JOURNAL OF FUNCTIONAL ANALYSIS 23, 218–238 (1976)

On the Decoupling of Finite Singularities from the Question of Asymptotic Completeness in Two Body Quantum Systems

P. DEIFT* AND B. SIMON†

Department of Physics, Princeton University, Princeton, New Jersey 08540

Communicated by Tosio Kato

Received July 7, 1975

Let V be a multiplication operator, whose negative part, $V_-(V_- \leqslant 0)$ obeys $-\Delta + (1+\epsilon)V_- \geqslant -c$ for some ϵ, $c > 0$. Let $W = V\chi$ where χ is the characteristic function of the *exterior* of a ball. Our main result asserts that the scattering for $-\Delta + V$ is complete if and only if that for $-\Delta + W$ is complete. Our technical estimates exploit Wiener integrals and the Feynman–Kac formula. We also make an application to acoustical scattering.

1. INTRODUCTION

Since the original papers of Cook [5], Jauch [14], and Kuroda [22], the scattering theory of two body Schrödinger operators has been extensively studied. A common thread running through much of this work is the idea that only the behavior at infinity is critical for scattering and the finite singularities are merely an inessential technical complication. As far as existence of the wave operators is concerned, this idea is probably best expressed in the result of Kupsch–Sandhas [21] (not stated in exactly the form below; see also [37]):

PROPOSITION 1. *Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^n)$ and let H be a self-adjoint operator so that for any $\phi \in \mathscr{S}(\mathbb{R}^n)$ with support of ϕ outside some ball B, $H\phi = -\Delta\phi + V\phi$ where V is a multiplication operator. Let χ be the*

* Research supported in part by AFOSR under Contract Number F44620-71-C-0108; Present address: Courant Institute, New York University, New York, New York.

† A. Sloan Fellow; partially supported by the National Science Foundation under Grant Number GP-39048.

characteristic function of the exterior of B *and suppose for a dense set* D *in* C_0^∞, $W = XV$ *obeys the Cook condition*:

$$\int_{-\infty}^{\infty} \| We^{-iH_0t}\phi \| \, dt < \infty; \qquad \phi \in D.$$

Then the wave operators $s\text{-}\lim_{t\to\mp\infty} e^{iHt}e^{-iH_0t} = \Omega^{\pm}(H, H_0)$ *exist.*

Our goal in this paper is to prove a result of Kupsch–Sandhas genre allowing one to conclude completeness of wave operators, i.e., $\operatorname{Ran} \Omega^{\pm}(H, H_0) = \mathscr{H}_{\text{ac}}(H)$, the absolutely continuous space for H. In seeking such a result, one subtlety that one must bear in mind is that finite singularities can make a difference for the question of asymptotic completeness, a fundamental discovery of Pearson [31], who found an example of a potential V of compact support so that $H = -\Delta + V$ is essentially self-adjoint on $D(\Delta) \cap D(V)$, bounded below, and so that $\operatorname{Ran} \Omega^{+}(H, H_0) \neq \operatorname{Ran} \Omega^{-}(H, H_0)$. We will require a mild regularity condition on the negative part of the local singularity to eliminate the Pearson effect. Our main result is the following:

THEOREM 1. *Let* V *be a function on* $\mathbb{R}^n$ *which is locally* L^1 *away from a set* $G \subset \mathbb{R}^n$ *which is a closed set of measure zero. Suppose that* V_-, *the negative part of* V, *obeys an estimate*

$$-\Delta + (1 + \epsilon)\, V_- \geqslant -c \tag{1}$$

for some ϵ, $c > 0$, *as a sum of forms on* $C_0^\infty(\mathbb{R}^n)$. *Let* H *be the operator* $-\Delta + V$ *defined as the form closure of the sum of forms on* $C_0^\infty(\mathbb{R}^n \backslash G)$. *Let* W *be another function obeying* (1) *so that* $V - W$ *has compact support. Let* $H' = -\Delta + W$ *and* $H_0 = -\Delta$. *Then* $\Omega^{\pm}(H, H_0)$ *exist* (*resp. are complete*) *if and only if* $\Omega^{\pm}(H', H_0)$ *exist* (resp. *are complete*).

Remarks. 1. For discussion of form methods see Faris [7], Kato [18], or Reed–Simon [33, 34].

2. For the case of centrally symmetric potentials, results with a thrust related to Theorem 1 can be found in Pearson–Whould [32]; for related results see Amrein–Georgeseu [2].

3. Among the corollaries of the theorem is the existence and completeness of $\Omega^{\pm}(H, H_0)$ for a variety of H's; e.g., when $V \geqslant 0$ in $L^1_{\text{loc}}(\mathbb{R}^n \backslash G)$ has compact support. To obtain results when V does not have compact support, one controls $\Omega^{\pm}(H', H_0)$ by appealing to the various results for nonsingular potentials, e.g., Agmon [1], Kato–Kuroda [19].

4. As another corollary, we are able to obtain Robinson's extension [36] of Lavine's work on repulsive potentials, given Lavine's results [24].

Our main technique for isolating singularities is based on an idea in Pearson's paper [31]. This technique of Dirichlet decoupling is discussed in Section 2. Decoupling via Dirichlet boundary conditions has been used in a variety of mathematical physics situations going back at least as far as the Courant–Hilbert proof [6] of Weyl's theorem on the asymptotic number of eigenvalues of a vibrating membrane (see also Kac [17] and Reed–Simon [34]). More recent applications have been to statistical mechanics (Lieb [25], Robinson [35]), Schrödinger operators (Martin [29], Reed–Simon [34]), constructive quantum field theory (Glimm–Jaffe–Spencer [9], Guerra–Rosen–Simon [12]), and the connection of Thomas–Fermi theory with quantum mechanics (Lieb–Simon [26, 27]).

In Section 3, we use the ideas of Section 2 to prove a variety of results for central potentials generalizing those of [32] and also those of Theorem 1. Essentially the same results have been proven in [2] by related but different methods. In Section 4, we introduce the Wiener path integral ideas we will use to prove the estimates needed to verify Theorem 1 in the general case. We consider the special case of Theorem 1 where V, W are nonnegative. In Section 5, we extend this idea to prove Theorem 1 in the general case. In the appendix we describe an application to acoustical scattering and the relation of our work to some work of Birman.

Two remarks seem to be in order about possible ways of rewriting our methods in Sections 4, 5. First, it is likely that one can replace our use of the Feynman–Kac formula by the Trotter product formula and the positivity of various integral operator kernels. While this rewriting is "more elementary" in that it avoids the use of the Wiener integral, it also tends to obscure the intuition that led us to our results. Secondly, most of the estimates of Section 5 are expressed more naturally in terms of weighted L^2 spaces (see, e.g., Agmon [1]) which we have avoided for reasons of simplicity of exposition.

Finally, let us close this introduction with a few words about various technicalities we will slough over in Sections 4, 5. We will make various formally correct manipulations involving commutators. The reader may wonder if these manipulations are legitimate for the singular V we are considering. We finesse this question by viewing our estimates as a priori estimates. That is, the result we wish to prove is that certain operators are trace class. Our manipulations are certainly legitimate if V is in C_0^∞ and result in trace norm estimates on the objects of interest which only depend on the lower bound of $-\Delta + (1+\epsilon) V_-$. Now $-\Delta + V$ is the limit in strong resolvent sense of $-\Delta + V_n$ for suitable $V_n \in C_0^\infty$ (this may be established by appealing to monotone convergence theorems for forms [7, 18]). The trace class nature of the objects of interest can then be established by appealing to:

PROPOSITION 2. *Let $A_n \to A$ strongly for bounded operators, A_n, A. If each A_n is trace class with* $\sup \operatorname{Tr}(|A_n|) < \infty$, *then A is trace class, and* $\operatorname{Tr}(|A|) \leqslant \lim \operatorname{Tr}(|A_n|)$.

Proof. It follows by noting that A is trace class if and only if $|\operatorname{Tr}(AB)| \leqslant c \| B \|_{\mathrm{op}}$ for all finite real operators B. ∎

We also deal with integral kernels of various operators and it may not be clear that these operators have integral kernels. This problem can also be handled by a priori considerations of the type discussed above. Alternatively, we prove most of the objects that concern us are Hilbert–Schmidt or at least are Hilbert–Schmidt after multiplication by $(1 + x^2)^{-\rho}$ for suitable ρ. Thus these are direct proofs that many of the operators are integral operators. Finally, by the Dunford–Pettis Theorem (see, e.g., [40]), any continuous bilinear form on $L^1(\mathbb{R}^n)$ has an integral kernel in $L^\infty(\mathbb{R}^{2n})$. This can be used to prove e^{-tH} and $(H + \lambda)^{-1}$ are integral operators if $V \geqslant 0$.

2. DIRICHLET DECOUPLING

In Sections 4, 5 we will consider potentials $V \in L^1_{\mathrm{loc}}(\mathbb{R}^n \backslash G)$, where G is closed set of measure zero so that V_- is a form bounded perturbation of $-\Delta$ with relative bound less than 1. Under this condition it is easy to see that the form $h(\psi, \psi) = (\psi, -\Delta\psi) + (\psi, V\psi)$ with dense form domain $C_0^\infty(\mathbb{R}^n \backslash G)$ is semibounded and closable and so determines a self-adjoint operator H. Let S be a sphere in $\mathbb{R}^n$ and define $\tilde{H}$ to be the operator determined by closing the quadratic form h restricted to $C_0^\infty(\mathbb{R}^n \backslash (G \cup S))$. We say that $\tilde{H}$ has a Dirichlet B.C. (boundary condition) added at S. Now S divides $\mathbb{R}^n$ in two regions B and E (the interior of a ball and the exterior). The fundamental fact about $\tilde{H}$ is that:

PROPOSITION 3. *There are self-adjoint operators H_1 on $L^2(B)$ and* $H_2(\mathbb{R}^n) = L^2(B) \oplus L^2(E)$, $\tilde{H} = H_1 \oplus H_2$.

Proof. This follows directly from the fact that $C_0^\infty(\mathbb{R}^n \backslash (G \cup S)) =$

$C_0^\infty(B\backslash G) + C_0^\infty(E\backslash G)$ (for more details, the reader can consult [34]). ∎

We also recall some elementary facts about relative wave operators (see Kato [18]). If A and B are self-adjoint operators and $P_{ac}(A)$ (resp. $P_{ac}(B)$) is the projection onto the absolutely continuous space for A (resp. B), then we say that $\Omega^\pm(A, B)$ exists if the

$$\underset{t\to\mp\infty}{s\text{-lim}}\, e^{itA}e^{-itB}P_{ac}(B) \equiv \Omega^\pm(A, B)$$

exists, and is complete if Ran $\Omega^\pm =$ Ran $P_{ac}(A)$.

(*Remark.* What we call $\Omega^\pm$, many call $\Omega^\mp$). The following result is an immediate consequence of the transitivity of wave operators:

PROPOSITION 4. *Suppose that $\Omega^\pm(A, B)$ exist and are complete. Then $\Omega^\pm(A, C)$ exist (are complete) if and only if $\Omega^\pm(B, C)$ exist (are complete).*

One also has the following basic result associated with the work of Birman, DeBranges, Kato, and Kuroda:

PROPOSITION 5. *Either of the following is sufficient for the existence and completeness of $\Omega^\pm(A, B)$:*

(a) *$(A + i)^{-1} - (B + i)^{-1}$ is trace class,*

(b) *$A, B \geqslant 0$ and $f(A) - f(B)$ trace class,*

for a C^2 function f on $[0, \infty]$ with strictly negative derivative.

THEOREM 2. *To prove Theorem 1, it suffices to prove that for any V obeying the hypothesis of the theorem, $e^{-H} - e^{-\tilde{H}}$ is trace class.*

Proof. By Proposition 4, it suffices to prove that $\Omega^\pm(\tilde{H}, H)$, $\Omega^\pm(\tilde{H}', H')$, and $\Omega^\pm(\tilde{H}, \tilde{H}')$ exist and are complete (for then $\Omega^\pm(H', H)$ exists and is complete). By hypothesis and Proposition 5, $\Omega^\pm(\tilde{H}, H)$ and $\Omega^\pm(\tilde{H}', H')$ exist and are complete. Now $\tilde{H} = H_1 \oplus H_2$ $\tilde{H}' = H_1' \oplus H_2'$ and for S chosen suitably $H_2 = H_2'$ (since $V - W = 0$ on E). Now

$$\begin{aligned}\tilde{H} &\geqslant H_0 + V_- = (1+\epsilon)^{-1}[H_0 + (1+\epsilon)V_-] + \epsilon(1+\epsilon)^{-1}H_0 \\ &\geqslant (1+\epsilon)^{-1}(\epsilon H_0 - c).\end{aligned}$$

(All statements are intended as form inequalities in the sense: $A \geqslant B$ if and only if $Q(A) \subset Q(B)$ and $(\phi, A\phi) \geqslant (\phi, B\phi)$ for all $\phi \in Q(A)$; it is sufficient to prove such an estimate on a form core for A. Notice in the first inequality it can happen that $Q(A) \neq Q(B)$.) Let $(H_0'')_1$ be obtained by closing $(\phi, -\Delta\phi)$ on $\mathscr{C}_0^\infty(B)$. Now $(H_0'')_1 \leqslant (H_0)_1$ as forms. Thus $(H_0)_1$ has compact resolvent. Hence, since $H_1 \geqslant (1+\epsilon)^{-1}(\epsilon(H_0)_1 - c)$ as above, so do H_1, and H_1', so $P_{\mathrm{ac}}(\tilde{H})$ and $P_{\mathrm{ac}}(\tilde{H}')$ have ranges in $L^2(E)$ and so $\Omega^{\pm}(\tilde{H}', \tilde{H}) = P_{\mathrm{ac}}(H_2) = P_{\mathrm{ac}}(H_2')$ exists. ∎

Remark. A direct calculation shows that $e^{-\tilde{H}'} - e^{-\tilde{H}}$ is trace class so that $e^{-H} - e^{-H'}$ is trace class under the hypotheses of the theorem.

For consideration in Section 3, we need a slightly different result than Theorem 2. This result is essentially contained in Pearson [31]:

THEOREM 3. *Let V be a central potential which is in $L^2_{\mathrm{loc}}(\mathbb{R}^n\backslash\{0\})$. Let H be self-adjoint operator commuting with rotations which is an extension of $-\Delta + V$ on $C_0^\infty(\mathbb{R}^n\backslash\{0\})$. Let H' be a similar operator associated with a potential W. Suppose that $V(x) = W(x)$ if $|x| > a$. Let H_1 (resp. H_1') be* any *rotationally invariant self-adjoint extension of $-\Delta + V$ on $C_0^\infty(0 < |x| < a)$* (resp. $-\Delta + W$). *If H_1 and H_1' have no absolutely continuous spectrum on each space of constant angular momentum, then $\Omega^{\pm}(H, H')$ exist and are complete.*

Proof. One need only prove that on each subspace of constant angular momentum that $\Omega^{\pm}(\tilde{H}, H)$ and $\Omega^{\pm}(\tilde{H}, \tilde{H}')$ exist and are complete. Pick H_2 to be an arbitrary self-adjoint extension of $-\Delta + V$ on $C_0^\infty(|x| > a)$. Let $\tilde{H} = H_1 \oplus H_2$. Then on such subspace, $(\tilde{H} + i)^{-1} - (H + i)^{-1}$ is an operator of rank at most 4 and so trace class. By hypothesis $\Omega^{\pm}(\tilde{H}, \tilde{H}') = \Omega^{\pm}(H_2, H_2') = P_{\mathrm{ac}}(H_2) = P_{\mathrm{ac}}(H_2')$. ∎

Remarks. 1. In Theorem 2 the easy part is that $\Omega^{\pm}(\tilde{H}, \tilde{H}')$ exist and in Theorem 3 that $\Omega^{\pm}(\tilde{H}, H)$ exist so the central case of Theorem 1 is very easy.

2. Note that if one particular choice for H_1 (respectively H_1') has no absolutely continuous spectrum, then the same is true for all choices for the self-adjoint extensions H_1 (respectively H_1') by the Kato–Birman theorem.

3. If V is central and in $L^1_{\mathrm{loc}}(\mathbb{R}^n\backslash\{0\})$, and its negative part is form small with respect to $-\Delta$, then of course Theorem 1 applies. If V is only $L^1_{\mathrm{loc}}(\mathbb{R}^n\backslash\{0\})$, then the limit point/limit circle method can still be used to construct rotationally invariant self-adjoint operators $H = -\Delta + V$. For such operators H, Theorem 3 is still true, though one needs more care in estimating $(\tilde{H} + i)^{-1} - (H + i)^{-1}$.

4. Theorem 3 makes assertions about *all* the self-adjoint extensions of $(-\Delta + V) \upharpoonright C_0^\infty(\mathbb{R}^n \backslash \{0\})$. If V is not necessarily central but satisfies, in addition to the requirements of Theorem 1, $V \in L^2_{\mathrm{loc}}(\mathbb{R}^n \backslash G)$ with G finite, then we conjecture that Theorem 1 extends to all self-adjoint extensions H of $(-\Delta + V) \upharpoonright C_0^\infty(\mathbb{R}^n \backslash G)$. If G is an arbitrary compact set of measure zero in $\mathbb{R}^n$, however, then the particular choice of the self-adjoint extension H does affect the scattering! For in $\mathbb{R}^3$, Pearson's [31] example of incompleteness with δ-functions is equivalent to taking $V = 0$ and requiring $-\Delta + V$ to satisfy particular boundary conditions on a countable number of spheres $S_i = \{| x | x | = a_i\}$, $\sup_i a_i < \infty$. If we were to take Dirichlet boundary conditions across these spheres, then Theorem 1 gives completeness. In the spirit of Theorem 3, Pearson's example shows us that for general compact G one self-adjoint extension H may be connected to a decomposition $\tilde{H} = H_1 \oplus H_2$ where the "core" H_1 has absolutely continuous spectrum, whereas another extension may be connected to a core without any absolutely continuous spectrum. The situation is not as simple as in Remark 2.

3. Central Potentials

In this section, we apply Theorem 3 to central potentials with compact support. We then use Pearson's decoupling to extend an approach due to Kuroda [22] for potentials satisfying a global integrability condition, to include potentials with a finite singularity.

Let $V = V(r)$ be a central potential in $\mathbb{R}^n$. Let $-\kappa_l$ be the lth eigenvalue of the Laplace–Beltrami operator on the $(n-1)$-sphere S_{n-1}: $\kappa_l \geqslant 0$. Where $a > 0$, let $H_{ln}^{(0,a)}$ be the operator $(-d^2/dr^2 + (((n-1)(n-3)/4) + \kappa_l)(1/r^2) + V(r)) \upharpoonright C_0^\infty(0, a)$. Rotationally invariant self-adjoint extensions H of $(-\Delta + V) \upharpoonright C_0^\infty(\mathbb{R}^n \backslash \{0\})$ are direct sums of self-adjoint extensions H_{ln} of $H_{ln}^{(0,\infty)}$. The self-adjoint Laplacian $H_0 = -\Delta$ on $\mathbb{R}^n$ is a direct sum of self-adjoint Dirichlet operators $H_{ln,0} \equiv -d^2/dr^2 + (((n-1)(n-3)/4) + \kappa_l)(1/r^2)$ on $L^2([0, \infty), dr)$. Scattering exists and is complete in $\mathbb{R}^n$ iff $\Omega^\pm(H_{ln}, H_{ln,0})$ exist and are complete for all l, n.

Theorem 3 immediately implies:

Theorem 4. *Let V be a central potential which has compact support B and which is in $L^2_{\mathrm{loc}}(\mathbb{R}^n \backslash \{0\})$. Let H and H_1 be as in Theorem 3, where a is any number for which $B \subset \{x: | x | \leqslant a\}$. Suppose that V satisfies at least one of the following conditions:*

(i) $V(r) + (((n-1)(n-3)/4) + \kappa_l)(1/r^2)$ *is in the limit circle case at* $r = 0$ *in each space of angular momentum* l;

(ii) $H_0 + (1+\epsilon)V \geqslant -c$ *on* $C_0^\infty(0, a)$ *for some* $\epsilon > 0$ *and some real* c;

(iii) V *is* H_0*-form bounded with bound* $\alpha < 1$, i.e., $Q(H_0) \subset Q(V)$ *and there exist* $\beta > 0$, $1 > \alpha \geqslant 0$ *such that*

$$|(\phi, V\phi)| \leqslant \alpha(\phi, H_0\phi) + \beta(\phi, \phi) \qquad \text{for all} \quad \phi \in Q(H_0),$$

(iv) $V \geqslant 0$.

Then H_1 *is discrete and* $\Omega^\pm(H, H_0)$ *exist and are complete.*

Proof. In the notation of Theorem 3, let H' be H_0. In $L^2\{x: |x| \leqslant a\}$ let H_1' be the (rotationally invariant) self-adjoint operator associated with the closure of the form $(\phi, H_0\phi)$ on $C_0^\infty\{x : 0 < |x| < a\}$. H_1' is discrete. Now if (i) is satisfied, then all rotationally invariant self-adjoint extensions H_1 of $(H_0 + V) \restriction C_0^\infty\{x: 0 < |x| < a\}$ are discrete (see Coddington and Levinson [4, pp. 242–244]). Also, the conditions (iii) and (iv) separately imply (ii), so we can assume $H_0 + (1+\epsilon)V \geqslant -c$ on $C_0^\infty(0, a)$. But if we define H_1 as in Section 2 by means of forms, we again have the forms inequality $H_1 = H_0 + V \geqslant (1+\epsilon)^{-1}(\epsilon H_0 - c)$, so H_1 is discrete. If $\bar{H}_1$ is some other (possibly unbounded from below) rotationally invariant, self-adjoint extension of $(H_0 + V) \restriction C_0^\infty\{x: 0 < |x| < a\}$, then in each space of angular momentum l, $[((\bar{H}_1))^2 + 1)^{-1} - ((H_1)^2 + 1)^{-1}]$ is at most a rank 4 operator. It follows then from the min–max principle and the spectral mapping theorem for self-adjoint operators that $\bar{H}_1$ is also discrete (and with a little more work, also bounded below). The result follows.

Remarks. 1. The conditions (ii) and (iii) are essentially due to Pearson and Whould [32].

2. Each "core" H_1 is discrete: this is of course more than is required for Theorem 3.

Theorem 4 gives an easy discussion of commonly occuring potentials, e.g., suppose that for $r < a$, $V(r) = \alpha r^\beta$ for some real α, β. Then near $r = 0$, $W(r) = (((n-1)(n-3)/4) + \kappa_l)(1/r^2) + \alpha r^\beta$ behaves as $\alpha' r^{-\beta'}$ for some reals α', β' with $\beta' \geqslant 2$. If $\alpha' < 0$, then $W(r)$ decreases as $r \to 0$ and so is limit circle at 0 (see, e.g., Titchmarsh [39, p. 127]). If $\alpha' \geqslant 0$, regard $W(r)$ as a potential in $\mathbb{R}^3$. Since $W(r)$ obeys hypothesis (iv) of Theorem 4, and since any self-adjoint extension on the zero angular momentum subspace can be extended to a rotationally invariant extension of $-\Delta + W$ in $\mathbb{R}^3$, the conclusion of Theorem 4 implies that any self-adjoint extension of

$$(-(d^2/dr^2) + W(r)) \restriction C_0^\infty(0, a)$$
$$= [(-d^2/dr^2 + ((n-1)(n-3)/4) + \kappa_l)(1/r^2)) + \alpha r^\beta] \restriction C_0^\infty(0, a)$$

has discrete spectrum. It follows that we have completeness for all rotationally invariant self-adjoint operators $-\Delta + \alpha r^\beta \chi$ where χ is the characteristic function of some ball.

At first glance one might think that for potentials of form $-r^{-n}$ ($n \geqslant 2$) near the origin, the classical phenomenon of fall-in to $r = 0$ is connected with asymptotic incompleteness. The preceding result shows, however, that this is not the case. In order to model the classical phenomenon quantum-mechanically, one must use non-self-adjoint extensions of $-\Delta - r^{-n}$ as discussed by Nelson [30] and Pearson [31]. To get breakdown of completeness for self-adjoint $(-\Delta + V)$, we must have $(H_1)_{\text{ac}} \neq 0$. Pearson's [31] construction gives a central potential V with compact support in $\mathbb{R}^3$ for which H_1 has precisely this property.

We now develop an approach due to Kuroda [22] and eventually prove:

THEOREM 5. *Let V be a central potential which is in $L^2_{\text{loc}}(\mathbb{R}^n\backslash\{0\})$. Let H and H_1 be as in Theorem* 3, *where a is any positive number. For each l, let H_{ln} be the component of H in the space of angular momentum l. Suppose that $\Omega^\pm(H, H_0)$ exist and that $(H_1)_{\text{ac}} = 0$. Then $\Omega^\pm(H, H_0)$ are* WAC [i.e., *weakly asymptotically complete*: $\operatorname{Ran} \Omega^+(H, H_0) = \operatorname{Ran} \Omega^-(H, H_0)$]. *If $\sigma_{\text{ac}}(H_{ln}) \subset \sigma_{\text{ac}}(H_{ln,0}) = [0, \infty)$, they are complete.*

In order to prove Theorem 5 we introduce some notions from real analysis. Let E be a Borel set in $\mathbb{R}$ and let $d\lambda$ be Lebesgue measure. If $x \in \mathbb{R}$ and $B(x, b)$ is the open ball $(x - b, x + b)$, then we say that x is a *point of density* of E (Stein [38, p. 12]) if

$$\lim_{b \to 0}(\lambda(E \cap B(x, b))/\lambda(B(x, b))) = 1.$$

Let $S(E)$ be the set of points of density of E.

PROPOSITION 2. (Stein [38]). *Almost every point $x \in E$ is a point of density of E.*

A self-adjoint operator T on a Hilbert space H is said to be spectrally simple (Reed–Simon [33, pp. 231–234]) if it is unitarily equivalent to multiplication by λ on $L^2(\mathbb{R}, d\nu)$ for some (regular) Borel measure $d\nu$. If in addition T is absolutely continuous then there exists a Borel set $E_T(\lambda - ae)$ with characteristic function $\chi_T(\lambda - ae)$ such that T is unitarily equivalent to multiplication by λ on $L^2(\mathbb{R}, \chi_T\, d\lambda)$. It is easy to see that on the space of simple, self-adjoint absolutely continuous operators T, the map $T \to S(E_T)$ is well-defined and 1–1. Also it follows from the proposition that the spectrum $\sigma(T) = \overline{S(E_T)}$. We call $S(E_T)$ the *spectral support* of T. The map $T \to \sigma(T)$, however, is not 1–1, even when restricted to the above space of operators, e.g., let $\{r_n\}_{n=1}^{\infty}$ be an enumeration of the rational in $[0, 1]$, let $E = [0, 1]$, and let $E' = \bigcup_{n=1}^{\infty} \{B(r_n, 2^{-n-2}) \cap [0, 1]\}$. Where χ (resp. χ') is the characteristic function of E (respectively E'), let T (resp. T') be multiplication by λ on $L^2(\mathbb{R}, \chi d\lambda)$ (resp. $L^2(\mathbb{R}, \chi' d\lambda)$). T and T' are self-adjoint, simple and absolutely continuous. As $\lambda(E') \leqslant \frac{1}{2} < 1$, we have $T \neq T'$. However $\mathrm{sp}(T) = \mathrm{sp}(T') = [0, 1]$!

We now prove a lemma of Kuroda which is fundamental in proving Theorem 5. Kuroda's argument in [22] is incomplete in that he does not distinguish between $\sigma(T)$ and $S(E_T)$.

We say that a Borel set E in $\mathbb{R}$ is closed (a.e.) if $\lambda(\bar{E} \backslash E) = 0$.

PROPOSITION 3. (Kuroda [22]). *Suppose A and B are self-adjoint operators in a Hilbert space $\mathscr{H}$. If both $\Omega^{\pm}(B, A)$ exist, and the absolutely continuous part of B is spectrally simple, then $\Omega^{\pm}(B, A)$ are* WAC. *If $\sigma_{\mathrm{ac}}(B) \subset \sigma_{\mathrm{ac}}(A)$, and if the spectral support of A_{ac} is closed* (a.e.), *then $\Omega^{\pm}(B, A)$ are complete.*

Proof. Let E_B, with characteristic function χ_B, be the Borel set for which B_{ac} is unitarily equivalent to multiplication by λ on $L^2(\mathbb{R}, \chi_B\, d\lambda)$. We have $\mathrm{Ran}\, \Omega^{\pm}(B, A) \subset \mathscr{H}_{\mathrm{ac}}(B)$ and both $\mathrm{Ran}\, \Omega^{\pm}(B, A)$ reduce B. As the commutant of B_{ac} on $\mathscr{H}_{\mathrm{ac}}$ is the set of Borel functions of λ, it follows that the orthogonal projections $P^{\pm}$ onto $\mathrm{Ran}\, \Omega^{\pm}(B, A)$ respectively, are represented on $L^2(\mathbb{R}, \chi_B\, d\lambda)$ by multiplication by $\chi^{\pm}$ respectively, where $\chi^{\pm}$ are the characteristic function of two Borel sets $E_{p^{\pm}}$ respectively. We have $E_{p^{\pm}} \subset E_B$, i.e., $\chi^{\pm} = \chi^{\pm}\chi_B$ resp. Thus A_{ac} is unitarily equivalent to multiplication by λ on both $L^2(\mathbb{R}, \chi^{+}\, d\lambda)$ and $L^2(\mathbb{R}, \chi^{-} d\lambda)$. The essential uniqueness of the spectral representation [33], implies that $\chi^{+} = \chi^{-}$, i.e., $\mathrm{Ran}\, \Omega^{+}(B, A) = \mathrm{Ran}\, \Omega^{-}(B, A)$, so we have WAC. Let $E' = E_{p+} = E_{p-}$ and let $\chi' = \chi^{+} = \chi^{-}$. If we have $\sigma_{\mathrm{ac}}(B) \subset \sigma_{\mathrm{ac}}(A)$ and $E'()S = \overline{S(E')}$ (a.e.) then

$$S(E') \subset S(E_B) \subset \sigma_{\mathrm{ac}}(B) \subset \sigma_{\mathrm{ac}}(A) = \overline{S(E')} = S(E') \quad \text{(a.e.)}.$$

Thus $S(E') = S(E_B)$ a.e., so $E' = E_B$ (a.e.) by the previous proposition. ∎

In general the condition $\sigma_{ac}(B) \subset \sigma_{ac}(A)$ is not sufficient for completeness: for let E', χ' be as in the example preceding Proposition 3. In $\mathscr{H} = L^2([0, 1], d\lambda)$, let B be multiplication by λ and A be multiplication by $\lambda\chi'$. Then $\Omega^{\pm}(B, A)$ exist and equal χ' and $\sigma_{ac}(A) = \sigma_{ac}(B) = [0, 1]$. But $\operatorname{Ran} \Omega^{\pm}(B, A) = \chi'\mathscr{H} \neq L^2[0, 1] = \mathscr{H}_{ac}(B)$. Of course the spectral support $S(E')$ of A_{ac} is not closed (a.e.). We have, however:

Theorem 6. *Let V, H, H_1, H_{ln} be as in Theorem 5. Suppose also that $(H_1)_{ac} = 0$, Then $(H_{ln})_{ac}$ is spectrally simple.*

Proof. Let $H = H_1 + H_2$ be the decoupling across the ball Ba. It follows from the proofs of Theorems 3 and 4 that the absolutely continuous part of H is unitarily equivalent to $(H)_{ac} = (H_2)_{ac} + (H_1)_{ac} = (H_2)_{ac}$. Thus it suffices to prove that for each l, the component $H_{2,ln}$ of H_2 in the space of angular momentum l, is simple. But in limit point/limit circle terminology [(4, Chap. X]), only the point at infinity is singular for $H_{ln}^{(a,\infty)}$. The limit point/limit circle method then explicitly exhibits each self-adjoint extension $H_{2,ln}$ of $H_{l,n}^{(a,\infty)}$ as a simple operator. ∎

Theorem 5 now follows from Proposition 3, Theorem 6, and the fact that $s(H_{ln,0}) = (0, \infty) = [0, \infty)$ a.e.

In a later paper [23], Kuroda proves existence and completeness in $\mathbb{R}^3$ for central potentials satisfying $\int_0^a r \mid V(r)\mid dr + \int_a^\infty \mid V(r)\mid dr < \infty$ for some $a > 0$. His method is easily combined with Theorem 3 to prove:

Corollary. *Let V, H, H_1, H_{ln} be as in Theorem 5. Suppose there exists $a > 0$ such that $\int_a^\infty \mid V(r)\mid dr < \infty$. Suppose also that $(H_1)_{ac} = 0$. Then $\sigma_{ac}(H_{ln}) = \sigma_{ac}(H_{ln,0}) = [0, \infty)$ and $\Omega^{\pm}(H, H_0)$ exist. Hence they are complete.*

Remark. Results for V with $\int_a^\infty \mid V(r)\mid dr < \infty$ are also in Lundquist [28], Green and Lanford [11], Pearson and Whould [32], and Amrein and Georgescu [2].

4. Positive Potentials

In this section, we illustrate a number of the ideas we will exploit in the proof of Theorem 1 by proving:

THEOREM 7. *Let V be a positive function in $L^1(\mathbb{R}^n\backslash G)$. Let $H = -\Delta + V$ and $\tilde{H}$ be H with an added Dirichlet boundary condition on the sphere $\{x \mid |x| = R\}$. Then, if $\alpha \geqslant 2$ and $\alpha > n/2$, $(H+1)^{-\alpha} - (\tilde{H}+1)^{-\alpha}$ is a trace class operator.*

Remarks. 1. By a simple modification in the statement of Theorem 2, this result implies Theorem 1 in case V is positive.

2. The first difference of the above form that one might try to prove trace class is when $\alpha = 1$. However, when $V = 0$, $(H_0+1)^{-1} - (\tilde{H}_0+1)^{-1}$ is a positive operator with positive integral kernel $\delta G_0(x,y)$ which one can show has an $(|x| - R)^{2-n}$ singularity as $|x| \to R$ if $n \geqslant 3$ (and only a $\log(|x| - R))$ singularity if $n = 2$) so the $\alpha = 1$ result is only true if $n \leqslant 2$. For $\alpha < n/2$ and $V = 0$, the singularity should only be $(|x| - R)^{2\alpha-n}$ so the condition $\alpha > n/2$ can probably be replaced with $\alpha > (n-1)/2$ but its proof seems to be a little simpler when $\alpha > n/2$. The requirement $\alpha \geqslant 2$ is probably not necessary but is convenient.

3. One difficulty that confronts us is that for $\alpha > 1$, $(H_0+1)^{-\alpha} - (\tilde{H}_0+1)^{-\alpha}$ still has an integral kernel $\delta K(x,y)$ which is positive but it is no longer a positive operator. Thus it is not sufficient to prove $\int \delta K(x,x)\,dx < \infty$ to conclude that the difference is trace class. For this reason, we resort to proving certain operators are Hilbert–Schmidt and writing $(H_0+1)^{-\alpha} - (\tilde{H}_0+1)^{-\alpha}$ as a sum of products of Hilbert–Schmidt operators:

LEMMA 1. *If* $\alpha > n/4$ and $\alpha \geqslant 1$, *then for any real* m, $E > 0$; $(x^2+1)^{m/2}[(H_0+E)^{-\alpha} - (\tilde{H}_0+E)^{-\alpha}]$ *is Hilbert–Schmidt.*

Proof. Let $\delta K_{\alpha,E}$ be the integral kernel of $(H_0+E)^{-\alpha} - (\tilde{H}_0+E)^{-\alpha}$. Then for $\alpha > 0$:

$$(\delta K_{\alpha,E})(x,y) = C_\alpha \int_0^\infty dt\, t^{\alpha-1} e^{-tE}[e^{-tH_0} - e^{-t\tilde{H}_0}](x,y)$$

for a constant C_α. Since the integral kernel for $e^{-tH_0} - e^{-t\tilde{H}_0}$ is positive (see the discussion of path integrals below) we see that $\delta K_{\alpha,E} \geqslant 0$ and if $\alpha > \beta$, $E > E'$, $\delta K_{\alpha,E} \leqslant (\delta K_{\beta,E'})$ (const.) (since $t^{\alpha-\beta}e^{-t(E-E')}$ is bounded). Thus we may suppose that $\alpha < n/2$. The required estimate $\int (x^2+1)^m \,|\delta K_{\alpha,E}(x,y)|^2\,dx\,dy$ clearly follows from the hypothesis $\alpha > n/2$ and the pair of estimates $(C, D > 0)$:

$$|\delta K_{\alpha,E}(x,y)| \leqslant C\,|x-y|^{-n+2\alpha} \qquad \text{all} \quad x, y$$

$$|\delta K_{\alpha,E}(x,y)| \leqslant C\exp[-D(|x| + |y|)] \qquad \text{if} \quad |x| \quad \text{or} \quad |y| \geqslant R+1.$$

Since $e^{-t\tilde{H}_0}$ has a positive integral kernel

$$0 \leqslant \delta K_{\alpha,E}(x, y) \leqslant C_\alpha \int_0^\infty t^{\alpha-1} e^{-tE} (e^{-tH_0})(x, y)\, dt$$
$$\leqslant C_\alpha \int_0^\infty t^{\alpha-1} e^{-tH_0}(x, y)\, dt = H_0^{-\alpha}(x, y)$$
$$= \text{const.}\, | x - y |^{-n+2\alpha}$$

since $\alpha > n/2$. This proves the first required estimate.

Since $\alpha \geqslant 1$, $\delta K_{\alpha,E}(x, y) \leqslant (\delta K_{1,E/2}(x, y))$ (const), so we need only prove the second estimate when $\alpha = 1$. By a simple application of the maximum principle for harmonic functions (see, e.g., [12]) for any $| y | > R + 1$ and all x:

$$| \delta K_{1,E}(x, y)| \leqslant \max_{|x|=R} G_0(x, y) \leqslant C_1 \exp(-\beta\, | y |)$$

where $G_0(x, y)$ is the kernel of $(H_0 + R)^{-1}$ which is convolution with a function falling as $\exp(-(E^{1/2})\, | x |)$ as $| x | \to \infty$. Thus for $| x | \leqslant R + 1$ we certainly have

$$| \delta K_1(x, y)| \leqslant C \exp(-\tfrac{1}{2}\beta\, | y |)$$

and for $| x | \geqslant R + 1$, by symmetry of δK:

$$| \delta K_1(x, y)| \leqslant [C_1 \exp(-\beta\, | x |)]^{1/2}\, [C_1 \exp(-\beta\, | y |)]^{1/2},$$

proving the second estimate. ∎

LEMMA 2. *If* $\alpha > n/4$, $(H_0 + 1)^{-\alpha}(x^2 + 1)^{-\alpha}$ *and* $(\tilde{H}_0 + 1)^{-\alpha}(x^2 + 1)^{-\alpha}$ *are Hilbert–Schmidt operators.*

Proof. Since $\alpha > n/4$, $(p^2 + 1)^{-\alpha} \in L^2(\mathbb{R}^n)$, so its Fourier transform is in L^2. It follows that $(H_0 + 1)^{-\alpha}(x^2 + 1)^{-\alpha}$ has an integral kernel in $L^2(\mathbb{R}^n \times \mathbb{R}^n)$. Since the integral kernels, K_α and $\tilde{K}_\alpha$, of $(H_0 + 1)^{-\alpha}$ and $(\tilde{H}_0 + 1)^{-\alpha}$ obey $0 \leqslant \tilde{K}_\alpha(x, y) \leqslant K_\alpha(x, y)$ (as above), $(\tilde{H}_0 + 1)^{-\alpha}$ $(x^2 + 1)^{-\alpha}$ also has a square integrable kernel. ∎

LEMMA 3. *If* $\alpha > n/2$ *and* $\alpha \geqslant 2$, *then* $(H_0 + 1)^{-\alpha} - (\tilde{H}_0 + 1)^{-\alpha}$ *is trace class.*

Proof. Write $(H_0 + 1)^{-\alpha} - (\tilde{H}_0 + 1)^{-\alpha} = AB + (CB)^*$ where $A = (H_0 + 1)^{-\alpha/2}(x^2 + 1)^{-\alpha/2}$, $C = (\tilde{H}_0 + 1)^{-\alpha/2}(x^2 + 1)^{-\alpha/2}$ and $B = (x^2 + 1)^{\alpha/2}[(H_0 + 1)^{-\alpha/2} - (\tilde{H}_0 + 1)^{-\alpha/2}]$ and appeal to Lemmas 1 and 2. ∎

Our proof of Theorem 7 is based on the Feynman–Kac formula of Kac [15]; see also Kac [16], Nelson [30], and Reed–Simon [34]. The n-dimensional conditional Weiner measure $d\mu_{x,y,t}$ is a positive measure on those continuous functions, ω, from $[0, t]$ to $\mathbb{R}^n$ with $\omega(0) = x$ and $\omega(t) = y$ of total mass $(4\pi t)^{-n/2} \exp(- | x - y |^2/4t)$; see Ginibre [8], Ito–MacKean [13], or Nelson [30] for a precise description. The Feynman–Kac formula asserts that for H and $\tilde{H}$ as we have defined them (by means of form sums on $C_0^\infty(\mathbb{R}^n \backslash G)$ and $C_0^\infty(\mathbb{R}^n \backslash (G \cup \{x \mid | x | = R\}))$

$$(e^{-tH})(x, y) = \int_{\{\omega \mid \omega(s) \notin G, \text{all } s\}} \exp\left(-\int_0^t V(\omega(s))\, ds\right) d\mu_{x,y;t},$$

$$(e^{-t\tilde{H}})(x, y) = \int_{\{\omega \mid \omega(s) \notin G, |\omega(s)| \neq R, \text{all } s\}} \exp\left(-\int_0^t V(\omega(s))\, ds\right) d\mu_{x,y;t}.$$

Before proving Theorem 7, we introduce the notation $A \mathrel{\underset{\cdot}{\leqslant}} B$ for operators A, B on $L^2(\mathbb{R}^n)$ to indicate that $B - A$ is an integral operator with a positive kernel (note the dot in $\underset{\cdot}{\leqslant}$).

Proof of Theorem 7. By the Feynman–Kac formula

$$\begin{aligned}
&(e^{-tH} - e^{-t\tilde{H}})(x, y) \\
&\quad = \int_{\{\omega \mid \omega(s) \notin G \text{ all } s, |\omega(s)| = R, \text{ some } s\}} \exp\left(-\int_0^t V(\omega(s))\, ds\right) d\mu_{x,y;t} \\
&\quad \mathrel{\underset{\cdot}{\leqslant}} \int_{\{\omega \mid |\omega(s)| = R \text{ some } s\}} d\mu_{x,y;t} = (e^{-tH_0} - e^{-t\tilde{H}_0})(x, y)
\end{aligned}$$

where we have used $V \geqslant 0$ in the inequality and the Feynman–Kac formula with $V = 0$, $G = \phi$ in the last step. Thus, since $\int e^{-tA} e^{-t} t^{\alpha-1}\, dt = C_\alpha^{-1}(A + 1)^{-\alpha}$,

$$0 \mathrel{\underset{\cdot}{\leqslant}} (H + 1)^{-\alpha} - (\tilde{H} + 1)^{-\alpha} \mathrel{\underset{\cdot}{\leqslant}} (H_0 + 1)^{-\alpha} - (\tilde{H}_0 + 1)^{-\alpha}.$$

So, by Lemma 1, if $\alpha \geqslant 1$, $\alpha > n/4$, m real,

$$(x^2 + 1)^{m/2} [(H + 1)^{-\alpha} - (\tilde{H} + 1)^{-\alpha}]$$

is Hilbert–Schmidt. By a simpler use of Feynman–Kac than above (and $V \geqslant 0$), $0 \mathrel{\underset{\cdot}{\leqslant}} (H + 1)^{-\alpha} \mathrel{\underset{\cdot}{\leqslant}} (H_0 + 1)^{-\alpha}$ and $0 \mathrel{\underset{\cdot}{\leqslant}} (\tilde{H} + 1)^{-\alpha} \mathrel{\underset{\cdot}{\leqslant}} (\tilde{H}_0 + 1)^{-\alpha}$. Thus by Lemma 2, if $\alpha > n/4$, $(x^2 + 1)^{-\alpha}(H + 1)^{-\alpha}$ and $(x^2 + 1)^{-\alpha}(\tilde{H} + 1)^{-\alpha}$ are Hilbert–Schmidt. As in the proof of Lemma 3, we conclude that $\alpha \geqslant 2$ and $\alpha > n/2$, then $(H + 1)^{-\alpha} - (\tilde{H} + 1)^{-\alpha}$ is trace class.

5. Proof of Theorem 1: General Case

The basic idea of the proof will be to use the Feynman–Kac formula to handle the positive part of V. In order to establish the analog of Lemma 1, we will use the Feynman–Kac formula and the analog of Lemma 2, which is our first goal. Thus we first prove that if $\alpha > n/4$ is an integer, then $(x^2 + 1)^{-\alpha}(H_0 + V_- + c)^{-\alpha}$ is Hilbert–Schmidt for suitable c.

We require the following general interpolation result:

Proposition 4. *Let I_p denote the family of operators with* $\operatorname{Tr}(|A|^p) < \infty$ *where* $|A| = (A^*A)^{1/2}$, *for* $p < \infty$. *Let I_∞ denote the compact operators and $\tilde{I}_\infty$ the bounded operators. Let D be a dense set in $\mathscr{H}$ and suppose that for each complex z with* $0 \leqslant \operatorname{Re} z \leqslant 1$, *we are given a quadratic form t_z on $D \times D$ so that*

(1) *for* $\phi, \psi \in D$, $t_z(\phi, \psi)$ *is continuous on* $0 \leqslant \operatorname{Re} z \leqslant 1$, *analytic on* $0 < \operatorname{Re} z < 1$;

(2) *for each* $\phi, \psi \in D$, $\ln |t_z(\phi, \psi)| \leqslant C_{\phi,\psi} \exp(k_{\psi,\phi} |\operatorname{Im} z|)$ with $k_{\psi,\phi} < \pi$.

(3) *If* $\operatorname{Re} z = 0$ (resp $= 1$), *there is an operator T_z in I_{p_0}* (resp. I_{p_1}) *with* $t_z(\phi, \psi) = (\phi, T_z\psi)$, *all* $\phi, \psi \in D$.

(4) *For suitable m,* $\sup_y(1 + |y|)^{-m} \| T_{iy} \|_{p_0} < \infty$ *and* $\sup_y(1 + |y|)^{-m} \| T_{1+iy} \|_{p_1} < \infty$.

Then, for any z, there is a bounded operator T_z so that $(\phi, T_z\psi) = t_z(\phi, \psi)$ *(all ϕ, ψ) and if* $\operatorname{Re} z = t$, *then* $T_z \in I_{p_t}$ *where* $p_t^{-1} = tp_1^{-1} + (1 - t)p_0^{-1}$. *The results remains true if I_∞ is replaced by $\tilde{I}_\infty$ everywhere.*

Interpolation results of this type go back to Kunze [20] and Calderon [3]; see also Gohberg–Krein [10] and Reed–Simon [34]. This particular result when $m = 0$ follows from the proof of Gohberg–Krein if one restricts oneself to operators K of the form $\sum_1^N \lambda_n(\phi\lambda\ , \cdot)\, \psi_n$ with $\phi_n, \psi_n \in D$. By replacing t_z with $(1 + z)^{-m}t_z$ the general result follows from the $m = 1$ result.

Lemma 4. *Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^n)$. Let $\alpha > n/4$. Then for any real m, y;* $(x^2 + 1)^m(H_0 + 1)^{-\alpha+iy}(x^2 + 1)^{-m-\alpha}$ *is Hilbert–Schmidt with Hilbert–Schmidt norm bounded independently of y.*

Proof. Suppose first that m is a positive integer and let $A_t = (x^2+1)^m e^{-tH_0}(x^2+1)^{-m-\alpha}$. Then A_t has integral kernel

$$Q_t(x, y) = (x^2+1)^m (4\pi t)^{-n/2} \exp(-|x-y|^2/4t)(y^2+1)^{-m-\alpha}$$
$$\leqslant C \sum_{j=0}^{m} t^{-n/2} \exp(-z^2/4t) \binom{m}{j} (z^2)^j (y^2+1)^{-j-\alpha}$$

where $z = x - y$. Thus Q_t is in L^2 with a norm bounded by (const) $[t^{-n/4}][1 + t^m]$. Thus since $\alpha > n/4$, $\int_0^\infty \| A_t \|_{\mathrm{HS}} e^{-t} t^{\alpha-1}\, dt < \infty$ so $C_\alpha \int A_t e^{-t} t^{\alpha-iy-1}\, dt$ is Hilbert–Schmidt. This proves the result for m a positive integer. We get the general m result by duality and interpolation with $D = \mathscr{S}(\mathbb{R}^n)$). ∎

LEMMA 5. *Let $H_0 = -\Delta$. For any real y, m; $(x^2+1)^m(H_0+1)^{iy}$ $(x^2+1)^{-m}$ is a bounded operator with a norm bounded in y by $(1 + |y|)^k$ for suitable k.*

Proof. By interpolation, we need only consider the case where m is a positive integer. In that case by passing to the representation with $x = id/dp$ we obtain the result by explicitly commuting the x's through. ∎

LEMMA 6. For any real m, and any p with $p > n$, $(x^2+1)^m$ $(H_0+1)^{-1/2}(x^2+1)^{-m-(1/2)}$ *is an I_p operator on $L^2(\mathbb{R}^n)$.*

Proof. Follows from Lemmas 4 and 5 by interpolation (with $D = \mathscr{S}(\mathbb{R}^n)$). ∎

LEMMA 7. *Let $A = (x^2+1)^m$ with m a positive integer and $B = (p^2+E)^{1/2}$. Then $[B, A]\, A^{-1}B^{-1}$ and $AB^{-1}A^{-1}[B, A]\, A^{-1}$ are bounded operators whose norms go to zero as E goes to infinity.*

Proof. Passing to the representation with $x = id/dp$, this is an immediate computation. ∎

LEMMA 8. *Let W be a multiplication operator so that $(p^2+E)^{-1/2}$ $W(p^2+E)^{-1/2}$ is a bounded operator whose norm approaches $\alpha < 1$ as $E \to \infty$. Then for any positive integer m, there is an E_0 so that $(x^2+1)^\rho(1 + (p^2+E)^{-1/2}W(p^2+E)^{-1/2})^{-1}(x^2+1)^{-\rho}$ is bounded for all ρ with $|\rho| \leqslant m$ and $E > E_0$.*

Proof. By interpolation and duality, we need only consider the case $\rho = m$. By choosing E_0 sufficiently large, we can suppose that $(1 + (p^2+E)^{-1/2}W(p^2+E)^{-1/2})^{-1}$ is given by the geometric series

$\sum_{k=0}^{\infty}(-1)^k[(p^2+E)^{-1/2}W(p^2+E)^{-1/2}]^k$. It thus suffices to prove that $D=(x^2+1)^m(p^2+E)^{-1/2}W(p^2+E)^{-1/2}(x^2+1)^{-m}$ is bounded with norm less than 1 for $E>E_0$. Let $A=(x^2+1)^m$, $B=(p^2+E)^{+1/2}$, $C=B^{-1}WB^{-1}$. Then, using the fact that A commutes with W one finds that

$$D = C + \delta C + D\epsilon$$

where $\delta = AB^{-1}A^{-1}[B, A]A^{-1}$ and $C=[B, A]A^{-1}B^{-1}$. It follows that if $\| \epsilon \| < 1$, then D is bounded and

$$\| D \| \leqslant (1 - \| \epsilon \|)^{-1} (1 + \| \delta \|) \| C \|.$$

Since $\| \epsilon \|$, $\| \delta \| \to 0$ as $E \to \infty$ (by Lemma 7), $\| D \| \to \alpha < 1$ as $E \to \infty$. ∎

LEMMA 9. *Let W be a multiplication operator where $(p^2+E)^{-1/2}W(p^2+E)^{-1/2}$ is bounded with norm strictly less than 1 for E sufficiently large. Then for any sufficiently large E, and any integer α, $(x^2+1)^{-\alpha}(H_0+W+E)^{-\alpha}$ is an operator in I_p so long as $\alpha p > \frac{1}{2}n$.*

Proof. It suffices to prove that $(x^2+1)^{-m}(H_0+W+E)^{-1}(x^2+1)^{m-1}$ is in I_p for any $p > n/2$. But this follows from Lemmas 6 and 8 by writing

$$(x^2+1)^{-m}(H_0+W+E)^{-1}(x^2+1)^{m-1} = ABC$$

with

$$A = (x^2+1)^{-m}(p^2+1)^{-1/2}(x^2+1)^{m-(1/2)}$$

and

$$C = (x^2+1)^{-m+(1/2)}(p^2+1)^{-1/2}(x^2+1)^{m-1}$$

in I_{2p} and

$$B = (x^2+1)^{-m+(1/2)}(1+(p^2+E)^{-1/2}W(p^2+E)^{-1/2})^{-1}(x^2+1)^{m-(1/2)}$$

in $\tilde{I}_\infty$ and using Hölder's inequality for the spaces I_{2p}. ∎

LEMMA 10. *If W obeys the hypotheses of Lemma 9, then for any integer $\alpha > n/4$, $(x^2+1)^{-\alpha}e^{-t(H_0+W)}$ is Hilbert–Schmidt for all $t > 0$.*

Proof. It follows from Lemma 9 by writing

$$(x^2+1)^{-\alpha}e^{-tH} = (x^2+1)^{-\alpha}(H+E)^{-\alpha}[(H+E)^{\alpha}e^{-tH}]. \quad ∎$$

Proof of Theorem 1. By Theorem 2, it suffices to prove that $(x^2+1)^{-\alpha}e^{-H/2}$, $(x^2+1)^{-\alpha}e^{-\hat{H}/2}$ and $(x^2+1)^{+\alpha}(e^{-H/2}-e^{-\hat{H}/2})$ are all Hilbert–Schmidt (and then follow the proof of Lemma 3). By the Feynman–Kac formula, we can bound the objects when $H = H_0 + V$ by the objects with $H = H_0 + V_-$, i.e., we may suppose $G = \phi$ and $V_+ = 0$. By Lemma 10 for $\alpha > n/4$, $(x^2+1)^{-\alpha}e^{-H/2}$ has a Hilbert–Schmidt kernel and thus so does $(x^2+1)^{-\alpha}e^{-\hat{H}/2}$. For some $\beta > 1$, $H = H' + \beta V_-$ also has $(x^2+1)^{-\alpha}e^{-H'/2}$ Hilbert–Schmidt. Let K' be the kernel for $e^{-H'/2}$. Let δG be the kernel for $e^{-H_0/2} - e^{-\hat{H}_0/2}$. Then, by Hölder's inequality:

$$
\begin{aligned}
0 &\leqslant (e^{-H/2} - e^{-\hat{H}/2})(x, y)\\
&= \int_{\{\omega \mid |\omega(s)|=R,\text{some } s\}} \exp\left(-\int_0^{1/2} V_-(\omega(s))\, ds\right) d\mu_{x,y;t=1/2}\\
&\leqslant [K'(x, y)]^{1/\beta}\, [\delta G(x, y)]^{1-1/\beta}.
\end{aligned}
$$

Since $(1+x^2)^{-\alpha}K' \in L^2$ and $(1+x^2)^m \delta G \in L^2$ for all m, again using Hölder's inequality, we see that $(1+x^2)^m[e^{-H/2} - e^{-\hat{H}/2}]$ is Hilbert–Schmidt for any m. ∎

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Appendix

Application to Acoustical Scattering

In this appendix, we wish to describe an application of our ideas to acoustical scattering. We wish to prove:

Theorem A.1. *Let G be a bounded set whose boundary has measure 0. Then the two Hilbert-space wave operators of Kato* [A2] (*see also Wilcox* [A5]) *for acoustical scattering exist and are complete.*

Remarks. 1. Kato [A2], using results of Birman [A1] has proven a similar theorem when G has a boundary which is a C^2 manifold.

2. Birman's results in [A1] are similar to some of ours. They are weaker in their smoothness restrictions on G and V but stronger in allowing more general boundary conditions than Dirichlet. He does not seem to use decoupling to do Schrödinger scattering theory.

3. For more details on acoustical scattering, see Lax–Phillips [A3] and Wilcox [A4].

By Kato's methods, Theorem A.1 follows from:

Lemma A.1. *Let Γ $(= \partial G)$ be a bounded closed set of measure zero. Then, for any $t > 0$:*

$$e^{+t\Delta} - e^{+t\Delta_\Gamma} \tag{A.1}$$

where $-\Delta_\Gamma$ is the Laplacian with Dirichlet conditions on Γ, is trace class.

Proof. As in the method of Section 4, (A.1) follows if we prove that

$(1 + x^2)^k(e^{+t\Delta} - e^{+t\Delta_\Gamma})$ is Hilbert–Schmidt. Let S be a sphere which surrounds Γ. Then

$$e^{t\Delta} - e^{t\Delta_\Gamma} \leqslant e^{t\Delta} - e^{t\Delta_{\Gamma \cup S}}$$

$$= (e^{t\Delta} - e^{t\Delta_S}) + (e^{t\Delta_S} - e^{t\Delta_{\Gamma \cup S}}).$$

Now $(1 + x^2)^k(e^{t\Delta} - e^{t\Delta_S})$ is Hilbert–Schmidt by our methods in Sections 4, 5. Now $e^{t\Delta_S} - e^{t\Delta_{S \cup \Gamma}}$ is zero on $L^2(\mathbb{R}^n \backslash B)$ where B is the ball with $\partial B = S$. Moreover, $(1 + x^2)^k$ is bounded on $L^2(B)$ and $e^{t\Delta_S} - e^{t\Delta_{S \cup \Gamma}} \leqslant e^{t\Delta_S}$ is Hilbert–Schmidt on $L^2(B)$. ∎

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