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Expansions in Generalized Eigenfunctions of Selfadjoint Operators

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1. Introduction

1.1. Physical Motivation

a) One of the fundamental assertions in quantum mechanics is as follows: For every selfadjoint operator H representing an observable quantity, any state function f has an expansion in the generalized eigenfunctions of H (cf. [Sch], Chap. 3, Sect. 10, and [J], Chap. 2, Sect. 2.6.3.1),

$$f(x)=\sum \alpha_n \Phi_n(x)+\int \alpha(\lambda)\,\Psi_\lambda(x)\,d\lambda. \tag{1}$$

Here the $\Phi_n \in L_2$ are eigenfunctions corresponding to eigenvalues $a(n)$ of H, and the $\Psi_\lambda \notin L_2$ are "generalized eigenfunctions" corresponding to values $a(\lambda)$ in the continuous spectrum of H. The coefficients in (1) are

$$\alpha_n=\int \overline{\Phi_n(x)}\,f(x)\,dx=\langle \Phi_n, f\rangle, \tag{2}$$

respectively

$$\alpha(\lambda)=\int \overline{\Psi_\lambda(x)}\,f(x)\,dx=\langle \Psi_\lambda, f\rangle. \tag{3}$$

Let a quantum mechanical system be in the normalized state f; measuring the observable quantity which is represented by H, we have the probability $|\alpha_n|^2$ to find the value $a(n)$ and the probability density to find $a(\lambda)$ in the continuous spectrum is $|\alpha(\lambda)|^2$.

b) Let for example $H=-\Delta+V$ be a one-body Hamiltonian (i.e. $V(x)\to 0$ for $|x|\to\infty$). We expect the Ψ_λ to be bounded or at most slowly increasing (plane waves for $V=0$). On the other hand, for values $E\notin\sigma(H)$ the solutions Ψ of $(-\Delta+V)\Psi=E\Psi$ should grow fast (exponentially) at infinity. These conjectures can be summarized to

$$\sigma(H)=\{E\colon \text{there is an at most slowly increasing solution of } (-\Delta+V)\Psi=E\Psi\}. \tag{4}$$

1.2. Approach to a Mathematical Treatment

If the operator H has an orthonormal basis of eigenfunctions, i.e. the spectrum is pure point, the assertion in a) is correct; in this case the integral term in (1) vanishes. Now let H be an arbitrary selfadjoint operator in a Hilbert space $\mathscr{H}$ and $E(\cdot)$ its spectral resolution. For every $f \in \mathscr{H}$ we have

$$f = \int_{\sigma(H)} dE(\lambda) f. \tag{5}$$

Suppose that the ($B(\mathscr{H})$-valued) function $\lambda \mapsto E(\lambda)$ is differentiable in some sense with derivative $E'(\lambda)$; then formally (5) becomes

$$f = \int_{\sigma(H)} E'(\lambda) f \, d\lambda \quad \text{where} \quad HE'(\lambda) f = \lambda E'(\lambda) f, \tag{6}$$

i.e. f can be expanded in the "generalized eigenfunctions" $E'(\lambda) f$ of H.

This idea has been developed rigorously in [B] for abstract selfadjoint operators and in [S], Chap. C5 for Schrödinger operators.

In this paper we will use another (more direct) approach to expansions in eigenfunctions; in the case of ordinary differential operators this method was used in [W 2], Theorem 8.4.

Our approach is motivated by the following example: Consider the momentum operator $p = -i d/dx$ in $L_2(\mathbb{R})$; the inverse Fourier transform is an expansion for p in the sense of a):

$$f(x) = \operatorname*{l.i.m.}_{N \to \infty} \int_{-N}^{N} \hat{f}(\lambda) e_\lambda(x) \, d\lambda \qquad \text{for all } f \in L_2(\mathbb{R}), \tag{7}$$

where $e_\lambda(x) = (2\pi)^{-1/2} e^{i\lambda x}$, $-i \dfrac{d}{dx} e_\lambda = \lambda e_\lambda$ and

$$\hat{f}(\lambda) = \operatorname*{l.i.m.}_{N \to \infty} \int_{-N}^{N} \overline{e_\lambda(x)} f(x) \, dx. \tag{8}$$

The Fourier transform is a spectral representation for p.

Actually, every selfadjoint operator H possesses a spectral representation

$$U = (U_j) \colon \mathscr{H} \to \bigoplus_j L_2(\mathbb{R}, d\rho_j), \qquad f \mapsto (U_j f)$$

([W 1], Theorem 7.18). It should be possible to write this representation in a form similar to (8), i.e.

$$(U_j f)(\lambda) = \langle \varphi_j(\lambda), f \rangle \qquad \text{for suitable } f \text{ and all } j. \tag{9}$$

Inserting a Hilbert-Schmidt operator $A \in B(\mathscr{H})$, we get

$$(U_j A g)(\lambda) = \langle u_j(\lambda), g \rangle \qquad \text{for all } g \in \mathscr{H} \tag{10}$$

([W 1], Th. 6.12). If A is invertible we get formally

$$(U_j f)(\lambda) = \langle (A^{-1})^* u_j(\lambda), f\rangle \quad \text{for all } f \in D(A^{-1}) \tag{11}$$

which is the desired result.

In general the $(A^{-1})^* u_j(\lambda)$ will not be elements of $\mathscr{H}$, and therefore the meaning of the right hand side of (11) needs some explanation.

In Sect. 2 we introduce the generalized inner product which will be used to justify (11); then we construct a special form of the spectral representation reflecting the spectral multiplicities of the operator.

Our eigenfunction expansion for selfadjoint operators H is formulated as Theorem 1 in Sect. 3. There we use $A = \gamma(H) T^{-1}$, where T is selfadjoint, $T \geqq 1$ and γ is continuous and bounded with $|\gamma| > 0$ on $\sigma(H)$. Our result coincides with those of [B] and [S]. However, our method of proof seems to be new and it has essentially two advantages: it leads more directly to the expansions and it allows to prove Theorem 2 which shows some additional properties of the generalized eigenfunctions.

Section 4 deals with applications to Schrödinger operators $H = -\Delta + V$ in $L_2(\mathbb{R}^m)$. The aim of this section is merely to give some examples for realizing the assumptions of our theorems in concrete cases and to give a concrete form of our abstract expansion. More general results can be found in [S]; see also the literature cited there. As an application of Theorem 2 we get the weak differentiability of the generalized eigenfunctions without using any results on the regularity of weak solutions of the Schrödinger equation. Applications to more general Schrödinger operators than those studied in [S] will be presented in [St].

In addition to the cited results on spectral representations, we use some basic facts from the theory of the Bochner-integral without further reference (cf. [HP], Ch. III.1).

2. Preliminaries

Let $(\mathscr{H}, \langle \cdot, \cdot \rangle)$ be a separable Hilbert space, T a selfadjoint operator in $\mathscr{H}$ with $T \geqq 1$. With the scalar product $\langle u, v\rangle_+ := \langle Tu, Tv\rangle$, $D(T)$ is a Hilbert space which will be denoted by $\mathscr{H}_+(T)$. We have $T^{-1} > 0$ so that $\langle f, g\rangle_- := \langle T^{-1} f, T^{-1} g\rangle$ defines a scalar product on $\mathscr{H}$. For the completion of $(\mathscr{H}, \langle \cdot, \cdot \rangle_-)$ we will write $\mathscr{H}_-(T)$. The triple $\mathscr{H}_+(T) \subset \mathscr{H} \subset \mathscr{H}_-(T)$ is called the *T-triple of* $\mathscr{H}$.

Lemma 1. *a) Let* $u \in \mathscr{H}_+(T), f \in \mathscr{H}_-(T)$; *for every sequence* $(f_n) \subset \mathscr{H}$ *with* $\|f_n - f\|_- \to 0$ *the limit* $\langle f, u\rangle := \lim \langle f_n, u\rangle$ *exists and it is independent of the choice of the sequence.*

b) Let $\hat{T}$ *be* T *considered as an operator with values in* $\mathscr{H}_-(T)$; *the closure* $\tilde{T}$ *of* $\hat{T}$ *is an isometric operator from* $\mathscr{H}$ *into* $\mathscr{H}_-(T)$.

c) For $u \in \mathscr{H}_+(T)$ *and* $f \in \mathscr{H}$ *we have* $\langle \tilde{T} f, u\rangle = \langle f, Tu\rangle$.

Proof. a) From

$$|\langle f_n - f_m, u\rangle| = |\langle T T^{-1}(f_n - f_m), u\rangle| = |\langle T^{-1}(f_n - f_m), Tu\rangle| \leqq \|f_n - f_m\|_- \, \|Tu\|$$

it follows that $(\langle f_n, u\rangle)$ is a Cauchy-sequence, hence it is convergent. The independence of the choice of the sequence can be shown by mixing two such sequences.

b) We have $\|\hat{T}u\|_- = \|Tu\|_- = \|T^{-1}Tu\| = \|u\|$ so that $\hat{T}$ is isometric and densely defined. Hence $\hat{T}$ has an isometric closure $\tilde{T} \in B(\mathscr{H}, \mathscr{H}_-(T))$.

c) Choose a sequence $(f_n) \subset \mathscr{H}_+(T)$ with $\|f_n - f\| \to 0$; consequently $\|\tilde{T}f_n - \tilde{T}f\|_- \to 0$. We conclude

$$\langle f, Tu\rangle = \lim \langle f_n, Tu\rangle = \lim \langle Tf_n, u\rangle = \lim \langle \tilde{T}f_n, u\rangle = \langle \tilde{T}f, u\rangle$$

where we use part a) for the last equality. □

Let H be a selfadjoint operator in $\mathscr{H}$ with spectral resolution $E(\cdot)$. A Borel measure ρ on $\mathbb{R}$ is called a *spectral measure of H* (cf. [S], p. 501) provided that for Borel sets Δ the following equivalence holds:

$$\rho(\Delta) = 0 \Leftrightarrow E(\Delta) = 0. \tag{12}$$

Let U be a unitary operator of the form

$$U = (U_j)\colon \mathscr{H} \to \bigoplus_{j=1}^{N} L_2(\mathbb{R}, d\rho_j), \qquad Uf = (U_j f)_{j=1,2,\ldots,N} \quad (N \in \mathbb{N} \cup \{\infty\}) \tag{13}$$

with bounded Borel measures ρ_j which are different from zero. U is called a *spectral representation of H* if $UHU^{-1} = M_{\mathrm{id}}$. For every selfadjoint operator there exists a spectral representation. In fact it is possible to chose the ρ_j such that ρ_{j+1} is absolutely continuous with respect to ρ_j for $j = 1, 2, \ldots$; in this case U is called an *ordered* spectral representation of H (cf. [W 2], Theorem 8.1).

The *spectral multiplicity of H* is the least number of elements $u_1, \ldots, u_i \in \mathscr{H}$ for which the span of $\{E(t)u_k\colon k = 1, \ldots, i;\ t \in \mathbb{R}\}$ is dense in $\mathscr{H}$. For an E-measurable set $M \subset \mathbb{R}$ (i.e., M is measurable with respect to the measure $d\|E(\cdot)f\|^2$ for every $f \in \mathscr{H}$) we define the *spectral multiplicity of H on M* as the spectral multiplicity of $H|_{R(E(M))}$.

Lemma 2. *a) Any two spectral measures ρ and μ of H are mutually absolutely continuous.*

b) For every selfadjoint operator H there exists a spectral measure.

c) For every spectral measure μ of H there exists a spectral representation of H of the form

$$U = (U_j)\colon \mathscr{H} \to \bigoplus_{j=1}^{N} L_2(\mathbb{R}, \chi_{M_j} d\mu) = \bigoplus_{j=1}^{N} L_2(M_j, d\mu), \tag{14}$$

where the sets M_j are μ-measurable with $M_{j+1} \subset M_j (j = 1, \ldots, N-1)$. The M_j are uniquely determined (up to μ-nullsets) and independent of the spectral measure μ.

d) If $\mu(M_j \setminus M_{j+1}) > 0$ then H has spectral multiplicity j on $M_j \setminus M_{j+1}$ for $j = 0, 1, \ldots$ (here $M_0 := \mathbb{R}$).

Proof. a) is clear from the definition.

b) Consider an ordered spectral representation

$$V=(V_j)\colon \mathscr{H}\to \bigoplus_{j=1}^{N} L_2(\mathbb{R}, d\rho_j)$$

of H. ρ_j is absolutely continuous with respect to $\rho:=\rho_1$ $(j=1,2,\ldots)$; therefore we have $d\rho_j=h_j d\rho$ with $h_j\in L_{1,\mathrm{loc}}(\mathbb{R}, d\rho)$ and $h_j\geqq 0$ $(\rho-\text{a.e.})$.

ρ is a spectral measure of H: Using

$$\int_\Delta d\|E(\lambda)f\|^2=\int_\Delta d\|VE(\lambda)V^{-1}Vf\|^2=\sum_{j=1}^{N}\int_\Delta |V_j f)(\lambda)|^2 d\rho_j(\lambda)$$

we conclude

$$\begin{aligned} E(\Delta)=0 &\Leftrightarrow \{\int_\Delta d\|E(\lambda)f\|^2=0\ \forall f\in\mathscr{H}\}\\ &\Leftrightarrow \left\{\sum_{j=1}^{N}\int_\Delta |g_j|^2 d\rho_j=0\ \forall g=(g_1,g_2,\ldots)\in\bigoplus_j L_2(\mathbb{R}, d\rho_j)\right\}\\ &\Leftrightarrow \{\rho_j(\Delta)=0\ \forall j\}\Leftrightarrow \rho(\Delta)=0.\end{aligned}$$

c) First, we construct a spectral representation of the desired form for the spectral measure which we have found in b):

For every h_j we choose some representative with $h_j(\lambda)\geqq 0$ for all $\lambda\in\mathbb{R}$ and set $M_j:=\{\lambda\in\mathbb{R}\colon h_j(\lambda)>0\}$; M_j is measurable. The absolute continuity of ρ_{j+1} with respect to ρ_j yields $M_{j+1}\subset M_j$ (where we change the M_j by ρ-nullsets if necessary).

Then the map $\tilde U_j\colon L_2(\mathbb{R}, d\rho_j)\to L_2(M_j, d\rho)$, $\tilde U_j g:=h_j^{1/2}g$ is unitary; we have $\tilde U_j M_{\mathrm{id}}\tilde U_j^{-1}=M_{\mathrm{id}}$ (the M_{id} on the left hand side is in $L_2(\mathbb{R}, d\rho_j)$, the other one in $L_2(M_j, d\rho)$).

Let $U'_j:=\tilde U_j V_j\colon \mathscr{H}\to L_2(M_j, d\rho)$; then $U':=(U'_j)\colon \mathscr{H}\to\bigoplus_j L_2(M_j, d\rho)$ is a spectral representation of the desired form.

For an arbitrary spectral measure μ of H we have $d\mu=h\,d\rho$ with $h\neq 0$ (ρ-a.e.). $W_j\colon L_2(M_j, d\rho)\to L_2(M_j, d\mu)$, $W_j g:=h^{-1/2}g$ is unitary; taking $U_j:=W_j U'_j$, the map $U=(U_j)$ has all the properties stated in c).

The uniqueness of the M_j and their independence of the spectral measure μ are consequences of part d) which we will prove now.

d) Without loss of generality we may assume that $\mu(\mathbb{R})<\infty$ (if necessary, multiply μ with a suitable weightfunction).

$H|_{R(E(M_j\setminus M_{j+1}))}$ is unitary equivalent to M_{id} on $\mathscr{H}_j:=\bigoplus_{k=1}^{j} L_2(M_j\setminus M_{j+1}, d\mu)$ $=L_2(M_j\setminus M_{j+1})^j$, therefore the two operators have the same spectral multiplicity. For the latter one, the spectral multiplicity is equal to j:

Define $h_1,\ldots,h_j\in\mathscr{H}_j$, $h_k=(h_{k,n})_{n=1}^{j}$ by $h_{k,k}=1$ and $h_{k,n}=0$ for $k\neq n$; then the span of $\{\chi_{(-\infty,t]}h_k\colon t\in\mathbb{R};\ k=1,\ldots,j\}$ is dense in $\mathscr{H}_j$. On the other hand $\{h_k\colon k=1,\ldots,j\}$ is a minimal system. To prove this, let $f_1,\ldots,f_i\in\mathscr{H}_j$ with $i<j$. For

$\lambda \in M_j \setminus M_{j+1}$ let $P(\lambda) \neq 0$ be the orthogonal projection on span$\{f_1(\lambda), \ldots, f_i(\lambda)\}^{\perp}$ in $\mathbb{C}^j$. $P(\cdot)$ is measurable, and $(Pf)(\lambda) := P(\lambda) f(\lambda)$ defines an orthogonal projection P in $\mathscr{H}_j$. There exists an $m \in \{1, \ldots, j\}$ with $P h_m \neq 0$; otherwise we would have $P(\lambda) = 0$ for μ-a.e. λ. Since by construction of P we have $\langle P h_m, \chi_{(-\infty, t]} f_k \rangle = 0$ for all $t \in \mathbb{R}$ and $k = 1, \ldots, i$, the span of $\{\chi_{(-\infty, t]} f_k : t \in \mathbb{R}; k = 1, \ldots, i\}$ is not dense.

This proves d), from which the independence of the M_j of the spectral measure follows. □

A spectral representation of the form (14) is called a *μ-spectral representation of H.*

3. The Expansion Theorem

Theorem 1. *Let $\mathscr{H}_+(T) \subset \mathscr{H} \subset \mathscr{H}_-(T)$ be a T-triple and H a selfadjoint operator in $\mathscr{H}$. Let μ be a spectral measure for H, U a μ-spectral representation of H and $\mathscr{E} := \{f \in \mathscr{H}_+(T) \cap D(T) : Hf \in \mathscr{H}_+(T)\}$. Suppose there is a bounded continuous function $\gamma: \mathbb{R} \to \mathbb{C}$ with $|\gamma| > 0$ on $\sigma(H)$ such that $\gamma(H) T^{-1}$ is a Hilbert-Schmidt operator. Then there exist μ-measurable functions $\varphi_j: M_j \to \mathscr{H}_-(T)$, $j = 1, 2, \ldots$, such that*

a) $(U_j f)(\lambda) = \langle \varphi_j(\lambda), f \rangle$ for $f \in \mathscr{H}_+(T)$ and μ-a.e. $\lambda \in M_j$.
b) $\langle \varphi_j(\lambda), Hf \rangle = \lambda \langle \varphi_j(\lambda), f \rangle$ for $f \in \mathscr{E}$ and μ-a.e. $\lambda \in M_j$.
c) For every $g = (g_j) \in \bigoplus_j L_2(M_j, d\mu)$ we have

$$U^{-1} g = \lim_{\substack{n \to N \\ E \to \infty}} \sum_{j=1}^{n} \int_{\{|\lambda| \leq E\} \cap M_j} g_j(\lambda) \varphi_j(\lambda) \, d\mu(\lambda), \tag{15}$$

and therefore for every $f \in \mathscr{H}$

$$f = \lim_{\substack{n \to N \\ E \to \infty}} \sum_{j=1}^{n} \int_{\{|\lambda| \leq E\} \cap M_j} (U_j f)(\lambda) \varphi_j(\lambda) \, d\mu(\lambda). \tag{16}$$

The limit is taken in $\mathscr{H}$; the integrals $\int_{\{|\lambda| \leq E\} \cap M_j} (U_j f)(\lambda) \varphi_j(\lambda) \, d\mu(\lambda)$ represent elements of $\mathscr{H}$, although the $\varphi_j(\lambda)$ are contained in $\mathscr{H}_-(T)$ only.

Remarks. (i) Because of b), the $\varphi_j(\lambda)$ are called *generalized eigenfunctions* corresponding to λ, but this notion makes sense only if $\mathscr{E}$ is a core for H; then (16) is the *eigenfunction expansion.* (15) is a generalization of the Fourier inversion formula.

(ii) Theorem 1 holds similarly for an arbitrary spectral representation of H. We have chosen a special U to emphasize the connection between the spectral multiplicity and the eigenfunction expansion.

(iii) One can always find an operator T of the desired form such that $\gamma(H) T^{-1}$ is a Hilbert-Schmidt operator: Choose for T^{-1} a selfadjoint injective

Hilbert-Schmidt operator with $0 < T^{-1} \leqq 1$. For a bounded function γ, the operator $\gamma(H)$ is bounded and therefore $\gamma(H)T^{-1}$ is a Hilbert-Schmidt operator, too.

(iv) On the other hand, if $\gamma(H)T^{-1}$ is a Hilbert-Schmidt operator for *every* selfadjoint operator H then T^{-1} itself must be a Hilbert-Schmidt operator: Take a bounded selfadjoint operator H, then $\gamma(H)^{-1}$ is bounded and therefore $T^{-1} = \gamma(H)^{-1}(\gamma(H)T^{-1})$ is a Hilbert-Schmidt operator.

In our applications to Schrödinger operators we will only have the product $\gamma(H)T^{-1}$ to be a Hilbert-Schmidt operator, i.e. we will make use of some properties of H. This will yield a connection between properties of H and the form of its generalized eigenfunctions.

Proof of Theorem 1. For continuous functions $\gamma: \mathbb{R} \to \mathbb{C}$ we have ([W 1], Theorem 7.15)

$$U\gamma(H)U^{-1} = M_\gamma.$$

For every j, $M_\gamma U_j T^{-1} = U_j \gamma(H) T^{-1}$ is a Hilbert-Schmidt operator from $\mathscr{H}$ into $L_2(M_j, d\mu)$ (since U_j is bounded and $\gamma(H)T^{-1}$ is Hilbert-Schmidt). Therefore by [W 1], Theorem 6.12 there exists a measurable function $u_j(\cdot)$: $M_j \to \mathscr{H}$, $\|u_j(\cdot)\| \in L_2(M_j, d\mu)$, satisfying

$$\gamma(\lambda)(U_j T^{-1} g)(\lambda) = (M_\gamma U_j T^{-1} g)(\lambda) = \langle u_j(\lambda), g\rangle \quad \text{for } g \in \mathscr{H}, \mu\text{-a.e. } \lambda \in M_j.$$

Setting $w_j(\lambda) := \gamma(\lambda)^{-1} u_j(\lambda)$ we get

$$(U_j T^{-1} g)(\lambda) = \langle w_j(\lambda), g\rangle \quad \text{for } g \in \mathscr{H} \quad \text{and} \quad \mu\text{-a.e. } \lambda \in M_j.$$

Then $\varphi_j(\lambda) := \tilde{T} w_j(\lambda) \in \mathscr{H}_-(T)$ are the desired functions: For $f \in \mathscr{H}_+(T)$ and μ-a.e. $\lambda \in M_j$ we conclude

$$(U_j f)(\lambda) = (U_j T^{-1})(Tf)(\lambda) = \langle w_j(\lambda), Tf\rangle = \langle \tilde{T} w_j(\lambda), f\rangle = \langle \varphi_j(\lambda), f\rangle.$$

The function φ_j: $M_j \to \mathscr{H}_-(T)$ is measurable since u_j: $M_j \to \mathscr{H}$ is measurable, $1/\gamma$ is continuous and $\tilde{T}$: $\mathscr{H} \to \mathscr{H}_-(T)$ is bounded.

b) From part a) it follows for $f \in \mathscr{E}$ and μ-a.e. $\lambda \in M_j$

$$\begin{aligned}\langle \varphi_j(\lambda), Hf\rangle &= \langle \tilde{T} w_j(\lambda), Hf\rangle = \langle w_j(\lambda), THf\rangle = (U_j T^{-1})(THf)(\lambda)\\ &= (U_j Hf)(\lambda) = \lambda(U_j f)(\lambda) = \lambda\langle \varphi_j(\lambda), f\rangle.\end{aligned}$$

c) First we show that

$$w_j(\cdot) \in L_{2,\mathrm{loc}}(M_j, d\mu; \mathscr{H}) \quad \text{and} \quad \varphi_j(\cdot) \in L_{2,\mathrm{loc}}(M_j, d\mu; \mathscr{H}_-(T)):$$

We know already that $w_j(\cdot)$ and $\varphi_j(\cdot)$ are measurable. From $1/\gamma \in L_{\infty,\mathrm{loc}}(\mathbb{R})$ and $\|u_j(\cdot)\| \in L_2(M_j, d\mu)$ it follows that $\|w_j(\cdot)\| = |\gamma(\cdot)|^{-1} \|u_j(\cdot)\| \in L_{2,\mathrm{loc}}(M_j, d\mu)$, $j = 1, \ldots, N$. The statement for $\varphi_j(\cdot)$ now follows from

$$\|\varphi_j(\cdot)\|_- = \|\tilde{T} w_j(\cdot)\|_- \leqq \|\tilde{T}\| \, \|w_j(\cdot)\|.$$

Now let $v \in \mathscr{H}_+(T)$, $g=(g_j) \in \bigoplus_j L_2(M_j, d\mu)$ with $g_j = 0$ for $j > j_0$ and $g_j(\lambda)=0$ for $|\lambda| > R, j=1, \ldots, j_0$. We have

$$\langle U^{-1}g, v\rangle = \langle g, Uv\rangle = \sum_{j=1}^{j_0} \int_{M_j} \overline{g_j(\lambda)}(U_j v)(\lambda)\, d\mu(\lambda) = \sum_{j=1}^{j_0} \int_{M_j} \overline{g_j(\lambda)} \langle \varphi_j(\lambda), v\rangle\, d\mu(\lambda)$$

$$= \sum_{j=1}^{j_0} \int_{M_j} \overline{g_j(\lambda)} \langle w_j(\lambda), Tv\rangle\, d\mu(\lambda) = \left\langle \sum_{j=1}^{j_0} \int_{M_j} g_j(\lambda)\, w_j(\lambda)\, d\mu(\lambda), Tv \right\rangle$$

(where we have used that $g_j(\cdot)\, w_j(\cdot)$ is Bochner-integrable)

$$= \left\langle \tilde{T} \sum_{j=1}^{j_0} \int_{M_j} g_j(\lambda)\, w_j(\lambda)\, d\mu(\lambda), v \right\rangle = \left\langle \sum_{j=1}^{j_0} \int_{M_j} g_j(\lambda)\, \varphi_j(\lambda)\, d\mu(\lambda), v \right\rangle.$$

Since $\mathscr{H}_+(T)$ is dense in $\mathscr{H}$ this implies

$$U^{-1} g = \sum_{j=1}^{j_0} \int_{M_j} g_j(\lambda)\, \varphi_j(\lambda)\, d\mu(\lambda),$$

and the integrals on the right hand side represent elements of $\mathscr{H}$. Part c) of the theorem follows by a limiting argument. □

With an additional assumption, we get more information about the generalized eigenfunctions:

Theorem 2. *In addition to the assumptions of Theorem 1, let S be an injective operator in $\mathscr{H}$ such that $S^{-1} \in B(\mathscr{H})$ and $\gamma(H)\, T^{-1} S$ is the restriction of a Hilbert-Schmidt operator to $D(S)$. Then the generalized eigenfunctions $\varphi_j(\lambda)$ lie in the range of $\tilde{T}(S^{-1})^*$.*

Proof. Using the argument in the proof of Theorem 1, we get the existence of functions $\tilde{u}_j(\cdot)\colon M_j \to \mathscr{H}$ with $\|\tilde{u}_j(\cdot)\| \in L_2(M_j, d\mu)$ and

$$\gamma(\lambda)(U_j T^{-1} S g)(\lambda) = \langle \tilde{u}_j(\lambda), g\rangle \quad \text{for } g \in D(S).$$

With $\tilde{w}_j(\lambda) = \gamma(\lambda)^{-1} \tilde{u}_j(\lambda)$ and $\varphi_j(\cdot)$ from Theorem 1 we have for $f \in \mathscr{H}_+(T)$

$$\langle \varphi_j(\lambda), f\rangle = (U_j f)(\lambda) = (U_j T^{-1} S)(S^{-1} Tf)(\lambda) = \langle \tilde{w}_j(\lambda), S^{-1} Tf\rangle$$
$$= \langle (S^{-1})^* \tilde{w}_j(\lambda), Tf\rangle = \langle \tilde{T}(S^{-1})^* \tilde{w}_j(\lambda), f\rangle,$$

i.e. $\varphi_j(\lambda) = \tilde{T}(S^{-1})^* \tilde{w}_j(\lambda)$. □

4. Applications to Schrödinger Operators

We define $k_z\colon \mathbb{R}^m \to \mathbb{R}$ by $k_z(x) := (1+|x|^2)^{z/2}$ for $z \in \mathbb{C}$ and

$$L_{2,s}(\mathbb{R}^m) := \{f\colon \mathbb{R}^m \to \mathbb{C} \text{ with } k_s f \in L_2(\mathbb{R}^m)\} \quad \text{for } s \in \mathbb{R}.$$

In our applications, T will be the multiplication by $k_s (s>0)$. With $\mathscr{H}=L_2(\mathbb{R}^m)$ this yields $\mathscr{H}_+(T)=L_{2,s}(\mathbb{R}^m)$ and $\mathscr{H}_-(T)=L_{2,-s}(\mathbb{R}^m)$. In this case the generalized scalar product for $f\in L_{2,-s}(\mathbb{R}^m)$ and $u\in L_{2,s}(\mathbb{R}^m)$ (see Lemma 1) is of the form $\langle f, u\rangle=\int\overline{f(x)}\,u(x)\,dx$. By $B_2(L_2(\mathbb{R}^m))$ we denote the set of Hilbert-Schmidt operators in $L_2(\mathbb{R}^m)$.

The following lemma verifies the assumptions of Theorem 1.

Lemma 3. Let $m\leqq 3$, $V\colon \mathbb{R}^m\to\mathbb{R}$ Δ-bounded with relative bound less than 1, $H:=-\Delta+V$ in $L_2(\mathbb{R}^m)$ and $s>m/2$. Then $(H-z)^{-1}k_{-s}\in B_2(L_2(\mathbb{R}^m))$ for every $z\in\rho(H)$.

Proof. We have

$$(-\Delta+1)^{-1}k_{-s}\in B_2(L_2(\mathbb{R}^m)): \tag{17}$$

For $m\leqq 3$, $g(x)=(|x|^2+1)^{-1}\in L_2(\mathbb{R}^m)$ and therefore the convolution theorem for L_2-functions yields

$$\begin{aligned}((-\Delta+1)^{-1}k_{-s}f)(x)&=F^{-1}(gF(k_{-s}f))(x)=(h*(k_{-s}f))(x)\\&=\int h(x-y)\,k_{-s}(y)\,f(y)\,dy,\end{aligned}$$

where $h=F^{-1}g\in L_2(\mathbb{R}^m)$; thus $(-\Delta+1)^{-1}k_{-s}$ has the integral kernel $t(x,y)=h(x-y)\,k_{-s}(y)$. Since $t(\cdot,\cdot)$ lies in $L_2(\mathbb{R}^m\times\mathbb{R}^m, dx\times dy)$, $(-\Delta+1)^{-1}k_{-s}$ is a Hilbert-Schmidt operator. Now the lemma follows from the second resolvent identity:

$$(H-z)^{-1}k_{-s}=(-\Delta+1)^{-1}k_{-s}-(H-z)^{-1}(V-z+1)(-\Delta+1)^{-1}k_{-s}.$$

The first term on the right hand side is Hilbert-Schmidt by (17), the second is a product of a bounded operator and a Hilbert-Schmidt operator. □

By $k_z(p)$ we denote the Fourier transform of the multiplication by $k_z(\cdot)$, i.e. $k_z(p):=F^{-1}k_zF$; we will use Theorem 2 with $S=k_1(p)$ to prove regularity properties of the generalized eigenfunctions.

Lemma 4. *Let V and H be as in Lemma 3 and $\mu\in\rho(H)$; then $\overline{k_1(p)(H-\mu)^{-1}k_1(p)}$ is bounded.*

Proof. Let $f, g\in C_0^\infty(\mathbb{R}^m)$; for $0\leqq \operatorname{Re} z\leqq 1$ we use the abbreviation

$$F_{f,g}(z):=\langle f, k_{2z}(p)(H-\mu)^{-1}k_{2-2z}(p)g\rangle=\langle k_{2\bar{z}}(p)f, (H-\mu)^{-1}k_{2-2z}(p)g\rangle.$$

$F_{f,g}$ is analytic in $\{z: 0<\operatorname{Re} z<1\}$ and continuous on the closure of this strip, since the maps $z\mapsto k_{2\bar{z}}(p)f$ and $z\mapsto k_{2-2z}(p)g$ have these properties. Using

$$k_2(p)(H-\mu)^{-1}=(-\Delta+1)(H-\mu)^{-1}=(H+1)(H-\mu)^{-1}-V(H-\mu)^{-1}$$

and taking adjoints we see that $k_2(p)(H-\mu)^{-1}$ and $\overline{(H-\mu)^{-1}k_2(p)}$ are bounded. We have

$$|F_{f,g}(z)| \leqq \|f\| \, \|(H-\mu)^{-1}k_2(p)\| \, \|g\| = C\|f\| \, \|g\| \quad \text{for } \operatorname{Re} z = 0,$$

and

$$|F_{f,g}(z)| \leqq \|f\| \, \|k_2(p)(H-\mu)^{-1}\| \, \|g\| = C\|f\| \, \|g\| \quad \text{for } \operatorname{Re} z = 1.$$

Now Hadamard's Three-Line-Theorem ([RS II], appendix to IX.4) yields for $0 \leqq \operatorname{Re} z \leqq 1$

$$|F_{f,g}(z)| \leqq \|f\| \, \|g\| \, \|(H-\mu)^{-1}k_2(p)\|^{1-\operatorname{Re} z} \|k_2(p)(H-\mu)^{-1}\|^{\operatorname{Re} z} = C\|f\| \, \|g\|.$$

The boundedness of $k_{2z}(p)(H-\mu)^{-1}k_{2-2z}(p)$ follows from

$$\|k_{2z}(p)(H-\mu)^{-1}k_{2-2z}(p)\| = \sup\{|F_{f,g}(z)| : f, g \in C_0^\infty(\mathbb{R}^m), \|f\| = \|g\| = 1\} \leqq C;$$

taking $z = 1/2$ yields the lemma. □

Now we are in the position to verify the assumptions of Theorem 2 for the Schrödinger operator of Lemma 3.

Lemma 5. *Under the assumptions of Lemma 3, let $z \in \rho(H)$ and $s > m/2$; then we have*

$$\overline{(H-z)^{-2}k_{-s}k_1(p)} \in B_2(L_2(\mathbb{R}^m)).$$

Proof. Restricted to $C_0^\infty(\mathbb{R}^m)$, the following equality holds:

$$\begin{aligned}(H-z)^{-2}k_{-s}k_1(p) &= (H-z)^{-1}k_{-s}(H-z)^{-1}k_1(p) \\ &\quad + (H-z)^{-1}[(H-z)^{-1}, k_{-s}]\,k_1(p).\end{aligned}$$

The first term on the right hand side is (the restriction of) a Hilbert-Schmidt operator. Next we calculate the commutator in the second term and get

$$\begin{aligned}[(H-z)^{-1}, k_{-s}] &= (H-z)^{-1}[\Delta, k_{-s}](H-z)^{-1} \\ &= (H-z)^{-1}\{(\Delta k_{-s}) + 2\langle(\operatorname{grad} k_{-s}), \operatorname{grad}\rangle\}(H-z)^{-1}.\end{aligned}$$

Thus it suffices to show that

$$(H-z)^{-2}(\Delta k_{-s})(H-z)^{-1}k_1(p) + 2(H-z)^{-2}\langle(\operatorname{grad} k_{-s}), \operatorname{grad}\rangle(H-z)^{-1}k_1(p) \quad (18)$$

is a Hilbert-Schmidt operator. Following the argument in the proof of Lemma 3 and using $|\Delta k_{-s}| \leqq c k_{-s-2}$, we see that the first term in (18) is Hilbert-Schmidt. For the second term we examine $(H-z)^{-1}(\partial_j k_{-s})\partial_j(H-z)^{-1}k_1(p)$ $(j = 1, \ldots, m)$. These operators are in $B_2(L_2(\mathbb{R}^m))$ since by $|\partial_j k_{-s}| \leqq c k_{-s}$ this is true for $(H-z)^{-1}(\partial_j k_{-s})$ and $\partial_j(H-z)^{-1}k_1(p) = \partial_j k_{-1}(p)\,k_1(p)(H-z)^{-1}k_1(p)$ is bounded by Lemma 4. □

Now we can formulate the following theorem on the expansion in generalized eigenfunctions of Schrödinger operators:

Theorem 3. *Let $m \leqq 3$, $V: \mathbb{R}^m \to \mathbb{R}$ uniformly locally in $L_2(\mathbb{R}^m)$, and $H := -\Delta + V$ in $L_2(\mathbb{R}^m)$; let μ be a spectral measure of H, U a μ-spectral representation of H, and $s > m/2$. Then there exist μ-measurable functions φ_j: $M_j \to L_{2,-s}(\mathbb{R}^m) \cap W_{2,1,\mathrm{lok}}(\mathbb{R}^m)$, with:*

a) $(U_j f)(\lambda) = \operatorname*{l.i.m.}_{R\to\infty} \int_{|x|\leqq R} \overline{\varphi_j(\lambda, x)} f(x)\,dx,\ f \in L_2(\mathbb{R}^m)$.

b) *$\varphi_j(\lambda, \cdot)$ is a weak solution of $H\varphi = \lambda\varphi$ (for μ-a.e. $\lambda \in M_j$).*

c) *For $f \in L_2(\mathbb{R}^m)$ we have*

$$f(x) = \operatorname*{l.i.m.}_{n\to N, E\to\infty} \sum_{j=1}^{n} \int_{\{|\lambda|\leqq E\}\cap M_j} (U_j f)(\lambda)\,\varphi_j(\lambda, x)\,d\mu(\lambda).$$

d) *For μ-measurable sets $I \subset \mathbb{R}$ and for $f \in L_2(\mathbb{R}^m)$ we have*

$$\langle f, \chi_I(H) f\rangle = \sum_{j=1}^{N} \int_{M_j \cap I} |U_j f(\lambda)|^2\,d\mu(\lambda).$$

Proof. V is Δ-bounded with relative bound zero ([RSIV], Theorem XIII.96) so that the Lemmas 3, 4 and 5 are applicable. Using Lemma 5 we see that the assumptions of Theorem 2 are fulfilled with $\gamma(\lambda) = (\lambda - z)^{-2}$ for a $z \in \rho(H)$ and $S = k_1(p)$. Therefore Theorem 1 is applicable with functions $\varphi_j(\lambda, \cdot) \in k_s W_{2,1}(\mathbb{R}^m) \subset L_{2,-s}(\mathbb{R}^m) \cap W_{2,1,\mathrm{lok}}(\mathbb{R}^m)$. a) and c) follow immediately. Part b) follows from Theorem 1.b) since we can check easily $C_0^\infty(\mathbb{R}^m) \subset \mathscr{E}$. Part d) follows from

$$\langle f, \chi_I(H) f\rangle = \|\chi_I(H) f\|^2 = \|U \chi_I(H) f\|^2 = \|M_{\chi_I} U f\|^2. \quad \square$$

Remarks. (i) All statements of Theorem 3 except $\varphi_j(\lambda, \cdot) \in W_{2,1,\mathrm{lok}}(\mathbb{R}^m)$ are already consequences of Theorem 1 and Lemma 3.

(ii) Theorem 3 is the mathematical version of the fundamental assertion in quantum mechanics which was formulated in Sect. 1.1.a), when the observable is chosen to be the energy: Part c) corresponds to Eq. (1), part b) expresses the fact that the functions $\varphi_j(\lambda, \cdot)$ are generalized eigenfunctions, and part a) corresponds to the Eq. (2) and (3). Part d) is just the statement about the probability densities: For a system in the state f the probability to measure an energy value in I is given by $\langle f, \chi_I(H) f\rangle$, i.e. the function $\sum_j |\chi_M U_j f|^2$ is the probability density with respect to μ.

In the case of a typical one-body potential V we have $\sigma_d(H) = \{\lambda_j : j \in \mathbb{N}\}$ with $\lambda_j < 0$ and $\lambda_j \to 0$ for $j \to \infty$, $\sigma_{ac}(H) = [0, \infty)$ and $\sigma_{sc}(H) = \emptyset$, so that we can choose

$$d\mu = \sum_{j=1}^{\infty} \delta_{\lambda_j} + \chi_{[0,\infty)}\,d\lambda$$

as a spectral measure. In this case the expansion in c) has the same form as the corresponding one in Eq. (1), except for the additional sum in front of the integral.

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