SCHRÖDINGER OPERATORS IN THE TWENTIETH CENTURY

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Dedicated to Tosio Kato (1917–1999),
father of the modern theory of Schrödinger operators

Contents

1. Introduction

The twentieth century is the century of science. In a century that has seen special and general relativity, quantum electrodynamics and chromodynamics, a total revamping of our understanding of molecules and of the cosmos, plate tectonics, and the rise of microbiology, one can make the case that the most spectacular scientific development was the discovery of nonrelativistic quantum mechanics in the first quarter of the century. Its aftermath not only changed the physicist's view of matter but it set the stage for the

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revolutions in chemistry, our understanding of stars, biology, and practical electronics.

In what is one of the more striking cases of serendipity, just as Heisenberg and Schrödinger were discovering the "new" quantum theory, von Neumann was developing the theory of unbounded self-adjoint operators and Weyl the representations of compact Lie groups—two subjects of great relevance to the mathematics underlying nonrelativistic quantum mechanics. In short order they produced books (von Neumann [271] and Weyl [275]) that used this mathematics to give a mathematical foundation to the framework of quantum mechanics. With later additions, notably by Bargmann, Wigner, and Mackey, the basic foundations are mathematically firm.

This is analogous to having formulated classical mechanics as Hamiltonian flows on symplectic manifolds. What remains is what might be called the second-level foundations—existence of solutions of the time-dependent Schrödinger equation (which is equivalent to self-adjointness of these operators) and general qualitative issues in dynamics. It is this subject, essentially born fifty years ago, that I will review here. The subject matter is vast with hundreds of contributors and thousands of papers. Each section of this paper is a proxy for what deserves a book or at least a very long review article. In attempting to overview such a vast area in a few pages, I have had to focus on the high points. No proofs are given and I have settled for usually quoting the initial or especially significant papers. I have no doubt that I have left out some important papers, and if so, I ask the forgiveness of the reader (and their authors!).

To keep this paper a reasonable size, I have focused almost entirely on the general basics of Schrödinger operators and some simple applications to atomic and molecular Hamiltonians. That means, among other areas, I haven't considered general second-order operators on $\mathbb{R}^n$ and on general manifolds (but see Davies-Safarov [57], Davies [55], and Kenig [154]) nor have I considered some of the detailed papers on perturbations of Hamiltonians with periodic potential (see, e.g., Deift-Hempel [58] and Gesztesy-Simon [91]) nor the extensive literature on Dirac operators nor the considerable work on Schrödinger operators in a bounded region with some boundary conditions including subtle results on what happens at irregular boundary points (see Davies [55]) nor the results on phenomena like the quantum Hall effect that apply and extend the general theory to results in condensed matter physics. While there are a few results about $-\Delta + V$ for cases where $V(x) \to \infty$ as $|x| \to \infty$, again there is a large literature we won't attempt to review. While Section 10 has a brief discussion of constant magnetic field, we have not attempted to discuss the recent extensive literature on nonconstant magnetic fields.

There is a companion piece to this one on open problems (Simon [260]).

I would like to thank Michael Aizenman, Brian Davies, Percy Deift, Fritz Gesztesy, Dirk Hundertmark, Walter Hunziker, and Rowan Killip for useful input.

2. Mathematical Tools and Issues

The mathematics most relevant to the modern theory of Schrödinger operators is functional, real, harmonic, and complex analysis. In this section, we will briefly set the stage to fix notation. For more details, see Reed-Simon [214, 211].

Quantum Hamiltonians are unbounded operators, defined on a dense subspace rather than the whole Hilbert space. Physics books tend to emphasize the symmetry ("Hermiticity") of the Hamiltonian; that is, that $\langle H\varphi, \psi\rangle = \langle \varphi, H\psi\rangle$ for all φ, ψ in $D(H)$. But more important is a property called self-adjointness. The adjoint H^* of an operator H is defined to be the maximal operator so that $\langle H^*\varphi, \psi\rangle = \langle \varphi, H\psi\rangle$ for all $\psi \in D(H)$, $\varphi \in D(H^*)$. Hermiticity says only that H^* is an extension of H.

We say H is self-adjoint if $H = H^*$, H is called essentially self-adjoint if and only if H is symmetric and has a unique self-adjoint extension. This holds if and only if H^* is self-adjoint. Self-adjointness is important in the first place because if H is self-adjoint, one can form the unitary group e^{-itH} and so solve $i\,\dot\varphi_t = H\varphi_t$ (as $\varphi_t = e^{-itH}\varphi$) for initial conditions $\varphi \in D(H)$. Indeed, Stone's theorem says that any one-parameter continuous unitary group is associated to a self-adjoint operator. Secondly, self-adjointness implies the spectral theorem. There is for each Borel set $A \subset \mathbb{R}$, a projection, $E_A(H)$, so that $H = \int \lambda\, dE_\lambda$ and $e^{-itH} = \int e^{-itH}\, dE_\lambda$. One defines spectral measures $d\mu_\varphi^H$ by

$$\mu_\varphi^H(A) = (\varphi, E_A(H)\varphi) \tag{2.1}$$

so that

$$\int e^{-it\lambda} d\mu_\varphi^H(\lambda) = (\varphi, e^{-itH}\varphi) \tag{2.2}$$

and

$$\int \frac{d\mu_\varphi^H(\lambda)}{\lambda - z} = (\varphi, (H-z)^{-1}\varphi). \tag{2.3}$$

$\sigma(H)$, the spectrum of H is precisely, $\cup_\varphi \operatorname{supp}(d\mu_\varphi^H)$.

Much of what we discuss in this paper involves two distinct decompositions of the spectrum of H. The first is

$$\begin{aligned}\sigma_{\rm disc}(H) = \{\lambda \mid \lambda &\text{ is an eigenvalue of finite multiplicity}\\ &\text{and an isolated point of } \sigma(H)\}\\ \sigma_{\rm ess}(H) = \sigma(H)&\backslash\sigma_{\rm disc}(H).\end{aligned}$$

Equivalently, $\lambda \in \sigma_{\rm disc}(H)$ if and only if for some $\varepsilon > 0$, $\dim E_{(\lambda-\varepsilon,\lambda+\varepsilon)}(H)$ is finite and for all $\varepsilon > 0$, $E_{(\lambda-\varepsilon,\lambda+\varepsilon)}(H) \neq 0$. $\sigma_{\rm disc}(H)$ captures the notion of bound states.

The second breakup involves the fact that any measure $d\mu$ on $\mathbb{R}$ has a decomposition

$$d\mu = d\mu_{\rm pp} + d\mu_{\rm ac} + d\mu_{\rm sc},$$

where $d\mu_{\rm pp}$ is a pure point measure (sum of delta functions), $d\mu_{\rm ac}$ is $F(\lambda)\,d\lambda$, with F a nonnegative locally integrable density, and $d\mu_{\rm sc}$ is a singular continuous measure (like the Cantor measure). I will define $\sigma_{\rm pp}(H)$ to be the set of eigenvalues of H; it is not the union of the supports of $\mu_{\rm pp}$ because it may not be closed

$$\sigma_{\rm ac}(H) = \bigcup_\varphi \operatorname{supp}(d\mu_\varphi^H)_{\rm ac}$$

$$\sigma_{\rm sc}(H) = \bigcup_\varphi \operatorname{supp}(d\mu_\varphi^H)_{\rm sc}.$$

One often defines a refined set $\Sigma_{\rm ac}$ with $\overline{\Sigma}_{\rm ac} = \sigma_{\rm ac}(H)$, the essential support of the a.c. measure. Basically, the essential support of the a.c. measure $F(\lambda)\,d\lambda$ is $\{\lambda \mid F(\lambda) \neq 0\}$. It is defined modulo sets of Lebesgue measure zero. $\Sigma_{\rm ac}$ is the union of the essential support of $(d\mu_\varphi^H)_{\rm ac}$ over a countable dense set of φ's.

3. Self-Adjointness

The theory of Schrödinger operators was born with Kato's famous self-adjointness theorem for atomic Hamiltonians. His theorem abstracted says the following:

Theorem 3.1. (Kato [144]) *Let $\mathcal{H} = L^2(\mathbb{R}^{3N})$ where $x \in \mathbb{R}^{3N}$ is written $(x_1, \dots, x_N)$ with $x_i \in \mathbb{R}^3$. Let Δ_i be the Laplacian in x_i and let V_i, V_{ij} be functions on $\mathbb{R}^3$ in $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Let*

$$H_0 = -\sum_{i=1}^N (2\mu_i)^{-1}\Delta_i \tag{3.1}$$

$$V = \sum_{i=1}^N V_i(x_i) + \sum_{i<j} V_{ij}(x_i - x_j) \tag{3.2}$$

and let $H = H_0 + V$. Then H defined on $D(H_0)$ is self-adjoint and is essentially self-adjoint on $C_0^\infty(\mathbb{R}^{3N})$.

Remarks. 1. See Reed-Simon [211] for a proof.

2. The basic idea of the proof is a perturbation theoretic one. There is a general theorem (the Kato-Rellich theorem) that if A is a self-adjoint operator and B is a symmetric operator with $D(B) \supset D(A)$ and for some $\alpha < 1$ and $\beta > 0$ and all $\varphi \in D(A)$, that

$$\|B\varphi\| \leq \alpha\|A\varphi\| + \beta\|\varphi\|, \tag{3.3}$$

then $A+B$ is self-adjoint on $D(A)$ and essentially self-adjoint on any domain of essential self-adjointness for A. If (3.3) holds, we will say B is A-bounded. The infimum over all α is called the relative bound of B with respect to A.

3. If one looks at a general bound of type (3.3) with $\alpha < 1$ where $A = -\Delta$ on $L^2(\mathbb{R}^k)$ and B is multiplication by V, then in terms of requirements that $V \in L^p_{\text{loc}}(\mathbb{R}^k)$, one needs

$$p \geq 2 \qquad k = 1, 2, 3 \tag{3.4a}$$

$$p > 2 \qquad k = 4 \tag{3.4b}$$

$$p \geq \tfrac{k}{2} \qquad k \geq 5 \tag{3.4c}$$

by using Sobolev estimates (see, e.g., Cycon et al. [53])

4. If $k = 3N$ and we use *only* the L^p requirements of Remark 3, Coulomb potentials stop working already at $N = 2$. Thus, for Kato's theorem, it is critical to use Sobolev estimates in subsets of variables as Kato did.

An industry developed in understanding when $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$. An illustrative example is

Example. Let $H = -\Delta - c|x|^{-2}$ on $C_0^\infty(\mathbb{R}^k)$ with $n \geq 5$ (needed for $H\varphi \in L^2$ for all $\varphi \in C_0^\infty(\mathbb{R}^k)$). Then it can be seen (Reed-Simon [211, Example 4 in Section X.2]) that if $c > c_0 = \frac{(n-4)n}{4}$, then H is not self-adjoint on C_0^∞. This is a quantum analog of the classical fact that if $V = -c|x|^{-2}$ for any $c > 0$, a set of initial conditions of positive measure falls into $x = 0$ in finite time ($c_0 > 0$ is a reflection of an uncertainly principle repulsion).

This example shows that for pure L^p requirements, one cannot do better than (3.4) since $|x|^{-2} \in L^p + L^\infty$ if $p < \frac{k}{2}$. But it turns out this is only so if V is allowed to have any sign. For $V \geq 0$, one can do much better. The best result of this genre is

Theorem 3.2. (Leinfelder-Simader [173]) *Let* $V \geq 0$, $V \in L^2_{\text{loc}}(\mathbb{R}^k)$, $\{a_j\}_{j=1}^k \in L^4_{\text{loc}}(\mathbb{R}^k)$ *with* $\nabla \cdot a \in L^2_{\text{loc}}(\mathbb{R}^k)$ (distributional derivatives). Then

$$H = \sum_{j=1}^k (i\partial_j - a_j)^2 + V \tag{3.5}$$

is essentially self-adjoint on $C_0^\infty(\mathbb{R}^k)$.

Remarks. 1. For a proof, see Cycon et al. [53].

2. This is essentially a best possible result. If $a = 0$, H is defined on C_0^∞ if and only if $V \in L^2_{\text{loc}}$; so the result says for positive V, we have essential self-adjointness if and only if H is defined. Similarly, unless there are cancellations, $a_j \in L^4_{\text{loc}}$ and $\nabla \cdot a \in L^2_{\text{loc}}$ is required for H to be defined on C_0^∞.

3. It was Simon [239] who first realized that for $V \geq 0$, there only needed to be local L^2 conditions. However, he required a global condition $\int |V(x)|^2 e^{-bx^2}\, dx < \infty$ for some $b > 0$. It was Kato [152] who proved the

general $a = 0$ result (and also allowed for smooth a's). Kato's paper used the distributional inequality, now called Kato's inequality

$$\Delta|u| \geq \operatorname{Re}(\operatorname{sgn} u \Delta u) \tag{3.6}$$

that is also critical to the Leinfelder-Simader proof.

4. (3.6) is essentially equivalent to the fact that $e^{t\Delta}$ is positivity preserving. The version of (3.6) with magnetic fields is equivalent to diamagnetic inequalities:

$$|(e^{-tH}\varphi)(x)| \leq (e^{t\Delta}|\varphi|)(x) \tag{3.7}$$

for the H of (3.5) (with $V \geq 0$). These ideas were discovered by Nelson [198], Simon [241, 247], and Hess-Schrader-Uhlenbrock [119].

While there are best possible self-adjointness results for magnetic fields and positive potentials, the results for V's which can be negative are not in such a definitive form. All the basic principles are understood but I'm not aware of a single result that puts them all together (one of the best results is in Kato's paper [151] although, as we will see, it is not quite optimal with regard to local singularities). So I will present the general principles that are understood in this case.

(a) $-|x|^2$ *borderline for behavior at infinity.* Negative potentials V of compact support for which $H = -\Delta + V$ is essentially self-adjoint on C_0^∞ normally obey a global estimate of the form (3.3) (with $A = -\Delta$, $B = V$) and, in particular, H is bounded from below. However, if V is not of compact support, it can go to minus infinity at infinity without destroying self-adjointness. More or less, the borderline for keeping self-adjointness is $-|x|^2$. For example, it can be proven (see, e.g., Reed-Simon [211, Theorem X.9]) that $-\frac{d^2}{dx^2} - |x|^\alpha$ on $L^2(-\infty, \infty)$ is essentially self-adjoint on $C_0^\infty(-\infty, \infty)$ if and only if $\alpha \leq 2$. This is attractive since a classical particle with the same potential reaches infinity in finite time if and only if $\alpha > 2$. Nelson has examples (see Reed-Simon [211], p. 156) of $V(x)$ with $V(x) \leq -cx^4$ so $-\frac{d^2}{dx^2} + V(x)$ is still essentially self-adjoint and thus, the borderline won't be if and only if, but the general version of this is that if $V(x) \geq -cx^2$ in some averaged sense, then $-\Delta + V(x)$ will be essentially self-adjoint on C_0^∞. The earliest version of this is Ikebe-Kato [130]. My favorite theorem of this genre is due to Faris and Lavine [80] (see Reed-Simon [211, Theorem X.38]). In particular, Stark Hamiltonians where $V = \vec{c} \cdot \vec{x} + V_0$ are essentially self-adjoint for suitable V_0. In any event, I will focus henceforth on cases where $-\Delta + V$ is not unbounded from below.

(b) *Stability of relative boundedness under adding $V \geq 0$ or a magnetic field.* Suppose $A \geq 0$. Then (3.3) holds for some $\alpha < 1$ if and only if

$$\lim_{\gamma \to \infty} \|B(A + \gamma)^{-1}\| < 1.$$

On the other hand, (3.7) implies that for $V \geq 0$, any $\vec{a}$ and any multiplication operator W:

$$\|W(H+\gamma)^{-1}\| \leq \|W(-\Delta+\gamma)^{-1}\|$$

and so the second principle is that in studying the negative part of V, one can assume V is negative and then add back an arbitrary positive $L^2_{\rm loc}$ positive V. While this is true, it ignores situations where there are cancellations between the positive and negative parts which can occur (see, e.g., Combescure-Ginibre [48]).

(c) *Relative bounds need only hold uniformly locally.* The following proposition holds:

Proposition 3.3. *Suppose V is a function on $\mathbb{R}^d$ so that for some α, β and every y,*

$$\|V\chi(\cdot - y)\varphi\| \leq \alpha\|-\Delta\varphi\| + \beta\|\varphi\|, \tag{3.8}$$

where χ is the characteristic function of the unit cube. Then for any $\tilde{\alpha} > \alpha$, there is some $\tilde{\beta}$ so that

$$\|V\varphi\| \leq \tilde{\alpha}\|-\Delta\varphi\| + \tilde{\beta}\|\varphi\|. \tag{3.9}$$

This result is proven by a variant of an idea of Sigal [231]. Find a "partition of unity" $\{j_\mu\}_\mu$ so that $\sum j_\mu^2 = 1$, each j_μ is supported in some unit cube (so $j_\mu\chi(\cdot - y_\mu) = j_\mu$ for some j_μ), and the j_μ's are locally finite, $\sum(\vec{\nabla} j_\mu)^2$ is uniformly bounded (the j_μ's can be translates of a single j_μ) and $\sum|\Delta j_\mu|$ is uniformly bounded. If $H_0 = -\Delta$, we have (where C is related to $\|\sum(\nabla j_\mu)^2\|_\infty$ and $\|\sum(\Delta j_\mu)\|_\infty$)

$$\sum_\mu [j_\mu, [j_\mu, H_0^2]] \leq C(H_0+1)$$

and from this that

$$\sum \|H_0 j_\mu\varphi\|^2 \leq (1+\varepsilon)\|H_0\varphi\|^2 + C_\varepsilon\|\varphi\|^2. \tag{3.10}$$

Thus

$$\begin{aligned}
\|V\varphi\|^2 &= \sum_\mu \|V\chi(\cdot - y_\mu) j_\mu\varphi\|^2 \\
&\leq (1+\varepsilon)\alpha^2 \sum_\mu \|H_0 j_\alpha\varphi\|^2 + (1+\varepsilon^{-1})\beta^2\|\varphi\|^2 \qquad \text{(by (3.8)} \\
&\leq (1+\varepsilon)^2\alpha^2\|H_0\varphi\|^2 + ((1+\varepsilon^{-1})\beta^2 + C_\varepsilon)\|\varphi\|^2 \quad \text{(by (3.10)}
\end{aligned}$$

which yields (3.9).

Proposition 3.3 says that the proper condition on V to yield a $-\Delta$ bound is a uniform local condition.

(d) *Convolution results are the proper local condition.* As discussed earlier, L^p conditions on V do not properly control functions on subspaces. Explicitly, let $\pi : \mathbb{R}^k \to \mathbb{R}^\ell$ be a projection and $V(x) = W(\pi(x))$. Then for V to

be $-\Delta$ bounded (assuming $k \geq \ell \geq 5$), we need $W \in L^p_{\text{loc}}(\mathbb{R}^\ell)$ for $p \geq \frac{\ell}{2}$ and so $V \in L^p_{\text{loc}}(\mathbb{R}^k)$ with $p \geq \frac{\ell}{2}$. But if V is not a function of a subset of variables, in general we need $p \geq \frac{k}{2}$. It is a discovery of Stummel [262] that by stating conditions in terms of convolution estimates, one can find conditions that respect subsets of variables. In particular, the following is a space, S_ν, introduced in Stummel [262]: Let V be a function on $\mathbb{R}^\nu$; we say $V \in S_\nu$ if and only if

$$\lim_{\alpha \downarrow 0} \left[\sup_x \int_{|x-y| \leq \alpha} |x-y|^{4-\nu} |V(y)^2| \, d^\nu y \right] = 0 \quad \text{if } \nu \geq 5$$

$$\lim_{\alpha \downarrow 0} \left[\sup_x \int_{|x-y| \leq \alpha} \ln(|x-y|^{-1}) |V(y)|^2 \, d^\nu y \right] = 0 \quad \text{if } \nu = 4$$

$$\sup_x \int_{|x-y| \leq 1} |V(y)|^2 \, d^\nu y < \infty \quad \text{if } \nu \leq 3.$$

This class respects functions of subvariables in the sense that if $\pi : \mathbb{R}^k \to \mathbb{R}^\ell$ is a projection, $V(x) = W(\pi(x))$ and $W \in S_\ell$, then $V \in S_k$. Moreover, it is not hard to show (see, e.g., Cycon et al. [53]) that if $V \in S_\nu$, then V is $-\Delta$-bounded with relative bound zero. Moreover (see Cycon et al. [53], Thm. 1.9), if for some $a, b > 0$ and δ with $0 < \delta < 1$ and all $0 < \varepsilon < 1$ and $\varphi \in D(H_0)$

$$\|V\varphi\|^2 \leq \varepsilon \|\Delta\varphi\|^2 + a \exp(b\varepsilon^{-\delta}) \|\varphi\|^2, \tag{3.11}$$

then V is in S_ν. See Schechter [226] for more on Stummel conditions.

(3) *The Kato class and going beyond relative boundedness.* In his inequality paper [152], Kato introduced a form analog, K_ν of S_ν: Let V be a function on $\mathbb{R}^\nu$; we say $V \in K_\nu$ if and only if

$$\lim_{\alpha \downarrow 0} \left[\sup_x \int_{|x-y| \leq \alpha} |x-y|^{2-\nu} |V(y)| \, d^\nu y \right] = 0 \quad \text{if } \nu \geq 3 \tag{3.12a}$$

$$\lim_{\alpha \downarrow 0} \left[\sup_x \int_{|x-y| < \alpha} \ln(|x-y|^{-1}) |V(y)| \, d^\nu y \right] = 0 \quad \text{if } \nu = 2 \tag{3.12b}$$

$$\sup_x \int_{|x-y| \leq 1} |V(y)| \, d^\nu y < \infty \quad \text{if } \nu = 1. \tag{3.12c}$$

Then Kato [151] proved if $\max(-V, 0) \in K_\nu$ and $V \in L^2_{\text{loc}}(\mathbb{R})$, then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^\nu)$. While it is not Kato's proof, this is intimately connected with the semigroup result discussed in the next section. Defining the form sum, H, one knows $\exp(-tH) : L^2 \to L^\infty$ so $L^\infty \cap L^2 \cap D(H)$ is a domain of essential self-adjointness. It is not hard to then show $L_0^\infty \cap D(H)$, the L^∞ functions of compact support are a domain of essential self-adjointness. Then convolution allows one to get C_0^∞ approximations.

(f) *Logarithmic improvements.* Neither S_ν nor K_ν is quite the ideal space for essential self-adjointness. For example, if $\nu \geq 5$ and $V(x) = |x|^{-2}(1 +$

$|\log|x|\,|)^{-\alpha}$, V is in K_ν only if $\alpha > 1$, in S_ν only if $\alpha > \frac{1}{2}$, but $-\Delta$-bounded with relative bound zero if $\alpha > 0$.

Analogous to the issue of self-adjointness is a question of whether maximal and minimal forms agree. This is discussed in Kato [152] and Simon [248] (see Thm. 1.13 in Cycon et al. [53]).

4. Properties of Eigenfunctions, Green's Functions, Semigroups, and All That

I wrote a long review of these subjects twenty years ago (Simon [250]) and the situation has hardly changed since then, although there has been extensive interesting work on what happens for general elliptic operators and for bounded regions (see, e.g., Davies [55]). So it will suffice to hit a few major themes. The basic theorem is

Theorem 4.1. *Let $V_+ \in L^1_{\rm loc}(\mathbb{R}^\nu)$ and $V_- \in K_\nu$, the space of* (3.12). *Let $H = -\Delta + V$ as a form sum. Then for any $p \le q$, e^{-tH} maps L^p to L^q and for $t \le 1$,*

$$\|e^{-tH}\|_{p,q} \le C\, t^{-\alpha}, \tag{4.1}$$

where

$$\alpha = \frac{\nu}{2}\left(\frac{1}{p} - \frac{1}{q}\right). \tag{4.2}$$

Remarks. 1. Semigroup L^p bounds were first found by Davies [54], Herbst-Sloan [118], and Kovalenko-Semenov [161] with further developments by Carmona [41], Simon [246], and Aizenman-Simon [12].

2. In particular, it was Aizenman-Simon [12] who found that K_ν is the natural class for L^p bounds. Indeed, they not only proved Theorem 4.1 in this form but also showed that if $V \le 0$ and $\exp(-tH)$ maps L^∞ to itself with $\lim_{t\downarrow 0} \|e^{-tH}\|_{\infty,\infty} = 1$, then $V \in K_\nu$.

3. The result holds when magnetic fields are added (by a diamagnetic inequality).

4. Most of these authors use a combination of path integral estimates and L^p-interpolation theory. In particular, the Feynman-Kac and Feynman-Kac-Itô formulae (see Simon [246] for extensive discussion) are useful tools in studying Schrödinger operators. See Simon [259] for an extension to cases when $V(x) \ge -cx^2$.

5. In fact, e^{-tH} takes L^p not only into L^∞ but into the continuous functions (see Simon [250, Thm. B.3.1]).

6. (4.1)/(4.2) are precisely the best results for $H = -\Delta$.

7. This theorem says that H can be defined as the generator of a semigroup on each L^p space. The spectrum has been shown to be L^p independent in Hempel-Voight [113]. For a general discussion of L^p Schrödinger operators, see Davies [56].

Once one has these estimates, they can be used to derive:

(a) *Sobolev estimates*: As in the free case if V obeys the conditions of Theorem 4.1, then $(H-z)^{-\nu}$ takes L^p to L^q if

$$p^{-1} - q^{-1} < \left(\frac{2\alpha}{\nu}\right). \tag{4.3}$$

The result (see Simon [250, Thm. B.2.1],) is obtained by integrating the semigroup bound. (4.3) comes from (4.2) and the requirement of integrability at $t = 0$.

(b) *Integral kernels*: Bounded operators from L^1 to L^∞ have bounded integral kernels and so Theorem 4.1 can be used (see Simon [250, Thm. B.7.1]) to prove e^{-tH}, $(H-z)^{-\alpha}$ $(\alpha > \frac{\nu}{2})$ are integral operators with continuous integral kernels. One can also show (Simon [250, Thm. B.7.2]) that for $0 < \alpha < \frac{\nu}{2}$, $(H-z)^{-\alpha}$ is an integral operator with an integral kernel that is continuous away from $x = y$ with a precise singularity at $x = y$.

(c) *Eigenfunctions*: Since global eigenfunctions (i.e., $\varphi \in L^2$ that obey $H\varphi = E\varphi$) are in $\mathrm{Ran}(e^{-tH})$, Theorem 4.1 implies such eigenfunctions are in L^∞. In fact, all this can be done locally. Any eigenfunction (distributional solution of $H\varphi = E\varphi$) is automatically continuous and one can prove Harnack inequalities and subsolution estimates. This is discussed in detail in Aizenman-Simon [12] and Simon [250].

We end this section with a discussion of some issues involving eigenfunctions. There is a huge literature on when Schrödinger operators have positive solutions. This was begun by Allegretto [13] and Piepenbrink [206] with later results by Agmon [5] and Pinchover [207].

Here is a typical theorem (Simon [250, Thm. C.8.1]):

Theorem 4.2. *Let $V_- \in K_\nu$ and $K_+ \in K_\nu^{\mathrm{loc}}$. Then $Hu = Eu$ has a nonzero distributional solution which is everywhere positive if and only if* $\inf \mathrm{spec}(H) \geq E$.

There is also a huge literature on the issue of exponential decay of eigenfunctions. One result (see Simon [250, Thm. C.3.1]) says that any L^2 eigenfunction actually goes to zero pointwise—of interest only for eigenfunctions of embedded eigenvalues. For discrete spectrum, the decay is at least exponential under minimal regularity hypothesis on V. The original key papers on this theme are by O'Connor [200] and Combes-Thomas [47]. From their ideas, one obtains (see Section C.3 of Simon [250]);

Theorem 4.3. *Let $V_- \in K_\nu$, $V_+ \in K_\nu^{\mathrm{loc}}$ and let $H = -\Delta + V$ and let $Hu = Eu$ with $u \in L^2$. Then*

$$|u(x)| \leq C\, e^{-A|x|}, \tag{4.4}$$

where:

(i) *For general E in the discrete spectrum,* (4.4) *holds for some $A > 0$ and $C > 0$.*
(ii) *If H has compact resolvent, then* (4.4) *holds in the sense for any $A > 0$, there is a suitable $C > 0$.*
(iii) *If $\Sigma_{\rm ess} = \inf \sigma_{\rm ess}(H)$ and $E < \Sigma_{\rm ess}$, then* (4.4) *holds in the sense that for any $A \leq \sqrt{E - \Sigma_{\rm ess}}$, there is a suitable $C > 0$.*

One can go beyond this to get fairly detailed behavior on decay in cases when H has compact resolvent or for N-body potentials. In one dimension, one can justify under some regularity conditions the WKB formula that says when $V(x) \to \infty$, eigenfunctions decay like

$$V(x)^{-1/4} \exp\biggl(- \int_a^x \sqrt{V(y) - E}\, dy \biggr). \tag{4.5}$$

It was Agmon [4] who realized the proper higher-dimensional analog for this involves what is now called the Agmon metric: $\rho(x)$ is the geodesic distance of x to 0 in the Riemannian metric $\rho_{ij}(x) = \delta_{ij}(V(x) - E)_+ \, d^2x$. There is a related but more subtle definition for N-body systems. See Agmon [4] and Deift et al. [59] for further discussions. See Simon [253] and Helffer-Sjöstrand [111] for an application to tunnelling probabilities.

Eigenfunctions play a critical role in explicit spectral representations of Schrödinger operators. The basic ideas go back to work of Browder [39], Garding [88], Gel'fand [89], Kac [137], and especially Berezanskii [29, 30]. See Section C.5 of Simon [250] and Last-Simon [170] for some addditional one-dimensional results.

Finally, we mention issues of cusps and nodes of eigenfunctions. Kato [148] has a famous paper on cusps at Coulomb singularities for atomic eigenfunctions. See Hoffmann-Ostenhof et al. [108, 120, 121] for recent developments in this area.

5. One-Dimensional Decaying Potentials

One-dimensional Schrödinger operators

$$-\frac{d^2}{dx^2} + V(x) \tag{5.1}$$

on $L^2(-\infty, \infty)$ and $L^2(0, \infty)$ and their discrete analogs

$$hu(n) = u(n+1) + u(n-1) + V(u)u(n) \tag{5.2}$$

on $\ell^2(-\infty, \infty)$ and $\ell^2[0, \infty)$ have been heavily studied for two reasons. First, ODE/difference equation methods allow one to study them in much greater detail than one can the higher-dimensional analogs. Second, if $V(x) = V(|x|)$ is a spherically symmetric function on $\mathbb{R}^\nu$, then $-\Delta + V$ is unitarily equivalent to a direct sum of operators on $L^2(0, \infty)$ or the form (5.1) where the effective V's have the form $V_\ell(x) = \kappa_\ell |x|^{-2} + V(x)$ for suitable κ_ℓ's. The details can be found, for example, in Reed-Simon [211], Example 4 to the Appendix for X.1.

The one-dimensional theory has been in and out of vogue. It was extensively studied from 1930–1950 with important contributions by Titchmarsh, Kodaira, Gel'fand, Hartman-Wintner, Levinson, Coddington-Levinson, and Jost. Significant developments during the next twenty-five years were mainly in the area of inverse spectral theory (a major exception was Weidmann's work [273], to be discussed shortly) which will be discussed in Section 6 below. From about 1975 starting with work of Goldsheid, Molchanov, and Pastur [98] and Pearson [204], this has been an active area with extensive study of the one-dimensional case, especially with long-range and with ergodic potentials.

One special feature of one dimension is that one can limit spectral multiplicities under very general conditions on V:

Theorem 5.1. (a) *Let $H = -\frac{d^2}{dx^2} + V(x)$ on $L^2(0,\infty)$ with fixed $hu(0) + u'(0) = 0$ boundary conditions and suppose H is essentially self-adjoint on $C_0^\infty[0,\infty)$. Then H has simple spectrum (multiplicity 1).*

(b) *Let $H = -\frac{d^2}{dx^2} + V(x)$ on $L^2(-\infty,\infty)$ and suppose H is essentially self-adjoint on $C_0^\infty(-\infty,\infty)$. Then*

(i) *The a.c. spectrum of H is of multiplicty at most 2.*
(ii) *The singular spectrum of H is of multiplicity 1.*

Remarks. 1. All one needs for local regularity of V is $V \in L^1[0,R]$ for all $R > 0$ or $L^1_{\text{loc}}(-\infty,\infty)$.

2. The result holds even if H is not essentially self-adjoint (V limit circle at $\pm\infty$) so long as a boundary condition is imposed at ∞ or at $-\infty$.

3. The only subtle part of the result is that the s.c. spectrum is simple on the real line. This is a theorem of Kac [138, 139]; see also Berezanskii [29, 30]. My preferred proof is due to Gilbert [95, 96].

In this section, we will discuss the case where $V(x) \to 0$ at infinity. In the next section, we will discuss inverse spectral theory, and in the section after that, we will discuss ergodic potentials. (These two subjects are mainly one-dimensional.) The issue of the asymptotic eigenvalue distribution when $V \to \infty$ as $\pm\infty$ is discussed in Section 14 on the quasiclassical limit.

This section will discuss (5.1)/(5.2) in situations where $V(x)$ (or $V(n)$) goes to zero (at least in an average sense) as $x \to \infty$ (or $n \to \infty$). The interesting thing is that there are three natural breaks in behavior. Expressed in terms of $|x|^{-\alpha}$ behavior, they are

(i) At $\alpha = 2$, we shift between a finite number of bound states ($\alpha > 2$) or an infinite number ($\alpha < 2$) at least if $V(x) < 0$.
(ii) At $\alpha = 1$ ($V \in L^1$), we shift between a pure scattering situation for positive energies ($\alpha > 1$) and the possibility of positive energy bound states ($\alpha < 1$).
(iii) At $\alpha = \frac{1}{2}$, ($V \in L^2$), we shift from there being a.c. spectrum for a.e. positive energy ($\alpha > \frac{1}{2}$) to at least the possibility of very different spectrum.

(i) and (ii) have been known since the earliest days of quantum mechanics. The $\alpha = \frac{1}{2}$ borderline first occurred in Simon [251] who found that random decay potentials had point spectrum when $\alpha < \frac{1}{2}$. Delyon, Simon, and Souillard [64] then showed if $\alpha = \frac{1}{2}$, there may be some nonpoint spectrum. As we will see, subsequent results confirmed this borderline.

The negative spectrum for decaying potentials is easy: So long as $\int_x^{x+1} |V(y)|\, dy \to 0$, H is bounded below and has $[0, \infty)$ as essential spectrum by Weyl's criterion (see, e.g., Reed-Simon [213, Section XIII.4]), which means that $(-\infty, 0)$ has only discrete eigenvalues of finite multiplicity, which can only accumulate at energy 0. Indeed, by Theorem 5.1, the point spectrum is of multiplicity 1. Once these basics are established for the discrete spectrum, a number of detailed questions about it arise:

(a) *Is σ_{disc} finite or infinite?* The borderline, as mentioned above, is r^{-2} decay. Explicitly, one has Bargmann's bound [24] that the number of eigenvalues on a half-line with $u(0) = 0$ boundary conditions is bounded by $\int x|V(x)|\, dx$ and on a whole line by $1 + \int_{-\infty}^{\infty} |x|\, |V(x)|\, dx$ (see Simon [240] for a review of bounds on the number of bound states). On the other hand, if $\overline{\lim}_{x\to\infty} |x|^2 V(x) \leq -\frac{1}{4}$, one can prove that H has an infinity of bound states (see, e.g., Reed-Simon [213, Thm. XIII.6]).

(b) *If σ_{disc} is infinite, how does $\lim_{\lambda\uparrow 0} \dim E_{(-\infty,\lambda)}(H)$ diverge?* This is a quasiclassical limit and discussed in Section 14 below.

(c) *Bounds on moments of eigenvalues.* Lieb and Thirring [186], motivated in part by their work on the stability of matter [185], initiated extensive study on the best constant $L_{\gamma,1}$ in

$$\sum_j |e_j|^\gamma \leq L_{\gamma,1} \int |V(x)|^{\gamma+1/2}\, dx,$$

which holds if $\gamma \geq \frac{1}{2}$. Here $\{e_j\}$ are the negative eigenvalues of H. For $\gamma \geq \frac{3}{2}$, the constant $L_{\gamma,1}$ is known to be quasiclassical (Aizenman-Lieb [9]). For $\gamma \in [\frac{1}{2}, \frac{3}{2})$, it is known that $L_{\gamma,1}$ is strictly larger than the quasiclassical result [186]. It is conjectured to be the optimal value for a single bound state, as explained in Lieb-Thirring [186], but this is still open (except at $\gamma = \frac{1}{2}$ (Hundertmark-Lieb-Thomas [125])).

(d) *Is there a bound state for weak coupling?* In one (and two) dimensions, H has bound states even for very weak coupling. The result (Simon [242]) is that if $\int |x|\, |V(x)|\, dx < \infty$ and $\int V(x)\, dx \leq 0$ and $V \neq 0$, then H always has a bound state and the binding energy of $-\Delta + \mu V$ is $\sim c\mu^2$ as $\mu \downarrow 0$ (if $\int V(x)\, dx < 0$; it is $\sim c\mu^4$ if $\int V(x) = 0$).

As for positive energies, the situation is simple if $V \in L^1$:

Theorem 5.2. *Let $V \in L^1(-\infty, \infty)$ or $L^1(0, \infty)$. Then $HE_{(0,\infty)}(H)$ is unitarily equivalent to $-\frac{d^2}{dx^2}$ (on $L^2(-\infty, \infty)$ or $L^2(0, \infty)$ with $u(0) = 0$ boundary conditions).*

Remarks. 1. This result is essentially due to Titchmarsh [267].

2. In terms of $r^{-\alpha}$ falloff, $V \in L^1$ means $\alpha > 1$.

3. Using scattering theoretic ideas, one can prove wave operators exist and are complete (see Section 8).

4. This says there is no point of singular continuous spectrum at positive energies and that the a.c. spectrum has essential support $(0, \infty)$ with multiplicity 2 or 1.

5. We have stated the result for $u(0) = 0$ boundary condition for simplicity; it holds for all boundary conditions at 0.

As for slower decay than L^1, if one has control of derivatives, one can still conclude the positive spectrum is purely absolutely continuous. The simplest result of this genre is

Theorem 5.3. (Weidmann [273]) *Let $V = V_1 + V_2$ where V_1 is in L^1, $V_2(x) \to 0$ as $x \to \pm\infty$, and V_2 is of bounded variation. Then, $HE_{(0,\infty)}(H)$ is unitarily equivalent to $-\frac{d^2}{dx^2}$ (on $L^2(-\infty, \infty)$ or on $L^2(0, \infty)$ with $u(0) = 0$ boundary conditions).*

Remarks. 1. V_2 of bounded variation with $V_2 \to 0$ at infinity essentially says that $-\frac{dV_2}{dx} \in L^1$; in fact, any V_2 of bounded variation can be written $V_3 + V_4$ with $V_3 \in L^1$ and V_4 a C^1 function with $\frac{dV_4}{dx} \in L^1$.

2. Pure power potentials $r^{-\alpha}$ for any $\alpha > 0$ are included in this theorem; indeed, any monotone function $V(x)$ with $V(x) \to 0$ as $x \to \infty$ is of bounded variation.

For a short proof of Theorems 5.2/5.3, see Simon [256]. Both theorems can be understood as coming from the fact that all solutions of $-u'' + Vu = \lambda u$ with $\lambda > 0$ are bounded. That such a conclusion implies the spectrum is purely absolutely continuous was first indicated by Carmona [42] (who required some kind of uniformity in λ). Important later developments that capture this idea are due to Gilbert-Pearson [97], Last-Simon [170], and Jitomirskaya-Last [135]. The tools in those papers are also important for the proofs of the results of Section 7.

Once one allows decay slower than $r^{-1-\varepsilon}$ for both V and V', the conclusion of Theorems 5.2/5.3 can fail because of embedded point spectrum. The original examples of this were found by von Neumann-Wigner [272]. Basically, if $V(x) = \gamma |x|^{-1} \sin(x)$ for x large and $\gamma > 1$, then $-u'' + Vu = \frac{1}{4}u$ has a solution which is L^2 at infinity (see, e.g., Theorem XI.67 in Reed-Simon [213]). By adjusting V at finite x, one can arrange for any boundary condition one wants at $x = 0$. In fact, if one allows slightly slower decay than $|x|^{-1}$, one can arrange dense point spectrum. Naboko [197] and Simon [257] have shown that for any sequence $\{\lambda_n\}_{n=1}^{\infty}$ of energies in $(0, \infty)$ (Naboko has a mild restriction on the λ's) and any $g(r)$ obeying $\lim_{r\to\infty} r\, g(r) = \infty$, there is a $V(x)$ obeying:

(i) $|V(x)| \le g(|x|)$ for x large

(ii) $-u'' + Vu = \lambda_n u$ has a solution L^2 at infinity

and obeying a prescribed boundary condition at $x = 0$.

Remark. It is an interesting open question about whether there exist potentials decaying faster than $|x|^{-1/2-\varepsilon}$ with dense singular continuous spectrum (rather than dense point spectrum).

The interesting fact is that even though potentials of Naboko-Simon type have dense point spectrum, they may also have lots of a.c. spectrum. The best result is:

Theorem 5.4. (Deift-Killip [60]) *Let $V \in L^2$. Then the essential support of the a.c. spectrum of $H = -\frac{d^2}{dx^2} + V$ is $[0, \infty)$.*

Remarks. 1. In terms of $r^{-\alpha}$ decay, this result requires $\alpha > \frac{1}{2}$.

2. This result is optimal in that it is known for any Orlicz space strictly larger than L^2 in terms of behavior at infinity, there are V's whose associated H has no a.c. spectrum.

3. The first result of this genre was found by Kiselev [156] who proved the conclusion of this theorem for $|V(x)| \leq C\, x^{-3/4-\varepsilon}$. There were subsequent improvements of this by Kiselev [157], Christ-Kiselev [46], and Remling [218].

4. Killip [155] has a partially alternate proof of Theorem 5.4.

Once the decay is allowed to be slower than $r^{-1/2}$, one can have much different spectrum in $[0, \infty)$:

(i) If W is a suitable family of random homogeneous potentials and $V(x) = |x|^{-\alpha} W(x)$ with $\alpha < \frac{1}{2}$, then H has only dense point spectrum in $(0, \infty)$. This was first proven in the discrete case by Simon [251] and later in the continuum case by Kotani-Ushiroya [160].

(ii) Generic potentials decaying like $|x|^{-\alpha}$ ($\frac{1}{2} > \alpha > 0$) produce singular continuous spectrum as discovered by Simon [255]. For example, in $\{V \in \mathbb{C}(\mathbb{R}) \mid \sup_x |x|^\alpha |V(x)| \equiv \|V\|_\alpha\}$ viewed as a complete metric space in $\|\cdot\|_\alpha$, a dense G_δ of V's are such that $-\frac{d^2}{dx^2} + V(x)$ has purely singular continuous spectrum on $[0, \infty)$.

(iii) Much more is known in the borderline $\alpha = \frac{1}{2}$ case, at least for the discrete Schrödinger operator (5.2). For example, if a_n are independent, identically distributed random variables uniformly distributed in $[-1, 1]$ and $V(n) = \mu n^{-1/2} a_n$, then for suitable coupling constants μ and energies E in $[-2, 2]$, the spectral measures have fractional Hausdorff dimension with an exactly computable local dimension. This is discussed in Kiselev-Last-Simon [158]. There are earlier results on this model by Delyon-Simon-Souillard [64] and Delyon [62].

(iv) A very different class of decaying potentials was studied by Pearson [204]. His potentials are of the form

$$V(x) = \sum_{n=1}^{\infty} a_n\, W(x - x_n), \tag{5.3}$$

where $W \geq 0$, $a_n \to 0$, and $x_n \to \infty$ very rapidly so the bumps are sparse. He showed that for suitable a_n, x_n, the corresponding H has purely singular spectrum—providing the first explicit examples of such spectrum. Strong versions of his results were found by Remling [217] and Kiselev-Last-Simon [158]. In particular, the latter authors proved if $\frac{x_{n+1}}{x_n} \to \infty$ (e.g., $x_n = n!$), then potentials of the form (5.3) lead to H's with purely singular spectrum if $\sum a_n^2 = \infty$ and to ones with purely a.c. spectrum if $\sum a_n^2 < \infty$.

6. Inverse Spectral Theory

One area related to Schrödinger operators, especially in one dimension, is the question of inverse theory: How does one go from spectral or scattering information to the potential. There is a huge literature, including three books I would like to refer the reader to: Chadan-Sabatier [45], Levitan [176], and Marchenko [190]. I will only touch some noteworthy ideas here.

In one dimension, a key role is played by the Weyl m-function and the associated spectral measure, $d\rho$. Given a potential V so that H is self-adjoint with $u(0) = 0$ boundary conditions, for each z with $\operatorname{Im} z > 0$, there is a solution $u(x; z)$ of $-u'' + Vu = zu$ which is L^2 at infinity. The m-function is defined by

$$m(z) = \frac{u'(0; z)}{u(0, z)}. \tag{6.1}$$

$\operatorname{Im} m(z) > 0$ in $\operatorname{Im} z > 0$ so by the Herglotz representation theorem

$$m(z) = B + \int d\rho(\lambda) \left[\frac{1}{\lambda - z} - \frac{\lambda}{1 + \lambda^2} \right] \tag{6.2}$$

for a suitable constant B. $d\rho$ is called the spectral measure for H. One can recover $d\rho$ from m by

$$\frac{1}{\pi} \operatorname{Im} m(\lambda + i\varepsilon)\, d\lambda \to d\rho(\lambda) \tag{6.3}$$

weakly as $\varepsilon \downarrow 0$ and (6.2) allows the recovery of m from $d\rho$ given the known asymptotics (Atkinson [15], Gesztesy-Simon [93])

$$m(-\kappa^2) = -\kappa + o(1) \tag{6.4}$$

as $|\kappa| \to \infty$ with $\delta < \operatorname{Arg} \kappa < \frac{\pi}{2} - \delta$. $d\rho$ really is a spectral measure for let $\tilde{\varphi}(x, \lambda)$ solve $-\tilde{\varphi}'' + V\tilde{\varphi} = \lambda\tilde{\varphi}$ with boundary conditions $\tilde{\varphi}(0, \lambda) = 0$,

$\tilde\varphi'(0,\lambda) = 1$, and define for $f \in C_0^\infty(0,\infty)$

$$(Uf)(\lambda) = \int \tilde\varphi(x,\lambda) f(x)\, dx. \tag{6.5}$$

Then U is a unitary map of $L^2(0,\infty,dx)$ to $L^2(\mathbb{R}, d\rho(\lambda))$; in particular,

$$\int |(U(f)(\lambda)|^2\, d\rho(\lambda) = \int |f(x)|^2\, dx \tag{6.6}$$

or formally

$$\int \varphi(x,\lambda)\varphi(y,\lambda)\, d\rho(\lambda) = \delta(x-y). \tag{6.7}$$

Moreover, $(UHf)(\lambda) = \lambda(Uf)(\lambda)$. $d\rho$ and its equivalent function m is therefore close to spectral information. One way of seeing this explicitly is if $V(x) \to \infty$. In that case, m is meromorphic, the poles of m are precisely the eigenvalues of H with $u(0) = 0$ boundary conditions and by definition of m, the zeros are precisely the eigenvalues with $u'(0) = 0$ boundary conditions. m is uniquely determined by these two sets of eigenvalues.

In many ways, the fundamental result in inverse theory is the following one:

Theorem 6.1. (Borg [37]-Marchenko [188]) *m determines q, that is, if q_1 and q_2 have equal m's, then $q_1 = q_2$.*

Recently, the following local version of the Borg-Marchenko theorem was proven

Theorem 6.2. *Let q_1 and q_2 be potentials and m_1 and m_2 their m-functions. Then $q_1 = q_2$ on $[0,a]$ if and only if*

$$|m_1(-\kappa^2) - m_2(-\kappa^2)| = O(e^{-2a\kappa})$$

as $\kappa \to \infty$ for κ obeying $\delta \le \arg\kappa \le \frac{\pi}{2} - \delta$.

Remarks. 1. This result was first proven by Simon [258] when q_1 and q_2 are bounded from below.

2. The general result which even allows q_i to be limit circle at infinity was first obtained by Gesztesy-Simon [93].

3. A simple proof of Theorem 6.2 was subsequently obtained by Gesztesy-Simon [94].

Given the uniqueness result, it is natural to ask about concrete methods of determining q given m. There are two approaches for the general case. The first is due to Gel'fand-Levitan [90] and depends on the orthogonality relation (6.7), while the other, due to Simon [258], is a kind of continuum analog of the continued fraction approach to solving the moment problem.

The Gel'fand-Levitan approach depends on a representation of the solutions φ due to Povzner [208] and Levitan [175]:

$$\varphi(x,\lambda) = \frac{\sin(kx)}{k} + \int_0^x K(x,y)\, \frac{\sin(ky)}{k}\, dy, \tag{6.8}$$

where $\lambda = k^2$. In essence, (6.7) leads to a linear Volterra integral equation for K whose kernel is determined by ρ. Once one has K, one can determine V from (6.8) and $-\varphi'' + V\varphi = \lambda\varphi$ or from more direct relations of K to V.

The approach of Simon depends on a representation of m as a Laplace transform:

$$m(-\kappa^2) = -\kappa - \int_0^a A(\lambda)\, e^{-2\kappa a}\, d\alpha + O(e^{-2a\kappa}), \tag{6.9}$$

which determines A given m (there is also a direct relation of A to ρ given in Gesztesy-Simon [93]). One can introduce a second variable and function $A(x,\alpha)$ so $A(x=0,\alpha) \equiv A(\alpha)$. A obeys

$$\frac{\partial A}{\partial x} = \frac{\partial A}{\partial \alpha} + \int_0^\beta A(x,\beta) A(x,\alpha-\beta)\, d\beta \tag{6.10}$$

and

$$\lim_{\alpha\downarrow 0} A(x,\alpha) \equiv V(x). \tag{6.11}$$

In this approach, m determines $A(x=0,\,\cdot\,)$ by (6.9); the differential equation (6.10) determines $A(x,\alpha)$, and then (6.11) determines V.

Inverse spectral theory is connected to inverse scattering for short-range potentials since $d\rho$ on $[0,\infty)$ is determined by scattering data. Scattering data also determine the positions of the negative eigenvalues. One needs to supplement that with the weight of the pure points at these negative eigenvalues known as norming constants. Marchenko [190, 189] has an approach to inverse scattering related to the Gel'fand-Levitan approach by using a different representation than (6.8). When $\int_0^\infty x|V(x)|\, dx < \infty$, Levin [174] has proven that in $\operatorname{Im} k > 0$, there is a solution $\psi(x,k)$ of $-\psi'' + V\psi = k^2\psi$ given by

$$\psi(x,k) = e^{ixk} + \int_x^\infty \tilde{K}(x,y)\, e^{iky}\, dy.$$

Krein [162, 163, 164] also developed an approach to inverse problems. A different approach to inverse scattering is due to Deift-Trubowitz [61]. For another approach to inverse problems, see Melin [195]. Inverse theory for periodic potentials also has an extensive literature starting with Dubrovin-Matveev-Novikov [70], Its-Matveev [132], McKean-van Moerbeke [193], McKean-Trubowitz [192], and Trubowitz [268].

As for higher-dimensional inverse scattering, these scattering data overdetermine the potential. For example, for short-range V's, the scattering amplitude at fixed momentum transfer approaches the Fourier transform of V at large energy, so the large energy asymptotics of scattering determine V. There is considerable literature on recovering V from partial scattering data, which we will not try to summarize here.

One reason for the interest in inverse theory is the connection it sets up between spectral theory of Schrödinger operators and the analysis of certain

nonlinear PDEs like KdV (see Dodd et al. [68], Novikov et al. [199], and Belokolos [26]).

7. Ergodic Potentials

Let Ω be a compact metric space with probability measure $d\gamma$ and T_t with $t \in R^\nu$ or T_n with $n \in \mathbb{Z}^\nu$ be an ergodic family of measure-preserving transformations. Let $f : \Omega \to \mathbb{R}$ be continuous. For $\omega \in \Omega$, define

$$V_\omega(x) = f(T_x\omega) \tag{7.1}$$

and

$$H_\omega = -\Delta + V_\omega. \tag{7.2}$$

Note: To allow unbounded V's as seen, for example, in Gaussian random potentials, one wants to extend this picture to either allow f to be discontinuous and/or take values in $\mathbb{R} \cup \{\infty\}$, and/or allow Ω to be noncompact; for simplicity, we will discuss this model for motivation.

H_ω is a family of Schrödinger operators, not a single one, but by the ergodicity and an obvious translation covariance $V_{T_y\omega}(x) = V_\omega(x+y)$, many spectral properties occur with probability one. So one can speak of typical properties. In particular, it is known that the full spectrum Σ, the essential support of the absolutely continuous spectrum Σ_{ac}, the closure of the point spectrum $\overline{\Sigma}_{\text{pp}}$, and the singular continuous spectrum Σ_{sc} are a.e. constant in ω (see, e.g., Theorems 9.2 and 9.4 in Cycon et al. [53] for proofs; the result for Σ is due to Pastur [202] and the other results to Kunz-Souillard [165]). Note only $\overline{\Sigma}_{\text{pp}}$ is a.e. constant; Σ_{pp}, the actual set of eigenvalues is not.

Examples. 1. Let $\Omega = [a, b]^{\mathbb{Z}^\nu}$ and let $d\gamma$ be the infinite product of normalized Lebesgue measure on $[a, b]$. Let $(T_m\omega)_n = \omega_{n+m}$. The corresponding discrete Schrödinger operator is called the Anderson model and is typical of random potential models.

2. If Ω is a compact Abelian group with $\mathbb{Z}^\nu$ or $\mathbb{R}^\nu$ as dense subgroup, $d\gamma$ is Haar measure and T_x is group translate, then V is a periodic or almost periodic function. A frequently discussed example is

$$V(n) = \lambda \cos(\pi\alpha n + \theta), \tag{7.3}$$

where α is irrational, θ runs in $[0, 2\pi)$ (which is Ω), and λ is a parameter. The corresponding discrete Schrödinger operator is called the almost Mathieu model.

The simplest example of this framework—which is atypical in many ways—is the periodic potential. The basic facts in this case go back to the physics literature at the start of quantum mechanics (Bloch, Brillouin, Kramer, and Wigner) and, in one dimension, to work on Hill's equation (Floquet, Lyapunov, Hamel, and Haupt). A critical early mathematical paper on the multidimensional case is Gel'fand [89]. The key result is that for periodic V's

with a mild local regularity condition, $H = -\Delta + V$ has purely absolutely continuous spectrum. This result is discussed in detail in Reed-Simon [212, Section XIII.16]. The only subtle part of the argument is to eliminate the possibility of what are called flat bands, a result of Thomas [264].

In the mathematical physics literature, the period from 1975 onwards has seen enormous interest in the study of almost periodic and random models and special cases thereof. Three books that discuss this are part of Carmona-Lacroix [44], Cycon et al. [53], and Pastur-Figotin [203]. We will only touch some of the general principles, leaving the details—especially of detailed models—to the books and the vast literature. We will make references to the Lyapunov exponent without defining it; see Cycon et al. [53], Section 9.3.

For random potentials, the most interesting results concern localization. While the spectrum is typically an interval (e.g., for the Anderson model in ν-dimensions, it is $[a - 2\nu, b + 2\nu]$), the spectrum is pure point with eigenvalues dense in the interval and exponentially decaying eigenfunctions.

In one dimension, localization was first rigorously proven by Goldsheid, Molchanov, and Pastur [98] with a later alternative by Kunz-Souillard [165]. Following an idea of Kotani [159], Simon-Wolff [261] and Delyon-Levy-Souillard [63] found another proof. Typical is

Theorem 7.1. *For the one-dimensional Anderson model, the spectrum is* $[a - 2, b + 2]$ *and is pure point with probability one with eigenfunctions decaying at the Lyapunov rate.*

Carmona-Klein-Martinelli [43] and Shubin-Vakilian-Wolff [228] have approaches that work if the single site distribution is discrete (the other quoted approaches require an absolutely continuous component for this distribution).

In higher dimensions, the two main approaches to localization are due to Fröhlich-Spencer [87] (see also von Dreifus-Klein [270]) and to Aizenman-Molchanov [10]. (See also Aizenman-Graf [8] and Aizenman et al. [11].) Basically, these authors and the many papers that extend their ideas prove dense point spectrum in regimes where the coupling constant is large or one is near the edge of the spectrum. It is believed—but not proven—that in suitable regimes when $\nu \geq 3$, there is absolutely continuous spectrum.

For almost periodic models, one can have any kind of spectral type. The almost Mathieu model has been almost entirely analyzed and the spectral type shows a great variety. Recall this is the discrete model with potential

$$V_{\alpha,\lambda,\theta}(n) = \lambda \cos(\pi\alpha n + \theta),$$

where λ, α are fixed parameters and θ runs through Ω. Then

(i) If $\lambda < 2$, there is always (i.e., for any irrational α) lots of a.c. spectrum and it is known for some α and believed for all α that is all there is (see Last [169], Gesztesy-Simon [92], Gordon et al. [100], Jitomirskaya [134]; the earliest results of this genre are due to Dinaburg-Sinai [67]).

(ii) If $\lambda = 2$ and α is an irrational whose continued fraction integers are unbounded (almost all α have this property), then the spectrum is known to be purely singular continuous for almost all θ (see Gordon et al. [100]).

(iii) If $\lambda > 2$ and α is an irrational with good Diophantine properties ($|\alpha - \frac{p}{q}| \geq C\, q^{-\ell}$ for some C, ℓ and all $p, q, \in \mathbb{Z}$), then for a.e. θ, the spectrum is dense pure point (Jitomirskaya [134]; see also Bourgain-Goldstein [38].

(iv) If $\lambda > 2$ and α is irrational, there are always lots of θ (a dense G_δ) for which the spectrum is purely singular continuous (Jitomirskaya-Simon [136]). For some α, like those in (iii), the set while a dense G_δ has measure 0. For Liouville α (irrational α's with $\underline{\lim}\, \frac{1}{q} \ln |\sin \pi \alpha q| = -\infty$), the spectrum is purely singular continuous (Avron-Simon [22] using results of Gordon [99]).

In general, for almost periodic models, the spectral type is dependent on the number theoretic properties of the frequencies.

Among the general spectral results known for almost periodic models is that the spectrum is everywhere constant on Ω (rather than only almost everywhere constant; Avron-Simon [22]) and that the essential support of the a.c. spectrum is everywhere constant (Last-Simon [170]). It is known (see (iv) above) that $\bar{\sigma}_{\rm pp}$ and $\sigma_{\rm sc}$ may only be almost everywhere constant and fail to be constant on all of Ω.

8. Two-Body Hamiltonians

Hamiltonians of the form $-\Delta + V$ where $V(x) \to 0$ at infinity are often referred to as two-body Hamiltonians since the Hamiltonian of two particles with a potential $W(\vec{r}_1 - \vec{r}_2)$ reduces to $-\Delta + V$ (where V is a multiple of W depending on the masses) after removal of the center of mass. The issues are essentially the same as for one-dimensional decaying potentials as discussed in Section 5.

With regard to the negative spectrum, again Weyl's criterion easily shows that $\sigma_{\rm ess}(H) = [0, \infty)$ so that H has only discrete spectrum of finite multiplicity in $(-\infty, 0)$ and only 0 can be an accumulation point. Typical is:

Theorem 8.1. *For $\alpha \in \mathbb{Z}^\nu$, let χ_α be the characteristic function of the unit cube about α. Let $V : \mathbb{R} \to \mathbb{R}$. Suppose $V \in K_\nu$ and that as $\alpha \to \infty$, $\|\chi_\alpha V\|_{K_\nu} \to 0$. Then $\sigma_{\rm ess}(-\Delta + V) = [0, \infty)$.*

As for whether $N(V)$, the number of negative bound states (counting multiplicity, i.e., $N(V) = \dim E_{(-\infty,0)}(H)$), is finite or infinite, there is a considerable literature. The earliest bound is due to Birman [32] and Schwinger [227] for $\nu = 3$. It says

$$N(V) \leq \frac{1}{(4\pi)^2} \int \frac{|V(x)|\, |V(y)|}{|x-y|^2}\, dx\, dy \qquad (\nu = 3). \tag{8.1}$$

Perhaps the most famous bound is that of Cwickel [52], Lieb [177], and Rosenbljum [220]:

$$N(V) \leq L_{0,\nu} \int |V(x)|^{\nu/2}\, dx \qquad (\nu \geq 3). \tag{8.2}$$

One reason this is of special interest is that for nice V's as $\lambda \to \infty$, $N(\lambda V)/\int |\lambda V|^{\nu/2}\, dx$ converges to a universal constant (see Section 14). In particular, (8.1) has the wrong large λ behavior while (8.2) has the right such behavior. (Simon [243] had the first bounds with the right large λ behavior for nice enough V's; he also conjectured (8.2).)

As in the one-dimensional case, there are Lieb–Thirring-type bounds on the moments of the negative eigenvalues e_j of $-\Delta + V$

$$\sum_j |e_j|^\gamma \leq L_{\gamma,\nu} \int dx\, |V(x)|^{\gamma+\nu/2}\, d^\nu x$$

for $\gamma > 0$ if $\nu = 2$ and $\gamma \geq 0$ if $\nu \geq 3$. These were proven first in Lieb-Thirring [185]. There has been considerable literature on best values of $L_{\gamma,\nu}$. In particular, a recent pair of papers of Laptev-Weidl [168] and Hundertmark-Laptev-Weidl [124] has obtained a breakthrough in understanding the ν-dependence of $L_{\gamma,\nu}$. In particular, they show that for $\gamma \geq \frac{3}{2}$, $L_{\gamma,\nu}$ is given by the quasiclassical value. On the other hand, it is known that $L_{\gamma=0,\nu} > L^{\text{q.c.}}_{\gamma=0,\nu}$, the quasiclassical value for all ν (Helffer-Robert [109, 110]).

For a review of the literature on bounds on the number of eigenvalues, especially the subtle two-dimensional case, see Birman-Solomyak [36].

The absence of eigenvalues at positive energies is a specialized issue largely independent of the rest of the analysis of positive spectrum. Given the examples of Wigner-von Neumann and related ones of Naboko and Simon discussed in Section 5, one needs some condition on the falloff or lack of oscillations. Here is a simple result:

Theorem 8.2. *Let $V(x) = V_1(x) + V_2(x)$ where $|x|\,|V_1(x)| \to 0$ and $|(x \cdot \nabla)V_2(x)| \to 0$. Then $-\Delta + V$ has no eigenvalues in $[0, \infty)$.*

Remarks. 1. The stated theorem requires local regularity (V_1 bounded near infinity and V_2 is C^1), but there are extensions that allow local singularities.

2. Rellich [216] proved that if V has compact support, there are no positive energy eigenvalues. Theorem 8.2 when $V_2 = 0$ is due to Kato [150] and the full result to Agmon [2] and Simon [235].

3. See Froese et al. [86] for another result of this genre; we will discuss their result further in Section 9.

The methods we will discuss below typically show that $\sigma_{\text{pp}} \cap (0, \infty)$ is finite; one can then usually use Theorem 8.2 to prove that the set is actually empty.

As for positive spectrum, it is intimately related to scattering theory. Given two self-adjoint operators A, B, one says the wave operators exist if

$$\Omega^{\pm}(A,B) = \operatorname*{s-lim}_{t\to\mp\infty} e^{itA}e^{-itB}P_{\mathrm{ac}}(B)$$

exists where P_{ac} is the projection onto the a.c. subspace for B. We say they are complete if $\operatorname{Ran}\Omega^{\pm}(A,B) = \operatorname{Ran}P_{\mathrm{ac}}(A)$, in which case $\Omega^{\pm}(A,B)$ are unitary maps of $\operatorname{Ran}P_{\mathrm{ac}}(B)$ to $\operatorname{Ran}P_{\mathrm{ac}}(A)$ which intertwine A and B. See Reed-Simon [213], Baumgärtel-Wollenberg [25], or Yafaev [277] (or many other books) for a discussion of the physics involved.

The development of abstract scattering theory is closely intertwined (pun intended) to its applications to Schrödinger operators. Fundamental work was done by Jauch [133], Cook [51], Rosenblum [221], Kato [149], Birman [33], and Birman-Krein [35].

The basic result for positive spectrum for "short-range" potentials is:

Theorem 8.3. *Let V be such that $(1+|x|)^{1+\varepsilon}V(x) \in L^p + L^\infty(\mathbb{R}^\nu)$ for $\max(2,\frac{\nu}{2}) < p < \infty$ and let $H = -\Delta + V$ and $H_0 = -\Delta$. Then $\Omega^{\pm}(H,H_0)$ exist and are complete. Moreover, H has no singular continuous spectrum and any eigenvalues in $(0,\infty)$ are isolated (from other eigenvalues) and of finite multiplicity.*

Remarks. 1. The first results on absence of singular continuous spectrum depended on eigenfunction expansions and were obtained by Povzner [209] (V's of compact support) and Ikebe [129] (V's which were $O(|x|^{-2-\varepsilon})$ at infinity). The earliest results on completeness of wave operators depended on the trace class theory of scattering (of Rosenblum [221] and Kato [149]) and were obtained by Kuroda [166, 167]. From 1960 to 1972, the decay was successively improved until Agmon [3] obtained the $O(|x|^{-1-\varepsilon})$ result quoted.

2. Enss [77] has a different, quite physical, approach to this result. Enss' work depends in part on an earlier geometric characterization of the continuous subspace of a Schrödinger operator by Ruelle [222] and Amrein-Georgescu [14]. This is sometimes called the RAGE theorem after the initials of the authors.

3. It is known (e.g., Dollard [69]) that if $V(x) = O(|x|^{-1})$, $\Omega^{\pm}(H,H_0)$ may not exist.

For long-range behavior decaying slower than $O(|x|^{-1})$, there are results if ∇V decays faster than $O(|x|^{-1-\varepsilon})$. Basically, there is only a.c. spectrum at positive energy if $V = V_1 + V_2$ with $V_1 = O(|x|^{-1-\varepsilon})$ and $x\cdot\nabla V_2 = O(|x|^{-\varepsilon})$. For details, see Lavine [172], Agmon-Hörmander [6], and Hörmander [122]. These works use modified wave operators as introduced by Dollard [69].

9. N-Body Hamiltonians

Let $\widetilde{H}$ be the Hamiltonian of N particles in $\mathbb{R}^\nu$. Explicitly, $\widetilde{H}$ is an operator on $L^2(\mathbb{R}^{\nu N})$ given by $\widetilde{H} = \widetilde{H}_0 + V$ where

$$\widetilde{H}_0 = -\sum_{j=1}^{N} \frac{1}{2m_j}\,\Delta_{x_j}$$

with $x = (x_1, \dots, x_N)$ a point in $\mathbb{R}^{\nu N} = \mathbb{R}^\nu \times \mathbb{R}^\nu \times \cdots \times \mathbb{R}^\nu$ (N times) and

$$V = \sum_{i<j} V_{ij}(x_i - x_j)$$

with V_{ij} a function in $\mathbb{R}^N$ which decays at infinity. There is a standard way of removing the center of mass and getting an associated Hamiltonian H on $L^2(\mathbb{R}^{\nu(N-1)})$. For a more extensive review of the subject than this brief discussion, see Hunziker-Sigal [128].

For any partition a of $\{1, \dots, N\}$ into disjoint subsets, one defines $I(a) = \sum_{(i,j)\not\subset a} V_{ij}$ over the pairs (i, j) in distinct clusters and $H(a) = H - I(a)$.

The issues one faces are similar to those in the two-body case but often more subtle. The first thing one needs to establish about N-body systems is where the essential spectrum of H lies. The result involves

$$\Sigma(a) = \inf \operatorname{spec}(H(a)) \tag{9.1}$$

$$\Sigma = \min_{\#a \geq 2} (\Sigma(a)). \tag{9.2}$$

Σ is the minimum energy the system can have after it is broken into two pieces moved very far from each other. That makes the following physically attractive:

Theorem 9.1. (HVZ Theorem) *Suppose each V_{ij} viewed as an operator on $L^2(\mathbb{R}^\nu)$ obeys $V_{ij}(-\Delta_{ij} + 1)^{-1}$ is compact. Then*

$$\sigma_{\text{ess}}(H) = [\Sigma, \infty).$$

Remarks. 1. The name "HVZ" comes from work of Hunziker [126], van Winter [269], and Zhislin [280] who first proved it.

2. The original proofs used resolvent equations; a geometric proof was later found by Enss [76] and Simon [244].

The next issue is whether the discrete spectrum is finite or infinite. A great deal of attention has been paid to atomic or ionic Hamiltonians. Define on $L^2(\mathbb{R}^{3N})$:

$$H_M(N, Z) = \sum_{i=1}^{N} \left(-\Delta_i - \frac{Z}{|x_i|} \right) + \frac{1}{M} \sum_{i<j} \nabla_i \cdot \nabla_j + \sum_{i<j} \frac{1}{|x_i - x_j|}$$

which describes N electrons moving around a nucleus of charge Z and mass M. A basic result says that neutral atoms and positive ions always have an infinite number of bound states:

Theorem 9.2. (Zhislin [280]) *If $N \leq Z$, $\dim E_{(-\infty,\Sigma)}(H_M(N,Z)) = \infty$ for any M (including $M = \infty$).*

Remarks. 1. The first result of this genre was Kato [145] who proved the result if $N = Z = 2$ and $M = \infty$ (Helium). He did not properly handle $M < \infty$ because he did not use the right coordinate systems. As shown by Simon [236], Kato's idea, which involved placing $N-1$ electrons in the ground states for the $N-1$ ion and the Nth in a hydrogen-like state around the core, can prove Theorem 9.2.

2. This result holds even if one adds Fermi statistics (see, e.g., Simon [236]).

3. If Z is not restricted to be an integer, the proper condition is $N < Z+1$.

As for negative ions, we have

Theorem 9.3. (Zhislin [281]) $\dim E_{(-\infty,\Sigma)}(H_M(Z+1,Z)) < \infty$

Remarks. 1. This result also has a geometric proof by Sigal [231] and Simon [244].

2. This result may not be true for fermion electrons because the $N-1$ problem may have a degenerate ground state which allows one with a nonzero dipole moment.

3. While it is presumably true that $\dim E_{(-\infty,\Sigma)}(H_M(N,Z)) < \infty$ for all $N \geq Z+1$, that is not known.

Finally, with regard to bound states of atoms, there is the issue of when $\dim E_{(-\infty,\Sigma)} = 0$. The result is the following:

Theorem 9.4. *Let $M = \infty$.*

(a) (Ruskai [223, 224] and Sigal [231, 232]) *For any Z, there is an $N_0(Z)$ so that for $N \geq N_0(Z)$, there is no spectrum in $(-\infty, \Sigma)$. $N_0(Z)$ denotes the smallest N_0 for which this true.*

(b) (Lieb et al. [181]) *For fermions, $N_0(Z)/Z \to 1$ as $Z \to \infty$.*

(c) (Benguria-Lieb [28]) *Without Fermi statistics, $N_0(Z) > 1.2Z$ for Z large.*

(d) (Lieb [178]) $N_0(Z) \leq 2Z$.

Remarks. 1. If $N \geq N_0$, then $\inf \operatorname{spec}(H(N,Z)) = \inf \operatorname{spec}(H(N_0,Z)) < \inf \operatorname{spec}(H(N_0-1,Z))$.

2. Some of these results hold if $M < \infty$.

With short-range potentials, the situation is simple if the bottom of the essential spectrum is two body. Define

$$\Sigma_3 = \min_{\#(a)\geq 3}(\Sigma(a)).$$

Then (see Cycon et al. [53, Section 3.9]),

Theorem 9.5. (Sigal [231]) *Suppose $\Sigma_3 > \Sigma$, $\nu \geq 3$, and each V_{ij} lies in $L^{\nu/2}(\mathbb{R}^\nu)$. Then $\dim E_{(-\infty,\Sigma)}(H) < \infty$.*

On the other hand, if $\Sigma_3 = \Sigma$, there can be an infinite number of bound states even if the V_{ij}'s have compact support (in x_{ij}). In particular, if $N = 3$, $V_{12} = V_{23} = V_{13} = -c\chi_1$ with χ the characteristic function of a unit ball and c chosen so that $\inf \operatorname{spec}(H) = 0$ but $\inf \operatorname{spec}(H + \varepsilon V) < 0$ for all $\varepsilon > 0$, it is known that $\dim E_{(-\infty,0)}(H) = \infty$. This is known as the Efimov effect after work of Efimov [74, 75]. For proofs of this phenomenon, see Yafaev [276] and Ovchinnikov-Sigal [201].

In analyzing the spectrum of H on $[\Sigma, \infty)$, a particular class of physically significant energies occurs, the thresholds. For each partition a of $\{1, \dots, N\}$ with $\#a \geq 2$, there is a natural decomposition of $L^2(\mathbb{R}^{\nu(N-1)}) = \mathcal{H}_a \otimes \mathcal{H}^a$ where $\mathcal{H}_a$ are functions of $x_i - x_j$ with i and j in the same cluster of a and $\mathcal{H}^a$ are functions of $R_\alpha - R_\beta$ where R_α is the center of mass of a cluster (see [128] for an elegant way of doing this kinematics). Under the decomposition $H(a) = H_a \otimes I + I \otimes T^a$. H_a is the internal energy of the cluster and T^a the kinetic energy of the cluster centers of mass. $\mathcal{I}(a)$ is the set of eigenvalues of H_a (with the condition that if $\#(a) = N$, so H_a is 0 on $\mathbb{C}$, then $\mathcal{I}(a) = \{0\}$. The set of thresholds is defined to be

$$\mathcal{I} = \bigcup_a \mathcal{I}(a).$$

Note: An energy in $\mathcal{I}(a)$ is a sum of eigenvalues of individual cluster Hamiltonians. In particular, the statement in the theorems below that the set of thresholds is a closed countable set follows by induction from the other statement that eigenvalues can only accumulate at thresholds.

The three-body problem turns out to have some aspects that make it simpler than the general N-body problem, and Faddeev [79] and later Enss [78] (using very different methods) have fairly complete results on spectral and scattering theory for $N = 3$. We will focus here on results that apply for all N.

Historically, the first aspect of the continuous spectrum for general N-body systems controlled was the absence of singular continuous spectrum. The earliest result required analyticity of the potentials but included atoms:

Theorem 9.6. (Balslev-Combes [23]) *Suppose each $V_{ij}(x) = f_{ij}(x_i - x_j)$ where f_{ij} is a function on $\mathbb{R}^\nu \backslash \{0\}$ that obeys*

$$A(\theta) = V(e^\theta x)(-\Delta + 1)^{-1}$$

is compact and has an analytic continuation from $\theta \in \mathbb{R}$ to $\{\theta \mid |\operatorname{Im} \theta| < \varepsilon\}$ for some $\varepsilon > 0$. Then $\sigma_{\mathrm{sc}}(H) = \emptyset$.

Moreover,

(i) *Any eigenvalue of H in $\mathbb{R} \backslash \mathcal{I}$ is of finite multiplicity, and eigenvalues can only accumulate at thresholds.*
(ii) *The set of eigenvalues union thresholds is a closed countable set.*

Remarks. 1. Such potentials are called dilation analytic.

2. This result was first proven for two-body systems by Aguilar-Combes [7].

3. See Simon [237, 238] for extensions of this result.

The most general results on absence of singular continuous spectrum depend on ideas of Mourre [196].

Theorem 9.7. *Suppose $V_{ij}(x) = f_{ij}(x_i - x_j)$ where f_{ij} is a function on $\mathbb{R}^\nu$ that obeys (as operators on $L^2(\mathbb{R}^\nu)$)*

(i) *$f_{ij}(x)(-\Delta + 1)^{-1}$ is compact*

(ii) *$(-\Delta + 1)^{-1} x \cdot \nabla f_{ij}(-\Delta + 1)^{-1}$ is compact.*

Then $\sigma_{\text{ess}}(H)$ is empty. Moreover, any eigenvalue in $\mathbb{R}\backslash\mathcal{I}$ is discrete, eigenvalues can only accumulate at thresholds, and the set of eigenvalues and thresholds is a closed countable set.

Remarks. 1. This theorem was proven for $N = 3$ by Mourre [196]. His methods were extended and elucidated by Perry-Sigal-Simon [205] who obtained the general N-body result. Substantial simplifications of the proof were found by Froese-Herbst [85].

2. Condition (ii) does not require that f_{ij} be smooth because $\nabla f_{ij} = [\nabla, f_{ij}]$ and $\nabla(-\Delta + 1)^{-1}$ is bounded. Basically, (i), (ii) hold if $f_{ij} = f_{ij}^{(1)} + f_{ij}^{(2)}$ where $x f_{ij}^{(1)}(-\Delta + 1)^{-1}$ is compact and $f_{ij}^{(2)}$ is smooth with $(x \cdot \nabla) f_{ij}^{(2)}(-\Delta + 1)^{-1}$ and $f_{ij}^{(2)}(-\Delta + 1)^{-1}$ compact.

3. Froese-Herbst [85] have some general results that imply that $\mathcal{I} \cap (0, \infty) = \emptyset$ (see Thm. 4.19 in Cycon et al. [53]).

Finally, there has been extensive study of scattering theory and completeness. For each cluster with $\#(a) \geq 2$, let P_a on $\mathcal{H}_a$ be the projection onto the point spectrum of H_a and let $P(a) = P_a \otimes I$, the projection onto vectors which are bound within the clusters and arbitrary for the centers of mass coordinates. The cluster wave operators are defined by

$$\Omega^{\pm}(a) = \operatorname*{s-lim}_{t \to \mp\infty} e^{+itH} e^{-itH(a)} P(a). \tag{9.3}$$

$\text{Ran}(\Omega^+(a))$ are those states which in the distant past look like bound clusters (coresponding to the partition a) moving freely relative to one another.

The existence of cluster wave operators (9.3) was proven first by Hack [103]. It is not hard to see (e.g., Theorem XI.36 in Reed-Simon [213]) that for $a \neq b$, $\text{Ran}\,\Omega^+(a)$ is orthogonal to $\text{Ran}\,\Omega^+(b)$. Asymptotic completeness is the statement that

$$\bigoplus_{\#(a) \geq 2} \text{Ran}(\Omega^+(a)) = \mathcal{H}_{\text{ac}}(H),$$

where $\mathcal{H}_{\text{ac}}(H)$ is the absolutely continuous subspace for H. After fairly general results for $N = 3$ (Faddeev [79] and Enss [78]) and for general N with weak coupling (Iorio-O'Carroll [131]) and repulsive potentials (Lavine [171]), Sigal and Soffer [233] solved the general result. Their theorem is

Theorem 9.8. (Sigal-Soffer [233]) *If each* $V_{ij}(x) = f_{ij}(x_i - x_j)$ *where* $|(D^\alpha f_{ij}(x)| \leq C(1+|x|)^{-|\alpha|-\varepsilon-1}$ *for all multi-indices with* $|\alpha| \leq 2$, *then asymptotic completeness holds.*

Extensions and clarifications of this work are due to Graf [101], Hunziker [127], and Yafaev [278]. Long-range potentials are discussed in Derezinski [65], Sigal-Soffer [234], and Derezinski-Gerard [66].

10. Constant Electric and Magnetic Fields

Quantum mechanics with a potential and constant electric or magnetic field played a critical role experimentally and theoretically in the earliest days of the subject, and there has been considerable mathematical literature on the spectral properties of these operators. The basic Stark Hamiltonian on $L^2(\mathbb{R}^\nu)$ is

$$H = -\Delta + Ex_1 + V(x), \tag{10.1}$$

where V is short range. A key role has been played by an explicit formula of Avron-Herbst [18] for the operator when $V = 0$, viz.,

$$\exp(-it(-\Delta + x_1)) = \exp(-it^3/3)\exp(-itx_1)\exp(-it\Delta + ip_1t^2), \tag{10.2}$$

where $p_1 = \frac{1}{i}\frac{\partial}{\partial x_1}$. Classically in an electric field, a particle has $x_1 = N - ct^2$ as $t \to \infty$ and (10.2) realizes this with the p_1t^2 term. It means the borderline for short range is $|x|^{-1/2-\varepsilon}$ rather than $|x|^{-1-\varepsilon}$. The result is

Theorem 10.1. *Suppose* $|V(x)| \leq C(1+|x|)^{-\varepsilon}(1+|x_1|)^{-1/2-\varepsilon}$. *Then* H *given by* (10.1) *has complete wave operators and empty singular continuous spectrum. Eigenvalues are isolated and of finite multiplicity.*

This result and ones similar to it are discussed by Herbst [114], Yajima [279], and Simon [249]. Multiparticle completeness in electric fields has been studied by Herbst-Møller-Skibsted [116], and Adachi-Tamura [1].

There is a large literature on both constant and variable magnetic fields but an extensive review of it is beyond the scope of this article. One can begin looking at the literature by consulting a series by Avron, Herbst, and Simon [19, 20, 21] and Chapter 6 of Cycon et al. [53] and references therein. See also Section 12.

11. Coulomb Energies

While much of the mathematical theory of nonrelativistic quantum mechanics has focused on general potentials, nature uses the Coulomb potential and there is considerable literature on binding energies of Coulomb systems, especially as some parameter goes to infinity. Section 9 (see Theorem 9.4) already discussed one such result. We will only introduce some seminal themes; consult Lieb [179] for a review of the subject.

The most famous of these results is the stability of matter. In its simplest form, it concerns the Hamiltonian

$$H(N,M;R_1,\dots,R_M) = \\ -\sum_{i=1}^{N}\Delta_i - \sum_{i,\alpha}\frac{1}{|x_i-R_\alpha|} + \sum_{i<j}\frac{1}{|x_i-x_j|} + \sum_{\alpha<\beta}\frac{1}{|R_\alpha-R_\beta|}$$

of N electrons moving in the field of M infinitely massive protons. Let $\mathcal{H}_f$ be the functions on $L^2(\mathbb{R}^{3N})$ thought of as functions $\psi(x_1,\dots,x_N)$ of N variables in $\mathbb{R}^3$ which are antisymmetric, that is,

$$\psi(x_{\pi(1)},\dots,x_{\pi(n)}) = (-1)^\pi\psi(x_1,\dots,x_N)$$

for any permutation, π; that is, $\mathcal{H}_f$ is the wave function with Fermi statistics (we ignore spin which is easily accommodated). Define

$$E(N,M) = \inf_{\substack{\psi\in\mathcal{H}_f \\ R_1,\dots,R_M}} \langle\psi, H(N,M;R_1,\dots,R_M)\psi\rangle.$$

Stability of matter says that

$$E(N,M) \geq -c(N+M). \tag{11.1}$$

Among other things, this bound is important because it is equivalent to the fact that the radius of a chunk of matter with $N = M$ does not shrink to zero as $N\to\infty$.

The first proof of (11.1) was obtained by Dyson-Lenard [72, 73] with a constant C that was many powers of ten too large. Lieb-Thirring [186] found an elegant proof with a constant C that is on the order of magnitude of Rydbergs. The result (11.1) fails if one does not impose Fermi statistics (see Dyson [71] and Conlon-Lieb-Yau [50]). Extensions that involve relativistic kinetic energy, magnetic and/or radiation fields can be found in Conlon [49], Lieb-Loss-Solovej [180], and Fefferman-Fröhlich-Graf [81].

Another Coulomb energy problem that has been extensively studied is the total binding energy in the limit of large of Z. One defines

$$H(N,Z) = \sum_{i=1}^{N}\left(-\Delta_i - \frac{Z}{|x_i|}\right) + \sum_{i<j}\frac{1}{|x_i-x_j|}$$

on $\mathcal{H}_f$ and

$$E(N,Z) = \inf_{\psi\in\mathcal{H}_f}\langle\psi, H(N,Z)\psi\rangle$$

and

$$E(Z) = \min_N E(N,Z).$$

One knows that

$$E(Z) = \alpha Z^{7/3} + \beta Z^2 + \gamma Z^{5/3} + o(Z^{5/3}). \tag{11.2}$$

The α term is given by Thomas-Fermi theory and this leading asymptotics was proven by Lieb-Simon [182]. The β term is called the Scott correction and it was established by a combination of ideas of Hughes [123] and Siedentop-Weikard [229, 230]. The full asymptotics (11.2) was obtained by Fefferman-Seco [82]. Results for large Z and large magnetic field can be found in Lieb-Solovej-Yngvason [183, 184].

12. Eigenvalue Perturbation Theory

Some of Schrödinger's earliest papers on quantum mechanics concerned eigenvalue perturbation theory. Kato's book [153] is a source of detailed information on what we will call regular and asymptotic perturbation theory below. A review of some of the other aspects can be found in Reed-Simon [212] and Simon [254].

If A is self-adjoint and B is A-bounded in the sense of (3.3), and if E_0 is a simple eigenvalue of A, then for β small, $A+\beta B$ has a unique eigenvalue $E(\beta)$ near E_0 and $E(\beta)$ is analytic in β. This is a result of Rellich [215] and Kato [142, 143]. An example is

$$-\Delta_1 - \Delta_2 - \frac{1}{|x_1|} - \frac{1}{|x_2|} - \frac{1}{Z}\,\frac{1}{|x_1 - x_2|} \tag{12.1}$$

about $\frac{1}{Z} = 0$ which is equivalent after scaling (of space and energy) to

$$-\Delta_1 - \Delta_2 - \frac{Z}{|x_1|} - \frac{Z}{|x_2|} + \frac{1}{|x_1 - x_2|}\,.$$

The numerical radius of convergence in $|\frac{1}{Z}|$ is about 1.06 so $H(Z=2)$ and $H(Z=1)$ are both included. Kato [147] developed the theory for form perturbations. Rellich and Kato included degenerate eigenvalues.

Titchmarsh [265, 266] and Kato [146] also developed the theory of asymptotic situations like the anharmonic oscillator

$$-\frac{d^2}{dx^2} + x^2 + \beta x^4, \tag{12.2}$$

where each eigenvalue $E_n(\beta)$ for $\beta > 0$ has an asymptotic series

$$E_n(\beta) \sim \sum_{n=0}^{\infty} a_n \beta^n$$

even though this series can be divergent (and is for the case (12.2), as shown by Bender-Wu [27]). See Herbst-Simon [117] for an example where an asymptotic series converges but to the wrong answer! See Simon [252] for a study of multiwell problems.

In some cases, including (12.2), it is known that the divergent perturbation series can be made to give the right eigenvalue with a summability method, either Padé approximation (Loeffel et al. [187]) or Borel summation (Graffi et al. [102]). Borel summability is also known to work for the

Zeeman series for hydrogen-hydrogen perturbed by turning on a constant magnetic field; see Avron-Herbst-Simon [21] and Avron et al. [17].

In certain cases, eigenvalues are perturbed into resonances, the subject of Section 13. For eigenvalues embedded in continuous spectrum under regular perturbations (like (12.1)), the convergence of the perturbation series for a resonance and its related time-dependent perturbation theory and the Fermi golden rule is discussed in Simon [237, 238]. For Stark Hamiltonians, the basic paper is Herbst [115]. Harrell-Simon [107] found the leading resonance asymptotics in this case.

13. Resonances

Almost everything we have discussed so far has involved a single operator and properties invariant under unitary transformations. The notion of resonances has got to involve additional structure. For example, the operators $-\Delta - |x|^{-1} - Fx = H(F)$ are unitarily equivalent for all $F \neq 0$. But according to the physics lore, there is a resonance with an F-dependent position. We will not emphasize the extra structure, but it is there. We will focus on two definitions of resonances: one suitable for potentials that decay very rapidly (see Zworski [284, 285] for reviews) and the method of complex scaling already discussed in a different context in Section 9. (See Reed-Simon [212] and Simon [245] for reviews.)

Let ν be an odd dimension, let V be a bounded potential of compact support on $\mathbb{R}^\nu$, and for $\operatorname{Re}\kappa > 0$, define

$$B(\kappa) = |V|^{1/2}(-\Delta + \kappa^2)^{-1}V^{1/2},$$

where $V^{1/2} = |V|^{1/2}\operatorname{sgn}(V)$. Then $-\kappa^2$ is an eigenvalue of $-\Delta + V$ if and only if -1 is an eigenvalue of $B(\kappa)$. Since ν is odd, $B(\kappa)$ has an analytic continuation as a compact operator-valued function of κ to all of $\mathbb{C}$ (when $\nu = 1$, there is a simple pole at $\kappa = 0$ but $\kappa B(\kappa)$ is entire). If $\operatorname{Re}\kappa < 0$ and -1 is an eigenvalue of $B(\kappa)$, we say $-\kappa^2$ is a resonance of $-\Delta + V$.

Froese [83] has a lovely formula that relates resonances defined by this method to scattering theory. For all κ, $B(\kappa) - B(-\kappa)$ is trace class so $(1 + B(-\kappa))(1 + B(\kappa))^{-1}$ is 1 plus trace class and has a determinant as an operator on $L^2(\mathbb{R}^\nu)$. For k real and $S(k)$, the S-matrix on $L^2(S^{\nu-1})$,

$$\det(S(k)) = \det((1 + B(-ik))(1 + B(ik))^{-1}),$$

so resonances are related to poles of the analytic continuation of S.

There has been considerable literature on the number of resonances. Let $N(R)$ be the number of resonances with energy E obeying $|E| < R$. In one dimension, one has a complete result:

Theorem 13.1. (Zworski [282]) *Let $\nu = 1$ and suppose $[a, b]$ is the convex hull of the support of V. Then*

$$\lim_{R\to\infty} R^{-1/2}N(R) = \frac{2}{\pi}\,|b - a|.$$

Remarks. 1. The result depends on a theorem of Titchmarsh and Cartwright on the zeros of Fourier transforms of functions of compact support.

2. Froese [83] has obtained some results for cases when a potential decays faster than any exponential but may not have compact support.

In higher dimensions, much less is known. Zworski [283] proved that for V of compact support, $N(R) \leq C(R+1)^{\nu/2}$ (see also Froese [84]). On the other hand for general V's, it is only known (Sá Barreto-Zworski [225]) that $\lim_{R\to\infty} N(R) = \infty$.

Suppose V is a dilation analytic potential in the sense of Theorem 9.6. Let

$$H(\theta) = -e^{-2\theta}\Delta + V(e^{\theta}r).$$

Because of the analyticity assumption, $H(\theta)$ is analytic in $\{\theta \mid |\operatorname{Im}(\theta)| < \alpha\}$ for some α. Then Aguilar-Combes [7] found the essential spectrum of $H(\theta)$ for $N = 2$ and Balslev-Combes [23] for general N:

Theorem 13.2. $\sigma_{\text{ess}}(H(\theta)) = \cup_{E\in\mathcal{I}(\theta)}(E + e^{-2\theta}\mathbb{R})$

Remarks. 1. $\mathcal{I}(\theta)$ is the thresholds of $H(\theta)$ defined analogously to the case $\theta = 0$. It is not hard to see that $\sigma_{\text{ess}}(H(\theta))$ and $\mathcal{I}(\theta)$ depend only on $\operatorname{Im}\theta$.

2. If $\operatorname{Im}\theta > 0$, $\sigma_{\text{ess}}(H(\theta)) \cap \mathbb{R}$ consists precisely of $\mathcal{I}$. Basically as we increase $\operatorname{Im}\theta$ from 0, the essential spectrum rotates about the thresholds. In doing that, it can uncover resonances.

Resonances defined by this method have been used by quantum chemists for numerical calculations as well as a theoretical tool. Simon [237, 238] used it to study the Fermi golden rule and Harrell-Simon [107] to prove various one-dimensional tunnelling estimates.

Avron [16] used these ideas to study large-order perturbation theory for Hydrogen in a magnetic field; a rigorous proof of his results was obtained by Helffer-Sjöstrand [112].

Herbst [115] has extended the ideas to Hamiltonians with constant electric field. Among his results is the surprising one that if $0 < \operatorname{Im}\theta < \frac{\pi}{3}$, then $-e^{-2\theta}\Delta + e^{\theta}x$ has empty spectrum!

14. The Quasiclassical Limit

There has been considerable literature on the connection between quantum and classical mechanics. Much of it has focused on what happens as $\hbar \to 0$, but there are other limiting situations where a classical or semiclassical picture is appropriate—for example, the large Z limit of atoms. We will touch on some of the subjects considered, but the literature is vast. Robert [219] has an excellent review of those results obtained for very smooth potentials using the Fourier integral operator methods pioneered by Hörmander and Maslov. Therefore, I will not try to cover these results here. We note that in Section 11, we referenced the Thomas-Fermi limit, which is quasiclassical.

Consider first the $\hbar \downarrow 0$ limit. Let $H_\hbar = -\frac{\hbar^2}{2m}\Delta + V$. Kac [140, 141] had the idea that the small $\hbar$ limit of $\exp(-sH_\hbar)$ was the same as the zero time limit in Brownian motion. This allows one to prove under great generality that the quantum partition function $\mathrm{Tr}(\exp(-sH_\hbar))$ approaches a classical partition function as $\hbar \downarrow 0$; see, for example, Theorem 10.1 in Simon [246]. The earliest results I know of on this subject are due to Berezin [31].

Quantum dynamics, $e^{-isH_\hbar/\hbar}\psi_\hbar$, on suitable states $\psi_\hbar$ make an elegant classical limit—one takes $\psi_\hbar$ to be a coherent state which collapses to a single point in phase space as $\hbar \downarrow 0$. Such results were found by Hagedorn [104, 105, 106] (similar methods were developed independently by Ralston [210]).

Since $-\hbar^2\Delta + V = \hbar^2[-\Delta + \hbar^{-2}V]$, the small $\hbar$ limit is the same as the large coupling constant limit for $-\Delta + \lambda V$. In particular, if $N(V) = \dim E_{(-\infty,0)}(-\Delta + V)$, the quantity discussed in Section 8, one has

Theorem 14.1. *Let $\nu \geq 3$ and $V \in L^{\nu/2}(\mathbb{R}^\nu)$. Then $\lim_{\lambda\to\infty} N(\lambda V)/\lambda^{\nu/2} = (2\pi)^{-\nu}\tau_\nu \int_{V\leq 0}(-V(x)^{\nu/2}\, d^\nu x$ where τ_ν is the volume of a unit ball in $\mathbb{R}^\nu$.*

Remarks. 1. This theorem is quasiclassical since the right side is $(2\pi)^{-\nu}$ times the volume of the classical phase space region where $p^2 + V(x) \leq 0$.

2. The historical thread for this theorem goes back to a celebrated paper of Weyl [274] on Dirichlet Laplacians. Theorems like 14.1 with stronger conditions on V are due to Birman-Borzov [34], Kac [141], Martin [191], and Tamura [263]. See Reed-Simon [212, Theorem XIII.80] for the proof under the stated assumptions.

Let $V(x) \to \infty$ as $|x| \to \infty$ in a fairly regular way (e.g., suppose V is an elliptic polynomial). Then $-\Delta + V$ has discrete spectrum and the asymptotics of the number of eigenvalues $\dim E_{(-\infty,\alpha]}(-\Delta + V)$ as $\alpha \to \infty$ is determined by phase space. Results of this type go back to Titchmarsh [267]; see also Reed-Simon [212, Theorem XIII.81]. Similarly, if $V(x) \to 0$ but so slowly that $N(V) = \infty$, for example, $V(x) \sim -|x|^{-\beta}$ with $0 < \beta < 2$, then the divergence of $\dim E_{(-\infty,\alpha]}(-\Delta + V)$ as $\alpha \uparrow 0$ is sometimes given by quasiclassical considerations; see Brownell-Clark [40], McLeod [194], and Reed-Simon [212, Theorem XIII.82].

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