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AN INTRODUCTION TO THE SELF-ADJOINTNESS AND SPECTRAL ANALYSIS OF SCHRÖDINGER OPERATORS

by

B. SIMON
Departments of Mathematics and Physics
Princeton University
Princeton, N.J.08540
USA

§1. INTRODUCTION

We will give an introduction to the study of Schrödinger operators, $-\Delta+V$. Even though I can skip general features of N-body systems and of scattering which will be discussed in detail by the other speakers, I will still only be able to scratch the surface of an extensive subject with a large literature. For references until 1966, the reader can consult the excellent review article of Kato [19] – we will mainly give more recent references. Among the monograph references, we recommend Faris [14], Kato [20], Reed-Simon [29,30,31] and Thirring [44].

The two aspects of the study of Schrödinger operators we discuss are "self-adjointness" and "spectral analysis". These rather forbidding mathematical terms are really code words for two important elements of the physics of quantum systems. "Self-adjointness" is equivalent to the unique solvability of the time-dependent Schrödinger equation $i\dot{\psi}_t = H\psi_t$ for all times. "Spectral analysis" is the abstract study of the eigenfunctions of H - both discrete and continuous. I need hardly remind you that Schrödinger's original series of papers [33] was entitled "Quantization as an Eigenvalue Problem".

It is a great honor to speak at this symposium on the 50th anniversary of Schrödinger's equation and I am glad to dedicate this review first to the memory of E. Schrödinger, first founder of the subject. I should like to point out that this is a double anniversary. This year is also the 25th anniversary of the publication of Kato's basic paper [18] on the self-adjointness of atomic Hamiltonians - his paper, by shifting emphasis from abstract to concrete problems gave birth to the theory of Schrödinger operators, a theory, to which he has continued to make important contributions. It is a pleasure to dedicate this review also to Tosio Kato, our subject's second founder.

I have tried to write this review in a way that it might be readable to a physicist with relatively little mathematical sophistification. Unfortunately I have found it impossible not to occasionally fall into the jargon of spaces, Hilbert spaces and even simple operator theory (see §I,II,VI of [29]).

§2. SELF-ADJOINTNESS - WHAT'S IT ALL ABOUT

In this section, I want to explain the basic results about self-adjointness from a point of view different from the more usual presentation (see e.g. §VIII of [29]). The more usual presentation depends on the notion of adjoint - it seems to me that its use in virtually all pedagogic treatments is a legacy of the original development of the theory by Stone [41] and von Neumann [45]. Our treatment will emphasize the connection with solvability of the Schrödinger equation. The sophisticated reader will note how similar the theory then looks to the theory of contraction semigroups on a Banach space (§X.8 of [30]).

Definition. A unitary one-parameter group is a family $U(t)$ (one for each real t) of linear operators on a Hilbert space, $\mathcal{H}$, so that

(i) $t \to U(t)\psi$ is continuous for each ψ in $\mathcal{H}$,

(ii) $U(t+s) = U(t)\,U(s)$; $U(0) = 1$,

(iii) $\|U(t)\psi\| = \|\psi\|$, all t, all ψ in $\mathcal{H}$.

The intuitive model for such families is the following. For each "nice" $\psi \in \mathcal{H}$, we solve the equation $i\dot{\psi}_t = H\psi_t$ with initial condition $\psi_{t=0} = \psi$ and then set $U(t)\psi$ to be ψ_t. (iii) which expresses "conservation of probability" can then be used to extend $U(t)$ from "nice" ψ to all ψ. According to Schrödinger, the Hamiltonian, H, of a system in units with $\hbar = 2m = 1$ is $H = -\Delta+V$. It is not a priori clear for which vectors ψ, $H\psi$ makes sense, but the presence of the differential operator suggests that not all vectors are allowed. We must therefore be prepared to deal only with densely defined operators, i.e. operators, H, with a domain $D(H)$ dense in $\mathcal{H}$.

Definition. An operator, H, is called symmetric (also called Hermitian) if and only if $(\phi,H\psi) = (H\phi,\psi)$ for all ϕ, $\psi \in D(H)$

Definition. An operator, H, is called self-adjoint if and only if there is a unitary one-parameter group, $U(t)$, so that $D(H) = \{\phi | t \to U(t)\phi \text{ is differentiable}\}$ with $d(U(t)\phi)/dt = -iHU(t)\phi$.

Remarks. 1. The equivalence of this definition to the usual one is the content of Stone's theorem (§VIII.4 of [29]).
2. It is not hard to see that any self-adjoint operator is symmetric. But the converse is not true, which is the reason why symmetry is not enough despite its emphasis in most physics texts.

Theorem 2.1. A necessary and sufficient condition that an operator, H, be self-adjoint is that it is symmetric and $\mathrm{Ran}(H+i) = \mathrm{Ran}(H-i) = \mathcal{H}$, the entire Hilbert space.

Rather than give a detailed proof of this result (which the reader can find in §VIII.2 of [29]) let us give an intuition which explains why the condition $\mathrm{Ran}(H+i) = \mathrm{Ran}(H-i) = \mathcal{H}$ should enter naturally in the construction of solutions of $\dot{\psi}_t = -iH\psi_t$. The solution is formally nothing but $e^{-iHt}\psi$ as we all know, but how can we construct e^{-iHt} from H? The "compound interest" formula:

$$e^{-iHt} = \lim_{n\to\infty} (1 + \frac{iHt}{n})^{-n} = \lim[(\pm 1)^{-n}(\frac{|t|H}{n} \mp i)^{-n}]$$

is an attractive possibility. One first notes that for any real $\alpha > 0$:

$$\|(\alpha H \pm i)\phi\|^2 = \langle\phi, (\alpha^2 H^2 + 1)\phi\rangle \pm \langle\alpha H\phi, i\phi\rangle \pm \langle i\phi, \alpha H\phi\rangle =$$

$$= \langle\phi, (\alpha^2 H^2 + 1)\phi\rangle \geq \|\alpha\|^2$$

for any symmetric H. This means one can define an operator, $A = (\alpha H \pm 1)^{-1}$ from $\mathrm{Ran}(\alpha H \pm i)$ to $D(H)$ with $\|A\phi\| \leq \|\phi\|$. If $\mathrm{Ran}(\alpha H + i)$ is not all of $\mathcal{H}$ then, in general, $(\alpha H \pm i)^{-n}$ will be defined on smaller and smaller spaces as $n \to \infty$. Thus, the condition $\mathrm{Ran}(\alpha H \pm i) = \mathcal{H}$ for all $\alpha > 0$ is very natural. The final fact needed to finish the explanation of the Theorem is that $\mathrm{Ran}(\alpha H + i) = \mathcal{H}$ for one $\alpha > 0$ if and only if it equals $\mathcal{H}$ for all $\alpha > 0$ (see e.g. Theorem X.1 of [30]). The reader should consult Kato [20] for a proof of Theorem 2.1 (in the context of contraction semigroup theory) along the intuitive lines discussed above.

Suppose that $\mathrm{Ran}(H \pm i)$ are only dense and not all of $\mathcal{H}$. Then $(H+i)^{-1}$ is defined and bounded from a dense subset of $\mathcal{H}$ to $D(H)$ and so it can be extended to all $\mathcal{H}$ with a range $\bar{D}$. The operator $\bar{H}$ with domain $\bar{D}$ given by $\bar{H}\phi = [((H+i)^{-1})^{-1} - i]\phi$ can then be shown to be symmetric with $\mathrm{Ran}(\bar{H} \pm i)$ all of $\mathcal{H}$. In this situation, we call H <u>essentially self-adjoint:</u> while it does not quite meet our definition of self-adjoint, it does determine in a unique way a natural set of solutions of the Schrödinger equation.

Most quantum Hamiltonian, H, are bounded below in the sense that $(\phi, H\phi) \geq -\alpha(\phi, \phi)$ for some number α and all $\phi \in D(H)$. Under such circumstances Theorem 2.1 has a useful extension:

<u>Theorem 2.2.</u> Let H obey $(\phi, H\phi) \geq -\alpha(\phi, \phi)$. Then a necessary and sufficient condition for H to be self-adjoint (resp. essentially self-adjoint) is that $\mathrm{Ran}(H + \alpha + 1)$ be all of $\mathcal{H}$ (resp. dense)..

Much of the development of bounded operator theory by Hilbert and his students was in terms of explicit matrices and their quadratic forms. Von Neumann and Stone found that the development of unbounded operators was severely hampered by matrix language and so developed abstract operator theory. It is an irony of history that somehow in this revolution of concept, the quadratic form ideas got lost. So far as I know, the abstract theory of quadratic forms of self-adjoint operators was developed in the 50's and only systematically applied to quantum mechanics in the 60's in work of Faris, Kato, Kuroda, Nelson and Simon, among others. It is now clear that in most cases, aspects of the theory of Schrödinger operators can be developed in two parallel tracks - one emphasizing operators, the other forms. Since, depending on the situation, either one can be technically simpler than the other, the thory is made richer and more elegant by the dual presentation.

Definition. A (symmetric) quadratic form a is a function of two vectors ϕ, ψ defined when ϕ, ψ lie in some dense set $Q(a)$ so that $a(\phi,\cdot)$ is linear for each fixed ϕ, $a(\cdot,\psi)$ is antilinear for each fixed ψ and $a(\phi,\psi) = \overline{a(\psi,\phi)}$. a is called semibounded, if and only if $a(\phi,\phi) \geq -\alpha\|\phi\|^2$ for some real α. a is then called closed if $Q(a)$ is a Hilbert space in the norm $\|\phi\|_H = \sqrt{a(\phi,\phi) + (\alpha+1)(\phi,\phi)}$.

Definition. Let H be a self-adjoint operator which is bounded below. Its quadratic form domain, $Q(H)$ is those ϕ with $(\phi,U(t)\phi)$ differentiable for all t where $U(t) = e^{-iHt}$. For ϕ, $\psi \in Q(H)$ we define

$$h(\phi,\psi) = i \frac{d}{dt}(\phi,U(t)\psi)\Big|_{t=0} .$$

Remarks. 1. Implicit in this last definition is the fact that if $(\phi,U(t)\phi)$ and $(\psi,U(t)\psi)$ are differentiable, so is

$(\phi, U(t)\psi)$.

2. The canonical example of a quadratic form without any closed extension is that with $q(a) = C_0^\infty(\mathbb{R})$ and $a(\phi,\psi) = \overline{\phi(0)}\psi(0)$.

3. One often abuses notation and writes $(\phi, H\psi)$ for $h(\phi,\psi)$. Since there are $\psi \in Q(H)$, not in $D(H)$ this is technically "illegal notation" and it can lead to dangerous errors if one forgets that it is shorthand. I have even been known to go further and define $(\phi, H\phi)$ to be $h(\phi,\phi)$ if $\phi \in Q(H)$ and to be ∞ if $\phi \notin Q(H)$.

4. It can be shown that a self-adjoint operator is uniquely determined by its quadratic form, i.e. there is at most one self-adjoint operator with a given quadratic form.

Theorem 2.3. A semibound quadratic form is the quadratic form of a self-adjoint operator if and only if it is closed.

This remarkable result has a rather simple proof (see §VIII.6 of [29]) reducing it to Theorem 2.2. I must confess, nevertheless, to not really understanding it! I regard self-adjointness as equivalent to solvability of a Schrödinger equation and I do not see on any heuristic level why closure of quadratic form should imply solvability of the associated Schrödinger equation.

§3. SELF-ADJOINTNESS OF SCHRÖDINGER OPERATORS - FOUR METHODS

Mike Reed and I devoted a chapter in [30] with 217 pages to the question of self-adjointness (actually other material is included, but even a conservative count of pages yields almost 90) so I am certainly not going to give a complete account of the subject here. But I should like to describe four methods that define self-adjoint Hamiltonians for most Schrödinger operators, $-\Delta+V$ with $V \to 0$ or $+\infty$ at infinity. The most interesting cases I will not discuss are the Hamiltonians in the presence of uniform electric or magnetic fields - after important early work of Stümmel [43], general results for these situations were found by Kato and Ikebe [23] - my preferred methods for obtaining these results use Kato's inequality for magnetic fields (see [21,36] or §X.4 of [30]) and the method of Faris and Lavine [15] for electric fields (see §X.5 of [30]). With some reluctance, I will be cavalier about questions like giving the domain of $-\Delta$ etc. See [30] for further details.

Method 1: Operator Perturbation Theory

Definition: Let A be a self-adjoint operator and B a symmetric operator. We say that B is relatively A-bounded if and only if $D(B) \supset D(A)$ and these are α and β so that

$$\|B\phi\| \leq \alpha\|A\phi\| + \beta\|\phi\| \tag{1}$$

for all $\phi \in D(A)$. The infimum of those α for which (1) holds is called the relative bound of B.

Theorem 3.1. If A is self-adjoint and B is symmetric and relatively A-bounded with relative bound $\alpha < 1$, then A+B, defined with domain D(A), is self-adjoint.

Let us sketch the proof. As we have already shown, $\|(A+i\lambda)\phi\|^2 = \|A\phi\|^2 + \lambda^2\|\phi\|^2$ so that letting $\phi = (A+i\lambda)^{-1}\psi$:

$$\|A(A+i\lambda)^{-1}\psi\|^2 + \lambda^2\|(A+i\lambda)^{-1}\psi\|^2 = \|\psi\|^2$$

so that $\|A(A+i\lambda)^{-1}\| \leq 1$, $\|(A+i\lambda)^{-1}\| \leq |\lambda|^{-1}$. Thus by (1)

$$\|B(A+i\lambda)^{-1}\| \leq \alpha + \beta|\lambda|^{-1} .$$

Taking $|\lambda|$ large, $\|B(A+i\lambda)^{-1}\| < 1$, so by using a geometric series, $1 + B(A+i\lambda)^{-1}$ is invertible and, in particular $\mathrm{Ran}(1 + B(A+i\lambda)^{-1}) = H$. Writing

$$A + B + i\lambda = [1 + B(A+i\lambda)^{-1}](A + i\lambda)$$

we see that $\mathrm{Ran}(A+B+i\lambda) = H$. This proves the theorem.

Example 1. In non-relativistic quantum mechanics, $A = H_o$, the free Hamiltonian, $-\Delta$, and B is the operator V of multiplication by a real-valued (measurable) function, $V(x)$. (1) is then what has become known mathematically as "an inhomogeneous Sobolev estimate" - physically it is somehow a kind of sharp form of the uncertainty principle. Kato's original application [18] is so simple, we can give it in detail. Suppose that V is the sum of a bounded function and a square integrable function on R^3; for example let $V = |r|^{-1}$. Then we can write $V = V_1 + V_2$ with $\|V_1\|_2 = (\int |V_1|^2 dx)^{1/2} \leq \varepsilon$ and $\|V_2\|_\infty = \sup|V_2(x)| = D < \infty$. By the Fourier inversion formula $\phi(x) = (2\pi)^{-3/2} \int e^{-ikx} \hat{\phi}(k) d^3k$ and, by the Plancherel theorem $\|\phi\|_2 = \|\hat{\phi}\|_2$. Thus:

$$\begin{aligned}
\|\phi\|_\infty &\leq (2\pi)^{-3/2} \int |\hat{\phi}(k)| \, d^3k \\
&\leq C[\int |\hat{\phi}(k)|^2 (1+k^2)^2]^{1/2} \\
&\leq C(\|H_o\phi\|_2 + \|\phi\|_2)
\end{aligned}$$

where we have used the Schwartz inequality and $\int d^3k(1+k^2)^{-2} < \infty$ in the second step and $H_o\phi = k^2\hat{\phi}$ in the last. By the trivial estimate $\|fg\|_2 \leq \|f\|_2 \|g\|_\infty$, we have:

$$\|V\phi\|_2 \leq \|V_1\|_2 \|\phi\|_\infty + \|V_2\|_\infty \|\phi\|_2 \leq$$

$$\leq \varepsilon C \| H_o\phi\| + (\varepsilon C + D)\|\phi\|_2 .$$

Thus V is relatively H-bounded with relative bound zero, and so H_o+V is self-adjoint on $D(H_o)$.

Example 2. It is not hard to show that if an estimate like (1) holds for a given V with $H_o = -\Delta$ on $L^2(\mathbb{R}^3)$, it continues to hold (up to factors of 2 and such) if V is the some potential viewed as an interparticle potential and $H_o = -\Delta$ on $L^2(\mathbb{R}^{3N})$. Thus the considerations of Example 1 and Theorem 3.1 lead to self-adjointness results for atomic Hamiltonians. This is really very striking. It is not known if the corresponding classical (Newtonian) equations of motion have global solutions for all time! Quantum mechanics is nicer than classical mechanics in this way. This is true essentially for the same reason that atoms are stable - the "uncertainty principle" prevents collapse.

Example 3. The problem of extending the result of Example 1 from $\mathbb{R}^3$ to $\mathbb{R}^n$ is not only of obvious mathematical interest. It is also of considerable use in understanding what is going on! The first general study of the n-dimensional case was by Stümmel [43] who introduced spaces that now bear his name. I have no fondness for these spaces much preferring the L^p-space language. The sharpest L^p results are due to Faris [13] who used the best Sobolev estimates: for V to be $-\Delta$ bound with relative bound zero it suffices that $V \in L^p(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)$ where $p = 2$ if $n \leq 3$, $p > 2$ if $n = 4$ and $p = n/2$ if $n \geq 5$; moreover, this is no longer true if any smaller value of p is chosen. (Note that if $q > p$, $L^q+L^\infty \subset L^p+L^\infty$). We should also mention Strichartz' improvements [42] of the Sobolev estimates: First he allows potentials to be "uniformly locally L^p" with p as above thereby including various unbounded periodic potentials (see §XIII.16 of [31]) and secondly various "weak L^p" spaces.

Method 2: Form Perturbation Theory

Definition. Let a be the quadratic form of a semibounded self-adjoint operator and b a symmetric quadratic form. We say that b is relatively a-form bounded if and only if $Q(b) \supset Q(a)$ and there are γ and δ so that

$$|b(\phi,\phi)| \leq \gamma \; a(\phi,\phi) + \delta\|\phi\|^2. \tag{2}$$

The infimum of those γ for which (2) holds is called the relative form bound of b.

Theorem 3.2. If a is the quadratic form of a semibounded self-adjoint operator and b is symmetric and relatively a-form bounded with relative bound $\gamma < 1$, then a+b, defined with form domain $Q(a)$ is the quadratic form of a self-adjoint operator.

Let us sketch the proof. Without loss one can suppose that $a \geq 0$. Then letting $\|\phi\|_{+1} = (a(\phi,\phi) + \|\phi\|^2)^{1/2}$ and $\|\phi\|'_{+1} = (a(\phi,\phi) + b(\phi,\phi) + (\delta+1)\|\phi\|^2)^{1/2}$, we know by (2) that

$$(\|\phi\|'_{+1})^2 \geq (1+\gamma)a(\phi,\phi)+(2\delta+1)\|\phi\|^2 \leq (1+\gamma+2\delta)\|\phi\|^2_{+1}$$

and

$$(\|\phi\|_{+1})^2 \geq (1-\gamma)a(\phi,\phi) + \|\phi\|^2$$

so that $\|\phi\|^2_{+1} \leq [1 + (1-\gamma)^{-1}](\|\phi\|'_{+1})^2$. It follows that $\|\cdot\|_{+1}$ and $\|\cdot\|'_{+1}$ are equivalent norms on $Q(a)$. Since $Q(a)$ is complete in the first norm, it is complete in the second so the Theorem follows from Theorem 2.3.

Remarks. 1. It is striking that while the statements of Theorem 3.1 and 3.2 are parallel, the proofs are completely different.

2. b in Theorem 3.2 need not be associated with any operator. The canonical example is $a = -d^2/dx^2$ and $b = \delta(x)$ so that one can give a real mathematical meaning to the common pedagogical example $-d^2/dx^2 + \delta(x)$.

Example 4. The astute reader may have noticed that while physicists know that in three dimensions $-r^{-\alpha}$ shouldn't be singular until $\alpha = 2$, it stops meeting the operator criteria which require V in L^2 locally when $\alpha = 3/2$. For $3/2 \leq \alpha < 2$, one can define the Hamiltonian by using Theorem 3.2. The quantum mechanics of potentials of a class including these is developed in [35].

Method 3. Kato's Inequality

A beautiful proof of the self-adjointness of various potentials which are positive and more singular than what is allowed by operator perturbation theory is based on:

Lemma 3.3. (Kato [21]). Suppose that $u \in L^1_{loc}(\mathbb{R}^n)$ and the distributional Laplacian $\Delta u \in L^1_{loc}(R^n)$. Then

$$\Delta|u| \geq \text{Re}\,[\text{sgn}(u)\ \Delta u] \qquad (3)$$

where $\text{sgn}\, u = u^*/|u|$.

Let us sketch the proof. By an approximation argument, one need only prove (3) for $u \in D(H_0)$. This can be done by suitably clever differentiation [21] but we prefer an argument from [39] which emphasizes the general reason why (3) holds. The operator e^{-tH_0} is convolution with the positive function $(4\pi t)^{-n/2} \exp(-|x|^2/4t)$ so that for any u:

$$|(e^{-tH_o}u)(x)| \leq (e^{-tH_o}|u|)(x)$$

and thus for $f \geq 0$ in $C_o^\infty(R^n)$:

$$\text{Re } [((\text{sgn } u)^* f, e^{-tH_o}u)] \leq (f, e^{-tH_o}|u|). \qquad (4)$$

Equality holds in (4) when $t = 0$, so subtracting the $t = 0$ result, dividing by t and taking $t \downarrow 0$ we have:

$$\text{Re } ((\text{sgn } u)^* f, (-H_o)u)) \leq -(H_o f, |u|)$$

since $u, f \in D(H_o)$. This is just (3).

Theorem 3.4. (Kato [21]). If $V \in L^2_{loc}(\mathbb{R}^n)$ is positive, then $-\Delta+V$ is essentially self-adjoint on $C_o^\infty(\mathbb{R}^n)$.

We sketch the proof. By Theorem 2.2, it suffices to prove that $(-\Delta+V+1)[C_o^\infty]$ is dense. If it is not, then there is a non-zero $u \in L^2$ orthogonal to it so that

$$(-\Delta+V+1)u = 0$$

in distribution sense. In particular, $\Delta u = (V+1)u \in L^1_{loc}$ so by (3)

$$(-\Delta+1)|u| \leq \text{Re } ((\text{sgn } u)(-Vu)) = -V|u| \leq 0.$$

Now $(-\Delta+1)^{-1}$ is a map on the tempered distributions which takes positive distributions into themselves, so that $|u| \leq 0$ and thus $u = 0$. This condition shows that $(-\Delta+V+1)[C_o^\infty]$ is indeed dense.

One can allow V to have a negative relatively bounded part with relative bound $\alpha < 1$; see Kato [21] or §X.4 of [30]. See Kato [22], Simon [37] and Kalf-Walter [17] for further applications.

Method 4. The Form Sum

Theorem 3.5. Let a and b be positive quadratic forms which are the forms of self-adjoint operators. Suppose that $Q(a) \cap Q(b)$ is dense. Then the sum $c = a+b$ defined on $Q(c) = Q(a) \cap Q(b)$ is the quadratic form of a self-adjoint operator.

Suppose that $\phi_n \in Q(a) \cap Q(b)$ and $c(\phi_n-\phi_m,\phi_n-\phi_m) \to 0$ as $n, m \to \infty$. Then since a and b are positive, $\|\phi_n-\phi_m\| \to 0$, $a(\phi_n-\phi_m,\phi_n-\phi_m) \to 0$ and $b(\phi_n-\phi_m,\phi_n-\phi_m) \to 0$. Since a and b are closed, it follows that $\phi_n \to \phi$ in H with $\phi \in Q(a)$ and $\phi \in Q(b)$, $a(\phi_n-\phi,\phi_n-\phi) \to 0$ and $b(\phi_n-\phi,\phi_n-\phi) \to 0$ so that $c(\phi_n-\phi,\phi_n-\phi) \to 0$. We have thus shown that c is closed. The theorem now follows from Theorem 2.3.

Example 5. If $V \in L^1_{loc}(\mathbb{R}^n)$ is positive, then $-\Delta+V$ can be defined as a form sum. $Q(-\Delta) \cap Q(V)$ is dense since it contains $C_o(\mathbb{R}^n)$.

One can allow a negative part of V as long as it is $-\Delta$ form bounded with relative bound $\gamma < 1$.

§4. TYPES OF SPECTRA

Definition. The spectrum, $\sigma(H)$, of a self-adjoint operator is the set of complex λ so that $(H-\lambda)^{-1}$ is not invertible.

By the calculation $\|(H-\lambda)\phi\| \geq |\text{Im } \lambda| \; \|\phi\|$ and Theorem 2.1, $\sigma(H) \subset \mathbb{R}$. The spectrum of H has the interpretation of possible values of the energy. To get more information about H, it is often useful to refine the spectrum further. There are two useful breakups of $\sigma(H)$, one into σ_{ess} and σ_{disc}; the other into σ_{pp}, σ_{ac} and σ_{sing} - see /VII of [29] for more details.

Definition. $\lambda \in \sigma(H)$ is said to be discrete if and only if λ is an isolated point of $\sigma(H)$ and an eigenvalue of finite multiplicity. The set of discrete points is denoted $\sigma_{disc}(H)$. The essential spectrum, $\sigma_{ess}(H)$, is $\sigma(H)\setminus\sigma_{disc}(H)$.

The point of singling out σ_{ess} is that it has some simple stability properties under sufficiently nice perturbations. This will be further discussed in §5 below; see also §XIII.4 of [31].

Given a self-adjoint operator H and any $\phi \in \mathcal{H}$, there is a measure $d\mu_\phi$ determined by:

$$(\phi, e^{-itH}\phi) = \int e^{-itx}\, d\mu_\phi(x) \quad .$$

Corresponding to the fact that any measure $d\mu$ is a sum of a pure point part (a piece $d\mu_{pp} = \sum c_i\ \delta(x-x_i)$), a part absolutely continuous with respect to Lebesgue measure (a piece $d\mu_{ac} = F(x)\ dx$) and a singular continuous part (a piece $d\nu$ with $d\nu(\{x\}) = 0$ for all x but with A obeying $\nu[\mathbb{R}\setminus A] = 0$; $\int_A dx = 0$) one has (see §VII of [29]):

Theorem 4.1. Given any self-adjoint operator H on $\mathcal{H}$, there is a unique decomposition $\mathcal{H} = \mathcal{H}_{ac} + \mathcal{H}_{pp} + \mathcal{H}_{sing}$ so that H leaves each subspace invariant and $\phi \in \mathcal{H}_{ac}$ (resp. $\mathcal{H}_{pp}$ or $\mathcal{H}_{sing}$) if and only if $d\mu_\phi$ is absolutely continuous (resp. pure point or singular continuous).

Definition. $\sigma_{ac}(H) = \sigma(H\restriction\mathcal{H}_{ac})$, $\sigma_{sing}(H) = \sigma(H\restriction\mathcal{H}_{sing})$,

$\sigma_{pp} = \{\lambda | \lambda$ is an eigenvalue of H$\}$.

Note that σ_{ac}, σ_{sing} and σ_{pp} need not be disjoint and that σ may not equal $\sigma_{ac} \cup \sigma_{sing} \cup \sigma_{pp}$ (although $\sigma = \sigma_{ac} \cup \sigma_{sing} \cup \bar{\sigma}_{pp}$).

For quantum Hamiltonians, σ_{pp} (or at least σ_{disc}!) has the interpretation of bound states. As I am sure you will hear, σ_{ac} is the study of scattering states - thus one of the hard problems in the study of Schrödinger operators is that of showing $\sigma_{sing}(H) = \emptyset$. For example, it is still not proven that a system with 4 or more particles and square well potentials (or even potentials in C_0^∞) has $\sigma_{sing} = \emptyset$!

We complete our "review" of Schrödinger operators with finding $\sigma_{ess}(H)$ in the two body case and by discussing qualitative information on $\sigma_{disc}(H)$ in the two body case.

§5. THE ESSENTIAL SPECTRUM IN THE TWO BODY CASE

Weyl [46] first proved various stability statements for the essential spectrum of ordinary differential operators under change of boundary condition. It has been realized that the general invariance principle behind Weyl's results is the following: If A and B are self-adjoint and $(A+i)^{-1} - (B+i)^{-1}$ is compact (to be defined shortly), then $\sigma_{ess}(A) = \sigma_{ess}(B)$. In this section, we want to describe how to prove the special case where $A = -\Delta$ and $B = -\Delta+V$ which has some simplifying features; the general case can be found in §XIII.4 of [31]. I hope the description I give will set the stage for beautiful results which Hunziker will describe in the next lecture.

Definition. A bounded operator, A, is called finite rank if and only if

$$A\phi = \sum_{n=1}^{N} \psi_n(\phi_n,\phi)$$

for some $\phi_1,\ldots,\phi_N$, $\psi_1,\ldots,\psi_N$. A is called compact if and only if it is a limit in operator norm of finite rank operators.

In many ways, compact operators behave like finite dimensional matrices. For example, if f(z) is a finite dimensional matrix-valued analytic function on an open connected set, Ω, then $1 - f(z)$ is either never invertible or it is invertible except for a discrete subset D of Ω (i.e. D has no limit points in Ω) for either $\det(1 - f(z))$ is identically zero or it has a discrete set of zeros. This result extends to compact valued functions (see §VI.5 of [29] for a proof):

Theorem 5.1. ("The Analytic Fredholm Theorem"). Let f(z) be an analytic function from a connected set, Ω of the complex numbers to the compact operators on some Hilbert space. Then either $1 - f(z)$ is invertible for no z in Ω or else it is invertible except for a discrete subset, D, of Ω. In the latter case, $(1 - f(z))^{-1}$ is analytic on $\Omega\setminus D$ and about each point $z_0 \in D$ there is a Laurent expansion

$$(1 - f(z))^{-1} = \sum_{n=-N}^{\infty} a_n(z - z_0)^n$$

with N finite and $a_{-N}, \ldots, a_{-1}$ all finite rank.

To apply this theorem, one needs criteria for an operator to be compact.

Definition. An operator, A, on $L^2(\mathbb{R}^n)$ is called Hilbert-Schmidt if and only if there is a function K in $L^2(\mathbb{R}^{2n})$ (note 2n, not n) so that

$$(Af)(x) = \int K(x,y)\, f(y)\, dy.$$

K is called the kernel of A.

Theorem 5.2. (a) Every Hilbert-Schmidt operator is compact. (b) Any norm-limit of compact operators is compact.

Let us sketch the proof. If $\phi_n(x)$ is a basis for $L^2(\mathbb{R}^n)$, then $\phi_n(x)\overline{\phi_m(y)}$ is a basis for $L^2(\mathbb{R}^{2n})$, so that $K(x,y) = \sum \alpha_{nm}\phi_n(x)\overline{\phi_m(y)}$ with $\sum |\alpha_{nm}|^2 < \infty$. Let A_N be the operator with kernel

$$\sum_{n,m\leq N} \alpha_{nm}\, \phi_n(x)\, \overline{\phi_m(y)} .$$

The A_N are clearly finite rank and one can show that

$$\|A_N - A\| \leq \Big(\sum_{n>N \text{ or } m>N} |\alpha_{nm}|^2\Big)^{1/2}$$

goes to zero. This proves (a). To prove (b), let $A_n \to A$ with A_n compact. Given m, find $A_{n(m)}$ so that $\|A_{n(m)} - A\| < \frac{1}{2}m^{-1}$ and let B_m finite rank so that $\|B_m - A_{n(m)}\| < \frac{1}{2}m^{-1}$. Then $B_m \to A$ in norm.

Example 1. Let $L^2 + L^\infty_\varepsilon$ denote the set of those potentials, V, which for any ε, can be decomposed as $V = V_{1,\varepsilon} + V_{2,\varepsilon}$ with $V_{1,\varepsilon} \in L^2$ and $V_{2,\varepsilon} \in L^\infty$ with $\|V_{2,\varepsilon}\|_\infty \leq \varepsilon$. Any locally L^2 function going to zero at infinity such as $V(r) = r^{-1}$ on R^3 is clearly in $L^2 + (L^\infty)_\varepsilon$. We claim that for $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)_\varepsilon$ and any complex z not in $\sigma(-\Delta) = [0,\infty)$, $V(-\Delta-z)^{-1}$ is compact. Suppose first that $V \in L^2$. Choose μ so that $\mu^2 = -z$ and Re $\mu > 0$. Then $V(-\Delta-z)^{-1}$ has the explicit kernel

$$V(x) \exp(-\mu|x-y|)/4\pi|x-y|$$

which is Hilbert-Schmidt. If now V is in $L^2 + L^\infty_\varepsilon$ and $V_{1,\varepsilon} + V_{2,\varepsilon}$ is the decomposition above, then $V_{1,\varepsilon}(-\Delta-z)^{-1}$ goes to $V(-\Delta-z)^{-1}$ in norm and so the latter is compact.

We now have the tools for:

<u>Theorem 5.3.</u> Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)_\varepsilon$. Then $-\Delta+V$ has essential spectrum $[0,\infty)$, i.e. $\sigma(-\Delta+V)$ is $[0,\infty)$ together with a (possibly empty) set of negative numbers whose only possible limit point is zero and each negative eigenvalue has finite multiplicity.

<u>Proof.</u> Let $f(z) = -V(H_0 - z)^{-1}$ for z complex not in $[0,\infty)$. Then f(z) has compact values and is analytic. Moreover, as in Example 1 of Section 3, $\|f(z)\| < 1$ for $z = i\mu$ with $|\mu|$ large. It follows that $1 - f(z)$ is sometimes invertible, and thus by Theorem 5.1, it is invertible for all z not in a discrete set, D. It follows that $(H-z) = (1 - f(z))(H_0-z)$ is invertible for all z in $C\backslash D \cup [0,\infty)$ so $\sigma(H) \subset D \cup [0,\infty)$. Since $(H-z)^{-1}$ has finite rank residues at points in D, one can show that points in D are eigenvalues of finite multiplicity. Thus $\sigma_{ess}(H) \subset [0,\infty)$.

If $\sigma_{ess}(H)$ is not equal to $[0,\infty)$, there is some interval $(a,b) \subset [0,\infty)$ with $(a,b) \cap \sigma(H) = \emptyset$. We now turn the above argument around. Letting $g(z) = V(H-z)^{-1}$ so that

$$(H_o - z) = (1 - g(z))(H - z)$$

by mimicking the above, we prove that $\sigma_{ess}(H) \cap (a\ b) = \emptyset$. Since this is false, $\sigma_{ess}(H)$ must be all of $[0,\infty)$.

§6. BOUNDS ON THE NUMBER OF BOUND STATES

Since I have recently written a review article [40] on this subject with fairly complete references, I will settle for describing without proof some of the main results and for giving the reader some references to the Russian literature [1,4-10,24,32] which through ignorance I did not list in [40] - I should like to thank Prof.M.S. Birman for bringing these to my attention.

Bounds on $n_\ell(V)$

Let V be a central potential on $\mathbb{R}^3$ and let $n_\ell(V)$ be the number of negative eigenvalues of $-\Delta+V$ with angular momentum ℓ, not counting the multiplicity $(2\ell+1)$. The first general bound on $n_\ell(V)$ is that of Bargmann [2]:

Theorem 6.1. $n_\ell(V) \leq (2\ell+1)^{-1}\int_0^\infty r|V(r)|\,dr$ while the best bound I know is that of G^2MT [16]:

Theorem 6.2. $n_\ell(V) \leq B(\ell,\alpha)\int_0^\infty r^{2\alpha-1}|V(r)|^\alpha dr$ for $1 < \alpha < \infty$ and

$$B(\ell,\alpha) = \frac{(\alpha-1)^{\alpha-1}\Gamma(2\alpha)}{\alpha^\alpha\Gamma^2(\alpha)(2\ell+1)^{2\alpha-1}} \quad .$$

Remarks. 1. As $\alpha \to 1$, G^2MT yields Bargmann's bound.
2. Both bounds are best possible in that given any ε, ℓ and N there is a V with $n_\ell(V) = N$ and with the right side of the bounds less than $N+\varepsilon$.

Bounds on N(V) - 1 and 2 dimensions

Let N(V) be the number of negative eigenvalues counting multiplicity of $-\Delta+V$ on $\mathbb{R}^{\nu}$. For $\nu = 1,2$ the basic result is negative [40]:

Theorem 6.3. For $\nu = 1,2$: (a) Let $\|\cdot\|$ be a translation invariant norm. Then for any N, and $\varepsilon > 0$, there is a V with $\|V\| \leq \varepsilon$ and $N(V) \geq N$. (b) For no norm is $N(V) \leq \|V\|^{\alpha}$ with $\alpha > 0$.

The basic reason that Theorem 6.3 holds is that for any negative V, $-\Delta+V$ has bound states in $\nu = 1,2$ dimensions for any $\lambda > 0$. See [38,11] for additional information on this state.

Theorem 6.4. For $\nu = 1$, $N(V) \leq 1 + \int_{-\infty}^{\infty} |x| |V(x)| \, dx$.

Remark. Theorem 6.4 is proven in [40] with 1 replaced by 2. That 1 can be used follows by noting that if $G_{\alpha}(x,y)$ is the kernel for $(-d^2/d^2x + \alpha^2)^{-1}$ and $K_{\alpha}(x,y)$ is the kernel with a Dirichlet boundary condition then $G_{\alpha} - K_{\alpha}$ is the rank one operator

$$(2\alpha)^{-1} \exp -\alpha(|x| + |y|) \quad .$$

Bounds on N(V) - 3 or more dimensions

The first general bound is that obtained independently by Birman [3] and Schwinger [34]:

Theorem 6.5. For $\nu = 3$:

$$N(V) \leq (4\pi)^{-2} \int |x-y|^{-2} |V(x)| |V(y)| \, d^3x \, d^3y.$$

Recently, Cwickel [12], Lieb [25] and Rosenbljum [32] have independently proven the bound:

Theorem 6.6. For any $\nu \geq 3$

$$N(V) \leq c_\nu \int |V(x)|^{\nu/2} d^\nu x.$$

Remark. The constant in Theorem 6.5 is best possible in the sense of Remark 2 after Theorem 6.2. The constant c_ν in Theorem 6.6 is different in the papers of the three authors (and not even explicit in [32]). Lieb's constant seems to be the best of the three. It is probably not best possible but it cannot be improved by more than about 33 % without violating some explicit examples of [16].

Among the interesting subjects I will not discuss are the large λ behavior of $N(\lambda V)$, the pathologics in the multiparticle case and the connection of Theorem 6.6 to the problem of "stability of matter". See [40] for the first two topics and Lieb-Thirring [27,28] for the second.

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