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General Theory of Potential Scattering with Absorption at Local Singularities

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Abstract. The mathematical theory of potential scattering is generalised to allow real singular potentials for which there is a non-zero probability of absorption of the particle by the scattering centre at large (positive or negative) times. That such potentials exist has already been shown by the present author.

The usual identification of $M_{\mathrm{a.c.}}(H)$ with the subspace of scattering states need no longer hold. Instead for each limit $t \to \pm\infty$ we have a canonical decomposition of $M_{\mathrm{a.c.}}(H)$ into two mutually orthogonal subspaces, one being the scattering subspace and the other consisting of states which are absorbed.

The general theory applies equally to short and long range potentials, but for short range potentials the scattering subspaces may be identified with the ranges of corresponding wave operators, which are known to exist even if the potential is highly singular.

I. Introduction

The customary picture of quantum mechanical scattering of a single particle by a local potential $V(\mathbf{r})$ is of a particle initially (i.e. at large negative times) moving freely far from the scattering region, subsequently to be scattered by the potential and finally (at large positive times) again moving freely and receding to a great distance from the scattering region.

Such a picture of the physical scattering process is to be related to a corresponding mathematical description in which the states are represented by elements of the Hilbert space $L^2(\mathbb{R}^3)$, and the evolution of states by the one parameter family of unitary operators, of which the generator is the total Hamiltonian H; H is some self-adjoint extension of the differential operator $-\Delta + V$. An important initial step in constructing this mathematical picture of the scattering is to define the subspaces of scattering states $M_\infty^\pm$, for which two definitions have recently been proposed. Both definitions have the merit of relating to observable properties of the evolution of states in position space.

The first is to define $M_\infty^\pm$ to consist of states for which the mean squared probability of finding the particle in any bounded region of $\mathbb{R}^3$ approaches zero as $t \to \pm\infty$ [1, 2].

Because of the existence of bound states, $M_\infty^\pm$ will generally be a proper subspace of the entire Hilbert space, and contained in M_c, the subspace of continuity for the total Hamiltonian. Physically one would expect to have $M_\infty^\pm = M_c$, and indeed this result has been proved for a very large class of potentials [2].

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An alternative and complementary approach, which will be adopted here, is to take $M_\infty^\pm$ to be a subspace of the space of absolute continuity $M_{a.c.}$ of the total Hamiltonian, consisting of states for which the probability itself of finding the particle in any bounded region of $\mathbb{R}^3$ approaches zero [2, 3].

This definition is particularly appropriate when one studies the way in which scattering states have asymptotically free evolution. The mathematical expression of this depends on the behaviour of the potential at large distances, the simplest case being that of short-range potentials. (For long-range potentials see, for example, [4, 5].) In this case, scattering states become free in the limit $t \to \pm\infty$ in the very precise sense that they approach in norm states for which the evolution is given by the unitary group generated by the free Hamiltonian $H_0 = -\Delta$ [6]. This result, called asymptotic completeness, is equivalent to the equality of $M_{a.c.}$ with the ranges of the wave operators $\Omega_\pm(H, H_0)$, and has again been proved for a wide class of singular and non-singular potentials [5, 7, 8].

However, highly singular potentials have now been found [9] such that there are states in $M_{a.c.}$ which are asymptotically free at $t = -\infty$ but which have non-zero probability of absorption into the scattering centre at time $t = +\infty$. Such potentials violate asymptotic completeness, and the results mentioned above do not apply to them. (Whether these potentials should be regarded as pathological is not yet clear.)

The purpose of the present paper is to establish a framework for the mathematical description of potential scattering which is sufficiently general to allow absorption at local singularities. We considered it important to deal with as wide as possible a class of potentials; we therefore consider potentials not necessarily spherically symmetric nor short-range, and which may be singular on some arbitrary bounded set Σ of measure zero.

An important aid to studying the asymptotic behaviour of states in position space is an analysis of local domain properties of H, and closely related to this the use of compactness methods. (Roughly we say that f is in the local domain of H if, away from the singularities of $V(\mathbf{r})$, f is equal to some element in the domain of H.) We rely heavily on the method and results of Ikebe and Kato [10] which, though applying to non-singular potentials, may be extended in part to the class of potentials considered here. The use of compactness is already apparent in [2]. In Section 2 we give a fairly systematic analysis of local domain properties, the results being summarised by Lemmas 1–5.

A first consequence (Section 3, Theorem 1) is that for any state in $M_{a.c.}$ the probability of finding the particle in any compact region *not* containing singularities of $V(\mathbf{r})$ approaches zero. (One may show that, for states in M_c, the mean-squared probability approaches zero). This leads us to define subspaces $M_\Sigma^\pm$, consisting of states which as $t \to \pm\infty$ asymptotically approach the singularities of V. Analogous subspaces may be defined by the asymptotic behaviour of states in momentum space, viz. $N_\infty^\pm$ consisting of states for which the kinetic energy (or free energy) tends to infinity and a corresponding orthogonal subspace $N_f^\pm$. (For precise definitions see equations 13–14.) The relevance of these definitions appears from Theorem 2, showing that

(i) $M_{a.c.} = M_\Sigma^\pm \oplus M_\infty^\pm$, and

(ii) Subspaces defined by asymptotic behaviour respectively in position and momentum space are in fact identical; for example $M_\Sigma^\pm = N_\infty^\pm$.

In Section 4 we turn to the description of free particle states in the case that V is short-range, and prove (Theorem 3) that in this case $M_\infty^\pm$ is identical to the range of the wave operator $\Omega_{\mp}(H, H_0)$. Asymptotic completeness then holds if and only if $M_{\Sigma}^{\pm}$ is empty, implying that all states in $M_{\text{a.c.}}$ move asymptotically to infinity in position space as $t \to \pm\infty$. This confirmation of a result which is physically very reasonable has as a by-product a proof of asymptotic completeness for semi-bounded Hamiltonians under extremely weak conditions (Corollary to Theorem 3).

We have succeeded, then, in establishing a more general framework for potential scattering, with the usual scattering theory for non-singular potentials as a special case. In addition to the scattering states, there are states which are asymptotically absorbed, for which the kinetic energy necessarily tends to infinity. (Either at $t = -\infty$, or at $t = +\infty$, or conceivably in both limits). A correct formulation must take these states into account. For example, in defining the wave operators $\Omega_{\pm}(H_0 + V_1, H_0 + V_2)$ by a strong limit it must be realised that the evolutions generated by $H_0 + V_1$ and $H_0 + V_2$ may be comparable only in regions free of singularities; the strong limits, suitably redefined, may then be proved to exist for short range potentials (Remark 2, Section 4), and to define partial isometries. However, in general $H_0 + V_1$, $H_0 + V_2$, acting in their respective absolutely continuous subspaces, need not be unitarily equivalent. In several respects the theory of scattering by absorptive potentials presents a richer structure, and we believe one that deserves the further attention of mathematicians and physicists.

II. Local Domain Properties of $-\Delta + V$

The differential operators $-i\partial_k$ ($\equiv -i\partial/\partial x_k$, $k = 1,2,3$) and $-\Delta$ ($\equiv -\sum_{k=1}^{3} \partial^2/\partial x_k^2$), defined on all C^∞ functions having compact support in $\mathbb{R}^3$, are known to be essentially self-adjoint, and we denote by P_k and H_0 respectively their self-adjoint extensions, acting in $L^2(\mathbb{R}^3)$.

We suppose that there is a compact subset of $\mathbb{R}^3$, denoted by Σ, having zero Lebesgue measure and such that the potential V is locally L^2 in the complement of Σ. (This means that every point of $\mathbb{R}^3 \backslash \Sigma$ has an open neighbourhood N with $V \in L^2(N)$). We denote by $\hat{H}$ the operator $-\Delta + V$ with domain $D(\hat{H})$ consisting of all C^∞ functions ϕ on $\mathbb{R}^3$ such that supp. ϕ is compact and is contained in the complement of Σ. It is easily seen that $D(\hat{H})$ is dense in $L^2(\mathbb{R}^3)$ and that $\hat{H}$ is symmetric. Since every self-adjoint extension of $\hat{H}$ is a restriction of $\hat{H}^*$ (the adjoint of $\hat{H}$), it is important to study the domain of $\hat{H}^*$.

Let us denote by $D^{(\mathrm{loc})}(T)$ the *local domain* of a self-adjoint operator T, defining this by

$$f \in D^{(\mathrm{loc})}(T) \Leftrightarrow \rho f \in D(T) \qquad \forall \rho \in D(\hat{H}).$$

(With some abuse of notation, we shall employ the same symbol for the *function* ρ as for the *operator* of multiplication by ρ).

Now let f be any element belonging to $D^{(\mathrm{loc})}(H_0)$. Then any point in the complement of Σ has an open neighbourhood N for which we can find $\rho \in D(\hat{H})$ such that $\rho|_N \equiv 1$. Δf may now be defined as an element of $L^2(N)$ by

$$(\Delta f)(\mathbf{r}) = (-H_0 \rho f)(\mathbf{r}) \qquad (\mathbf{r} \in N).$$

The right-hand side is independent of the particular choice of ρ, since if $\rho = \rho_1, \rho_2$, say, then

$$\langle H_0(\rho_1 - \rho_2)f, \phi\rangle = \langle(\rho_1 - \rho_2)f, \hat{H}_0\phi\rangle = 0$$

for any $\phi \in D(\hat{H}_0)$ having supp. $\phi \subset N$; such ϕ are dense in $L^2(N)$, so that $H_0(\rho_1 - \rho_2)f = 0$ as an element of $L^2(N)$. Now the assumption that Σ is of measure zero, and the observation that the open sets N cover $\mathbb{R}^3 \backslash \Sigma$, enable us to construct a function (or more exactly an equivalence class of functions), defined a.e. on $\mathbb{R}^3$, and which we denote by $(\Delta f)(\cdot)$, which agrees with the above definition on each local neighbourhood N. If $f \in D(H_0)$ then $f \in D^{(\mathrm{loc})}(H_0)$ and $\Delta f \in L^2(\mathbb{R}^3)$, whereas the converse implication is in general false. We may similarly define $-i\partial_k f$ for $f \in D^{(\mathrm{loc})}(P_k)$.

Jörgens [11] has pointed out that the arguments of Ikebe and Kato in [10] may be extended and used to obtain local domain properties of $\hat{H}^*$ even for potentials having local singularities. Thus for any $f \in D(\hat{H}^*)$ an integral representation may be derived for $f(\mathbf{r})$ in an open neighbourhood N of each point in the complement of Σ. This integral representation (c.f. [10], equation (A2)) may be regarded as a local analogue of the relation

$$f(\mathbf{r}) = \frac{1}{4\pi} \int \frac{(\Delta f)(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}\, dV'$$

giving the solution of Laplace's equation in potential theory. We find, from the integral representation, that f is bounded locally in the complement of Σ. Again, by differentiation we obtain an integral representation for $(\partial f/\partial x_k)(\mathbf{r})$, from which it follows that $\partial f/\partial x_k \in L^2(N)$ for each N. Given any $\rho \in D(\hat{H})$, a compactness argument shows that supp ρ may be covered by a *finite* set of neighbourhoods N. Hence we readily obtain $f \in D(P_k)\ \forall \rho \in D(\hat{H}),\ f \in D(\hat{H}^*)$, which in the notation introduced above gives

$$D(\hat{H}^*) \subset D^{(\mathrm{loc})}(P_k) \qquad (k = 1, 2, 3) \tag{1}$$

In fact, noting $D^{(\mathrm{loc})}(H_0) \subset D^{(\mathrm{loc})}(P_k)$, a stronger result than (1) holds, namely

Lemma 1

$$D(\hat{H}^*) \subset D^{(\mathrm{loc})}(H_0) \tag{1'}$$

Proof. Suppose $f \in D(\hat{H}^*)$ and $\rho \in D(\hat{H})$. We first prove $\rho f \in D(\hat{H}^*)$. For $\psi \in D(\hat{H})$ we have

$$\begin{aligned}\langle \hat{H}\psi, \rho f\rangle &= \langle(-\Delta + V)\psi, \rho f\rangle \\ &= \langle(-\Delta + V)\bar{\rho}\psi, f\rangle + \langle\psi\Delta\bar{\rho}, f\rangle + 2\sum_{k=1}^{3}\left\langle\frac{\partial\psi}{\partial x_k}\cdot\frac{\partial\bar{\rho}}{\partial x_k}, f\right\rangle\end{aligned} \tag{2}$$

The first term on the r.h.s. is

$$\langle \hat{H}\bar{\rho}\psi, f\rangle = \langle\psi, \rho\hat{H}^* f\rangle.$$

The second term may be written

$$\langle\psi, (\Delta\rho)f\rangle,$$

and the third term is

$$2\sum_{k=1}^{3}\langle iP_k\psi, (\partial\rho/\partial x_k)f\rangle = 2\sum_{k=1}^{3}\langle i\psi, P_k(\partial\rho/\partial x_k)f\rangle,$$

where we have used (1) and noted that $\partial\rho/\partial x_k \in D(\hat{H})$.

From the Cauchy-Schwarz inequality applied to each term of the right-hand side of (2) it follows that

$$|\langle \hat{H}\psi, \rho f\rangle| \leqslant \text{const}\|\psi\| \qquad \forall\psi \in D(\hat{H}), \tag{3}$$

where the constant is independent of ψ, so that we indeed have $\rho f \in D(\hat{H}^*)$.

Now let ϕ be an arbitrary C^∞ function having compact support in $\mathbb{R}^3$. The open sets $\mathbb{R}^3\backslash\text{supp}\,\rho$ and $\mathbb{R}^3\backslash\Sigma$ together cover $\mathbb{R}^3$, so that by a standard result on partitions of unity (see for example [12]) we can find real non-negative C^∞ functions ρ_k $(k = 1, 2)$ satisfying $\rho_1 + \rho_2 = 1$, with

$$\text{supp}\,\rho_1 \subset \mathbb{R}^3\backslash\text{supp}\,\rho;\ \text{supp}\,\rho_2 \subset \mathbb{R}^3\backslash\Sigma. \tag{4}$$

Writing $\phi = \phi_1 + \phi_2$, where $\phi_k = \rho_k\phi$, and defining

$$\left.\begin{aligned}\tilde{V}(\mathbf{r}) &= V(\mathbf{r})\\ &= 0\end{aligned}\right\}\begin{aligned}&\mathbf{r}\in\text{supp}\,\rho\\ &\text{otherwise,}\end{aligned} \tag{5}$$

we have

$$\begin{aligned}\langle(-\Delta + \tilde{V})\phi, \rho f\rangle &= \langle(-\Delta + V)\phi_2, \rho f\rangle\\ &= \langle \hat{H}\phi_2, \rho f\rangle = \langle\phi_2, \hat{H}^*\rho f\rangle,\end{aligned}$$

where we have used

i) $\phi_1 = 0$ and $V = \tilde{V}$ on supp ρ,

ii) $\phi_2 \in D(\hat{H})$,

iii) $\rho f \in D(\hat{H}^*)$.

Hence

$$|\langle(-\Delta + \tilde{V})\phi, \rho f\rangle| \leqslant \text{const}\|\phi_2\| \leqslant \text{const}\,\|\phi\|,$$

so that ρf belongs to the domain of the adjoint of the operator $-\Delta + \tilde{V}$ defined on C^∞ functions having compact support in $\mathbb{R}^3$. But, by a compactness argument, $\tilde{V} \in L^2(\mathbb{R}^3)$, and it is known [13] in that case that $-\Delta + \tilde{V}$ with this domain is essentially self-adjoint, the self-adjoint extension being $H_0 + \tilde{V}$, defined as an operator sum on $D(H_0)$. It follows that $\rho f \in D(H_0)$ $(\forall\rho \in D(\hat{H}))$, so that (1′) holds and we have proved the lemma.

Following the discussion of the local definition of Δ at the beginning of this section, we also have

Corollary. If $f \in D(\hat{H}^*)$, then

$$(\hat{H}^*f)(\mathbf{r}) = (-\Delta f)(\mathbf{r}) + V(\mathbf{r})f(\mathbf{r}) \qquad \text{a.e.,} \tag{6}$$

where both terms on the right-hand side are locally L^2 in $\mathbb{R}^3\backslash\Sigma$.

Lemma 2. Let ρ be any C^∞ function with supp $\rho \subset \mathbb{R}^3\backslash\Sigma$, such that $\rho(\mathbf{r}) = \text{const}$ for sufficiently large $|\mathbf{r}|$. Then

$$f \in D(\hat{H}^*) \Rightarrow \rho f \in D(\hat{H}^*).$$

Further, if there exists $R > 0$ such that $V \in L^2 + L^\infty$ in the region

$$|\mathbf{r}| \geqslant R, \quad \text{then} \quad f \in D(\hat{H}^*) \Rightarrow \rho f \in D(H_0),\ D(\hat{H}^{**}).$$

Proof. For the first part of the Lemma, and to prove $\rho f \in D(H_0)$ under the additional hypothesis, follow the proof of Lemma 1, replacing the hypothesis $\rho \in D(\hat{H})$ by the weaker assumptions on ρ. Observe that

(i) $\partial\rho/\partial x_k \in D(\hat{H})$,

(ii) If $\tilde{V}$ is defined by (5), the condition on V implies $\tilde{V} \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, so that again $-\Delta + \tilde{V}$, defined on C^∞ functions having compact support in $\mathbb{R}^3$, is essentially self-adjoint.

To prove $\rho f \in D(\hat{H}^{**})$, consider a general member g of $D(\hat{H}^*)$. Then

$$\langle \hat{H}^* g, \rho f \rangle = \langle \hat{H}^* \rho_2 g, \rho f \rangle,$$

where we have written $g = \rho_1 g + \rho_2 g$, and the C^∞ functions ρ_k satisfy (4). If ρ has compact support, then ρ_2 may be chosen to have compact support, whereas if $\rho(\mathbf{r}) =$ const $\neq 0$ for large $|\mathbf{r}|$ then ρ_1 has compact support, so that $\rho_2(\mathbf{r}) = 1 - \rho_1(\mathbf{r}) = 1$ for large $|\mathbf{r}|$. Hence in either case, by the first part of Lemma 2, $\rho_k g \in D(\hat{H}^*)$ $(k = 1, 2)$. Also, from the Corollary to Lemma 1 we have

$$\langle \hat{H}^* \rho_1 g, \rho f \rangle = \langle (-\Delta\rho_1 g)(\cdot) + (V\rho_1 g)(\cdot), \rho f \rangle = 0,$$

since $\rho_1 = 0$ wherever $\rho \neq 0$.

We also have $\rho_2 g \in D(H_0) \cap D(V)$, so that

$$\begin{aligned}\langle \hat{H}^* g, \rho f \rangle &= \langle (H_0 + V)\rho_2 g, \rho f \rangle = \langle \rho_2 g, (H_0 + V)\rho f \rangle \\ &= \langle g, (H_0 + V)\rho f \rangle, \qquad \text{since } \rho_2 = 1 \text{ wherever } \rho \neq 0.\end{aligned}$$

Since g is an arbitrary member of $D(\hat{H}^*)$, it follows that $\rho f \in D(\hat{H}^{**})$, and Lemma 2 is proved. It is also useful to note at this point that

$$\hat{H}^* \supset H_0 + V \tag{7}$$

where the r.h.s. is defined on $D(H_0) \cap D(V)$ by the operator sum. To verify (7), we need only observe that, if $\phi \in D(\hat{H})$ and

$$h \in D(H_0) \cap D(V), \quad \text{then} \quad \langle \hat{H}\phi, h \rangle = \langle (H_0 + V)\phi, h \rangle = \langle \phi, (H_0 + V)h \rangle.$$

Lemma 2 applies to a wide class of short- and long-range singular potentials. For the second part of the lemma, the behaviour of V for large $|\mathbf{r}|$ must be such that $-\Delta + \tilde{V}$ is essentially self-adjoint, and for this the assumptions on V could be modified or weakened somewhat. If ρ has compact support, all the conclusions of Lemma 2 are obtained without making use of any assumptions on V beyond the property that V is locally L^2 in $\mathbb{R}^3 \backslash \Sigma$. Restating the lemma in this case gives

Lemma 3

$$D(\hat{H}^*) \subset D^{(\mathrm{loc})}(\hat{H}^{**}) \subset D^{(\mathrm{loc})}(\hat{H}^*). \tag{8}$$

Each self-adjoint extension of $\hat{H}$ is a restriction of $\hat{H}^*$, and may be defined by specifying a core. The following result shows that, for a wide class of potentials, there is a core consisting precisely of those members of the domain of the extension which, as elements of $L^2(\mathbb{R}^3)$, have compact support.

Lemma 4. Suppose $V \in L^2 + L^\infty$ in the region $|\mathbf{r}| \geqslant R$, for some $R > 0$, and let H be a self-adjoint extension of $\hat{H}$. Define a set Λ of C^∞ functions on $\mathbb{R}^3$ by $\rho \in \Lambda$

iff $\text{supp}(1 - \rho)$ is compact and $\text{supp}\,\rho \subset \mathbb{R}^3\backslash\Sigma$. Then $\{(1 - \rho)f;\, \rho \in \Lambda, f \in D(H)\}$ is a core for H.

Proof. From Lemma 2, we have $\rho f \in D(\hat{H}^{**}) \subset D(H)$, so that certainly $(1 - \rho)f \in D(H)$. Now let g satisfy

$$\langle (H \pm i)(1 - \rho)f, g\rangle = 0, \qquad \forall \rho \in \Lambda, f \in D(H). \tag{9}$$

Then $D(\hat{H}) \subset D(H)$, so that if $\phi \in D(\hat{H})$ we have

$$\langle (\hat{H} \pm i)(1 - \rho)\phi, g\rangle = 0, \qquad \text{for all } \rho \in \Lambda. \tag{9'}$$

Since ρ may be chosen to vanish on $\text{supp}\,\phi$, (9′) implies

$$\langle (\hat{H} \pm i)\phi, g\rangle = 0, \qquad \forall \phi \in D(\hat{H}). \tag{9''}$$

But, from Lemma 2 again, $\rho f \in D(\hat{H}^{**})$, and $\hat{H}^{**}$ is just the closure of $\hat{H}$, so that from (9″) we obtain

$$\langle (H \pm i)\rho f, g\rangle = 0, \quad \forall \rho \in \Lambda, f \in D(H).$$

Combining this result with (9), we now have

$$\langle (H \pm i)f, g\rangle = 0, \qquad \forall f \in D(H),$$

so that $g = 0$, since H is self-adjoint. Hence there is no non-trivial g satisfying (9), and the lemma follows.

It may happen that the set of points Σ on which V is singular may be further subdivided, and we conclude this section by exhibiting a class of self-adjoint extensions of $\hat{H}$ in that case.

Lemma 5. Suppose $\Sigma = \Sigma_1 \cup \Sigma_2$, where Σ_1, Σ_2 are compact disjoint subsets of $\mathbb{R}^3$ having zero Lebesgue measure. Writing $V = V_1 + V_2$, suppose that $V_1(V_2)$ is essentially bounded in some open set containing $\Sigma_2(\Sigma_1)$, and that V_k $(k = 1, 2)$ is $L^2 + L^\infty$ in the region $|\mathbf{r}| \geqslant R$, for some $R > 0$, and is L^2 locally in $\mathbb{R}^3\backslash\Sigma_k$. Denote by $\hat{H}_k$ $(k = 1, 2)$ the operator $-\Delta + V_k$ defined on all C^∞ functions having compact support contained in $\mathbb{R}^3\backslash\Sigma_k$, and let H_k $(k = 1, 2)$ be self-adjoint extensions of $\hat{H}_k$. Let H denote the closure of the operator $-\Delta + V$ defined on all $\rho_k g_k$ $(k = 1, 2)$ (and on linear combinations), provided $g_k \in D(H_k)$ and the C^∞ functions ρ_k have compact support and satisfy $\text{supp}\,\rho_1 \subset \mathbb{R}^3\backslash\Sigma_2$, $\text{supp}\,\rho_2 \subset \mathbb{R}^3\backslash\Sigma_1$, $\text{supp}(1 - \rho_k) \subset \mathbb{R}^3\backslash\Sigma_k$.

Then (i) H is self-adjoint, and (ii) If $f \in D(H)$ and ρ_k $(k = 1, 2)$ satisfies the conditions above, then $\rho_k f \in D(H_k) \cap D(H)$.

Proof. The proof, of which we shall give a sketch only, uses the results of the preceeding lemmas. Thus, for example, $\rho_1 g_1 \in D(H_1)$ (from Lemma 4), and $H\rho_1 g_1 = H_1\rho_1 g_1 + V_2\rho_1 g_1$. Using a similar expression for $H\rho_2 g_2$, one may verify that H is symmetric.

Moreover, if f is in the domain of H (or of some self-adjoint extension of H), and $g_1 \in D(H_1)$, we may write

$$\langle H_1 g_1, \rho_1 f\rangle = \langle H_1\psi g_1, \rho_1 f\rangle + \langle H_1(1 - \psi)g_1, \rho_1 f\rangle \tag{10}$$

where ψ is a C^∞ function chosen such that $\text{supp}(1 - \psi) \subset \mathbb{R}^3\backslash\Sigma_1$ and such that $\rho_1 \equiv 1$ on $\text{supp}\,\psi$. The first term on the r.h.s. of (10) may be written

$$\langle H\psi g_1, f\rangle - \langle V_2\psi g_1, f\rangle = \langle g_1, \bar{\psi} H f\rangle - \langle g_1, V_2\bar{\psi} f\rangle,$$

so that certainly $|\langle H_1\psi g_1, \rho_1 f\rangle| \leqslant \text{const}\|g_1\|$. Similarly one may show that

$$|\langle H_1(1-\psi)g_1, \rho_1 f\rangle| \leqslant \text{const}\|g_1\|,$$

so that from (10) we have

$$|\langle H_1 g_1, \rho_1 f\rangle| \leqslant \text{const}\|g_1\| \; \forall g_1 \in D(H_1).$$

Hence $\rho_1 f \in D(H_1)$, since H_1 is self-adjoint, and it follows easily that $\rho_1 f \in D(H)$. Similarly we find $\rho_2 f \in D(H_2) \cap D(H)$.

The self-adjointness of H is a straightforward application of Lemma 4.

III. Behaviour of States as $t \to \pm\infty$

We consider a single quantum-mechanical particle moving in the potential V, and suppose throughout this section that V is L^2 locally in $\mathbb{R}^3\backslash\Sigma$, that $V \in L^2 + L^\infty$ in the region $|\mathbf{r}| > R$, and that Σ is contained in the region $|\mathbf{r}| < R$.

The total Hamiltonian H is some self-adjoint extension of the operator $\hat{H}$ defined in Section II, and H_0 is the free Hamiltonian. $\hat{H}$ is in general not essentially self-adjoint (and indeed may well have infinite deficiency indices), and we know of no mathematical or physical principle which in all cases selects any one self-adjoint extension in preference to the others. We have already seen, however, that certain domain properties are common to *all* self-adjoint extensions of $\hat{H}$, and we shall find that it is precisely these domain properties which determine the behaviour of states for large times. A preliminary result of this kind is the following.

Theorem 1. Given a bounded measurable subset B of $\mathbb{R}^3$, such that the closure of B is contained in $\mathbb{R}^3\backslash\Sigma$, define the corresponding projection operator $E_{\mathbf{r}\in B}$ by

$$\left.\begin{aligned} (E_{\mathbf{r}\in B}f)(\mathbf{r}) &= f(\mathbf{r}) && \mathbf{r} \in B \\ &= 0 && \text{otherwise} \end{aligned}\right\} \tag{11}$$

Then for any f in $M_{\text{a.c.}}(H)$ (the subspace of absolute continuity for H) we have

$$\underset{t\to\pm\infty}{s\text{-lim}}\; E_{\mathbf{r}\in B}e^{-iHt}f = 0. \tag{12}$$

Proof. It will be sufficient to prove (12) for a dense set of elements f in $M_{\text{a.c.}}(H)$. Since the range of $E_{|H|<c}$, as c is varied over the interval $(0, \infty)$, is also dense, we need only show that

$$\underset{t\to\pm\infty}{s\text{-lim}}\; E_{\mathbf{r}\in B}e^{-iHt}E_{|H|<c}f = 0, \tag{12'}$$

where (with a fairly obvious notation) $E_{|H|<c}$ denotes the spectral projection of H associated with the interval $(-c, c)$.

Now certainly $E_{|H|<c}f \in D(H) \subset D(\hat{H}^*)$, and it follows from Lemma 1 that $\rho E_{|H|<c}f \in D(H_0)$, where ρ is a C^∞ function of compact support, chosen to satisfy $\rho(\mathbf{r}) \equiv 1$ for $\mathbf{r} \in B$, and such that $\operatorname{supp}\rho \subset \mathbb{R}^3\backslash\Sigma$.

Thus $(H_0 + 1)\rho E_{|H|<c}$ is defined on the entire Hilbert space and must, by the closed graph theorem, be bounded. Moreover, it may be verified that $E_{\mathbf{r}\in B}(H_0 + 1)^{-1}$ is compact (in fact Hilbert-Schmidt). The product of a compact operator and a bounded operator being itself compact, we see that $E_{\mathbf{r}\in B}\rho E_{|H|<c}$ is compact.

By a version of the Riemann-Lebesgue lemma,

$$w\text{-}\lim_{t\to\pm\infty} \exp(-iHt)f = 0, \quad \text{so that} \quad s\text{-}\lim_{t\to\pm\infty} E_{\mathbf{r}\in B}\rho E_{|H|<c}e^{-iHt}f = 0.$$

Equation (12′) follows immediately on observing that $E_{\mathbf{r}\in B} = E_{\mathbf{r}\in B}\rho$, and the Theorem is proved.

Let us now define eight subspaces $M_\Sigma^\pm$, $M_\infty^\pm$, $N_\infty^\pm$, $N_f^\pm$, of $M_{\text{a.c.}}(H)$ as follows, where in each case g is assumed to belong to $M_{\text{a.c.}}(H)$.

$$g \in M_\Sigma^\pm \quad \text{iff} \quad s\text{-}\lim_{t\to\pm\infty} E_{|\mathbf{r}|>a}e^{-iHt}g = 0, \qquad \forall a > R \tag{13}$$

$$g \in M_\infty^\pm \quad \text{iff} \quad s\text{-}\lim_{t\to\pm\infty} E_{|\mathbf{r}|<a'}e^{-iHt}g = 0, \qquad \forall a' > R \tag{13'}$$

$$g \in N_\infty^\pm \quad \text{iff} \quad s\text{-}\lim_{t\to\pm\infty} E_{H_0<b}e^{-iHt}g = 0, \qquad \forall b > 0 \tag{14}$$

$g \in N_f^+$ (respectively N_f^-) iff, given any $\epsilon > 0$, there exist $\beta, T > 0$ such that $\|E_{H_0>b'}\exp(-iHt)g\| < \epsilon$, $\forall b' > \beta$, $t > T$ (respectively $t < -T$).

Remark 1. It is sufficient to verify (13) for a single value of a, $a = a_1$ say, since if $R < a_2 < a_1$ then from Theorem 1 we have

$$s\text{-}\lim_{t\to\pm\infty} E_{a_2<|\mathbf{r}|\le a_1}\exp(-iHt)g = 0.$$

Similarly, (13′) need be verified only for a single value of a'.

Remark 2. With the help of Theorem 1 we find that $M_\Sigma^\pm$ consists of states which (with probability 1) approach Σ asymptotically as $t \to \pm\infty$. $M_\infty^\pm$ consists of scattering states, that is states for which the particle moves asymptotically to a large distance from Σ as $t \to \pm\infty$.

$N_\infty^\pm$ contains states for which (with probability 1) the kinetic energy tends to infinity as $t \to \pm\infty$, whereas for states belonging to $N_f^\pm$ the kinetic energy remains essentially finite.

The following theorem gives the relationship between the subspaces defined above, and shows that they reduce H.

Theorem 2

(i) $M_\Sigma^+ \perp M_\infty^+;\ M_\Sigma^- \perp M_\infty^-$ (15)

(ii) $M_\Sigma^\pm = N_\infty^\pm;\ M_\infty^\pm = N_f^\pm$ (16)

(iii) Denoting by $P_\Sigma^\pm$ and $P_\infty^\pm$ the orthogonal projections onto $M_\Sigma^\pm$ and $M_\infty^\pm$ respectively, we have

$$\left.\begin{aligned} P_\Sigma^\pm &= s\text{-}\lim_{t\to\pm\infty} e^{iHt}E_{|\mathbf{r}|<a'}e^{-iHt}P_{\text{a.c.}}(H) \\ &\text{and} \\ P_\infty^\pm &= s\text{-}\lim_{t\to\pm\infty} e^{iHt}E_{|\mathbf{r}|>a}e^{-iHt}P_{\text{a.c.}}(H) \end{aligned}\right\} \tag{17}$$

where a, $a' > R$, and $P_{\text{a.c.}}(H)$ is the orthogonal projection onto $M_{\text{a.c.}}(H)$.

(iv) $M_{\text{a.c.}}(H) = M_\Sigma^\pm \oplus M_\infty^\pm$, (18)

and the subspaces reduce H.

Proof. (i) Suppose $g \in M_\Sigma^\pm$ and $h \in M_\infty^\pm$. Then

$$\langle g, h\rangle = \langle E_{|\mathbf{r}|>a}e^{-iHt}g, e^{-iHt}h\rangle + \langle e^{-iHt}g, E_{|\mathbf{r}|<a}e^{-iHt}h\rangle. \tag{19}$$

But, from (13) and (13′), the r.h.s. of (19) converges to zero in the limit as $t \to \pm\infty$. Hence $\langle g, h\rangle = 0$, and we have verified (15).

(ii) Suppose $g \in M_\Sigma^\pm$. Then

$$E_{H_0<b}e^{-iHt}g = E_{H_0<b}E_{|\mathbf{r}|<a}e^{-iHt}g + E_{H_0<b}E_{|\mathbf{r}|>a}e^{-iHt}g.$$

On the right-hand side, the first term tends to zero as $t \to \pm\infty$ since $E_{H_0<b}E_{|\mathbf{r}|<a}$ is compact (in fact Hilbert-Schmidt), and equation (13) implies that the second term also tends to zero. Hence $g \in N_\infty^\pm$, and we have proved $M_\Sigma^\pm \subseteq N_\infty^\pm$.

Now suppose conversely that $g \in N_\infty^\pm$. Given any $\epsilon > 0$, we can choose c sufficiently large that $\|E_{|H|>c}g\| < \epsilon/2$. Given any $a > R$, we can find a C^∞ function ρ, with $0 \leqslant \rho \leqslant 1$, such that $\rho(\mathbf{r}) \equiv 1$ for $|\mathbf{r}| \geqslant a$, and supp $\rho \subset \mathbb{R}^3\backslash\Sigma$. From Lemma 2 we have $\rho E_{|H|\leqslant c}g \in D(H_0)$, so that $H_0\rho E_{|H|\leqslant c}$ is bounded (c.f. the proof of Theorem 1). Also $\|E_{H_0>b}(H_0 + 1)^{-1}\| = (1 + b)^{-1}$, so that we may choose b sufficiently large that

$$\|E_{H_0>b}(H_0 + 1)^{-1}(H_0 + 1)\rho E_{|H|\leq c}\exp(-iHt)g\| = \\ \|E_{H_0>b}\rho E_{|H|\leq c}\exp(-iHt)g\| < \epsilon/2 \qquad \text{for all } t.$$

But $\|E_{H_0>b}\rho E_{|H|>c}\exp(-iHt)g\| < \epsilon/2$, and hence

$$\|E_{H_0>b}\rho\exp(-iHt)g\| < \epsilon \qquad \text{(for sufficiently large } b). \tag{20}$$

We also have

$$E_{H_0<b}\rho e^{-iHt}g = E_{H_0<b}(\rho - 1)e^{-iHt}g + E_{H_0<b}e^{-iHt}g.$$

On the right-hand side, the first term tends to zero as $t \to \pm\infty$ since $E_{H_0<b}(\rho - 1)$ is compact (in fact Hilbert-Schmidt), and equation (14) implies that the second term also tends to zero. Hence

$$\operatorname*{s\text{-}lim}_{t\to\pm\infty} E_{H_0<b}\rho\exp(-iHt)g = 0,$$

and since ϵ in (20) is arbitrary we have $s\text{-}\lim_{t\to\pm\infty}\rho\exp(-iHt)g = 0$. Now (13) follows immediately on noticing that $E_{|\mathbf{r}|>a}\rho = E_{|\mathbf{r}|>a}$, and we have proved $g \in M_\Sigma^\pm$.

We have, then, $N_\infty^\pm \subseteq M_\Sigma^\pm$, so that we may conclude $M_\Sigma^\pm = N_\infty^\pm$. The proof that $M_\infty^\pm = N_f^\pm$ follows by very similar arguments.

(iii) Let ρ be a C^∞ function with supp $\rho \subset \mathbb{R}^3\backslash\Sigma$, and such that $\rho(\mathbf{r}) \equiv 1$ for $|\mathbf{r}| \geqslant R$. With $a > R$, define $\tilde{V}(\cdot) \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ by

$$\left.\begin{aligned} \tilde{V}(\mathbf{r}) &= V(\mathbf{r}), \qquad && |\mathbf{r}| \geqslant a \\ &= 0, && \text{otherwise} \end{aligned}\right\} \tag{21}$$

and let $\tilde{H}$ denote the (unique) self-adjoint extension of $-\Delta + \tilde{V}$ acting on C^∞ functions of compact support [13].

Now let A_1, A_2 be any pair of self-adjoint operators such that

$$A_1E_{|A_1|<c_1}TE_{|A_2|<c_2} - E_{|A_1|<c_1}TA_2E_{|A_2|<c_2}$$

is of trace class for some bounded operator T. Then $s\text{-}\lim_{t\to\pm\infty} E_{|A_1|<c_1} e^{iA_1t} T e^{-iA_2t} E_{|A_2|<c_2}$ exists on $M_{\text{a.c.}}(H_2)$ and has range contained in $M_{\text{a.c.}}(A_1)$.

We shall apply this result, which is a slight generalisation of a theorem of Belopolskii and Birman [14] on a two Hilbert space formalism of scattering theory, to the case $A_1 = H$, $A_2 = \tilde{H}$, $T = \rho$. A proof of the result, based on methods developed in [15], will be published elsewhere. (An alternative approach to the present application is to use methods based on smoothness; see [16, 17]).

We have to show, then, that $E_{|H|<c_1}(H\rho - \rho\tilde{H})E_{|\tilde{H}|<c_2}$ is of trace class. (Using Lemma 2,

$$f \in D(\hat{H}) \Rightarrow \rho f \in D(H_0) \cap D(\tilde{V}),$$

so that $\rho f \in D(V)$ also. With (7), we have $\rho f \in D(\hat{H}^*)$, and $\rho f \in D(H)$ on a further application of Lemma 2, since $H \supset \hat{H}^{**}$. Hence we are justified in writing

$$HE_{|H|<c_1}\rho E_{|\tilde{H}|<c_2} = E_{|H|<c_1} H\rho E_{|\tilde{H}|<c_2}.)$$

Setting $H = -\Delta + V$ and $\tilde{H} = -\Delta + \tilde{V}$, we have

$$H\rho - \rho\tilde{H} = \rho(V - \tilde{V}) - \Delta\rho - 2\sum_{k=1}^{3} \partial\rho/\partial x_k \cdot \partial/\partial x_k. \tag{22}$$

Now let ψ be a C^∞ function with $\operatorname{supp}\psi \subset \mathbb{R}^3\backslash\Sigma$, and such that $\psi(\mathbf{r}) = 1$ for $\mathbf{r} \in \operatorname{supp} \partial\rho/\partial x_k$ $(k = 1, 2, 3)$ and $\psi(\mathbf{r}) = 0$ for $|\mathbf{r}| > a$.

If $f \in D(\tilde{H})$ then $\psi f \in D(P_k)$ (c.f. equation (1)) so that we can write

$$-iE_{|H|<c_1} \frac{\partial\rho}{\partial x_k}\left(\frac{\partial}{\partial x_k}\right) E_{|\tilde{H}|<c_2} = E_{|H|<c_1} \psi \frac{\partial\rho}{\partial x_k} P_k \psi E_{|\tilde{H}|<c_2}.$$

From Lemma 1, $f \in D(H) \Rightarrow \bar{\psi} f \in D(H_0)$, so that $(H_0 + 1)\bar{\psi}E_{|H|<c_1}$ is bounded (c.f. proof of Theorem 1).

If $f \in D(\tilde{H})$, then $\psi f \in D(\tilde{H})$, and writing $\tilde{H} = -\Delta + \tilde{V}$ we obtain

$$\tilde{H}\psi f = \psi\tilde{H}f + (\Delta\psi)f - 2\sum_{k=1}^{3} \partial/\partial x_k(\partial\psi/\partial x_k f).$$

If $f \in D(\tilde{H}^2)$, then the first two terms on the right-hand side belong to $D(\tilde{H}) = D(H_0)$ and $\partial\psi/\partial x_k f \in D(H_0)$, so that the third term on the right-hand side belongs to $D(P_k)$. Hence certainly $f \in D(\tilde{H}^2) \Rightarrow \psi f \in D(P_k\tilde{H})$. But $\tilde{H}\psi f = H_0\psi f$ (since $\tilde{V} \equiv 0$ on $\operatorname{supp}\psi$), so that $\psi f \in D(P_k H_0)$, and it follows that $P_k(H_0 + 1)\psi E_{|\tilde{H}|<c_2}$ is bounded.

We now have

$$E_{|H|<c_1}\psi \frac{\partial\rho}{\partial x_k} P_k \psi E_{|\tilde{H}|<c_2}$$
$$= [(H_0 + 1)\bar{\psi}E_{|H|<c_1}]^*(H_0 + 1)^{-1} \frac{\partial\rho}{\partial x_k}(H_0 + 1)^{-1}[P_k(H_0 + 1)\psi E_{|\tilde{H}|<c_2}].$$

But $\partial\rho/\partial x_k \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$, so that $(H_0 + 1)^{-1}\,\partial\rho/\partial x_k(H_0 + 1)^{-1}$ is of trace class (see [18]), and we have shown that the contribution of the third term of (22) to $E_{|H|<c_1}(H\rho - \rho\tilde{H})E_{|\tilde{H}|<c_2}$ is of trace class. The remaining terms of the right-hand side of equation (22) similarly give rise to trace class contributions, since both $\rho(V - \tilde{V})$

and $\Delta\rho$ belong to $L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$. (For these terms we need use only the boundedness of $(H_0 + 1)\bar{\psi}E_{|H|<c_1}$ and of $(H_0 + 1)\psi E_{|\tilde{H}|<c_2}$.)

Hence $E_{|H|<c_1}(H\rho - \rho\tilde{H})E_{|\tilde{H}|<c_2}$ is of trace class, and we have proved the existence of the limit $s\text{-}\lim_{t\to\pm\infty} E_{|H|<c_1}e^{iHt}\rho e^{-i\tilde{H}t}E_{|\tilde{H}|<c_2}$ on $M_{\text{a.c.}}(\tilde{H})$. Moreover, one may verify that

$$\|E_{|H|\geqslant c_1}\rho E_{|\tilde{H}|<c_2}\| = \|E_{|H|\geqslant c_1}(|H| + 1)^{-1}(|H| + 1)\rho E_{|\tilde{H}|<c_2}\|$$

may be made arbitrarily small by taking c_1 sufficiently large ($\|E_{|H|\geqslant c_1}(|H| + 1)^{-1}\| \leqslant (1 + c_1)^{-1}$, and $(|H| + 1)\rho E_{|\tilde{H}|<c_2}$ is bounded.) We may deduce the existence on $M_{\text{a.c.}}(\tilde{H})$ of $s\text{-}\lim_{t\to\pm\infty} \exp(iHt)\rho\exp(-i\tilde{H}t)E_{|\tilde{H}|<c_2}$ and since, as c_2 is varied over the interval $(0, \infty)$, the range of $E_{|\tilde{H}|<c_2}$ is dense in $M_{\text{a.c.}}(\tilde{H})$, the existence of $s\text{-}\lim_{t\to\pm\infty} \exp(iHt)\rho\exp(-i\tilde{H}t)$ on $M_{\text{a.c.}}(\tilde{H})$ follows. As $\tilde{V}$ is a non-singular potential and $(1 - \rho)$ is of compact support, Theorem 1 implies $s\text{-}\lim_{t\to\pm\infty}(1 - \rho)\exp(-i\tilde{H}t) = 0$ on $M_{\text{a.c.}}(\tilde{H})$.

Hence the wave operators $s\text{-}\lim_{t\to\pm\infty} \exp(iHt)\exp(-i\tilde{H}t)P_{\text{a.c.}}(\tilde{H})$ exist. Since the trace conditions which we have verified are symmetric between A_1 and A_2, an identical argument proves the existence of $s\text{-}\lim_{t\to\pm\infty} \exp(i\tilde{H}t)\rho\exp(-iHt)P_{\text{a.c.}}(H)$.

By Theorem 1, if χ is the characteristic function of the intersection of supp ρ with the region $|\mathbf{r}| \leqslant a$, then $s\text{-}\lim_{t\to\pm\infty} \chi\exp(-iHt)P_{\text{a.c.}}(H) = 0$, so that we may conclude the existence of the limits $s\text{-}\lim_{t\to\pm\infty} \exp(i\tilde{H}t)E_{|\mathbf{r}|>a}\exp(-iHt)P_{\text{a.c.}}(H)$. The ranges of these limits lie in $M_{\text{a.c.}}(\tilde{H})$, and the existence of the limits on the right-hand side of equation (17) follow from transitivity; for example

$$\underset{t\to\pm\infty}{s\text{-}\lim}\ e^{iHt}E_{|\mathbf{r}|>a}e^{-iHt}P_{\text{a.c.}}(H) = \underset{t\to\pm\infty}{s\text{-}\lim}\ (e^{iHt}e^{-i\tilde{H}t})(e^{i\tilde{H}t}E_{|\mathbf{r}|>a}e^{-iHt}P_{\text{a.c.}}(H). \tag{23}$$

(For the remaining limit, substitute $E_{|\mathbf{r}|<a'} = 1 - E_{|\mathbf{r}|>a'}$.) The limiting operators have ranges in $M_{\text{a.c.}}(H)$ and are self-adjoint. To show that they are projection operators we need only use transitivity again to verify that in each case $P^2 = P$. If P denotes the limit in equation (23) and g is in the range of P, so that $g = s\text{-}\lim_{t\to\pm\infty} \exp(iHt)E_{|\mathbf{r}|>a} \times\exp(-iHt)P_{\text{a.c.}}(H)h$, say, then $s\text{-}\lim_{t\to\pm\infty} E_{|\mathbf{r}|<a'}e^{-iHt}g = s\text{-}\lim_{t\to\pm\infty} E_{|\mathbf{r}|\in(a,a')}\times e^{-iHt}P_{\text{a.c.}}(H)h = 0$, so that equation (13′) is satisfied and $g \in M^{\pm}_{\infty}$. Conversely, if $g \in M^{\pm}_{\infty}$ we may verify $Pg = g$. Hence the limit in equation (23) gives precisely $P^{\pm}_{\infty}$, and similarly $P^{\pm}_{\Sigma}$ is the other limit in equation (17).

(iv) Taking $a = a'$ in equation (17) we have $P^{\pm}_{\Sigma} + P^{\pm}_{\infty} = P_{\text{a.c.}}(H)$, and equation (18) follows. Moreover, e^{iHs} commutes with $P^{\pm}_{\Sigma}$ and with $P^{\pm}_{\infty}$, and it follows that the two subspaces on the r.h.s. of equation (18) reduce H; this completes the proof of Theorem 2.

Theorem 2 shows that $M_{\text{a.c.}}(H)$ is the direct sum of two orthogonal subspaces, the first consisting of states which approach Σ asymptotically as $t \to \pm\infty$, and for which the kinetic energy tends to infinity, the second consisting of scattering states for which the kinetic energy remains finite. There are two decompositions of $M_{\text{a.c.}}(H)$, one corresponding to the limit $t \to +\infty$ and the other corresponding to $t \to -\infty$.

It may happen that there is a further canonical decomposition of $M^{\pm}_{\Sigma}$ or $M^{\pm}_{\infty}$. For example, if $\Sigma = \Sigma_1 \cup \Sigma_2$, where Σ_1, Σ_2 are compact disjoint subsets of $\mathbb{R}^3$ having zero Lebesgue measure, and if H belongs to the class of self-adjoint extensions defined by Lemma 5, then using conclusion (ii) of Lemma 5 and following an argument similar to the proof of Theorem 2, we find $M^{\pm}_{\Sigma} = M^{\pm}_{\Sigma_1} \oplus M^{\pm}_{\Sigma_2}$, each subspace reducing H, where $M^{\pm}_{\Sigma_k}$ consists of states which approach Σ_k asymptotically as $t \to \pm\infty$. This result need not hold for a self-adjoint extension corresponding to boundary conditions which 'mix' the singularities Σ_1 and Σ_2, for which (ii) of Lemma 5 is not valid.

IV. Singular short-range potentials

The preceding results have been obtained without having to make any assumptions which would imply the existence of the wave operators $\Omega_{\pm}(H, H_0)$. Assuming these wave operators to exist, it is not difficult to show [2] that the ranges of the wave operators are contained in corresponding subspaces of scattering states; i.e.

$$\operatorname{range}(\Omega_{\pm}(H, H_0)) \subseteq M^{\mp}_{\infty}. \tag{24}$$

If the potential V is of short range, a stronger result holds.

Theorem 3. Suppose that, for sufficiently large $|\mathbf{r}|$ and for some $\epsilon > 0$, V satisfies $|V(\mathbf{r})| \leqslant \text{const}|\mathbf{r}|^{-(1+\epsilon)}$. Then

$$\operatorname{range}(\Omega_{\pm}(H, H_0)) = M^{\mp}_{\infty}. \tag{24$'$}$$

Proof. The existence of $\Omega_{\pm}(H, H_0)$ has been proved by Kupsch and Sandhas [19]. Indeed if $a > R$ we have $s\text{-}\lim_{t\to\pm\infty} E_{|\mathbf{r}|<a}e^{-iH_0t} = 0$, so that

$$\Omega_{\pm}(H,H_0) = \underset{t\to\mp\infty}{s\text{-}\lim}\ e^{iHt}e^{-iH_0t} = \underset{t\to\mp\infty}{s\text{-}\lim}\ e^{iHt}E_{|\mathbf{r}|>a}e^{-iH_0t} \tag{25}$$

The potential $\tilde{V}$ in equation (21) is both short-range and non-singular, so that defining $\tilde{H}$ as in the proof of (iii) in Theorem 2 we may conclude the existence of

$$\underset{t\to\mp\infty}{s\text{-}\lim}\ \exp(iH_0t)\exp(-i\tilde{H}t)P_{\text{a.c.}}(\tilde{H}).\ ([5])$$

But we have already proved the existence of $s\text{-}\lim_{t\to\mp\infty} e^{i\tilde{H}t}E_{|\mathbf{r}|>a}e^{-iHt}P_{\text{a.c.}}(H)$, so that by transitivity we may deduce the existence of $s\text{-}\lim_{t\to\mp\infty}\exp(iH_0t)E_{|\mathbf{r}|>a}\times \exp(-iHt)P_{\text{a.c.}}(H)$. In fact, comparing with equation (25), we have

$$\Omega^{*}_{\pm}(H, H_0) = \underset{t\to\mp\infty}{s\text{-}\lim}\ e^{iH_0t}E_{|\mathbf{r}|>a}e^{-iHt}P_{\text{a.c.}}(H). \tag{26}$$

By a further application of transitivity, equations (25) and (26) imply

$$\underset{t\to\mp\infty}{s\text{-}\lim}\ e^{iHt}E_{|\mathbf{r}|>a}e^{-iHt}P_{\text{a.c.}}(H) = \Omega_{\pm}(H, H_0)\Omega^{*}_{\pm}(H, H_0). \tag{27}$$

The right-hand side of equation (27) is the projection onto the range of $\Omega_{\pm}(H, H_0)$, and from equation (17) the left-hand side is just $P^{\mp}_{\infty}$, the projection onto $M^{\mp}_{\infty}$. Hence we have proved equation (24′).

Remark 1. Unitarity of the scattering operator $S(H, H_0)$ $(\equiv \Omega^{*}_{-}(H, H_0)\Omega_{+}(H, H_0))$ is equivalent to equality of the ranges of $\Omega_{+}(H, H_0)$ and $\Omega_{-}(H, H_0)$. Theorem 3 shows that $S(H, H_0)$ is unitary iff the states in $M_{\text{a.c.}}(H)$ which become asymptotically free as $t \to +\infty$ are precisely those states which are asymptotically free as $t \to -\infty$. Asymptotic completeness (the equality of the ranges of $\Omega_{\pm}(H, H_0)$ with $M_{\text{a.c.}}(H)$) holds if *all* states in $M_{\text{a.c.}}(H)$ are asymptotically free both as $t \to +\infty$ and as $t \to -\infty$. The use of Theorem 3 to prove strong asymptotic completeness may be illustrated by the following.

Corollary. Suppose that, for some $g > 1$, $-\Delta + gV$, regarded as a bilinear form on $D(\hat{H}) \times D(\hat{H})$, is bounded below. (Hence $\hat{H}$ is similarly bounded below, since we can write

$$\hat{H} = -\Delta + V = (1 - g^{-1})(-\Delta) + g^{-1}(-\Delta + gV)) \tag{28}$$

Then, if H is the Friedrichs extension ([20], p. 329) of $\hat{H}$, the wave operators $\Omega_\pm(H, H_0)$ satisfy strong asymptotic completeness.

Proof. Every f belonging to $D(H)$, by the definition of the Friedrichs extension, is the strong limit of a sequence $\{f_n\}$ such that

$$\lim_{m,n\to\infty} \langle \hat{H}(f_m - f_n), (f_m - f_n)\rangle = 0.$$

Choosing $c > 0$ such that $-\Delta + gV + c \geqslant 0$, we have

$$\lim_{m,n\to\infty} \langle (\hat{H} + cg^{-1})(f_m - f_n), (f_m - f_n)\rangle = 0,$$

so that using equation (28) and writing $-\Delta f_n = H_0 f_n$, we see that

$$\lim_{m,n\to\infty} \langle H_0(f_m - f_n), (f_m - f_n)\rangle = 0.$$

It follows that f is in the domain of $(H_0 + 1)^{1/2}$, and we have $D(H) \subset D((H_0 + 1)^{1/2})$. Hence, by the closed graph theorem, $(H_0 + 1)^{1/2} E_{|H| < \text{const}}$ is bounded. But $E_{|\mathbf{r}| < a}(H_0 + 1)^{-1/2}$ is compact, so that the compactness of $E_{|\mathbf{r}| < a} E_{|H| < \text{const}}$ follows. Any $h \in M_{\text{a.c.}}(H)$ is a limit of elements of the form $E_{|H| < \text{const}} h$, and we may deduce that $s\text{-}\lim_{t\to\pm\infty} E_{|\mathbf{r}| < a} \exp(-iHt)h = 0$. Hence $M_\Sigma^\pm(H)$ is empty and $M_\infty^\pm(H) = M_{\text{a.c.}}(H)$, so that the wave operators satisfy strong asymptotic completeness. This generalises a result of Robinson ([21]) on positive potentials.

Remark 2. From the existence of $\Omega_\pm(H, H_0)$ and of the limit in equation (26) we may use transitivity to deduce the existence of

$$\omega_\pm(H_V, H_W) \equiv \underset{t\to\mp\infty}{s\text{-}\lim}\ e^{iH_V t} E_{|\mathbf{r}| > a} e^{-iH_W t} P_{\text{a.c.}}(H_W) \tag{29}$$

where H_V and H_W correspond to short range singular potentials V and W respectively. Equation (29) defines $\omega_\pm$ as a strong limit even if the wave operators $\Omega_\pm(H_V, H_W)$ fail to exist; $\omega_\pm$ is a partial isometry with initial set $M_\infty^\pm(H_W)$ and final set $M_\infty^\pm(H_V)$, and satisfies the usual intertwining and transitivity properties of wave operators. If $g \in M_\infty^\pm(H_W)$ we have

$$\underset{t\to\mp\infty}{s\text{-}\lim}\ E_{|\mathbf{r}| > a}(\exp(-iH_V t)h - \exp(-iH_W t)g) = 0,$$

where

$$h = \omega_\pm(H_V, H_W)g \in M_\infty^\pm(H_V),$$

so that $\omega_\pm$ gives the relation between two asymptotically free states (corresponding to an evolution $e^{-iH_V t}$ and $e^{-iH_W t}$ respectively) which become asymptotically equal in the region $|\mathbf{r}| > a$, i.e. away from the singularities of the potential.

Remark 3. If $\Sigma = \Sigma_1 \cup \Sigma_2$, where Σ_1, Σ_2 are compact disjoint subsets of $\mathbb{R}^3$ having zero Lebesgue measure, and if H belongs to the class of self-adjoint extensions defined by Lemma 5, where (in the notation of Lemma 5) V_1 and V_2 are short-range singular potentials, we may prove the existence of $s\text{-}\lim_{t\to\pm\infty} e^{iH_k t}\chi_k e^{-iHt}P_{\text{a.c.}}(H)$, where χ_k ($k = 1, 2$) are characteristic functions of disjoint bounded open sets containing Σ_1 and Σ_2 respectively. If $\Omega_\pm(H_k, H_0)$ are asymptotically complete then this limit is zero (since $w\text{-}\lim_{t\to\pm\infty} P_{\text{a.c.}}(H_k)e^{iH_k t}\chi_k = 0$), so that $s\text{-}\lim_{t\to\pm\infty} \chi_k e^{-iHt}P_{\text{a.c.}}(H) = 0$ ($k = 1, 2$), from which it follows that $\Omega_\pm(H, H_0)$ are complete. A similar argument proves the converse to be true, so that strong asymptotic completeness of $\Omega_\pm(H, H_0)$ is equivalent to strong asymptotic completeness of $\Omega_\pm(H_k, H_0)$ for $k = 1, 2$. This result enables us in some cases to reduce the question of completeness for a potential having a number of singularities to that for a potential having a single singularity only.

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REFERENCES

[1] D. Ruelle, Nuovo Cimento *61A*, 655 (1969).
[2] W. Amrein and V. Georgescu, Helv. Phys. Acta *46*, 635 (1973).
[3] C. Wilcox, J. Funct. Anal. *12*, 257 (1973).
[4] J. Dollard, J. Math. Phys. *5*, 729 (1964).
[5] B. Simon, *Quantum Mechanics for Hamiltonians defined as Quadratic forms* (Princeton University Press), Princeton, N.J. 1971).
[6] J. Jauch, Helv. Phys. Acta *31*, 127 (1958).
[7] D. Pearson, Helv. Phys. Acta *47*, 249 (1974).
[8] W. Amrein and V. Georgescu, Helv. Phys. Acta *47*, 517 (1974).
[9] D. Pearson, Comm. Math. Phys. *40*, 125 (1975).
[10] T. Ikebe and T. Kato, Arch. Rat. Mech. Anal. *9*, 77 (1962).
[11] K. Jörgens, Math. Scand. *15*, 5 (1964).
[12] J. Dieudonné, *Treatise on Analysis* (Academic Press, N.Y., 1970), Vol. II.
[13] T. Kato, Trans. Amer. Math. Soc. *70*, 195 (1951).
[14] A. Belopolskii and M. Birman, Math. USSR Izv. *2*, 1117 (1968).
[15] D. Pearson, J. Math. Phys. *13*, 1490 (1972).
[16] T. Kato, Math. Ann. *162*, 258 (1966).
[17] R. Lavine, Indiana Univ. Math. J. *21*, 643 (1972).
[18] S. Kuroda, Nuovo Cimento *12*, 431 (1959),
[19] J. Kupsch and W. Sandhas, Comm. Math. Phys. *2*, 147 (1966).
[20] F. Riesz and B. Sz.-Nagy, *Functional Analysis* (Ungar, N.Y. 1955).
[21] D. Robinson, Ann. Inst. Henri Poincaré *21*, 181 (1975).