorphisms** of $\mathscr{L}(\mathsf{H})$. In other words, every h_g is an ortho-automorphisms of $\mathscr{L}(\mathsf{H})$ such that

$$h_e = id , \quad h_g h_{g'} = h_{g \cdot g'} .$$

(2) The *dual action* $G \ni g \mapsto h'_g$ is, instead, a **left representation of G by ortho-automorphisms** of $\mathscr{L}(\mathsf{H})$. That is to say, every h_g is an ortho-automorphisms of $\mathscr{L}(\mathsf{H})$ satisfying

$$h'_e = id\,, \quad h'_g h'_{g'} = h'_{g' \cdot g}$$

(notice the reversed order of g and g'.)

Evidently, if G is Abelian the dual action is an 'ordinary' representation (in the sense of Definition 7.9).

Remark 7.11

(a) It is easily proved that every unitary-projective representation $g \mapsto U_g$ is always equivalent to a normalized representation. It is sufficient to redefine $U'_g := \chi_g U_g$ with $\chi_g = 1$ for $g \neq e$ and $\chi_e = \omega(e,e)^{-1}$, and remember the general formula $\omega'(g,e) = \omega'(e,g) = \omega'(g',e)$.
(b) Being equivalent is evidently an equivalence relation among unitary-projective representations. It is clear that two projective unitary representations are equivalent if and only if they are made of the same Wigner (or Kadison) symmetries, since the latter disregard the phases multiplying the unitary operators describing them. ■

7.2.2 Representations Comprising Anti-Unitary Operators

Up to now, we have only considered the case where the operators V_g of a unitary-projective representation are unitary. We may however wonder if it is possible to construct a map $G \ni g \mapsto V_g$ where the V_g, which we assumed represent quantum symmetries on the Hilbert space H with $\dim \mathsf{H} > 1$, are all anti-unitary, or even some unitary and some anti-unitary, and the group operations are preserved up to phase as in (7.7). Notice that the unitary or anti-unitary nature of V_g is fixed by the corresponding g (since it defines the quantum symmetry) and Theorem 7.6 holds. If every $g \in G$ can be written as $g = h{\cdot}h$ for some h depending on g, or more generally every $g \in G$ can be written as a finite product of elements $g_1, \ldots, g_n$ where each is a square $g_k = h_k \cdot h_k$, then the U_g must be unitary. In fact, $V_g = \omega(h,h)^{-1} V_h V_h$ is necessarily linear no matter whether U_h is linear or anti-linear.

The argument above is valid in particular if G is a *connected* Lie group,[1] because: (a) there exists a sufficiently small neighbourhood O of the neutral element such that any $g \in O$ has the form $g = \exp(t_g T_g)$ for some $T_g \in \mathfrak{g}$ (the Lie algebra of G) and $t_g \in \mathbb{R}$, so that $h = \exp((t_g/2)T_g)$; furthermore, (b) every $g \in G$

[1] A Lie group is a second-countable Hausdorff real-analytic manifold, locally homeomorphic to $\mathbb{R}^n$, and equipped with smooth group operations. Real analyticity can be replaced by smoothness.

can be written as a finite product of elements $g_1, \ldots, g_n \in O$. As a matter of fact, there exist generalized unitary-projective representations where anti-unitary operators show up. These representations can be treated as particular cases. For instance, when representing the complete (non-connected) Poincaré group $\mathcal{P}$ for quantum systems with non-negative squared mass and non-negative energy, the *time-reversal symmetry* is necessarily anti-unitary. Observe that time reversal does not belong to the connected component in $\mathcal{P}$ of the identity.

When talking about unitary-projective representations of groups of quantum symmetries in this work, we shall stick to unitary operators only.

7.2.3 Unitary-Projective Representations of Lie Groups and Bargmann's Theorem

As stressed above, a technical problem is to check whether a given unitary-projective representation is equivalent to a unitary representation. The point is that unitary representations are much simpler to handle. This is a difficult problem [Var07, Mor18], that has been addressed especially when G is a *topological group* or even better a *Lie group* (see [NaSt82] and [Var84] for classical treatises emphasizing the analytic structure of Lie groups, and [HiNe13] for a complete, up-to-date and modern report on the smooth structure). In these cases the representation satisfies the following, physically natural, *continuity property*. It refers to the *transition probability* of two pure states, which is a physically measurable quantity.

Definition 7.12 A unitary-projective representation $G \ni g \mapsto U_g$ of the topological group G on the Hilbert space H is called **continuous** if the map

$$G \ni g \mapsto |\langle \psi | U_g \phi \rangle|$$

is continuous for every $\psi, \phi \in \mathsf{H}$. ■

Remark 7.13 In presence of superselection rules, continuous symmetries representing a connected topological group *cannot* swap coherent sectors when acting on pure states, for topological reasons [Mor18]. ■

A well-known cohomological condition ensuring that every unitary-projective representation of a *Lie group* is equivalent to a unitary one is due to Bargmann [BaRa84, Mor18].

Theorem 7.14 (Bargmann's Criterion) *Let G be a (real, finite-dimensional) connected and simply connected Lie group with Lie algebra $\mathfrak{g}$. Every continuous unitary-projective representation of G on a Hilbert space H is equivalent to a strongly-continuous unitary representation of G on H if, for every bilinear skew-symmetric map $\Theta : \mathfrak{g} \times \mathfrak{g} \to \mathbb{R}$ such that*

$$\Theta([u, v], w) + \Theta([v, w], u) + \Theta([w, u], v) = 0\,, \quad \forall u, v, w \in \mathfrak{g}\,, \tag{7.16}$$

there exists a linear map $\alpha : \mathfrak{g} \to \mathbb{R}$ *such that*

$$\Theta(u, v) = \alpha([u, v]) \quad \textit{for all } u, v \in \mathfrak{g}. \tag{7.17}$$

Remark 7.15 The condition is equivalent to demanding that the *second real cohomology group* $H^2(\mathfrak{g}, \mathbb{R})$ be trivial. ■

Example 7.16 Let us prove that the group $SU(2)$ satisfies Bargmann's Theorem 7.14. As is well known (e.g., see [HiNe13]), $SU(2)$ is connected and simply connected. We must prove that condition (7.17) holds. The Lie algebra $su(2)$ of $SU(2)$ is made by all skew-Hermitian 2×2 matrices. As a real vector space, it is three-dimensional and, in particular, it admits a basis T_1, T_2, T_3 of skew-Hermitian matrices given by $T_k := -\frac{i}{2}\sigma_k$. Therefore $[T_a, T_b] = \sum_{c=1}^{3} \epsilon_{abc} T_c$, where $\epsilon_{abc} \in \mathbb{R}$ is totally skew-symmetric in $a, b, c \in \{1, 2, 3\}$ and $\epsilon_{123} = 1$. Now consider a skew-symmetric bilinear map $\Theta : su(2) \times su(2) \to \mathbb{R}$. It is completely determined by the numbers $\Theta_{ab} := \Theta(T_a, T_b) = -\Theta_{ba}$. In fact, considering generic vectors $u = \sum_{a=1}^{3} t_a T_a$ and $v = \sum_{b=1}^{3} s_b T_b$, we have

$$\Theta(u, v) = \Theta\left(\sum_{a=1}^{3} t_a T_a, \sum_{b=1}^{3} s_b T_b\right) = \sum_{a=1}^{3}\sum_{b=1}^{3} t_a s_b \Theta_{ab} \,.$$

By direct inspection one sees that, as $\Theta_{ab} = -\Theta_{ba}$, we also have $\Theta_{ab} = \sum_{c=1}^{3} \alpha_c \epsilon_{cab}$, where $\alpha_1 = \Theta_{23}$, $\alpha_2 := \Theta_{31}$, $\alpha_3 := \Theta_{12}$. Finally observe that, letting $\alpha : su(2) \to \mathbb{R}$ be

$$\alpha\left(\sum_{a=1}^{3} t_a T_a\right) := \sum_{a=1}^{3} \alpha_a t_a \,, \quad \text{with } \alpha_a := \alpha(T_a),$$

we have

$$\alpha\left(\left[\sum_{a=1}^{3} t_a T_a, \sum_{b=1}^{3} s_b T_b\right]\right) = \sum_{a=1}^{3}\sum_{b=1}^{3} t_a s_b \alpha\left([T_a, T_b]\right) = \sum_{a,b,c=1}^{3} t_a s_b \epsilon_{abc} \alpha\left(T_c\right)$$

$$= \sum_{a,b,c=1}^{3} t_a s_b \epsilon_{abc} \alpha_c \,.$$

Now, notice that $\sum_{c=1}^{3} \epsilon_{abc}\alpha_c = \sum_{c=1}^{3} \epsilon_{cab}\alpha_c$, so that

$$\alpha([u, v] = \alpha\left(\left[\sum_{a=1}^{3} t_a T_a, \sum_{b=1}^{3} s_b T_b\right]\right) = \sum_{a,b,c=1}^{3} t_a s_b \alpha_c \epsilon_{cab} = \sum_{a,b} t_a s_b \Theta_{ab}$$

$$= \Theta\left(\sum_{a=1}^{3} t_a T_a, \sum_{b=1}^{3} s_b T_b\right) = \Theta(u, v) \,.$$

We have proved that (7.17) for all $u, v \in su(2)$. We stress that we have not even imposed constraint (7.16),

$$\Theta([u,v],w) + \Theta([v,w],u) + \Theta([w,u],v) = 0\,, \quad \forall u,v,w \in su(2)\,,$$

since this is automatically true in our case, as the reader can prove. ■

Remark 7.17 The hypothesis of *simply connectedness* in Bargmann's theorem is not that fundamental. If the connected Lie group G is not simply connected, every continuous unitary-projective representation $G \ni g \mapsto V_g$ can be viewed as a continuous unitary-projective representation of the universal covering $\widetilde{G}$ (which has the same Lie algebra as G). One must use the *covering map* $\pi : \widetilde{G} \to G$ (which is a surjective Lie-group homomorphism and a local Lie-group isomorphism) to define

$$\widetilde{G} \ni h \mapsto U_h := V_{\pi(h)}\,.$$

Notice also that if V is irreducible, U is irreducible as well, since irreducibility depends on the images of U and V which are identical. By definition $\widetilde{G}$ is connected and simply connected, so if the remaining assumptions in Bargmann's theorem are true, U can be made unitary. In this case, by knowing all (irreducible) strongly-continuous unitary representations of $\widetilde{G}$ we also know *up to equivalence* all (irreducible) continuous unitary-projective representations of G. ■

Example 7.18 Recall that the Lie group $SO(3)$ is connected but not simply connected. Besides, not all *irreducible* continuous unitary-projective of $SO(3)$ can be made unitary, and annoying phases show up. The discussion above contains the reason why they can nevertheless be obtained as *irreducible* strongly-continuous unitary representations of the universal covering $SU(2)$ (which satisfies Bargmann's hypotheses, see Example 7.16).

Let us briefly analyse the structure of the representations arising thus. Since (e.g., see [HiNe13]) the universal covering map $\pi : SU(2) \to SO(3)$ has $ker(\pi) = \{\pm I\}$, two cases are possible for a given irreducible unitary representation $SU(2) \ni g \mapsto U_g$. Starting from $U_{-I}U_g = U_{-I\cdot g} = U_{g\cdot(-I)} = U_g U_{-I}$ for every $g \in SU(2)$, since the representation is irreducible Schur's lemma (Theorem 6.19) implies $U_{-I} = \chi I_{\mathfrak{B}(\mathsf{H})}$ for some $\chi \in \mathbb{T}$. As $I_{\mathfrak{B}(\mathsf{H})} = U_I = U_{-I\cdot(-I)} = \chi^2 I_{\mathfrak{B}(\mathsf{H})}$ we conclude that either $U_{-I} = I_{\mathfrak{B}(\mathsf{H})}$ or $U_{-I} = -I_{\mathfrak{B}(\mathsf{H})}$. Now let us consider irreducible *strongly-continuous* unitary representations $U : SU(2) \to \mathfrak{B}(\mathsf{H})$.

(1) If $U_{-I} = I_{\mathfrak{B}(\mathsf{H})}$, then $SU(2) \ni g \mapsto U_g$ can be seen as irreducible unitary representation $SO(3) \ni R \mapsto V_R$ as well, where $V_R := U_{\pi^{-1}(R)}$. This is well defined since $\pi^{-1}(R) = \{\pm g_R\}$, but $U_{-g_R} = U_{-Ig_R} = U_{-I}U_{g_R} = U_{g_R}$. Note that $SO(3) \ni R \mapsto U_{\pi^{-1}(R)}$ is also strongly-continuous if U is, because

$SO(3)$ is homeomorphic to the *quotient*[2] $SU(2)/ker(\pi)$, and $V \circ \pi = U$. These unitary representations of $SU(2)$ are called **integer spin representations**.

(2) If $U_{-I} = -I_{\mathfrak{B}(\mathsf{H})}$ the picture is different. In this case, $V_R := U_{\pi^{-1}(R)}$ would be ill-defined because $\pi^{-1}(R) = \{\pm g_R\}$, but $U_{g_R} = -U_{-g_R}$. However, by choosing one between $\pm g_R$ for every given R, we obtain a unitary-projective representation of $SO(3)$ whose multipliers take values in $\{\pm 1\}$. The ensuing map $V : SO(3) \to \mathfrak{B}(\mathsf{H})$ satisfies $|\langle\psi|V_{\pi(g)}\phi\rangle| = |\langle\psi|U_g\phi\rangle|$, and the latter is continuous as $g \in SU(2)$ varies. By definition of quotient topology, as $SO(3)$ is homeomorphic to $SU(2)/ker(\pi)$ the map $SO(3) \ni R \mapsto |\langle\psi|V_R\phi\rangle|$ is continuous. Hence, $V : SO(3) \to \mathfrak{B}(\mathsf{H})$ is continuous as a unitary-projective representation. These irreducible representations of $SU(2)$ are called **half-integer spin representations**.

Due to Remark 7.17, all irreducible continuous unitary-projective representation of $SO(3)$ are constructed in this way up to equivalence, and necessarily belong in one of the two classes defined above. The (half-integer spin) unitary-projective representations of $SO(3)$ are often interpreted as *multi-valued* unitary representations.

As observed in Sect. 7.3.1, the Peter-Weyl theorem says that all strongly-continuous unitary representations of $SU(2)$ are direct sums of *irreducible* strongly-continuous and finite-dimensional unitary representations of $SU(2)$. Therefore considering irreducible representations is not restrictive.

It is finally important to stress that the use of unitary representations of $SU(2)$ is only based on mathematical convenience, but there is no physical reason to prefer them over unitary-projective representations of $SO(3)$ where multipliers show up. The group of symmetries in physics is $SO(3)$, not $SU(2)$, and the action of $SO(3)$ on states and observables is not affected by multipliers, as is evident from (7.13)–(7.15). ■

Back to the general case, there exist unitary-projective representations of a connected and simply connected Lie group G that cannot be made unitary, and one has to deal with them. There is nonetheless an overall way to circumvent this (merely technical) problem, which consists in viewing them as unitary representations of *another* group. Given a unitary-projective representation $G \ni g \mapsto U_g$ with multiplier ω, let us put on $U(1) \times G$ the product

$$(\chi, g) \circ (\chi', g') = (\chi\chi'\omega(g, g'), g \cdot g')$$

and indicate by $\hat{G}_\omega$ this group. The map $\hat{G}_\omega \ni (\chi, g) \mapsto \chi U_g =: V_{(\chi,g)}$ is a *unitary representation* of $\hat{G}_\omega$. If the initial representation is normalized, $\hat{G}_\omega$ is a **central extension of** G by $U(1)(= \mathbb{T})$ [Var07, Mor18]. Indeed, its elements (χ, e) commute with everything in $\hat{G}_\omega$ and thus they belong to the centre of the group. It is possible to prove that, with a suitable topology (different from the product topology

[2] A set $A \subset SU(2)/ker(\pi) = SO(3)$ is open if and only if $\pi^{-1}(A) \subset SU(2)$ is open.

in general), $\hat{G}_\omega$ turns into a topological/Lie group if G is a topological/Lie group [Var07, Mor18].

Unitary representations of $U(1)$-central extensions play a remarkable role in physics. With a particular choice of ω, $\hat{G}_\omega$ is sometimes viewed as the *true* group of symmetries at the quantum level, whereas G is the *classical group* of symmetries.

7.2.4 Inequivalent Unitary-Projective Representations and Superselection Rules

The notion of equivalence given in (7.12) can be extended to pairs of unitary-projective representations $G \ni g \mapsto U_g \in \mathfrak{B}(\mathsf{H})$ and $G \ni g \mapsto U'_g \in \mathfrak{B}(\mathsf{H}')$ defined on *different* Hilbert spaces H and H'. Again, two such representations are said to be **equivalent** if there is an assignment $G \ni g \mapsto \chi_g \in \mathbb{T}$ such that multipliers obey (7.12).

Such a pair of unitary-projective representations, *once the multipliers have been redefined to become identical*, can be added together giving rise to a unitary-projective representation on the Hilbert space $\mathsf{K} := \mathsf{H} \oplus \mathsf{H}'$,

$$G \ni g \mapsto U_g \oplus U'_g \in \mathfrak{B}(\mathsf{H} \oplus \mathsf{H}') .$$

This map is a well-behaved unitary-projective representation: if the multipliers ω and ω' of U and U' are equal, then for any $g, h \in G$,

$$(U_g \oplus U'_g)(U_h \oplus U'_h) = U_g U_h \oplus U'_g U'_h = \omega(g,h)U_{g\cdot h} \oplus \omega'(g,h)U'_{g\cdot h}$$
$$= \omega(g,h)\left(U_{g\cdot h} \oplus U'_{g\cdot h}\right) .$$

If, conversely, the representations are not equivalent, it is impossible to arrange phases in order to define a unitary-projective representation on the sum K, and G cannot be interpreted as symmetry group for a quantum system described on K (through a unitary-projective representation which reduces to U and U' on the subspaces H and H').

There is however a way out when suitable *Abelian superselection rules occur* (Sect. 6.3.1).

Sometimes it happens that the system's Hilbert space is an orthogonal sum $\mathsf{H} = \bigoplus_{j\in J} \mathsf{H}_j$ of closed subspaces which are invariant under respective unitary-projective representations $G \ni g \mapsto U^{(j)}_g \in \mathfrak{B}(\mathsf{H}_j)$ of a common group G of quantum symmetries. If some pairs of representations are not equivalent, the group does not act (as sum of the representations) on the entire Hilbert space, since as already observed this sum cannot define a unitary-projective representation. So, if H is the *Hilbert space of the system*, i.e. every orthogonal projector $P \in \mathscr{L}(\mathsf{H})$ represents an elementary observable of the system, G cannot be interpreted directly as a group of symmetries. But if each H_j is a *superselection sector* or, more weakly, the *Hilbert sum of superselection sectors*, then the orthogonal projectors representing observables belong to the lattice $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ of the system's von Neumann algebra of observables $\mathfrak{R}$ (see Sect. 6.3.1), and hence $P = \oplus_{j\in J} P_j$, where $P_j \in \mathscr{L}(\mathsf{H}_j)$. In this case, the global action of G given by

$$h_g : \oplus_{j\in J} P_j \mapsto \oplus_{j\in J} h_g^{(j)}(P_j) = \oplus_{j\in J} U_g^{(j)} P_j U_g^{(j)-1}$$

is legit. This action is *not* induced by a unitary-projective representation of G on H, but it works well anyway as a representation of G made of *automorphisms of* $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$. In fact, the different phases arising when composing the representations of different elements g, g' cancel each other:

$$\begin{aligned} h_g\left(h_{g'}\left(\oplus_{j\in J} P_j\right)\right) &= \oplus_{j\in J} U_g^{(j)} U_{g'}^{(j)} P_j U_g^{'(j)*} U_g^{(j)*} \\ &= \oplus_{j\in J} \omega^{(j)}(g, g')\overline{\omega^{(j)}(g, g')} U_{g\cdot g'}^{(j)} P_j U_{g\cdot g'}^{(j)*} \\ &= \oplus_{j\in J} U_{g\cdot g'}^{(j)} P_j U_{g\cdot g'}^{(j)*} = h_{g\cdot g'}\left(\oplus_{j\in J} P_j\right) . \end{aligned}$$

Here are two important examples of this situation to do with *continuous unitary-projective representations.*

Example 7.19

(1) A superselection rule arises as soon as we represent the group of spatial rotations $SO(3)$. According to Example 7.18 these representations can be seen as continuous unitary-projective representations of $SU(2)$, and the irreducible ones are divided in two equivalence classes in accordance with the value of an observable of the quantum system, the *total angular momentum squared* J^2. Its spectrum is a point spectrum and its eigenvalues are $\hbar j(j + 1)$, where $j = 0, 1/2, 1, 3/2, 2, \ldots$ Every eigenspace of J^2 is invariant and irreducible (or a direct sum of irreducible closed subspaces where J^2 has the same value) for the action of a suitable unitary-projective representation of $SO(3)$. All irreducible representations associated with $j = 0, 1, 2, \ldots$ are equivalent (also with different values of j of said type); they are also *proper* strongly-continuous unitary representations of $SO(3)$, being *integer spin representations* by Example 7.18. All irreducible representations associated with $j = 1/2, 3/2, 5/2, \ldots$ are similarly equivalent, but the representations of the first type are not equivalent to those of the second type, which is made of *half-integer spin representations* (Example 7.18). A superselection rule occurs if we split the Hilbert space in two sectors, which are sums of irreducible closed subspaces associated to integer or half-integer values of j. Following the discussion of Sect. 6.3.1 we may associate a superselection charge to this structure. For instance, eigenvalue 0 to the space of half-integer j and eigenvalue 1 to the integer j space. Obviously, this superselection rule

may be accompanied by further compatible rules (e.g., the electrical charge superselection rule), thus producing a finer structure of sectors.

(2) Another important case of superselection rule is related to inequivalent unitary-projective representations of the (universal covering of the) *Galilean group* G—the group of coordinate transformations between inertial reference frames in classical physics, viewed as *active* transformations. As clarified by Bargmann (see, e.g.,[Mor18]), the only physically relevant continuous unitary-projective representations of G in QM are those *not* equivalent to unitary representations! Furthermore there are infinitely many non-equivalent classes of such representations. The multipliers encapsulate the information about the *mass* m of the system: they take the form $\omega_m(g, g') = e^{imf(g,g')}$ with $f : G \times G \to \mathbb{R}$ a universal smooth function. Different values $m \in (0, +\infty)$ produce inequivalent continuous unitary-projective representations. This phenomenon, according to the discussion above, gives rise to a famous superselection structure on the Hilbert space of quantum systems admitting the Galilean group as a symmetry group, known as *Bargmann's superselection rule* (see [Mor18] for a summary). The superselection charge can be defined as the *mass* of the system *provided the values are discrete*. In other words, superselection sectors are labelled by distinct *eigenvalues* m of the mass, whereby we think of the mass as a proper quantum observable, a selfadjoint operator M. Differently from the electric charge, however, the eigenvalues of the mass are not proportional to a given elementary mass m_0. Therefore, if we intend to use the mass operator M (divided by some unit of mass) as the superselection charge Q appearing in the exponent of (6.13), no *compact* global gauge group will describe this Abelian superselection rule (Sect. 6.3.2). Still, we may employ a representation $\mathbb{R} \ni r \mapsto e^{irM}$ of the non-compact Abelian group $\mathbb{R}$, see the beginning of Sect. 6.3.2. Further compatible superselection rules, if present, would refine the sector decomposition. ■

7.2.5 Continuous Unitary-Projective and Unitary Representations of $\mathbb{R}$

An important consequence of Bargmann's theorem is the following crucial result, which describes strongly-continuous one-parameter unitary groups as a central tool in Quantum Theory. This theorem could be proved independently of Bargmann's theorem [Mor18], but the proof is quite technical.

Theorem 7.20 *Let* $\gamma : \mathbb{R} \ni r \mapsto U_r$ *be a continuous unitary-projective representation of the additive group* $\mathbb{R}$ *on the Hilbert space* H. *Then*

(a) γ *is equivalent to a strongly-continuous unitary representation* $\mathbb{R} \ni r \mapsto V_r$ *of* $\mathbb{R}$ *on* H.

(b) *A strongly continuous unitary representation* $\mathbb{R} \ni r \mapsto V'_r$ *is equivalent to* γ *if and only if*

$$V'_r = e^{icr} V_r \quad \textit{for some constant } c \in \mathbb{R} \textit{ and all } r \in \mathbb{R}.$$

Proof

(a) Let us embed the connected, simply connected group $(\mathbb{R}, +)$ in $GL(2, \mathbb{R})$ as a Lie group: for this we represent with $r \in \mathbb{R}$ by the 2×2 matrix

$$A_r := \begin{bmatrix} 1 & r \\ 0 & 1 \end{bmatrix}.$$

Observe that

$$\begin{bmatrix} 1 & a \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & b \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & a+b \\ 0 & 1 \end{bmatrix},$$

making $\mathbb{R} \ni r \mapsto A_r \in GL(2, \mathbb{R})$ a continuous, injective homomorphism and a homeomorphism on its image. The two groups are therefore isomorphic as topological groups. As the set of matrices A_r is a closed subgroup of $GL(2, \mathbb{R})$, by a theorem of Cartan it is a Lie subgroup of $GL(2, \mathbb{R})$. In this picture, the Lie algebra of $\mathbb{R}$ is $\mathbb{R}$ itself, represented as one-dimensional subspace of the Lie algebra $\mathfrak{gl}(2, \mathbb{R})$ with elements

$$T_a := \begin{bmatrix} 0 & a \\ 0 & 0 \end{bmatrix}$$

for $a \in \mathbb{R}$. In fact this is the vector space of derivatives at the origin of differentiable curves $r \mapsto A_r$ such that $A_0 = I$. The commutator in the Lie algebra $\mathbb{R}$ is the restriction of the Lie bracket of $GL(2, \mathbb{R})$, $[T_a, T_b] = T_a T_b - T_b T_a = 0$. As the Lie algebra is one-dimensional (it coincides with $\mathbb{R}$ itself as a vector space), any skew-symmetric map $\Theta : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ is zero, so Bargmann's condition is satisfied trivially for the Lie group $\mathbb{R}$.

(b) If $\mathbb{R} \ni t \mapsto V_t$ is strongly-continuous and $c \in \mathbb{R}$, evidently $\mathbb{R} \ni t \mapsto V'_t := e^{ict} V_t$ is still strongly-continuous, and equivalent to the same unitary-projective representation of V. Let us prove the converse. Suppose that V' and V are strongly-continuous unitary representation obtained from the continuous unitary-projective representation U of $\mathbb{R}$. Then $V'_t = \chi(t) V_t$ for some map $\chi : \mathbb{R} \to \mathbb{T} = \{z \in \mathbb{C} \mid |z| = 1\}$. If $x, y \in \mathsf{H}$ with $\langle x|y\rangle \neq 0$, we also have $\chi(t)\langle x|y\rangle = \langle x|V_{-t} V'_t y\rangle = \langle V_t x|V'_t y\rangle$, and therefore χ is continuous. Now (a) and (b) in Theorem 7.25 (which is independent of the present proposition) prove that there exists a dense domain of vectors x such that $\mathbb{R} \ni t \mapsto V_t x$ is differentiable at $t = 0$ in the topology of H. The same happens for $V'_t y$. Choosing a pair of such vectors with $\langle x|y\rangle \neq 0$ (possible in view of density),

$\chi(t)\langle x|y\rangle = \langle V_t x|V'_t y\rangle$ also implies that $\chi(t)$ admits derivative at $t = 0$. From $V'_t V'_{t'} = \chi(t)\chi(t')V_t V_{t'}$ we deduce $V'_{t+t'} = \chi(t)\chi(t')V_{t+t'}$, that is $\chi(t+t')V_{t+t'} = \chi(t)\chi(t')V_{t+t'}$, and then $\chi(t+t') = \chi(t)\chi(t')$ since $V_{t+t'}$ is invertible. As the reader can easily prove, then, $\frac{d\chi}{dt} = \frac{d\chi}{dt}|_{t=0}\chi(t)$. This differential equation has the unique solution $\chi(t) = e^{at}$, where $a = \frac{d\chi}{dt}|_{t=0}$. But $|\chi(t)| = 1$ forces $a = ic$ for some $c \in \mathbb{R}$, and $\chi(t) = e^{ict}$.

□

The above unitary representations of $\mathbb{R}$ include the *strongly-continuous one-parameter unitary groups* encountered in Propositions 3.61–3.62, where we treated what appeared to be a particular case.

Definition 7.21 If H is a Hilbert space, a representation $V : \mathbb{R} \ni r \mapsto V_r \in \mathfrak{B}(\mathsf{H})$ such that

(i) V_r is unitary for every $r \in \mathbb{R}$
(ii) $V_0 = I$ and $V_r V_s = V_{r+s}$ for all $r, s \in \mathbb{R}$,
is a **one-parameter unitary group**. It is called a **strongly-continuous one-parameter unitary group** if, in addition,
(iii) V is strongly continuous: $V_r\psi \to V_{r_0}\psi$ for $r \to r_0$ and every $r_0 \in \mathbb{R}$ and $\psi \in \mathsf{H}$. ■

An elementary but important proposition holds.

Proposition 7.22 *For a one-parameter unitary group* $U : \mathbb{R} \ni r \mapsto U_r \in \mathfrak{B}(\mathsf{H})$, *strong continuity is equivalent to each of the conditions below:*

(a) *U is weakly continuous;*
(b) *U is strongly continuous at $r = 0$;*
(c) *U is weakly continuous at $r = 0$;*
(d) $\langle\psi|U_r\psi\rangle \to \langle\psi|\psi\rangle$ *as* $r \to 0$ *for every given* $\psi \in \mathcal{D}$, *where* $\mathcal{D} \subset \mathsf{H}$ *is a set such that* $\overline{span(\mathcal{D})} = \mathsf{H}$.

Proof Evidently, strong continuity implies (a), (b), (c), (d). The fact that (b) implies strong continuity follows from $||U_r\psi - U_s\psi|| = ||U_{-s}(U_r\psi - U_s\psi)|| = ||U_{r-s}\psi - \psi||$, since $r \to s$ implies $r - s \to 0$. (c) implies strong continuity because

$$||U_r\psi - \psi||^2 = ||U_r\psi||^2 + ||\psi||^2 - \langle\psi|U_r\psi\rangle - \langle U_r\psi|\psi\rangle = 2||\psi||^2 - 2Re\langle\psi|U_r\psi\rangle \to 0$$

when $r \to 0$, and (b) implies strong continuity. (a) implies (c) which in turn forces strong continuity. Let us finally prove that (d) implies strong continuity. If $\phi \in \mathsf{H}$, then

$$||U_r\phi - \phi|| \leq \left|\left|U_r\sum_{k=1}^{N} c_k\psi_k - U_r\phi\right|\right| + \left|\left|U_r\sum_{k=1}^{N} c_k\psi_k - \sum_{k=1}^{N} c_k\psi_k\right|\right| + \left|\left|\sum_{k=1}^{N} c_k\psi_k - \phi\right|\right| .$$

Using the density of span$\mathcal{D}$, we can fix $N \in \mathbb{N}$, the numbers $c_k \in \mathbb{C}$ and the vectors $\psi_k \in \mathcal{D}$ so that $||U_r \sum_{k=1}^N c_k\psi_k - U_r\phi|| = || \sum_{k=1}^N c_k\psi_k - \phi|| < \epsilon/2$. The formula used for part (c) now gives

$$\left|\left|U_r \sum_{k=1}^N c_k\psi_k - \sum_{k=1}^N c_k\psi_k\right|\right| \le \sum_{k=1}^N |c_k|||U_r\psi_k - \psi_k||$$

$$\le C \sum_{k=1}^N \sqrt{2||\psi_k||^2 - 2Re\langle\psi_k|U_r\psi_k\rangle} \le \epsilon/2$$

for $C = \max\{|c_1|, \dots, |c_N|\}$, $|r| < \delta$ and $\delta > 0$ small enough. Hence $||U_r\phi - \phi|| < \epsilon$ if $|r| < \delta$, proving (b) and hence the claim. □

7.2.6 Strongly Continuous One-Parameter Unitary Groups: Stone's Theorem

Theorem 7.20 certifies that when we deal with continuous unitary-projective representations of $\mathbb{R}$ we can always restrict to strongly-continuous one-parameter unitary groups. On a separable Hilbert space there are very few one-parameter unitary groups that are not strongly continuous, by the following result of von Neumann (for a proof see, e.g., [Sim76, Mor18]).

Theorem 7.23 *On a separable complex Hilbert space* H*, a one-parameter unitary groups* $V : \mathbb{R} \ni r \mapsto V_r \in \mathfrak{B}(\mathsf{H})$ *is strongly continuous if and only if the maps* $\mathbb{R} \ni r \mapsto \langle\psi|V_r\phi\rangle$ *are Borel measurable for all* $\psi, \phi \in \mathsf{H}$.

Let us come to Stone's celebrated characterization of strongly-continuous one-parameter unitary groups (and we stress again that *strong* continuity is here equivalent to *weak* continuity, by Proposition 7.22), whereby these groups always correspond to observables. We already know that if A is a selfadjoint operator on a Hilbert space, $U_t := e^{itA}$, for $t \in \mathbb{R}$, defines a strongly-continuous one-parameter unitary group (Propositions 3.62 and 3.63). The main content of Stone's remarkable achievement is that the result can be turned the other way around: for every strongly continuous one-parameter unitary group $\{U_t\}_{t\in\mathbb{R}}$ there exists exactly one selfadjoint operator A such that $U_t = e^{itA}$, for $t \in \mathbb{R}$.

Before we take the plunge let us prove a general result on uniformly bounded, weakly continuous maps $\mathbb{R} \ni t \mapsto V_t \in \mathfrak{B}(\mathsf{H})$. $C_c(X)$ henceforth denotes the space of complex-valued continuous maps on a topological space X with compact support.

Proposition 7.24 *Let* H *be a Hilbert space, take* $f \in C_c(\mathbb{R})$ *and* $\psi \in \mathsf{H}$*. If* $\mathbb{R} \ni t \mapsto V_t \in \mathfrak{B}(\mathsf{H})$ *is a weakly continuous map such that* $||V_t|| < K$ *for all* $t \in \mathbb{R}$ *and some* $K < +\infty$*, then the following facts hold.*

(a) *There exists a unique vector, denoted by* $\int_{\mathbb{R}} f(t)V_t\psi dt$*, such that*

$$\left\langle \phi \middle| \int_{\mathbb{R}} f(t)V_t \; \psi dt \right\rangle = \int_{\mathbb{R}} f(t)\langle\phi|V_t\psi\rangle dt \quad \textit{for all } \phi \in \mathsf{H}.$$

(b) *For every* $B \in \mathfrak{B}(\mathsf{H})$*,*

$$B\int_{\mathbb{R}} f(t)V_t\psi dt = \int_{\mathbb{R}} f(t)BV_t\psi dt \; .$$

(c) *We have the estimate*

$$\left|\left|\int_{\mathbb{R}} f(t)V_t\psi dt\right|\right| \leq \int_{\mathbb{R}} |f(t)|||V_t\psi||dt \; .$$

(d) *If* $g \in C_c(\mathbb{R})$ *and* $a, b \in \mathbb{C}$*, then*

$$\int_{\mathbb{R}} (af(t) + bg(t))V_t\psi dt = a\int_{\mathbb{R}} f(t)V_t\psi dt + b\int_{\mathbb{R}} g(t)V_t\psi dt \; .$$

Proof

(a) By hypothesis, $\mathsf{H} \ni \phi \mapsto \int_{\mathbb{R}} f(t)\langle\phi|V_t\psi\rangle dt$ is well defined as the integrand function is continuous and compactly supported. This map is anti-linear in ϕ and also continuous because, by the Cauchy-Schwartz inequality, $|\int_{\mathbb{R}} f(t)\langle\phi|V_t\psi\rangle dt| \leq \int_{\mathbb{R}} |f(t)||\langle\phi|V_t\psi\rangle|dt \leq ||\phi||||\psi||K\int_{\mathbb{R}} |f(t)|dt$. Riesz's lemma therefore implies that it can be written as $\mathsf{H} \ni \phi \mapsto \langle\phi|\psi_{V,f,t}\rangle$ for a unique $\psi_{V,f,t} \in \mathsf{H}$. By definition, $\int_{\mathbb{R}} f(t)V_t\psi dt := \psi_{V,f,t}$.

(b) Observe that $\mathbb{R} \ni t \mapsto BV_t \in \mathfrak{B}(\mathsf{H})$ is weakly continuous and $||BV_t|| \leq ||B||K$, so $\int_{\mathbb{R}} f(t)BV_t\psi dt$ is well defined. From (a)

$$\left\langle \phi \middle| B\int_{\mathbb{R}} f(t)V_t \; \psi dt \right\rangle = \left\langle B^*\phi \middle| \int_{\mathbb{R}} f(t)V_t \; \psi dt \right\rangle = \int_{\mathbb{R}} f(t)\langle B^*\phi|V_t\psi\rangle dt$$
$$= \int_{\mathbb{R}} f(t)\langle\phi|BV_t\psi\rangle dt \; .$$

Using (a) again, we conclude $B\int_{\mathbb{R}} f(t)V_t\psi dt = \int_{\mathbb{R}} f(t)BV_t\psi dt$.

(c) Using (a) twice and the Cauchy-Schwartz inequality in the penultimate passage,

$$\begin{aligned}
\left|\left|\int_{\mathbb{R}} f(t)V_t\psi dt\right|\right|^2 &= \left|\left\langle \int_{\mathbb{R}} f(s)V_s\psi ds \,\middle|\, \int_{\mathbb{R}} f(t)V_t \ \psi dt\right\rangle\right| \\
&= \left|\int_{\mathbb{R}} f(t)\left\langle \int_{\mathbb{R}} f(s)V_s\psi ds \,\middle|\, V_t\psi\right\rangle dt\right| \\
&= \left|\int_{\mathbb{R}}\int_{\mathbb{R}} \overline{f(s)} f(t)\langle V_s\psi|V_t\psi\rangle ds dt\right| \\
&\leq \int_{\mathbb{R}}\int_{\mathbb{R}} |\overline{f(s)}||f(t)|||V_s\psi||||V_t\psi||ds dt \\
&= \left(\int_{\mathbb{R}} |f(t)|||V_t\psi||dt\right)^2 .
\end{aligned}$$

The proof of (d) is evident from (a) and the inner product's linearity. □

And here is Stone's theorem.

Theorem 7.25 (Stone's Theorem) *Let* $\mathbb{R} \ni t \mapsto U_t \in \mathfrak{B}(\mathsf{H})$ *be a strongly continuous one-parameter unitary group on the Hilbert space* H.

(a) *There exists a selfadjoint operator* A *on* H*, defined on a dense domain* $D(A)$*, such that*

$$U_t = e^{itA}, \quad \forall t \in \mathbb{R}. \tag{7.18}$$

(b) *If (7.18) holds for some selfadjoint operator* A*, then*

$$D(A) = \left\{\psi \in \mathsf{H} \,\middle|\, \exists \lim_{t\to 0}\frac{1}{t}(U_t - I)\psi \in \mathsf{H}\right\} \quad \text{and} \quad A\psi = -i\lim_{t\to 0}\frac{1}{t}(U_t - I)\psi . \tag{7.19}$$

(c) *The operator* A*, called the* ***selfadjoint (infinitesimal) generator*** *of* U*, is unique.*
(d) $U_t(D(A)) = D(A)$ *for all* $t \in \mathbb{R}$ *and*

$$AU_t\psi = U_tA\psi \quad \text{if } \psi \in D(A) \text{ and } t \in \mathbb{R}.$$

Proof We have to prove (a), (b) and (c), since (d) was established in Propositions 3.62 and 3.63.

(a) We first construct a candidate generator for U on a special dense subspace D. By Proposition 7.24 we define D to contain all finite linear combinations of functions $\psi_f := \int_{\mathbb{R}} f(t)U_t\psi dt$ for every $f \in C_c^\infty(\mathbb{R})$ and $\psi \in \mathsf{H}$. In view of part (d) of the Proposition D coincides with the set of the ψ_f. We claim this subspace is dense in H. To prove it, observe that by taking $V_t := U_t - I$ in Proposition 7.24,

$$||\psi_f - \psi|| = \left|\left|\int_{\mathbb{R}} f(t)(U_t - I)\psi dt\right|\right| \leq \int_{\mathbb{R}} |f(t)|||(U_t - I)\psi||dt$$

$$\leq \int_{\mathbb{R}} |f(t)|dt \sup_{t\in \mathrm{supp}(f)} ||(U_t - I)\psi|| \,.$$

For every $\epsilon > 0$, we can now define $f_\epsilon(x) := \frac{1}{\epsilon}g(x/\epsilon)$ where $g \in C_c^\infty(\mathbb{R})$ satisfies $\mathrm{supp}(g) \subset [-1, 1]$ and $\int_{\mathbb{R}} g dt = 1$, so that $\int_{\mathbb{R}} f_\epsilon dt = 1$ and $\mathrm{supp}(f_\epsilon) \subset [-\epsilon, \epsilon]$. Inserting this choice in the inequality,

$$0 \leq ||\psi_{f_\epsilon} - \psi|| \leq \sup_{t\in[-\epsilon,\epsilon]} ||(U_t - I)\psi|| \,.$$

As $\mathbb{R} \ni t \mapsto U_t$ is strongly continuous and $U_0 = I$, we obtain that $\psi_{f_\epsilon} \to \psi$ as $\epsilon \to 0$ for every $\psi \in$ H. Hence D is dense in H.

Next we prove that the strong derivative of U at $t = 0$ can be computed on D. Let us assume $s \in [-\epsilon, \epsilon]$ for some $\epsilon > 0$. With ψ_f as above and $K = [-a, a]$ such that $\mathrm{supp}(f) \subset [-a, a]$ for a sufficiently large $a > 0$, plus Proposition 7.24,

$$\frac{1}{s}(U_s - I)\,\psi_f = \frac{1}{s}(U_s - I)\int_K f(t)U_t\psi dt = \frac{1}{s}\int_K f(t)U_{t+s}\psi dt - \frac{1}{s}\int_K f(t)U_t\psi dt$$

$$= \frac{1}{s}\int_{K_\epsilon} f(t-s)U_t\psi dt - \frac{1}{s}\int_K f(t)U_t\psi dt = \frac{1}{s}\int_{K_\epsilon} f(t-s)U_t\psi dt - \frac{1}{s}\int_{K_\epsilon} f(t)U_t\psi dt$$

$$= \int_{K_\epsilon} \frac{f(t-s) - f(t)}{s} U_t\psi dt \,, \tag{7.20}$$

where $K_\epsilon := [-a-\epsilon, a+\epsilon] \supset K$. Now, assuming that f is real, the mean value theorem implies that $\left|\frac{f(t-s)-f(t)}{s}\right| = |f'(\xi_{t,s})| < C < +\infty$ where $\xi_{t,s} \in K_\epsilon$, and C does not depend on t, s since the continuous map f' is bounded on the compact set K_ϵ. The result trivially extends to f complex by looking at its real and imaginary parts. Dominated convergence proves that, for $s \to 0$,

$$\left|\left|\frac{1}{s}(U_s - I)\,\psi_f - \psi_{-f'}\right|\right| = \left|\left|\int_{K_\epsilon}\left(\frac{f(t-s) - f(t)}{s} + f'(t)\right)U_t\psi dt\right|\right|$$

$$\leq \int_{K_\epsilon}\left|\frac{f(t-s) - f(t)}{s} + f'(t)\right| ||U_t\psi||dt = ||\psi||\int_{K_\epsilon}\left|\frac{f(t-s) - f(t)}{s} + f'(t)\right| dt \to 0 \,.$$

We can therefore define the operator $\widetilde{A} : D \to D \subset \mathsf{H}$ by means of

$$\widetilde{A}\psi_f := -i \lim_{s\to 0} \frac{1}{s} (U_s - I)\, \psi_f = -i\psi_{-f'}\,, \tag{7.21}$$

and extend linearly to finite combinations of ψ_f. Observe that

$$U_u(D) = D \quad \text{and} \quad U_u\widetilde{A} = \widetilde{A}U_u \quad \forall u \in \mathbb{R}\,. \tag{7.22}$$

The first relation comes from the definition of D and Proposition 7.24 (b), alongside $U_u^{-1} = U_{-u}$. The second formula is an immediate consequence of the first, the definition of $\widetilde{A}$ in (7.21), the continuity of U_u and Proposition 7.24(b) once more.

Let us now show that $\widetilde{A}$ is essentially selfadjoint. First observe that it is symmetric because it is densely defined and Hermitian:

$$\begin{aligned}\langle\psi_g|\widetilde{A}\psi_f\rangle &= \left\langle\psi_g \left| -i \lim_{s\to 0}\frac{1}{s}(U_s - I)\,\psi_f\right.\right\rangle = \lim_{s\to 0}\left\langle i\frac{1}{s}\left(U_s^* - I\right)\psi_g\right|\left.\psi_f\right\rangle\\ &= \lim_{s\to 0}\left\langle i\frac{1}{s}(U_{-s} - I)\,\psi_g\right|\left.\psi_f\right\rangle = \lim_{s\to 0}\left\langle -i\frac{1}{-s}(U_{-s} - I)\,\psi_g\right|\left.\psi_f\right\rangle\\ &= \left\langle -i\lim_{s\to 0}\frac{1}{s}(U_s - I)\,\psi_g\right|\left.\psi_f\right\rangle = \langle\widetilde{A}\psi_g|\psi_f\rangle\,.\end{aligned}$$

Concerning essentially selfadjointness, we employ Proposition 2.47 (b) directly. Suppose there exist $\phi_\pm \in D(\widetilde{A}^*)$ such that $\widetilde{A}^*\phi_\pm = \pm i\phi_\pm$. As a consequence, using (7.22) and (7.21), if $\psi \in D = D(\widetilde{A})$

$$\begin{aligned}\frac{d}{dt}\langle U_t\psi|\phi_\pm\rangle &= \lim_{s\to 0}\left\langle\frac{1}{s}(U_s - I)U_t\psi\right|\left.\phi_\pm\right\rangle = \langle i\widetilde{A}U_t\psi|\phi_\pm\rangle = \langle iU_t\psi|\widetilde{A}^*\phi_\pm\rangle\\ &= \pm\langle U_t\psi|\phi_\pm\rangle\,.\end{aligned}$$

Hence $\mathbb{R} \ni t \mapsto \langle U_t\psi|\phi_\pm\rangle$ is continuously differentiable and satisfies the differential equation, so

$$\langle U_t\psi|\phi_\pm\rangle = \langle U_0\psi|\phi_\pm\rangle e^{\pm t} = \langle\psi|\phi_\pm\rangle e^{\pm t} \quad \forall t \in \mathbb{R}\,.$$

The left-most side is bounded as $|\langle U_t\psi|\phi_\pm\rangle| \leq ||\psi||||\phi_\pm||||U_t|| = ||\psi||||\phi_\pm||$, whereas the right-most term is unbounded unless $\langle\psi|\phi_\pm\rangle = 0$. But the formula must be true for every $\psi \in D$, and since D is dense, we conclude that $\phi_\pm = 0$. Therefore $\widetilde{A}$ is essentially selfadjoint on D by Proposition 2.47 (b), and we denote by A its unique selfadjoint extension.

To conclude, we can define the strongly continuous one-parameter group of unitary operators $\mathbb{R} \ni t \mapsto e^{itA}$ according to Proposition 3.62. We want to prove that, if $\psi, \phi \in D$, then $\langle \phi | U_{-t} e^{itA} \psi \rangle = \langle \phi | \psi \rangle$. To this end it is sufficient to show

$$\frac{d}{dt} \langle \phi | U_{-t} e^{itA} \psi \rangle = \frac{d}{dt} \langle U_t \phi | e^{itA} \psi \rangle = 0 \,.$$

Set $V_t := e^{itA}$. The domain D is U_t-invariant, and also V_t-invariant by Proposition 3.62 (since $D \subset D(A)$), so the second derivative is

$$\begin{aligned}
&\lim_{h \to 0} \frac{1}{h} \left(\langle U_{t+h}\phi | \, V_{t+h}\psi \rangle - \langle U_t\phi | \, V_t\psi \rangle \right) \\
&= \lim_{h \to 0} \frac{1}{h} \left(\langle U_h U_t\phi | \, V_h V_t\psi \rangle - \langle U_t\phi | \, V_t\psi \rangle \right) \\
&= \lim_{h \to 0} \left\langle U_h U_t \phi \left| \frac{1}{h}(V_h - I) V_t \; \psi \right.\right\rangle + \lim_{h \to 0} \left\langle \frac{1}{h}(U_h - I) U_t \phi \right| \left. V_t \psi \right\rangle \\
&= \langle U_t\phi | iAV_t\psi \rangle + \langle iAU_t\phi | V_t\psi \rangle i \langle AU_t\phi | V_t\psi \rangle - i \langle AU_t\phi | V_t\psi \rangle = 0 \,.
\end{aligned}$$

We exploited the fact that A is selfadjoint and Proposition 3.63. All-in-all, $\langle \phi | (U_{-t} e^{itA} - I) \psi \rangle = 0$ for all $t \in \mathbb{R}$, so $U_{-t} e^{itA} = I$ because $\phi, \psi \in D$ which is dense. In summary, we have proved that $U_t = e^{itA}$ for every $t \in \mathbb{R}$ and a selfadjoint operator A, concluding the proof of existence.

(b) Consider a strongly continuous one-parameter group of unitary operators $U_t = e^{itA}$, where A is some selfadjoint operator. We known that if $\psi \in D(A)$, then $-i \lim_{t \to 0} \frac{1}{t}(U_t - I)\psi = A\psi$ by Proposition 3.63. We intend to prove that, if $\lim_{t \to 0} \frac{1}{t}(U_t - I)\psi$ exists, then $\psi \in D(A)$ and the limit coincides with $iA\psi$. Let us define $B\psi := \lim_{t \to 0} \frac{1}{t}(U_t - I)\psi$ for all $\psi \in \mathsf{H}$ such that the right-hand side exists. It is easy to see that B is linear and $D(B)$ is a dense subspace, for it contains $D(A)$. Furthermore, exactly as we did for $\widetilde{A}$, we immediately obtain that B is Hermitian. So B is a symmetric extension of the selfadjoint operator A, and Proposition 2.39 (a) tells $B = A$, concluding the proof.

(c) Suppose that $U_t = e^{itB} = e^{itA}$ for all $t \in \mathbb{R}$ and a pair of selfadjoint operators A and B. Applying (7.19) we have $D(A) = D(B)$ and $A\psi = B\psi$ for every $\psi \in D(A) = D(B)$. The proof is over.

□

Corollary 7.26 *Let $A : D(A) \to \mathsf{H}$ be a selfadjoint operator on the Hilbert space $\mathsf{H} \supset D(A)$. Suppose that $S \subset D(A)$ is a dense subspace such that $e^{itA}S \subset S$ for every $t \in \mathbb{R}$. Then $A\restriction_S$ is essentially selfadjoint and its unique selfadjoint extension $\overline{A\restriction_S}$ is A itself. In other words, S is a core for A.*

Proof Along the lines of Stone's proof we replace the dense e^{itA}-invariant domain $D \subset D(A)$ by the dense e^{itA}-invariant domain $S \subset D(A)$, and $\widetilde{A}$ by $-i \frac{d}{dt}|_{t=0} e^{itA}\restriction_S = A\restriction_S$ (strong derivative). Then $A\restriction_S$ is essentially selfadjoint on S. Since $A \supset A\restriction_S$ is selfadjoint, necessarily $\overline{A\restriction_S} = A$. □

7.2.7 Time Evolution, Heisenberg Picture and Quantum Noether Theorem

The perspective of quantum symmetries allows us to settle certain issues raised in Sect. 3.4.3 and justify more firmly several notions.

Consider a quantum system described on the Hilbert space H in some *inertial* reference frame. Suppose that, physically speaking, the system is either isolated or interacts with some external *stationary* environment. These hypotheses guarantee temporal homogeneity, and the time evolution of states is axiomatically described by a continuous symmetry: more precisely, a *continuous unitary-projective representation* $\mathbb{R} \ni t \mapsto V_t$.

In view of Theorems 7.20 and 7.25, this group is equivalent to a strongly continuous one-parameter group of unitary operators $\mathbb{R} \ni t \mapsto U_t$, and there is a selfadjoint operator H, called the **Hamiltonian operator**, such that (notice the sign in the exponent)

$$U_t = e^{-\frac{i}{\hbar}tH}\,, \quad t \in \mathbb{R}\,, \tag{7.23}$$

where for once we have included the constant $\hbar$. By Theorems 7.20 and 7.25 V determines H *up to additive real constants*: the selfadjoint operator $H + cI$ defines the same continuous symmetry V. H is usually thought of as *the energy of the system* in the reference frame, and $c \in \mathbb{R}$ can be fixed using some physical case-by-case argument.

Within this picture, if $T \in \mathscr{S}(\mathsf{H})$ is the state of the system at $t = 0$, the state at time t is

$$T_t = U_t T U_t^{-1}\,.$$

If the initial state is pure and represented by the unit vector $\psi \in \mathsf{H}$, the state at time t is $\psi_t := U_t\psi$. As mentioned in Sect. 3.4.3, $\psi \in D(H)$ implies $\psi_t \in D(H)$ for every $t \in \mathbb{R}$ by Theorem 7.25 (b)–(d):

$$i\hbar\frac{d\psi_t}{dt} = H\psi_t\,. \tag{7.24}$$

where the derivative is computed in the topology of H. One recognizes in Equation (7.24) the general form of **Schödinger's equation**. From now on shall set $\hbar = 1$.

Remark 7.27 It is possible to study quantum systems interacting with a non-stationary external system. In this case the Hamiltonian observable depends parametrically on time, see Sect. 1.2.1. A Schrödinger-type equation is supposed to describe the time evolution of the system, giving rise to a groupoid of unitary operators [Mor18]. We shall not tackle this technical issue here. ■

In this framework, called **Schrödinger picture**, observables do not evolve whereas states do. There is another approach to describe time evolution, called **Heisenberg picture**. In that representation, states do not evolve in time, but observables evolve under the *dual action* (7.4) of the symmetries induced by U_t. In this sense, if A is an observable at $t = 0$, its evolution at time t is the observable

$$A_t := U_t^{-1} A U_t \ .$$

Obviously $D(A_t) = U_t^{-1}(D(A)) = U_{-t}(D(A)) = U_t^*(D(A))$. As already observed in the case general case, by Proposition 3.60 (j) the spectral measure of A_t is

$$P_E^{(A_t)} = U_t^{-1} P_E^{(A)} U_t ,$$

as expected. The probability that, at time t, the observable A produces the outcome E, when the normal state is represented by the quantum-state operator $T \in \mathscr{S}(\mathsf{H})$ at $t = 0$, can be computed using either the standard (Schrödinger) picture, where states evolve as $tr(P_E^{(A)} T_t)$, or the Heisenberg picture where observables evolve as $tr(P_E^{(A_t)} T)$. Indeed

$$tr(P_E^{(A)} T_t) = tr(P_E^{(A)} U_t^{-1} T U_t) = tr(U_t P_E^{(A)} U_t^{-1} T) = tr(P_E^{(A_t)} T) \ .$$

The two pictures are completely equivalent for the purpose of describing non-relativistic quantum physics. In relativistic quantum physics and QFT in particular, though, Heisenberg's picture (extended covariantly to include spatial translations) is preferable, due to the existence of a plethora of different notions of time evolution. The Heisenberg picture grants us the following important definition, see also Sect. 3.4.3.

Definition 7.28 Let H be a the Hilbert space and $\mathbb{R} \ni t \mapsto U_t$ a strongly-continuous unitary one-parameter group representing time evolution. An observable A is said to be a **constant of motion** with respect to U if $A_t := U_t^{-1} A U_t$ does not depend on t, i.e. $A_t = A_0$ for every $t \in \mathbb{R}$. ■

The definition can be further improved by considering a possible *temporal dependence already in Schrödinger's picture*.

Definition 7.29 Let H be a the Hilbert space and $\mathbb{R} \ni t \mapsto U_t$ a strongly-continuous unitary one-parameter group representing time evolution. A family of observables $\{A(t)\}_{t\in\mathbb{R}}$, parametrized by and also depending on time, is called a **parametrically time-dependent constant of motion** with respect to U if $A_t := U_t^{-1} A(t) U_t$ does not depend on t, i.e. $A_t = A_0$ for every $t \in \mathbb{R}$. ■

The meaning of the two definitions should be clear: even if the state evolves, the probability to obtain an outcome E, when measuring a constant of motion, remains stationary. Expectation values and standard deviations do not change in time either.

We are now ready to state the analogue of *Noether's theorem* in QM.

Theorem 7.30 (Quantum Noether Theorem I) *Consider a quantum system described on the Hilbert space* H *and a strongly continuous unitary one-parameter group* $\mathbb{R} \ni t \mapsto U_t$ *representing time evolution. If* A *is an observable represented by a (generally unbounded) selfadjoint operator* A *on* H*, the following facts are equivalent.*

(a) *A is a constant of motion: $A_t = A_0$ for all $t \in \mathbb{R}$.*
(b) *The one-parameter group of symmetries generated by A, $\mathbb{R} \ni s \mapsto e^{-isA}$, is a* **group of dynamical (quantum) symmetries**, *i.e. it commutes with time evolution:*

$$e^{-isA}U_t = U_t e^{-isA} \quad \textit{for all } s, t \in \mathbb{R}\,. \tag{7.25}$$

In particular, it transforms the time evolution of a pure state into the evolution of (another) pure state, i.e. $e^{-isA}\, U_t\psi = U_t\, e^{-isA}\psi$.
(c) *The dual action on observables (7.4) (or equivalently the inverse dual action (7.5)) of the one-parameter group of symmetries $\mathbb{R} \ni s \mapsto e^{-isA}$ generated by A, leaves H invariant:*

$$e^{-isA}He^{isA} = H\,, \quad \textit{for all } s \in \mathbb{R}\,.$$

Proof Suppose that (a) holds. By definition $U_t^{-1}AU_t = A$. From Proposition 3.69 we have $U_t^{-1}e^{-isA}U_t = e^{-isA}$ which is equivalent to (b). If (b) is true, we have $e^{-isA}e^{-itH}e^{isA} = e^{-itH}$. Proposition 3.69 yields $e^{-isA}He^{isA} = H$. Finally, suppose that (c) is valid. Again Proposition 3.69 produces $e^{-isA}U_te^{isA} = U_t$, which can be written $U_t^{-1}e^{-isA}U_t = e^{-isA}$. Eventually, Proposition 3.69 leads to $U_t^{-1}AU_t = A$ which is (a), concluding the proof. □

It is possible to define **dynamical (quantum) symmetries**, as of Exercise 7.33 (2), in agreement with the notion introduced above. The theorem can be extended to *parametrically time-dependent* observables $\{A(t)\}_{t\mathbb{R}}$.

Theorem 7.31 (Quantum Noether Theorem II) *Consider a quantum system described on the Hilbert space* H *equipped with a strongly continuous unitary one-parameter group representing time evolution* $\mathbb{R} \ni t \mapsto U_t$*. If* $\{A(t)\}_{t\in\mathbb{R}}$ *is a family of observables represented by a (generally unbounded) selfadjoint operator depending on* t*, the following facts are equivalent.*

(a) *$\{A(t)\}_{t\in\mathbb{R}}$ is a parametrically time-dependent constant of motion: $A_t = A_0$ for all $t \in \mathbb{R}$.*
(b) *The one-parameter group of symmetries generated by every $A(t)$, $\mathbb{R} \ni s \mapsto e^{-isA(t)}$, defines a* **group of dynamical symmetries depending parametrically on time**:

$$e^{-isA(t)}U_t = U_t e^{-isA(0)} \quad \textit{for all } s, t \in \mathbb{R}\,. \tag{7.26}$$

In particular it transforms the evolution of a pure state into the evolution of (another) pure state, i.e. $e^{-isA(t)}\, U_t\psi = U_t\, e^{-isA(0)}\psi$.

Proof The proof is trivial by Proposition 3.69: $A_t = A_0$ means $U_t^{-1}A(t)U_t = A(0)$ which, in turn, implies $U_t^{-1}e^{-isA(t)}U_t = e^{-isA(0)}$, namely $e^{-isA(t)}U_t = U_t e^{-isA(0)}$. So (a) implies (b). But all implications are reversible, and from the last equation we obtain $U_t^{-1}A(t)U_t = A(0)$, hence (b) implies (a). □

There is a suitable version of Theorem 7.30 (c) for observables depending parametrically on time. But exactly as in classical Hamiltonian mechanics, it has a more complicated interpretation [Mor18].

In physics' textbooks the above statements are almost inevitably stated using time derivatives and commutators. This approach is cumbersome, useless and it involves all the subtleties concerning the domains of the operators. ■

Example 7.32

(1) As we explained in Example 3.76, for the free particle in the rest space $\mathbb{R}^3$ of an inertial reference frame, the momentum along x_1 is a constant of motion, as a consequence of translational invariance along that axis. Let $\{U_u\}$ be the unitary group representing x_1-translations, $(U_u\psi)(x) = \psi(x - u\mathbf{e}_1)$ if $\psi \in L^2(\mathbb{R}^3, d^3x)$. The Hamiltonian $H = \frac{1}{2m}\sum_{j=1}^{3} P_j^2$ commutes with U_u, because the group is generated by P_1 itself: $U_u := e^{-iuP_1}$. Theorem 7.30 yields the thesis.

(2) An example of a parametrically time-dependent constant of motion is the generator of the boost along the axis $\mathbf{n}$, i.e. the one-parameter subgroup $\mathbb{R}^3 \ni x \mapsto x + tv\mathbf{n} \in \mathbb{R}^3$ of the Galilean group, where the speed $v \in \mathbb{R}$ is the group's parameter. The generator is [Mor18] the unique selfadjoint extension of

$$K_{\mathbf{n}}(t) = \sum_{j=1}^{3} n_j (mX_j|_D - tP_j|_D)\,, \tag{7.27}$$

where $m > 0$ is the system's mass and D is the *Gårding* or *Nelson* domain of the representation of the (central extension of the) Galilean group. The details will appear later in the book.

(3) In QM there exist symmetries described by operators which are simultaneously selfadjoint and unitary, meaning they are observables and they can be measured. Among them we have the **parity inversion**, or **spatial reflection**: $(\mathcal{P}\psi)(x) := \eta\psi(-x)$ for any particle described on $L^2(\mathbb{R}^3, d^3x)$, where $\eta = \pm 1$ does not depend on ψ. They are constants of motion ($U_t^{-1}\mathcal{P}U_t = \mathcal{P}$) if and only if they are dynamical symmetries ($\mathcal{P}U_t = U_t\mathcal{P}$). This phenomenon has no classical correspondent.

(4) The **time-reversal** symmetry, described by an anti-unitary operator $\mathcal{T}$, is supposed to satisfy $\mathcal{T}H\mathcal{T}^{-1} = H$. (See Exercise 7.33 (3) for the definition). Its anti-linearity implies (exercise) $\mathcal{T}e^{-itH}\mathcal{T}^{-1} = e^{+it\mathcal{T}H\mathcal{T}^{-1}}$, so $\mathcal{T}U_t = U_{-t}\mathcal{T}$, as expected physically. We stress that $\mathcal{T}$ *is a symmetry, but not a dynamical*

symmetry. There is no conserved quantity associated with this operator (it is not selfadjoint, nor linear!). ■

Exercise 7.33

(1) Prove that a Hamiltonian observable that does not depend on time is a constant of motion.

Solution The time translation is described by $U_t = e^{itH}$ and, trivially, it commutes with U_s. Noether's theorem allows to conclude. □

(2) If $U_t = e^{-itH}$ is the time time-evolution operator of a quantum system, a ***dynamical quantum symmetry*** (if any) is a Wigner symmetry represented by a unitary or anti-unitary operator $V : \mathsf{H} \to \mathsf{H}$ such that, recalling that pure states are unit vectors up to phase,

$$\chi_t^{(\psi)} V U_t \psi = U_t V \psi$$

for all $t \in \mathbb{R}$ and every unit $\psi \in \mathsf{H}$, where $\chi_t^{(\psi)} \in \mathbb{C}$ with $|\chi_t^{(\psi)}| = 1$.

Prove that $\chi_t^{(\psi)}$ does not depend on ψ and has the form $\chi_t = e^{ict}$ for some $c \in \mathbb{R}$. Furthermore, if $\sigma(H)$ is bounded below but not above, show that $\chi_t^{(\psi)} = 1$, V is unitary and $VHV^{-1} = H$.

Solution By the same argument of the proof of Theorem 7.6 it is not hard to see that $\chi_t^{(\psi)}$ does not depend on ψ. Next observe that $\chi_t U_t = VU_tV^{-1}$, the right-hand side being a strongly-continuous one-parameter group of unitary operators. Mimicking the proof of Theorem 7.20 (b) we find $\chi_t = e^{ict}$ for some $c \in \mathbb{R}$. If the operator V is anti-unitary, $e^{ict}U_t = VU_tV^{-1}$ implies $-VHV^{-1} = H - cI$ and therefore, with obvious notation, $\sigma(VHV^{-1}) = -\sigma(H) + c$. Proposition 3.4 immediately yields $\sigma(H) = -\sigma(H) + c$, which contradicts the boundedness. Hence V must be unitary, and $\sigma(H) = \sigma(H) - c$. Since $\sigma(H)$ is bounded below, $c = 0$. □

(3) If $U_t = e^{-itH}$ is the time time-evolution operator of a quantum system, ***time reversal*** (if present) is a Wigner symmetry represented by a unitary or anti-unitary operator $\mathcal{T} : \mathsf{H} \to \mathsf{H}$ such that, according to the fact that pure states are unit vectors up to phase,

$$\chi_t^{(\psi)} \mathcal{T} U_t \psi = U_{-t} \mathcal{T} \psi$$

for all $t \in \mathbb{R}$ and every unit $\psi \in \mathsf{H}$, where $\chi_t^{(\psi)} \in \mathbb{C}$ with $|\chi_t^{(\psi)}| = 1$.

Prove that, $\chi_t^{(\psi)}$ does not depend on ψ and has the form $\chi_t = e^{ict}$ for some $c \in \mathbb{R}$. Furthermore, if $\sigma(H)$ is bounded below but not above, show that $\chi_t^{(\psi)} = 1$, $\mathcal{T}$ is anti-unitary, and $\mathcal{T} H \mathcal{T}^{-1} = H$.

Solution With the same argument of Theorem 7.6, $\chi_t^{(\psi)}$ does not depend on ψ. In $\chi_t U_t = \mathcal{T} U_{-t} \mathcal{T}^{-1}$ the right-hand side is a strongly-continuous one-parameter group of unitary operators. Inspired by the proof of Theorem 7.20 (b), we obtain $\chi_t = e^{ict}$ for some $c \in \mathbb{R}$. If the operator $\mathcal{T}$ is unitary, $e^{ict}U_t = \mathcal{T}U_{-t}\mathcal{T}^{-1}$ implies $\mathcal{T}H\mathcal{T}^{-1} = -H + cI$ and therefore, with obvious notation, $\sigma(\mathcal{T}H\mathcal{T}^{-1}) = -\sigma(H) + c$. Proposition 3.4 immediately yields $\sigma(H) = -\sigma(H) + c$, which is false if $\sigma(H)$ is bounded below but not above. Hence $\mathcal{T}$ is anti-unitary and $\sigma(H) = \sigma(H) + c$. Since $\sigma(H)$ is bounded below, $c = 0$. □

(4) Consider the spinless particle, and prove that if $V : L^2(\mathbb{R}^3, d^3x) \to L^2(\mathbb{R}^3, d^3x)$ is unitary, selfadjoint, and satisfies $VX_kV^{-1} = -X_k$, $VP_kV^{-1} = -P_k$ for $k = 1, 2, 3$, then $V = \mathcal{P}$, with $\mathcal{P}$ defined in Example 7.32 (3).

Solution If V and V' satisfy the given conditions, then $V^{-1}V'$ commutes with X_k and P_k for $k = 1, 2, 3$. According to Example 6.28 (3), $V^{-1}V' = cI$ for some $c \in \mathbb{C}$. That V and V' are selfadjoint and unitary respectively implies $c \in \mathbb{R}$ and $c \in \mathbb{T}$, hence $c = \pm 1$. To conclude, observe that the $\mathcal{P}$ of Example 7.32 (3) satisfies the hypothesis. □

(5) With reference to the spinless particle, suppose $\mathcal{T} : L^2(\mathbb{R}^3, d^3x) \to L^2(\mathbb{R}^3, d^3x)$ is anti-unitary and satisfies

$$\mathcal{T}X_k\mathcal{T}^{-1} = X_k\,, \quad \mathcal{T}P_k\mathcal{T}^{-1} = -P_k \quad \text{for } k = 1, 2, 3.$$

Show that $(\mathcal{T}\psi)(x) := \eta\overline{\psi(x)}$ for every $\psi \in L^2(\mathbb{R}^3, d^3x)$, and where η is a phase independent of ψ.

Solution Observe that $(V\psi)(x) := \overline{\psi(x)}$ and ηV satisfy the hypotheses, for every fixed $\eta \in \mathbb{T}$. If $\mathcal{T}$ is another anti-unitary operator satisfying the hypotheses then $\mathcal{T}V^{-1}$ is unitary and commutes with X_k and P_k for $k = 1, 2, 3$. Exactly as for the previous exercise, necessarily $\mathcal{T}V^{-1} = \eta I$ for some $\eta \in \mathbb{T}$, proving the assertion. □

7.3 More on Strongly Continuous Unitary Representations of Lie Groups

Symmetry Lie groups arise naturally in physics when one considers the whole group of symmetries for a given quantum system [BaRa84]. For instance, in classical physics the (proper orthochronous) *Galilean group* (where $SU(2)$ is used in place of $SO(3)$) is taken to be the group of continuous symmetries of every isolated quantum system studied in an inertial reference frame. Actually every strongly-continuous unitary representation of the Galilean group is trivial, and not accidentally those used in quantum physics are strongly-continuous unitary representations of a *central extension* of the Galilean group. This happens for reasons of physical and mathematical nature: the mass of the system is necessary to describe the action of the boost in quantum physics, and this piece of information is not retained by the Galilean group (but it can be encoded in the multipliers when constructing central extensions). Mathematically speaking, the Galilean group violates the cohomological obstruction of Bargmann's theorem. The (proper orthochronous) *Poincaré group* (with $SU(2)$ instead of $SO(3)$) replaces the Galilean group in the relativistic realm, and its continuous unitary-projective representations can always be made unitary because Bargmann's constraint is satisfied [BaRa84].

From an abstract point of view, the groups of symmetries of a quantum system—excluding discrete symmetries if any—are by definition *topological groups*. We can always suppose that the group is connected by looking at the connected component of the identity. There are a bunch of assumptions of physical significance in addition to the continuity of the group operations, namely that the topology is (1) Hausdorff,[3] (2) second countable, and (3) locally Euclidean (every element of the group has compatible local coordinate charts, which create a local identification with $\mathbb{R}^n$). If all of this happens, the celebrated *Gleason-Montgomery-Zippin* theorem (see [Mor18] for a concise discussion) implies that the topological group is actually a *Lie group* [HiNe13], whose unique smooth (analytic) structure underlies the C^0 structure.

It is worth stressing that the general group of continuous symmetries of a quantum system in particular contains *time evolution* as a subgroup. (Even *different notions of* time *evolution*, corresponding to different choices of the reference frame in the relativistic context.)

Sometimes these Lie groups can be represented in terms of proper unitary representations, in particular when Bargmann's theorem holds. When not, the central extensions that have the structure of Lie groups can be represented unitarily and strongly continuously [Var07, Mor18]. Therefore it is not too restrictive to limit ourselves to *strongly-continuous* unitary representations of *Lie* groups only.

General reference texts on unitary and projective-unitary representations of topological and Lie groups with relevance in physics include: [BaRa84] (albeit not always rigorously written), [Var07], and for a concise summary on some topics [Mor18]. A fairly complete mathematical treatise on continuous representations (also of algebras) is [Schm90].

7.3.1 Strongly Continuous Unitary Representations

Before we examine Lie groups, let us tackle strongly-continuous representations of general *topological groups*. Sometimes *strongly-continuous representations* are simply called *continuous representations*. This is due to the following elementary result.

[3]From the experimental point of view, a Hausdorff topology means that we can distinguish different elements of the group even if our knowledge is affected by experimental errors.

Proposition 7.34 *If G is a topological group with neutral element e and $U : G \ni g \mapsto U_g \in \mathfrak{B}(\mathsf{H})$ is a unitary representation on the Hilbert space H, each of the following facts is equivalent to the strong continuity of U.*

(a) *U is weakly continuous;*
(b) *U is strongly continuous at e;*
(c) *U is weakly continuous at e;*
(d) *$\langle\psi|U_g\psi\rangle \to \langle\psi|\psi\rangle$ as $g \to e$ for every $\psi \in \mathcal{D}$, where $\mathcal{D} \subset \mathsf{H}$ satisfies $\overline{span(\mathcal{D})} = \mathsf{H}$.*

Proof Observing that $||U_g x - U_f x|| = ||U_{f^{-1}\cdot g} x - Ix||$ and $f^{-1}\cdot g \to e$ if $g \to f$, the proof is identical to that of Proposition 7.22. □

The theory of strongly-continuous unitary representations of topological groups is an important part of Representation Theory (see in particular [NaSt82] for a classical treatise on the subject and [BaRa84] for physical applications). An important result due to *Peter and Weyl* concerns compact Hausdorff groups (see [Mor18] for the full statement and proof).

Theorem 7.35 (Peter-Weyl's Basic Statement) *Let G be a compact Hausdorff group—a compact Lie group in particular—and $G \ni g \mapsto U_g \in \mathfrak{B}(\mathsf{H})$ a strongly-continuous unitary representation on the Hilbert space $\mathsf{H} \neq \{0\}$.*

(a) *If U is irreducible, then H is finite-dimensional.*
(b) *If U is not irreducible, then the orthogonal Hilbert decomposition $\mathsf{H} = \bigoplus_{k\in K} \mathsf{H}_k$ holds, where H_k are pairwise-orthogonal and non-trivial closed subspaces of finite dimension, all invariant under U. Furthermore every map $U\restriction_{\mathsf{H}_k} : \mathsf{H}_k \to \mathsf{H}_k$ is an irreducible representation of G.*

This result applies in particular to compact Lie groups like $SU(n)$ and $SO(n)$, whose irreducible strongly-continuous unitary representations are therefore always finite-dimensional. The theory of the *spin* deals with strongly-continuous unitary irreducible representations of $SU(2)$ which, as physicists know very well, are finite-dimensional by the Peter-Weyl theorem.

Another technical general result is the following one, that links a representation's irreducibility to the Hilbert space's separability. As before, we state it in a more general fashion which includes Lie groups.

Proposition 7.36 *Let $G \ni g \mapsto U_g \in \mathfrak{B}(\mathsf{H})$ be a strongly-continuous unitary representation of a separable topological group G—a Lie group in particular—on the Hilbert space H. If the representation is irreducible, then H is separable.*

Proof As G is separable, let $V \subset G$ be a dense countable set. Pick $\psi \in \mathsf{H} \setminus \{0\}$. Since every $U_g : \mathsf{H} \to \mathsf{H}$ is continuous, the closure H_0 of the set of finite combinations of elements $U_g\psi$ for $g \in G$ is invariant under the action of U. The representation is irreducible and $\mathsf{H}_0 \neq \{0\}$, so $\mathsf{H}_0 = \mathsf{H}$. By the strong continuity of $G \ni g \mapsto U_g$, every element in H_0 is the limit of finite linear combinations with rational (complex) coefficients of elements $U_h\psi$ where $h \in V$.

If G is a Lie group, in particular it is a second-countable and therefore separable. Given a topological basis $\{B_n\}_{n\in\mathbb{N}}$ of G—where we assume $B_n \neq \varnothing$—choose $b_n \in B_n$ for every $n \in \mathbb{N}$. Then $C := \{b_n \mid n \in \mathbb{N}\}$ is countable and dense, because every open neighbourhood O_g of $g \in G$ necessarily contains some B_p, so $O_g \ni b_p \in C$. □

7.3.2 From the Gårding Space to Nelson's Theorem

We henceforth restrict our study to Lie groups.

Remark 7.37 In the rest of the chapter we consider only *finite-dimensional real Lie groups* G, with Lie algebra $\mathfrak{g}$ and Lie bracket $\{\ ,\ \}$. ■

A fundamental technical fact is that strongly-continuous unitary representations of (connected) Lie groups are associated with representations of the Lie algebras in terms of (anti-)selfadjoint operators. These operators are often interpreted physically as constants of motion (in general depending parametrically on time) when the Hamiltonian of the system belongs to the representation of the Lie algebra. We want to study the relationship between representations of G and representations of $\mathfrak{g}$. First of all, we define the operators representing the Lie algebra.

Definition 7.38 Let G be a Lie group and consider a strongly continuous unitary representation U of G on the Hilbert space H. Let $\mathbb{R} \ni s \mapsto \exp(s\mathsf{A}) \in G$ be the one-parameter Lie subgroup generated by $\mathsf{A} \in \mathfrak{g}$. The **selfadjoint generator associated with** A,

$$A : D(A) \to \mathsf{H},$$

is the generator of the strongly continuous one-parameter unitary group

$$\mathbb{R} \ni s \mapsto U_{\exp\{s\mathsf{A}\}} = e^{-isA}$$

in the sense of Theorem 7.25. ■

The expectation is that these generators (with a factor $-i$) define a *representation of the Lie algebra* of the group. The major reason is that they are associated with unitary one-parameter subgroups exactly as the elements of the Lie algebra are associated with one-parameter Lie subgroups. In particular, we expect the Lie bracket to correspond to the commutator of operators. The problem is that the generators A may have different domains. We therefore seek a common invariant domain (the commutator must be defined on it), where all generators make simultaneous sense. This domain should retain all information on the operators A, disregarding the fact that they may be defined on larger domains. In other words, we would like each generator's domain to be a *core* (Definition 2.30 (3)). There are several candidates for this space, and one of the most appealing is the *Gårding space*.

Definition 7.39 Let G be a Lie group and consider a strongly continuous unitary representation U of G on the Hilbert space H. If $f \in C_c^\infty(G)$ (compactly-supported smooth complex functions on G) and $x \in \mathsf{H}$, define

$$x[f] := \int_G f(g) U_g x \, dg \tag{7.28}$$

where dg is the left-invariant Haar measure on G and integration is defined in a weak sense via Riesz's lemma: since the anti-linear map $\mathsf{H} \ni y \mapsto \int_G f(g)\langle y|U_g x\rangle dg$ is continuous, $x[f]$ is the unique vector in H such that

$$\langle y|x[f]\rangle = \int_G f(g)\langle y|U_g x\rangle dg \,, \quad \forall y \in \mathsf{H} \,.$$

The finite span of vectors $x[f] \in \mathsf{H}$ with $f \in C_c^\infty(G)$ and $x \in \mathsf{H}$ is called the **Gårding space** of the representation, and we indicate by $D_G^{(U)}$. ■

The subspace $D_G^{(U)}$ enjoys very remarkable properties that we list in the next theorem. In the following $L_g : C_c^\infty(G) \to C_c^\infty(G)$ denotes the standard left action of $g \in G$:

$$(L_g f)(h) := f(g^{-1}h) \quad \forall h \in G \,, \tag{7.29}$$

and, if $\mathsf{A} \in \mathfrak{g}$, $X_\mathsf{A} : C_c^\infty(G) \to C_c^\infty(G)$ is the smooth vector field on G (smooth differential operator):

$$(X_\mathsf{A}(f))\,(g) := \lim_{t\to 0} \frac{f(\exp\{-t\mathsf{A}\}g) - f(g)}{t} \quad \forall g \in G \,. \tag{7.30}$$

Thus

$$\mathfrak{g} \ni \mathsf{A} \mapsto X_\mathsf{A} \tag{7.31}$$

defines a representation of $\mathfrak{g}$ on $C_c^\infty(G)$ by vector fields (differential operators). We conclude with the following theorem [Schm90, Mor18], whereby the Gårding space has all the expected properties.

Theorem 7.40 *Referring to Definitions 7.38 and 7.39, $D_G^{(U)}$ satisfies the following properties.*

(a) $D_G^{(U)}$ *is dense in* H.
(b) $U_g(D_G^{(U)}) \subset D_G^{(U)}$ *for every $g \in G$. More precisely, if $f \in C_c^\infty(G)$, $x \in \mathsf{H}$, $g \in G$, then*

$$U_g x[f] = x[L_g f] \,. \tag{7.32}$$

(c) *If* $\mathsf{A} \in \mathfrak{g}$*, then* $D_G^{(U)} \subset D(A)$ *and* $A(D_G^{(U)}) \subset D_G^{(U)}$*. More precisely*

$$-iAx[f] = x[X_{\mathsf{A}}(f)] \tag{7.33}$$

(d) *The map*

$$\mathfrak{g} \ni \mathsf{A} \mapsto -iA|_{D_G^{(U)}} =: u(\mathsf{A}) \tag{7.34}$$

is a Lie algebra representation by skew-symmetric operators defined on the common dense and invariant domain $D_G^{(U)}$*. In other words, the map is* $\mathbb{R}$*-linear and*

$$[u(\mathsf{A}), u(\mathsf{A}')] = u(\{\mathsf{A}, \mathsf{A}'\}) \quad \textit{if } \mathsf{A}, \mathsf{A}' \in \mathfrak{g}.$$

(e) $D_G^{(U)}$ *is a core for every selfadjoint generator* A *with* $\mathsf{A} \in \mathfrak{g}$*, that is*

$$A = \overline{A|_{D_G^{(U)}}}\,, \quad \forall \mathsf{A} \in \mathfrak{g}\,. \tag{7.35}$$

Now we wish to address the converse problem. Suppose we are given a representation of a Lie algebra $\mathfrak{g}$ in terms of skew-symmetric operators defined on common invariant subspace of a Hilbert space H. We wonder whether or not it is possible to lift the representation to a unitary strongly-continuous representation of the unique simply connected Lie group G with Lie algebra $\mathfrak{g}$. This is a much more difficult problem. It was solved by Nelson [Nel69], who introduced a special domain in the Hilbert space of the representation.

Given a strongly continuous representation U of a Lie group G, there is another space $D_N^{(U)}$ with similar features to $D_G^{(U)}$ (see, e.g., [Mor18]). This space ends up being more useful than the Gårding space to *build* the representation U by exponentiating the Lie algebra representation. The domain $D_N^{(U)}$ consists of vectors $\psi \in \mathsf{H}$ such that $G \ni g \mapsto U_g\psi$ is *analytic* in g, i.e. expandable in power series of (real) analytic coordinates around any point of G. The elements of $D_N^{(U)}$ are called **analytic vectors of the representation** U and $D_N^{(U)}$ is the **space of analytic vectors of the representation** U. It turns out that $D_N^{(U)}$ is invariant under every U_g and that $D_N^{(U)} \subset D_G^{(U)}$ (this is by no means trivial and follows from the deep *Dixmier-Mallievin theorem* [Mor18], whereby $\psi \in D_G^{(U)}$ if and only if $G \ni g \mapsto U_g\psi$ is smooth).

There is a remarkable relationship between $D_N^{(U)}$ and Definition 2.52. Nelson proved the following important result [Schm90, Mor18], which implies that $D_N^{(U)}$ is dense in H, because analytic vectors for a selfadjoint operator are dense (Exercise 3.78). An operator crops up that we call *Nelson operator*.

Proposition 7.41 *Let G be a Lie group and $G \ni g \mapsto U_g$ a strongly-continuous unitary representation on the Hilbert space H. Take a basis $\mathsf{A}_1, \dots, \mathsf{A}_n \in \mathfrak{g}$ and define the* **Nelson operator** *on $D_G^{(U)}$ by*

$$\Delta_N := -\sum_{k=1}^{n} u(\mathsf{A}_k)^2 ,$$

where, as earlier, $iu(\mathsf{A}_k)$ are the selfadjoint generators A_k restricted to the Gårding domain $D_G^{(U)}$. Then

(a) *Δ_N is essentially selfadjoint on $D_G^{(U)}$.*
(b) *Every analytic vector of the selfadjoint operator $\overline{\Delta_N}$ is analytic and belongs in $D_N^{(U)}$. In particular $D_N^{(U)}$ is dense.*
(c) *Every vector in $D_N^{(U)}$ is analytic for every selfadjoint operator $i\overline{u(\mathsf{A}_k)}$, which is therefore essentially selfadjoint in $D_N^{(U)}$ by Nelson's criterion (Theorem 2.53)*

Now that we possess the necessary notions, we can eventually state the well-known theorem of Nelson that associates representations of the only simply connected Lie group with a given Lie algebra to representations of that Lie algebra.

Theorem 7.42 (Nelson's Theorem) *Consider a real n-dimensional Lie algebra V of operators $-iS$, where each S is symmetric on the Hilbert space H, defined on a common invariant and dense subspace $\mathcal{D} \subset \mathsf{H}$, with the usual commutator as Lie bracket.*

Let $-iS_1, \cdots, -iS_n \in V$ be a basis of V and define Nelson's operator with domain $\mathcal{D}$:

$$\Delta_N := \sum_{k=1}^{n} S_k^2 .$$

If Δ_N is essentially selfadjoint, there exists a strongly-continuous unitary representation

$$G_V \ni g \mapsto U_g$$

on H of the unique connected, simply-connected Lie group G_V with Lie algebra V.

U is uniquely determined by the fact that the closures $\overline{S}$, for every $-iS \in V$, are the selfadjoint generators of the representations of the one-parameter subgroups of G_V in the sense of Definition 7.38. In particular, the symmetric operators S are essentially selfadjoint on $\mathcal{D}$.

Our version is slightly more than what is necessary, for it is known that the hypotheses can be relaxed (see [Mor18], also for further results on Nelson's theory).

Exercise 7.43 Let H be a Hilbert space and A, B selfadjoint operators with common invariant dense domain $D \subset \mathsf{H}$ where they are symmetric and commute. Prove that if $A^2 + B^2$ is essentially selfadjoint on D, then the spectral measures of A and B commute.

Solution Exploit Nelson's theorem after noticing that A, B define the Lie algebra of the Abelian Lie group $(\mathbb{R}^2, +)$ (which is connected and simply-connected) and that D is a core for A and B, since they are essentially selfadjoint on D by Nelson's theorem. ∎

Example 7.44

(1) Using polar coordinates, the Hilbert space $L^2(\mathbb{R}^3, d^3x)$ factorizes as

$$L^2([0, +\infty), r^2 dr) \otimes L^2(\mathbb{S}^2, d\Omega) ,$$

where $d\Omega$ is the standard rotationally-invariant Borel measure on the unit sphere $\mathbb{S}^2$ in $\mathbb{R}^3$ normalized by $\int_{\mathbb{S}^2} 1 d\Omega = 4\pi$. In particular a Hilbert basis of $L^2(\mathbb{R}^3, d^3x)$ is made of the products $\psi_n(r)Y^l_m(\theta, \phi)$ where $\{\psi_n\}_{n\in\mathbb{N}}$ is any Hilbert basis in $L^2([0, +\infty), r^2 dr)$ and $\{Y^l_m \mid l = 0, 1, 2, \dots , m = 0, \pm 1, \pm 2, \dots \pm l\}$ is the standard Hilbert basis of *spherical harmonics* of $L^2(\mathbb{S}^2, d\Omega)$ [BaRa84]. The ψ_n are smooth functions with compact support, whose derivatives at 0 vanish at every order. Since the Y^l_m are smooth on $\mathbb{S}^2$, the ψ_n can be chosen so that $\mathbb{R}^3 \ni x \mapsto (\psi_n \cdot Y^l_m)(x)$ are elements of $C^\infty(\mathbb{R}^n)$ (and therefore also of $\mathscr{S}(\mathbb{R}^3)$). Now consider the three symmetric operators, defined on the common dense invariant domain $\mathscr{S}(\mathbb{R}^3)$,

$$\mathscr{L}_k = \sum_{i,j=1}^{3} \epsilon_{kij} X_i P_j|_{\mathscr{S}(\mathbb{R}^3)} ,$$

where ϵ_{ijk} is totally skew-symmetric in ijk and $\epsilon_{123} = 1$. By direct inspection one sees that

$$[-i\mathscr{L}_k, -i\mathscr{L}_h] = \sum_{r=1}^{3} \epsilon_{khr}(-i\mathscr{L}_r)$$

so that the real span of the operators $-i\mathscr{L}_k$ is a representation of the Lie algebra of the simply connected real Lie group $SU(2)$ (the universal covering of $SO(3)$). Define the Nelson operator $\mathscr{L}^2 := \sum_{k=1}^{3} \mathscr{L}_k^2$ on $\mathscr{S}(\mathbb{R}^3)$. Obviously this is a symmetric operator. A well-known computation proves that

$$\mathscr{L}^2\, \psi_n(r)Y^l_m = l(l+1)\, \psi_n(r)Y^l_m .$$

We conclude that $\mathscr{L}^2$ admits a Hilbert basis of eigenvectors. Corollary 2.54 implies $\mathscr{L}^2$ is essentially selfadjoint. Therefore we can apply Theorem 7.42, and define a strongly continuous unitary representation $SU(2) \ni M \mapsto U_M$ (an $SO(3)$-representation actually, since $U_{-I} = I$). The three selfadjoint operators $L_k := \overline{\mathscr{L}_k}$ are the generators of the one-parameter group of rotations around the orthogonal Cartesian axes x_k, $k = 1, 2, 3$. The one-parameter subgroup of rotations around the generic unit vector $\mathbf{n}$, with components n_k, has selfadjoint generator $L_{\mathbf{n}} = \overline{\sum_{k=1}^{3} n_k \mathscr{L}_k}$. The observable $L_{\mathbf{n}}$ has the physical meaning of the $\mathbf{n}$-*component of the angular momentum* of the particle described on $L^2(\mathbb{R}^3, d^3x)$. It turns out that, for $\psi \in L^2(\mathbb{R}^3, d^3x)$,

$$(U_M\psi)(x) = \psi(\pi(M)^{-1}x) \,, \quad M \in SU(2) \,, x \in \mathbb{R}^3 \tag{7.36}$$

where $\pi : SU(2) \to SO(3)$ is the covering map. Equation (7.36) describes the action of the 3D rotation group on pure states in terms of quantum symmetries. This representation is, in fact, a subrepresentation of the unitary $IO(3)$-representation of Example 7.8 (1).

(2) Given a quantum system, a quite general situation is that where the quantum symmetries of the systems are described by a strongly continuous representation $V : G \ni g \mapsto V_g$ on the Hilbert space H of the system, and time evolution is the representation of a one-parameter Lie subgroup with generator $\mathsf{H} \in \mathfrak{g}$:

$$V_{\exp(t\mathsf{H})} = e^{-itH} =: U_t \,.$$

This is the case, for instance, of relativistic quantum particles, where G is the *special orthochronous Poincaré group*, i.e. the semi-direct product $SO(1,3)_+ \ltimes \mathbb{R}^4$ (or its universal covering $SL(2,\mathbb{C}) \ltimes \mathbb{R}^4$). To describe non-relativistic quantum particles, the relevant group G is a $U(1)$-central extension of the universal covering of the (connected, orthochronous) Galilean group.

In this situation, every element of $\mathfrak{g}$ determines a constant of motion. There are actually two cases.

(i) If $\mathsf{A} \in \mathfrak{g}$ and $\{\mathsf{H}, \mathsf{A}\} = 0$, the Lie subgroups $\exp(t\mathsf{H})$ and $\exp(s\mathsf{A})$ commute by the *Baker-Campbell-Hausdorff* formula (see [NaSt82, Mor18], for instance). Consequently A is a constant of motion because $V_{\exp(t\mathsf{H})} = e^{-itH}$ and $V_{\exp(s\mathsf{A})} = e^{-isA}$ commute as well and Theorem 7.30 holds. In this case e^{-isA} defines a dynamical symmetry by Noether's theorem. This picture applies, for a free particle, to $A = J_{\mathbf{n}}$, the observable describing the total angular momentum along the unit vector $\mathbf{n}$ in an inertial frame.

(ii) If $\mathsf{A} \in \mathfrak{g}$ but $\{\mathsf{H}, \mathsf{A}\} \neq 0$ the situation is slightly more complicated, and we exploit Theorem 7.31. A defines a constant of motion in terms of selfadjoint operators (observables) belonging to the representation of $\mathfrak{g}$. The difference with the previous case is that now the constant of motion *depends parametrically on time*. We therefore have a collection of observables $\{A(t)\}_{t\in\mathbb{R}}$ in the Schrödinger picture, such that $A_t := U_t^{-1}A(t)U_t$ are the corresponding observables in the Heisenberg picture. The equation of the constant of motion is therefore $A_t = A_0$.

By exploiting the natural action of the one-parameter Lie subgroups on $\mathfrak{g}$ we define elements

$$\mathsf{A}(t) := \exp(t\mathsf{H})\mathsf{A}\exp(-t\mathsf{H}) \in \mathfrak{g}\ , \quad t \in \mathbb{R}$$

parametrised by time. If $\{\mathsf{A}_k\}_{k=1,\dots,n}$ is a basis of $\mathfrak{g}$,

$$\mathsf{A}(t) = \sum_{k=1}^{n} a_k(t)\mathsf{A}_k \tag{7.37}$$

for some real-valued smooth maps $a_k = a_k(t)$. By construction, the corresponding selfadjoint generators $A(t)$, $t \in \mathbb{R}$, define a parametrically time-dependent constant of motion. Indeed, since (exercise)

$$\exp(s\exp(t\mathsf{H})\mathsf{A}\exp(-t\mathsf{H})) = \exp(t\mathsf{H})\exp(s\mathsf{A})\exp(-t\mathsf{H})\ ,$$

we have

$$-iA(t) = \frac{d}{ds}|_{s=0}V_{\exp(s\exp(t\mathsf{H})\mathsf{A}\exp(-t\mathsf{H}))} = \frac{d}{ds}|_{s=0}V_{\exp(t\mathsf{H})\exp(s\mathsf{A})\exp(-t\mathsf{H})}$$

$$= \frac{d}{ds}|_{s=0}V_{\exp(t\mathsf{H})}V_{\exp(s\mathsf{A})}V_{\exp(-t\mathsf{H})} = -iU_tAU_t^{-1}\ .$$

Therefore, as claimed, we end up with a constant of motion that depends parametrically upon time,

$$A_t = U_t^{-1}A(t)U_t = U_t^{-1}U_tAU_t^{-1}U_t = A = A_0\ .$$

By Theorem 7.40, as the map $\mathfrak{g} \ni A \mapsto A|_{D_G^{(V)}}$ is a Lie algebra isomorphism, we can recast (7.37) for selfadjoint generators

$$A(t)|_{D_G^{(V)}} = \sum_{k=1}^{n} a_k(t)A_k|_{D_G^{(V)}} \tag{7.38}$$

(where $D_G^{(V)}$ could be replaced by $D_N^{(V)}$ as the reader can easily establish, using Proposition 7.41 and Theorem 7.42). Since $D_G^{(V)}$ (resp. $D_N^{(V)}$) is a core for $A(t)$,

$$A(t) = \overline{\sum_{k=1}^{n} a_k(t)A_k|_{D_G^{(V)}}}\ , \tag{7.39}$$

the bar denoting the closure of an operator, as usual. (The same is valid with $D_N^{(V)}$ in place of $D_G^{(V)}$.)

A relevant case, both for the non-relativistic and the relativistic framework is the selfadjoint generator $K_{\mathbf{n}}(t)$ associated with the *Galilean boost transformation* along the unit vector $\mathbf{n}$ in $\mathbb{R}^3$ (the rest space of the inertial frame where the boost is viewed as an active transformation). Indeed, consider the generators of the connected orthochronous Galilean group (or a ($U(1)$-central extension of its universal covering). Then

$$\{h, k_{\mathbf{n}}\} = -p_{\mathbf{n}} \neq 0\,,$$

where $p_{\mathbf{n}}$ is the generator of spatial translations along $\mathbf{n}$, corresponding to the momentum observable along the axis $\mathbf{n}$ when passing to selfadjoint generators. The non-relativistic expression of $K_{\mathbf{n}}(t)$, for a single particle, appears in (7.27). For an extended discussion on the non-relativistic case consult [Mor18]. A pleasant and physically exhaustive discussion encompassing the relativistic case appears in [BaRa84]. ■

Theorem 7.45 (Stone-von Neumann-Mackey Theorem) *Let H be a Hilbert space and suppose that there are $2n$ symmetric operators $Q_1, \ldots, Q_n$ and $M_1, \ldots, M_n$ on H satisfying the following requirements.*

(1) *There is a common, dense, invariant subspace $D \subset \mathsf{H}$ where the CCRs*

$$[Q_h, M_k]\psi = i\hbar\delta_{hk}\psi\,, \quad [Q_h, Q_k]\psi = 0\,, \quad [M_h, M_k]\psi = 0\,, \tag{7.40}$$

with $\psi \in D$, $h, k = 1, \ldots, n$, hold.

(2) *The representation is irreducible in the sense that there is no proper non-zero closed subspace $\mathsf{K} \subset \mathsf{H}$ such that $P_{\mathsf{K}}\overline{Q_k} \subset \overline{Q_k}P_{\mathsf{K}}$ and $P_{\mathsf{K}}\overline{M_k} \subset \overline{M_k}P_{\mathsf{K}}$ where $P_{\mathsf{K}} : \mathsf{H} \to \mathsf{H}$ is the orthogonal projector onto K.*

(3) *The operator $\sum_{k=1}^n Q_k^2|_D + M_k^2|_D$ is essentially selfadjoint.*

Under these conditions, Q_k and M_k are essentially selfadjoint on D, which turns out to be a common core, and there exists a Hilbert-space isomorphism (a surjective linear isometry) $U : \mathsf{H} \to L^2(\mathbb{R}^n, d^n x)$ such that

$$U\overline{Q_k}U^{-1} = X_k \quad \textit{and} \quad U\overline{M_k}U^{-1} = P_k \quad k = 1, \ldots, n \tag{7.41}$$

where X_k and P_k are the standard position (2.22) and momentum (2.23) selfadjoint operators on $L^2(\mathbb{R}^n, d^n x)$. In particular H is separable.

If only (1) and (3) are valid, then H decomposes as an orthogonal Hilbert sum $\mathsf{H} = \oplus_{r\in R}\mathsf{H}_r$ where R is finite, or countable if H is separable, the $\mathsf{H}_r \subset \mathsf{H}$ are closed with

$$P_{\mathsf{H}_r}\overline{Q_k} \subset \overline{Q_k}P_{\mathsf{H}_r} \quad \textit{and} \quad P_{\mathsf{H}_r}\overline{M_k} \subset \overline{M_k}P_{\mathsf{H}_r}\,,$$

where $P_{\mathsf{H}_r} : \mathsf{H} \to \mathsf{H}$ *is the orthogonal projector onto* H_r, $k = 1, \ldots, n$ *and the restrictions of* $\overline{Q_k}$ *and* $\overline{M_k}$ *to each* H_r *satisfy (7.41) for suitable surjective linear isometries* $U_r : \mathsf{H}_r \to L^2(\mathbb{R}^n, d^n x)$.

Proof If (1) holds, the restrictions to D of Q_k, M_k define symmetric operators (since they are symmetric and D is dense and contained in their domains), and also their squares are symmetric, since D is invariant. Adding (3), Nelson's theorem (the symmetric operator $I|_D^2 + \sum_{k=1}^n Q_k^2|_D + M_k^2|_D$ is essentially selfadjoint if $\sum_{k=1}^n Q_k^2|_D + M_k^2|_D$ is), says there is a strongly continuous unitary representation $W \ni g \mapsto V_g \in \mathfrak{B}(\mathsf{H})$ of the simply connected $(2n + 1)$-dimensional Lie group W whose Lie algebra is spanned by $-iI, -iQ_k, -iM_k$ subject to (7.40) and $[-iQ_h, -iI] = [-iM_k, -iI] = 0$, where $-iI$ is restricted to D. W is the *Weyl-Heisenberg* group [Mor18]. Due to Theorem 7.42, the selfadjoint generators of this representation are just the selfadjoint operators $\overline{Q_k|_D}$ and $\overline{P_k|_D}$ (and I). Since $\overline{Q_k|_D} \subset \overline{Q_k}$, where the former is selfadjoint and the latter symmetric, necessarily $\overline{Q_k|_D} = \overline{Q_k}$ and $\overline{M_k|_D} = \overline{M_k}$. D is therefore a common core. If, furthermore, the Lie algebra representation is irreducible (as in (2)), the unitary representation is irreducible, too: if $\mathsf{K} \subset \mathsf{H}$ were invariant under the unitary operators, by Stone's theorem it would be invariant (again, as in (2)) under the selfadjoint generators $\overline{Q_k}$, $\overline{P_k}$ of the one-parameter Lie groups associated to each Q_k and P_k. This is impossible if the representation is irreducible, as we are assuming. The standard version of the Stone-von Neumann theorem [Mor18] implies that there exists an isometric surjective operator $U : \mathsf{H} \to L^2(\mathbb{R}^n, d^n x)$ such that $W \ni g \mapsto UV_gU^{-1} \in \mathfrak{B}(L^2(\mathbb{R}^n, d^n x))$ is the standard unitary representation of W on $L^2(\mathbb{R}^n, d^n x)$, generated by X_k and P_k (and I). Stone's theorem immediately yields (7.41). The last statement follows easily from the standard form of Mackey's theorem, which completes the Stone-von Neumann result [Mor18]. □

With hindsight the result furnishes a strong justification for requiring the Hilbert space of an elementary quantum system, like a particle in non-relativistic quantum mechanics, must be *separable*. Separability also arises from Proposition 7.36 in the relativistic case when, following Wigner's ideas, we think of elementary particles as described by irreducible strongly-continuous unitary representations of the (universal covering of the special orthochronous) Poincaré group.

7.3.3 Pauli's Theorem

Physically meaningful Hamiltonian operators have lower-bounded spectrum to avoid thermodynamical instability. This fact prevents the existence of a "time operator" canonically conjugated to H. This result is sometimes quoted as *Pauli's theorem*. As a consequence, the meaning of Heisenberg's inequality $\Delta E \Delta T \geq \hbar/2$ differs from the meaning of the analogous relationship of position and momentum. Yet it is possible to define a sort of time observable simply by passing from PVMs to POVMs (positive-operator valued measures) [Mor18]. POVMs are employed to describe concrete physical phenomena related to measurement procedures, especially in quantum information theory [Bus03, BGL95].

Theorem 7.46 (Pauli's Theorem) *If the spectrum of the (selfadjoint) Hamiltonian operator H of a quantum system described on the Hilbert space H is bounded below, there is no selfadjoint operator T satisfying*

$$[T, H]\psi = i\hbar\psi \quad \textit{for } \psi \in D$$

where $D \subset \mathsf{H}$ is dense, invariant and such that $H|_D^2 + T|_D^2$ is essentially selfadjoint.

Proof The pair H, T should be mapped to corresponding P, X in $L^2(\mathbb{R}, dx)$, or a direct sum of such spaces, by a Hilbert space isomorphism due to Theorem 7.45. In either case the spectrum of H should coincide with the spectrum of P, namely $\mathbb{R}$. But this is forbidden right from the start. □

Chapter 8
The Algebraic Formulation

This last chapter is devoted to introduce the so-called *algebraic formulation* of Quantum Theories, an advanced formulation where the protagonist role is played by observables and not by the (Hilbert) space of the states. It is particularly useful in the study of Quantum Field Theory [Haa96, Ara09], especially in external classical background, typically in curved spacetime, and in statistical mechanics [BrRo02]. After some introductory motivation we shall describe the fundamental theoretical tools and some applications, with particular attention to the description of symmetries.

8.1 Physical Motivations

The fundamental Theorem 7.45 of Stone-von Neumann and Mackey is stated in the jargon of theoretical physics as follows:

> all irreducible representations of the CCRs with a finite, and fixed, number of degrees of freedom are unitarily equivalent.

The expression *unitarily equivalent* refers to the existence of a Hilbert-space isomorphism U, and the finite number of freedom degrees is the dimension of the Lie algebra spanned by the generators I, X_k, P_k. What happens in infinite dimensions then?

Jumping from the finite-dimensional case to the infinite-dimensional one corresponds to passing from Quantum Mechanics to Quantum Field Theory (possibly relativistic, and on curved spacetime [KhMo15]). This is the case when one deals with *quantum fields*, where the $2n + 1$ generators I, X_k, P_k , $k = 1, 2, \ldots, n$, are replaced by the identity operator and a *continuum* of generators. These are the so-called quantum **field operators at fixed time** and the **conjugated momentum operators at fixed time** $I, \phi(f), \pi(g)$, which are *smeared* with arbitrary *real* functions $f, g \in C_0^\infty(\mathbb{R}^3; \mathbb{R})$. In this sense one says that there are infinite

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dimensions (a different operator for every function), compared to the $2n + 1$ operators of the CCRs. More precisely

$$C_c^\infty(\mathbb{R}^3; \mathbb{R}) \ni f \mapsto \phi(f)\,, \quad C_c^\infty(\mathbb{R}^3; \mathbb{R}) \ni g \mapsto \pi(g) \tag{8.1}$$

are linear maps associating test functions f, g to *essentially selfadjoint* operators $\phi(f), \pi(g)$ defined on a dense invariant domain D in a Hilbert space H. These observables admit time evolution and the entire picture can be recast in a completely covariant way, but here we shall consider them at fixed time in a fixed Minkowski frame. $\mathbb{R}^3$ is, in fact, the rest space of a given reference frame in Minkowski spacetime. The field operators satisfy commutation relations, called **bosonic commutation relations** (bCCR),

$$[\phi(f), \phi(f')] = [\pi(f), \pi(f')] = 0\,, \quad [\phi(f), \pi(f')] = i \int_{\mathbb{R}^3} f(x) f'(x) d^3x \, I\restriction_D\,, \tag{8.2}$$

similar to the ones of X_k and P_k (e.g., see [Haa96, Ara09, BrRo02] and [KhMo15] in curved spacetime). Now the Stone-von Neumann theorem no longer holds and theoretical physicists say that

there exist irreducible non-equivalent bCCR representations.

In practice, it means that there exist pairs of *isomorphic* *-algebras of field operators: the one generated by $I, \phi(f), \pi(g)$ (made of finite complex linear combinations of finite products of these operators) on the Hilbert space H, and another generated by $I', \phi'(f), \pi'(g)$ on a Hilbert space H'. They admit *no Hilbert-space* isomorphism $U : \mathsf{H}' \to \mathsf{H}$ satisfying:

$$U\phi'(f)\, U^{-1} = \phi(f)\,, \quad U\pi'(g)\, U^{-1} = \pi(g) \quad \text{for any pair } f, g \in C_c^\infty(\mathbb{R}^3).$$

Pairs of this kind are called *unitarily inequivalent*. It is worth stressing that everything can be reformulated at the level of C^*-algebras of operators, thus getting rid of annoying technicalities concerning domains which refer to the unital C^*-algebra (the concrete *Weyl* C^*-algebra of quantum fields) generated by the exponentiated unitary operators $e^{i\overline{\phi(f)}}$, $e^{i\overline{\pi(g)}}$ (see Example 8.25 below). The presence of non-equivalent representations of one single physical system shows that a formulation in a fixed Hilbert space is quite inadequate, if nothing because it insists on *one* fixed Hilbert space, whereas the physical system is characterized by a more abstract object, namely an algebra of observables which may be represented on *different* Hilbert spaces in terms of operators. These representations are not unitarily equivalent, and none of them can be considered more fundamental than the others. We should relinquish the structure of Hilbert space in order to lay the foundations of quantum theories in broader generality. This programme has been widely developed (see e.g., [BrRo02, Stro05, Haa96, Ara09, BrRo02]), starting from the pioneering work of von Neumann himself, and is nowadays called *algebraic formulation of quantum (field) theories*.

Within this framework it was possible to formalise rigorously, for instance, field theories in curved spacetime (see [BDFY15] for a recent review) in relation to the quantum phenomenology of black-hole thermodynamics, such as Hawking's radiation (see, e.g., [DMP11, MP12]).

Regarding general algebraic approaches to QFT, it is worth stressing that another notion of (bosonic) field operators is used more often in place of $\phi(f)$ and $\pi(g)$, where the functions f and g are defined on a spacelike 3-surface. Especially on a curved spacetime M, it is more convenient [BeDa15, KhMo15] to think of the quantum field as a smeared operator $\Phi(h)$ with smooth functions $h : C_0^\infty(M) \to \mathbb{R}$, without referring to preferred spacelike 3-surfaces. In *globally hyperbolic spacetimes* [BeDa15], the field operators $\Phi(h)$ generate a unital *-algebra that retains the full information of the unital *-algebra generated by ϕ and π.

8.2 Observables and States in the Algebraic Formalism

The algebraic formulation prescinds, anyway, from the nature of the quantum system and may be given also for systems with finitely many degrees of freedom as well [Stro05]. The new point of view, in the general case, trades on the two assumptions [Haa96, Ara09, Stro05, Mor18] listed below.

8.2.1 The C-Algebra Case*

We first examine the more rigid case of C^*-algebras, and later we will relax the structure to a *-algebra.

A1. A physical system S is described by its **observables**, viewed as selfadjoint elements in a certain C^*-algebra $\mathfrak{A}_S$ with unit $\mathbb{1}$ associated to S.

A2. An **algebraic state** on $\mathfrak{A}_S$ is a linear functional $\omega : \mathfrak{A}_S \to \mathbb{C}$ such that:

$$\omega(a^*a) \geq 0 \quad \forall\, a \in \mathfrak{A}_S, \qquad \omega(\mathbb{1}) = 1\,,$$

that is, **positive** and **normalized**.

The pair $(\mathfrak{A}_S, \omega)$ is called a **quantum probability space**.

$\mathfrak{A}$ is not understood as a concrete C^*-algebra of operators (a von Neumann algebra, for instance) on a given Hilbert space, but it remains an abstract object.

The values ω takes on selfadjoint elements of $\mathfrak{A}_S$, *the observables* of the system, completely fix ω, by linearity. Physically speaking, $\omega(a)$ is interpreted as the *expectation value* of the observable $a = a^* \in \mathfrak{A}_S$ in the state ω. Section 8.2.3 discusses mathematical issues ensuing from this interpretation.

The most conspicuous a posteriori justification for the algebraic approach lies in its powerfulness [Haa96]. There have nonetheless been a myriad attempts to account for assumptions A1 and A2 and their physical meaning in full generality (see the studies of [Emc72, Ara09, Stro05], and especially the work of I.E. Segal [Seg47] based on *Jordan algebras*). Still, none of these seems to be definitive [Stre07]. From general physical assumptions what is difficult to fully justify is the *-algebra structure of the space of observables, in particular the existence of an associative product between non-commuting elements.

Remark 8.1

(a) $\mathfrak{A}_S$ is usually called **the algebra of observables of** S although, properly speaking, the observables are the selfadjoint elements of $\mathfrak{A}_S$.
(b) Differently from the Hilbert space formulation, the algebraic approach may be adopted to account for *both classical and quantum systems*. The two cases are distinguished on the base of the commutativity of the algebra of observables $\mathfrak{A}_S$: a commutative algebra is assumed to describe a classical system, whereas a non-commutative one a quantum system.
(c) We mentioned in Definition 3.8 that the **resolvent** (set) and **spectrum** of an element a in a C^*-algebra $\mathfrak{A}$, with unit element $\mathbb{1}$, are defined in analogy to the operator case [BrRo02, Mor18]:

$$\rho(a) := \{\lambda \in \mathbb{C} \mid \exists (a - \lambda\mathbb{1})^{-1} \in \mathfrak{A}\}\,, \quad \sigma(a) := \mathbb{C} \setminus \rho(a)\,, \tag{8.3}$$

where $\rho(a)$ is open and $\sigma(a) \neq \varnothing$ is compact in $\mathbb{C}$. We know from Proposition 3.80 that

$$||a|| = \sup_{\lambda \in \sigma(a)} |\lambda| \qquad \text{if } a \in \mathfrak{A} \text{ is } \textbf{normal} : a^*a = aa^*\,. \tag{8.4}$$

When a is not normal, a^*a is selfadjoint and hence normal, and the C^*-property $||a||^2 = ||a^*a||$ entitles us to compute $||a||$ in terms of the spectrum of a^*a. As the spectrum is a completely algebraic notion, we conclude that it is impossible to change the norm of a C^*-algebra and preserve its C^* nature: *a unital *-algebra admits at most one C^*-norm.* ■

Proposition 8.2 *Let $\mathfrak{A}$ and $\mathfrak{B}$ be unital C^*-algebras and $\phi : \mathfrak{A} \to \mathfrak{B}$ a *-homomorphism (by Definition 2.15 it preserves the unit but disregards norms). Then*

(a) *$\phi(\mathfrak{A})$ is a unital C^*-subalgebra of $\mathfrak{B}$.*
(b) *ϕ is norm-decreasing ($||\phi(a)||_{\mathfrak{B}} \leq ||a||_{\mathfrak{A}}$), hence continuous.*
(c) *$\sigma_{\mathfrak{B}}(\phi(a)) \subset \sigma_{\mathfrak{A}}(a)$ if $a \in \mathfrak{A}$, with $=$ if ϕ is injective.*
(d) *ϕ is isometric if and only if it is injective. In particular, *-isomorphisms between unital C^*-algebras are isometric.*
(e) *If $\mathfrak{A} \subset \mathfrak{B}$ is a unital C^*-subalgebra of $\mathfrak{B}$, then $\sigma_{\mathfrak{A}}(a) = \sigma_{\mathfrak{B}}(a)$.*

Proof See [Mor18, Theorem 8.22 (b)] for statement (a). Properties (b)–(e) [Mor18, Theorems 8.22 and 8.23] are straightforward from (8.3), (8.4), the C^*-property $||a^*a|| = ||a||^2$, and Theorem 3.82. □

Properties (a),(b),(c),(d) apply in particular to representations (Definition 2.27) of unital C^*-algebras on Hilbert spaces: $\pi : \mathfrak{A} \to \mathfrak{B}(\mathsf{H})$.

Example 8.3 von Neumann algebras $\mathfrak{R}$ on a Hilbert space H are special instances of unital C^*-algebras. A von Neumann algebra $\mathfrak{R}$ can be characterised abstractly as a unital C^*-algebra which is the Banach dual of a certain Banach space $\mathfrak{R}_*$. An important achievement of Sakai [Tak10] says that $\mathfrak{R}_*$ is uniquely determined by $\mathfrak{R}$, and is called the *pre-dual* of $\mathfrak{R}$. In this abstract context, von Neumann algebras are more often called W^***-algebras** and their Hilbert space representations (the *-algebras of operators called von Neumann algebras in this book) are said **concrete** W^***-algebras**.

The algebraic notion of state on $\mathfrak{R}$ is weaker than the notion of normal state on $\mathfrak{R}$ (the Hilbert space one, so to speak, given in terms of positive unit-trace nuclear operators of $\mathfrak{R}$; see Sect. 6.3.4). A normal state T induces an associated algebraic state $\omega_T : \mathfrak{R} \to \mathbb{C}$, $\omega_T(A) := tr(AT)$ for $A \in \mathfrak{R}$. These special algebraic states, whose set is called the *folium* of $\mathfrak{R}$, become σ-additive measures when restricted to $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ when H is separable, or *completely additive* measures when H is not separable. Conversely, generic algebraic states restricted to $\mathscr{L}_{\mathfrak{R}}(\mathsf{H})$ give rise to just *additive* measures, which are not necessarily σ-additive. Notice that every algebraic state ω is necessarily continuous in the uniform topology of $\mathfrak{B}(\mathsf{H})$ by the GNS Theorem (see Theorem 8.7 below). Note that uniform continuity is not enough to warrant σ-additivity. The appropriate form of continuity to that end would be *strong continuity*, which is not always guaranteed. This is the reason why algebraic states on a von Neumann algebra are more abundant than normal states, and the notion of algebraic state is less restrictive than that of normal state. ■

8.2.2 The *-Algebra Case

In the rest of the chapter we shall often assume that the algebra of observables is a C^*-algebra with unit; however, several results remain valid if one relaxes the topological constraints and uses a *-algebra with unit instead. Physically speaking, within the algebraic formulation of bosonic QFT the use of a *-algebra is appropriate when the elementary objects are the field operators $\phi(f)$, $\pi(g)$ rather than their formal exponentials $e^{i\phi(f)}$, $e^{i\pi(f)}$.

When we use unital *-algebras, we shall therefore loosen things up and impose the following conditions, which subsume A1, A2 since unital C^*-algebras are unital *-algebras.

A1′. A physical system S is described by its **observables**, viewed now as selfadjoint elements in a certain *-algebra $\mathfrak{A}_S$ with unit $\mathbb{1}$ associated to S.

A2′. An **algebraic state** on $\mathfrak{A}_S$ is a linear functional $\omega : \mathfrak{A}_S \to \mathbb{C}$ such that:

$$\omega(a^*a) \geq 0 \quad \forall a \in \mathfrak{A}_S, \qquad \omega(\mathbb{1}) = 1 ,$$

that is, **positive** and **normalized**.

The pair $(\mathfrak{A}_S, \omega)$, often also assuming that $\mathfrak{A}_S$ is positive, is a **quantum probability space**.

Again, the values of ω on selfadjoint elements of $\mathfrak{A}_S$ determine ω completely, by linearity. Physically speaking, $\omega(a)$ is the *expectation value* of the observable $a = a^* \in \mathfrak{A}_S$ in the state ω. Section 8.2.3 discusses mathematical issues of this interpretation.

8.2.3 *Consistency of a Probabilistic Interpretation*

An evident difference with standard QM, where a state is a *probability measure* on the lattice of elementary propositions, is that here a state is a positive linear map that computes the *expectation values* of observables directly.

Actually, this identification is natural in the Hilbert space formulation. As said, there the class of observables includes elementary observables, which are represented by orthogonal projectors P and correspond to yes/no statements. The expectation value $\omega(P)$ of such an observable coincides with the probability that the measurement returns"yes". The set of all those probabilities defines a quantum state of the system, as we know, provided a suitable continuity condition for ω is satisfied to ensure σ-additivity (see Example 8.3 below). In particular when such a measure is restricted to the PVM $P^{(A)}$ of an observable A, we obtain a σ-additive Borel probability measure $\mathscr{B}(\mathbb{R}) \ni E \mapsto w_\omega^{(A)}(E) := \omega(P^{(A)}(E))$ (supported on $\sigma(A)$), which gives the probability of a certain outcome $E \in \mathscr{B}(\mathbb{R})$, measuring A, when the quantum state is determined by ω. By construction, $\omega(A) = \int_{\mathbb{R}} \lambda d w_\omega^{(A)}(\lambda)$.

By dropping the Hilbert space structure the picture changes dramatically. Unless $\mathfrak{A}$ is a von Neumann algebra, the analogues of elementary propositions do not generally belong to the unital *-algebra (or unital C^*-algebra) of observables in the algebraic formulation. Therefore the identification of $\omega(a)$ with an *expectation value* seems quite formal, because it is by no means obvious what is (if any) the probability distribution one uses to compute that expectation value!

Nevertheless, this is not an insurmountable obstruction. What we need, for a given observable $a = a^* \in \mathfrak{A}$ and a state $\omega : \mathfrak{A} \to \mathbb{C}$ defined according to A2 and A2′, is a (Borel) probability measure $w_\omega^{(a)} : \mathscr{B}(\mathbb{R}) \to [0, 1]$. Its physical meaning amounts to saying that $w_\omega^{(a)}(E)$ is the probability that the outcome of measuring a in state ω belongs to (is) the Borel set $E \subset \mathbb{R}$. From the mathematical viewpoint, this $\omega(a)$ has to coincide with the expectation value of $w_\omega^{(a)}$. This sole requirement is not enough to fix $w_\omega^{(a)}$. But the physical interpretation implies that $w_\omega^{(a)}$ is also naturally related to the real Abelian unital algebra of observables generated by a, made of the *real polynomials* $p(a)$. (When $\mathfrak{A}$ is a unital C^*-algebra, this object would be the real Abelian unital C^*-algebra generated by a and made of *continuous* functions $f(a)$, according to Theorem 3.82.) We are committed to viewing $p(a)$ as the observable with values $p(\lambda)$ for all values $\lambda \in \mathbb{R}$ attained by a. Hence the physical meaning of $w_\omega^{(a)}$ implies $w_\omega^{(p(a))}(E) := w_\omega^{(a)}(p^{-1}(E))$, and therefore

$$\int_{\mathbb{R}} p(\lambda) dw_\omega^{(p(a))}(\lambda) = \omega(p(a)) \tag{8.5}$$

is assumed to hold. In particular, we can focus on the *moments* $\omega(a^n)$, $n \in \mathbb{N}$:

$$\int_{\mathbb{R}} \lambda^n dw_\omega^{(a^n)}(\lambda) = \omega(a^n)\ . \tag{8.6}$$

From the theory of the *Hamburger moment problem*, we have a crucial result [ReSi75, Theorem X4 and Example 4, p.205] (beware this reference has a gap in the proof of uniqueness, fixed in [Sim98, Proposition 1.5]).

Proposition 8.4 *Let* $\{m_n\}_{n=0,1,2,\ldots} \subset \mathbb{R}$ *be a sequence of real numbers.*

(a) *There exists a positive* σ*-additive Borel measure* $\mu : \mathscr{B}(\mathbb{R}) \to [0, +\infty)$ *whose moments are the given* m_n*, i.e.,* $\int_{\mathbb{R}} \lambda^n d\mu(\lambda) = m_n$*, if and only if*

$$\sum_{i,j=0,1,\ldots}^{N} \overline{c_i} c_j m_{i+j} \geq 0 \tag{8.7}$$

for every set $\{c_k\}_{k=0,1,2,\ldots,N} \subset \mathbb{C}$ *with* $N \in \mathbb{N}$.

(b) *The measure* μ *is unique if* $|m_n| \leq CD^n n!$ *for some constants* $C, D \geq 0$ *and* $n = 0, 1, 2, \ldots$.

This result has an important consequence for the consistency of the algebraic formulation.

Proposition 8.5 *Let* $\mathfrak{A}$ *be a unital* **-algebra (or unital* C^**-algebra) and* $\omega : \mathfrak{A} \to \mathbb{C}$ *an algebraic state. If* $a = a^* \in \mathfrak{A}$*, there exists a Borel probability measure* $w_\omega^a : \mathscr{B}(\mathbb{R}) \to [0, 1]$ *satisfying (8.5) for every (typically complex) polynomial* $p : \mathbb{R} \to \mathbb{R}$*. If* $\mathfrak{A}$ *is a* C^**-algebra,* w_ω^a *is unique.*

Proof Set $m_n := \omega(a^n)$. There exists $w_\omega^{(a)}$ satisfying (8.6) because (8.7) is true, since

$$\sum_{i,j=0,1,\ldots}^{N} \overline{c_i} c_j \omega(a^{i+j}) = \omega\left(\left(\sum_i^N c_i a_i\right)^* \left(\sum_j^N c_j a_j\right)\right) \geq 0$$

(we exploited the linearity and positivity of ω assumed in A2 and A2$'$, and $a^* = a$). Since $m_0 = \omega(a^0) = \omega(\mathbb{1}) = 1$, the positive measure is a probability measure. Finally, (8.6) implies (8.5) by linearity. The uniqueness of $w_\omega^{(a)}$ is brought about by Lemma 8.17 when $\mathfrak{A}$ is a unital C^*-algebra: the continuity of ω and its unit norm imply $|m_n| = |\omega(a^n)| \leq ||a^n|| \leq ||a||^n \leq ||a||^n n!$, so Proposition 8.4 (b) is satisfied. □

We will explicitly construct the measure $w_\omega^{(a)}$ for a unital C^*-algebra $\mathfrak{A}$ in Remark 8.8, and prove its support is at least contained in $\sigma(a)$. Since $\sigma(a)$ is compact in that case, by the Stone-Weierstrass theorem it is easy to extend (8.5) to continuous (generally complex) functions f. Remark 8.11 (b) shows the procedure to construct $w_\omega^{(a)}$ for $a = a^* \in \mathfrak{A}$ when $\mathfrak{A}$ is a *-algebra but not a C^*-algebra. However, uniqueness is more delicate in that case.

All this can be generalised: if $a_1, \ldots, a_N \in \mathfrak{A}$ are pairwise commuting selfadjoint elements and $\omega : \mathfrak{A} \to \mathbb{C}$ a given state, one would expect to be able to define a (possibly unique) *joint measure* $w_\omega^{(a_1,\ldots,a_N)}$ on $\mathbb{R}^n$ such that

$$\omega(p(a_1, \ldots, a_N)) = \int_{\mathbb{R}^n} p(\lambda_1, \ldots, \lambda_N) dw_\omega^{(a_1,\ldots,a_N)}(\lambda_1, \ldots, \lambda_N) \qquad (8.8)$$

for every polynomial p of finite degree. This is an even more difficult problem, which for unital *-algebras has been tackled by a few authors, and is related to the choice of a suitable family of seminorms on $\mathfrak{A}$.

8.3 The GNS Constructions and Their Consequences

Surprisingly, most of the abstract apparatus introduced, given by a *- or C^*-algebra and its algebraic states, admits elementary Hilbert space representations *when a reference algebraic state is given*. In particular, not only is there a probability measure $w_\omega^{(a)}$ for every fixed observable $a \in \mathfrak{A}$, but there even exists an overall *quantum probability measure* on a suitable Hilbert space where all elements of $\mathfrak{A}$ are represented as operators. This structure is unique (up to isomorphism). This is by virtue of a celebrated procedure that Gelfand, Najmark and Segal invented [Haa96, Ara09, Stro05, Mor18] (see, in particular, [Schm90] for general *-algebras). Before we split the C^*-algebra and *-algebra cases, let us prove a lemma common to both.

Lemma 8.6 *If $\omega : \mathfrak{A} \to \mathbb{C}$ is a positive linear functional on a unital *- algebra $\mathfrak{A}$, then $\omega(a^*) = \overline{\omega(a)}$ for every $a \in \mathfrak{A}$.*

Proof If $b = b^*$, we have $0 \leq \omega((\mathbb{1} + b)^*(\mathbb{1} + b)) = \omega((\mathbb{1} + b)(\mathbb{1} + b)) = \omega(\mathbb{1}) + 2\omega(b) + \omega(b^2) \in \mathbb{R}$. From $\omega(\mathbb{1}) = \omega(\mathbb{1}^*\mathbb{1}) \geq 0$ and $\omega(b^2) = \omega(b^*b) \geq 0$ we infer $\omega(b) \in \mathbb{R}$. Decompose $a \in \mathfrak{A}$ as $a = \frac{1}{2}(a+a^*)+\frac{i}{2}(ia^*-ia)$. Since $a+a^*$

and $ia^* - ia$ are selfadjoint, $\overline{\omega(a)} = \overline{\frac{1}{2}\omega(a + a^*) + \frac{i}{2}\omega(ia^* - ia)} = \frac{1}{2}\omega(a+a^*) - \frac{i}{2}\omega(ia^* - ia) = \omega(a^*)$. □

8.3.1 The GNS Reconstruction Theorem: The C-Algebra Case*

Relatively to representations of unital C^*-algebras (Definition 2.27) we have the following paramount result.

Theorem 8.7 (GNS Reconstruction Theorem) *Let $\mathfrak{A}$ be a C^*-algebra with unit $\mathbb{1}$ and $\omega : \mathfrak{A} \to \mathbb{C}$ a positive linear functional with $\omega(\mathbb{1}) = 1$. Then the following hold.*

(a) *There exist a triple $(\mathsf{H}_\omega, \pi_\omega, \Psi_\omega)$, where*

  (1) *H_ω is a Hilbert space,*
  (2) *$\pi_\omega : \mathfrak{A} \to \mathfrak{B}(\mathsf{H}_\omega)$ is a continuous (norm-decreasing) representation of unital *-algebras,*
  (3) *$\Psi_\omega \in \mathsf{H}_\omega$ has unit norm,*

  such that:

  (i) *Ψ_ω is **cyclic** for π_ω, namely $\pi_\omega(\mathfrak{A})\Psi_\omega$ is dense in H_ω,*
  (ii) *$\langle\Psi_\omega|\pi_\omega(a)\Psi_\omega\rangle = \omega(a)$ for every $a \in \mathfrak{A}$.*

(b) *If another triple (H, π, Ψ) satisfies (1),(2),(3),(i),(ii) for ω, then there exists a unitary (i.e., isometric surjective) operator $U : \mathsf{H}_\omega \to \mathsf{H}$ such that*

$$\Psi = U\Psi_\omega \quad \textit{and} \quad \pi(a) = U\pi_\omega(a)U^{-1} \quad \textit{for every } a \in \mathfrak{A},$$

Proof

(a) Consider the map $\mathfrak{A} \times \mathfrak{A} \ni (a, b) \mapsto s(a, b) := \omega(a^*b)$, viewing $\mathfrak{A}$ as a complex vector space. The map s is sesquilinear (right-linear and $s(a, b) = \overline{s(b, a)}$ due to Lemma 8.6) and positive: $s(a, a) \geq 0$ for $a \in \mathfrak{A}$. So it satisfies the Cauchy-Schwartz inequality $|s(a, b)|^2 \leq s(a, a)s(b, b)$. Consequently $G_\omega := \{a \in \mathfrak{A} \mid s(a, a) = 0\}$ is a subspace of $\mathfrak{A}$ with the further property that $ba \in G_\omega$ if $a \in G_\omega$ and $b \in \mathfrak{A}$, because

$$|s(ba, ba)|^2 \leq |\omega((ba)^*ba)|^2 = |\omega(((ba)^*b)a)|^2 = |s((ba)^*b, a)|^2$$
$$\leq s((ba)^*b, (ba)^*b)s(a, a)\,.$$

G_ω is therefore a left ideal called **Gelfand ideal**. At this point, it is easy to prove that $\langle[a]|[b]\rangle := \omega(a^*b)$ is a well-defined (strictly positive!) Hermitian inner product on the quotient vector space $\mathfrak{A}/G_\omega \ni [a], [b]$. We define the

Hilbert space H_ω to be the completion of $\mathfrak{A}/G_\omega$. Next set $\Psi_\omega = [\mathbb{1}]$ and $\pi_\omega(a)[b] := [ab]$ for $[b] \in \mathfrak{A}/G_\omega$. The map $\pi(a) : \mathfrak{A}/G_\omega \to \mathfrak{A}/G_\omega$ is well defined since, if $b' \in [b]$, then $[ab] - [ab'] = [a(b - b')]$ has zero norm because $b - b' \in G_\omega$, so $[ab] = [ab']$. In particular, $\pi(\mathfrak{A})\Psi_\omega = \{[a] \mid a \in \mathfrak{A}\}$ is dense in H_ω. Moreover, by construction, $\pi(a) : \mathfrak{A}/G_\omega \to \mathfrak{A}/G_\omega$ is linear for every $a \in \mathfrak{A}$. Furthermore, $\mathfrak{A} \ni a \mapsto \pi(a)$ is linear and satisfies $\pi(a)\pi(b) = \pi(ab)$, $\pi(\mathbb{1}) = I$, $\langle \pi(b)\Psi_\omega | \pi(a)\pi(c)\Psi_\omega \rangle = \omega(b^*ac) = \omega((a^*b)^*c) = \langle \pi(a^*)\pi(b)\Psi_\omega | \pi(c)\Psi_\omega \rangle$ (so that $\pi(a^*) \subset \pi(a)^*$) and finally $\langle \Psi_\omega | \pi(a)\Psi_\omega \rangle = \langle [\mathbb{1}] | [a\mathbb{1}] \rangle = \omega(\mathbb{1}a) = \omega(a)$. If we assume $||\pi(a)|| \leq ||a||$, all properties extend by continuity to the whole H_ω. This completes the proof of (a), if we define $\pi_\omega(a)$ as the unique continuous extension of $\pi(a)$ from the dense set $\pi(\mathfrak{A})\Psi_\omega$ $(= \pi_\omega(\mathfrak{A})\Psi_\omega)$ to H_ω according to Proposition 2.18. To conclude the proof of (a) there remains to show $||\pi(a)|| \leq ||a||$ for $a \in \mathfrak{A}$. Referring to Theorem 3.82, let $\Psi : C(\sigma(a^*a)) \to \mathfrak{A}$ be the norm-preserving *-homomorphism associated to the selfadjoint element $a^*a \in \mathfrak{A}$ (this was a in Theorem 3.82). Consider the bounded, continuous real-valued maps $\alpha_\pm(x) := ||a^*a|| \pm x$ with $x \in \sigma(a^*a)$. Since $\sigma(a^*a) \subset [-||a^*a||, ||a^*a||]$ by Proposition 3.80), we have $\alpha_\pm(x) \geq 0$ and the real-valued continuous bounded maps $\sigma(a^*a) \ni x \mapsto \sqrt{\alpha_\pm(x)} =: \beta_\pm(x)$ are well defined. Exploiting again Theorem 3.82, the elements $b_\pm := \Psi(\beta_\pm) \in \mathfrak{A}$ satisfy $b_\pm = b_\pm^*$ and $b_\pm^* b_\pm = ||a^*a||\mathbb{1} \pm a^*a$. For every positive linear functional $\phi : \mathfrak{A} \to \mathbb{C}$, we consequently find $\phi(||a^*a||\mathbb{1} \pm a^*a) = \phi(b_\pm^* b_\pm) \geq 0$, so that $-||a^*a||\phi(\mathbb{1}) \leq \phi(a^*a) \leq ||a^*a||\phi(\mathbb{1})$, namely, $|\phi(a^*a)| \leq \phi(\mathbb{1})||a^*a||$. Applying this to the linear positive functional $\phi : \mathfrak{A} \ni a \mapsto \phi(a) = \omega(b^*ab)$ where $b \in \mathfrak{A}$ is given, the result above implies

$$
\begin{aligned}
||\pi(a)\pi(b)\Psi_\omega||^2 = |\omega(b^*a^*ab)| = |\phi(a^*a)| &\leq \phi(\mathbb{1})||a^*a|| \\
&= \omega(b^*b)||a^*a|| = ||\pi(b)\Psi_\omega||^2||a||^2 .
\end{aligned}
$$

In other words, $\pi(a) : \mathfrak{A}/G_\omega \to \mathsf{H}_\omega$ satisfies $||\pi(a)|| \leq ||a||$ as wanted. The proof of (a) is over.

(b) The operator $U'\pi_\omega(a)\Psi_\omega := \pi(a)\Psi$, $a \in \mathfrak{A}$, maps $\mathfrak{A}/G_\omega$ to $\pi(\mathfrak{A})\Psi$ and is well defined (every element has a unique image) because $||(\pi(a) - \pi(a'))\Psi||^2 = \omega((a - a')^*(a - a')) = ||(\pi_\omega(a) - \pi_\omega(a'))\Psi_\omega||^2$. For the same reason U' is isometric. It admits inverse (isometric) operator $V\pi(a)\Psi := \pi_\omega(a)\Psi_\omega$ for $a \in \mathfrak{A}$. By Proposition 2.18 the unique continuous extension U of U' to H_ω is isometric and surjective (the analogous extension of V being its right inverse) and satisfies all the requirements in (b). □

Remark 8.8

(a) If $a = a^* \in \mathfrak{A}$ and a state $\omega : \mathfrak{A} \to \mathbb{C}$ is given on the unital C^*-algebra $\mathfrak{A}$, the GNS construction provides a probability measure on $\mathscr{B}(\mathbb{R})$, which is supported on $\sigma(\pi_\omega(a))$, and satisfies (8.6). Trivially

$$w_\omega^{(a)}(E) := \langle \Psi_\omega | P^{(\pi_\omega(a))}(E) \Psi_\omega \rangle$$

where $P^{(\pi_\omega(a))}$ is the PVM of the selfadjoint operator $\pi_\omega(a) \in \mathfrak{B}(\mathsf{H}_\omega)$. This probability measure is *unique*, by Proposition 8.5. Referring to the final comment in Sect. 8.2.3, the joint PVM $P^{(\pi_\omega(a_1),\ldots,\pi_\omega(a_1))}$ of commuting selfadjoint operators $\pi_\omega(a_k) \in \mathfrak{B}(\mathsf{H}_\omega)$, where $k = 1, \ldots, N$, when the corresponding selfadjoint elements $a_k \in \mathfrak{A}$ commute, gives rise to a joint probability measure

$$w_\omega^{(a_1,\ldots,a_N)}(F) := \langle \Psi_\omega | P^{(\pi_\omega(a_1),\ldots,\pi_\omega(a_1))}(F) \Psi_\omega \rangle \ ,$$

for every Borel set $F \in \mathbb{R}^n$. It is easy to prove that this measure satisfies (8.8). What is more, a careful analysis based on [Schm17] shows it is the unique Borel σ-additive probability measure satisfying (8.8).

(b) The GNS representation $\pi_\omega : \mathfrak{A} \to \mathfrak{B}(\mathsf{H}_\omega)$ is a *-homomorphism and therefore Proposition 8.2 applies. Physically meaningful representations of the algebra of observables are generally expected to be *faithful*, i.e., injective (though non-injective cases exist and may have a physical interpretation). In this case, according to Proposition 8.2, π_ω is isometric and preserves the spectra of the elements. A sufficient (not necessary in general) condition for having π_ω faithful is that the Gelfand ideal of ω be trivial: from the proof above this amounts to say that $\omega(a^*a) = 0$ implies $a = 0$ (and in this case ω is said to be **faithful**). If $a \in \mathfrak{A}$ is selfadjoint $\pi_\omega(a)$ is a selfadjoint *operator*, and its spectrum has the well-known quantum meaning according to (a) above. This meaning, in view of the permanence of the spectrum (Proposition 8.2) for π_ω faithful, can be attributed directly to the spectrum of $a \in \mathfrak{A}$: *if $a \in \mathfrak{A}$ represents an abstract observable, $\sigma(a) = \sigma(\pi_\omega(a))$ is the set of possible values of a*. If π_ω is not faithful, we still have $\sigma(\pi_\omega(a)) \subset \sigma(a)$ from Proposition 8.2 (d). In any case $\sigma(\pi_\omega(a))$ is a compact subset of $\mathbb{R}$. ■

*8.3.2 The GNS Reconstruction Theorem: The *-Algebra Case*

Let us pass to *-algebras, where the GNS theorem holds but in a weaker form.

Theorem 8.9 (GNS Construction for *-Algebras) *If $\mathfrak{A}$ is a complex unital *-algebra and $\omega : \mathfrak{A} \to \mathbb{C}$ is a state, the following facts hold.*

(a) *There exists a quadruple $(\mathsf{H}_\omega, \mathcal{D}_\omega, \pi_\omega, \Psi_\omega)$ where*

  (1) *H_ω is a Hilbert space,*

(2) $\mathcal{D}_\omega \subset \mathsf{H}_\omega$ *is a dense subspace,*
(3) $\pi_\omega : \mathfrak{A} \ni a \to \pi(a)$ *is a* **-representation of* $\mathfrak{A}$ *on* H_ω *with domain* $\mathcal{D}_\omega$*, in the sense that*

 (i) $\pi_\omega(a) : \mathcal{D}_\omega \to \mathsf{H}_\omega$ *is a linear operator such that* $\pi_\omega(a)(\mathcal{D}_\omega) \subset \mathcal{D}_\omega$ *for every* $a \in \mathfrak{A}$*,*
 (ii) $\pi_\omega(\alpha a + \beta b) = \alpha\pi_\omega(a) + \beta\pi_\omega(b)$ *and* $\pi_\omega(ab) = \pi_\omega(a)\pi_\omega(b)$ *for* $\alpha, \beta \in \mathbb{C}$ *and* $a, b \in \mathfrak{A}$*,*
 (iii) $\pi_\omega(\mathbb{1}) = I_{\mathcal{D}}$*, where* $\mathbb{1}$ *is the unit of* $\mathfrak{A}$*,*
 (iv) $\pi_\omega(a^*) = \pi_\omega(a)^*\restriction_{\mathcal{D}_\omega}$ *if* $a \in \mathfrak{A}$ *(the second* * *is the adjoint in* H_ω*).*

(4) $\pi_\omega(\mathfrak{A})\Psi_\omega = \mathcal{D}_\omega$*,*
(5) $\omega(a) = \langle\Psi_\omega|\pi_\omega(a)\Psi_\omega\rangle$ *for every* $a \in \mathfrak{A}$*.*

(b) *If* $(\mathsf{H}'_\omega, \mathcal{D}'_\omega, \pi'_\omega, \Psi'_\omega)$ *satisfies (1)–(5), there exists a surjective isometric map* $U : \mathsf{H}_\omega \to \mathsf{H}'_\omega$ *such that*

 (i) $U\Psi_\omega = \Psi'_\omega$*,*
 (ii) $U(\mathcal{D}_\omega) = \mathcal{D}'_\omega$*,*
 (iii) $U\pi_\omega(a)U^{-1} = \pi'_\omega(a)$ *if* $a \in \mathfrak{A}$ *.*

Proof Define $\mathcal{D}_\omega := \{[a] \mid a \in \mathfrak{A}\}$, so that $\mathcal{D}_\omega = \pi_\omega(\mathfrak{A})\Psi_\omega$. Then the proof is identical to that of Theorem 8.7, dropping the part concerning the continuity of π_ω. □

Regarding the faithfulness of π_ω, we remark that if $\omega(a^*a) = 0$ implies $a = 0$, the GNS representation is faithful exactly as in the C^* case. But if we impose the weaker condition $\omega(a^*a) = 0 \Longrightarrow a^*a = 0$, then π_ω may not be faithful, in contrast to the C^* case, unless $\mathfrak{A}$ is positive.

Since $\mathcal{D}_\omega$ is dense, $\pi_\omega(a)^*$ is always well defined, actually densely defined by Theorem 8.9 (a)(3). In particular, every operator $\pi_\omega(a) : \mathcal{D}_\omega \to \mathsf{H}_\omega$ is closable. It is not hard to show that the operators $\pi_\omega(a)$ defined on $\mathcal{D}_\omega$ form a positive unital *-algebra equipped with the involution $\pi(a)^\star := \pi(a^*) = \pi(a)^*\restriction_{\mathcal{D}_\omega}$. Yet the interplay of the two notions of selfadjointness—on $\mathfrak{A}$ and on the GNS Hilbert space—is not very clear. If $a = a^*$, $\pi_\omega(a)$ is at least symmetric. The precise technical conditions, and their physical significance, under which an operator $\pi_\omega(a)$, with $a = a^*$, is (essentially) selfadjoint on $\mathcal{D}_\omega$ are poorly explored in the literature (see however [Schm90]), and the problem deserves further investigation. For *-algebras which are not C^* there seems to be an embarrassing mismatch between the notions of observable in the algebraic sense ($a = a^*$) and in the sense of Hilbert-space theory ($\pi_\omega(a)$ selfadjoint, or at least essentially selfadjoint), when a state ω is given.

The next result is rather general but requires quite strong hypotheses.

Proposition 8.10 *Let* $\mathfrak{A}$ *be a unital* **-algebra and* $a = a^* \in \mathfrak{A}$*.*

(a) *If* $(a \pm i\mathbb{1})b_\pm = \mathbb{1}$ *(equivalently,* $b_\pm(a \pm i\mathbb{1}) = \mathbb{1}$*) for some pair* $b_\pm \in \mathfrak{A}$*, then* $\pi_\omega(a)$ *is essentially selfadjoint for every state* $\omega : \mathfrak{A} \to \mathbb{C}$*.*

(b) *If, for a given state* $\omega : \mathfrak{A} \to \mathbb{C}$*, there exists a pair of operators* $B_\pm : \mathcal{D}_\omega \to \mathcal{D}_\omega$ *such that* $(\pi_\omega(a) \pm iI)B_\pm = I_{\mathcal{D}_\omega}$*, then* $\pi_\omega(a)$ *is essentially selfadjoint.*

Proof (a) (First things first, $(a \pm i\mathbb{1})b_\pm = \mathbb{1}$ is equivalent to $b_\pm(a \pm i\mathbb{1}) = \mathbb{1}$ by taking adjoints and renaming $b_\pm$). $\pi_\omega(a)$ is symmetric and, from the hypotheses, $(\pi_\omega(a) \pm iI)\pi_\omega(b_\pm)\mathcal{D}_\omega = \mathcal{D}_\omega$. In particular, $\overline{Ran(\pi_\omega(a) \pm iI)} = \overline{\mathcal{D}_\omega} = \mathsf{H}_\omega$. Proposition 2.47 (b) proves the claim. As for part (b), by using $B_\pm$ in place of $\pi_\omega(b_\pm)$ the proof becomes identical to that of (a). □

Remark 8.11

(a) For all $a = a^* \in \mathfrak{A}$ such that $\overline{\pi_\omega(a)}$ is selfadjoint (i.e., $\pi_\omega(a)$ is essentially selfadjoint), the GNS construction provides a canonical way to define a probability distribution of the observable a in state ω satisfying (8.6):

$$\mathscr{B}(\mathbb{R}) \ni E \mapsto w_\omega^{(a)}(E) := \langle \Psi_\omega | P_E^{(\overline{\pi_\omega(a)})} \Psi_\omega \rangle \;, \tag{8.9}$$

where $\mathscr{B}(\mathbb{R})$ is the Borel σ-algebra on $\mathbb{R}$ and $P^{(\overline{\pi_\omega(a)})}$ the PVM of $\overline{\pi_\omega(a)}$. Notice that $\Psi_\omega \in D(\pi(a)^n)$ for every $n \in \mathbb{N}$. However it is not obvious that (8.9) is the unique probability distribution to satisfy (8.6) for the given a, since we cannot exploit Proposition 8.4 (b) as we did for C^*-algebras. The uniqueness of this measure is related to the essential selfadjointness of $\pi_\omega(a)$ on suitable domains.

(b) In any case, we know from Proposition 8.5 that probability measures $w_\omega^{(a)}$ satisfying (8.6) exist for every $a = a^* \in \mathfrak{A}$ and a given state ω, regardless of the essential selfadjointness of $\pi_\omega(a)$. For instance, let $\mathsf{H}_a \subset \mathsf{H}_\omega$ be the complex span of the vectors $\pi_\omega(a)^n\Psi_\omega$, $n \in \mathbb{N}$. It is invariant under $\pi_\omega(a)$, which therefore defines a symmetric operator on the closed subspace $\overline{\mathsf{H}_a}$, viewed as a Hilbert space, and commutes with the unique conjugation on $\overline{\mathsf{H}_a}$ such that $C : \pi_\omega(a)^n\Psi_\omega \mapsto \pi_\omega(a)^n\Psi_\omega$. Due to Proposition 2.50, $\pi_\omega(a)\restriction_{\mathsf{H}_a}$ admits selfadjoint extensions on $\overline{\mathsf{H}_a}$. The PVM of each such selfadjoint extension $\pi_\omega(a)_s$ gives rise to a probability measure $w_\omega^{(a)}$ satisfying (8.6) and defined as in (8.9), with $\pi_\omega(a)_s$ in place of $\overline{\pi_\omega(a)}$.

(c) If Ψ_ω is *analytic* for $\pi_\omega(a)$ (Definition 2.52) when $a = a^* \in \mathfrak{A}$, then $|\omega(a^n)| \leq CD^n n!$ (condition (b) in Proposition 8.4) holds by the GNS theorem since, for some $t \neq 0$,

$$\frac{|t|^n}{n!}|\omega(a^n)| = \frac{|t|^n}{n!}|\langle \Psi_\omega | \pi_\omega(a)^n \Psi_\omega \rangle| \leq \frac{|t|^n}{n!}||\pi_\omega(a)^n\Psi_\omega|| \to 0, \text{ for } n \to +\infty.$$

In this special case, therefore, there is a *unique* probability measure $w_\omega^{(a)} : \mathscr{B}(\mathbb{R}) \to [0, 1]$ satisfying (8.6). ■

Definition 8.12 The **weak commutant** $\pi(\mathfrak{A})'_w$ of a *-representation π of $\mathfrak{A}$ on H with domain $\mathfrak{D}$ (in the sense of Theorem 8.9 (a)(3)) is

$$\pi(\mathfrak{A})'_w := \{A \in \mathfrak{B}(\mathsf{H}) \mid \langle\psi|A\pi(a)\phi\rangle = \langle\pi(a)^*\psi|A\phi\rangle \quad \forall a \in \mathfrak{A}, \forall\psi, \phi \in \mathfrak{D}\} . \tag{8.10}$$

We say that π is **weakly irreducible** if its weak commutant is trivial ($\pi(\mathfrak{A})'_w = \mathbb{C}I$). ■

Remark 8.13 From of Theorem 8.9 (a)(3) it follows that $\pi(\mathfrak{A})'_w$ is *-closed and contains I, so its own commutant $\pi(\mathfrak{A})''_w$ is a von Neumann algebra. Furthermore, if $\mathfrak{A}$ is a unital C^*-algebra and $\omega : \mathfrak{A} \to \mathbb{C}$ an algebraic state, then $\pi_\omega(\mathfrak{A})'_w = \pi_\omega(\mathfrak{A})'$ trivially. ■

8.3.3 *Normal States*

As we initially said, when we deal with a C^*-algebra $\mathfrak{A}$ different algebraic states ω, ω' generally give rise to *unitarily inequivalent* GNS representations $(\mathsf{H}_\omega, \pi_\omega, \Psi_\omega)$ and $(\mathsf{H}_{\omega'}, \pi_{\omega'}, \Psi_{\omega'})$. There is no isometric surjective operator $U : \mathsf{H}_{\omega'} \to \mathsf{H}_\omega$ such that

$$U\pi_{\omega'}(a)U^{-1} = \pi_\omega(a) \quad \forall a \in \mathfrak{A} .$$

An analogous observation is valid for *-algebras. The fact that one can handle all these inequivalent representations simultaneously is a manifestation of the power of the algebraic approach over the Hilbert space framework.

However, we may choose to focus on states referred to a fixed GNS representation. If ω is an algebraic state on the unital C^*-algebra $\mathfrak{A}$, every *normal state* (Sect. 6.3.4 and Example 8.3) on the von Neumann algebra $\pi_\omega(\mathfrak{A})''$ in the GNS representation of ω—i.e. every positive, trace-class operator with unit trace $T \in \mathfrak{B}_1(\mathsf{H}_\omega)$—determines an algebraic state $\mathfrak{A} \ni a \mapsto tr\,(T\pi_\omega(a))$ when we restrict from $\pi_\omega(\mathfrak{A})''$ to $\pi_\omega(\mathfrak{A})$. This is true, in particular, for a unit vector $\Phi \in \mathsf{H}_\omega$, in which case the above definition reduces to $\mathfrak{A} \ni a \mapsto \langle\Phi|\pi_\omega(a)\Phi\rangle$.

Definition 8.14 Let ω be an algebraic state on the C^*-algebra $\mathfrak{A}$ with unit. A **normal state** on $\mathfrak{A}$, relative to ω and its GNS representation $(\mathsf{H}_\omega, \pi_\omega, \Psi_\omega)$, is the restriction to $\pi_\omega(\mathfrak{A})$ of a normal state of the von Neumann algebra $\pi_\omega(\mathfrak{A})'' \supset \pi_\omega(\mathfrak{A})$. The set of normal states $Fol(\omega)$ is called the **folium** of the algebraic state ω. ■

$Fol(\omega)$ also depends on the GNS representation we pick out of the fixed ω. Part (b) of the GNS theorem for C^*-algebras, however, says that when we change representation but keep ω, the normal states of ω change only through a unitary equivalence, so they are fixed if viewed as algebraic states.

In the context of *-algebras the notion of folium is a bit more complicated, since $tr\,(T\pi_\omega(a))$ is generally undefined due to problems with the domain of each $\pi_\omega(a)$. Yet it is possible to replace $\pi_\omega(\mathfrak{A})''$ by $\pi_\omega(\mathfrak{A})''_w := (\pi_\omega(\mathfrak{A})'_w)'$, and define the folium of ω as the set of *normal states of the von Neumann algebra* $\pi_\omega(\mathfrak{A})''_w$.

Definition 8.15 Let ω be an algebraic state on the *-algebra $\mathfrak{A}$ with unit. A **normal state** on $\mathfrak{A}$, relative to ω and its GNS representation $(\mathsf{H}_\omega, \mathcal{D}_\omega, \pi_\omega, \Psi_\omega)$, is a normal state of the von Neumann algebra $\pi_\omega(\mathfrak{A})''_w$. The set of normal states $Fol(\omega)$ is the **folium** of the algebraic state ω. ■

Since $\pi_\omega(\mathfrak{A})''_w = \pi_\omega(\mathfrak{A})''$ if $\mathfrak{A}$ is a C^*-algebra, this definition extends the notion given for C^*-algebras.

Remark 8.16 If $\mathfrak{A}$ is not C^*, some of the normal states of ω still define algebraic states on $\mathfrak{A}$: if $b \in \mathfrak{A}$, then $\Psi_b := \pi_\omega(b)\Psi_\omega \in \mathcal{D}_\omega$, so the new algebraic state

$$\mathfrak{A} \ni a \mapsto \omega_b(a) := \omega(b^*ab) = \langle \Psi_b | \pi_\omega(a)\Psi_b \rangle$$

is well defined. It is the trivial restriction of a normal state of $\pi_\omega(\mathfrak{A})''_w$. ■

8.3.4 The Gelfand-Najmark Theorem

We discuss an important, though purely mathematical, consequence of the GNS construction whereby a unital C^*-algebra is always isomorphic to some concrete C^*-algebra of operators. But first

Lemma 8.17 *A linear functional $\omega : \mathfrak{A} \to \mathbb{C}$ on the unital C^*-algebra $\mathfrak{A}$ is positive if and only if: (1) ω is continuous and (2) $||\omega|| = \omega(\mathbb{1})$.*

Proof That positivity implies (1) and (2) when $\omega(\mathbb{1}) = 1$ follows from statements (2) and (ii) in Theorem 8.7 (a): $|\omega(a)| \leq ||\Psi_\omega||^2||\pi_\omega(a)|| \leq 1||a||$. In particular, $||\omega|| \leq 1$. Since $\omega(\mathbb{1}) = 1$ we also have $||\omega|| = 1 = \omega(\mathbb{1})$. In the general case, let ω be linear and positive, so $\omega(\mathbb{1}) = \omega(\mathbb{1}^*\mathbb{1}) \geq 0$. If $\omega(\mathbb{1}) = c > 0$, redefining $\omega'(a) := c^{-1}\omega(a)$ and applying the argument to ω', we obtain $||\omega|| = c = \omega(\mathbb{1})$. If $\omega(\mathbb{1}) = 0$, then the Cauchy-Schwartz inequality ($|\omega(a)|^2 = |\omega(\mathbb{1}^*a)|^2 \leq \omega(\mathbb{1}^*\mathbb{1})\omega(a^*a) = 0$) forces $\omega = 0$, so $||\omega|| = 0 = \omega(\mathbb{1})$ again.

Let us prove that (1) and (2) imply positivity. Take $a \in \mathfrak{A}$ with $||a||(= ||a^*a||^2) = 1$. Passing to the representation of a^*a on $C(\sigma(a^*a))$ of Theorem 3.82 and using $\sigma(a^*a) \subset [-||a^*a||, ||a^*a||]$, it is easy to prove that $||\mathbb{1} - a^*a|| = ||1 - \alpha||_\infty \leq 1$, where $\Psi(\alpha) = a^*a$. Summing up, $|\omega(a^*a) - 1| = |\omega(\mathbb{1} - a^*a)| \leq ||\omega||||\mathbb{1} - a^*a|| = ||\mathbb{1} - a^*a|| \leq 1$. Hence $-1 \leq \omega(a^*a) - 1 \leq 1$ and, in particular, $0 \leq \omega(a^*a)$. □

Theorem 8.18 (Gelfand-Najmark Theorem) *Given any unital C^*-algebra $\mathfrak{A}$, there exist a Hilbert space H and a faithful isometric representation $\pi : \mathfrak{A} \to \mathfrak{B}(\mathsf{H})$ of unital *-algebras.*

Proof Consider the set S of algebraic states and the orthogonal Hilbert sum of GNS representations (one for every state) $\mathsf{H} := \bigoplus_{\omega\in S}\mathsf{H}_\omega$. S is not empty because it contains the trivial state $\omega(\mathbb{1}) = 1$ and $\omega(a) = 0$ if $a \neq \mathbb{1}$. Next define, for $a \in \mathfrak{A}$, $\pi(a) := \bigoplus_{\omega\in S}\pi_\omega(a)$. This is a well-defined representation of unital *-algebras which is also continuous since, trivially, $||\pi(a)\oplus_\omega x_\omega||^2 = \sum_\omega ||\pi_\omega(a)x_\omega||^2 \leq ||a||^2||\oplus_\omega x_\omega||$, using Proposition 8.2 (b). The fact that π is isometric follows from Proposition 8.2 (d), since we shall show π is injective. It is sufficient to prove that if $a \neq a' \in \mathfrak{A}$ then there is $\omega \in S$ with $\omega(a - a') \neq 0$, so that $\langle\Psi_\omega|(\pi_\omega(a) - \pi_\omega(a'))\Psi_\omega\rangle \neq 0$ and $\pi_\omega(a) \neq \pi_\omega(a')$, which implies $\pi(a) \neq \pi(a')$. Write $a - a' = b_1 + ib_2$ with $b_k = b_k^*$ and assume that $b_1 \neq 0$ (the other case is analogous). It suffices to find $\omega \in S$ with $(Re(\omega(a - a')) =)\ \omega(b_1) \neq 0$. By Theorem 3.82 we may write $b_1 = \Psi(\beta)$ where $\beta \in C(\sigma(b_1)) \setminus \{0\}$ and $\Psi : C(\sigma(b_1)) \to \mathfrak{A}$ is an isometric *-homomorphism. $\omega'(\gamma) := (\int_{\sigma(b_1)}|\beta(x)|dx)^{-1}\int_{\sigma(b_1)}|\beta(x)|\gamma(x)dx$ is a positive linear functional on $C(\sigma(b_1))$ with $||\omega'|| = \omega'(1) = 1$. The *Hahn-Banach theorem* (see, e.g.,[Rud86]) implies there exists a bounded functional on $\mathfrak{A}$ which extends ω' (viewed as bounded functional on the closed subspace $\Psi(C(\sigma(b_1)))$) such that $||\omega|| = ||\omega'||$. Since $\omega(b_1) = \omega'(b_1) \neq 0$ and $\omega(\mathbb{1}) = \omega'(\mathbb{1}) = 1$, the proof is completed once we establish ω is positive. But this is an immediate consequence of Lemma 8.17 since $||\omega|| = ||\omega'|| = 1 = \omega'(\mathbb{1}) = \omega(\mathbb{1})$. □

8.3.5 *Pure States, Irreducible Representations and Superselection Rules*

As in the standard formulation, we can define *pure algebraic states* as the extremal elements of the convex body of algebraic states of unital *-algebras (including unital C^*-algebras).

Definition 8.19 An algebraic state $\omega : \mathfrak{A} \to \mathbb{C}$ on a *-algebra $\mathfrak{A}$ with unit is **pure** if it is extremal in the set of algebraic states: if $\omega = \lambda\omega_1 + (1-\lambda)\omega_2$ for a pair of algebraic states ω_1, ω_2 and $\lambda \in (0, 1)$, then $\omega = \omega_1$ (or $\omega = \omega_2$). An algebraic state that is not pure is **mixed**. ■

We explain now how pure states are characterized in the algebraic framework. To this end we have the following pivotal result.

Theorem 8.20 (Characterization of Pure Algebraic States) *Let ω be an algebraic state on the C^*-algebra $\mathfrak{A}$ with unit and $(\mathsf{H}_\omega, \pi_\omega, \Psi_\omega)$ a corresponding GNS triple. Then ω is pure if and only if π_ω is irreducible ($\pi_\omega(\mathfrak{A})' = \mathbb{C}I$, i.e. $\pi_\omega(\mathfrak{A})'' = \mathfrak{B}(\mathsf{H}_\omega)$).*

Proof Let us prove that π_ω irreducible implies ω pure. Assume that π_ω is irreducible and $\omega = \lambda\omega_1 + (1-\lambda)\omega_2$ for $\lambda \in (0, 1)$ and a pair of states ω_1, ω_2. The goal is establishing that $\omega = \omega_1 = \omega_2$. As a consequence of the positivity property and $||\omega|| = 1$ we have $0 \leq \lambda\omega_1(a^*a) \leq \omega(a^*a) \leq ||a||^2$. The sesquilinear map $S(\pi_\omega(a)\Psi_\omega, \pi_\omega(b)\Psi_\omega) := \lambda\omega_1(a^*b)$ on the dense subspace $\pi_\omega(\mathfrak{A})\Psi_\omega \subset \mathsf{H}_\omega$ is positive, so it satisfies the Cauchy-Schwartz inequality. The previous inequality implies $S(\Phi, \Phi') \leq ||\Phi||\,||\Phi'||$. A straightforward application of the Riesz theorem shows that there exists a bounded operator $T \in \mathfrak{B}(\mathsf{H}_\omega)$ such that $S(\Phi, \Phi') = \langle \Phi | T\Phi' \rangle$. As a consequence, $\lambda\omega_1(a^*b) = \langle \Psi_\omega | \pi_\omega(a^*) T \pi_\omega(b)\Psi_\omega\rangle$ if $a, b \in \mathfrak{A}$. In particular,

$$\langle \pi_\omega(a)\Psi_\omega | T\pi_\omega(b)\pi_\omega(c)\Psi_\omega\rangle = \lambda\omega_1(a^*bc) = \lambda\omega_1((b^*a)^*c) = \langle \pi_\omega(a)\Psi_\omega | \pi_\omega(b) T \pi_\omega(c)\Psi_\omega\rangle \,.$$

By the cyclic property of Ψ_ω, that is equivalent to saying that $T\pi_\omega(b) = \pi_\omega(b)T$ for every $b \in \mathfrak{A}$. Since π_ω is irreducible, Schur's lemma implies that $T = \mu I$ for some $\mu \in \mathbb{C}$. Here, $\lambda\omega_1(a^*b) = \langle \Psi_\omega | \pi_\omega(a^*) T \pi_\omega(b)\Psi_\omega\rangle$ yields $\lambda\omega_1(a^*b) = \mu\omega(a^*b)$, so in particular for $a = b = \mathbb{1}$ we find $\lambda = \mu$. In summary $\omega_1 = \omega$ and the decomposition $\omega = \lambda\omega_1 + (1-\lambda)\omega_2$ is trivial, proving that ω is pure. Let us prove that if π_ω is reducible then ω is not pure. Indicate by $P \neq 0, I$ the orthogonal projector onto a proper, non-trivial and π_ω-invariant subspace of H_ω. By hypothesis $P\pi_\omega(a)P = \pi_\omega(a)P$, so taking adjoints we have $\pi_\omega(a)P = P\pi_\omega(a)$, because a is arbitrary. Hence, the cyclic property of Ψ_ω implies both $P\Psi_\omega \neq 0$ and $(I-P)\Psi_\omega \neq 0$. Furthermore, $\pi_\omega(a)P = P\pi_\omega(a)$ leads to $P\pi_\omega(\mathfrak{A})(I-P) = (I-P)\pi_\omega(\mathfrak{A})P = 0$. Hence we can decompose the right-hand side of $\omega(a) = \langle (P + I - P)\Psi_\omega | \pi_\omega(a)(P + I - P)\Psi_\omega\rangle$:

$$\omega(a) = \langle P\Psi_\omega | \pi_\omega(a) P\Psi_\omega\rangle + \langle (I-P)\Psi_\omega | \pi_\omega(a)(I-P)\Psi_\omega\rangle = \lambda\omega_1(a) + (1-\lambda)\omega_2(a)\,,$$

where $\lambda := ||P\Psi_\omega||^2 = \langle P\Psi_\omega | P\Psi_\omega\rangle \in (0, 1)$. Let us prove that $\omega_1 \neq \omega$ and therefore ω is not pure. The relation $\omega_1 = \omega$ reads

$$\langle \Psi_\omega | \pi_\omega(a)\Psi_\omega\rangle = \left\langle \frac{P\Psi_\omega}{||P\Psi_\omega||} \middle| \pi_\omega(a) \frac{P\Psi_\omega}{||P\Psi_\omega||} \right\rangle \quad \text{for every } a \in \mathfrak{A}.$$

Since $PP = P = P^*$, P commutes with $\pi(a)$, and replacing $\pi(a)$ by $\pi(a^*b)$ we get

$$\langle \pi(a)\Psi_\omega | \pi_\omega(b)\Psi_\omega\rangle = \langle \pi(a)\Psi_\omega | ||P\Psi_\omega||^{-2} P\pi_\omega(b)\Psi_\omega\rangle \quad \text{for every } a, b \in \mathfrak{A}.$$

Since Ψ_ω is cyclic, we have $I = ||P\Psi_\omega||^{-2}P$. This is impossible because the operators have different range, by hypothesis. Hence ω is not pure and the proof ends. □

Remark 8.21 The theorem is also valid for unital *-algebras by replacing *irreducibility* with *weak irreducibility* (Definition 8.12, see [Schm90, Corollary 8.6.7]). ■

The algebraic notion of pure state fits well with the Hilbert space formulation, since pure states are represented by unit vectors (in the absence of superselection rules). The following proposition sets up a comparison between the two notions.

Proposition 8.22 *Let ω be a pure state on the unital C^*-algebra $\mathfrak{A}$ and $\Phi \in \mathsf{H}_\omega$ a unit vector. Then*

(a) *the functional $\mathfrak{A} \ni a \mapsto \langle\Phi|\pi_\omega(a)\Phi\rangle$ defines a pure algebraic state and $(\mathsf{H}_\omega, \pi_\omega, \Phi)$ is a GNS triple for it. (In particular, GNS representations of algebraic states given by unit vectors in H_ω are all unitarily equivalent, trivially).*

(b) *Unit vectors $\Phi, \Phi' \in \mathsf{H}_\omega$ give the same (pure) algebraic state if and only if $\Phi = c\Phi'$ for some $c \in \mathbb{C}$, $|c| = 1$, i.e. if Φ and Φ' belong to the same ray.*

Proof (a) $(\mathsf{H}_\omega, \pi_\omega, \Phi)$ is a GNS triple for ω_Φ because it satisfies the GNS theorem. In particular, since π_ω is irreducible, $\pi_\omega(\mathfrak{A})\Phi$ must be dense, otherwise its closure would be a proper closed invariant subspace. In particular Φ is pure because its GNS representation π_ω is irreducible by hypothesis. Regarding (b), observe that $\pi_\omega(\mathfrak{A})'' = \mathfrak{B}(\mathsf{H}_\omega)$ since the representation is irreducible. Hence $\langle\Phi|\pi_\omega(a)\Phi\rangle = \langle\Phi'|\pi_\omega(a)\Phi'\rangle$ for every $a \in \mathfrak{A}$ implies, by weak continuity, that $\langle\Phi|A\Phi\rangle = \langle\Phi'|A\Phi'\rangle$ for every $A \in \mathfrak{B}(\mathsf{H}_\omega)$ (by the double commutant theorem, $\mathfrak{B}(\mathsf{H}_\omega) = \pi_\omega(\mathfrak{A})''$ is the weak closure of $\pi_\omega(\mathfrak{A})$). This can be written $tr(AP) = tr(AP')$ for every $A \in \mathfrak{B}(\mathsf{H}_\omega)$, where P and P' are the orthogonal projectors onto the spans of Φ and Φ' respectively. Choosing $A = \langle\Psi|\cdot\rangle\Psi$, $tr(A(P - P')) = 0$ reads $\langle\Psi|(P - P')\Psi\rangle = 0$ for every $\Psi \in \mathsf{H}_\omega$, which implies $P = P'$. But this means exactly $\Phi = c\Phi'$ for some $c \in \mathbb{C}$, $|c| = 1$. □

Pure states give rise to *unitarily inequivalent* representations when $\mathfrak{A}$ contains non-trivial elements q commuting with every element of $\mathfrak{A}$ (this is to say the *center* of $\mathfrak{A}$ is not the trivial subalgebra $\mathbb{C}\mathbb{1}$). If ω, ω' are algebraic states, so that the representations π_ω and $\pi_{\omega'}$ are irreducible, Schur's lemma implies $\pi_\omega(q) = cI_{\mathsf{H}_{\omega'}}$ and $\pi_{\omega'}(q) = c'I_{\mathsf{H}_\omega}$ for some $c, c' \in \mathbb{C}$. It is therefore evident that, if $c \neq c'$, there cannot be any Hilbert space isomorphism $U : \mathsf{H}_\omega \to \mathsf{H}_{\omega'}$ with $U\pi_\omega(a)U^{-1} = \pi_{\omega'}(a)$ for every $a \in \mathfrak{A}$: taking $a = q$ would produce a contradiction. Assuming $q = q^*$ (if the initial q is not selfadjoint we can use $q + q^*$ and $i(q - q^*)$), we can think of q as a *superselection charge*, viewing H_ω and $\mathsf{H}_{\omega'}$ as *(Abelian) superselection sectors* labelled by different values of the superselection charge—an approach similar to that of Sect. 6.3.1. This is a way to introduce the idea of superselection rules in the algebraic formalism (see, e.g., [Haa96, Mor18]).

The correspondence pure (algebraic) states vs. state vectors, automatic in the standard formulation, holds on Hilbert spaces of GNS representations of pure algebraic states, but in general not for mixed algebraic states. The following exercise focuses on this apparent problem.

Exercise 8.23

(1) Consider, in the standard (non-algebraic) formulation, a physical system described on the Hilbert space H and a quantum-state operator $T \in \mathscr{S}(\mathsf{H}) \setminus \mathscr{S}_p(\mathsf{H})$. The map $\omega_T : \mathfrak{B}(\mathsf{H}) \ni A \mapsto tr(TA)$ defines an algebraic state on the C^*-algebra $\mathfrak{B}(\mathsf{H})$. By the GNS theorem, there exist another Hilbert space H_{ω_T}, a representation $\pi_{\omega_T} : \mathfrak{B}(\mathsf{H}) \to \mathfrak{B}(\mathsf{H}_{\omega_T})$ and a unit vector $\Psi_{\omega_T} \in \mathsf{H}_{\omega_T}$

such that $tr(TA) = \langle \Psi_{\omega_T} | \pi_{\omega_T}(A)\Psi_{\omega_T}\rangle$ for $A \in \mathfrak{B}(\mathsf{H})$. Therefore it would seem that the initial mixed state has been transformed into a pure state! How is this fact explained?

Solution There is no transformation from mixed states to pure states because the mixed state is represented by a vector, Ψ_{ω_T}, living in a different Hilbert space H_{ω_T}. Moreover, there is no Hilbert space isomorphism $U : \mathsf{H} \to \mathsf{H}_{\omega_T}$ with $UAU^{-1} = \pi_{\omega_T}(A)$, such that $U^{-1}\Psi_{\omega_T} \in \mathsf{H}$. In fact the representation $\mathfrak{B}(\mathsf{H}) \ni A \mapsto A \in \mathfrak{B}(\mathsf{H})$ is irreducible, whereas π_{ω_T} cannot be irreducible (it would, provided U existed), because the state T is not an extremal point in the space of non-algebraic states, and so it cannot be extremal in the larger space of algebraic states.

(2) Consider $T \in \mathscr{S}(\mathsf{H})$ defining the algebraic state $\omega_T : \mathfrak{B}(\mathsf{H}) \to \mathbb{C}$ by means of $\omega_T(A) := tr(TA)$. Construct explicitly a GNS representation of ω_T and prove that π_{ω_T} is irreducible if and only if $T \notin \mathscr{S}_p(\mathsf{H})$.

Solution Decompose spectrally $T = \sum_{j=1}^{N} p_j \langle \psi_j | \ \rangle \psi_j$, where $N \subset (\mathbb{N} \setminus \{0\}) \cup \{+\infty\}$, $p_j > 0$, $\sum_{j=1}^{N} p_j = 1$, and N contains more than one element iff $T \notin \mathscr{S}_p(\mathsf{H})$. Consider the Hilbert direct sum $\mathsf{H}_{\omega_T} := \bigoplus_{j=1}^{N} \mathsf{H}$, define $\Psi_{\omega_T} := \oplus_{j=1}^{N} \sqrt{p_j}\psi_j$, and eventually set $\pi_{\omega_T}(A) := \bigoplus_{j=1}^{N} A$. It is easy to prove that all requirements for a GNS triple of ω_T are satisfied. In particular, use the fact that $AP_k\psi_h = \delta_{kh}A\psi_h$ is dense in $\mathfrak{B}(\mathsf{H})$, for every fixed $k = h$, when $A \in \mathfrak{B}(\mathsf{H})$ and where P_k is the orthogonal projector onto span$\{\psi_k\}$. Finally, every copy of H in the space $\mathsf{H}_{\omega_T} := \bigoplus_{j=1}^{N} \mathsf{H}$ is invariant under $\pi_{\omega_T}(A)$ for all $A \in \mathfrak{B}(\mathsf{H})$, whence the representation is not irreducible if $N > 1$. If $N = 1$, it is irreducible since $\pi_{\omega_T}(\mathfrak{B}(\mathsf{H})) = \mathfrak{B}(\mathsf{H})$ is irreducible. ■

8.4 Examples: Weyl C^*-Algebras

A real **symplectic space** is a vector space V equipped with a **symplectic form**, that is a skew-symmetric bilinear map $\sigma : \mathsf{V} \times \mathsf{V} \to \mathbb{R}$. The 2-form σ is **weakly non-degenerate** whenever $\sigma(x, y) = 0$ for every $x \in \mathsf{V}$ implies $y = 0$. This structure is related with various versions of the canonical commutation relations in QM and QFT. As a *finite-dimensional* example, consider

$$\mathsf{V} := \mathbb{R}^n \times \mathbb{R}^n \quad \text{and} \quad \sigma((u, v), (u', v')) := u \cdot v' - v \cdot u' , \tag{8.11}$$

where $\cdot$ is the standard inner product of $\mathbb{R}^n$. This symplectic form is related to the *position* and *momentum operators* on $\mathbb{R}^n$ discussed in Example 2.59. If, for $u, v \in \mathbb{R}^n$, we define

$$u \cdot X := \sum_{k=1}^{n} u_k X_k \quad \text{and} \quad v \cdot P := \sum_{k=1}^{n} v_k P_k ,$$

then, on the common invariant and dense domain $\mathscr{S}(\mathbb{R}^n)$, the commutation relations of X_k and P_k immediately produce

$$[u\cdot X+v\cdot P, u'\cdot X+v'\cdot P]\restriction_{\mathscr{S}(\mathbb{R}^3)}= i(u\cdot v'-v\cdot u')I_{\mathscr{S}(\mathbb{R}^3)} = i\sigma((u,v),(u',v'))I_{\mathscr{S}(\mathbb{R}^3)}.$$

If $\dim \mathsf{V} < +\infty$ and σ is weakly non-degenerate, then $\dim \mathsf{V}$ has to be even. Furthermore, it is always possible to fix a basis in V so σ reads as in (8.11) (see, e.g., [Mor18]).

An *infinite-dimensional* example related with QFT in Minkowski spacetime is:

$$\mathsf{V} := C_c^\infty(\mathbb{R}^3,\mathbb{R})\times C_c^\infty(\mathbb{R}^3,\mathbb{R}) \quad \text{and} \quad \sigma((f,g),(f',g')) := \int_{\mathbb{R}^3}(fg'-f'g)d^3x\,.$$

(This can be variously generalized, especially in curved spacetime: see, e.g., [KhMo15].) Now, referring to (8.1), the commutation relation (8.2) on the dense invariant domain D yields

$$[\phi(f)+\pi(g),\phi(f')+\pi(g')]\restriction_D = i\int_{\mathbb{R}^3}(fg'-gf')I_D = i\sigma((f,g),(f',g'))I_D\,.$$

The symplectic forms are weakly non-degenerate in both cases (exercise!). The symplectic formalism allows one to define abstract unital *-algebras associated to the symplectic structures canonically (see, e.g., [KhMo15]). At present though we are more interested in a C^*-algebra description.

The first remark which relates symplectic spaces to the theory of C^*-algebras is that if we exponentiate unitary operators, thus avoiding domain issues, the commutation relations of $e^{\overline{iu\cdot X+iv\cdot P}}$ and $e^{\overline{i\phi(f)+i\pi(g)}}$[1] are again described by the corresponding symplectic forms (see, e.g., [Stro05, Mor18] for the former case and [ReSi75, BrRo02] for the latter):

$$e^{\overline{iu\cdot X+iv\cdot P}}e^{\overline{iu'\cdot X+iv'\cdot P}} = e^{-i\sigma((u,v),(u',v'))/2}e^{\overline{i(u+u')\cdot X+i(v+v')\cdot P}}$$

and

$$e^{\overline{i\phi(f)+i\pi(g)}}e^{\overline{i\phi(f')+i\pi(g')}} = e^{-i\sigma((f,g),(f',g'))/2}e^{\overline{i\phi(f+f')+i\pi(g+g')}}\,.$$

[1]We are assuming that the symmetric operator $\phi(f)+\pi(g)$ is essentially selfadjoint on D, as it happens in many physically relevant cases [BrRo02]. Instead, $u\cdot X+v\cdot P$ is essentially selfadjoint on $\mathscr{S}(\mathbb{R}^n)$ as the reader can prove by establishing the existence of a dense set of analytic vectors [Mor18].

The second noteworthy observation is that relationships of that type uniquely determine a unital C^*-algebra, called the Weyl C^*-algebra associated to (V, σ), thus promoting the theory to the same league as the algebraic formulation. Indeed, given a real symplectic space (V, σ) with σ non-degenerate, a **Weyl C^*-algebra** $\mathcal{W}(\mathsf{V}, \sigma)$ associated with (V, σ) is a unital C^*-algebra such that

(1) there exists a set of non-zero elements $W(x) \in \mathcal{W}(\mathsf{V}, \sigma)$ for every $x \in \mathsf{V}$, called **generators**, satisfying the **Weyl (commutation) relations**

$$W(x)W(y) = e^{-i\sigma(x,y)/2}W(x+y)\,, \quad W(x)^* = W(-x)\,, \quad x, y, \in \mathsf{V}\,; \tag{8.12}$$

(2) $\mathcal{W}(\mathsf{V}, \sigma)$ is actually **generated** by the $W(x)$, i.e., the linear span of finite combinations of finite products of the $W(x)$ is dense in $\mathcal{W}(\mathsf{V}, \sigma)$.

In this way $W(0)$ becomes the unit $\mathbb{1}$ of the algebra (since it commutes with every element, and the unit is unique) and the generators are *unitary*: $W(-x) = W(x)^* = W(x)^{-1}$ for $x \in \mathsf{V}$. It is possible to prove that Weyl C^* algebras exist for every given (V, σ) (e.g., [Mor18]). The very remarkable result is however that $\mathcal{W}(\mathsf{V}, \sigma)$ is uniquely determined (up to isomorphism) by (V, σ) (e.g., [Mor18, Theorems 11.48 and 14.40]).

Theorem 8.24 *Consider a real symplectic space* (V, σ) *with non-degenerate symplectic form, and associated Weyl C^*-algebras:* $\mathcal{W}(\mathsf{V}, \sigma)$ *generated by* $W(x)$*,* $\mathcal{W}'(\mathsf{V}, \sigma)$ *generated by* $W'(x)$*. Then there exists a unique (isometric)* **-isomorphism* $\gamma : \mathcal{W}(\mathsf{V}, \sigma) \to \mathcal{W}'(\mathsf{V}, \sigma)$ *such that* $\gamma(W(x)) = W'(x)$ *for every* $x \in \mathsf{V}$.

Example 8.25

(1) If $\mathcal{W}(\mathsf{V}, \sigma)$ is a Weyl C^* algebra, an algebraic state $\omega : \mathcal{W}(\mathsf{V}, \sigma) \to \mathbb{C}$ is called **regular** if $\mathbb{R} \ni t \mapsto \pi_\omega(W(tx))$ is strongly continuous at $t = 0$ for every $x \in \mathsf{V}$ (the requirement is independent of the chosen GNS representation by item (b) in the GNS theorem). Since (8.12) imply that $\mathbb{R} \ni t \mapsto \pi_\omega(W(tx))$ is a unitary one-parameter group of operators on H_ω, exploiting Stone's theorem it is possible to define **selfadjoint generators** $A_\omega(x)$ such that $\pi_\omega(W(x)) = e^{iA_\omega(x)}$, simply by taking the strong derivative of $\pi_\omega(W(tx))$ at $t = 0$, recasting the operators X_k, P_h and the field operators $\phi(f), \pi(g)$ in the two examples seen above. However, a fundamental difference shows up when we restrict to *pure states* ω, i.e., irreducible GNS representations. If $\dim(V) = 2n < +\infty$ and ω, ω' are pure states on $\mathcal{W}(\mathsf{V}, \sigma)$, then π_ω and π'_ω are unitarily equivalent, and they are unitarily equivalent to the standard representation of $\mathcal{W}(\mathsf{V}, \sigma)$ on $L^2(\mathbb{R}^n, d^n x)$ where $W(u, v) = e^{\overline{iu\cdot X + iv\cdot P}}$. This is an immediate consequence of the celebrated *Stone-von Neumann theorem* (see, e.g., [Mor18, Theorem 11.43]), of which Theorem 7.45 is a different version. If $\dim \mathsf{V}$ is not finite, as is in the second example considered in (1) (quantum fields), irreducible inequivalent representations crop up, as we said at the beginning of the chapter.

(2) An important class of regular states, especially relevant in QFT, are **Gaussian** states $\omega_\mu : \mathcal{W}(\mathsf{V}, \sigma) \to \mathbb{C}$ (also known as **quasi-free** states). They are defined by requiring that

$$\omega_\mu(W(x)) = e^{-\mu(x,x)/2} \quad \text{if } x \in \mathsf{V} \tag{8.13}$$

where $\mu : \mathsf{V} \times \mathsf{V} \to \mathbb{R}$ is a fixed real inner product satisfying

$$\frac{1}{4}|\sigma(x, y)|^2 \le \mu(x, x)\mu(y, y) \quad \text{for } x, y \in \mathsf{V}.$$

(An equivalent way would be to say σ is induced by a bounded operator S with $||S|| \le 1$ on the real Hilbert space obtained by completing V under $\mu(x, Sy) = \frac{1}{2}\sigma(x, y)$). It is possible to prove that, for a fixed such μ, there exists exactly one algebraic state on $\mathcal{W}(V, \sigma)$ satisfying (8.13) and such that the GNS representation of ω_μ is (unitarily equivalent to) the familiar (bosonic) *Fock representations* used in QFT, where Ψ_ω is the *vacuum state* [BrRo02, KhMo15].

(3) We finally observe that every Weyl C^*-algebra $\mathfrak{A}$ is **simple** (see, e.g., [Mor18, Theorem 14.40]). In other words, it does not admit (non-trivial proper) closed *two-sided* **-ideals* (meaning *-invariant subspaces $J \subset \mathfrak{A}$ such that $ab, ba \in J$ for $a \in J$ and $b \in \mathfrak{A}$). As a consequence, every (not necessarily GNS) representation of unital *-algebras $\pi : \mathfrak{A} \to \mathfrak{B}(\mathsf{H})$ must be *faithful*. This is because $\ker\pi$ is a closed two-sided *-ideal as the reader can immediately prove (notice that π is necessarily continuous by Proposition 8.2). Furthermore $\ker\pi \neq \mathfrak{A}$, because otherwise $\pi(\mathbb{1}) = 0$, which is impossible because representations of unital *-algebras have $\pi(\mathbb{1}) = I$. ■

Exercise 8.26 Prove that a state $\omega : \mathcal{W}(\mathsf{V}, \sigma) \to \mathbb{C}$ is regular iff $\omega(W(tf)) \to 1$ as $t \to 0$ for all $f \in \mathsf{V}$. Conclude that every Gaussian state is regular.

Solution If ω is regular, then $\omega(W(tf)) = \langle\Psi_\omega|\pi_\omega(W(tf))\Psi_\omega\rangle \to \langle\Psi_\omega|\pi_\omega(W(0))\Psi_\omega\rangle = \langle\Psi_\omega|\pi_\omega(\mathbb{1})\Psi_\omega\rangle = \langle\Psi_\omega|\Psi_\omega\rangle 1$ as $t \to 0$ for all $f \in \mathsf{V}$. Since $\{\pi_\omega(W(tf))\}_{t\in\mathbb{R}}$ is a one-parameter group of unitary operators, from Proposition 7.22 (d) we know that strong continuity is equivalent to the requirement that $\langle\Psi|\pi_\omega(W(tf))\Psi\rangle \to \langle\Psi|\pi_\omega(W(0))\Psi\rangle = 1$ for all $\Psi \in \mathcal{D}$, where $\mathcal{D} \subset \mathsf{H}_\omega$ is such that span$(\mathcal{D})$ is dense in H_ω. But $\mathcal{D} := \{\pi_\omega(W(g))\Psi_\omega \mid g \in \mathsf{V}\}$ has dense span, since it is closed under products up to coefficients arising from Weyl's relations, and linear combinations of those products are dense in H_ω by the GNS theorem. If $\Psi = \pi_\omega(W(g))\Psi_\omega$, we have $\langle\Psi|\pi_\omega(W(tf))\Psi\rangle = \langle\Psi_\omega|\pi_\omega(W(g))^*\pi_\omega(W(tf))\pi_\omega(W(g))\Psi_\omega\rangle = \langle\Psi_\omega|\pi_\omega(W(-g)W(tf)W(g))\Psi_\omega\rangle = e^{it\sigma(g,f)}\langle\Psi_\omega|\pi_\omega(W(tf))\Psi_\omega\rangle = e^{it\sigma(g,f)}\omega(W(tf))$, which is continuous by hypothesis when $t \to 0$. The proof of the last statement now follows from (8.13). ■

8.5 Symmetries and Algebraic Formulation

Symmetries in the algebraic approach are direct generalizations of symmetries in the Hilbert space formulation.

8.5.1 Symmetries and Spontaneous Symmetry Breaking

Definition 8.27 Let $\mathfrak{A}_S$ be the unital *-algebra of observables of the quantum system S with unit element $\mathbb{1}$. An **(algebraic quantum) symmetry** of S is an **automorphism** or an **anti-automorphism** of $\mathfrak{A}_S$. In other words, a map $\alpha : \mathfrak{A}_S \to \mathfrak{A}_S$ which is

(i) bijective,
(ii) linear or anti-linear, respectively,[2]
(iii) unit-preserving: $\alpha(\mathbb{1}) = \mathbb{1}$,
(iv) multiplicative: $\alpha(ab) = \alpha(a)\alpha(b)$, for $a, b \in \mathfrak{A}_S$,
(v) *-preserving: $\alpha(a^*) = \alpha(a)^*$, for $a \in \mathfrak{A}_S$,
(vi) isometric if $\mathfrak{A}_S$ is a C^*-algebra. ■

Remark 8.28 Actually, (vi) is automatic under (i)–(v) if $\mathfrak{A}_S$ is a unital C^*-algebra, as a consequence of Proposition 8.2 (d). (To include the anti-linear case we also need (8.4)). ■

Example 8.29 With reference to a Weyl C^*-algebra $\mathcal{W}(\mathsf{V}, \sigma)$ (Sect. 8.4), suppose that $\Gamma : \mathsf{V} \to \mathsf{V}$ is linear, bijective and preserves the symplectic form: $\sigma(\Gamma x, \Gamma y) = \sigma(x, y)$ for every $x, y \in \mathsf{V}$. Using Theorem 8.24 it is easy to prove [Mor18] that there exists a unique automorphism $\gamma : \mathcal{W}(\mathsf{V}, \sigma) \to \mathcal{W}(\mathsf{V}, \sigma)$ such that $\gamma(W(x)) := W(\Gamma(x))$ if $x \in \mathsf{V}$. In a manner of speaking, it is the geometry of V that brings about the algebraic symmetry. This sort of background-induced symmetries play an important role in QFT on curved spacetime (see, e.g., [KhMo15]). What happens if $\sigma(\Gamma x, \Gamma y) = -\sigma(x, y)$ for every $x, y \in \mathsf{V}$, but we keep the other hypotheses? ■

In the rest of the chapter, unless specified differently, $\mathfrak{A}_S$ will be a unital *-algebra, so that the unital C^*-algebra case in automatically included.

Definition 8.30 An algebraic state $\omega : \mathfrak{A}_S \to \mathbb{C}$ is said to be **invariant** under a symmetry $\alpha : \mathfrak{A}_S \to \mathfrak{A}_S$ if

$$\omega(\alpha(a)) = \omega(a) , \qquad \text{for every } a^* = a \in \mathfrak{A}_S .$$

(The requirement extends to every element of $\mathfrak{A}_S$, by the (anti-)linearity of α.) ■

[2] An anti-automorphism can be alternatively defined as a *linear* map satisfying (i), (iii), (v), (vi) and $\alpha(ab) = \alpha(b)\alpha(a)$ in place of (iv). If so, the anti-linear map $\alpha' : \mathfrak{A} \ni a \mapsto \alpha(a)^* \in \mathfrak{A}$ satisfies (i)–(vi), and conversely.

When an α-invariant state exists, the action of α is implementable unitarily by means of the *inverse dual action* (7.5) of a Wigner-Kadison symmetry on the GNS Hilbert space, as we shall prove now.

Theorem 8.31 *Suppose that* $\alpha : \mathfrak{A}_S \to \mathfrak{A}_S$ *is a symmetry and the state* $\omega : \mathfrak{A}_S \to \mathbb{C}$ *is invariant under* α. *Consider the GNS quadruple* $(\mathsf{H}_\omega, \mathcal{D}_\omega, \pi_\omega, \Psi_\omega)$ *(if* $\mathfrak{A}_S$ *is unital* C^**-algebra we take the GNS triple* $(\mathsf{H}_\omega, \pi_\omega, \Psi_\omega)$*). Then*

(1) α *is* **(anti-)unitarily implementable**: *there exists an isometric surjective map* $U : \mathsf{H}_\omega \to \mathsf{H}_\omega$*, linear or anti-linear in agreement with* α*, such that*

$$U\pi_\omega(a)U^{-1} = \pi_\omega(\alpha(a)) \qquad \forall a \in \mathfrak{A} .$$

(2) $U\Psi_\omega = \Psi_\omega$.

The (anti-)unitary operator U *is uniquely determined by (1), (2) and satisfies* $U(\mathcal{D}_\omega) = \mathcal{D}_\omega$.

Proof By direct inspection one sees that the required operator is the unique continuous extension U, to the whole H_ω, of the map

$$U'\pi(a)\Psi_\omega := \pi_\omega(\alpha(a))\Psi_\omega \quad \forall a \in \mathfrak{A}_S \tag{8.14}$$

defined on the dense subspace $\pi_\omega(\mathfrak{A})\Psi_\omega$. The fact that the map is isometric (hence bounded) comes from

$$||\pi_\omega(\alpha(a))\Psi_\omega||^2 = \langle\Psi_\omega|\pi_\omega(\alpha(a^*a))\Psi_\omega\rangle = \omega(\alpha(a^*a)) = ||\pi_\omega(a)\Psi_\omega||^2 ,$$

Using its (anti-)linearity, guaranteed by the (anti-)linearity of $\pi_\omega \circ \alpha$, the above formula simultaneously proves that U' is well defined (single-valued). Observing that the isometric map $V\pi(a)\Psi_\omega := \pi_\omega(\alpha^{-1}(a))\Psi_\omega$, $a \in \mathfrak{A}_S$, is the inverse of U' on $\pi_\omega(\mathfrak{A})\Psi_\omega$, and $U'V = VU' = I_{\pi_\omega(\mathfrak{A})\Psi_\omega}$ extends continuously to the identity on H_ω, we also obtain surjectivity. Uniqueness holds by construction: if U satisfies both (1) and (2), the latter implies $U^{-1}\Psi_\omega = \Psi_\omega$ and the former $U\pi(a)\Psi_\omega := \pi_\omega(\alpha(a))\Psi_\omega$ for every $a \in \mathfrak{A}$. Thus we find just the operator constructed above. $U(\mathcal{D}_\omega) = \mathcal{D}_\omega$ is evident, since $\mathcal{D}_\omega = \pi_\omega(\mathfrak{A}_S)\Psi_\omega$. □

The algebraic approach permits us to deal with a physically important situation where a symmetry exists only at the level of the algebra of observables, but it 'breaks down' at the level of states. This situation is usually called *spontaneous breakdown of symmetry*. There are several interpretations of this idea (see [Lan17] for a broad, up-to-date review on the subject and [Haa96, Stro08] for more specific results in relativistic local QFT). Generally speaking, the **spontaneous breakdown of symmetry** occurs when the *-algebra of observables $\mathfrak{A}_S$ admits a symmetry α described by an (anti-)automorphism, but there is no state invariant under α in any class of states of physical relevance. In particular,

Definition 8.32 The symmetry $\alpha : \mathfrak{A}_S \to \mathfrak{A}_S$ is said to be **spontaneously broken** by a given algebraic state $\omega : \mathfrak{A}_S \to \mathbb{C}$ if ω is *not* invariant under α. ■

In this case α could still be implemented in the GNS representation of ω: (1) Theorem 8.31 might hold for some (anti-)unitary operator U on H_ω, although U does not satisfy (2). This situation calls for a stronger version of symmetry breakdown.

Definition 8.33 The symmetry $\alpha : \mathfrak{A}_S \to \mathfrak{A}_S$ is **spontaneously broken** by an algebraic state $\omega : \mathfrak{A}_S \to \mathbb{C}$ in **strong sense**, if α cannot be implemented in the GNS representation of ω: no (anti-)unitary operator U on H_ω satisfies Theorem 8.31 (1) (hence in particular ω cannot be invariant under α, by Theorem 8.31). ■

Exercise 8.34 Consider an algebraic state $\omega : \mathfrak{A}_S \to \mathbb{C}$ on the unital C^*-algebra (or unital *-algebra) $\mathfrak{A}_S$ and an algebraic (linear) symmetry $\alpha : \mathfrak{A}_S \to \mathfrak{A}_S$. Prove that ω spontaneously breaks α in strong sense iff π_ω and $\pi_{\omega\circ\alpha}$ are not unitarily equivalent.

Solution To fix ideas let us consider C^*-algebras, for the other case is essentially identical. The claim is equivalent to saying that α can be unitarily implemented in H_ω iff π_ω and $\pi_{\omega\circ\alpha}$ are unitarily equivalent. Let us prove this statement. First observe that the representation $\pi_{\omega\circ\alpha}\circ\alpha^{-1} : \mathfrak{A}_S \to \mathfrak{B}(\mathsf{H}_{\omega\circ\alpha})$ satisfies $\langle \Psi_{\omega\circ\alpha}|\pi_{\omega\circ\alpha}\circ \alpha^{-1}(a)\Psi_{\omega\circ\alpha}\rangle = \omega(\alpha(\alpha^{-1}(a)) = \omega(a)$. Hence $(\mathsf{H}_{\omega\circ\alpha}, \pi_{\omega\circ\alpha}\circ\alpha^{-1}, \Psi_{\omega\circ\alpha})$ is a GNS triple for ω (the remaining conditions are satisfied trivially). The final part of the GNS theorem shows that there is a surjective isometric operator $V : \mathsf{H}_{\omega\circ\alpha} \to \mathsf{H}_\omega$ such that $V\pi_{\omega\circ\alpha}(\alpha^{-1}(a))V^{-1} = \pi_\omega(a)$ for all $a \in \mathfrak{A}_S$. Namely, $\pi_{\omega\circ\alpha}(a) = V^{-1}\pi_\omega(\alpha(a))V$ for all $a \in \mathfrak{A}_S$. To conclude, observe that π_ω and $\pi_{\omega\circ\alpha}$ are unitarily equivalent iff there exist a surjective isometry $U : \mathsf{H}_{\omega\circ\alpha} \to \mathsf{H}_\omega$ with $U\pi_{\omega\circ\alpha}(a)U^{-1} = \pi_\omega(a)$ for all $a \in \mathfrak{A}_S$, that is to say $UV^{-1}\pi_\omega(\alpha(a))VU^{-1} = \pi_\omega(a)$ for all $a \in \mathfrak{A}_S$. This is the same as saying that $V^{-1}U$ implements α in H_ω. ■

8.5.2 *Groups of Symmetries in the Algebraic Approach*

To wrap up, we consider topological (or Lie) groups of symmetries. We will only examine symmetries represented by *linear* *-algebra automorphisms for the same reasons evoked for Hilbert spaces, see Sect. 7.2.2. Suppose $\alpha : G \ni g \mapsto \alpha_g$ associates every element g of the group with an automorphism $\alpha_g : \mathfrak{A}_S \to \mathfrak{A}_S$ of unital *-algebras, and that this map represents the group, i.e., $\alpha_e = id$ and $\alpha_g \circ \alpha_{g'} = \alpha_{g\cdot g'}$. In this sense G is a **group of algebraic symmetries**. If the state $\omega : \mathfrak{A}_S \to \mathbb{C}$ is α-invariant, in view of (8.14) in Theorem 8.31 there exists a map $G \ni g \mapsto U_g \in \mathfrak{B}(\mathsf{H}_\omega)$ that can be proved to be a *unitary representation* of G and satisfies

(1) $U_g\pi_\omega(a)U_g^{-1} = \pi_\omega(\alpha_g(a))$ for every $a \in \mathfrak{A}$ and every $g \in G$.
(2) $U_g\Psi_\omega = \Psi_\omega$ for every $g \in G$.

Remark 8.35 If $\mathfrak{A}_S$ is not C^* and hence the GNS theorem uses the quadruple $(\mathsf{H}_\omega, \mathcal{D}_\omega, \pi_\omega, \Psi_\omega)$, (1) and (2) imply also $U_g(\mathcal{D}_\omega) = \mathcal{D}_\omega$ for every $g \in G$. ■

If G is topological group, the physically natural requirement on the continuity of α with respect to ω (which can be immediately stated in terms of seminorms) is that

$$G \ni g \mapsto \omega\left(b^*\alpha_g(a)b\right) \quad \text{is continuous for every } a^* = a \text{ and } b \text{ in } \mathfrak{A}_S. \tag{8.15}$$

This is because the right-hand side satisfies $\omega(b^*cb) = \langle \pi_\omega(b)\Psi_\omega | \pi_\omega(c)\pi_\omega(b)\Psi_\omega\rangle$ and this is the expectation value of $\pi_\omega(c)$ (for $c = c^*$) up to normalization,[3] in a state represented by a unit vector in H_ω. There is however another mathematically natural notion of continuity with reference to ω[4]:

$$G \ni g \mapsto \omega\left(a^*\alpha_g(a)\right) \qquad \text{is continuous for all } a \in \mathfrak{A}_S. \tag{8.16}$$

At last, also the strong continuity of $G \ni g \mapsto U_g \in \mathfrak{B}(\mathsf{H}_\omega)$ is relevant when describing the theory on the GNS Hilbert space. The following result links the three types of continuity.

Theorem 8.36 *Let $\omega : \mathfrak{A}_S \to \mathbb{C}$ be an invariant state under the representation $G \ni g \mapsto \alpha_g : \mathfrak{A}_S \to \mathfrak{A}_S$ in terms of (linear) automorphisms of unital *-algebras. The following facts hold.*

(a) *There exists a unitary representation $G \ni g \mapsto U_g \in \mathfrak{B}(\mathsf{H}_\omega)$ such that*

  (i) $U_g\Psi_\omega = \Psi_\omega$,
  (ii) $U_g\pi_\omega(a)U_g^{-1} = \pi_\omega(\alpha_g(a))$ *(where $U_g(\mathcal{D}_\omega) = \mathcal{D}_\omega$ if $\mathfrak{A}_S$ is not C^*)*

  for every $g \in G$ and every $a \in \mathfrak{A}_S$

(b) *(8.15) $\Longleftrightarrow$ the representation $G \ni g \mapsto U_g \in \mathfrak{B}(\mathsf{H}_\omega)$ is strongly continuous $\Longleftrightarrow$ (8.16).*

Proof (a) Everything can be proved immediately by the same argument of Theorem 8.31, and we leave the elementary details to the reader. Let us pass to (b). It is clear that, in view of the group structure, continuity at $g_0 \in G$ is equivalent to continuity at e, so we consider the latter only. Since U_g is unitary,

$$\begin{aligned} ||(U_g - I)\pi_\omega(a)\Psi_\omega||^2 &= 2||\pi_\omega(a)\Psi_\omega||^2 - 2Re\langle \pi_\omega(a)\Psi_\omega | U_g\pi_\omega(a)\Psi_\omega\rangle \\ &= 2\omega(a^*a) - 2Re\,\omega(a^*\alpha_g(a)) \, . \end{aligned}$$

If (8.15) holds, then the right-hand side vanishes as $g \to e$. This proves strong continuity (as $g \to e$) when U_g is restricted to the dense subspace $\pi_\omega(\mathfrak{A}_S)\Psi_\omega$. The

[3] True if $\omega(b^*b) \neq 0$. If not, the right-hand side of (8.15) is 0 and continuity holds trivially.

[4] Using the GNS theorem, the term $\omega\left(a^*\alpha_g(a)\right)$ appearing in (8.16) can be replaced by the apparently more general $\omega\left(b\alpha_g(a)\right)$ for all $a, b \in \mathfrak{A}_S$, preserving the introduced notion of continuity.

result easily extends to the whole space by a standard procedure involving $||U_g - I|| \leq 2$. Hence (8.15) implies strong continuity. Now observe that

$$\omega\left(b^*\alpha_g(a)b\right) = \langle U_{g^{-1}}\pi_\omega(b)\Psi_\omega|\pi_\omega(a)U_{g^{-1}}\pi_\omega(b)\Psi_\omega\rangle \,.$$

Therefore the strong continuity of U (together with the continuity of the inner product) implies (8.16). To conclude we show that (8.16) implies (8.15). To this end observe that, if $a = a^*$, then $\mathfrak{A} \times \mathfrak{A} \ni (c, d) \mapsto \omega(c^*\alpha_g(a)d)$ is sesquilinear, so we have the polarization formula. Then the continuity of $G \ni g \mapsto \omega(b^*\alpha_g(a)b)$ implies the continuity of $G \ni g \mapsto \omega(c^*\alpha_g(a)d)$. By linearity, this map is also continuous if $a \neq a^*$ (it suffices to write a as linear combination of selfadjoint elements). Choosing $c = a$ and $d = \mathbb{1}$, we obtain (8.15) from (8.16), concluding the proof. □

Remark 8.37

(a) Suppose that $G = \mathbb{R}$ in the theorem above, that ω is $\mathbb{R}$-invariant, and $\{\alpha_t\}_{t\in\mathbb{R}}$ is continuous with respect to ω. We call ω a **ground (algebraic) state** if the selfadjoint generator H of the associated unitary $\mathbb{R}$-representation $U_t = e^{-itH}$ in the GNS representation of ω satisfies $\sigma(H) \subset [0, +\infty)$. From (a) above $H\Psi_\omega = 0$, so that $0 \in \sigma_p(H)$.

(b) When the group is $\mathbb{R}$, the representation $\{\alpha_t\}_{t\in\mathbb{R}}$ by $\mathfrak{A}$-automorphisms can have the meaning of a group of **dynamical evolution** of the observables. If $\mathfrak{A}$ is a unital C^*-algebra, a stronger requirement than (8.16) is the continuity of $\mathbb{R} \ni t \mapsto \alpha_t$ in the topology of $\mathfrak{A}$. It is easy to prove that if ω is α-invariant, the associated one-parameter unitary group $\{U_t\}_{t\in\mathbb{R}}$ is *uniformly continuous*, and the selfadjoint generator H belongs to $\mathfrak{B}(\mathsf{H}_\omega)$. ■

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