Some Aspects of the Theory of Schrödinger Operators *

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In these notes, we will survey a part of theory of the operator $-\Delta + V$. More extensive surveys can be found in [1,2,3] and in [4].

1. Self-adjointness, properties of eigenfunctions and all that

There is an enormous literature on the basic issue of giving a domain where $-\Delta + V$ is self-adjoint or essentially self-adjoint. To a large extent, I think one can single out two results as the most important: (1) The basic perturbation results of Kato-Rellich which accomodate virtually all cases of physical interest (2) "Kato's inequality," which, at least among positive V, is definitive. We will describe the first result briefly (for background on definition of self-adjoint, etc., see [5,6,7]; for a discussion of Kato's inequality, see [1,8,9,10]).

Theorem 1.1 (The Kato-Rellich theorem [11,12]) Let A be a self-adjoint operator on a Hilbert space, $\mathcal{H}$, and let B be symmetric. Suppose that $D(B) \supset D(A)$ and for some $a < 1$ and $b < \infty$,

$$\|B\varphi\| \leq a\|A\varphi\| + b\|\varphi\| \tag{1.1}$$

for all $\varphi \in D(A)$. Then $A+B$ is self-adjoint on $D(A)$ and any core for A is a core for $A+B$.

For a proof, see [1], pp. 162-163.

To apply this to $-\Delta + V$, we set $A = -\Delta$, $B = V$ and study (1.1). In this form, (1.1) is related to Sobolev estimates. Kato studied when (1.1) held in terms of L^p-spaces a point of view I long preferred, but I have come around to prefer a point of view introduced by Stummel [13].

Definition Fix $\nu \geq 4$, and $0 < \alpha < 4$ and let $S_\alpha^{(\nu)}$ be the set of functions, V, on R^ν obeying

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$$\sup_{x} \int_{|y-x|\leq 1} |x-y|^{-(\nu-4+\alpha)} |V(y)|^2 dy < \infty \tag{1.2}$$

If $\nu \leq 3$, we define $S_\alpha^{(\nu)}$ in terms of (1.2) with $|x-y|^{-(\nu-4+\alpha)}$ replaced by 1 (independently of α).

With these definitions, it is not hard to prove the following pair of results (see Stummel [13]).

Theorem 1.2 If $V \in S_\alpha^{(\nu)}$, then (1.1) holds on $D(-\Delta)$ where $B = V$, $A = -\Delta$ and a can be taken arbitrarily close to zero.

Theorem 1.3 If $g \in S_\alpha^{(\mu)}$, $\nu > \mu$ and $V(x) = g(\pi x)$ where π is a linear map of R^ν *onto* R^μ, then $V \in S_\alpha^{(\nu)}$.

Thm. 1.2 is proven by noting that for $\nu \geq 4$, the integral of $(-\Delta+\kappa^2)^{-2}$ goes to $|x-y|^{-(\nu-4)}$ for $|x-y|$ small and as $e^{-\kappa|x-y|}$ for $|x-y|$ large and for $\nu \leq 3$, the kernel is bounded at small distances. As a result, $\|V(-\Delta+\kappa^2)^{-2}V\| \to 0$ as $\kappa \to \infty$. Theorem 1.3 follows by noting that $|x-y|^{-(\nu-4+\alpha)}$ integrated over $\nu-\mu$ variables (and cutoff at large distances) is bounded by $|x-y|^{-(\mu-4+\alpha)}$.

The most important special case of Thm. 1.3 is to take μ fixed ($\mu=3$ is the physical case), $\nu = \mu N$, write a point in R^ν as $x = (x_1,\ldots,x_N)$ with $x_j \in R^\mu$ and let $Tx = x_i - x_j$. Thus picking, for all pairs i,j, a function $\upsilon_{ij} \in S_\alpha^{(\mu)}$ and letting $V_{ij}(x) = \upsilon_{ij}(x_i - x_j)$, we see that $V_{ij} \in S_\alpha^{(\nu)}$. Therefore, the operator

$$\tilde{H} = \tilde{H}_0 + V;\ \tilde{H}_0 = \sum_{j=1}^{N} -(2m_j)^{-1}\Delta_j;\ V = \sum_{i<j} V_{ij}\ . \tag{1.3}$$

called an *N-body Hamiltonian* obeys

Theorem 1.4 Any N-body Hamiltonian with $\upsilon_{ij} \in S_\alpha^{(\mu)}$ defines an operator $\tilde{H}$ self-adjoint on $D(-\Delta)$ and essentially self-adjoint on $C_0^\infty(R^\nu)$.

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We used $\tilde{H}$ for the operator in (1.3) because there is a closely related operator, H, on $L^2(R^{\mu(N-1)})$ called the *operator with center of mass removed.* Here are two ways of understanding this change:

(1) Let $R = \sum m_i x_i / \sum m_i$ and let $\zeta_1,\ldots,\zeta_{N-1}$ be $N-1$ additional μ-component coordinates (i.e. linear functions of the x's), so that (i) ζ_j is invariant under $x_j \to x_j + a$ for any a (ii) $x_j \to R, \zeta_j$ is an invertible transformation. For example, one might take

$$\zeta_j = r_j - r_N \qquad j=1,\ldots,N-1 \tag{1.4}$$

Then by writing $R^{\mu N} = R^{\mu} \times R^{\mu(N-1)}$ by the coordinates $R, \zeta, L^2(R^{\mu N})$ decomposes into $\mathcal{H}_{cm} \otimes \mathcal{H} \equiv L^2(R^{\mu}) \otimes L^2(R^{\mu(N-1)})$ (functions of R tensored by functions of ζ). Under this decomposition

$$\tilde{H} = H_{0,cm} \otimes 1 + 1 \otimes H \tag{1.5}$$

where $H_{0,cm} = -2(\sum m_i)^{-1} \Delta_R$ and $H = H_0 + V$. The precise form of H_0 depends on the choice of local coordinates. For example, in the coordinate system (1.4),

$$H_0 = -\sum_{j=1}^{N-1} (2\mu_j)^{-1} \Delta_{\zeta_j} + m_N^{-1} \sum_{i<j} \nabla_i \cdot \nabla_j \tag{1.6}$$

with $\mu_j = (m_N^{-1} + m_j^{-1})^{-1}$.

(2) ([14,15]) View $\tilde{H}_0$ as one half the Laplace Beltrami operator associated to the metric $\|dx\|^2 = \sum m_i (dx_i)^2$. Let $X = \{x \mid \sum m_i x_i = 0\}$. Then in the metric, $X^{\perp} = \{x \mid x_1 = x_2 = \cdots = x_N\}, \mathcal{H}_{cm} = L^2(X^{\perp}), \mathcal{H} = L^2(X)$ and H_0 is just the Laplace-Beltrami operator on X in the induced metric.

For later purposes, we introduce some additional notation to describe N-body systems. A partition of $\{1,\ldots,N\}$, i.e. a family $C_1,\ldots,C_k$ of disjoint subsets of $\{1,\ldots,N\}$ which exhaust $\{1,\ldots,N\}$ is called a *cluster decomposition*. We write $a = \{C_1,\ldots,C_k\}$; $k \equiv \#(a)$. The family of cluster decompositions is important because in various aspects of the study of N-body Hamiltonians, one expects that we want to analyze what happens as $|x| \to \infty$ with $\sum m_i x_i = 0$. This happens if the system breaks up into distinct clusters; i.e. we can find numbers $R_1,\ldots,R_k$ and a decomposition a so $|x_i - R_j|$ stays bounded if $i \in C_j$ and so each $|R_i - R_j|$ goes to infinity.

Given a, we pick coordinates $\zeta_1,\ldots,\zeta_k$ involving differences of center of mass of clusters in a, and "internal coordinates," $\zeta^1,\ldots,\zeta^{N-1-k}$, i.e. coordinates left invariant by the transformations $x_i \to x_i + R_{j(i)}$ where $j(i)$ is that j with $x_i \in C_j$. (Put differently, $\zeta^1,\ldots,\zeta^{N-1-k}$ are coordinates for the plane $X^a = \{x \mid \sum_{i\in C_j} m_i x_i = 0, \text{ all } j\}$ and $\zeta_1,\ldots,\zeta_k$ for its orthogonal complement, X_a, in X). If we decompose $\mathcal{H} = \mathcal{H}^a \otimes \mathcal{H}_a$ corresponding to functions of ζ^a and ζ_a (i.e. $\mathcal{H}^a = L^2(X^a), \mathcal{H}_a = L^2(X_a)$), then we have

$$V = V(a) + I(a);\; I(a) = \sum_{(ij)\not\subset a} V_{ij};\, V(a) = \sum_{(ij)\subset a} V_{ij}$$

(where $(ij)\subset a$ means i and j are in the same cluster), and

$$H \equiv H(a) + I(a)$$

$$H(a) = H^a \otimes I + I \otimes T_a$$

where T_a has no potentials and is exactly the kinetic energy of relative motion of the clusters. Eigenvalues of H^a with $\#(a) \geq 2$ are called *thresholds*.

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[16] contains extensive discussion of properties of eigenfunctions of $-\Delta + V$. Here we state some of the most important results. For many purposes, the natural class of potentials, V, for this study is K^ν defined by:

<u>Definition</u> Let $\nu \geq 3$; $V \in K^\nu$ if and only if

$$\lim_{\alpha\downarrow 0} \sup_x \int_{|x-y|\leq\alpha} |x-y|^{-(\nu-2)} |V(y)| d^\nu y = 0$$

If $\nu = 2$, K^ν is defined with $|x-y|^{-(\nu-2)}$ replaced by $\ln(|x-y|^{-1})$ and if $\nu = 1$, $V \in K^\nu$ if and only if $\sup_x \int_{|x-y|\leq 1} |V(y)| d^\nu y < \infty$.

$V \in K^\nu$ does *not* imply that $-\Delta + V$ is essentially self-adjoint on C_0^∞, but one can [16] always define a self-adjoint operator "$-\Delta + V$" by a method of forms: This meaning agrees with that obtained by closing the operator on C_0^∞ in case the operator sum is self-adjoint there. The following three results are discussed (either proofs or references given) in [16]. If $Hu = Eu$, then $(-\Delta + (V-E))u = 0$, so by changing V, we can look at functions with $Hu = 0$ and obtain information on general eigenfunctions.

<u>Theorem 1.5</u> (Sobolev estimates for H) Let $H = -\Delta + V$ with $V_- \equiv \max(-V,0)$ in K^ν and $V_+ = \max(V,0)$ in K^ν_{loc}. Let $k > \nu/4$. Then any function in $D(|H|^k)$ is a bounded continuous function.

<u>Theorem 1.6</u> (Subsolution estimate for H) Let H obey the hypotheses of Thm. 1.5. Let u obey $Hu = 0$ in distributional sense (u *not* necessarily in L^2). Then

$$|u(x)| \leq C \int_{|x-y|\leq 1} |u(y)| d^\nu y$$

for a constant C depending only on K^ν norms of V_-.

<u>Theorem 1.7</u> (Harnack's inequality for H) Let $V \in K^\nu_{loc}$. Let Ω be a bounded open set and K compact in Ω. Then, there is a constant C depending only on K^ν norms of $V\chi_\Omega$ so that every solution, u, of $Hu = 0$ in Ω with u non-negative on Ω, obeys

$$C^{-1} u(x) \leq u(y) \leq C u(x)$$

for all x,y.

We will not indicate in detail the proofs of the last two theorems. In many ways, the key is the study of the Poisson kernel for H, i.e. for a small open ball, B, about a point x, one can study the map, M_V^B from continuous functions f on ∂B to functions on B defined by $M_V^B(f) = u$ obeys $Hu = 0$ in distributional sense on B and $u(x) \to f(y)$ as $x \to y$ on ∂B. It happens that $(M_V^B f)(x) = \int_{\partial B} P_V^B(x,y) f(y) d\omega(y)$. The last two theorems are proven by showing that P is bounded above and away from zero as x runs through a compact subset of B and y runs through ∂B. This is precisely what Aizenman-Simon [17] do. Recently, Zhao [18] and Brossard [19] have actually proven more subtle estimates showing that $P_V^B(x,y)/P_{V=0}^B(x,y)$ is bounded above and below uniformly in x and y (i.e. they show the boundary behavior of P is essentially V independent).

2. Bound state problems

"Bound states" is the name given to eigenfunctions of eigenvalues in the discrete spectrum (isolated points of the spectrum of finite multiplicity). There are various aspects of the study of eigenfunctions: (i) Identify $\sigma_{ess}(H)$ $(=\sigma(H)\backslash\sigma_{disc}(H))$ (ii) Let N denote the sum of the dimensions of the eigenspaces associated to all points in σ_{disc}. Is N finite or infinite? (This is the same as asking if $\#(\sigma_{disc})$ is finite or infinite.) (iii) If N is finite, can one obtain effective bounds on it? (iv) When is $N = 0$?

For two body systems, $-\Delta + V$ with V decaying at ∞, there is a large literature on these questions, summarized in [20]. We will single out two results for special mention, but first we need to find $\sigma_{ess}(-\Delta+V)$ in this case.

Definition Let A be a self-adjoint operator. B is called *A-compact* if and only if $D(B) \supset D(A)$ and $B(A+i)^{-1}$ is compact.

The methods of the proof of Thm. 1.2 imply easily that

Proposition 2.1 If $\nu \leq 3$ and $\lim_{|x|\to\infty} \int_{|y-x|\leq 1} |V(y)|^2 dy = 0$ or if $\nu \geq 4$ and

$$\lim_{|x|\to\infty} \int_{|x-y|\leq 1} |y-x|^{-(\nu-4+\alpha)} |V(y)|^2 dy = 0 \text{ for some } \alpha > 0, \text{ then } V \text{ is } -\Delta\text{-compact.}$$

We write S^{ν}_{comp} for the V's given in Prop. 2.1.

Proposition 2.2 If A is self-adjoint, and if B is A-compact and symmetric, then $\sigma_{ess}(A+B) = \sigma_{ess}(A)$.

Proof A simple theorem of Weyl (see [3]) says that $E \in \sigma_{ess}(C)$ if and only if there exists a sequence of vectors $\varphi_n \in D(C)$ with $\varphi_n \to 0$ *weakly* and $\|(C-E)\varphi_n\| \to 0$, $\|\varphi_n\| \to 0$. Given $E \in \sigma_{ess}(A)$, find such a sequence, let $\psi_n = (E^2+1)(A^2+1)^{-1}\varphi_n$. It is not hard to show that $\psi_n \to 0$ weakly, $\|(A+B-E)\psi_n\| \to 0$, $\|\psi_n\| \to 1$. Thus, $E \in \sigma_{ess}(A+B)$ and we conclude that $\sigma_{ess}(A) \subset \sigma_{ess}(A+B)$. Using $(A+B+i)^{-1} = (A+i)^{-1}(1+B(A+i)^{-1})^{-1}$, one can show that B is $(A+B)$-compact. Thus, $\sigma_{ess}(A+B) \subset \sigma_{ess}(A)$ by repeating the above argument. ■

Corollary 2.3 If V lies in S^{ν}_{comp}, then $\sigma_{ess}(-\Delta+V) = [0,\infty)$.

We return now to N for $-\Delta + V$ which we denote by $N(V)$. We want to single out two results:

Theorem 2.4 (Quasiclassical bounds on $N(V)$) Let $\nu \geq 3$. There is a universal constant C_ν so for all $V \in L^{\nu/2}$,

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

This theorem is particularly important because the semiclassical approximation for $N(V)$ is to take the volume in phase space where $p^2 + V(x)$ is negative and divide it by $(2\pi)^\nu$ (for $\hbar=1$, so h is 2π). Thus if $V(x) \leq 0$:

$$N_{c\ell}(V) = \frac{\tau_\nu}{(2\pi)^\nu} \int |V(x)|^{\nu/2} d^\nu x$$

where τ_ν is the volume of the unit sphere in R^ν. As a result, Thm. 2.3 says that the quantum $N(V)$ is bounded by a multiple of $N_{c\ell}(V)$. There is also a connection with Sobolev estimates (see [21,22]). Thm. 2.1 was proven independently (with different C_ν) by Rosenbljum [23], Cwickel [24] and Lieb [25] (see [21,26] for expositions of [25,24]) with newer proofs by Li-Yau [27] and Fefferman-Phong [28]. Theorem 2.4 is in some sense especially accurate for "large" V:

Theorem 2.5 (Quasiclassical limit for $N(V)$). Let $\nu \geq 3$, $V \in L^{\nu/2}$. Then

$$\lim_{\lambda\to\infty} N(\lambda V)/N_{c\ell}(\lambda V) = 1$$

Since $-\Delta + \lambda V = (-\lambda^{-1}\Delta+V)\lambda$, the $\lambda \to \infty$ limit is "equivalent" to the $\hbar \to 0$ limit, which is "why" the semiclassical result is asymptotically correct. Thm. 2.4 is used to show that Thm. 2.5 need only be proven when $V \in C_0^\infty$ where Thm. 2.5 was proven independently by Birman-Borzov [29], Martin [30] and Tamura [31] (see [3,21] for pedagogic discussions). A multiparticle analog of Thm. 2.4 can be found in [32].

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Now we want to describe some results on bound states for multiparticle systems. The first basic result describes $\sigma_{ess}(H)$. We first use the partition notation described in Section 1.

Theorem 2.6 (HVZ theorem) Let H be the Hamiltonian (with C.M. motion removed) of an N-body system on $L^2(R^{\mu(N-1)})$ with two body potential in S^{μ}_{comp}. Let

$$\Sigma = \inf_{a|\#(a)\geq 2} [\min \sigma(H(a))]$$

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

In order to understand this result, it is useful to know

Theorem 2.7 (Persson's theorem [33]) Let $V_- \varepsilon K^{\nu}$, $V_+ \varepsilon K^{\nu}_{loc}$. Then

$$\inf \sigma_{ess}(-\Delta+V) = \lim_{R\to\infty} \inf\{(\varphi,(-\Delta+V)\varphi) | \varphi\in C_0^{\infty}(R^{\nu}); \|\varphi\|=1; \operatorname{supp}\varphi\subset\{x| |x|>R\}\}$$

For a proof, see also Agmon [34,35] or Cycon et al. [4]. What Persson's theorem suggests is that essential spectrum is associated with vectors living near infinity (this is basically because $(H+i)^{-1}$ times the characteristic function of a bounded set is compact). Thus, in the N-body case, essential spectrum is associated with states near infinity where the system must break up into two or more subsets. Thus, one should expect

$$\sigma_{ess}(H) = \bigcup_{a|\#(a)\geq 2} \sigma(H(a))$$

which is just a restatement of Thm. 2.6.

Thm. 2.6 has two parts in a natural sense: (i) $[\Sigma,\infty) \subset \sigma(H)$ and (ii) $\sigma(H) \cap (-\infty,\Sigma)$ is discrete. (i) is the "easy" half and (ii) will be what we concentrate on (see e.g. Garding [36] for the "easy" half). The name HVZ recognizes contributions of Hunziker [37], van Winter [38] and Zhislin [39]. Zhislin used geometric ideas together with rather extensive machinery, so for some years the integral equation proof of van Winter and Zhislin was considered the more elementary (see e.g. [3] for that proof), but with the work of Enss [40] and Simon [41], the geometric proof has come into fashion, and it is Sigal's version of it [42] that we will sketch.

We begin with a basic result on localization called the "IMS localization formula" due to contributions of Ismigilov, Morgan, Simon and I.M. Sigal, who first appreciated its great usefulness.

Proposition 2.8 Let $\{j_a\}$ be a finite family of functions with distributional gradients in L^∞ obeying $\sum j_a^2 = 1$. Let $H = -\Delta + V$ on $L^2(R^\nu)$ have C_0^∞ as a form core. Then

$$H = \sum j_a H j_a - \sum (\nabla j_a)^2 \tag{2.1}$$

Remark (2.1) is intended in the sense of expectation values with $(\varphi, j_a H j_a \varphi) \equiv (j_a\varphi, H j_a \varphi)$. If the j's are sufficiently smooth, it holds in operator sense.

Proof By a limiting argument, we can suppose the j's are C^∞. Then $[j_a,[j_a,H]] = [j_a,[j_a,-\Delta]] = -2(\nabla j_a)^2$. Thus

$$\sum_a j_a^2 H + H j_a^2 = 2\sum_a j_a H j_a - 2\sum_a \nabla j_a^2$$

which yields (2.1) given $\sum j_a^2 = 1$. ■

Next, we need the existence of a special partition of unity for N-body system: A *Ruelle-Simon partition of unity* of an N-body system is a set of functions $\{j_a\}$ on X (the CM=0 space) labeled by partitions, a, with $\#(a) = 2$ obeying (i) j_a is C^∞ (ii) $\sum j_a^2 = 1$ (iii) if $\lambda > 1$ and $\|x\| > 1$, then $j_a(\lambda x) = j_a(x)$ (iv) for some $C > 0$,

$$[\operatorname{supp} j_a \cap \{x \mid \|x\| > 1\}] \subset \bigcup_{(ij)\not\subset a} \{x \mid \|x_i - x_j\| \geq C\|x\|\}$$

Thus j_a lives in the region where particles in different clusters of a are far from each other as $\|x\| \to \infty$. (The norm of x is measured in any convenient way.)

Proposition 2.9 Ruelle-Simon partitions of unity exist.

Sketch of proof Let $S_a = \{x \mid \|x\| = 1,\ x_i = x_j \text{ for some } (ij) \subset a\}$. We claim that $\bigcap_a S_a = \phi$. For if $\|x\| = 1$, $x_i \neq x_j$ for some pair i,j (since $\sum m_i x_i = 0$). Let $a = \{C_1, C_2\}$ with $C_1 = \{x \mid x = x_i\}$ and $C_2 = \{1,\ldots,N\} \setminus C_1$. Then $x \notin S_a$. Since the S_a are closed and $\bigcap_a S_a = \phi$, it is not hard to find $C^\infty \tilde{j}_a$ on $\{x \mid \|x\| = 1\}$ so that $\sum \tilde{j}_a^2 = 1$ and $\tilde{j}_a$ vanishes in a neighborhood of S_a. Now let $j_a(x) = \tilde{j}_a(x/\|x\|)$ if $\|x\| \geq 1$ and continued to be smooth near 0. ■

One can actually estimate the constant C; see [41].

Proposition 2.10 Let H be an N-body Hamiltonian of the type described in Thm. 2.6, and let $\{j_a\}$ be a Ruelle-Simon partition of unity. Then:

(a) $(\nabla j_a)^2$ is H-compact for any a

(b) $I(a)j_a$ is H-compact for any a.

Proof $(\nabla j_a)^2$ is bounded and goes to zero at ∞ (as $|x|^{-2}$) so (a) is easy. If $(ij) \not\subset a$, $|x_i - x_j| \to \infty$ as $|x| \to \infty$, so it is not hard to show that $V_{ij}j_a$ is H-compact (see e.g. [41]). ∎

We are now ready for

Proof of Thm. 2.6 [42] (Hard direction) Pick a Ruelle-Simon partition of unity. Write

$$H = \hat{H} + W, \ \hat{H} = \sum_{\#(a)=2} j_a H(a) j_a$$

$$W = \sum j_a I(a) j_a - \sum (\nabla j_a)^2$$

W is H-compact, so $\sigma_{ess}(H) = \sigma_{ess}(\hat{H})$ by Prop. 2.2. Since $H(a) \geq \Sigma$ for all a, we have for any φ in L^2 that

$$(\varphi, \hat{H}\varphi) \geq \sum_a (j_a^2\varphi, \Sigma\varphi) = \Sigma(\varphi,\varphi)$$

so $\sigma_{ess}(\hat{H}) \subset \sigma(H) \subset [\Sigma, \infty)$. ∎

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These geometric methods have been extremely useful in studying bound state problems in N-body systems. Here are some results which we quote without detailed proofs:

Theorem 2.11 Let $\nu \geq 3$. Let H be the Hamiltonian of an N-body system with potentials V_{ij} obeying $|V_{ij}(x)| \leq C(1+|x|)^{-2-\varepsilon}$. Suppose that the bottom of the continuum is two body in the sense that

$$\inf_{\#(a)\geq 3} \sigma(H(a)) > \inf_{\#(a)\geq 2} \sigma(H(a))$$

Then H has only a finite discrete spectrum.

Theorems of this genre go back to Zhislin and collaborators, see e.g. [43,44]. This result is proven by geometric means in Sigal [42].

Theorem 2.12 For any N,Z let H(N,Z) be the operator on $L^2_a(R^{3N})$ (≡ function on $R^{3N} = \{x=(x_1,\ldots,x_N)|x_i \in R^3\}$ antisymmetric in the x_i's) given by

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

Let $E(N,Z) \equiv \inf \operatorname{spec} H(N,Z)$. Then, there exists N(Z), so that

$$E(N+1,Z) = E(N,Z) \qquad \text{if } N \geq N(Z)$$

This result says that a nucleus of charge Z bonds at most N(Z) electrons (we will take N(Z) to be the smallest N(Z) obeying the above). Thm. 2.12 with L^2_a replaced by L^2 was proven by Ruskai [45]; Thm. 2.12 was proven by Sigal [42]. Recently, Lieb [46] has found an elegant direct proof that $N(Z) \leq 2Z$ for all Z. Using Sigal's method, Lieb et al. [47] have proven that $\lim_{Z\to\infty} N(Z)/Z = 1$.

3. The basic notions of scattering theory

We will introduce here some of the simplest notions in scattering theory; Enss, in his lectures, will discuss much more involved ideas. See [2] for an extensive discussion of scattering theory.

Given A,B, we want to find pairs φ,ψ so

$$e^{-itA}\varphi - e^{-itB}\psi \to 0 \quad \text{as} \quad t \to +\infty \tag{3.1}$$

It turns out that for general B, one shouldn't normally expect that a φ exists for every ψ. For example, if $B\psi = 0$, one must have $\varphi = \psi$ and $A\psi = 0$ for the limit (3.1) to occur. Thus, we only try to find φ for $\psi \in \mathcal{H}_{a.c.}(B)$, the absolutely continuous subspace for B. Note (3.1) is equivalent to

$$\varphi = \lim_{t\to\infty} e^{itA}e^{-itB}\psi \tag{3.2}$$

This motivates

Definition Given two self-adjoint operators, A,B we say that the *wave operators* $\Omega^{\pm}(A,B)$ exist if and only if $\text{s-lim}_{t\to\mp\infty} e^{itA}e^{-itB}P_{a.c.}(B)$ exists.

Notice that if s is fixed and we replace t by $t-s$, the limit is the same. Thus:

$$e^{-isA}\Omega^{\pm}(A,B) = \Omega^{\pm}(A,B)e^{-isB} \tag{3.3}$$

This implies that B restricted to $\text{Ran } P_{a.c.}(B)$ and A restricted to $\text{Ran } \Omega^{\pm}(A,B)$ are unitarily equivalent. In particular, $\text{Ran } \Omega^{\pm}(A,B) \subset \text{Ran } P_{a.c.}(A)$. It is clearly natural to single out:

Definition Let $\Omega^{\pm}(A,B)$ exist. We say they are *complete* if and only if $\text{Ran } \Omega^{\pm}(A,B) = \text{Ran } P_{a.c.}(A)$.

If $\Omega^{\pm}$ exist and are complete, then the association (3.1) sets up a one-one correspondence between $\mathcal{H}_{a.c.}(A)$ and $\mathcal{H}_{a.c.}(B)$. Given the fact that (3.1) is symmetric in A and B, it is not hard to show:

Proposition 4.1 Let $\Omega^{\pm}(A,B)$ exist. Then, they are complete if and only if

$\Omega^{\pm}(B,A)$ exist.

Remark Deift-Simon [48] have an N-body analog of Prop. 4.1.

Proposition 4.1 suggests that one look for a condition symmetric in A,B which implies that $\Omega^{\pm}(A,B)$ exist. The strongest such result seems to be:

Theorem 4.2 Let A,B be self-adjoint operators with $(A+i)^{-1} - (B+i)^{-1}$ compact and so that for any interval, Δ: $E_{\Delta}(A)(A-B)E_{\Delta}(B)$ is trace class (where $E_{\Delta}(\cdot)$ is a spectral projection). Then $\Omega^{\pm}(A,B)$ exist and are trace class.

Theorems of this genre go back to Kato and Rosenbljum, with later contributions of note by Kato, Birman, Pearson and Davies. This result follows from an observation of Davies [49] and a theorem of Birman which appears as Cor. 6.7 in [26].

As far as the abstract theory is concerned, Thm. 4.2 is quite elegant. However, in the concrete situation of $A = -\Delta + V$ and $\Omega = -\Delta$ on $L^2(R^{\nu})$, it breaks down when V decays more slowly than $|x|^{-\nu}$ while one expects that $\Omega^{\pm}(A,B)$ and are complete so long as V only has $|x|^{-1-\varepsilon}$ decay. Various methods exist for proving that this compactness result (existence is easy, see [2], Sect. XI.4 and references therein):

(a) The method of weighted L^2 estimates developed by Agmon and Kuroda and discussed in Section XIII.8 of [3].

(b) The Enss method discussed in Section XI.17 of [2], and the book of Perry [50].

(c) Combining the Mourre estimates, to be described in the next section, with the smoothness techniques of Kato and Lavine (see e.g. Perry, Sigal, Simon [51]).

For N-body systems, the notion of completeness requires a more elaborate definition. Let H^a be the Hamiltonian describing internal motion for the clustering a and let P^a denote the projection onto the span of the eigenvectors of H^a, and let $P(a) = P^a \otimes I$. One defines for any a

$$\Omega_a^{\pm} = \lim_{t \to \mp\infty} e^{itH} e^{-itH(a)} P(a)$$

Under suitable hypotheses, it is not hard to show that $\Omega_a^{\pm}$ exist (see Thm. XI.35 in [2], but note the arguments there require modification if $\nu = 1,2$). $\Omega_a^{\pm}\varphi = \eta$ is a state with $e^{-itH}\eta$ asymptotic as $t \to -\infty$ to a state with *bound* clusters in a moving relatively freely. It is thus reasonable and not hard to prove ([2], Thm. XI.36(b)) that

$$\text{Ran}\ \Omega_a^{+} \perp \text{Ran}\ \Omega_b^{+} \qquad a \neq b$$

Completeness now reads

$$L^2(R^{(N-1)\nu}) = \bigoplus_a (\text{Ran}\ \Omega_a^{\pm}) \tag{3.4}$$

Notice that if a_1 is the unique clustering with $\#(a_1) = 1$ (so $H(a_1) = H$), then $\Omega_{a_1}^{\pm} = P(a_1)$ is the projection onto the point spectral subspace H, and that by the intertwining relation

$$e^{itH}\Omega_a^{\pm} = \Omega_a^{\pm} e^{itH(a)}$$

$\text{Ran}\ \Omega_a^{\pm} \subset \mathcal{H}_{a.c.}(H)$ if $\#(a) \geq 2$. Thus (3.4) implies that H has empty singular continuous spectrum.

Thus far, there are fairly general results on three body completeness [52,53,54] but only very specialized results for N-body, see e.g. [55,56,57,58]. It has been emphasized to me by I.M. Sigal that the following result which extends an idea of Deift-Simon [48] should be very useful in a possible inductive proof of completeness:

<u>Proposition 4.3</u> Let $\{A(a)\}_{\#(a)\geq 2}$ be bounded operators with $\sum_a A(a) = 1$. Suppose that (i) Each H^a with $\#(a)\geq 2$ is complete (ii) The operators $\lim_{t\to\mp\infty} e^{itH(a)}A(a)e^{-itH}P_{a.c.}(H) \equiv W_a^{\pm}$ exist. (iii) $\mathcal{H}_{sing}(H) = \phi$. Then H is complete.

<u>Proof</u> Let $\eta \in \text{Ran}\ P_{a.c.}(H)$. Then

$$e^{-itH}\eta = \sum_a A(a)e^{-itH}\eta \sim \sum_a e^{-itH(a)}W_a^{\pm}\eta$$

where $\sim$ means the difference goes to zero as $t \to \mp\infty$. Since H^a is complete, $e^{-itH(a)}\varphi$ is asymptotically a sum of vectors of the form $e^{-itH(b)}P(b)\varphi_b$ with $b \leq a$, so we have completeness for H. ■

4. Mourre estimates

Eric Mourre, in a deep paper [59], singled out certain estimates which he showed have important spectral consequences, and which he proved for a large class of two and three body systems. Perry, Sigal, Simon [51] then gave an involved proof of these estimates for general N-body systems. Subsequently, Froese-Herbst [80] found a rather simple proof of these PSS results.

Let H be a self-adjoint operator, and A a second self-adjoint operator. We will not be explicit about all domains referring the reader to [59,51] for explicit hypotheses. Under such hypotheses, one can define $-i[A,H] = B$ originally on a suitable core for H and then as an "operator" from $D(H)$ to $D^{-1}(H)$ (equal abstract dual of $D(H)$) i.e. $(H+i)^{-1}B(H+i)^{-1}$ is a bounded operator. We say that H obeys a *Mourre estimate* at a point E_0, if there is an open interval Δ about E_0 so that

$$E_\Delta B E_\Delta \geq \alpha E_\Delta^2 + E_\Delta K E_\Delta \tag{4.1}$$

for a *compact* operator K, and some $\alpha > 0$.

Theorem 4.1 Under suitable domain hypotheses (including a bound on $[A,B]$), if a Mourre estimate holds for any $E_0 \in I$, an open interval, then

(i) H has no singular continuous spectrum in I

(ii) In any compact $J \subset I$, there are finitely many eigenvalues of H and each eigenvalue has finite multiplicity.

(iii) For any compact $J \subset I$ and $\delta > 0$, $\sup_{\substack{0 \leq \varepsilon < 1 \\ E \in J}} \|(|A|+1)^{-\frac{1}{2}-\delta}(H-E-i\varepsilon)^{-1}(|A|+1)^{-\frac{1}{2}-\delta}\|$ $< \infty$.

The result is essentially due to Mourre [59], although the above include refinements of [51]. While we will not give the proof in detail, we note the basic idea behind (ii). Using the unstated domain conditions, one verifies a Virial theorem: If $H\varphi = E\varphi$, then $(\varphi, B\varphi) = 0$. Thus, if $H\varphi_n = E_n\varphi_n$ with $E_n \to E_0 \in \Delta$ and φ_n is orthonormal, then, by (4.1)

$$0 \geq \alpha\|\varphi_n\|^2 + (\varphi_n, K\varphi_n)$$

which is impossible since K is compact and $\varphi_n \to 0$ weakly.

Mourre [61] (see also [62]) has also proven interesting propagation estimates when Mourre estimates hold.

When does an estimate like (4.1) hold? Mourre had the idea of taking $A = \frac{1}{2}(x\cdot p+p\cdot x)$ (with $p = -i\nabla$), the generator of dilations. For two body operators, $H = H_0 + V$

$$-i[A,H] = 2H_0 - x\cdot\nabla V = 2H + W$$

where

$$W = -x\cdot\nabla V - 2V$$

If $K = E_\Delta(H)WE_\Delta(H)$ is compact, and if $\Delta = [a,b]$ with $a > 0$, then $E_\Delta BE_\Delta \geq 2aE_\Delta^2 + E_\Delta KE_\Delta$, so a Mourre estimate holds.

<u>Proposition 4.2</u> If $V = V_1 + V_2$ with $V_1(H_0+i)^{-1}$, $x\cdot\nabla V_1(H_0+i)^{-1}$ and $(1+|x|)V_2(H_0+i)^{-1}$ all compact, then a Mourre estimate holds for $A = \frac{1}{2}(x\cdot p+p\cdot x)$; $H = -\Delta + V$ and $E_0 > 0$.

<u>Proof</u> Note first that $D(H) = D(H_0)$, so $(H_0+i)E_\Delta(H)$ is bounded. Thus, $E_\Delta W_1 E_\Delta$ is obviously compact as is $E_\Delta V_2 E_\Delta$. As for $-i[A,V_2]$, we can write that as $-\sum_i [\nabla_i, x_i V_2] + \nu V_2$ and $E_\Delta[(\nabla_i)(x_i V_2)]E_\Delta$ is compact. ■

Mourre [59] showed how to do this for three-body systems and then PSS [51] proved:

<u>Theorem 4.3</u> If each $V_{ij} = V_{ij}^{(1)} + V_{ij}^{(2)}$, where as operators on $L^2(R^\nu)$, $V^{(1)}(h_0+i)^{-1}$, $x\cdot\nabla V^{(1)}(h_0+i)^{-1}$ and $(1+|x|)V^{(2)}(h_0+i)^{-1}$ are all compact on ($h_0 = -\Delta$ on R^ν), then a Mourre result holds for any $E_0 \neq$ threshold (and α is twice the distance from E_0 to the threshold of next lowest energy).

To conclude (i) and (iii) in Thm. 4.1, we also need control on [A,B] which requires V_{ij} have more decay than in the above theorem (e.g. $(1+x^2)V^{(2)}(h_0+i)^{-1}$ $V^{(1)}(h_0+i)^{-1}$ and $x^2\nabla\nabla V^{(1)}(h_0+i)^{-1}$ compact will do); see e.g. [51]. Froese-Herbst [60] have a simple proof of Thm. 4.3.

Froese-Herbst [63] have proven the following theorems using Mourre estimates:

<u>Theorem 4.4</u> [63] Let V_{ij} obey the hypotheses of Theorem 4.3, and suppose that $H\varphi = E\varphi$, with $\varphi \in L^2$. Let $|x|$ denote the norm of x in X (i.e. $(\sum m_i x_i^2)^{\frac{1}{2}}$ if $\sum m_i x_i = 0$). Define

$$\alpha = \sup\{a \,|\, e^{a|x|}\varphi \in L^2\}$$

Then either $\alpha = \infty$ or $\alpha^2 + E$ is a threshold.

By using results [64] which imply $\alpha = \infty$ is not allowed:

<u>Theorem 4.5</u> [63] If the V_{ij} obey the hypotheses of Theorem 4.3, and for all $\varepsilon > 0$

$$y \cdot \nabla V_{ij}(y) \leq \varepsilon h_0 + C_\varepsilon$$

then $H\varphi = E\varphi$ has no L^2 solutions with $E > 0$.

5. An Introduction to the Theory of Stochastic Jacobi Matrices

In this final section, we consider another topic currently of intense interest, namely Schrödinger operators with random or almost periodic potentials. For technical simplicity, we will restrict ourselves to $\nu = 1$ and we will discretize space, i.e. replace R by Z and $-d^2/dx^2$ by a second difference operator. See [65] for an extensive bibliography including papers dealing with the continuum case and with $\nu > 1$.

We should take h_0 to be the finite difference analog of $-d^2/dx^2$, namely $(h_0 u)(n) = \delta^{-2}[2u(n) - u(n+1) - u(n)]$. First of all, we take $\delta = 1$ for convenience. Then, we replace h_0 by $h_0 - 2$ which won't change any spectral properties. Then we make the unitary transformation $u(n) \to (-1)^n u(n)$ which means that instead, we take

$$(h_0 u)(n) = u(n+1) + u(n-1) \tag{5.1}$$

on $\ell^2(Z)$. We will study not individual operators but whole classes: Let (Ω, μ) be a probability measure space and let $T : \Omega \to \Omega$ be an invertible, measure preserving ergodic transformation. Let $f : \Omega \to R$ be a bounded measurable function. Given $\omega \in \Omega$, define

$$V_\omega(n) = f(T^\alpha \omega) \tag{5.2}$$

and

$$h_\omega = h_0 + V_\omega \tag{5.3}$$

We ask about properties of h_ω that hold for a.e. ω.

Examples 1. $\Omega = \mathop{X}\limits_{n=-\infty}^{\infty} [a,b]$, $d\mu = \bigotimes_{n=-\infty}^{\infty} d\nu(x_n)$ where $d\nu$ is a probability measure on $[a,b]$. Let $(Tx)_n = x_{n+1}$ and $f(x) = x_0$. Then the variables $V_\omega(n)$ are precisely independent identically distributed (i.i.d.) random variables with common density $d\nu$. This is conventionally called "random potentials." The case $d\nu(x) = (b-a)^{-1}\chi_{(a,b)}(x)dx$ is called *the Anderson model.*

2. Let Ω be the k torus $\{(\theta_1, \ldots, \theta_k);\ 0 \le \theta < 1\}$ with its structure as a group (addition of components, mod. 1) and Haar measure $\prod_1^k d\theta_i$. Let f be

a continuous function on Ω and let $(T\theta)_i = \theta_i + \alpha_i$ (mod 1) where $\alpha_1,\ldots,\alpha_k$ are numbers so that $1,\alpha_1,\ldots,\alpha_k$ are independent over the rationals. Then $V_\theta(n) = f(\alpha_i n+\theta_i)$ is quasiperiodic. A good example is $V_\theta(n) = \lambda \cos(2\pi\alpha n+\theta)$ (now θ runs through $[0,2\pi)$) called *Harper's equation* or the *almost Mathieu equation*. An interesting example (see [66,67,68]) which doesn't quite fit into this framework is $V_\theta(n) = \lambda \tan(\pi\alpha n+\theta)$. This is called the *Maryland model* and has the feature of being exactly soluble in a certain sense.

It makes sense to study the totality of the operators $\{h_\omega\}$ for one has the following consequence of ergodicity.

Theorem 5.1 ([69]) The following sets are constant for a.e. ω (i.e. there is a set $S \subset \Omega$ whose complement has measure zero, so that if $\omega, \omega' \in S$ all the objects below are equal for ω and ω'): $\sigma(h_\omega)$, $\sigma_{a.c.}(h_\omega)$, $\sigma_{pp}(h_\omega)$ ($\equiv$ *closure* of set of eigenvalues), $\sigma_{s.c.}(h_\omega)$. Moreover, $\sigma_{disc}(h_\omega) = \phi$ and $\sigma(h_\omega)$ has *no* isolated points.

Remark $\sigma_{disc}(h_\omega) = \phi$ also in the higher dimensional case; it is also true in that case that $\sigma(h_\omega)$ has no isolated points, but this is more subtle (see [70,71]).

Here are some typical results illustrating the subtle spectral properties of stochastic Jacobi matrices:

Theorem 5.2 Let h_ω have a random potential ($V_\omega(n)$ i.i.d.'s) with $d\nu(x) = F(x)dx$ (supported on $[a,b]$). Then, for a.e. ω,

$$\mathrm{spec}(h_\omega) = [-2,2] + \mathrm{supp}(F)$$

and h_ω has a complete set of eigenfunctions.

For proofs see [69,72]. For related continuum results, see [73,74]. For the study of $h_0 + (1+|n|)^{-\alpha}V_\omega(n)$, see [75,76].

Theorem 5.3 Let $\{a_n\} \in \ell_1(0,1,\ldots)$ and let $h(a_m) = h_0 + \sum_{m=0}^{\infty} a_m \cos(2\pi n/2^m)$. Then for a dense G_δ in ℓ_1, $h(a_m)$ has a nowhere dense spectrum and for a dense set in ℓ_1, $\sigma(h(a_m))$ is both nowhere dense and purely absolutely continuous.

See [77,78,79] for proofs; see [80] for a discussion of nowhere dense a.c. spectrum.

Theorem 5.4 Pick any $0 < \alpha < 1$. Then, there exists almost periodic potentials $V_\omega(n)$ so that $h_0 + V_\omega(n) = h_\omega$ has dense point spectrum and $\sigma(h_\omega)$ has Hausforff dimension α.

The basic idea is from Craig [81], although his examples are not strictly almost periodic; those are due to Poschel [82]. See also [83].

Sarnak [84] first suggested that spectral properties should depend on Diophantine properties of α:

Theorem 5.5 Let α be an irrational number for which there exist rational approximations p_n/q_n obeying $|\alpha - p_n/q_n| \leq n^{-q_n}$. Let $\lambda > 2$. Then

$$h_0 + \lambda \cos(2\pi\alpha n+\theta)$$

has purely singular continuous spectrum.

For a proof, see Avron-Simon [85]; important input comes from Aubry-André [86] and Gordon [87]. The set of α obeying the estimates is a dense G_δ in R (of Lebesgue measure zero).

Definition A stochastic process $V_\omega(n)$ is called *deterministic* if and only if $\{V_\omega(n)\}_{n\geq 0}$ is (a.e.) a measurable function of $\{V_\omega(n)\}_{n<0}$. For example, a.p. functions yield deterministic processes; random potentials do not.

Theorem 5.6 If h_ω is a stochastic Jacobi matrix and h_ω has some a.c. spectrum (for a.e. ω), then V_ω is a deterministic process.

This result in the continuum case is due to Kotani [88]; see Simon [89] for the discrete case.

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