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Commutators and Scattering Theory

I. Repulsive Interactions

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Abstract. We use commutators to find classes of operators which are smooth with respect to the Hamiltonian H for a system of quantum mechanical particles which repel each other. It follows that H is absolutely continuous, the wave operators are complete in many cases when they exist and limits of momentum observables as time approaches $\pm\infty$ exist even in cases where the long range of the interaction precludes existence of the wave operators.

1. Introduction

Let H_0 be the self adjoint operator in $\mathscr{K} = \mathscr{L}^2(\boldsymbol{R}^{3N})$ which represents the Hamiltonian for N free quantum mechanical particles, and H the Hamiltonian operator for the same system with repulsive interactions between pairs of particles and between each particle and a fixed center. Physically it is clear that if the potentials describing these interactions become small at large distances, for any initial state the interacting system should resemble the free system in the distant past and future, since no clustering of particles is possible. But even though the real complications of many particle scattering do not arise for purely repulsive interactions, the standard methods of scattering theory have failed to justify this physical certainty in some cases and do so only with difficulty in many others. The states φ which do appear free as $t \to \pm\infty$ in the sense that for some $\varphi_\pm$,

$$\|e^{-iHt}\varphi - e^{-iH_0 t}\varphi_\pm\| \to 0 \quad \text{as} \quad t \to \pm\infty$$

are just those in the range of both wave operators

$$\Omega_\pm = \underset{t\to\pm\infty}{s\text{-lim}}\, e^{iHt} e^{-iH_0 t}. \tag{1.1}$$

Thus what should be proved is that $\Omega_\pm$ exist and are complete in the sense that their ranges equal all of $\mathscr{K}$.

Problem 1. The wave operators can be shown to exist only if for all pair potentials $V: \boldsymbol{R}^3 \to \boldsymbol{R}$, $V(x) = 0(|x|^{-1-\varepsilon})$ as $|x| \to \infty$, $(\varepsilon > 0)$; thus the theory fails at the outset for potentials which do not decrease at infinity faster than the Coulomb potential. Alternative theories have been proposed for long range potentials by Dollard [3–7] and others [1, 2, 12] but these have only been shown to apply in special cases[1].

Problem 2. Techniques for showing completeness of the wave operators depend even more strongly on rapid decrease of the potential as $|x|\to\infty$; completeness is never easy to prove even in the case of one particle, and has been shown for many particles only for the case when the pair potentials decrease very rapidly at infinity [8].

Problem 3. The ranges of the wave operators are automatically contained in $\mathscr{K}_{ac}$, the subspace of absolute continuity for H, and some results in scattering theory state that $\mathscr{R}(\Omega_\pm)=\mathscr{K}_{ac}$. Thus a partial result would be that H is absolutely continuous, i.e. $\mathscr{K}=\mathscr{K}_{ac}$. Even this has not been shown in general, although Weidmann [16] has shown that there are no positive eigenvalues. The known results on absolute continuity are mostly for one body [2, 11, 15].

In this paper we use the theory of smooth operators and positive commutators due to Putnam [13] and Kato [9, 10] to solve some of these problems. This theory, which we describe partially in Section 2, says that if A is a bounded observable (self-adjoint operator) whose expectation value $\langle A e^{-iHt}\varphi, e^{-iHt}\varphi\rangle$ increases with time, then the commutator $i[H,A]$ is positive and its square root is "smooth" with respect to H in a sense (to be described) which is very useful in scattering theory [9]. In particular, if T is H-smooth the range of T^* is a subset of $\mathscr{K}_{ac}$, and if the potential $V=T^*S$ where T is H-smooth and S is H_0-smooth the wave operators exist and are complete. In Section 3 we find operators A such that $i[H,A]\geqq 0$ and deduce that certain classes of operators are H-smooth (thereby solving Problem 3). These results are applied in Section 4 to prove completeness of the wave operators for one particle if the potentials are $0(|x|^{-1-\varepsilon})$ as $|x|\to\infty$. (In the many body case we consider only spherically symmetric potentials and particles of equal mass for simplicity; here the potentials must be $0(|x|^{-3-\varepsilon})$ as $|x|\to\infty$.)

Since Dollard [3] has shown that the wave operators (1.1) do not exist for the Coulomb Hamiltonian, it is not clear what would constitute a solution to Problem 1, but his modified wave operators [3] provide as much information as one is likely to be able to get for this case. They tell as much about the unitary equivalence class of H as do the usual wave operators in the short range case, but their physical meaning is not as clear, and their existence has only been proved for $V(x)=0(|x|^{-3/4})$

[1] Further results have been obtained by Buslaev and Matveev, Teor. i Mat. Fiz **2**, 367—376.

as $|x| \to \infty$ [1]. We introduced in [12] an asymptotic condition to replace (1.1) for long range potentials. In the case at hand, where no bound states are possible, this can be written:

$$\underset{t \to \pm\infty}{s\text{-lim}}\, e^{iHt} A e^{-iHt} = \omega_{\pm}(A) \tag{1.2}$$

exists if A is a function of the momentum operators, $A = f(P_1, P_2, \ldots, P_{3N})$ where $f: \boldsymbol{R}^{3N} \to \boldsymbol{C}$ is continuous and approaches zero at infinity. (Similar proposals appear in [1, 2].) This condition was verified in [12] for potentials $V(|x|) = 0(|x|^{-\varepsilon})$, $\varepsilon > 0$, which are not necessarily repulsive, but the methods used there depend essentially on spherical symmetry and there a separate proof of absolute continuity is required. In Section 5 we show that (1.2) follows quite naturally from the results of Section 3. We also draw some conclusions from (1.2) to support the contention that it is a reasonable replacement for (1.1), and prove that the homomorphisms $\omega_{\pm}$ are injective.

Our approach here is completely time dependent. In part II we intend to investigate the use of positive commutators and the time-independent (or Fourier transform) theory of smooth operators to prove absolute continuity of the positive part of H, existence of the limits (1.2) and completeness (when the wave operators exist) for one particle with a non-repulsive potential.

2. H-smooth Operators and Positive Commutators

In this section we present the part of the theory of smooth operators and positive commutators which we shall need. This theory, due to Kato [9, 10], provides a new proof of results on absolute continuity of Putnam [13] which shows their connection with the behavior of e^{-iHt} at large times. Because the theorems we need are not stated in the literature in the most convenient form for us, we shall indicate their proofs below. (Also, this will indicate how brief and elementary a proof of completeness becomes using these ideas.)

Throughout this section H will denote a self-adjoint operator in a Hilbert space $\mathscr{H}$ with inner product $\langle\,,\rangle$; we shall write $\mathscr{D}(A)$ for the domain of an operator A in $\mathscr{H}$, $\mathscr{R}(A)$ for its range, and $A(t)$ for $e^{iHt} A e^{-iHt}$.

A bounded operator T is called *H-smooth* if

$$\|T\|_H^2 = \sup_{\varphi \neq 0} \frac{1}{2\pi} \int_{-\infty}^{\infty} \|T e^{-itH} \varphi\|^2 \, dt / \|\varphi\|^2 < \infty\,. \tag{2.1}$$

We call T *relatively H-smooth* if $\mathscr{D}(T) \supset \mathscr{D}(H)$ and

$$\int_{-\infty}^{\infty} \|T e^{-itH} \varphi\|^2 \, dt \leqq C(\|H\varphi\|^2 + \|\varphi\|^2) \tag{2.2}$$

for all $\varphi \in \mathscr{D}(H)$. Clearly T is relatively H-smooth if and only if $T(H+i)^{-1}$ is H-smooth. If B is a bounded operator commuting with H, smoothness of T implies smoothness of TB. The importance of smooth operators for the problems raised in the introduction is indicated by the following two theorems.

Theorem 2.1 (Kato [9]). *If T is H-smooth, then $\mathscr{R}(T^*) \subset \mathscr{K}_{ac}$.*

Proof. To show for $\varphi \in \mathscr{D}(T^*)$ that $T^*\varphi \in \mathscr{K}_{ac}$ it is sufficient to prove that measure $d\langle E_\lambda T^*\varphi, T^*\varphi\rangle$ is absolutely continuous with respect to Lebesgue measure (where E_λ is the spectral resolution of H). This will be true if the Fourier transform f of this measure is square integrable. But

$$\begin{aligned} |f(t)| &= \left| \int_{-\infty}^{\infty} e^{-it\lambda}\, d\langle E_\lambda T^*\varphi, T^*\varphi\rangle \right| \\ &= |\langle e^{-itH}\, T^*\varphi, T^*\varphi\rangle| \\ &\leqq \|T e^{-itH}\, T^*\varphi\|\ \|\varphi\|\,. \end{aligned}$$

So $\int_{-\infty}^{\infty} |f(t)|^2\, dt \leqq \|T\|_H^2\, \|T^*\varphi\|^2\, \|\varphi\|^2$. ▨

Theorem 2.2 (Kato [9, 10]). *Let H_1 and H_2 be self-adjoint operators on a common domain $\mathscr{D}$, and B a bounded operator which takes $\mathscr{D}$ into itself. Then*

$$\operatorname*{s-lim}_{t\to\pm\infty} e^{iH_1 t}\, B e^{-iH_2 t}$$

exists if $i(H_1 B - BH_2) = T_1^* T_2$ where T_j is H_j-smooth ($j=1,2$). The same is true if $i(H_1 B - BH_2)$ is a finite sum of such products.

Proof. It suffices to prove existence on $\mathscr{D}$. Let $\varphi \in \mathscr{D}$, $\psi \in \mathscr{K}$.

$$\begin{aligned} &|\langle (e^{iH_1 t} B e^{-iH_2 t} - e^{iH_1 s} B e^{-iH_2 s})\varphi, \psi\rangle| \\ &\quad = \left| \int_s^t \langle e^{iH_1 u}[H_1 B - BH_2]\, e^{-iH_2 u}\varphi, \psi\rangle\, du \right| \\ &\quad = \left| \int_s^t \langle T_2 e^{-iH_2 u}\varphi, T_1 e^{-iH_1 u}\psi\rangle\, du \right| \\ &\quad \leqq \left(\int_s^t \|T_2 e^{-iH_2 u}\varphi\|^2\, du \right)^{1/2} \left(\int_s^t \|T_1 e^{-iH_1 u}\psi\|^2\, du \right)^{1/2} \\ &\quad \leqq \left(\int_s^t \|T_2 e^{-iH_2 u}\varphi\|^2\, du \right)^{1/2} \|T_1\|_{H_1}\, \|\psi\|\,. \end{aligned}$$

The proof for sums of products is a trivial extension of this. ▨

There are two important cases: if $B=I$, $H_2=H_0$, $H_1=H=H_0+V$ we have existence of the wave operators, and by symmetry their completeness, if $V=T_1^* T_2$. If B is a function of momentum and $H_1=H_2=H$ we have existence of the limits (1.2) if $i[H,B]=T_1^* T_2$.

Conversely, the relation between limits as t tends to infinity and smoothness can be used to find smooth operators. The following is a version of a theorem of Kato [9] which is adapted to our purposes. (In our version, domain considerations obscure somewhat the striking simplicity of the original, where all operators are bounded.)

Theorem 2.3 *Let A be a symmetric operator with $\mathscr{D}(A)\supset\mathscr{D}(H)$ and $\mathscr{D}([H,A])$ a core of H. If B is an operator with $\mathscr{D}(B)\supset\mathscr{D}(H)$, and for all $\varphi\in\mathscr{D}([H,A])$*

$$\|B\varphi\|^2 \leqq \langle i[H,A]\varphi,\varphi\rangle$$

then B is relatively H-smooth.

Proof. Let $\varphi\in\mathscr{D}(H)$.

$$\frac{d}{dt}\langle A(t)\varphi,\varphi\rangle = i\langle Ae^{-iHt}\varphi, He^{-iHt}\varphi\rangle - i\langle He^{-iHt}\varphi, Ae^{-iHt}\varphi\rangle .$$

If $e^{-iHt}\varphi\in\mathscr{D}([H,A])$,

$$\frac{d}{dt}\langle A(t)\varphi,\varphi\rangle = \langle i[H,A]\, e^{-iHt}\varphi, e^{-iHt}\varphi\rangle \geqq \|Be^{-iHt}\varphi\|^2 .$$

Both the left and right members of this inequality are continuous in the graph norm on $\mathscr{D}(H)$, and $\{\varphi : e^{-iHt}\varphi\in\mathscr{D}([H,A])\}$ is a core of H, so this inequality holds for all $\varphi\in\mathscr{D}(H)$. Hence for $t<s$ and $\varphi\in\mathscr{D}(H)$,

$$\begin{aligned}\int_t^s \|Be^{-iHu}\varphi\|^2\,du &\leqq \int_t^s \frac{d}{du}\langle A(u)\varphi,\varphi\rangle\,du\\ &= \langle (A(s)-A(t))\varphi,\varphi\rangle\\ &\leqq 2\|A(H+i)^{-1}\|\;\|(H+i)\varphi\|^2 . \quad ▨\end{aligned}$$

Corollary 2.4. *If the situation of Theorem 2.3 occurs, the H is absolutely continuous on $\mathscr{R}(B^*)$.*

3. Classes of H-smooth Operators

In this section we find a self-adjoint operator A with $i[H,A]\geqq 0$ so that Theorem 2.3 can be applied. From the expression for $i[H,A]$ we shall be able to find classes of relatively H-smooth multiplication and differential operators.

If A is regarded as a quantum mechanical observable, the condition $i[H, A] > 0$ means that $\langle A(t)\varphi, \varphi\rangle$, its expectation value at time t, is constantly increasing, so we shall refer to such an operator as a "progress operator". One observable which tends to increase for a particle undergoing scattering is the scalar product $x \cdot p$ of position and momentum, for the change in x tends to be in the direction of p. The obvious choice of an operator for this observable is $-i(x \cdot \nabla + \nabla \cdot x)$, the generator of the unitary group of dilations. But the presence of the unbounded position operator means this operator is not H-bounded, and Theorem 2.3 cannot be applied. (It is an interesting question whether there is a theorem applying to this operator A which says that $i[H, A] > 0$ implies H is absolutely continuous. The use of the Virial Theorem by Weidmann [15] to prove absence of point spectrum can be considered a weaker version of such a theorem. This operator also enters into an interesting absolute continuity theorem of Combes [2].)

Our progress operator will be a modification of this operator, with x replaced by a bounded vector field $G(x): \boldsymbol{R}^n \to \boldsymbol{R}^n$. Let $h: [0, \infty) \to \boldsymbol{R}$ be a function in $\mathscr{L}^2([0, \infty))$ with $h(|x|) \in \mathscr{C}^\infty(\boldsymbol{R}^n)$, and let

$$g(r) = \int_0^r h^2(s)\, ds\,,$$

$$G(x) = \frac{x}{r} g(r) \qquad (r = |x|)\,.$$

We define A to be the symmetric operator defined for functions in $\mathscr{D}$, the set of $\mathscr{C}^\infty$ functions on $\boldsymbol{R}^n$ with compact support, by

$$A\varphi(x) = -i\{G(x) \cdot \nabla + \nabla \cdot G(x)\}\, \varphi(x)\,. \tag{3.1}$$

(Such an operator was used to prove absolute continuity in [11].) Let H_0 be the self-adjoint operator $-\Delta$ on its natural domain in $\mathscr{L}^2(\boldsymbol{R}^n)$, and V a Kato potential so that $H_0 + V = H$ is self-adjoint on $\mathscr{D}(H) = \mathscr{D}(H_0)$. It is clear from (3.1) that A can be extended to $\mathscr{D}(H)$, and is H-bounded.

It will be convenient to represent $\mathscr{L}^2(\boldsymbol{R}^n)$ as $\mathscr{L}^2([0, \infty); \mathscr{L}^2(S^{n-1}))$ where $S^{n-1} = \{x : |x| = 1\} \subset \boldsymbol{R}^n$, so that the function $\varphi \in \mathscr{L}^2(\boldsymbol{R}^n)$ is represented by $\Phi: [0, \infty) \to \mathscr{L}^2(S^{n-1})$,

$$\{\Phi(r)\}(u) = r^{(n-1)/2} \varphi(ru) \qquad (u \in S^{n-1},\ r \in [0, \infty))\,.$$

Then if f is a multiplication operator on $\mathscr{L}^2(\boldsymbol{R}^n)$,

$$\{(f\Phi)(r)\}(u) = f(ru)\, \varphi(ru)$$

and

$$H_0 \Phi(r) = \frac{-d^2}{dr^2} \Phi(r) + \frac{(n-1)(n-3)}{4r^2} \Phi(r) + \frac{L}{r^2} \Phi(r)\,, \tag{3.2}$$

where L is the Laplace-Beltrami operator on S^{n-1}. We also have

$$A\,\Phi(r) = -i\left\{g(r)\frac{d\Phi(r)}{dr} + \frac{d}{dr}g(r)\,\Phi(r)\right\}. \tag{3.3}$$

Now we calculate $i[H, A]$.

Lemma 3.1. *Suppose H is as specified above, and $r\frac{\partial V}{\partial r}$ a Kato potential. Then $\mathscr{D}([H,A])\supset\mathscr{D}$ and if $\varphi\in\mathscr{D}$ is represented by $\Phi\in\mathscr{L}^2([0,\infty),\mathscr{L}^2(S^{n-1}))$*

$$\begin{aligned} i[H,A]\,\Phi = &-4h\frac{d^2}{dr^2}h\Phi + 2(h''h - h'^2)\Phi \\ &+ g\left\{\frac{(n-1)(n-3)}{r^3} + \frac{4L}{r^3} - 2\frac{\partial V}{\partial r}\right\}\Phi\,. \end{aligned} \tag{3.4}$$

Proof. It can be shown using Taylor's theorem that $g(|x|)/|x|$ is in $\mathscr{C}^\infty(\boldsymbol{R}^n)$. It follows that $\mathscr{D}(H\,A)\supset\mathscr{D}$, and multiplication by $g(|x|)\,\partial V/\partial r$ takes $\mathscr{D}$ into $\mathscr{L}^2(\boldsymbol{R}^n)$ so that $\mathscr{D}(A\,H)\supset\mathscr{D}$

$$i[H,A] = \left[-\frac{d^2}{dr^2} + \frac{(n-1)(n-3)}{4r^2} + \frac{L}{r^2} + V,\ \left\{g\frac{d}{dr} + \frac{d}{dr}g\right\}\right].$$

Let us calculate the terms involving multiplication operators in the left side of the commutator first:

$$\begin{aligned} &\left[\frac{(n-1)(n-3)}{4r^2} + \frac{L}{r^2} + V,\ g\frac{d}{dr} + \frac{d}{dr}g\right] \\ &\quad = \left[\frac{(n-1)(n-3)}{4r^2} + \frac{L}{r^2} + V,\ 2g\frac{d}{dr} + h^2\right] \\ &\quad = -2g\frac{d}{dr}\left\{\frac{(n-1)(n-3)}{4r^2} + \frac{L}{r^2} + V\right\} \\ &\quad = g\left\{\frac{(n-1)(n-3)}{r^3} + \frac{4L}{r^3} - 2\frac{\partial V}{\partial r}\right\}. \end{aligned}$$

We also have

$$\left[-\frac{d^2}{dr^2},\ g\frac{d}{dr}\right] = -\left\{g''\frac{d}{dr} + 2g'\frac{d^2}{dr^2}\right\},$$

and the adjoint of this equation gives

$$\left[-\frac{d^2}{dr^2},\ \frac{d}{dr}g\right] = \frac{d}{dr}g'' - 2\frac{d^2}{dr^2}g'\,.$$

Thus we have

$$\left[-\frac{d^2}{dr^2}, g\frac{d}{dr}+\frac{d}{dr}g\right] = -2\left(h^2\frac{d^2}{dr^2}+\frac{d^2}{dr^2}h^2\right)+\left[\frac{d}{dr}, (h^2)'\right]$$

$$= -4h\frac{d^2}{dr^2}h - 2\left[\frac{d^2}{dr^2}, h\right]h + 2h\left[\frac{d^2}{dr^2}, h\right]$$

$$+2(h'^2+h''h)$$

$$= -4h\frac{d^2}{dr^2}h$$

$$-4\frac{d}{dr}h'h + 2h''h$$

$$+4hh'\frac{d}{dr} + 2hh'' + 2(h'^2+h''h)$$

$$= -4h\frac{d^2}{dr^2}h - 4(hh')' + 4hh'' + 2(h'^2+h''h)$$

$$= -4h\frac{d^2}{dr^2}h + 2(h''h - h'^2). \quad ▨$$

To apply Theorem 2.3 we must have $i[H, A] \geqq 0$. If V is repulsive in the sense that $\frac{\partial V}{\partial r} \leqq 0$, all terms in (3.4) but $2(h''h - h'^2)$ will be non-negative if $n \geqq 3$. The next lemma shows that the first two terms of (3.4) taken together are positive for a certain choice of h.

Lemma 3.2. *Let* $h(r) = (1+r^2)^{-(1+\varepsilon)/4}$, $(0 < \varepsilon \leqq 1)$. *Then*

$$-2h\frac{d^2}{dr^2}h + h''h - h'^2 \geqq (2r)^{-2}(1+r^2)^{-(1+\varepsilon)/2}. \tag{3.5}$$

Proof. A calculation shows that

$$\frac{h''h - h'^2}{h^2} = \frac{(1+\varepsilon)(r^2-1)}{2(r^2+1)^2}.$$

Now it is known that $-d^2/dr^2 \geqq (2r)^{-2}$. (A simple proof: Let $f \in \mathscr{D}\left(\frac{d^2}{dr^2}\right)$.

$$0 \leqq \int_0^\infty \left|\left(-\frac{d}{dr}+\frac{1}{2r}\right)f(r)\right|^2 dr = \int_0^\infty \left\{\left(\frac{d}{dr}+\frac{1}{2r}\right)\left(-\frac{d}{dr}+\frac{1}{2r}\right)f(r)\right\}\overline{f(r)}\,dr$$

$$= -\int_0^\infty \left(f''(r)\overline{f(r)} + \frac{1}{4r^2}|f(r)|^2\right) dr.)$$

Therefore

$$-2\frac{d^2}{dr^2}+\frac{hh''-h'^2}{h^2}-\frac{1}{4r^2}\geqq\frac{1}{4r^2}+\frac{(1+\varepsilon)(r^2-1)}{2(r^2+1)^2}$$

$$=\frac{(r^2+1)^2+2(1+\varepsilon)r^2(r^2-1)}{4r^2(r^2+1)^2}=\frac{1-2\varepsilon r^2+(3+2\varepsilon)r^4}{4r^2(1+r^2)^2}$$

which is positive since $0<\varepsilon\leqq 1$ implies that $(2\varepsilon)^2<4(3+2\varepsilon)$. ▨

Now we apply these lemmas to find H-smooth operators.

Theorem 3.3. *If H satisfies the conditions of Lemma 3.1 and $\partial V/\partial r\leqq 0$, (with $n\geqq 3$) then operators of the following form are H-smooth:*

a) $f(x)(H+i)^{-1}$, *where*

$$|f(x)|^2\leqq C^2(1+r^2)^{-1/2}\left[-2r\frac{\partial V}{\partial r}+(2r)^{-2}(1+r^2)^{-\varepsilon/2}\right],$$

b) $\sqrt{H_0}\,f(x)(H+i)^{-1}$, *where* $|f(x)|^2\leqq C^2(1+x^2)^{-(1+\varepsilon)/2}$,

c) $D_r f(x)(H+i)^{-1}$, *where* $|f(x)|^2\leqq C^2(1+x^2)^{-(1+\varepsilon)/2}$

(where D_r is the symmetric operator on $\mathscr{D}(H_0)$ given in the representation $\mathscr{L}^2([0,\infty);\mathscr{L}^2(S^{n-1}))$ by $-id/dr$).

Proof. We apply Theorem 2.3. Let $B=f(x)/C$ and note that $\mathscr{D}(B)\supset\mathscr{D}(H)$. Then for $\varphi\in\mathscr{C}_0^\infty(\boldsymbol{R}^n)$,

$$\|B\varphi\|^2\leqq\left\langle\left\{-2(1+r^2)^{-1/2}r\frac{\partial V}{\partial r}+(2r)^{-2}(1+r^2)^{-(1+\varepsilon)/2}\right\}\varphi,\varphi\right\rangle.$$

Now $g'(r)=h^2(r)=(1+r^2)^{-1/2-\varepsilon/2}$ and

$$(r(1+r^2)^{-1/2})'=(1+r^2)^{-3/2} \tag{3.6}$$

so $g(r)\geqq r(1+r^2)^{-1/2}$, and we have

$$\|B\varphi\|^2\leqq\left\langle\left\{-2g(r)\frac{\partial V}{\partial r}+(2r)^{-2}(1+r^2)^{-(1+\varepsilon)/2}\right\}\varphi,\varphi\right\rangle$$

$$\leqq\langle i[H,A]\varphi,\varphi\rangle,$$

by (3.4) and (3.5). Therefore by Theorem 2.3, B is relatively H-smooth, and hence any multiple of B is relatively H-smooth. It follows that the operator a) is H-smooth.

For operators of the form b), we first note:

Lemma 3.4. *If A is given by (3.1)*

$$i[H_0,A]\geqq 4h\,H_0 h+2(h''h-h'^2)$$

$$\geqq 2h\,H_0 h.$$

Proof. Since by (3.6)

$$\frac{g(r)}{r} \geqq (1+r^2)^{-1/2} \geqq h^2(r)$$

we have

$$g(r)\left\{\frac{L}{r^3} + \frac{(n-3)(n-1)}{4r^3}\right\} \geqq h\left\{\frac{L}{r^2} + \frac{(n-3)(n-1)}{4r^2}\right\} h,$$

and therefore by (3.4) and (3.2),

$$i[H_0, A] \geqq 4h\, H_0 h + 2(h'' h - h'^2).$$

The second inequality follows from Lemma 3.2. ▨

To conclude the proof for b) observe

$$\|\sqrt{H_0}\, h\varphi\|^2 \leqq \langle i[H_0, A]\varphi, \varphi\rangle \leqq \langle i[H, A]\varphi, \varphi\rangle$$

since V is repulsive.

Smoothness for operators of the form c) follows directly from (3.4) and Lemma 3.2. ▨

Corollary 3.5. *The operator H of Theorem 3.3 is absolutely continuous.*

Proof. Let $T = (2r)^{-1}(1+r^2)^{-\varepsilon/4}(H+i)^{-1}$. Since T is H-smooth, $\mathscr{R}(T^*) \subset \mathscr{H}_{ac}$. But $T^* = (H-i)^{-1}(2r)^{-1}(1+r^2)^{-\varepsilon/4}$ has dense range, since the range of the multiplication is dense in $\mathscr{H}$, so that $(H-i)^{-1}$ takes it into a core of H. ▨

This improves the results of [11]. Its most important physical applications are to a single particle with repulsive potential ($n=3$) and to

$$H = -\Delta + \sum_{1 \leqq j < k \leqq N} V_{jk}(x_j - x_k)$$

where $V_{jk}: \boldsymbol{R}^3 \to \boldsymbol{R}$, $\partial V_{jk}/\partial r_{jk} \leqq 0$ and x_i is the position of the ith particle, $r_{jk} = |x_j - x_k|$, for

$$r\frac{\partial V_{jk}}{\partial r} = \sum_{i=1}^{3N} x_i \cdot \nabla_i V_{jk} = (x_j - x_k)\cdot \nabla V_{jk}$$
$$= r_{jk}\frac{\partial V_{jk}}{\partial r_{jk}}.$$

But for a more searching study of the many particle problem the smooth operators identified in Theorem 3.3 are not sufficient. We would like to know that operators like $V_{jk}(x_j - x_k)$ and its partial derivatives, which do not approach zero as $(x_1, \ldots, x_N)$ approaches infinity, are essentially products of H-smooth operators. Let us consider the case where there is no fixed center of force, but only interactions between pairs of particles, and assume that these potentials are spherically symmetric. In the Hilbert space $\mathscr{L}^2(\boldsymbol{R}^{3N})$

$$H = -\sum_{i=1}^{N} \Delta_i + \sum_{1 \leqq j < k \leqq N} V_{jk}(r_{jk}), \tag{3.7}$$

where Δ_i is the Laplacian with respect to x_i and V_{jk} is a Kato potential. Let P_{jk} represent twice the relative momentum between particles j and k:

$$P_{jk} = -i(\nabla_j - \nabla_k).$$

Note that if $f : \boldsymbol{R}^3 \to \boldsymbol{R}$,

$$[P_{jk}, f(x_j - x_k)] = -2i(\nabla f)(x_j - x_k).$$

We shall need a progress operator A_{jk} for each pair of particles:

$$A_{jk} = \{G(x_j - x_k) \cdot P_{jk} + P_{jk} \cdot G(x_j - x_k)\}$$

which operates only on the variables x_j and x_k. Note that $A_{jk} = A_{kj}$.

Theorem 3.6. *If H is given by* (3.7) *and for all $j < k \leqq N, 0 \geqq r_{jk}\, \partial V_{jk}/\partial r_{jk}$ is a Kato potential then operators of the following form are H-smooth:*

a) $f(x)(H+i)^{-1}$ *where*

$$|f(x)|^2 \leqq C^2(1 + r_{jk}^2)^{-1/2}\left[-2r_{jk}\frac{\partial V_{jk}}{\partial r_{jk}} + (2r_{jk})^{-2}(1 + r_{jk}^2)^{-\varepsilon/2}\right],$$

b) $\sqrt{P_{jk}^2}\, f(x)(H+i)^{-1}$ *where* $|f(x)|^2 \leqq C^2(1 + r_{jk}^2)^{-(1+\varepsilon)/2}$,

c) $D_{jk,r} f(x)(H+i)^{-1}$ *where* $|f(x)|^2 \leqq C^2(1 + r_{jk}^2)^{-(1+\varepsilon)/2}$

(where $D_{jk,r}$ is the symmetric operator on $\mathscr{D}(P_{jk}^2)$ given by d/dr_{jk} in the representation of functions of $x_j - x_k$ as $\mathscr{L}^2([0, \infty); \mathscr{L}^2(S^2))$).

Proof. Let $A = \sum_{1 \leqq j < k \leqq N} A_{jk}$. Then

$$\begin{aligned} i[H, A] &= \sum_{1 \leqq j < k \leqq N} i[H, A_{jk}] \\ &= -i \sum_{i=1}^{N} \sum_{j<k} [\Delta_i, A_{jk}] + i \sum_{l<m} \sum_{j<k} [V_{lm}, A_{jk}]. \end{aligned}$$

Consider first

$$-i \sum_{i=1}^{N} [\Delta_i, A_{jk}] = -i[\Delta_j + \Delta_k, A_{jk}].$$

Note that

$$-(\Delta_j + \Delta_k) = -\tfrac{1}{2}(\nabla_j + \nabla_k) \cdot (\nabla_j + \nabla_k) + \tfrac{1}{2} P_{jk} \cdot P_{jk}.$$

The first term on the right side commutes with A_{jk} so that

$$-i[\Delta_j + \Delta_k, A_{jk}] = \frac{i}{2}[P_{jk} \cdot P_{jk}, A_{jk}].$$

Then we have by Lemma 3.2,

$$-i[\Delta_j+\Delta_k, A_{jk}] \geqq (2r_{jk})^{-2}(1+r_{jk}^2)^{-(1+\varepsilon)/2}. \tag{3.8}$$

By Lemma 3.4,

$$-i[\Delta_j+\Delta_k, A_{jk}] \geqq h(r_{jk})\, P_{jk}^2\, h(r_{jk}). \tag{3.9}$$

Now let us look for fixed l, m, at

$$i\Big[V_{lm}, \sum_{j<k} A_{jk}\Big] = i[V_{lm}, A_{lm}] + \sum_{l \neq k \neq m} i[V_{lm}, A_{lk}+A_{km}].$$

Now

$$i[V_{lm}, A_{lm}] = -4g(r_{lm})\frac{\partial V_{lm}(r_{lm})}{\partial r_{lm}}. \tag{3.10}$$

We shall show that for any k, $l \neq k \neq m$,

$$i[V_{lm}, A_{lk}+A_{km}] \geqq 0.$$

We have

$$\begin{aligned} i[V_{lm}, A_{lk}+A_{km}] = &-2\left\{\frac{g(r_{lk})}{r_{lk}}(x_l-x_k)\cdot \nabla_l V_{lm}(|x_l-x_m|)\right.\\ &\left. -\frac{g(r_{km})}{r_{km}}(x_k-x_m)\cdot \nabla_m V_{lm}(|x_l-x_m|)\right\}\\ = &-2V'_{lm}(r_{lm})\frac{(x_l-x_m)}{r_{lm}}\cdot\left\{\frac{g(r_{lk})}{r_{lk}}(x_l-x_k)+\frac{g(r_{km})}{r_{km}}(x_k-x_m)\right\}\\ = &-2\frac{V'_{lm}(r_{lm})}{r_{lm}}[(x_l-x_k)+(x_k-x_m)]\cdot\left\{g(r_{lk})\frac{x_l-x_k}{r_{lk}}+g(r_{km})\frac{x_k-x_m}{r_{km}}\right\}. \end{aligned}$$

Now $-V'_{lm}(r_{lm})/r_{lm} \geqq 0$, and the scalar product of two vectors in $\boldsymbol{R}^3$ whose directions lie between the directions of the vectors $x_l - x_k$ and $x_k - x_m$, but closer to that of the longer one, must be nonnegative. Thus we have shown $i[V_{lm}, A_{lk}+A_{km}] \geqq 0$, and it follows from (3.10) that

$$i\Big[\sum_{l<m} V_{lm}, A\Big] \geqq -2\sum_{l<m} g(r_{lm})\frac{\partial V_{lm}}{\partial r_{lm}}(r_{lm}). \tag{3.11}$$

Using (3.8) and (3.11) we get for all $j<k$

$$i[H, A] \geqq (2r_{jk})^{-2}(1+r_{jk}^2)^{-(1-\varepsilon)/2} - 2g_{jk}(r_{jk})\frac{\partial V_{jk}}{\partial r_{jk}},$$

from which follows the smoothness of operators of the form a), and smoothness for operators of form b) is deduced from (3.9) as in the proof of Theorem 3.3. Operators like c) are smooth since $\|D_{jk,r}\varphi\|^2 \leqq \langle P_{jk}^2\varphi, \varphi\rangle$. ▨

The following lemma will be needed in our applications, and has some interest of its own since it says that each pair of particles separates as $t \to \pm\infty$. (We will get more information on the spatial behavior of $e^{-iHt}\varphi$ in Section 5.)

Lemma 3.7. *Let H be as in Theorem 3,6 and let χ_R be the characteristic function of the ball of radius R in $\boldsymbol{R}^3$. Then for $1 \leqq j < k \leqq N$,*

$$\operatorname*{s-lim}_{t\to\pm\infty} \chi_R(r_{jk})\, e^{-iHt} = 0\,.$$

Furthermore, if $V_{jk}(r_{jk}) \to 0$ as $r_{jk} \to \infty$ we have for $\varrho = \pm 1$

$$\operatorname*{s-lim}_{t\to\pm\infty} (H_0 + i\varrho)^{-1}\, V_{jk}\, e^{-iHt} = 0\,,$$

and

$$\operatorname*{s-lim}_{t\to\pm\infty} V_{jk}(H + i\varrho)^{-1}\, e^{-iHt} = 0$$

(i.e., $V_{jk}\, e^{-iHt}\varphi \to 0$ as $t \to \pm\infty$ for $\varphi \in \mathscr{D}(H)$).

Proof. By Theorem 3.6, for $\varphi \in \mathscr{D}(H)$

$$f(t) = \langle (1 + r_{jk}^2)^{-(3+\varepsilon)/2}\, e^{-iHt}\varphi, e^{-iHt}\varphi\rangle$$

is integrable. Furthermore f has a bounded derivative, so f is uniformly continuous. It follows that $f(t) \to 0$ as $t \to \pm\infty$. Since

$\chi_R(r_{jk}) \leqq c(1 + r_{jk}^2)^{-(3+\varepsilon)/2}$
we have

$$c^{-1}\|\chi_R(r_{jk})\, e^{-iHt}\varphi\|^2 \leqq f(t) \to 0 \quad \text{as} \quad t \to \pm\infty\,.$$

Since χ_R is bounded, we have convergence for all φ.

Now since $V_{jk}(r) \to 0$ as $r \to \infty$, given $\delta > 0$ one can find R such that

$$\begin{aligned}\|(H_0 \pm i)^{-1}\, V_{jk}\, e^{-iHt}\varphi\| &\leqq \|(H_0 \pm i)^{-1}\, V_{jk}\chi_R(r_{jk})\, e^{-iHt}\varphi\| + \delta\|\varphi\| \\ &\leqq \|(H_0 \pm i)^{-1}\, V_{jk}\|\, \|\chi_R(r_{jk}) e^{-iHt}\varphi\| + \delta\|\varphi\|\,.\end{aligned}$$

Finally, $V_{jk} = q_1 + q_2$ where $\|q_1(H + i)^{-1}\| < \delta$ and $\|q_2\| < C$. So we have

$$\begin{aligned}\|V_{jk}(H + i)^{-1}\, e^{iHt}\varphi\| \leqq\ &\|q_1(H + i)^{-1}\|\, \|\varphi\| \\ &+ \|q_2\|\, \|\chi_R e^{-iHt}(H + i)^{-1}\varphi\| \\ &+ \|(1 - \chi_R)\, q_2\|\, \|e^{-iHt}(H + i)^{-1}\varphi\|\,.\end{aligned}$$ ▨

4. Completeness of the Wave Operators

In this section we prove that the wave operators are complete for one-particle operators H with repulsive potentials $V(x) = 0(|x|^{-1-\varepsilon})$ as $|x| \to \infty$. In the many particle case we need $V_{jk}(x) = 0(|x|^{-3-\varepsilon})$ as $|x| \to \infty$.

Theorem 4.1. *Let* $H=-\Delta+V$, V *a Kato potential*, $r\,\partial V/\partial r\leqq 0$ *a Kato potential, and* $V=V_1+V_2$ *where*

$$|V_1(x)|\leqq b(2r)^{-2}(1+r^2)^{-(1+\varepsilon)/2}, \tag{4.1}$$

$$|V_2(x)|\leqq c(1+r^2)^{-(1+\varepsilon)/2}. \tag{4.2}$$

Then the wave operators exist and are complete. In fact

$$\Omega_\pm(H,H_0)=\operatorname*{s-lim}_{t\to\pm\infty} e^{iHt}e^{-iH_0t}$$

and

$$\Omega_\pm(H_0,H)=\operatorname*{s-lim}_{t\to\pm\infty} e^{iH_0t}e^{-iHt}=\Omega_\pm(H,H_0)^*$$

exist.

Remark. Of course the r^{-2} singularity permitted by (4.1) is not actually possible for the Kato potentials which we are considering, but these inequalities are all we use in the proof.

Proof. First we show that

$$\operatorname*{s-lim}_{t\to\pm\infty} B_t=\operatorname*{s-lim}_{t\to\pm\infty} e^{iH_0t}(H_0+i)^{-2}H_0(H+i)^{-1}e^{-iHt}$$

exists. By Theorem 2.2 it is sufficient to consider

$$\begin{aligned}
-H_0(H_0+i)^{-2}&H_0(H+i)^{-1}+(H_0+i)^{-2}H_0(H+i)^{-1}H\\
&=-(H_0+i)^{-2}H_0(H_0-H)(H+i)^{-1}\\
&=(H_0+i)^{-2}H_0V(H+i)^{-1}\\
&=H_0(H_0+i)^{-2}V_1(H+i)^{-1}+(H_0+i)^{-2}H_0V_2(H+i)^{-1}.
\end{aligned} \tag{4.3}$$

$$\begin{aligned}
(H_0+i)^{-2}H_0V_2(H+i)^{-1}&=(H_0+i)^{-2}H_0h(V_2/h)(H+i)^{-1}\\
&=(H_0+i)^{-2}\{hH_0(V_2/h)+[h,H_0](V_2/h)\}(H+i)^{-1}\\
&=(H_0+i)^{-2}\left\{hH_0(V_2/h)+\left(h''+2h'\frac{d}{dr}\right)(V_2/h)\right\}(H+i)^{-1}\\
&=[(H_0+i)^{-2}h\sqrt{H_0}]\,[\sqrt{H_0}(V_2/h)(H+i)^{-1}]\\
&\quad+[(H_0+i)^{-2}h''(1+r^2)^{1/2}]\,[(1+r^2)^{-1/2}(V_2/h)(H+i)^{-1}]\\
&\quad+2[(H_0+i)^{-2}h']\left[\frac{d}{dr}(V_2/h)(H+i)^{-1}\right].
\end{aligned}$$

These are all products of the required type by Theorem 3.3 (and the remarks following (2.2)) since

$$\begin{aligned}
V_2/h&\leqq c_1(1+r^2)^{-(1+\varepsilon)/4},\\
h'&\leqq c_2(1+r^2)^{-(3+\varepsilon)/4},\\
(1+r^2)^{1/2}h''&\leqq c_3(1+r^2)^{-(3+\varepsilon)/4}.
\end{aligned}$$

The remaining term in (4.3) is also such a product:

$$H_0(H_0+i)^{-2}\,V_1(H+i)^{-1}$$
$$=\{[H_0(H_0+i)^{-1}]\,[(H_0+i)^{-1}\,V_1^{1/2}]\}\,[V_1^{1/2}(H+i)^{-1}]\,.$$

But convergence of B_t implies convergence of $e^{iH_0t}\,e^{-iHt}$ on a dense set:

a) $e^{iH_0t}(H_0+i)^{-2}\,H_0(H+i)^{-1}\,e^{-iHt}=e^{iH_0t}(H_0+i)^{-2}\,H_0\,e^{-iHt}(H+i)^{-1}$
$$=e^{iH_0t}(H_0+i)^{-2}\,e^{-iHt}\,H(H+i)^{-1}-e^{iH_0t}(H_0+i)^{-2}\,Ve^{-iHt}$$

and compactness of $(H_0+i)^{-1}\,V$ implies the second term converges to zero, since H is absolutely continuous.

b) $e^{iH_0t}(H_0+i)^{-2}\,e^{-iHt}=e^{iH_0t}(H_0+i)^{-1}\,e^{-iHt}(H+i)^{-1}$
$$+\,e^{iH_0t}(H_0+i)^{-2}\,V(H+i)^{-1}\,e^{-iHt}\,,$$

and again the second term converges to zero.

c) $e^{iH_0t}(H_0+i)^{-1}\,e^{-iHt}$
$$=e^{iH_0t}\,e^{-iHt}(H+i)^{-1}+e^{iH_0t}(H_0+i)^{-1}\,V(H+i)^{-1}\,e^{-iHt}\,.$$

Therefore
$$\underset{t\to\pm\infty}{s\text{-}\lim}\,e^{iH_0t}\,e^{-iHt}(H+i)^{-3}\,H=\underset{t\to\pm\infty}{s\text{-}\lim}\,B_t\,.$$

Existence of $\Omega_\pm(H,H_0)$ could be proved similarly, but since this is a well-known theorem we omit it. ▨

Theorem 4.2. *Let H be as in Theorem 3.6 and*

$$|V_{jk}(r_{jk})|\leqq b(2r_{jk})^{-2}\,(1+r_{jk}{}^2)^{-(1+\varepsilon)/2}\,. \tag{4.4}$$

Then the wave operators exist and are complete.

Proof. First we shall show that

$$\underset{t\to\pm\infty}{s\text{-}\lim}\,e^{iH_0t}(H_0+i)^{-1}\,(H+i)^{-1}\,e^{-iHt} \tag{4.5}$$

exists. This is true by Theorem 2.2, since

$$H_0(H_0+i)^{-1}\,(H+i)^{-1}-(H_0+i)^{-1}\,(H+i)^{-1}\,H$$
$$=(H_0+i)^{-1}\,(H_0-H)\,(H+i)^{-1}$$
$$=-\sum_{j<k}(H_0+i)^{-1}\,V_{jk}(r_{jk})\,(H+i)^{-1}\,,$$

and (4.4) implies that $V_{jk}(r_{jk})^{1/2}(H_0+i)^{-1}$ is H_0-smooth and $V_{jk}(r_{jk})^{1/2}\cdot(H+i)^{-1}$ is H-smooth, by Theorem 3.6. But

$$e^{iH_0t}(H_0+i)^{-1}\,(H+i)^{-1}\,e^{-iHt}=e^{iH_0t}(H_0+i)^{-1}\,e^{-iHt}(H+i)^{-1}$$
$$=e^{iH_0t}\,e^{-iHt}(H+i)^{-2}$$
$$+\sum_{j<k}e^{iH_0t}(H_0+i)^{-1}\,V_{jk}\,e^{iHt}(H+i)^{-2}\,.$$

Since the second term converges strongly to zero as $t \to \pm\infty$ by Lemma 3.7, we have convergence of $e^{iH_0t} e^{-iHt}$ on a dense set, and therefore on all of $\mathscr{H}$. ▨

Remarks. 1. A time independent representation of the wave operators is also available from the theory of smooth operators [9].

2. A proof of completeness for the many particle case with potentials $V_{jk}(r_{jk}) = 0(r_{jk}^{-1-\varepsilon})$ along the lines of Theorem 4.1 would be possible using the theory to be developed in Section 5 if one knew that

$$\lim_{t \to \pm\infty} e^{iHt} P_{jk} \cdot P_{jk} e^{-iHt} \varphi \neq 0 \quad \text{for each} \quad \varphi \in \mathscr{D}(H).$$

5. Convergence of Momentum Observables

Now we prove that limits (1.2) of momentum observables exist. The following lemma shows that for this it is sufficient to prove that such limits exist for one type of operator.

Lemma 5.1. *If $H = H_0 + V$ in $\mathscr{L}^2(\mathbf{R}^n)$ and if for $\varrho = \pm 1$*

$$\operatorname*{s-lim}_{t \to \pm\infty} (H_0 + i\varrho)^{-1} V e^{-iHt} = 0$$

and for $j = 1, 2, \ldots, n$,

$$\operatorname*{s-lim}_{t \to \pm\infty} e^{iHt} (H - i)^{-1} P_j (H + i)^{-1} e^{-iHt} = B_j^{\pm}$$

exists, then the limits (1.2) *exist, and $\omega_{\pm}(f(H_0)) = f(H)$ if f is continuous and $f(\lambda) \to 0$ as $\lambda \to \infty$.*

Proof. First we show that because of the resolvent identity

$$(H_0 + i)^{-1} = (H + i)^{-1} + (H_0 + i)^{-1} V (H + i)^{-1} \tag{5.1}$$

we have

$$\operatorname*{s-lim}_{t \to \pm\infty} e^{iHt} (H_0 - i)^{-1} P_j (H_0 + i)^{-1} e^{-iHt} = B_j^{\pm}.$$

To see this, note that

$$\begin{aligned} &\{(H_0 - i)^{-1} P_j (H_0 + i)^{-1} - B_j^{\pm}\}(t) \\ &\quad = \{(H_0 - i)^{-1} P_j (H_0 + i)^{-1} - (H - i)^{-1} P_j (H + i)^{-1}\}(t) \\ &\qquad + \{(H - i)^{-1} P_j (H + i)^{-1} - B_j^{\pm}\}(t). \end{aligned}$$

The second term converges strongly to zero as $t \to \pm\infty$, and

$$\begin{aligned} &\{(H_0 - i)^{-1} P_j (H_0 + i)^{-1} - (H - i)^{-1} P_j (H + i)^{-1}\}(t) \\ &\quad = \{(H_0 - i)^{-1} P_j [(H_0 + i)^{-1} - (H + i)^{-1}]\}(t) \\ &\qquad + \{[(H_0 - i)^{-1} - (H - i)^{-1}] P_j (H + i)^{-1}\}(t) \\ &\quad = \{(H_0 - i)^{-1} P_j\}(t) \{(H_0 + i)^{-1} V (H + i)^{-1}\}(t) \\ &\qquad + \{(H_0 - i)^{-1} V\}(t) \{(H - i)^{-1} P_j (H + i)^{-1}\}(t). \end{aligned}$$

The first term is the product of an operator bounded uniformly in t with an operator which converges to zero, and the second term is the product of two strongly convergent operators, the first of which converges to zero.

The set of bounded operators A for which $A(t)$ converges strongly is clearly an algebra which is closed in the operator norm. By the Stone-Weierstrass theorem the operators $\{(H_0 - i)^{-1} P_j (H_0 + i)^{-1}\}(t)$ for which we have proved convergence generate an algebra whose closure (in norm) is the set of all operators represented as Fourier transforms of multiplication by a real valued continuous function approaching zero at infinity. The result follows immediately for complex-valued functions. (A similar argument appears in [12]). ▨

For the problem of one body and a repulsive potential we need to make stronger smoothness and repulsivity assumptions to prove (1.2) than were necessary for absolute continuity.

Theorem 5.2. *Let H be as in Theorem 3.3 and suppose that $\partial V/\partial r = 0(r^{-2})$ at $r=0$ and that the angle between the force $-\nabla V$ and the position vector x is bounded away from $\pi/2$, i.e., for some $\beta > 0$,*

$$|\nabla V| \leqq -\beta \frac{x}{|x|} \cdot \nabla V = -\beta \frac{\partial V}{\partial r}. \tag{5.2}$$

Assume also that $V(x) \to 0$ as $|x| \to \infty$. Then the limits (1.2) exist.

Proof. Since

$$\begin{aligned}\left|\frac{\partial V}{\partial x_j}\right| &\leqq |\nabla V| \leqq -\beta \frac{\partial V}{\partial r} \\ &\leqq c^2 (1+r^2)^{-1/2} \left[(-2r)\frac{\partial V}{\partial r} + (2r)^{-2}(1+r^2)^{-\varepsilon/2}\right],\end{aligned}$$

it follows from Theorem 3.3 that $|\partial V/\partial x_j|^{1/2}(H+i)^{-1}$ *is* H-smooth, so by Theorem 2.2, $\{(H-i)^{-1} P_j (H+i)^{-1}\}(t)$ converges as $t \to \pm\infty$, since $i[H, P_j] = -\partial V/\partial x_j$. Therefore by Lemma 5.1 we need only note that $(H_0 \pm i)^{-1} V e^{-iHt}$ converges strongly to zero since $(H_0 \pm i)^{-1} V$ is compact and H is absolutely continuous by Corollary 2.4. ▨

Theorem 5.3. *Let H be as in (3.7), with $V_{jk}(r_{jk}) \to 0$ as $r_{jk} \to \infty$, $0 \geqq V'_{jk} = O(r_{jk}^2)$ at $r_{jk} = 0$. Then the limits (1.2) exist.*

Proof. Since it has been shown in Lemma 3.7 that $(H_0 + i\varrho)^{-1} V e^{-iHt}$ converges to zero as $t \to \pm\infty$, by Lemma 5.1 it remains to show that $\{(H-i)^{-1}(-ie_i \cdot \nabla_k)(H+i)^{-1}\}(t)$ converges as $t \to \pm\infty$, where $e_j, j = 1,2,3$

are the standard basis vectors in $\boldsymbol{R}^3$ and $k=1,2,\ldots,N$. But

$$\begin{aligned}|i[H,(-ie_j\cdot \nabla_k)]| &= |e_j\cdot \nabla_k V|\\ &= \Big|\sum_{l<m} e_j\cdot \nabla_k V_{lm}\Big|\\ &\leqq \sum_{l<m}\Big|e_j\cdot\frac{(x_l-x_m)}{r_{lm}}V'_{lm}(r_{lm})\Big| \quad k=l \quad \text{or} \quad m\\ &\leqq \sum_{l<m}|V'_{lm}(r_{lm})|\,.\end{aligned}$$

The desired result then follows as in Theorem 5.2 from Theorems 3.6 and 2.2. ▨

It is clear that $\omega_\pm$ is a representation of the commutative C^*-algebra of operators of the form $f(P_1,\ldots,P_n)$ (f continuous, $f(p)\to 0$ as $|p|\to\infty$) into operators commuting with H. (See [12].) We can draw some conclusions about limits of other operators if we use the fact that for $\varphi\in\mathscr{D}(H)$, $Ve^{iHt}\varphi\to 0$ as $t\to\pm\infty$. (This is true by relative compactness of V in the one-particle case, and was proved in Lemma 3.7 for the many-particle case.)

Theorem 5.4. *Assume that the limits* (1.2) *exist and* $V(H+1)^{-1}e^{-iHt}$ *converges to zero as* $t\to\pm\infty$. *If* $f:\boldsymbol{R}^n\to\boldsymbol{C}$ *is continuous,* $f(p)(p^2+1)^{-1}$ *approaches zero as* $|p|\to\infty$, *and* $\varphi=(H+1)^{-1}\chi$, *then*

$$\lim_{t\to\pm\infty} e^{iHt}f(P_1,\ldots,P_n)e^{-iHt}\varphi=\omega_\pm(f(P_1,\ldots,P_n)(H_0+1)^{-1})\chi\,.$$

If f is real, such limits determine self-adjoint operators which are essentially self-adjoint on any core of H. These limits exist for all $\varphi\in\mathscr{L}^2(\boldsymbol{R}^n)$ if f is bounded.

Proof. Let $\varphi=(\mathrm{H}+1)^{-1}\chi$. Then

$$\begin{aligned}e^{iHt}f(P_1,\ldots,P_n)e^{-iHt}\varphi &= e^{iHt}f(P_1,\ldots,P_n)e^{-iHt}(H+1)^{-1}\chi\\ &= e^{iHt}f(P_1,\ldots,P_n)(H_0+1)^{-1}e^{-iHt}\chi\\ &\quad -\{e^{iHt}f(P_1,\ldots,P_n)(H_0+1)^{-1}\}V(H+1)^{-1}e^{-iHt}\chi\,.\end{aligned}$$

The first term converges to $\omega_\pm(f(P_1,\ldots,P_n)(H_0+1)^{-1})\chi$ and the second converges to zero. If f is bounded then the limit exists for all $\varphi\in\mathscr{L}^2(\boldsymbol{R}^n)$, since it already exists on a dense set.

Suppose f is real. Then

$$\lim_{t\to\pm\infty} e^{iHt}f(P_1,\ldots,P_n)e^{-iHt}\varphi=\omega_\pm(f(P_1,\ldots,P_n)(H_0+1)^{-1})(H+1)\varphi\,.$$

The product of the self-adjoint operator $H+1$ and a bounded self-adjoint commuting operator is essentially self-adjoint on any core of H. (This can be seen by representing them as multiplication operators.) ▨

The problem stated in Section 1 was to show that every state of the interacting system can be understood as a scattering state in the sense that the interacting system resembles the free system as $t \to \pm\infty$. We have proved that momentum observables are asymptotically constant, as in the free system. Now we shall show that position observables also behave as $t \to \pm\infty$ as they would in a free system. (See [6].)

Theorem 5.5. *Assume that H is as in Theorem 5.2 or 5.3. If $f: \boldsymbol{R}^n \to \boldsymbol{C}$ is a continuous function and $f(x) \to 0$ as $|x| \to \infty$, then*

$$\operatorname*{s\text{-}lim}_{t \to \pm\infty} e^{iHt} f\left(\frac{x}{t}\right) e^{-iHt} = \omega_{\pm}(f(2P_1, \ldots, 2P_n)).$$

We need a few lemmas for the proof of this theorem.

Lemma 5.6. *Let x_j be the self-adjoint operator of multiplication by the j^{th} coordinate in $\boldsymbol{R}^n$. If $\varphi \in \mathscr{D}(H) \cap \mathscr{D}(x_j)$ then for all t, $e^{-iHt}\varphi \in \mathscr{D}(H) \cap \mathscr{D}(x_j)$ and*

$$e^{iHt} x_j e^{-iHt} \varphi = x_j \varphi + 2 \int_0^t e^{iHs} P_j e^{-iHs} \varphi \, ds.$$

Proof. First note that

$$\begin{aligned} e^{iHt} e^{ix_j h} e^{-iHt} \varphi &= e^{ix_j h} \varphi + \int_0^t e^{iHs} i[H, e^{ix_j h}] e^{-iHs} \varphi \, ds \\ &= e^{ix_j h} \varphi + \int_0^t e^{iHs} [2ih e^{ix_j h} P_j + ih^2] e^{-iHs} \varphi \, ds, \end{aligned}$$

and

$$\begin{aligned} e^{iHt} x_j e^{-iHt} &= \frac{1}{i} \frac{d}{dh} \{e^{iHt} e^{ix_j h} e^{-iHt}\}_{h=0} \\ &= x_j + 2 \int_0^t e^{iHs} P_j e^{-iHs} \, ds. \end{aligned}$$

(Differentiation under the integral is justified by dominated convergence.) ▨

Lemma 5.7. *If the limits (1.2) exist and if $V(H+1)^{-1} e^{-iHt}$ converges to zero as $t \to \pm\infty$ then for $\varphi \in \mathscr{D}(H) \cap \mathscr{D}(x_j)$,*

$$\lim_{t \to \pm\infty} \frac{1}{t} e^{iHt} x_j e^{-iHt} \varphi = 2 \lim_{t \to \pm\infty} e^{iHt} P_j e^{-iHt} \varphi = 2P_j^{\pm} \varphi.$$

Proof. By Lemma 5.6

$$\frac{1}{t} e^{iHt} x_j e^{-iHt} \varphi - 2P_j^{\pm} \varphi = \frac{1}{t} x_j \varphi + \frac{2}{t} \int_0^t (P_j(s) - P^{\pm}) \varphi \, ds.$$

The right member of this equation clearly converges to zero as $t \to \pm\infty$. ▨

Proof of Theorem 5.5. Convergence of $f(e^{iHt}(x_j/t)e^{-iHt})$ (for f continuous, $f(x)\to 0$ as $|x|\to\infty$) follows from convergence of $e^{iHt}(x_j/t)e^{-iHt}\varphi$ to $2P_j^{\pm}\varphi$ for $\varphi \in \mathcal{D}(H)\cap\mathcal{D}(x_j)$ since $P_j^{\pm}$ is essentially self-adjoint on this domain ([14], § 135). But by the Stone-Weierstrass theorem, finite sums of products of continuous functions $f_j : \boldsymbol{R}\to\boldsymbol{C}$

$$f_1(x_1)\dots f_n(x_n), \quad f_j(x_j)\to 0 \quad \text{as} \quad |x|\to\infty$$

are dense in the uniform norm in the set of continuous functions $g : \boldsymbol{R}^n \to \boldsymbol{C}$ which approach zero at infinity. Therefore for such g,

$$\operatorname*{s\text{-}lim}_{t\to\pm\infty} e^{iHt} g\left(\frac{x}{t}\right) e^{-iHt} = \omega_{\pm}(g(2P_1, \dots, 2P_n)). \quad ▨$$

Theorem 5.8. *Let H be as in Theorem 5.5 and let $E^{\pm}(\cdot)$ be the projection valued measure on $\boldsymbol{R}^n$ obtained by simultaneous diagonalization of $2P_1^{\pm}, \dots, 2P_n^{\pm}$. Let B be a ball in $\boldsymbol{R}^n$ and B_δ the set of points of distance less than δ from B. If $\|E^{\pm}(B)\varphi\| = \|\varphi\| = 1$, the probability*

$$\int_{(x/t)\in B_\delta} |e^{-iHt}\varphi(x)|^2\, dx$$

of finding $x/t \in B_\delta$ at time t approaches 1 as $t\to\pm\infty$.

Proof. Let g be a continuous function with

$$g(x)=1 \quad \text{if} \quad x\in B$$
$$g(x)=0 \quad \text{if} \quad x\notin B_\delta$$
$$0 \leqq g(x) \leqq 1 .$$

Then

$$\int_{x/t\in B_\delta} |e^{-iHt}\varphi(x)|^2\, dx \geqq \int_{\boldsymbol{R}^n} g\left(\frac{x}{t}\right) |e^{-iHt}\varphi(x)|^2\, dx = \left\langle g\left(\frac{x}{t}\right) e^{-iHt}\varphi,\ e^{-iHt}\varphi\right\rangle$$

which converges to $\langle \omega_{\pm}(g(P_1, \dots, P_n))\varphi, \varphi\rangle$ as $t\to\pm\infty$. ▨

Such a system behaves very much as if it were free if (1.2) is satisfied, even though this condition is weaker than some others which have been proposed, where the algebra of operators A for which convergence of $A(t)$ is required is larger. In [1] and [2] this algebra is taken to contain all bounded measurable functions of momentum. We have not been able to prove convergence for all such operators (although convergence could be shown e.g. for the characteristic function of a box).

The algebra $\{H_0\}'$ of operators commuting with H_0 seems natural to consider (as is done in [1]), but it is not suitable for many body problems, and probably not for a potential which fails to be almost spherically symmetric. The physical reason for this is that if transverse forces persist far from the origin, such observables as the angular momentum may not be asymptotically constant. (Classically the asymptotic orbits would not be straight lines.) The formula (71) of [3] which is used by Dollard to obtain modified wave operators reveals the difficulties with the algebra $\{H_0\}'$ in the many body case.

The family of operators

$$e^{iHt}\, e^{-iH_0t}\, A\, e^{iH_0t}\, e^{-iHt} \tag{5.3}$$

for A in some irreducible algebra is also studied in scattering theory, especially for field theoretic problems, but the similarity between this approach and those of [1, 2, 12], and (1.2) is not deep. For long range potentials it is essential to consider a *reducible* algebra. Another difference is that (1.2) makes a statement about every vector φ for which convergence takes place, whereas for compact A, the limit of (5.3) is automatically zero on the orthocomplement of the range of the wave operator (if it exists). On the other hand the limits (1.2) do not answer the first question of scattering theory: can every type of free behavior be observed as $t \to \pm\infty$? The existence of the wave operators, or limits of (5.3), or Dollard's modified wave operators all answer this affirmatively.

This question can be put in a weak form: are momenta in any neighborhood in momentum space impossible to observe as $t \to \pm\infty$? One can imagine physical situations with infinite barriers where this does happen. (It is difficult to say how one would recognize physically the situation when this does not happen, but the Dollard wave operators do not exist.)

This question can be answered "no" if the homomorphisms $\omega_\pm$ are injective, for any neighborhood in momentum space supports a non-zero continuous function.

Theorem 5.9. *Let H be as in Theorem 5.2. Then $\omega_\pm$ is injective. In fact an inverse is given by*

$$\omega_\pm^{-1}(\omega_\pm(A)) = s\text{-}\lim_{t\to\pm\infty} e^{iH_0t}\,\omega_\pm(A)\, e^{-iH_0t}\,.$$

The idea of the proof is that for a state vector φ which describes a particle which is far away from the center and moving out, $f(P_1, P_2, P_3)\varphi$ should be close to $\omega_+(f(P_1, P_2, P_3))\varphi$, and therefore the latter can't vanish. Such a vector φ can be obtained by taking $\varphi = e^{-iH_0t}\chi$ for t large, and the extent to which φ is far away and moving out is effectively measured by the progress operator A. First we note:

Lemma 5.10. *In $\mathscr{L}^2(\boldsymbol{R}^3)$ let A be the operator defined by* (3.1), *and H as in Theorem 5.2. Then for $\varphi \in \mathscr{D}(H)$,*

$$\lim_{t\to\pm\infty} \langle A\, e^{-iHt}\varphi, e^{-iHt}\varphi\rangle = \pm\langle 2g(\infty)\sqrt{H}\,\varphi, \varphi\rangle\,.$$

Proof. First we show that

$$\lim_{t\to\pm\infty} e^{iHt}\frac{x_j}{r}g(r)\,e^{-iHt}\varphi = \pm g(\infty)\,P_j^{\pm}\,H^{-1/2}\varphi\,.$$

Let B_ε be a ball of center $p=(p_1,p_2,p_3)\neq 0$ and radius $\varepsilon<|p|$. Then by Theorem 5.8, one can make

$$\left\|\left\{\frac{x_j}{r}g(r)\mp\frac{p_j}{|p|}g(\infty)\right\}e^{-iHt}\,E(B_\varepsilon)\varphi\right\|\leqq\delta\|E(B_\varepsilon)\varphi\|$$

by choosing ε small and $\pm t$ large. But since H is absolutely continuous, it does not have 0 as eigenvalue and any φ can be approximated by a finite sum $\sum_{j=1}^{M} E(B_j)\varphi$ where each B_j is contained in such a ball. It follows that

$$\lim_{t\to\pm\infty} e^{iHt}(x_j/r)\,g(r)\,e^{-iHt}\varphi=\pm P_j^{\pm}\,H^{-1/2}\,g(\infty)\varphi\,.$$

Also,

$$\lim_{t\to\pm\infty} e^{iHt}\,P_j e^{-iHt}\varphi=P_j^{\pm}\,\varphi\,,$$

so

$$\begin{aligned}&\lim_{t\to\pm\infty}\langle e^{iHt}Ae^{-iHt}\varphi,\varphi\rangle\\ &\quad=\lim_{t\to\pm\infty}\sum_{j=1}^{3}2\,\mathrm{Re}\left\langle e^{iHt}\frac{x_j}{r}g(r)\,e^{-iHt}\varphi,\,e^{iHt}P_j^{\pm}\,e^{-iHt}\varphi\right\rangle\\ &\quad=\pm 2g(\infty)\,\langle H^{1/2}\varphi,\varphi\rangle\,.\end{aligned}$$ ▨

Proof of Theorem 5.9. First we note that since Ve^{-iH_0t} converges to zero we have for $\varphi\in\mathscr{D}(H)$,

$$\lim_{t\to\pm\infty} e^{iH_0t}\,H^{1/2}\,e^{-iH_0t}\varphi=H_0^{1/2}\,\varphi\,.$$

Using this and Lemma 5.10 (applied to H_0) we have for any ε there exists T such that for $t>T$

$$\frac{1}{2g(\infty)}\langle A\,e^{-iH_0t}\varphi,e^{-iH_0t}\varphi\rangle\geqq\langle H^{1/2}e^{-iH_0t}\varphi,e^{-iH_0t}\varphi\rangle-\varepsilon\,\|\varphi\|^2\,.$$

Let $\varphi(t)=e^{-iH_0t}\varphi$.

$$\begin{aligned}\|(P_i^+-P_i)\,\varphi(t)\|&=\sup_{\chi\neq 0}\frac{1}{\|\chi\|}\left|\int_0^\infty\left\langle\frac{\partial V}{\partial x_i}\,e^{-iHs}\varphi(t),e^{-iHs}\chi\right\rangle ds\right|\\ &\leqq C\sup_{\chi\neq 0}\left\{\int_0^\infty\langle i[H,A]\,(s)\,\varphi(t),\varphi(t)\rangle\,ds\right\}^{1/2}\\ &\qquad\cdot\left\{\frac{1}{\|\chi\|^2}\int_0^\infty\langle i[H,A]\,(s)\chi,\chi\rangle\,ds\right\}^{1/2}\\ &\leqq C'\{\langle A(\infty)\,\varphi(t),\varphi(t)\rangle-\langle A\,\varphi(t),\varphi(t)\rangle\}^{1/2}\\ &=C'\{g(\infty)\,2\langle H^{1/2}\varphi(t),\varphi(t)\rangle-\langle A\,\varphi(t),\varphi(t)\rangle\}^{1/2}\\ &\leqq C''\varepsilon^{1/2}\,\|\varphi\|\,.\end{aligned}$$

Thus for $\varphi \in \mathscr{D}(H)$

$$\lim_{t \to \infty} e^{iH_0 t} P_i^+ e^{-iH_0 t} \varphi = P_i \varphi$$

and therefore

$$s\text{-}\lim_{t \to \infty} e^{iH_0 t} f(P_1^+, P_2^+, P_3^+) e^{-iH_0 t} = f(P_1, P_2, P_3)$$

by an argument like that in the proof of Theorem 5.5. These limits provide an inverse to ω_+; similarly ω_- has an inverse. ▨

We hope we have made a case for the usefulness of positive commutators and the progress operator A in scattering theory. But there is still a long way to go in applying these ideas to more general problems.

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