MULTIDIMENSIONAL SCHRÖDINGER OPERATORS AND SPECTRAL THEORY

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Abstract. Here we present some fundamental theorems of Schrödinger operators and their spectral theory.

Contents

1. Introduction and Overview

The Schrödinger operator, also known as the Hamiltonian operator, completely determines the time evolution of a quantum system via the Schrödinger equation

$$i\hbar\partial_t\psi = H\psi,$$

where H is the Schrödinger operator and ψ is the wave function.

The Schrödinger operator is usually written as

$$H = -\frac{\hbar^2}{2m}\Delta + V(x), \tag{1.1}$$

where Δ is the Laplacian and $V(x)$ is a multiplication operator given by the potential field. In this exposition, we will, for simplicity, let $m = 1/2$ and $\hbar = 1$ in (1.1). The Schrödinger operator is then given by

$$H = -\Delta + V(x). \tag{1.2}$$

Multiplication operators are symmetric, and the negative of the Laplacian is self-adjoint on the Sobolev space $H^2(\mathbb{R}^n)$. However, since the collection of self-adjoint operators is not an algebra, it is not necessarily true that (1.2) is self-adjoint or even essentially self-adjoint on $\mathcal{H}$. Therefore, due to the physical importance of self-adjoint operators as observables, it is relevant to confirm that the Schrödinger operator H is self-adjoint or essentially self-adjoint. This depends upon the potential V, which is determined by the specific quantum system. The first important

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problem of the study of Schrödinger operators, then, is to find specific and realistic conditions for V under which H becomes self-adjoint or essentially self-adjoint.

The second big problem of Schrödinger operators is the determination of the spectrum, given the potential V. This is particularly important since the collection of eigenvalues describes the possible energy levels of the quantum system.

In this exposition, we will collect some of the most important techniques and theorems for finding the spectrum of H, along with the conditions under which H is (essentially) self-adjoint. I have tried to make this as self-contained as possible, although there were a few results of functional analysis upon which I was unable to further expound without considerably increasing the article's length. However, references [1], [2], and [4] do a particularly fine job of covering all necessary background material.

2. Sobolev Spaces and Elliptic Regularity

Often in quantum mechanics, the state space is some subset of $L^2(\mathbb{R}^n)$. Recall from the mathematical theory of quantum mechanics that an observable is a self-adjoint linear operator on the state space. Since the Hamiltonian is given by (1.2), a natural subset of $L^2(\mathbb{R}^n)$ in which to work would be a space in which not only the domain of H is in $L^2(\mathbb{R}^n)$, but the image of H must also be in $L^2(\mathbb{R}^n)$. This means that the second derivatives should also be in $L^2(\mathbb{R}^n)$ due to the Laplacian. The following construction creates a natural space in which this should occur.

Definition 2.1. Let $\alpha = (\alpha_1, \ldots, \alpha_n)$ be an n-tuple of integers. We say that α is a multi-index, and we define $|\alpha| = a_1 + \cdots + a_n$. A generalized derivative in $\mathbb{R}^n$ of order $k < n$ is defined to be the a derivative of the form $\partial^\alpha = \partial_{x_1}^{\alpha_1}\partial_{x_2}^{\alpha_2}\cdots\partial_{x_n}^{\alpha_2}$, where $\alpha = (\alpha_1, \cdots, \alpha_n)$ is an n-tuple and $|\alpha| = k$.

Using the notion of a generalized derivative, we can now define the Sobolev space $H^k(\mathbb{R}^n)$, which plays a very important and natural role in the theory of Schrödinger operators.

Definition 2.2. Let $k \in \mathbb{N}$. Then we define

$$H^k(\mathbb{R}^n) := \{f \in L^2(\mathbb{R}^n) : \partial^\alpha f \in L^2(\mathbb{R}^n)\, \forall |\alpha| \leq k\}.$$

Since in mathematical physics, we often want a derivative up to a particular order to be in $L^2(\mathbb{R}^n)$ (as in the case of the Hamiltonian with $k = 2$), the Sobolev spaces are rather vital to our exposition.

We introduce a scalar product in $H^k(\mathbb{R}^n)$ by setting

$$(f, g)_k := \sum_{|\alpha|<k} (\partial^\alpha f, \partial^\alpha g),$$

where $(\cdot, \cdot)$ is the scalar product in $L^2(\mathbb{R}^n)$. The corresponding norm is then

$$\|f\|_k = (f, f)_k^{1/2} = \left[\sum_{|\alpha|\leq k} \int_{\mathbb{R}^n} |\partial^\alpha f(x)|^2 dx\right]^{1/2}.$$

Theorem 2.3. *The scalar product $(f, g)_k$ makes $H^k(\mathbb{R}^n)$ into a separable Hilbert space.*

Proof. We first prove completeness. Let $\{f_m\}_{m=1}^{\infty}$ be a Cauchy sequence in $H^k(\mathbb{R}^n)$. Then all sequences $\{\partial^\alpha f_m\}_{m=1}^{\infty}$ for $|\alpha| \leq k$ are Cauchy in $L^2(\mathbb{R}^n)$. By the completeness of $L^2(\mathbb{R}^n)$, these all converge, that is,

$$\lim_{m\to\infty} \partial^\alpha f_m = g_\alpha$$

in $L^2(\mathbb{R}^n)$. In particular, letting $\alpha = 0$ gives us $f_m \to g_0$. But this means that $\partial^\alpha f_m \to \partial^\alpha g_0$ in $\mathcal{D}(\mathbb{R}^n)$, the space of distributions in $\mathbb{R}^n$. Hence, $g_\alpha = \partial^\alpha g_0$, so that $g_0 \in H^k(\mathbb{R}^n)$. This shows that $f_m \to g_0$ in H^k, which proves completeness.

For separability, we notice that the map $f \mapsto \{\partial^\alpha f\}_{|\alpha|\leq s}$ creates an isometric embedding of $H^k(\mathbb{R}^n)$ into a direct sum of copies of $L^2(\mathbb{R}^n)$. The separability of $H^k(\mathbb{R}^n)$ then follows from the separability of $L^2(\mathbb{R}^n)$. □

The definition of a Sobolev space is very direct for natural numbers. However, it is convenient to extend the definition of H^k to the case where $k \in \mathbb{R}$. We carry this out by performing a Fourier transformation. Recall that the Fourier transform is a unitary operator, and that it transforms $\partial^\alpha f(x)$ to $(i\xi)^\alpha \widetilde{f}(\xi)$, where $\widetilde{f}$ denotes the Fourier transform of f. Hence, the condition that $f \in H^k(\mathbb{R}^n)$ is equivalent to the condition that $\xi^\alpha \widetilde{f}(\xi) \in L^2(\mathbb{R}^n)$ for $|\alpha| \leq k$.

The above condition is in turn equivalent to the condition that

$$\sum_{|\alpha|\leq k} |\xi^\alpha|^2 |\widetilde{f}(\xi)|^2 \in L^1(\mathbb{R}^n).$$

Clearly, there exists a $C > 0$ independent of ξ such that the following holds:

$$C^{-1}(1+|\xi|^2)^k \leq \sum_{|\alpha|\leq k} |\xi^k|^2 \leq C(1+|\xi|^2)^k. \tag{2.4}$$

Hence, that $f \in H^k(\mathbb{R}^n)$ is equivalent to the condition that

$$(1+|\xi|^2)^{k/2}\widetilde{f}(\xi) \in L^2(\mathbb{R}^n)$$

and the norm $\|f\|_k$ may be written as

$$\|f\|_k = \left[\int (1+|\xi|^2)^k |\widetilde{f}(\xi)|^2 d\xi\right]^{1/2}. \tag{2.5}$$

There is one more definition we must make before we define the Sobolev space $H^k(\mathbb{R}^n)$, for $k \in \mathbb{R}$. Recall that the Schwartz space $\mathcal{S}(\mathbb{R}^n)$ is the function space of of all C^∞ functions on $\mathbb{R}^n$ such that all generalized derivatives, when multiplied by any power of $|x|$, converge to 0 as $|x| \to \infty$. More precisely,

$$\mathcal{S}(\mathbb{R}^n) = \{f \in C^\infty(\mathbb{R}^n) : \sup_{x\in\mathbb{R}^n} |x^\alpha \partial^\beta f(x)| < +\infty \text{ for all multi-indices } \alpha, \beta\}.$$

The Fourier transform is an automorphism of the Schwartz space $\mathcal{S}(\mathbb{R}^n)$. The following space is similar to the Schwartz space in the case of distributions, as the Fourier transform acts on it in a similar fashion.

Definition 2.6. The space of tempered distributions $\mathcal{S}'(\mathbb{R}^n)$ is defined to be the dual of the Schwartz space $\mathcal{S}(\mathbb{R}^n)$. That is, a distribution S is a tempered distribution if and only if $\lim_{m\to\infty} \sup_{x\in\mathbb{R}^n} |x^\alpha \partial^\beta \varphi_m(x)| = 0$ for all multi-indices α, β implies $\lim_{m\to\infty} S(\varphi_m) = 0$.

Let F be the Fourier transform, and let S be a tempered distribution. Then we define $(FS)(\varphi) = S(F\varphi)$, so that FS must also be a tempered distribution. In our definition of the Sobolev space, we want to be as general as possible while also yielding to common sense, noting that not all distributions have Fourier transforms. Tempered distributions provide a natural space, since the Fourier transform is a continuous, linear, bijective operator from the space of tempered distributions to itself.

Using the definition of tempered distributions, we can now make an appropriately general definition for $H^k(\mathbb{R}^n)$, for $k \in \mathbb{R}$.

Definition 2.7. Let $k \in \mathbb{R}$. Then we define

$$H^k(\mathbb{R}^n) := \{f \in \mathcal{S}'(\mathbb{R}^n) : (1 + |\xi|^2)^{k/2}\widetilde{f}(\xi) \in L^2(\mathbb{R}^n)\},$$

where $\mathcal{S}'(\mathbb{R}^n)$ is the collection of tempered distributions in $\mathbb{R}^n$. The norm is just (2.5) extended to all real numbers.

We now progress to a very famous result in analysis, the Sobolev embedding theorem. We first define a very important space to be used in the theorem.

Definition 2.8. Let $l \in \mathbb{N}$. Then we define

$$C_b^l(\mathbb{R}^n) := \{f \in C^l(\mathbb{R}^n) : \|\partial^\alpha f\|_\infty < +\infty \, \forall |\alpha| \leq k\}.$$

In $C_b^l(\mathbb{R}^n)$, we define the norm to be

$$\|f\|_{(l)} := \sum_{|\alpha| \leq k} \|\partial^\alpha f\|_\infty.$$

Theorem 2.9 (Sobolev Embedding Theorem)**.** *Let $k > n/2 + l$. Then we have the embedding $H^k(\mathbb{R}^n) \subset C_b^l(\mathbb{R}^n)$, where the embedding operator is continuous.*

Proof. We first show that

$$\|f\|_{(l)} \leq C\|f\|_k, \tag{2.10}$$

for $f \in \mathcal{S}(\mathbb{R}^n)$, where C is independent of f. The Fourier transform and the Inverse Fourier Transform Theorem imply that

$$\partial^\alpha f(x) = (2\pi)^{-n/2} \int (i\xi)^\alpha e^{ix\cdot\xi} \widetilde{f}(\xi) d\xi,$$

so that

$$|\partial^\alpha f(x)| \leq (2\pi)^{-n/2} \int |\xi^\alpha \widetilde{f}(\xi)| d\xi.$$

Therefore, using the C from (2.4), we obtain

$$\|u\|_{(l)} \leq C \int (1 + |\xi|^2)^{l/2} |\widetilde{f}(\xi)| d\xi.$$

Separating the integrand by using $(1 + |\xi|^2)^{k/2}$ brings us the following, after we apply the Cauchy-Schwartz inequality.

$$\|f\|_{(l)} \leq C \int (1 + |\xi|^2)^{(l-k)/2} (1 + |\xi|^2)^{k/2} |\widetilde{f}(\xi)| d\xi \leq$$
$$C \left(\int (1 + |\xi|^2)^{(l-k)} d\xi \right)^{1/2} \left(\int (1 + |\xi|^2)^{k/2} |\widetilde{f}(\xi)|^2 d\xi \right)^{1/2}.$$

The first of the two factors is finite, due to the convergence of the integral. The integral converges since $2(l-k) < -n$, so that the integrand decreases as $|\xi| \to +\infty$ faster than $|\xi|^{-n-\epsilon}$ for some sufficiently small $\epsilon > 0$. The second factor is $\|f\|_k$ by Definition 2.7. Therefore, Equation (2.10) holds as long as $k > l + n/2$.

We now show that $\mathcal{S}(\mathbb{R}^n)$ is dense in $H^k(\mathbb{R}^n)$ for any $k \in \mathbb{R}$. Consider the operator Λ_k that multiplies the Fourier transform $\widetilde{f}(\xi)$ by $(1+|\xi|^2)^{k/2}$. This is an isometric isomorphism of $H^k(\mathbb{R}^n)$ onto $L^2(\mathbb{R}^n)$ which takes $\mathcal{S}(\mathbb{R}^n)$ isomorphically onto $\mathcal{S}(\mathbb{R}^n)$. Hence, $\mathcal{S}(\mathbb{R}^n)$ is dense in $H^k(\mathbb{R}^n)$ since $\mathcal{S}(\mathbb{R}^n)$ is dense in $L^2(\mathbb{R}^n)$.

Let $g \in H^k(\mathbb{R}^n)$, $f_m \in \mathcal{S}(\mathbb{R}^n)$, and $f_m \to g$ in $H^k(\mathbb{R}^n)$. Then from Equation (2.10), $f_m \to g_1$ in $C_b^l(\mathbb{R}^n)$. But then g and g_1 coincide as distributions, so they should coincide almost everywhere. By continuity, (2.10) holds for any $f \in H^k(\mathbb{R}^n)$, proving the continuity of the embedding. □

We now introduce the space $H^k_{loc}(\mathbb{R}^n)$, which plays an important role in local elliptic regularity and the proof of Sear's Theorem.

Definition 2.11. Let $k \in \mathbb{R}$. Then we define

$$H^k_{loc}(\mathbb{R}^n) := \{f \in \mathcal{D}(\mathbb{R}^n) \text{ such that } \varphi f \in H^s(\mathbb{R}^n)\, \forall \varphi \in C_0^\infty(\mathbb{R}^n)\},$$

where $\mathcal{D}(\mathbb{R}^n)$ is the space of distributions on $\mathbb{R}^n$.

In fact, similar to the space $H^k(\mathbb{R}^n)$, this is a generalization of the case $k \in \mathbb{N}$. When $k \in \mathbb{N}$, the following definition is suitable.

Definition 2.12. Let $k \in \mathbb{N}$. Then $H^k(\mathbb{R}^n)$ is defined to be the set of $f \in \mathcal{D}(\mathbb{R}^n)$ such that $Pf \in L^2_{loc}(\mathbb{R}^n)$ for any differential operator P on $\mathbb{R}^n$ of order $\leq s$ with smooth coefficients.

There is one particular major result we should cover before progressing to the subject of self-adjointness. Consider the following partial differential equation:

$$-\Delta f + cf = g(x), \tag{2.13}$$

defined on a domain $\Omega \subset \mathbb{R}^n$, with $c \in \mathbb{R}$. Let $g \in H^{-1}_{loc}(\Omega)$. The function $f \in H^1_{loc}(\Omega)$ is called a weak solution of (2.13) if

$$\int_\Omega (\nabla f(x) \nabla \varphi(x) + cf(x)\varphi(x))dx = \langle g, \varphi \rangle$$

for every $\varphi \in C_0^\infty(\Omega)$. This definition leads us to the following important result.

Theorem 2.14. *Let $f \in H^1_{loc}(\Omega)$ be a weak solution of* (2.13)*, with $g \in H^k_{loc}(\Omega)$, where $k \in \mathbb{N}$. Then $f \in H^{k+2}_{loc}(\Omega)$.*

In particular, for $g \in L^2_{loc}(\Omega)$, we may conclude that $f \in H^2_{loc}(\Omega)$. We refer the reader to [3] for the proof of this theorem and for a more complete development of elliptic regularity in general.

3. Self-Adjointness

We recall the definitions of a symmetric and self-adjoint operator. A symmetric operator is an operator A the elements of the domain of which satisfy $\langle Af, g\rangle = \langle f, A^*g\rangle$ for all $f, g \in D(A)$, where A^* denotes the adjoint of A. A self-adjoint operator A is a symmetric operator that also satisfies $D(A) = D(A^*)$. Note that in general, we have the inclusion $D(A) \subset D(A^*)$, so to prove that a symmetric operator is self-adjoint, we need only prove the converse inclusion. An essentially self-adjoint operator is a symmetric operator with a unique self-adjoint extension.

Definition 3.1. We define an observable to be a densely-defined self-adjoint operator on a Hilbert space $\mathcal{H}$.

Notation 3.2. We will use the symbol $\mathcal{H}$ to represent the Hilbert space corresponding to the given quantum system. All Hilbert spaces are taken to be separable.

Definition 3.3. Let A and B be observables on a Hilbert space $\mathcal{H}$. Then B is said to be smaller than A in the sense of Kato (written $B <_K A$) if $D(A) \subset D(B)$, and there exist $a, b \in \mathbb{R}$, $a < 1$, such that the following inequality holds for all $\psi \in D(A)$:

$$\|B\psi\| \leq a\|A\psi\| + b\|\psi\|. \tag{3.4}$$

An equivalent condition for $B <_K A$ is if there exist $a, b \in \mathbb{R}$ with $a < 1$ satisfying

$$\|B\psi\|^2 \leq a\|A\psi\|^2 + b\|\psi\|^2$$

for all $\psi \in D(A)$.

The following theorem is one of the most important for confirming when the operator H is self-adjoint. We start with a lemma.

Lemma 3.5. *Let $\lambda \in \mathbb{R}$, and let A be a closed, symmetric operator in a Hilbert space $\mathcal{H}$. The following are equivalent:*

(1) A is self-adjoint
(2) $\exists \lambda \in \mathbb{R}$ s.t. $ker(A^* \pm \lambda i I) = \{0\}$
(3) $\exists \lambda \in \mathbb{R}$ s.t. $im(A \pm \lambda i I) = \mathcal{H}$

Proof. First, note that $\mathrm{im}(A \pm iI)$ is a closed subspace of $\mathcal{H}$. Since

$$(A \pm i\lambda I)^* = A^* \mp i\lambda I,$$

we have

$$\ker(A^* \mp i\lambda I) = [\mathrm{im}(A \pm i\lambda I)]^{\perp},$$

so (2) and (3) must be equivalent. Clearly, (1) implies (3), since the spectrum of any self-adjoint operator is real. It remains to show that (2) and (3) imply (1). Since $D(A) \subset D(A^*)$, we must show that $D(A^*) \subset D(A)$. Let $f \in D(A^*)$ and $\varphi = (A^* + iI)f$. By (3), there exists a $g \in D(A)$ satisfying $(A + iI)g = \varphi$. Since A is symmetric, $Ag = A^*g$. Therefore,

$$(A^* + i\lambda I)f = \varphi = (A^* + i\lambda I)g,$$

so that

$$(A^* + i\lambda I)(f - g) = 0.$$

By (2), $f = g$ and $f \in D(A)$. Therefore, $D(A) = D(A^*)$ and A is self-adjoint. □

This leads to another version of the same theorem.

Theorem 3.6. *Let A be a closed, non-negative, symmetric operator. Then A is self-adjoint if and only if there exists a $\lambda > 0$ such that*

$$\ker(A^* + \lambda I) = \{0\}.$$

Corollary 3.7. *Let A be a non-negative symmetric operator. Then A is essentially self-adjoint if and only if there exists a $\lambda > 0$ such that*

$$ker(A^* \pm \lambda I) = \{0\}.$$

Having established Lemma 3.5, we may prove the Kato-Rellich Theorem, one of the most important theorems in mathematical quantum physics for determining self-adjointness.

Theorem 3.8 (Kato-Rellich Theorem)**.** *Let A be an observable, and let B a symmetric operator. If $B <_K A$, then $H = A + B$ with $D(H) = D(A)$ is self-adjoint.*

Proof. By Lemma 3.5, H is self-adjoint iff $\text{im}(H \pm \eta I) = \mathcal{H}$ for some $\eta \in i\mathbb{R}$ (which further implies that this equation holds for all $\eta \in \mathbb{C} \setminus \sigma(H)$, where $\sigma(H)$ is the spectrum of H). Since A is self-adjoint, for each $\eta \in i\mathbb{R}$, $R_\eta = (A - \eta I)^{-1}$ is a bounded operator on $\mathcal{H}$ and $\text{im}R_\eta = D(A)$.

Now, $H - \eta I = (I + BR_\eta)(A - \eta I)$, so that $\text{im}(H - \eta I) = \mathcal{H}$ iff $\text{im}(I + BR_\eta) = \mathcal{H}$. The latter condition is true if there exists $N \in \mathbb{R}$ such that for all $|\eta| > N$, $\|BR_\eta\| < 1$, since then $I + BR_\eta$ is an invertible bounded operator.

To prove this, we first note that

$$\|R_\eta \varphi\| \leq \frac{1}{|\eta|}\|\varphi\| \text{ and } \|AR_\eta \varphi\| \leq \|\varphi\|.$$

These follow from the equation

$$\|(A - \eta I)\psi\|^2 = \|A\psi\|^2 + |\eta|^2\|\psi\|^2$$

by setting $\varphi = (A - \eta I)\psi$. Using Definition 3.3 with $\varphi = R_\eta \psi \in D(A)$, we have

$$\|BR_\eta \varphi\| \leq a\|AR_\eta \varphi\| + b\|R_\eta \varphi\| \leq (a + \frac{b}{|\eta|})\|\varphi\|,$$

so that $a < 1$ implies that $\|BR_\eta\| < 1$ for sufficiently large $|\eta|$.

The proof that $\text{im}(H + \eta I) = \mathcal{H}$ is almost identical. □

If we let $A = -\Delta$ and $B = V(x)$ in the Kato-Rellich Theorem, then as long as $V(x) <_K -\Delta$, H is self-adjoint. However, the inequality $<_K$ is somewhat foreign and not terribly intuitive. As a result, the Kato-Rellich theorem is not particularly useful to us by itself. On the other hand, we may derive some important theorems as corollaries, which we will in turn use to prove some physically critical results.

Theorem 3.9. *Let $V \in (L^p + L^\infty)(\mathbb{R}^n)$, where $p = 2$ if $n \leq 3$ and $p > n/2$ if $n \geq 4$. Then $H = -\Delta + V$ is a self-adjoint operator and $D(H) = H^p(\mathbb{R}^n)$.*

Proof. We may work within the confines of $C_0^\infty(\mathbb{R}^n)$ and use a density argument. It is sufficient to show that $V(x) <_K -\Delta$. We write $V(x) = V_p(x) + V_\infty(x)$. If $n \leq 3$ and $\psi \in D(-\Delta)$, then we have

$$\|V\psi\| \leq \|V_2\psi\| + \|V_\infty \psi\| \leq \|V_2\|\|\psi\|_\infty + \|V_\infty\|_\infty\|\psi\|.$$

We need to show that $\|V\psi\| \leq a\|-\Delta\psi\| + b\|\psi\|$, and we may do so by deriving an estimate for $\|\psi\|_\infty$. Let $h(p) := p^2$. Using the Fourier transform and the Cauchy-Schwartz inequality, we have

$$(2\pi)^{3/2}\|\psi\|_\infty = \sup_{x\in\mathbb{R}^3}\left|\int_{\mathbb{R}^3} e^{ipx}\widehat{\psi}(p)dp\right| \leq \|\widehat{\psi}\|_1 \leq \|(h+1)^{-1}\|\,\|(h+1)\widehat{\psi}\| \leq$$
$$C(\|h\widehat{\psi}\| + \|\widehat{\psi}\|) = C(\| - \Delta\psi\| + \|\psi\|).$$

We replace $\widehat{\psi}(p)$ by $\widehat{\psi}_r(p) := r^3\widehat{\psi}(rp)$, where $r > 0$. Since $\|\widehat{\psi}_r\|_\infty = \|\widehat{\psi}\|_\infty$, $\|\widehat{\psi}_r\|_1 = \|\widehat{\psi}\|_1$, $\|\widehat{\psi}_r\| = r^{3/2}\|\widehat{\psi}\|$, and $\|h\widehat{\psi}_r\| = r^{-1/2}\|h\widehat{\psi}\|$, we obtain

$$(2\pi)^{3/2}\|\psi\|_\infty \leq r^{-1/2}C(\| - \Delta\psi\| + r^2\|\psi\|),$$

where $r > 0$ is arbitrary. Now, if we choose r such that $a = r^{-1/2}(2\pi)^{-3/2}C\|V_1\| < 1$, then we have shown that $-\Delta >_K V$, completing the proof for $n \leq 3$.

If $n \geq 4$, we similarly obtain by Hölder's inequality:

$$\|V\psi\| \leq \|V_p\psi\| + \|V_\infty\psi\| \leq \|V_p\|_p\|\psi\|_q + \|V_\infty\|_\infty\|\psi\|,$$

where $\frac{1}{p} + \frac{1}{q} = 1$. In this case we can bound $\|\psi\|_q$ in a similar way to how we bounded $\|\psi\|_\infty$. We will not prove this result, but instead refer the reader to [5]. Once this is proven, the proof will be complete. □

The above theorem is considerably more intuitive than the Kato-Rellich Theorem itself, and we can easily observe some of its valuable consequences.

Example 3.10. The Hamiltonian of the hydrogen atom has potential

$$V(x) = -\frac{e^2}{|x|},$$

so that

$$H = -\Delta - \frac{e^2}{|x|}.$$

Let us prove that H is self-adjoint. Let B_1 be the unit ball in $\mathbb{R}^3$. Then we write $V = \chi_{B_1}V + (1 - \chi_{B_1})V$. The former term is in $L^2(\mathbb{R}^3)$ and the latter term is in $L^\infty(\mathbb{R}^3)$, so that by the previous theorem, H is necessarily self-adjoint.

Before proceeding to the next theorem, a few definitions need to be made. The first is the sign of a complex function. We define

$$(\text{sgn}(f))(x) := \begin{cases} 0 & \text{if } f(x) = 0 \\ \overline{f(x)}|f(x)|^{-1} & \text{if } f(x) \neq 0 \end{cases}$$

Essential in the proof of Kato's Inequality below will be the regularized absolute value of f, defined by

$$f_\epsilon(x) := (|f(x)|^2 + \epsilon^2)^{1/2}.$$

It is clear that $\lim_{\epsilon\to 0} f_\epsilon(x) = |f(x)|$ pointwise and $|f(x)| = (\text{sgn}f) \cdot f$, the same as in $\mathbb{R}$.

Theorem 3.11 (Kato's Inequality)**.** *Let $f \in L^1_{loc}(\mathbb{R}^n)$. Suppose that the distributional Laplacian $\Delta f \in L^1_{loc}(\mathbb{R}^n)$. Then*

$$\Delta|f| \geq Re[(sgn\ f)\Delta f] \tag{3.12}$$

in the distributional sense.

Proof. We begin with the assumption that $f \in C^\infty(\mathbb{R}^n)$. We would like to show that (3.12) holds pointwise except in the case that $|f|$ is not differentiable. For such f, we have

$$f_\epsilon\nabla f_\epsilon = \text{Re}\overline{f}\nabla f. \tag{3.13}$$

Since $f_\epsilon \geq |f|$, we obtain

$$|\nabla f_\epsilon| \leq \frac{|f|\,|\nabla f|}{f_\epsilon} \leq |\nabla f|. \tag{3.14}$$

Taking the divergence of (3.13), we get

$$|\nabla f_\epsilon|^2 + f_\epsilon \Delta f_\epsilon = |\nabla f|^2 + \mathrm{Re}\overline{f}\Delta f.$$

Together with (3.14), this shows that

$$f_\epsilon \Delta f_\epsilon \geq \mathrm{Re}\overline{f}\Delta f,$$

which, dividing both sides by f_ϵ leads to the equation

$$\Delta f_\epsilon \geq \mathrm{Re}\left[(\mathrm{sgn}_\epsilon f)\Delta f\right], \tag{3.15}$$

where we have defined $\mathrm{sgn}_\epsilon f := \overline{f} f_\epsilon^{-1}$. In fact, when $|f|$ is smooth, $\mathrm{sgn}_\epsilon f \to \mathrm{sgn} f$.

Now we use regularization to finish. Let $\varphi \in C_0^\infty(\mathbb{R}^n)$, $\varphi \geq 0$, and $\int \varphi = 1$. We define

$$\varphi_\delta(x) := \delta^{-n}\varphi(x/\delta)$$

and

$$(I_\delta f)(x) := (\varphi_\delta * f)(x) = \int_{\mathbb{R}^n} \varphi_\delta(x-y)f(y)dy.$$

(The family of operators I_δ, for $\delta > 0$, is called an approximate identity. See [4] for details.)

Replacing f with $I_\delta f$ in (3.15), we see that

$$\Delta(I_\delta f)_\epsilon \geq \mathrm{Re}[\mathrm{sgn}_\epsilon(I_\delta f)\Delta(I_\delta f)].$$

Letting $\delta \to 0$ and then $\epsilon \to 0$, we get (3.12), which completes the proof. □

Theorem 3.16. *Let $V \in L^2_{loc}(\mathbb{R}^n)$ and $V \geq 0$. Then H is essentially self-adjoint.*

Proof. H is clearly non-negative and symmetric. By Corollary 3.7, it suffices to prove that $\ker(H^* + I) = \{0\}$. Therefore, we need to show that there exists a unique solution for the PDE

$$-\Delta f + Vf + f = 0, \tag{3.17}$$

with $f \in L^2(\mathbb{R}^n)$, namely $f = 0$.

We observe that $f \in L^2(\mathbb{R}^n)$ and $V \in L^2_{loc}(\mathbb{R}^n)$ imply that $Vf \in L^1_{loc}(\mathbb{R}^n)$. Moreover, $f \in L^1_{loc}(\mathbb{R}^n)$. By (3.17), $\Delta f \in L^1_{loc}(\mathbb{R}^n)$.

We now apply Kato's inequality, thereby obtaining

$$\Delta|f| \geq \mathrm{Re}[(\mathrm{sgn} u)\Delta f] = \mathrm{Re}[(\mathrm{sgn} f)(V+1)f] = |f|(V+1) \geq 0.$$

As a result,

$$\Delta I_\delta|f| = I_\delta \Delta|f| \geq 0.$$

Now, $I_\delta|f| \geq 0$ clearly holds. Also, $I_\delta|f| \in D(\Delta)$. This follows from the facts that $|f| \in L^2(\mathbb{R}^n)$ and

$$(\partial_i I_\delta f) = \int \partial_i \varphi_\delta(x-y)f(y)dy.$$

Now,

$$(\Delta(I_\delta|f|), (I_\delta|f|)) = -\left\|\nabla(I_\delta|f|)\right\|^2_{L^2(\mathbb{R}^n)},$$

but since the LHS is ≥ 0, we obtain that $\nabla(I_\delta|f|) = 0$. Hence, $I_\delta|f| = c \geq 0$. Since $|f| \in L^2(\mathbb{R}^n)$, $c = 0$. Hence, $I_\delta|f| = 0$, which clearly implies that $|f| = 0$. □

In fact, a more general result using slightly different restraints on V is available by Sear's Theorem. We begin with a lemma, the proof of which is given in [1].

Lemma 3.18. *Let $V(x)$ satisfy $V(x) \geq -Q(|x|)$ for some increasing positive function $Q(x)$. Then if $f \in D(H^*)$,*

$$\int_{\mathbb{R}^n} \frac{|\nabla f(x)|^2}{Q(2|x|)} dx < +\infty \tag{3.19}$$

We may use this result to prove Sear's Theorem.

Theorem 3.20 (Sear's Theorem)**.** *Let the potential $V(x)$ satisfy the condition $V(x) \geq -Q(|x|)$, where $Q(x)$ is an increasing positive continuous function on $[0, +\infty)$ such that*

$$\int_0^\infty \frac{dx}{\sqrt{Q(2x)}} = +\infty. \tag{3.21}$$

Then H is essentially self-adjoint on $H^2(\mathbb{R}^n)$.

Proof. To show that H is essentially self-adjoint, it is sufficient to show that H^* is symmetric. Let $f_1, f_2 \in D(H^*)$, $g_i := -\Delta f_i + V(x) f_i$, so that $g_i \in L^2(\mathbb{R}^n)$. We need to show that

$$\int_{\mathbb{R}^n} f_1 \overline{g_2} = \int_{\mathbb{R}^n} g_1 \overline{f_2}. \tag{3.22}$$

Assuming that $f_i \in S(\mathbb{R}^n)$, we have

$$\begin{aligned} \int_{|x|\leq t} f_1\overline{g_2} - g_1\overline{f_2} &= -\int_{|x|\leq t} f_1 \Delta\overline{f_2} - \Delta f_1 \cdot \overline{f_2} \\ &= \int_{|x|\leq t} \nabla \cdot \left(\overline{f_2}\nabla f_1 - f_1 \nabla \overline{f_2}\right) \\ &= \int_{|x|=t} \left(\overline{f_2}\frac{\partial f_1}{\partial r} - f_1 \frac{\partial \overline{f_2}}{\partial r}\right). \end{aligned} \tag{3.23}$$

This formula also holds $f_1, f_2 \in H^2_{loc}(\mathbb{R}^n)$, and in particular, for all $f_1, f_2 \in D(H^*)$. Let

$$\rho(t) := \frac{1}{\sqrt{Q(2t)}}.$$

Now, multiplying (3.23) by $\rho(t)$, and integrating over $[0, T]$, we obtain

$$\int_0^T \rho(t) \left(\int_{|x|\leq t} (f_1\overline{g_2} - g_1\overline{f_2}) dx \right) dt = \int_0^T \rho(t) \left(\int_0^t I(\tau) d\tau \right) dt, \tag{3.24}$$

where $I(t) = \int_{|x|=t} (f_1\overline{g_2} - g_1\overline{f_2}) dS$, so that

$$\int_0^\infty |I(t)| dt < +\infty. \tag{3.25}$$

We now define

$$P(T) := \int_0^T \rho(t) dt.$$

The right-hand side of (3.24) takes the form

$$\int_0^T \rho(t) \left(\int_0^t I(\tau) d\tau \right) dt = \int_0^T I(\tau) \left(\int_\tau^T \rho(t) dt \right) d\tau = \int_0^T (P(T) - P(\tau)) I(\tau) d\tau.$$

Now, we estimate half of the RHS of (3.23) with the help of the Cauchy-Schwartz Inequality and Lemma 3.18:

$$\left|\int_0^T \rho(t)\left(\int_{|x|=t}\overline{f_2}\frac{\partial f_1}{\partial r}dS\right)dt\right| = \left|\int_{|x|\le T}\rho(|x|)\overline{f_2}(x)\frac{\partial f_1(x)}{\partial r}dx\right| \le$$
$$\left(\int_{|x|\le T}|f_2(x)|^2dx\right)^{1/2}\cdot\left(\int_{|x|\le T}\rho^2(|x|)\left|\frac{\partial f_1(x)}{\partial r}\right|^2dx\right)^{1/2} \le$$
$$\|f_2\|\cdot\int_{\mathbb{R}^n}Q^{-1}(|2x|)|\nabla f_1|^2dx \le C,$$

for some $C \in \mathbb{R}$. The other half works similarly, leading to the equation

$$\left|\int_0^T (P(T)-P(t))I(t)dt\right| < K. \tag{3.26}$$

for some $K \in \mathbb{R}$.

We divide both sides by $P(T)$ and let $T \to +\infty$. By (3.21), this implies that $P(T) \to +\infty$ as well. Hence, (3.26) shows that

$$\lim_{T\to+\infty}\int_0^T\left(1-\frac{P(t)}{P(T)}\right)I(t)dt = 0. \tag{3.27}$$

Our aim was originally to prove that $\int_0^\infty I(t)dt = 0$. This can clearly be derived by (3.27), since $\int |I(x)|dx < +\infty$. We choose $\epsilon > 0$ and take $R > 0$, so that $\int_R^\infty |I(t)|dt < \epsilon$. Fixing such R, if we take $T > R$, we have:

$$\left|\int_0^T\left(1-\frac{P(t)}{P(T)}\right)I(t)dt\right| \le \left|\int_0^T\left(1-\frac{P(t)}{P(T)}\right)I(t)dt\right| + \epsilon.$$

Then as $T \to +\infty$, we find by (3.27) that indeed $\int_0^\infty I(t)dt = 0$, and the proof is complete. □

4. Characterization of the Spectrum

Another big problem in mathematical quantum mechanics is the description of the spectral properties of the Schrödinger operator H. Some of the main results of the spectral theory of Schrödinger operators are presented here.

We begin with a relevant lemma that concerns variational principles, i.e., perturbation theory of operators. We recall that the spectral theorem allows us to identify a self-adjoint operator in a Hilbert space $\mathcal{H}$ with a collection of projection operators $\{E_\lambda\}$, called the spectral family of A, satisfying certain properties. (If the reader is unfamiliar with the spectral theorem, he may skip ahead to the next theorem and consult the results of the lemma.)

Recall that

$$E_{\lambda+0} = E_\lambda\, \forall\lambda \in \mathbb{R}$$

in the strong operator topology, and we define

$$E_{\lambda-0} := \lim_{\mu\to\lambda,\mu>\lambda} E_\mu.$$

The distribution function of the spectrum of A is defined by letting

$$N(\lambda) := \dim(E_\lambda\mathcal{H}).$$

$N(\lambda)$ actually represents the number of eigenvalues of A less than λ.

Lemma 4.1 (Glazman)**.** *Let D be a subspace of $D(A)$ such that an operator A in $\mathcal{H}$ is essentially self-adjoint on D. Then for any $\lambda \in \mathbb{R}$, we have*

$$N(\lambda - 0) = \sup\{\dim L : L \subset D, (Af, f) < \lambda(f, f) \text{ for } f \in L \setminus \{0\}\} =: M. \tag{4.2}$$

Proof. We begin by showing that if L is a subspace of D and $(Af, f) < \lambda(f, f)$ for all $f \in L \setminus \{0\}$, then $\dim L \leq N(\lambda - 0)$. In fact, if $\dim L > N(\lambda - 0)$, then $L \cap (E_{\lambda-0}\mathcal{H})^{\perp} \neq \{0\}$, since $L \cap (E_{\lambda-0}\mathcal{H})^{\perp} = \{0\}$ implies that $E_{\lambda-0}$ injectively maps L into $E_{\lambda-0}$, in turn implying that $\dim L \leq \dim(E_{\lambda-0}\mathcal{H}) = N(\lambda - 0)$. But if $f \in (E_{\lambda-0}\mathcal{H})^{\perp}$, then $(Af, f) \geq \lambda(f, f)$, so that the existence of a non-zero vector $f \in L \cap (E_{\lambda-0}\mathcal{H})^{\perp}$ is a contradiction of the definition of L. Hence, $\dim L \leq N(\lambda - 0)$, showing that $M \leq N(\lambda - 0)$.

We now confirm the converse inequality. Note that

$$E_{\lambda-0} = \lim_{N \to -\infty} E(N, \lambda),$$

where $E(N, \lambda) = E_{\lambda-0} - E_N$, so that

$$N(\lambda - 0) = \lim_{N \to -\infty} \dim\left[E(N, \lambda)\mathcal{H}\right].$$

Hence, it is sufficient to prove that $\dim E(N, \lambda)$ is not greater than M for any $N < \lambda$. In $E(N, \lambda)\mathcal{H}$, pick an orthonormal basis and let $\{e_1, \ldots, e_m\}$ be a finite number of vectors of this basis. It suffices to show that $m \leq M$. Since $E(N, \lambda) \subset D(A)$, $e_j \in D(A)\, \forall j = 1, \ldots, m$. Hence, for any $\epsilon > 0$, there exist vectors $\widehat{e_1}, \ldots, \widehat{e_m} \in D$ such that

$$\|e_j - \widehat{e_j}\| < \epsilon,\ \|Ae_j - A\widehat{e_j}\| < \epsilon\, \forall j = 1, \ldots, m,$$

since A is essentially self-adjoint on D. If L is the span of the set $\{\widehat{e_1}, \ldots, \widehat{e_m}\}$, then there is an $\epsilon > 0$ such that $\dim L = m$. (This follows from the non-degeneracy of the matrix $\|(\widehat{e_i}, \widehat{e_j})\|_{i,j=1}^{m}$ for small $\epsilon > 0$.) Furthermore, for $\epsilon > 0$, (4.2) holds for L. Hence, $m \leq M$, which finishes the proof. □

In fact, a slightly more specific result holds, which we shall use to prove the following theorem. The proof is exactly the same as that of the above theorem, except that it is unnecessary to approximate the vectors e_i by $\widehat{e_i}$.

Theorem 4.3. *Let D be a subspace of $D(A)$ such that A is essentially self-adjoint on D. Then for any $\lambda \in \mathbb{R}$, we have*

$$N(\lambda) = \sup\{\dim : L \subset D, (Af, f) < \lambda(f, f)\, \forall f \in L \setminus \{0\}\}. \tag{4.4}$$

Theorem 4.5. *Suppose that $V \in L^{\infty}_{loc}(\mathbb{R}^n)$ and*

$$\liminf_{|x| \to \infty} V(x) = \lim_{R \to \infty} \inf_{|x| \geq R} V(x) \geq a \tag{4.6}$$

for some $a \in \mathbb{R}$. Then the operator H is self-adjoint, bounded below, and, for all $a' < a$, only a finite number of eigenvalues of H of finite multiplicity exist in $\sigma(H) \cap (-\infty, a')$.

Proof. Clearly, $V(x) \geq -C$ for some C and therefore H is self-adjoint and bounded below.

Step 1. Let us initially consider

$$(H\psi, \psi) = \int_{\mathbb{R}^n} \left[-\Delta\psi + V(x)\psi\right] \overline{\psi} dx,\ \psi \in D(H).$$

We intend to show that

$$(H\psi, \psi) = \int_{\mathbb{R}^n} \left[|\nabla\psi|^2 + V(x)|\psi|^2 \right] dx, \; \psi \in D(H). \tag{4.7}$$

Now, (4.7) is obvious for $\psi \in C_0^\infty(\mathbb{R}^n)$. In the case that $\psi \in D(H)$, we initially show that

$$\int_{\mathbb{R}^n} \left[|\nabla\psi|^2 + V(x)|\psi|^2 \right] dx < +\infty. \tag{4.8}$$

Local elliptic regularity implies that if $\psi \in D(H)$, then $\psi \in H^2_{loc}(\mathbb{R}^n)$. Hence,

$$\int_B \left[|\nabla\psi|^2 + V(x)|\psi|^2 \right] dx < +\infty$$

for any $\psi \in D(H)$ and for any (bounded) ball B in $\mathbb{R}^n$.

Let $b \le \inf V(x) - 1$. Since $\psi \in L^2(\mathbb{R}^n)$, (4.8) is equivalent to:

$$H_b(\psi, \psi) := \int \left[|\nabla\psi|^2 + (V(x) - b)|\psi|^2 \right] dx < +\infty.$$

If the quadratic form H_b is finite, this means that

$$\int |\nabla\psi|^2 dx < +\infty \text{ and } \int (1 + |V(x)|)|\psi|^2 < +\infty. \tag{4.9}$$

The quadratic form H_b is actually generated by the inner product

$$H_b(\psi_1, \psi_2) = \int \left[\nabla\psi_1 \overline{\nabla\psi_2} + (V(x) - b)\psi_1\overline{\psi_2} \right] dx,$$

which is finite as long as ψ_1 and ψ_2 both satisfy (4.9).

If $\psi \in C_0^\infty(\mathbb{R}^n)$, we have

$$((H - bI)\psi, \psi) = H_b(\psi, \psi). \tag{4.10}$$

The LHS of the above equation is continuous with respect to the graph norm $\left(\|\psi\|^2 + \|H\psi\|^2 \right)^{1/2}$ on $D(H)$. Therefore, the same is true for $H_b(\psi, \psi)$ and, by continuity, H_b is well-defined on $D(H)$.

Now, we clearly have

$$\|\psi\|^2_{H^1(\mathbb{R}^n)} \le H_b(\psi, \psi)$$

for $\psi \in C_0^\infty(\mathbb{R}^n)$. Hence, the convergence of elements of $C_0^\infty(\mathbb{R}^n)$ with respect to the graph norm implies their convergence in $H^1(\mathbb{R}^n)$. Since $H^1(\mathbb{R}^n)$ is complete, $\psi \in D(H)$ implies that $\psi \in H^1(\mathbb{R}^n)$, so that the first inequality in (4.9) is true.

Similarly, the weighted L^2 space

$$L^2(\mathbb{R}^n, 1 + |V(x)|) := \left\{ \psi \in L^2(\mathbb{R}^n) : \int_{\mathbb{R}^n} (1 + |V(x)|) \, |\psi(x)|^2 dx < +\infty \right\}$$

is complete, therefore implying that $\psi \in L^2(\mathbb{R}^n, 1+|V(x)|)$ if $\psi \in D(H)$. Therefore, every $\psi \in D(H)$ satisfies (4.9). Since (4.8) and (4.9) are equivalent, every such ψ also satisfies (4.8).

Step 2. Now we use Theorem 4.3, keeping in mind that $N(\lambda)$ is the number of eigenvalues less than λ. To finish the proof of the theorem, we must show that if $a' < a$ and L is a subspace of $D(H)$ satisfying

$$(H\psi, \psi) \le a'(\psi, \psi) \tag{4.11}$$

for all $\psi \in L$, then $\dim(L) < +\infty$.

Due to step 1, we may rewrite (4.11) as

$$\int_{\mathbb{R}^n} \left[|\nabla\psi|^2 + (V(x) - a')|\psi|^2\right] dx \leq 0. \tag{4.12}$$

We let $\delta \in (0, a - a')$ and $R > 0$ be such that $V(x) \geq a' + \delta$ for $|x| \geq R$, and define

$$M := -\inf V(x).$$

If $C > 0$ and $C > M + a'$, then (4.12) implies that

$$\int_{|x|\leq R} |\nabla\psi|^2 dx + \int_{|x|\geq R} \left[|\nabla\psi|^2 + \delta|\psi|^2\right] dx \leq C \int_{|x|\leq R} |\psi|^2 dx, \tag{4.13}$$

for $\psi \in L$.

Now, consider an operator $A : L \to L^2(B_R)$ defined by $A : \psi \mapsto \psi|_{B_R}$, where B_R is the ball of radius R about the origin. We consider L with the topology induced from $L^2(\mathbb{R}^n)$. A is clearly continuous. Inequality (4.13) shows that $\ker(A) = \{0\}$. It then suffices to prove that $\widetilde{L} := AL$ is a finite dimensional subspace of $L^2(B_R)$. That $\widetilde{L} \subset H^1(B_R)$ is clear, and by (4.13), we have

$$\|\psi\|_{H^1(B_R)} \leq K\|\psi\|_{L^2(B_R)},$$

for $\psi \in \widetilde{L}$ and some $K \in \mathbb{R}$ independent of ψ.

Hence, the identity operator I in $\widetilde{L}$ may be written as a composition of the embedding $\widetilde{L} \subset H^1(B_R)$, which is continuous, and the embedding $H^1(B_R) \subset L^2(B_R)$, which is compact. It follows that I is a compact operator, since the collection of compact operators is an ideal in the collection of continuous operators. Therefore, $\dim(\widetilde{L}) < +\infty$, which finishes the proof. □

Corollary 4.14. *If $V(x) \in L^\infty_{loc}(\mathbb{R}^n)$ and $\lim_{|x|\to\infty} V(x) = +\infty$, then H has a discrete spectrum.*

Recall that the essential spectrum $\sigma_{ess}(H)$ consists of all non-isolated points of $\sigma(H)$ and eigenvalues of infinite multiplicity. Our first result regarding the essential spectrum claims that the essential spectrum is maintained under certain perturbations of the potential. We first introduce some results of functional analysis that are necessary in the proof of the theorem.

Lemma 4.15. *Let $\mathcal{H}$ be a Hilbert space. An operator $A : \mathcal{H} \to \mathcal{H}$ is relatively compact with respect to $B : \mathcal{H} \to \mathcal{H}$ if and only if it is compact as an operator from $D(B)$ into $\mathcal{H}$.*

Lemma 4.16. *Let A be a self-adjoint operator in $\mathcal{H}$ and B a symmetric operator into $\mathcal{H}$ with $D(B) \supset D(A)$. Suppose that B is relatively compact with respect to A. Then the operator $B = A + C$, with $D(B) = D(A)$, is self-adjoint and*

$$\sigma_{ess}(B) = \sigma_{ess}(A).$$

Lemma 4.17 (Rellich-Kondrashov Compactness Theorem)**.** *Let*

$$2 \leq p < \frac{2n}{n-2}.$$

Then the embedding $H^1(\mathbb{R}^n) \subset L^p(\mathbb{R}^n)$ is compact.

We may now prove a beneficial result, namely that under "small" variations of V, the essential spectrum remains the same.

Theorem 4.18. *Consider the operators* $H_0 := -\Delta + V_0$ *and* $H = -\Delta + V$*, where* $V = V_0 + V_1$*. Let* $V_0, V_1 \in L^\infty_{loc}(\mathbb{R}^n)$ *be bounded from below. Further assume that* $\lim_{|x|\to\infty} V_1(x) = 0$*. Then*

$$\sigma_{ess}(H) = \sigma_{ess}(H_0).$$

Proof. We prove that the multiplication operator V_1 is relatively compact with respect to H_0. The theorem will then follow by Lemma 4.16.

By Lemma 4.15, it is sufficient to prove that V_1 is a compact operator from the space $D(H_0)$, with the graph norm, into $L^2(\mathbb{R}^n)$. Since $D(H_0)$ can be continuously embedded into $H^1(\mathbb{R}^n)$, it suffices to show that V_1 is a compact operator from $H^1(\mathbb{R}^n)$ into $L^2(\mathbb{R}^n)$.

Let

$$S := \{V_1 f : f \in H^1(\mathbb{R}^n) \text{ and } \|f\|_{H^1(\mathbb{R}^n)} \le 1\}.$$

We must prove that S is a precompact set in $L^2(\mathbb{R}^n)$. Let $\epsilon > 0$. By assumption, there exists an $R > 0$ such that $|V(x)| \le \epsilon$ if $|x| \ge R$. Let B_R be the ball of radius R centered at the origin. Then we have

$$\|(1 - \chi_{B_R})Vf\|^2_{L^2(\mathbb{R}^n)} = \int_{B_R^c} |V(x)|^2 |f(x)|^2 dx \le \epsilon^2 \|f\|^2_{L^2(\mathbb{R}^n)} \le \epsilon^2. \tag{4.19}$$

Note that the set $S_\epsilon := \{\chi_{B_R} V_1 f : f \in S\}$ is precompact in $L^2(\mathbb{R}^n)$. This follows from the Rellich-Kondrashov Compactness Theorem, since the embedding $H^1(\mathbb{R}^n) \subset L^2_{loc}(\mathbb{R}^n)$ is compact and if $f \in S_\epsilon$, then $f(x) = 0$ for all $x \notin B_R$.

Now, S lies in a ϵ-neighborhood of S_ϵ, which is precompact, and $\epsilon > 0$ is arbitrary. Hence, S is precompact and the proof is complete. □

The following theorem shows that under certain conditions, the essential spectrum is in fact exactly the set of non-negative real numbers.

Theorem 4.20. *Let* $V(x) \in L^\infty_{loc}(\mathbb{R}^n)$ *and* $\lim_{|x|\to\infty} V(x) = 0$*. Then*

$$\sigma_{ess}(H) = [0, +\infty).$$

Proof. We know from Theorem 4.5 that H can have only isolated eigenvalues of finite multiplicity on $(-\infty, 0)$. It remains for us to show that $[0, +\infty) \subset \sigma(H)$. Let $\lambda \ge 0$ be fixed. The condition $\lambda \in \sigma(H)$ is equivalent to the existence of a sequence $\{\varphi_m\}_{m=1}^\infty$, $\varphi_m \in D(H)$, such that

$$\lim_{m\to+\infty} \frac{\|(H - \lambda I)\varphi_m\|}{\|\varphi_m\|} = 0. \tag{4.21}$$

We shall describe the construction of such a sequence. We consider the function $e^{ik\cdot x}$, where $|k| = \sqrt{\lambda}$. It satisfies the equation $(-\Delta)e^{ikx} = \lambda e^{ikx}$, so that since $\lim_{|x|\to\infty} V(x) = 0$, we have

$$\lim_{|x|\to\infty} [-\Delta + V(x) - \lambda] e^{ikx} = 0. \tag{4.22}$$

To obtain the sequence $\{\varphi_m\}$, we must choose cut-offs of the function e^{ikx} that approach infinity as m increases. Let $B \in C_0^\infty(\mathbb{R}^n)$ satisfy $B \ge 0$, $B(x) = 1$ for $|x| \le 1/2$, $B(x) = 0$ for $|x| \ge 2$. We set

$$B_m(x) := B\left(m^{-1/2}(x - m)\right).$$

Then we have

$$\operatorname{supp}(B_m) \subset \{x : |x - m| \le \sqrt{m}\}, \tag{4.23}$$

so that

$$\lim_{m\to+\infty}\sup_{x\in supp(B_m)}|V(x)|=0. \tag{4.24}$$

We now explicitly define

$$\varphi_m(x):=B_m(x)e^{ikx}.$$

We proceed to check that (4.21) holds for the above-defined $\{\varphi_m\}$. Note that

$$\|\varphi_m\|^2=\int|B_m(x)|^2dx=m^{n/2}\int|B(x)|^2dx=Cm^{n/2}, \tag{4.25}$$

where $C>0$. We clearly have

$$H\varphi_m=-(\Delta B_m)e^{ikx}-(\nabla B_m)(\nabla e^{ikx})+k^2B_me^{ikx}+V(x)B_me^{ikx}.$$

Therefore,

$$(H-\lambda I)\varphi_m=e^{ikx}[HB_m-ik\cdot\nabla B_m]. \tag{4.26}$$

Now,

$$|\nabla B_m|\leq Cm^{-1/2}\text{ and }|\Delta B_m|\leq\frac{C}{m}.$$

Noticing (4.24), we can now see from (4.26) that

$$\lim_{m\to+\infty}\sup_{x\in\mathbb{R}^n}|(H-\lambda I)\varphi_m(x)|=0.$$

But by (4.23), this implies that

$$\lim_{m\to+\infty}m^{-n/2}\|(H-\lambda I)\varphi_m\|^2=0.$$

Along with (4.25), this implies (4.21). This concludes the proof. □

5. Eigenvalue Bounds

Another critical area of mathematical quantum mechanics lies in finding bounds for the numbers of eigenvalues of H with a given potential. In this section, we will introduce three theorems involving eigenvalue bounds: the Birman-Schwinger bound, the Lieb-Cwikel-Rozenblum bound, and Kato's Theorem. We shall not prove our results, since they use more sophisticated methods than the rest of the theorems contained in this text.

We begin with the Birman-Schwinger bound. As we see, this is only to be used in the three-dimensional case, but since this is a physically important scenario, it is an invaluable method of eigenvalue bound calculation. It is quite an astounding result because of its generality (that is, it is easily computed given any $V\in L^\infty(\mathbb{R}^3)$) and because it is such a simple formula.

Theorem 5.1 (Birman-Schwinger)**.** *Suppose that $V(x)\in L^\infty(\mathbb{R}^3)$ and*

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{|V(x)V(y)|}{|x-y|^2}<+\infty. \tag{5.2}$$

If $N(H)$ is the total number of eigenvalues of H counted with multiplicities, then

$$N(H)\leq\frac{1}{16\pi^2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{|V(x)V(y)|}{|x-y|^2}. \tag{5.3}$$

The formula actually holds for a more general class of functions called the Rollnick class. See [6] for details.

A stronger result of Theorem 4.20 holds if V quickly goes to 0 as $|x| \to \infty$. Not only are there no negative numbers in the essential spectrum, there are no negative eigenvalues at all. This result is often referred to as Kato's Theorem, and instead of being an eigenvalue bound, it describes a case in which the conditions imposed on V are not too strong, but in which a powerful result exists. The proof is not provided, due to its length. However, a (rather long) proof is presented in [1].

Theorem 5.4 (Kato)**.** *Suppose that $V(x) \in L^\infty_{loc}(\mathbb{R}^n)$ and*

$$\lim_{|x|\to\infty} |x|V(x) = 0. \tag{5.5}$$

Then H has no positive eigenvalues.

Kato's Theorem brings forth an important question. Is there a general formula for the number of negative eigenvalues of an arbitrary Schrödinger operator similar to the one provided by the Birman-Schwinger bound? The answer to this question happens to be yes. In fact, there are many estimates of the number of negative eigenvalues of H (which we denote by $N_-(H)$), but there is one particularly well-known and valuable theorem that bounds $N_-(H)$ of a Schrödinger operator for dimension greater than three.

Theorem 5.6 (Lieb-Cwikel-Rozenblum)**.** *Let $V(x) \in L^\infty_{loc}(\mathbb{R}^n)$. If $N_-(H)$ is the number of negative eigenvalues of H counting multiplicities, then*

$$N_-(H) \le c_n \int_{\mathbb{R}^n} |\min[V(x), 0]|^{n/2}\, dx,$$

where c_n depends only on n.

Note that this theorem is in a way stronger for bounding negative eigenvalues than the Birman-Schwinger is for bounding both positive and negative eigenvalues. Whereas the Birman-Schwinger bound requires the dimension to be equal to three, the Lieb-Cwikel-Rozenblum bound has no restraints on dimension other than that it be greater than three.

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