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Quadratic Forms and Essential Self-Adjointness

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Abstract. Let H_0 and V be self-adjoint operators acting in a Hilbert space. Assume that $H_0 \geqslant 0$ and that $H = H_0 + V$ (where the sum is defined in the sense of quadratic forms) is self-adjoint and bounded below. The positive part of V need not be relatively bounded with respect to H_0. If $\exp(-H)$ sends a dense subspace of the Hilbert space into the domain of V, then H is essentially self-adjoint on the intersection of the domains of H_0 and V. The Trotter product formula for contraction semigroups may be used to verify the condition on $\exp(-H)$. This gives a general essential self-adjointness result for Schrödinger operators.

1. Introduction

Let H_0 and V be (unbounded) self-adjoint operators acting in a Hilbert space. Is the form sum $H = H_0 + V$ a uniquely defined self-adjoint operator? If so, is H essentially self-adjoint on the intersection of the domains of H_0 and V? If H is self-adjoint, then the unitary group $\exp(itH)$ is well defined. The importance of the latter question is that essential self-adjointness implies the Trotter product formula (unitary case)

$$\exp(itH) = \lim_{n\to\infty}\left(\exp\left(i\frac{t}{n}H_0\right)\exp\left(i\frac{t}{n}V\right)\right)^n \quad ([9], §8).$$

The purpose of this paper is to present sufficient conditions for essential self-adjointness.

The classical results for relatively small perturbations are based on a series expansion. They do not depend on the sign of V. Recent developments in quantum field theory have led to an interest in the case when $H_0 \geqslant 0$ and V is not smaller than H_0. The results do then depend on the sign of V. Quite generally, if only the negative part of V is relatively small, then H is self-adjoint and bounded below ([7], chap. VI). The essential self-adjointness results mostly have been obtained by L^p space techniques, in particular the theory of hypercontractive semigroups [11, 15]. In this paper it is shown how these results fit into the general framework of quadratic form perturbation theory.

The L^p space techniques were introduced in quantum field theory by Nelson in order to show that H is bounded below [8]. The mathematical study of quantum fields was carried much farther by Glimm and Jaffe [5]. In particular, they gave proofs of essential self-adjointness. The generality of the L^p space techniques was recognized by Segal [11]. He used the Trotter product formula (self-adjoint case)

$$\exp(-tH) = \lim_{n\to\infty}\left(\exp\left(-\frac{t}{n}H_0\right)\exp\left(-\frac{t}{n}V\right)\right)^n$$

in conjunction with the estimates of Nelson to prove that H is bounded below. Though essential self-adjointness is an entirely independent question, Segal showed that similar techniques may be used to prove essential self-adjointness. These results have been extended by Simon and Hoegh-Krohn in their survey article on hypercontractive semigroups [15].

The general theory may also be applied to Schrödinger operators $-\Delta + V$ acting in $L^2(\mathbb{R}^n, dx)$. Recently Simon showed that if V is bounded below and $V \in L^2(\mathbb{R}^n, \exp(-cx^2)dx)$, then $-\Delta + V$ is essentially self-adjoint [13]. Similar results have been obtained by partial differential equation methods; they indicate that it should be sufficient to assume that V is bounded below and locally in L^2. However, so far this has not been deduced from perturbation theory [13].

In this paper a generalization of the field theory techniques is applied to Schrödinger operators in a way which in certain respects improves Simon's result. The first sections of the paper are devoted to background material. We review the basic facts on self-adjointness of form sums (Theorem 2.1) and present abstract Hilbert space versions of some of Segal's techniques (corollary 3.1 and Theorem 4.1). In the main essential self-adjointness result (Theorem 4.2) $\exp(-tV)\exp(-tH_0)$ is assumed to be a contraction semigroup on a certain auxiliary Banach space $\mathscr{X}$ for $t \geqslant 0$. (The space $\mathscr{X}$ here plays the role of L^p.) The theory has also recently been abstracted by Segal in a somewhat different direction [12]. His approach is based on Duhamel's formula instead of quadratic forms.

The main result on Schrödinger operators (Theorem 6.1) is related to Simon's theorem; however V may not only be very much unbounded above but also unbounded below. In order to construct the auxiliary Banach space $\mathscr{X}$ we use a new representation of the Hilbert space which is adapted to the particular operator H.

2. Forms and Operators

Definition 2.1: Let $\mathscr{H}$ be a Hilbert space and A be a self-adjoint operator acting in $\mathscr{H}$. The domain $\mathscr{D} = \mathscr{D}(A)$ of A is the Hilbert space consisting of all $f \in \mathscr{H}$ such that $\|f\|_{\mathscr{D}}^2 = \|f\|^2 + \|Af\|^2$ is finite. The form domain $\mathscr{Q} = \mathscr{Q}(A)$ of A is the Hilbert space consisting of all f in $\mathscr{H}$ such that $\|f\|_{\mathscr{Q}}^2 = \|f\|^2 + \| \, |A|^{1/2} f\|^2$ is finite.

Definition 2.2: Let A be a self-adjoint operator with form domain $\mathscr{Q}$. The form dual $\mathscr{Q}^*$ is defined as the Hilbert space which is the completion of $\mathscr{H}$ in the norm $\|g\|_{\mathscr{Q}^*}^2 = \langle g, (1 + |A|)^{-1} g\rangle$.

The relation between these spaces is that $\mathscr{Q} \subset \mathscr{H} \subset \mathscr{Q}^*$ (and of course $\mathscr{D} \subset \mathscr{Q}$). If g is in $\mathscr{Q}^*$, then there is a natural definition (by continuity) of $\langle g,f\rangle$, $f \in \mathscr{Q}$, such that $|\langle g,f\rangle| \leqslant \|g\|_{\mathscr{Q}^*} \|f\|_{\mathscr{Q}}$. This is the sense in which $\mathscr{Q}^*$ is dual to $\mathscr{Q}$.

If A is a self-adjoint operator, then A extends by continuity to an operator $A : \mathscr{Q} \to \mathscr{Q}^*$, where $\mathscr{Q} = \mathscr{Q}(A)$ is the form domain of A and $\mathscr{Q}^*$ is the form dual. Similarly $|A|$ extends to an operator $|A| : \mathscr{Q} \to \mathscr{Q}^*$, in fact, $1 + |A| : \mathscr{Q} \to \mathscr{Q}^*$ is an isomorphism of Hilbert spaces. Thus we may write

$$\|f\|_{\mathscr{Q}}^2 = \langle (1 + |A|)f, f\rangle \quad \text{and} \quad \|g\|_{\mathscr{Q}^*}^2 = \langle g, (1 + |A|)^{-1} g\rangle.$$

Let A be a self-adjoint operator. If f and g are in $\mathscr{Q}(A)$, then $\langle Af,g\rangle$ is defined. This sesquilinear form is of course determined by the quadratic form $\langle Af,f\rangle$, $f \in D(\mathscr{Q})$.

Definition 2.3: Let A be a self-adjoint operator and let $\mathcal{Q}(A)$ be its form domain. The quadratic form of A is the quadratic form $\langle Af,f\rangle$, defined for $f \in \mathcal{Q}(A)$.

The quadratic form of a self-adjoint operator A will also be denoted simply by A.

Definition 2.4: Let A and B be self-adjoint operators. Then $A \leqslant B$ means that $\mathcal{Q}(A) \supset \mathcal{Q}(B)$ and $\langle Af,f\rangle \leqslant \langle Bf,f\rangle$ for all $f \in \mathcal{Q}(B)$.

Definition 2.5: Let $B \geqslant 0$ be a self-adjoint operator. The truncated operator B_n is defined to be the operator which is equal to B on the subspace where $B \leqslant n$ and equal to 0 on its orthogonal complement.

Proposition 2.1. Let $B \geqslant 0$ be a self-adjoint operator. Then $f \in \mathcal{Q}(B)$ if and only if $\langle B_n f,f\rangle$ is bounded as $n \to \infty$, and in that case $\langle B_n f,f\rangle \uparrow \langle Bf,f\rangle$ as $n \to \infty$.

Proof: This is an immediate consequence of the spectral theorem and the monotone convergence theorem.

Proposition 2.2 ([7], chap. VI, Theorem 2.21). Let A and B be self-adjoint operators which are bounded below and let c be a real number which is strictly less than the lower bounds. Then $A \leqslant B$ if and only if $(B-c)^{-1} \leqslant (A-c)^{-1}$.

Proof: By adding a constant we may suppose $c = 0$. Then $A \leqslant B$ says that $\|A^{1/2}f\|^2 \leqslant \|B^{1/2}f\|^2$, that is, $\|A^{1/2}B^{-1/2}\| \leqslant 1$. But $(A^{1/2}B^{-1/2})^* \supset B^{-1/2}A^{1/2}$, so $\|B^{-1/2}A^{1/2}\| \leqslant 1$. That is, $\|B^{-1/2}g\| \leqslant \|A^{-1/2}g\|$, $B^{-1} \leqslant A^{-1}$.

Proposition 2.3. Assume $0 < c \leqslant B \leqslant A$. Then $\log B \leqslant \log A$.

Proof: We first give the proof for the special case when B is bounded. (See for instance [10], proposition 2.5.8.)

We have

$$\int_0^r (t+A)^{-1}\,dt = \log(r+A) - \log A$$

and similarly for B. Hence

$$\begin{aligned}\log A - \log B &= \int_0^r [(t+B)^{-1} - (t+A)^{-1}]dt + \log(1+A/r) - \log(1+B/r)\\ &\geqslant -\log(1+B/r).\end{aligned}$$

Let $r \to \infty$. We see that $\log A \geqslant \log B$.

In the general case we have $B_n \leqslant B \leqslant A$, where B_n is the truncated operator. Hence $\log B_n \leqslant \log A$. Let $n \to \infty$. It follows that $\log B \leqslant \log A$.

Definition 2.6: Let A and B be self-adjoint operators acting in the Hilbert space $\mathscr{H}$. Let $A + B$ be the quadratic form defined on $\mathcal{Q}(A) \cap \mathcal{Q}(B)$ by adding the forms of A and B. If this is the quadratic form of a self-adjoint operator, then this operator will be called the form sum of A and B.

The self-adjoint operator which is the form sum of A and B will also be denoted $A + B$. The next theorems give criteria for the existence of the form sum.

Definition 2.7: Let A and B be self-adjoint operators. The operator B is said to be a relatively small form perturbation of A if there exist constants a and b with $a < 1$ such that $\pm B \leqslant a|A| + b$. It is said to be a relatively small perturbation of A if there exist a and b with $a < 1$ such that $B^2 \leqslant aA^2 + b$.

It is known that a relatively small perturbation is a relatively small form perturbation ([14], Lemma 1, has a nice proof).

Proposition 2.4 ([7], chap. V, Theorem 4.3). Let $\mathscr{H}$ be a Hilbert space and A and B be self-adjoint operators acting in $\mathscr{H}$. Assume that B is a relatively small perturbation of A. Then $\mathscr{D}(B) \supset \mathscr{D}(A)$, and $A + B$ is self-adjoint with domain $\mathscr{D}(A + B) = \mathscr{D}(A)$. The expansion $(A + B - z)^{-1} = (A - z)^{-1}[1 + B(A - z)^{-1}]^{-1}: \mathscr{H} \to \mathscr{D}$ in powers of $B(A - z)^{-1}: \mathscr{H} \to \mathscr{H}$ converges in norm for z sufficiently far from the spectrum of A.

Proposition 2.5 ([7], chap. VI, Theorem 3.11). Let $\mathscr{H}$ be a Hilbert space and A and B be self-adjoint operators acting in $\mathscr{H}$. Assume that B is a relatively small form perturbation of A. Then $A + B$ with form domain $\mathscr{Q} = \mathscr{Q}(A + B) = \mathscr{Q}(A)$ is the quadratic form of a self-adjoint operator. The expansion of $(A + B - z)^{-1} = (A - z)^{-1}$ $[1 + B(A - z)^{-1}]^{-1}: \mathscr{Q}^* \to \mathscr{Q}$ in powers of $B(A - z)^{-1}: \mathscr{Q}^* \to \mathscr{Q}^*$ converges in norm for z sufficiently far from the spectrum of A.

It should be observed that if $B: \mathscr{Q} \to \mathscr{Q}^*$ varies continuously in norm, the perturbation expansion shows that $(A + B - z)^{-1}: \mathscr{Q}^* \to \mathscr{Q}$ varies continuously in norm. In particular, the resolvent $(A + B - z)^{-1}: \mathscr{H} \to \mathscr{H}$ varies continuously in norm.

Notice that in proposition 2.5 there is no assumption that $A \geqslant 0$. However, in quantum mechanics it is very common to have a perturbation problem in which $A \geqslant 0$ is the kinetic energy and B is the potential energy. If $A + B$ is to represent the total energy it is desirable that $A + B$ be bounded below. This is closely related to the condition for a relatively bounded form perturbation. In fact, if $A \geqslant 0$ and B is a relatively bounded form perturbation of A, then $-B \leqslant aA + b \leqslant A + b$, so $A + B \geqslant -b$, $A + B$ is bounded below.

In the case of a negative perturbation there is an implication in the other direction. Assume that $A \geqslant 0$ and $B \leqslant 0$ and that for some $c > 1$, $A + cB$ is bounded below (on a dense subspace of $\mathscr{Q}(A)$). Then B is a relatively small form perturbation of A. In fact $-cB \leqslant A + b$, and if $c > 1$ this says that B is relatively small.

Proposition 2.6 ([7], chap. VI, Theorems 1.31 and 2.1). Let $\mathscr{H}$ be a Hilbert space and A and B be self-adjoint operators acting in $\mathscr{H}$. Assume that A and B are bounded below and that $\mathscr{Q}(A) \cap \mathscr{Q}(B)$ is dense in $\mathscr{H}$. Then the quadratic form $A + B$ defined on $\mathscr{Q}(A) \cap \mathscr{Q}(B)$ is the quadratic form of a self-adjoint operator.

Proof: We may assume that $A \geqslant 0$ and $B \geqslant 0$. Let $\mathscr{H}^1 = \mathscr{Q}(A) \cap \mathscr{Q}(B)$ with the inner product $\langle u, v \rangle_1 = \langle Ju, v \rangle$, where $J = 1 + A + B$. Then $\mathscr{H}^1$ is a Hilbert space and $\mathscr{H}^1 \subset \mathscr{H}$. Thus J is the form of a self-adjoint operator ([9], §7, Theorem 2).

The most important facts about self-adjointness of form sums are summarized in the following theorem.

Theorem 2.1. *Let $\mathscr{H}$ be a Hilbert space and $H_0 \geqslant 0$ be a self-adjoint operator acting in $\mathscr{H}$. Let V be a self-adjoint operator acting in $\mathscr{H}$, and write $V = V_+ - V_-$, where $V_+ \geqslant 0$, $V_- \geqslant 0$. Assume that $\mathscr{Q}(V_-) \supset \mathscr{Q}(H_0)$ and V_- is a relatively small form perturbation of H_0. Assume that $\mathscr{Q}(V_+) \cap \mathscr{Q}(H_0)$ is dense in $\mathscr{H}$. Then the form sum*

$$H = H_0 + V = (H_0 - V_-) + V_+$$

is a self-adjoint operator which is bounded below.

The following three propositions are used in the application of Theorem 2.1 to quantum field theory. They are presented here in order to show how naturally the field theory results may be obtained by quadratic form methods.

Proposition 2.7 [11]. Assume $\|\exp(V_-)\exp(-H_0/2)\|^2 \leqslant C$. Then V_- is a relatively small form perturbation of H_0.

Proof [15]: If $\exp(2V_-) \leqslant C\exp(H_0) = \exp(H_0 + b)$, then $2V_- \leqslant H_0 + b$, by proposition 2.3.

Proposition 2.8. Let $\mathscr{E} \subset \mathscr{H}$ be a dense linear subspace. Assume that $\exp(-H_0)\mathscr{E} \subset \mathscr{Q}(V)$. Then $\mathscr{Q}(H_0) \cap \mathscr{Q}(V)$ is dense in $\mathscr{H}$.

Proof: Clearly $\exp(-H_0)\mathscr{E} \subset \mathscr{D}(H_0) \subset \mathscr{Q}(H_0)$. Hence it is sufficient to show that $\exp(-H_0)\mathscr{E}$ is dense in $\mathscr{H}$. But if $u \perp \exp(-H_0)\mathscr{E}$, then $\exp(-H_0)u = 0$, so $u = 0$.

For the next proposition note that on a finite measure space $L^\infty \subset L^r \subset L^2$ for $2 \leqslant r \leqslant \infty$.

Proposition 2.9. Let $H_0 \geqslant 0$ be a self-adjoint operator acting in $L^2(M, \mu)$, where $\mu(M) = 1$. Assume that $\exp(-tH_0)$, $t \geqslant 0$, is bounded on L^∞. Let $r \geqslant 2$ and q be numbers with $1/r + 1/q = \frac{1}{2}$. Assume that $\exp(-\frac{1}{2}H_0): L^2 \to L^r$ is bounded. Let V be a real function in $L^1(M, \mu)$. Assume that $\exp(-V) \in L^q(M, \mu)$. Then the form sum $H = H_0 + V$ is a self-adjoint operator which is bounded below.

Proof: By Holder's inequality we have

$$\|\exp(V_-)\exp(-\tfrac{1}{2}H_0)f\|_2 \leqslant \|\exp(-V)\|_q \|\exp(-\tfrac{1}{2}H_0)f\|_r \leqslant \text{const}\|f\|_2.$$

Thus proposition 2.7 is applicable.

Now set $\mathscr{E} = L^\infty$. Then $\exp(-H_0)L^\infty \subset L^\infty \subset Q(V)$, since $V \in L^1$. Thus proposition 2.8 may be used.

The hypotheses of proposition 2.9 were verified by Nelson [8] and Glimm and Jaffe [5] for the case of a self-interacting boson field Hamiltonian in one space dimension with a space cutoff. Due to the Wick ordering V is unbounded below, but Nelson showed that nevertheless $\exp(-V) \in L^q$ for all $q < \infty$.

3. Strong Resolvent Convergence

Definition 3.1: Let $\mathscr{H}$ be a Hilbert space. Let A_n be a sequence of self-adjoint operators acting in $\mathscr{H}$. We say that the A_n converge to A in the sense of strong resolvent convergence if for some z (bounded away from the spectra of the A_n and A) $(A_n - z)^{-1} \to (A - z)^{-1}$ strongly.

Proposition 3.1. Let ϕ be a bounded continuous function on an open set containing the spectrum of A. Assume that $A_n \to A$ in the sense of strong resolvent convergence. Then $\phi(A_n) \to \phi(A)$ strongly.

Proof: Let $\psi(t) = \phi[(1/t) + z]$. Then

$$\phi(A_n) = \psi((A_n - z)^{-1}) \to \psi((A - z)^{-1}) = \phi(A)$$

by the result for bounded normal operators ([2], Theorem X.7.2).

It is well known that for bounded self-adjoint operators monotone weak convergence implies strong convergence. In fact, if $R_n \leqslant R$ and $R_n \to R$ weakly, then

$$\|(R - R_n)f\| \leqslant \|(R - R_n)^{1/2}\| \, \|(R - R_n)^{1/2} f\|$$

and

$$\|(R - R_n)^{1/2} f\|^2 = \langle (R - R_n)f, f\rangle \to 0.$$

The following two propositions are concerned with unbounded operators. Both are special cases of results due to Kato ([7], chap. VIII, §3). The proofs are presented for the convenience of the reader.

Proposition 3.2 ([7], chap. VIII, Theorem 3.6). Let A be a self-adjoint operator which is bounded below. Let A_n be self-adjoint operators such that $A \leqslant A_n$ and $Q(A_n) = Q(A)$. Assume that $\langle A_n f, f\rangle \to \langle Af, f\rangle$ for every f in $Q(A)$. Then $A_n \to A$ in the sense of strong resolvent convergence.

Proof: We may assume without loss of generality that $0 < c \leqslant A \leqslant A_n$. Then $A_n^{-1} \leqslant A^{-1} \leqslant c^{-1}$ and

$$\begin{aligned} |\langle (A^{-1} - A_n^{-1})f, g\rangle| &= |\langle (A_n - A)A_n^{-1} f, A^{-1} g\rangle| \\ &\leqslant \langle (A_n - A)A_n^{-1} f, A_n^{-1} f\rangle^{1/2} \langle (A_n - A)A^{-1} g, A^{-1} g\rangle^{1/2} \\ &\leqslant \langle f, A_n^{-1} f\rangle^{1/2} \langle (A_n - A)A^{-1} g, A^{-1} g\rangle^{1/2} \to 0. \end{aligned}$$

Hence $A_n^{-1} \to A^{-1}$ weakly. Since $A_n^{-1} \leqslant A^{-1}$, it follows that $A_n^{-1} \to A^{-1}$ strongly.

Proposition 3.3 ([7], chap. VIII, Theorem 3.13). Let A_n be a sequence of self-adjoint operators which are bounded below and increasing: $A_n \leqslant A_{n+1}$. Let A be a self-adjoint operator such that $A_n \leqslant A$ and such that whenever $f \in Q(A_n)$ and $\langle A_n f, f\rangle$ is bounded, then $f \in Q(A)$ and $\langle A_n f, f\rangle \uparrow \langle Af, f\rangle$. Then $A_n \to A$ in the sense of strong resolvent convergence.

Proof: We may assume that $0 < c \leqslant A_n$. Since the A_n^{-1} are decreasing and bounded below (by A^{-1}), it follows that the A_n^{-1} have a weak limit, hence a strong limit. Since this limit is bounded below by A^{-1}, it must have zero nullspace. Call it B^{-1}. Thus $A^{-1} \leqslant B^{-1} \leqslant A_n^{-1}$, which implies that $A_n \leqslant B \leqslant A$. Since $A_n \to B$ in the sense of strong resolvent convergence, we need only show that $B = A$.

The trick is to notice that $A_n^{-1} \to B^{-1}$ strongly implies that $A_n^{-1/2} \to B^{-1/2}$ strongly (proposition 3.1). Consider the space $\mathscr{Q} = \mathscr{Q}(B)$. Recall that we may identify

$\mathcal{Q} \subset \mathcal{H} \subset \mathcal{Q}^*$. Now $B^{1/2}: \mathcal{Q} \to \mathcal{H}$ is bounded and the $A_n^{1/2}: \mathcal{H} \to \mathcal{Q}^*$ are uniformly bounded (since $A_n \leqslant B$). Hence if $f \in \mathcal{Q}$,

$$(A_n^{1/2} - B^{1/2})f = A_n^{1/2}(B^{-1/2} - A_n^{-1/2})B^{1/2}f \to 0 \quad \text{in } \mathcal{Q}^*.$$

Since $A_n^{1/2}f \to B^{1/2}f$, $\langle A_n^{1/2}f,g\rangle \to \langle B^{1/2}f,g\rangle$ for all g in $\mathcal{Q} \subset \mathcal{H}$. But $\|A_n^{1/2}f\| \leqslant \|B^{1/2}f\|$ (since $A_n \leqslant B$). It follows that $A_n^{1/2}f \to B^{1/2}f$ in the weak topology of $\mathcal{H}$. But weak convergence and no loss of norm actually implies strong convergence, so $A_n^{1/2}f \to B^{1/2}f$ in $\mathcal{H}$.

In particular, if $f \in \mathcal{Q}(B)$, $\langle A_n f,f\rangle \uparrow \langle Bf,f\rangle$. It follows that $f \in \mathcal{Q}(A)$ and $\langle Af,f\rangle = \langle Bf,f\rangle$. Hence A extends B. But $B \leqslant A$, so $A = B$.

Theorem 3.1. *Let $H_0 \geqslant 0$ and $H = H_0 + V$ satisfy the conditions of Theorem 2.1. Write $V = V_+ - V_-$ and write V_+^m and V_-^n for the corresponding truncated operators. Set $V_{mn} = V_+^m - V_-^n$, $H_{mn} = H_0 + V_{mn}$.* Then

a) $H_{mn} \to H_m = H_0 + V_+^m - V_-$ as $n \to \infty$

in the sense of strong resolvent convergence, and

b) $H_m \to H = H_0 + V$ as $m \to \infty$

in the sense of strong resolvent convergence.

Proof:

a) Since $H_m \leqslant H_{mn}$, this follows from proposition 3.2.
b) Clearly $H_m \leqslant H$. Consider $f \in \mathcal{Q}(H_m) = \mathcal{Q}(H_0)$ with $\langle H_m f,f\rangle$ bounded. Then $\langle V_+^m f,f\rangle$ is bounded. Thus $f \in \mathcal{Q}(V_+)$ and $\langle V_+^m f,f\rangle \uparrow \langle V_+ f,f\rangle$, by proposition 2.1. Hence $f \in \mathcal{Q}(H) = \mathcal{Q}(H_0) \cap \mathcal{Q}(V_+)$ and $\langle H_m f,f\rangle \uparrow \langle Hf,f\rangle$. Thus the conclusion follows from proposition 3.3.

Corollary 3.1. The semigroup $\exp(-tH)$, $t \geqslant 0$, may be expressed as a strong limit as follows:

i) $\exp(-tH) = \lim_m \exp(-tH_m)$,

ii) $\exp(-tH_m) = \lim_n \exp(-tH_{mn})$,

iii) $\exp(-tH_{mn}) = \lim_k \left(\exp\left(-\frac{t}{k}H_0\right)\exp\left(-\frac{t}{k}V_{mn}\right)\right)^k.$

Proof: Parts i) and ii) follows from proposition 3.1. As for iii), it is just the Trotter product formula ([9], §8) for the case of a bounded perturbation V_{mn}.

4. Essential Self-Adjointness

Let A be a self-adjoint operator with domain $\mathcal{D}(A)$. Consider a linear subspace $\mathcal{D}_0 \subset \mathcal{D}(A)$. Let A_0 be the restriction of A to $\mathcal{D}_0$. Then it is equivalent to say that $\mathcal{D}_0$ is dense in $\mathcal{D}(A)$ (with the graph norm), or $\mathcal{D}_0$ is a core of A, or the closure of A_0 is A, or A_0 is essentially self-adjoint, or that A is essentially self-adjoint on $\mathcal{D}_0$. Thus essential self-adjointness is a property of a self-adjoint operator and a linear subspace of its domain.

Theorem 4.1. *Let $H_0 \geqslant 0$ and $H = H_0 + V \geqslant -b$ satisfy the conditions of Theorem 2.1. Assume that there is a linear subspace $\mathscr{E} \subset \mathscr{H}$ such that $\mathscr{E}$ is dense in $\mathscr{H}$ and such that either $\exp(-H)\mathscr{E} \subset \mathscr{D}(V)$ or $(H+c)^{-1}\mathscr{E} \subset \mathscr{D}(V)$ for some $c > b$. Then $H = H_0 + V$ is essentially self-adjoint on $\mathscr{D}(H_0) \cap \mathscr{D}(V)$.*

Proof: Let $\mathscr{D}_0 = \exp(-H)\mathscr{E}$ or $(H+c)^{-1}\mathscr{E}$. Then $\mathscr{D}_0$ is a core for H. To see this in the case when $\mathscr{D}_0 = \exp(-H)\mathscr{E}$, notice that if $u \in \mathscr{D}(H)$ and $\langle u, (H^2+1)\mathscr{D}_0\rangle = 0$, then $(H^2+1)\exp(-H)u = 0$, so $u = 0$. Thus $\mathscr{D}_0$ is dense in $\mathscr{D}(H)$.

Now $\langle Hf,g\rangle = \langle H_0 f,g)\rangle + \langle Vf,g\rangle$ for $f,g \in \mathscr{Q}(H)$. If $f \in \mathscr{D}_0$, then since $\mathscr{D}_0 \subset \mathscr{D}(H)$ and $\mathscr{D}_0 \subset \mathscr{D}(V)$, $Hf \in H$ and $Vf \in \mathscr{H}$. Hence $g \mapsto \langle H_0 f,g\rangle$ is continuous for g belonging to the dense set $\mathscr{Q}(H) \subset \mathscr{H}$. So $H_0 f \in \mathscr{H}$, $f \in \mathscr{D}(H_0)$.

Thus we have shown that $\mathscr{D}_0 \subset \mathscr{D}(H_0) \cap \mathscr{D}(V)$ and $\mathscr{D}_0 \subset \mathscr{D}(H)$ is a core. This proves the theorem.

Corollary 4.1. The unitary Trotter product formula holds:

$$\exp(itH) = \lim_{k\to\infty}\left(\exp\left(i\frac{t}{k}H_0\right)\exp\left(i\frac{t}{k}V\right)\right)^k$$

as a strong limit.

Proof: This follows from essential self-adjointness on $\mathscr{D}(H_0) \cap \mathscr{D}(V)$ ([9], §8).

Corollary 4.2. If V is bounded below, then the self-adjoint Trotter product formula holds:

$$\exp(-tH) = \lim_{k\to\infty}\left(\exp\left(-\frac{t}{k}H_0\right)\exp\left(-\frac{t}{k}V\right)\right)^k$$

as a strong limit for $t \geqslant 0$.

Definition 4.1. Let $\mathscr{H}$ be a Hilbert space and $\mathscr{X}$ be a Banach space such that the linear space $\mathscr{X} \cap \mathscr{H}$ is dense both in $\mathscr{X}$ and in $\mathscr{H}$. Then $\mathscr{X}^* \cap \mathscr{H}$ is defined to be the space of f in $\mathscr{H}$ such that $g \mapsto \langle f,g\rangle$, $g \in \mathscr{X} \cap \mathscr{H}$, extends by continuity to $\mathscr{X}$.

If $f \in \mathscr{X}^* \cap \mathscr{H}$ and defines the zero element of $\mathscr{X}^*$, then $f = 0$, since $\mathscr{X} \cap \mathscr{H}$ is dense in $\mathscr{H}$. Thus the correspondence is injective and the notation of the definition is justified.

In general, if $f \in \mathscr{X}^*$ and $g \in \mathscr{X}$ it is consistent to denote the value of f on g by $\langle f,g\rangle$. It may be useful to think of the example $\mathscr{H} = L^2$, $\mathscr{X} = L^1$, $\mathscr{X}^* = L^\infty$.

One important special case of the situation described in definition 4.1 is when $\mathscr{H} \subset \mathscr{X}$. It is assumed that the inclusion is continuous and that $\mathscr{H}$ is dense in $\mathscr{X}$. It is easy to see that in this case $\mathscr{X}^* \subset \mathscr{H}$ and that $\mathscr{X}^*$ is dense in $\mathscr{H}$. Thus we have $\mathscr{X}^* \subset \mathscr{H} \subset \mathscr{X}$. This corresponds to the situation in the example when the measure space is finite, so that $L^\infty \subset L^2 \subset L^1$.

Lemma 4.1. *Let $\mathscr{X} \cap \mathscr{H}$ be dense in both $\mathscr{X}$ and $\mathscr{H}$. Assume that $f_n \in \mathscr{X}^* \cap \mathscr{H}$, $f_n \to f$ in $\mathscr{H}$, and $\|f_n\|_{\mathscr{X}^*} \leqslant C$. Then $f \in \mathscr{X}^* \cap \mathscr{H}$, $\|f\|_{\mathscr{X}^*} \leqslant C$, and $f_n \to f$ in the weak * topology of $\mathscr{X}^*$.*

Proof: If $f_n \to f$ in the norm of $\mathscr{H}$, then in particular $f_n \to f$ in the weak topology of $\mathscr{H}$. Thus if $g \in \mathscr{X} \cap \mathscr{H}$

$$|\langle f, g\rangle| = \lim_n |\langle f_n, g\rangle| \leqslant C\|g\|_{\mathscr{X}},$$

so $f \in \mathscr{X}^* \cap \mathscr{H}$ and $\|f\|_{\mathscr{X}^*} \leqslant C$.

The weak $*$ convergence follows from the fact that $\mathscr{X} \cap \mathscr{H}$ is dense in $\mathscr{X}$.

Lemma 4.2. *Assume $S: \mathscr{H} \to \mathscr{H}$ is a bounded self-adjoint operator. Assume $\mathscr{X} \cap \mathscr{H}$ is dense in both $\mathscr{X}$ and $\mathscr{H}$. Then if $S: \mathscr{X} \cap \mathscr{H} \to \mathscr{X} \cap \mathscr{H}$ with $\|Sg\|_{\mathscr{X}} \leqslant M\|g\|_{\mathscr{X}}$, then $S: \mathscr{X}^* \cap \mathscr{H} \to \mathscr{X}^* \cap \mathscr{H}$ with $\|Sf\|_{\mathscr{X}^*} \leqslant M\|f\|_{\mathscr{X}^*}$.*

Proof: If $f \in \mathscr{X}^* \cap \mathscr{H}$ and $g \in \mathscr{X} \cap \mathscr{H}$, then

$$|\langle Sf, g\rangle| = |\langle f, Sg\rangle| \leqslant \|f\|_{\mathscr{X}^*}\|Sg\|_{\mathscr{X}} \leqslant M\|f\|_{\mathscr{X}^*}\|g\|_{\mathscr{X}}.$$

Hence $Sf \in \mathscr{X}^* \cap \mathscr{H}$ and $\|Sf\|_{\mathscr{X}^*} \leqslant M\|f\|_{\mathscr{X}^*}$.

Theorem 4.2. *Let $H_0 \geqslant 0$ and V be self-adjoint operators satisfying the conditions of Theorem 2.1. Let $\mathscr{X}$ be a Banach space such that $\mathscr{X} \cap \mathscr{H}$ is dense in $\mathscr{X}$ and in $\mathscr{H}$ and such that $\mathscr{X}^* \cap \mathscr{H}$ is dense in $\mathscr{H}$. Assume for $t > 0$ and for all values of the truncations m, n that* $\exp(-tV_{mn})\exp(-tH_0)$ *is a contraction on $\mathscr{X}$. Assume also that $\mathscr{X}^* \cap \mathscr{H} \subset \mathscr{D}(V)$. Then $H = H_0 + V$ is essentially self-adjoint on $\mathscr{D}(H_0) \cap \mathscr{D}(V)$.*

Proof: Let $\mathscr{E} = \mathscr{X}^* \cap \mathscr{H}$. We show that $\exp(-H)\mathscr{E} \subset \mathscr{D}(V)$. This permits the application of Theorem 4.1.

Let $f \in \mathscr{E} = \mathscr{X}^* \cap \mathscr{H}$. Then

$$\left\|\left(\exp\left(-\frac{1}{k}H_0\right)\exp\left(-\frac{1}{k}V_{mn}\right)\right)^k f\right\|_{\mathscr{X}^*} \leqslant \|f\|_{\mathscr{X}^*}$$

by Lemma 4.2 and the contraction property. Hence by corollary 3.1 and Lemma 4.1, $\exp(-H_{mn})f \in \mathscr{E}$, $\exp(-H_m)f \in \mathscr{E}$, $\exp(-H)f \in \mathscr{E}$. Thus $\exp(-H)\mathscr{E} \subset \mathscr{E} \subset \mathscr{D}(V)$.

Remark: If instead of requiring that $\exp(-tV_{mn})\exp(-tH_0)$ is a contraction we require that its norm be bounded by e^{bt} for some b, the same conclusion follows.

Throughout this paper when we consider spaces $L^p(M, \mu)$ we shall always assume that the measure is σ-finite. (Thus the dual space of $L^1(M, \mu)$ is indeed $L^\infty(M, \mu)$.)

Corollary 4.3 [6]. Let $H_0 \geqslant 0$ be a self-adjoint operator acting in $L^2(M, \mu)$. Assume that $\exp(-tH_0)$ is a contraction on $L^1(M, \mu)$ for $t \geqslant 0$. Let V be a function on M such that $V \geqslant 0$, $V \in L^2(M, \mu)$. Then $H = H_0 + V$ is essentially self-adjoint on $\mathscr{D}(H_0) \cap \mathscr{D}(V)$.

Proof: Take $\mathscr{X} = L^1$, $\mathscr{X}^* = L^\infty$ and $\mathscr{E} = L^\infty \cap L^2$. Apply proposition 2.8 and Theorem 4.2.

Notice that if $\mu(M) = 1$, then $L^\infty(M, \mu) \subset L^2(M, \mu) \subset L^1(M, \mu)$. This is the situation in the following proposition.

Proposition 4.1 [15]. Let $H_0 \geqslant 0$ be a self-adjoint operator acting in $L^2(M,\mu)$, where $\mu(M) = 1$. Assume that $f \geqslant 0$ implies $\exp(-tH_0)f \geqslant 0$ for $t \geqslant 0$ and that $H_0 1 = 0$. Then $\exp(-tH_0)$ is a contraction on $L^1(M,\mu)$ and on $L^\infty(M,\mu)$ for $t \geqslant 0$.

Proof: Let $f \geqslant 0$. Then $\exp(-tH_0)f \geqslant 0$ and

$$\|\exp(-tH_0)f\|_1 = \langle \exp(-tH_0)f, 1\rangle = \langle f, 1\rangle = \|f\|_1,$$

since $\exp(-tH_0)1 = 1$. Thus if $g = \Sigma_i c_i f_i$, where the $f_i \geqslant 0$ have disjoint supports, then

$$\|\exp(-tH_0)g\|_1 \leqslant \sum_i |c_i| \|\exp(-tH_0)f_i\|_1 = \sum_i |c_i| \|f_i\|_1 = \|g\|_1.$$

But such g are dense in L^1, so $\exp(-tH_0)$ is a contraction on L^1. By duality (Lemma 4.2) it is also a contraction on L^∞.

Part of the theory of hypercontractive semigroups used in quantum field theory may also be developed in the setting of quadratic forms.

Definition 4.2: Let $H_0 \geqslant 0$ be a self-adjoint operator acting in $L^2(M,\mu)$, where $\mu(M) = 1$. Then $\exp(-tH_0)$, $t \geqslant 0$, is said to be a hypercontractive semigroup if $\exp(-tH_0)$ is a contraction on L^1 and on L^∞, and if for all p with $1 < p < \infty$, there exists $q < \infty$ and $a < \infty$ such that $\exp(-tH_0): L^p \to L^r$, where $1/r = 1/p - t/q$, has norm bounded by $\exp(at)$ for t near zero.

Thus a hypercontractive semigroup sends an L^p space into a smaller space $L^r \subset L^p$ (with $r > p$).

Proposition 4.2 [11, 15]. Assume that $\exp(-tH_0)$ is hypercontractive and that V is a real function on M such that $\exp(-V) \in L^q$ for all $q < \infty$. Assume that there is an $s > 2$ such that $V \in L^s$. Then H is essentially self-adjoint on $\mathscr{D}(H_0) \cap \mathscr{D}(V)$.

Proof: The fact that H is a self-adjoint form sum and is bounded below follows from proposition 2.9. For the essential self-adjointness we may use Theorem 4.1 or Theorem 4.2. Consider the space $\mathscr{X}^* = L^p$, where $1/p + 1/s = \frac{1}{2}$. Then $2 \leqslant p < \infty$ and $L^p \subset L^2$; in fact $L^p \subset \mathscr{D}(V)$. Thus it is sufficient to show that $\exp(-H)L^p \subset L^p$.

Take $f \in L^p$. Then

$$\begin{aligned}\|\exp(-tV_{mn})\exp(-tH_0)f\|_p &\leqslant \|\exp(-tV_{mn})\|_{q/t} \|\exp(-tH_0)f\|_r \\ &\leqslant \|\exp(-V)\|_q^t \exp(at)\|f\|_p.\end{aligned}$$

This estimate permits use of corollary 3.1 and Lemma 4.1. Thus $\exp(-H)f \in L^p$.

In the quantum field theory of self-interacting bosons in one space dimension, the result of proposition 4.2 justifies the use of the Trotter product formula (unitary case). This is used to show the convergence of the field automorphisms as the space cut-off is removed [5, 11].

5. The Ground State

Definition 5.1: Let μ be a measure in M and consider the Hilbert space $L^2(M,\mu)$. Let $A: L^2 \to L^2$ be a linear operator. Then A is said to be positivity preserving if $f \in L^2$, $f \geqslant 0$ implies $Af \geqslant 0$.

Notice that the set of all $f \in L^2$ with $f \geqslant 0$ is a closed cone. In general it need have no interior points.

Definition 5.2: Let $S \subset M$ be a measurable subset. The position subspace of $L^2(M,\mu)$ corresponding to S is the closed subspace consisting of all $f \in L^2(M,\mu)$ such that $f(p) = 0$ for (almost every) $p \notin S$.

One version of the Perron–Frobenius theorem concerns a bounded self-adjoint operator $A: L^2 \to L^2$. It is assumed that $A \leqslant \lambda$ where λ is an eigenvalue of A. The theorem states that if A is positivity preserving and leaves invariant no non-trivial position subspace, then λ has multiplicity one. Further, the eigenspace corresponding to λ is spanned by a function $u \in L^2$ such that $u(p) > 0$ for almost every p [15].

Let H be a self-adjoint operator and P be a projection. It is clear from the spectral theorem that if P commutes with H, then $u \in \mathcal{Q}(H)$ implies $Pu \in \mathcal{Q}(H)$ and $\langle HPu, v\rangle = \langle Hu, Pv\rangle$ for all $u, v \in \mathcal{Q}(H)$. The converse is also true.

Lemma 5.1. *If $u \in \mathcal{Q}(H)$ implies $Pu \in \mathcal{Q}(H)$ and $\langle HPu, v\rangle = \langle Hu, Pv\rangle$ for all $u, v \in \mathcal{Q}(H)$, then P commutes with H.*

Proof: Assume $u \in \mathcal{D}(H)$. Then $Hu \in \mathcal{H}$ and $\langle HPu, v\rangle = \langle Hu, Pv\rangle = \langle PHu, v\rangle$. Since $PHu \in \mathcal{H}$, it follows that $Pu \in \mathcal{D}(H)$ and $HPu = PHu$.

Lemma 5.2. *If $H \geqslant 0$ and there is a dense subspace $\mathscr{E} \subset \mathcal{Q}(H)$ such that $u \in \mathscr{E}$ implies $Pu \in \mathscr{E}$ and such that $\langle HPu, v\rangle = \langle Hu, Pv\rangle$ for all $u, v \in \mathscr{E}$, then P commutes with H.*

Proof: For $u \in \mathscr{E}$,

$$\langle HPu, Pu\rangle \leqslant \langle HPu, Pu\rangle + \langle H(1-P)u, (1-P)u\rangle = \langle Hu, u\rangle.$$

This says that $u \mapsto Pu$ is continuous in the $\mathcal{Q}(H)$ sense on $\mathscr{E}$. Since $\mathscr{E}$ is dense in $\mathcal{Q}(H)$, it follows that $u \in \mathcal{Q}(H)$ implies $Pu \in \mathcal{Q}(H)$ and that P is actually a continuous operator on $\mathcal{Q}(H)$. Thus the relation $\langle HPu, v\rangle = \langle Hu, Pu\rangle$ must be in fact true for all u, v in $\mathcal{Q}(H)$ and Lemma 5.1 applies.

The following theorem is a slight improvement of results of Glimm and Jaffe [5] and of Segal [12].

Theorem 5.1. Let $\mathcal{H} = L^2(M,\mu)$. *Let $H_0 \geqslant 0$ be a self-adjoint operator acting in $\mathcal{H}$. Let V be multiplication by a real measurable function on M. Assume that $H = H_0 + V$ satisfies the conditions of Theorem 2.1. If* $\exp(-tH_0)$ *is positivity preserving for $t \geqslant 0$, then so is* $\exp(-tH)$. *Assume also that $\mathcal{Q}(H)$ is dense in $\mathcal{Q}(H_0)$. If for some $t > 0$* $\exp(-tH_0)$ *leaves invariant no position subspace, then for all $t > 0$* $\exp(-tH)$ *leaves invariant no position subspace.*

Proof: If $\exp(-tH_0)$ is positivity preserving, then so is $\exp(-tH)$, by corollary 3.1.

Let P be the projection on a position subspace. Assume that for some $t > 0$ P commutes with $\exp(-tH)$. Then P commutes with H. Hence $\langle HPu, v\rangle = \langle Hu, Pv\rangle$ for $u, v \in \mathcal{Q}(H)$. Since P commutes with V, it follows that $\langle H_0Pu, v\rangle = \langle H_0u, Pu\rangle$ for $u, v \in \mathcal{Q}(H)$. Since $\mathcal{Q}(H)$ is dense in $\mathcal{Q}(H_0)$, P commutes with H_0 (Lemma 5.2). Hence P commutes with $\exp(-tH_0)$ for all $t > 0$.

Corollary 5.1. Let $H = H_0 + V$ satisfy all the hypotheses of Theorem 5.1. If $H \geqslant \nu$ and ν is an eigenvalue of H, then ν has multiplicity one and the eigenspace of ν is spanned by a function $u \in L^2$ such that $u > 0$ almost everywhere.

Proof: Apply the Perron–Frobenius theorem to $A = \exp(-H)$.

6. Schrödinger Operators

Let $\mathscr{H} = L^2(\mathbb{R}^n, dx)$ and let $F: \mathscr{H} \to L^2(\mathbb{R}^n, (2\pi)^{-n}\,dk)$ be the Fourier transform. Let ϕ and γ be measurable functions on $\mathbb{R}^n$ and define the operators $\phi(Q)$ and $\gamma(P)$ acting in H by $\phi(Q)$ = multiplication by ϕ and $\gamma(P) = F^{-1}$ (multiplication by γ) F.

Proposition 6.1. Let ϕ and γ be in L^p for some p, $2 \leqslant p \leqslant \infty$. Then $\phi(Q)\gamma(P): L^2 \to L^2$ is bounded.

Proof: If $u \in L^2$, then $Fu \in L^2$ and $\gamma Fu \in L^q$, where $\frac{1}{2} + 1/p = 1/q$, and $1 \leqslant q \leqslant 2$. Thus $F^{-1}(\gamma Fu) \in L^r$, where $1/q + 1/r = 1$ and $2 \leqslant r \leqslant \infty$, by the Hausdorff–Young theorem. Finally $\phi F^{-1}(\gamma Fu) \in L^2$, since $1/r + 1/p = \frac{1}{2}$.

So $\|\phi F^{-1}(\gamma Fu)\|_2 \leqslant \|\phi\|_p \|\gamma\|_p \|u\|_2$.

Proposition 6.2. If ϕ and γ are in L^p for $2 \leqslant p < \infty$ or in the closure of $L^2 \cap L^\infty$, then $\phi(Q)\gamma(P): L^2 \to L^2$ is compact.

Proof: If ϕ and γ are in L^2, then $\phi(Q)\gamma(P)$ is Hilbert–Schmidt, hence compact. In the general case one may approximate ϕ and γ by L^2 functions, and use the fact that the norm limit of a sequence of compact operators is compact.

Proposition 6.3. Let $\mathscr{H} = L^2(\mathbb{R}^n, dx)$. Let $H_0 = -\Delta$ and let V be a real function on $\mathbb{R}^n$. Assume that there exists $p > n/2$, $p \geqslant 2$ such that $V \in L^p(\mathbb{R}^n)$. Then V is a relatively small perturbation of H_0 and $H = H_0 + V$ is self-adjoint with $\mathscr{D}(H) = \mathscr{D}(H_0)$. Further, if $p < \infty$, then V is a relatively compact perturbation.

Proof: The product $V(H_0 + c^2)^{-1}$ is of the form of proposition 6.1, where $V = \phi \in L^p$ and $\gamma(k) = (k^2 + c^2)^{-1} \in L^p$ for $p > n/2$. Since $\gamma \to 0$ in L^p as $c \to \infty$, we may choose c so that $\|V(H_0 + c^2)^{-1}\| \leqslant a < 1$. Then $V^2 \leqslant a^2(H_0 + c^2)^2$; V is a relatively small perturbation of H_0. If $p < \infty$ then $V(H_0 + c^2)^{-1}$ is compact (proposition 6.2) which says that V is relatively compact.

In the cases $n = 1, 2, 3$ one may allow stronger local singularity by using form sums [3].

Proposition 6.4. Let $\mathscr{H} = L^2(\mathbb{R}^n, dx)$. Let $H_0 = -\Delta$ and let V be a real function on $\mathbb{R}^n$. Assume that there exists $p > n/2$, $p \geqslant 1$ such that $V \in L^p(\mathbb{R}^n)$. Then V is a relatively small form perturbation of H_0 and $H = H_0 + V$ is self-adjoint with $\mathscr{Q}(N) = \mathscr{Q}(H_0)$.

Proof: The product $|V|^{1/2}(H_0 + c^2)^{-1/2}$ is of the form of proposition 6.1, where $|V|^{1/2} = \phi \in L^{2p}$ and $\gamma(k) = (k^2 + c^2)^{-1/2} \in L^{2p}$ for $p > n/2$. We may thus choose c such that $\||V|^{1/2}(H_0 + c^2)^{-1/2}\| \leqslant a < 1$, that is $|V| \leqslant a^2(H_0 + c^2)$.

Proposition 6.5. Let $\mathscr{H} = L^2(\mathbb{R}^n, dx)$. Let $H_0 = -\Delta$ and let V be a real function on $\mathbb{R}^n$. Write $V = V_+ - V_-$, where $V_+ \geqslant 0$, $V_- \geqslant 0$. Assume that there exists $p > n/2$, $p \geqslant 1$ such that $V_- \in L^p(\mathbb{R}^n)$. Assume that V_+ is in L^1 locally except on a closed set of measure zero. Then the form sum $H = H_0 + V$ is self-adjoint and bounded below.

Proof: To apply Theorem 2.1 we need only show that $\mathscr{Q}(H_0) \cap \mathscr{Q}(V_+)$ is dense in $\mathscr{H}$. Let V_+ be in L^1 locally on the complement of the closed set M. Let $\mathscr{E}$ be the space of C^1 functions with compact support in the complement of M. Then $\mathscr{E} \subset \mathscr{Q}(H_0) \cap \mathscr{Q}(V_+)$ and $\mathscr{E}$ is dense in $L^2(\mathbb{R}^n - M) = L^2(\mathbb{R}^n)$ if M is of measure zero.

Theorem 6.1. *Let $\mathscr{H} = L^2(\mathbb{R}^n, dx)$. Let $H_0 = -\Delta$ and let V be a real function on $\mathbb{R}^n$. Write $V = V_+ - V_-$, where $V_+ \geqslant 0$ and $V_- \geqslant 0$. Assume that $V_+ \exp(-a|x|) \in L^2(\mathbb{R}^n, dx)$ for some $a < \infty$. Assume that $V_- = Y + Z$, where $Y \exp(b|x|) \in L^p(\mathbb{R}^n, dx)$ for some $p > n/2$, $p \geqslant 2$, and $b > 0$, and where $Z \in L^\infty$. Then $H = H_0 + V$ is essentially self-adjoint on $\mathscr{D}(H_0) \cap \mathscr{D}(V)$.*

Proof: It follows from proposition 6.3 that $H_0 - V_-$ is a self-adjoint operator with $\mathscr{D}(H_0 - V_-) = \mathscr{D}(H_0)$. Thus it is sufficient to show that $H = (H_0 - V_-) + V_+$ is essentially self-adjoint on $\mathscr{D}(H_0 - V_-) \cap \mathscr{D}(V_+) \subset \mathscr{D}(H_0) \cap \mathscr{D}(V)$.

We may neglect the term $Z \in L^\infty$, since a bounded perturbation does not affect essential self-adjointness. Thus we may assume that $V_- = Y \in L^p$ with $p < \infty$. In this case V_- is a relatively compact perturbation, so $H_0 - V_-$ has the same essential spectrum as H_0 ([7], chap. IV, Theorem 5.35). In particular, the only strictly negative numbers in the spectrum are isolated eigenvalues of finite multiplicity.

We may also assume without loss of generality that $H_0 - V_-$ has a strictly negative eigenvalue. For there is surely a bounded function $W \geqslant 0$ with compact support such that $H_0 - W$ has such an eigenvalue. (Take W to be constant on a ball, zero elsewhere.) Since $H_0 - W - V_- \leqslant H_0 - W$, the lowest eigenvalue of $H_0 - W - V_-$ is even more negative. So we may write $H = H_0 - (V_- + W) + (V_+ + W)$. The same argument shows that the eigenvalue may be chosen as negative as we please.

Let $-c^2$ be the smallest eigenvalue of $H_0 - V_-$. By the Perron–Frobenius theorem (corollary 5.1) we know that the corresponding eigenfunction u may be chosen so that $u > 0$ almost everywhere. We may also require that $\|u\|_2 = 1$.

Let $\mathscr{K} = L^2(\mathbb{R}^n, u(x)^2 dx)$. Let $U: \mathscr{K} \to \mathscr{H}$ be multiplication by u. Then U is an isomorphism of Hilbert spaces which preserves the cone of positive functions.

Let $H_- = H_0 - V_- + c^2$. Our problem is to show that the self-adjoint operator $H_- + V_+$ acting in $\mathscr{H}$ is essentially self-adjoint on $\mathscr{D}(H_-) \cap \mathscr{D}(V_+)$. Let A be the operator acting in $\mathscr{K}$ defined by $A = U^{-1} H_- U$. Let B be multiplication by V_+ as an operator acting in $\mathscr{K}$. It is sufficient to show that $A + B$ acting in $\mathscr{K}$ is essentially self-adjoint on $\mathscr{D}(A) \cap \mathscr{D}(B)$, since this is isomorphic to the original problem.

Since $H_- \geqslant 0$ and $H_- u = 0$, it follows that $A \geqslant 0$ and $A1 = 0$. We know from Theorem 5.1 that $\exp(-tH_-)$ is positivity preserving. Thus $\exp(-tA) = U^{-1} \exp(-tH_0) U$ is also positivity preserving. Proposition 4.1 then shows that $\exp(-tA)$ is a contraction on $L^1(\mathbb{R}^n, u(x)^2 dx)$ for $t \geqslant 0$. By duality it is a contraction on L^∞ (Lemma 4.2).

In order to apply corollary 4.3 we need only show that $V_+ \in L^2(\mathbb{R}^n, u(x)^2 dx)$. This follows from propositions 7.1 and 7.2, the estimates on the eigenfunction u. In fact, if we choose the eigenvalue $-c^2$ so that $c > a$, we have

$$\begin{aligned} |V_+(x)| u(x) &= |V_+(x)| \exp(-a|x|) \exp(a|x|) u(x) \\ &\leqslant \text{const}\, V_+(x) \exp(-a|x|) \in L^2(\mathbb{R}^n, dx). \end{aligned}$$

Remark: In the special case when V_- is bounded the proof is much simpler. In particular we do not need the Perron–Frobenius theorem or the estimates of Section 7. In fact, without loss of generality we may take $V_- = W$, where W is constant on a ball, zero elsewhere. The ground-state eigenfunction u of $H_0 - W$ may be computed explicitly; it is of course positive and exponentially decreasing.

The following theorem is a variant which emphasizes the local regularity question.

Theorem 6.2. *Let $\mathscr{H} = L^2(\mathbb{R}^n, dx)$. Let $H_0 = -\Delta$ and let V be a real function on $\mathbb{R}^n$. Write $V = V_+ - V_- + Z$, where $V_+ \geqslant 0$ and $V_- \geqslant 0$. Assume that $V_+ \in L^2(\mathbb{R}^n, dx)$. Assume that $V_- \in L^p(\mathbb{R}^n, dx)$ for some $p > n/2$, $p \geqslant 2$. Finally, assume that $Z \in L^\infty$. Then $H = H_0 + V$ is essentially self-adjoint on $\mathscr{D}(H_0) \cap \mathscr{D}(V)$.*

Proof: The fact that $V_+ \in L^2(\mathbb{R}^n, u(x)^2 dx)$ follows now from the fact that u is bounded (proposition 7.1). Otherwise the proof is as before.

7. Estimates on Eigenfunctions

Proposition 7.1. Let V be a real function which is in $L^p(\mathbb{R}^n, dx)$ for some p with $p > n/2$ and $p \geqslant 2$. Let $u \in L^2(\mathbb{R}^n, dx)$ be an eigenfunction of $-\Delta + V$ with a strictly negative eigenvalue. Then $u \in L^\infty(\mathbb{R}^n, dx)$.

Proof: If $n = 1, 2$, or 3, then $u \in \mathscr{D}(-\Delta + V) = \mathscr{D}(-\Delta) \subset L^\infty$. Thus for low dimensions the result is immediate. The general case requires an iteration argument.

Assume $(-\Delta + V)u = -c^2 u$, $c > 0$. Then $u = -(-\Delta + c^2)^{-1} Vu$. Now $(-\Delta + c^2)^{-1}$ is convolution by a function g_c, where g_c is the inverse Fourier transform of $(k^2 + c^2)^{-1}$. But $g_c(x) = \text{const}\, K_{n/2-1}(c|x|)/|x|^{n/2-1}$ ([4], chap. III, §2.8). Thus $g_c(x)$ has a $1/|x|^{n-2}$ singularity at the origin (when $n \geqslant 3$) and is dominated by $\exp(-c|x|)$ at infinity. It follows that $g_c \in L^r$ whenever $1 - 2/n < 1/r \leqslant 1$.

Let $2 \leqslant a \leqslant \infty$ and consider $u \in L^a$. Then $Vu \in L^q$, where $1/a + 1/p = 1/q$, $1 \leqslant q \leqslant \infty$. Hence $u = -g_c * Vu \in L^b$, where $1/q + 1/r - 1 = 1/b$, provided that $1 \leqslant b \leqslant \infty$, by Young's inequality.

We have

$$\frac{1}{a} - \frac{1}{b} = 1 - \frac{1}{r} - \frac{1}{p} = \left(1 - \frac{2}{n} - \frac{1}{r}\right) + \left(\frac{2}{n} - \frac{1}{p}\right).$$

But r is subject only to $1 \geqslant 1/r > 1 - 2/n$, so we may choose r so as to give $1/a - 1/b$ an arbitrary value such that

$$-\frac{1}{p} \leqslant \frac{1}{a} - \frac{1}{b} < \frac{2}{n} - \frac{1}{p}.$$

But $2/n - 1/p > 0$ and we know that $u \in L^a$ implies $u \in L^b$ whenever $1/b \geqslant 0$. It follows by iteration that $u \in L^2$ implies $u \in L^\infty$.

The next proposition is a decay estimate for the eigenfunction u. More sophisticated estimates in various special cases may be found in the quantum chemistry literature [1].

Proposition 7.2. Let V be a real function on $\mathbb{R}^n$ such that for some $b > 0$, $V\exp(b|x|) \in L^p(\mathbb{R}^n, dx)$ with some $p > n/2$, $p \geqslant 2$. Let $u \in L^\infty$ be an eigenfunction of $-\Delta + V$ with a strictly negative eigenvalue $-c^2$, $c > 0$. Then $u\exp(a|x|) \in L^\infty$ for all $a < c$.

Proof: The important fact is that $g_c\exp(a|x|) \in L^r$ whenever $a < c$, where $1/p + 1/r = 1$. Since u is an eigenfunction we have

$$u(x) = -\int g_c(x-y)V(y)u(y)dy.$$

Thus

$$|u(x)|\exp(a|x|) \leqslant \int \{|g_c(x-y)|\exp(a|x-y|)\}\{|V(y)|\exp(a|y|)|u(y)|\}dy.$$

Write $a = b + d$ and insert this in the right-hand factor of the integrand. We then see that $u(y)\exp(d|y|) \in L^\infty$ implies $u(x)\exp(a|x|) \in L^\infty$, so long as $a < c$.

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