AN OVERVIEW OF RIGOROUS SCATTERING THEORY

B. Simon

We discuss the three main foundational problems of rigorous scattering theory: existence of wave operators, completeness of wave operators and absence of singular spectrum. We describe many of the mathematical techniques: Cook's method, the trace class theory of Kato and Birman, Kato's theory of smooth perturbations, the weighted L^2 method of Agmon and Kuroda and the new approach of V. Enss.

1 Introduction

The bulk of the rigorous work in scattering theory has concerned itself with three main problems; we begin by describing them in the simplest situation where $H = H_o + V$ with $H_o = -\Delta$ and V "short range", e.g. e^{-r}/r.

(a) Existence of Wave Operators We generally describe a prepared state in terms of parameters most suitable for a particle moving under the influence of H_o. Thus, if $e^{-itH_o}\phi$ is a free wave packet (think of ϕ as peaked about certain momenta), one wants an interacting wave packet, $e^{-itH}\psi$ so that

$$\| e^{-itH_o}\phi - e^{-itH}\psi\| \to 0 \text{ as } t \to -\infty . \tag{1.1}$$

Since e^{itH} is unitary

$$\psi = \lim_{t \to -\infty} e^{itH} e^{-itH_o} \phi . \tag{1.2}$$

If we deal only with physical (i.e. normalizable) states, we expect that the limit in (1.2) will exist for all ϕ in the basic Hilbert space of the problem, $L^2(R^3)$. In that case, the limit is said to exist in the strong operator topology and we write

$$\Omega^{\pm}(H,H_o) = \underset{t \to \mp\infty}{\text{s-lim}}\; e^{itH} e^{-itH_o} . \tag{1.3}$$

$\Omega^{\pm}$ are called the wave operators and the first problem is to show that the limit in (1.3) exists. We note that the strange convention on the $\pm$ in (1.3) is standard in the physics literature although it is only sometimes used in the more mathematical literature. It comes from the fact that $\Omega^{\pm}$ is connected with the resolvent $R(z) = (z - H)^{-1}$ for $z = x \pm i0$ (with x real) in the time-independent theory. Also note that since $e^{itH} e^{-itH_o}$ is unitary

$$\| \Omega^{\pm} \phi \| = \| \phi \| \quad . \tag{1.4}$$

(b) Completeness of Wave Operators It is a standard argument in quantum mechanics courses that unitarity of the S-matrix is merely an expression of conservation of probability. There is a hidden additional assumption that is being made here. After all, S is given by the condition that $|(\eta, S\phi)|^2$ is just the probability that a state which looks like $e^{-itH_o}\phi$ in the distant past and which moves under e^{-itH} will look like $e^{-itH_o}\eta$ in the distant future, i.e. $(\eta, S\phi)$ is the overlap of $\Omega^+\phi$ and $\Omega^-\eta$ which leads to

$$S = (\Omega^-)^* \, \Omega^+ \quad . \tag{1.5}$$

(1.4) immediately tells us how $(\Omega^{\pm})^*$ operate. They must be the inverse of $\Omega^{\pm}$ on $\mathrm{Ran}(\Omega^{\pm})$ since $(\Omega^+)^* \Omega^+ = (\Omega^-)^* \Omega^- = 1$ (by (1.4)). But suppose that $\eta \perp \mathrm{Ran}\, \Omega^+$. Then $(\eta, \Omega^+\phi) = 0$ for all ϕ so that $(\Omega^+)^*\eta \perp$ all ϕ so $(\Omega^+)^*\eta = 0$. Thus $(\Omega^+)^*$ is 0 on $(\mathrm{Ran}\, \Omega^+)^{\perp}$ and the inverse of Ω^+ on $\mathrm{Ran}\, \Omega^+$. This means that S preserves norms only if $\mathrm{Ran}\, \Omega^+ \subset \mathrm{Ran}\, \Omega^-$. Similarly S^* preserves norms only if $\mathrm{Ran}\, \Omega^- \subset \mathrm{Ran}\, \Omega^+$. Thus $S^*S = SS^* = 1$ if and only if

$$\mathrm{Ran}\, \Omega^+ = \mathrm{Ran}\, \Omega^- \quad . \tag{1.6}$$

Proving (1.6) is sometimes called the problem of weak asymptotic completeness. Physically, it corresponds to the assertion that any state which is asymptotically free in the past will also be of that type in the future; it is clear that such an assumption is tacitly made in deducing unitarity of S from "conservation of probability". How can (1.6) fail? It's not easy, but Pearson [22] has constructed a singular potential V so that $H = -\Delta + V$ is well-defined and physically reasonably (i.e. self-adjoint and bounded from below) and so that $\Omega^{\pm}$ exist but with (1.6) false! For his H, one can take a vector $\phi = \Omega^+\eta$ so that as $t \to +\infty$, $e^{-itH}\phi$ breaks into two pieces, one of which moves out to infinity; the other asymptotically approaches 0 which is where V is very singular. Often, one asks about a stronger property than (1.6), namely that

$$\mathrm{Ran}\, \Omega^+ = \mathrm{Ran}\, \Omega^- = \mathcal{H}_{pp}^{\perp} \tag{1.7}$$

where $\mathcal{H}_{pp}$ is the span of the eigenvectors of H. Physically (1.7), which is called asymptotic completeness asserts that any state is either bound (in $\mathcal{H}_{pp}$) or a scattering state (in $\mathrm{Ran}\, \Omega^+ = \mathrm{Ran}\, \Omega^-$); here, "either" is intended in the quantum mechanical sense, that is, we mean any state is a superposition of a bound and a scattering state.

(c) Absence of Singular Continuous Spectrum To describe the last problem requires a very short course in functional analysis; for a more detailed "course", see [25]. If H is any self-adjoint operator and ϕ is any vector, there is a measure $d\mu$ on $(-\infty, \infty)$ so that $(\phi, e^{-itH}\phi) = \int e^{-itx}\, d\mu(x)$. $d\mu$ is called the spectral measure (of ϕ, for H). To understand the kind of pathology about which one can worry, we need to consider a measure constructed by Cantor. First, Cantor constructed a function, f, as follows: $f = 0$ on $(-\infty, 0]$, $f = 1$ on $[1, \infty)$; f is only interesting on (0,1) where it is given by $f = \frac{1}{2}$ on (1/3, 2/3); f = 1/4 on (1/9, 2/9) and 3/4 on (7/9), 8/9), f = 1/8 on (1/27, 2/27) etc. Formally if $x = \sum_{n=1}^{\infty} a_n/3^n$ with each $a_n = 0,1,2$, then let N(x) = first n with $a_{n+1} = 1$ ($N = \infty$ if each $a_n = 0$ or 2) and

$$f(x) = 1/2 + \sum_{n=1}^{N(x)} (a_n - 1)/2^{n+1}$$

Notice that f is a queer function indeed: it is continuous and at any x with $N(x) < \infty$, f is differentiable with $f'(x) = 0$. The set of such points has size $1/3 + 2(1/9) + 4(1/27) + \ldots = 1$ but f is not constant! The Cantor measure is the Lebesgue Stieltjes measure df determined by f. Thus, for nice g, one can define $\int g\,df$ as one does the Riemann integral by $\lim_{n\to\infty} \sum_{k=1}^{2^n} g(k/2^n)$ $[f(k/2^n) - f((k-1)/2^n)]$. The Cantor measure has no pure points, i.e. $\lim_{\varepsilon\to 0} \int_{a-\varepsilon}^{a+\varepsilon} df = 0$ for all a but it still manages to live on a set of Lebesgue measure $1-1 = 0$. Such a pathological measure is called a singular continuous measure. The Lebesgue decomposition theorem asserts that any measure has the form $d\mu = d\mu_{pp} + d\mu_{ac} + d\mu_{sing}$ where $d\mu_{pp}$ is pure point, literally of the form $\sum_{n=1}^{\infty} a_n \delta(x-x_n)$, $d\mu_{ac}$ is of the form $g(x)dx$ and $d\mu_{sing}$ is singular continuous. Using this result, one shows that given any self-adjoint operator H on a Hilbert space $\mathcal{H}$, there is a decomposition $\mathcal{H} = \mathcal{H}_{pp} \oplus \mathcal{H}_{ac} \oplus \mathcal{H}_{sing}$ so that $\phi \in \mathcal{H}_{pp}$ (etc.) if and only if the spectral measure of ϕ for H is pure point (etc.). The last problem of the three is to prove that

$$\mathcal{H}_{sing} = \{0\} . \tag{1.8}$$

Why should we expect this? $\mathcal{H}_{pp}$ is precisely the span of the eigenvectors of H. Moreover, we claim that

$$\mathcal{H}_{ac} \supset \text{Ran}\ \Omega^{\pm} \tag{1.9}$$

so that (1.7) is equivalent to the pair of statements: (1.8) and

$$\text{Ran}\ \Omega^{+} = \text{Ran}\ \Omega^{-} = \mathcal{H}_{ac} . \tag{1.10}$$

(1.10) is often called completeness. To prove (1.9), we note that

$$e^{isH}\,\Omega^{\pm}\,e^{-isH_0} = \underset{t\to\mp\infty}{\text{s-lim}}\ e^{i(s+t)H}\,e^{-i(s+t)H_0} = \Omega^{\pm} ,$$

so

$$e^{isH}\,\Omega^{\pm} = \Omega^{\pm}\,e^{isH_0} , \tag{1.11}$$

and thus $(\Omega^{+}\phi,\ e^{isH}\,\Omega^{+}\phi) = (\phi,\ e^{isH_0}\,\phi)$. This says that the spectral measure of $\Omega^{+}\phi$ for H is the same as that of ϕ for H_0; this is just a sophisticated form of conservation of energy. Since $H_0 = -\Delta$ has purely absolutely continuous spectrum, (1.9) holds.

Pearson [23] has announced results on the existence of potentials V on $(-\infty, \infty)$ with V smooth and $V(x) \to 0$ at infinity so that $-\frac{d^2}{dx^2} + V$ has only singular continuous spectrum. It is worthwhile describing his example in some detail since it illustrates the kind of dynamical behavior that occurs when H has singular spectrum. Let V be an even function on $(-\infty, \infty)$, so that for x positive,

$$V(x) = \sum_{n=0}^{\infty} a_n\, f(x - y_n) ,$$

where f is a fixed non-negative C^{∞} function with support in $(-\frac{1}{2},\frac{1}{2})$, the a_n's obey $\Sigma a_n^{\,2} = \infty$ (but this can be done with $a_n \to 0$) and the y_n's are given by the condition

$$y_{n+1} - y_n = \exp(e^n) .$$

Pearson's statement is that for this V we have purely singular spectrum. Rather than try to describe his proof, let us give his argument as to why physically one expects the result. The canonical example of a potential which manages to have absolutely continuous states without V going to zero is a periodic potential with its Bloch wave packets. The particle manages to get through the infinity of bumps by cleverly building up coherences, i.e. the phases necessary for it to get through one bump help it get through the next. In this case, the enormous separation between y's causes the particle to "forget" any coherence it has built up; one can imagine the particle as successively undergoing independent collisions with potentials $a_n f$. By the Born approximation, for a_n small, the reflection from this potential is $O(a_n^2)$. The condition $\Sigma a_n^2 = \infty$ implies no particles reach infinity. Moreover, by tunnelling, the positivity of V and the inability to build up coherence, one expects no bound states. Thus, particles moving under H wander aimlessly about and this is precisely what corresponds to singular spectrum. Indeed, if $f(t) \equiv (\phi, e^{-itH}\phi) = \int e^{-ixt} d\mu(x)$ with $d\mu$ singular continuous, then f goes to zero in some average sense, since a theorem of Wiener assures that for the Fourier transform of any continuous measure:

$$\frac{1}{2T}\int_{-T}^{T} |f(t)|^2 \, dt \to 0 \tag{1.12}$$

On the other hand, f may not go to zero pointwise; for example, for the Cantor measure,

$$f(t) = e^{-\frac{1}{2}it} \prod_{n=1}^{\infty} \cos(3^{-n} t) ,$$

so that $|f(2\pi 3^m)| = |f(2\pi)| \neq 0$ for all m. This can only happen for singular measures; if μ is absolutely continuous, then the Riemann-Lebesgue lemma asserts that $f(t) \to 0$ as $t \to \infty$.

This completes our description of the three basic problems of rigorous scattering theory. In the rest of this paper, we will give a quick hit-and-run description of most of the major techniques of the subject. The one technique that we leave out is that of "complex scaling" or "dilation analyticity" - in part because it is not very scattering theoretic and, in part, because the proceedings of the March 1978 Sanibel Workshop [29] give a comprehensive overview of much of the subject. We also concentrate on the two body case with $r^{-1-\varepsilon}$ potentials where things are easier to describe. However, we should mention that wave operators in multiparticle situations had to be extended to consider channel

wave operators: a <u>channel</u>, α, of a N-body system, is a decomposition, $D(\alpha)$, of the particles into disjoint clusters $C_1,\ldots,C_k$ and bound states $\eta_1,\ldots,\eta_k$ of the Hamiltonian $H(C_i)$ of the internal motion of the clusters. One defines $H_D = H - I_D$ where H is the Hamiltonian of the whole system with center of mass motion removed and I_D is the sum of all potentials between particles in <u>different</u> clusters. Also one lets P_α be the projection onto all states of the form $(\Pi\eta_i)\phi$ with ϕ a function of the differences of the centers of mass of the cluster. Then, the <u>channel wave operator</u> is

$$\Omega_\alpha^\pm = \underset{t \to \mp\infty}{\text{s-lim}} \; e^{itH} e^{-itH_\alpha} P_\alpha \tag{1.13}$$

A result of Jauch [15] asserts that if one is careful about counting channels associated with degenerate eigenvalues of $H(C_i)$, then the Ran Ω_α^+ are mutually orthogonal. Asymptotic completeness then says that

$$\bigoplus_\alpha \text{Ran}\, \Omega_\alpha^+ = \bigoplus_\alpha \text{Ran}\, \Omega_\alpha^- = \mathcal{H}_{pp}^\perp \tag{1.14}$$

We should also mention that for $V = \lambda|r|^{-1}$, the s-lim (1.3) does not exist [8] because of the celebrated infinite phases of the Coulomb scattering problem. Rather one needs a modified dynamics, $U_D(t) = \exp(-if(-i\nabla,t))$, so chosen that

$$\Omega_D^\pm = \underset{t \to \mp\infty}{\text{s-lim}} \; e^{itH} U_D(t)$$

exists but so that (1.11) is still true (this will happen so long as $f(-i\nabla, t+s) - f(-i\nabla,t) \to s(-\Delta)$ as $t \to \infty$ with s fixed, e.g. $f(-i\nabla, t) = t(-\Delta) + t^\alpha g(\Delta)$ or $+ (\ln(t)g(\Delta))$. The proper physics will occur if $\int [|e^{-itH_0}\phi| - |U_D(t)\phi|]^2 \to 0$ so that up to "unimportant phases", $e^{-itH}\Omega_D^+\eta$ looks like $e^{-itH_0}\eta$ as $t \to -\infty$.

For a more detailed review of the status of the problems and more exhaustive presentation of the methods, see [26,27]. We note here that problem (a) has been solved in extremely great generality and the problems (b) and (c) for the two body case have also been solved. For the N-body case, problems (b) and (c) have only been solved in some special cases at the present instant (e.g. 3-bodies, or repulsive potentials, or weak coupling or "generic" dilation analytic potentials with sufficient fall off). However, Enss [10] is very close to extending his method described in Section 6 to N bodies and Combes [5] has a program based on the method of weighted L^2-space (Section 5) and some ideas of Deift-Simon [7], which appears promising. I hope that these problems will be solved soon and will free our energies for studying some of the more physical problems in the subject.

Finally I should attempt to explain why a practicing atomic theorist should care about the work on these questions which after all involve issues where any betting man would wager a great deal on the truth of the "obvious" answers. Let me give some reasons:

(a) Atomic physics should be a science and not an art: in studying a model like the purely Coulombic Hamiltonian, one should be able to derive basic properties like the unitarity of the S-matrix from first principles even if the derivation is not easy.

(b) These studies occasionally provide new insights into or even unexpected theorems about issues of direct experimental interest. I might mention, somewhat immodestly, my own theorem [30] concerning the absence of resonances in atomic systems at energies sufficient to completely ionize the atom.

(c) Occasionally, new calculational tools come from the rigorous work. The canonical example would be the famous work of Faddeev: he was motivated by wishing to solve the three basic problems we have described but his work has produced a computational industry!

"Rigorous" and "practical" atomic physics are two fields which have not interacted much with each other. Recently, there has been some attempts to change this and I regard this development as very exciting. The possibilities for cross-pollinization are very great indeed.

2 Cook's Method [6]

In virtually all Hilbert space theoretic scattering problems including optical and acoustical scattering as well as non-relativistic quantum scattering, one can solve the wave operator existence by a general method known as Cook's method or by one of its variants. One first notes that by a simple density argument (the $\varepsilon/3$ trick [25]), it suffices to prove that the limit (1.2) exists for a dense set of ϕ. Indeed, since $e^{+itH}e^{-itH_0}$ is linear, it need only be proven for a total set, i.e. a set whose finite linear combinations is dense. Using the completeness of a Hilbert space, we see that:

PROPOSITION 2.1 *Let $W(t) \equiv e^{+itH}e^{-itH_0}$. In order for the limit (1.2) to exist for all ϕ, it suffices that there is a total set $\mathcal{D}$ so that for any $\phi \in \mathcal{D}$:*

$$\lim_{t,s \to \pm\infty} \| [W(t) - W(s)]\phi \| = 0$$

How can we estimate $(W(t) - W(s))\phi$? Simple. Suppose that $W(t)\phi$ is differentiable. Then, for $s < t$

$$\| [W(t) - W(s)]\phi \| \leq \int_s^t \| \frac{d}{du} W(u)\phi \| \, du \tag{2.1}$$

by the fundamental theorem of calculus. Moreover if $H = H_0 + V$, then, at least formally

$$\frac{d}{dt} W(t)\phi = ie^{+itH} V e^{-itH_0} \phi \tag{2.2}$$

The technical domain conditions given below are chosen so that one can justify (2.2).

THEOREM 2.2 (Cook's method). Suppose that $H\phi - H_o\phi \equiv V\phi$ for $\phi \in D(H) \cap D(H_o)$. Suppose moreover, there is a total set $\mathcal{D} \subset D(H_o)$ so that $e^{-itH_o}\phi \in D(H)$ if $|t| \geq 1$ and that

$$\int_1^\infty \| V e^{\pm itH_o}\phi\| \, dt < \infty \tag{2.3}$$

for all $\phi \in \mathcal{D}$. Then $\Omega^\pm(H,H_o)$ exist.

Proof. (2.2) holds by the domain hypothesis. Thus, by (2.3) we have that the right side of (2.1) goes to zero as $s,t \to \infty$ or as $s,t \to -\infty$. Proposition 2.1 completes the proof. Q.E.D.

Cook's method has been generalized to accommodate local singularities [17] and to accommodate form perturbations [31]. We want to describe how an estimate like (2.3) can be proven for $H_o = -\Delta$ and V's behaving like $r^{-1-\epsilon}$ at infinity. There seem to be three general techniques:

(a) (Kuroda [18]) Take $\mathcal{D}$ to be the set of Gaussians $\phi_o = \exp(-a(x-x_o)^2)$ which are total. Using the explicit formula for $e^{-itH_o}\phi_o$, one easily proves (2.3) for any "reasonable" V.

(b) (Cook [6] used (2.5); the rest is folklore). Let ϕ be a nice smooth function with rapid falloff. Then certainly

$$\| e^{-itH_o}\phi\|_2 = \|\phi\|_2 \tag{2.4}$$

where

$$\|f\|_p = \left(\int |f(x)|^p dx\right)^{1/p}; \quad \|f\|_\infty = \text{ess.sup.}|f(x)|$$

Moreover, from the explicit integral kernel for e^{-itH_o}, i.e.

$$(e^{-itH_o}f)(x) = (4\pi it)^{-3/2}\int \exp(+(x-y)^2/2it) f(y)dy$$

one sees that

$$\| e^{-itH_o}\phi\|_\infty \leq t^{-3/2}\|\phi\|_1 \tag{2.5}$$

Hölder's inequality implies that

$$\|f\|_p \leq \|f\|_r^\theta \, \|f\|_q^{1-\theta} \quad ; \; p^{-1} = \theta r^{-1} + (1-\theta)q^{-1}$$

so, by (2.4) and (2.5)

$$\| e^{-itH_o}\phi\|_p \leq t^{-3(1/2-1/p)}\|\phi\|_1^{2/p}\|\phi\|_\infty^{1-2/p} \quad 2 \leq p \leq \infty \tag{2.6}$$

(Actually by using a more sophisticated tool, called complex interpolation, one can prove [2,7] that

$$\| e^{-itH_o}\phi\|_p \leq t^{-3(1/2-1/p)}\|\phi\|_{p'}$$

$$p' = (1-p^{-1})^{-1} \; ; \; 2 \leq p \leq \infty) \tag{2.6'}$$

Using the general Hölder inequality

$$\|V\eta\|_p \leq \|V\|_r \, \|\eta\|_q \qquad p^{-1} = r^{-1} + q^{-1}$$

one sees that for nice enough ϕ,

$$\| V e^{-itH_o}\phi\|_2 \leq C\, t^{-3/r}\|V\|_r \; ; \; r \geq 2 \tag{2.7}$$

As a result (2.3) holds for $H_o = -\Delta$ so long as $V \in L^2 + L^r$, $r < 3$. (Notice that $|r|^{-1-\epsilon}$ is just barely in $L^2 + L^{3-\delta}$).

(c) (Advocated by Haag [3], used in [17] in weak form, raised to high art in [13]). To explain the idea, we explain it in one dimension. Let $(e^{-itH_o}u)(x) = u(x,t)$. Then, in terms of the Fourier transform

$$u(x,t) = (2\pi)^{-\frac{1}{2}}\int e^{ikx - ik^2t}\,\hat{u}(k)\,dk \tag{2.8}$$

Now suppose that $\hat{u}$ is smooth and has support in some bounded set K.

Then, for $x/t \notin 2K = \{2k|\ k\varepsilon K\}$ and $k\varepsilon K$

$$\left(\frac{1}{ix - 2ikt}\frac{d}{dk}\right)^n e^{ikx - ik^2t} = e^{ikx - ik^2t}$$

Putting this in (2.8), and integrating by parts, one sees that

$$|u(x,t)| \le C_n (1 + |x| + |t|)^{-n};\ x/t \notin (2+\varepsilon) K$$

2K plays a special role here as the set of classically allowed velocities where the group velocity $\partial E(k)/\partial k$ is the relevant velocity. In three dimensions one has to break up $(\vec{x}, t, \vec{k})$ space into pieces since $(ix - 2ikt)^{-1}\ d/dk$ must be replaced by $[(ix - 2ikt)\cdot\rho]^{-1}\ d/d(k.\rho)$ for a suitable unit vector ρ, depending on where we are in $(\vec{x}, t, \vec{k})$ space. Being more explicit about the dependence of C_n on u, and using space translation invariance, one finds [13,32]:

$$|u(x,t)| \le C_{n,\theta}(1 + |x - x_o| + |t|)^{-n}$$
$$\|(1 + |x - x_o|)^n u\|_2\ ;\ (x - x_o/t) \notin \theta \quad (2.9)$$

where $\frac{1}{2}\theta$ is any set containing the support of $\hat{u}$. To use this estimate to prove (2.3), we follow an idea of Enss [9]. Let $F(|x| \le R)$ be the projection onto all functions supported in the set of x with $|x| \le R$ etc. Let us suppose that V is bounded and

$$\int_1^\infty \|V F(|x| \ge R)\|\ dR < \infty \quad (2.10)$$

(this allows no local singularities but there are modifications which do; roughly speaking (2.10) says that V is $O(R^{-1-\varepsilon})$). Then

$$\|V e^{-itH_o} u\| \le \|V F(|x| \ge \theta t)e^{-itH_o} u\|$$
$$+ \|V F(|x| \le at)\ e^{-itH_o} u\|$$
$$\le \|V F(|x| \ge at)\|\ \|u\| + \|V\|_\infty \|F(|x| \le at)e^{itH_o} u\|_2 \quad (2.11)$$

The second term in (2.11) is L^1 in t by (2.9) so long as $\hat{u}$ is supported away from 0 and $a < \inf\{2k|k\varepsilon \text{ supp } \hat{u}\}$ and the first is in L^1 by (2.10) if $a > 0$. Thus (2.3) holds.

We close this section by answering a question that may have occurred to the reader: if the Gaussian wave packet argument ((a) above) works, why bother with the more sophisticated arguments (b), (c) above? Here is the answer:

(i) By working for general V's or wave functions, the alternate methods can be useful in situations which go beyond mere existence of $\Omega^\pm$; see, for example, § 6 where (2.9) plays an important role.

(ii) The Gaussian proof depends on having $H_o = -\Delta$. If H_o was a free Dirac Hamiltonian or if we want to describe impurity scattering in a solid, one of the other approaches would be more useful.

3 The Kato-Birman Theory (Trace Class Method)

In this section we want to describe a method initiated by T. Kato with further developments by M. Rosenblum, S. Kuroda, L. DeBranges, D. Pearson and most especially M.S. Birman and T. Kato. The simplest proof of the basic result is due to Pearson [24] and can be used as the basis of the whole theory [26].

Definition (a) For any bounded operator, A, on a Hilbert space, one defines its absolute value, $|A|$ to be $\sqrt{A^*A}$.

(b) For any A, $\sum_{n=1}^{\infty}(\phi_n, |A|\ \phi_n)$ is independent of the orthonomal basis $\{\phi_n\}$ chosen. The trace class, $\mathcal{C}_1$, is the set of A with the sum finite.

(b) $\mathcal{C}_p$ is the set of A with $|A|^p$ trace class. $\mathcal{C}_2$ is called the Hilbert-Schmidt operators.

We warn the reader that there are lots of subtleties in the theory (see [33] for a pedagogical overview); for example, $|A + B| \le |A| + |B|$ (operator inequality) is false even for

2 x 2 matrices. Moreover, there are integral operators $(Af)(x) = \int K(x,y)\, f(y)dy$ with K continuous, and $\int |K(x,x)|dx < \infty$ but A not trace class. However, A is trace class if and only if A = BC with B,C Hilbert-Schmidt and an integral operator is Hilbert-Schmidt if and only if $\int |K(x,y)|^2\, dxdy < \infty$. Moreover, A trace class and B bounded implies AB trace class. The basic trace class scattering theorem depends on an abstract setup.

Definition Let A,B be self-adjoint operators and let $P_{ac}(A)$ be the projection onto the absolutely continuous subspace for A. Then, we say that $\Omega^{\pm}(B,A)$ exists if

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

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

THEOREM 3.1 Suppose that either
(a) B-A is trace class
or (b) $(B + i)^{-1} - (A + i)^{-1}$ is trace class
or (c) $A,B \geq -c$ and $(A + c + 1)^{-1} - (B + c + 1)^{-1}$ is trace class.
Then $\Omega^{\pm}(B,A)$ exist and are complete.

We will not give a complete proof or various extensions (see [26]) but we will describe a few of the input ideas. One simple but basic idea is

THEOREM 3.2 Suppose that $\Omega^{\pm}(B,A)$ exist. Then they are complete if and only if $\Omega^{\pm}(A,B)$ exist.

This theorem means that existence under a condition symmetric in A,B implies completeness; see [7] for a multiparticle analog. Another important element is the use of a so-called invariance principle: i.e. that $\Omega^{\pm}(\phi(A), \phi(B)) = \Omega^{\pm}(A,B)$ for suitable ϕ's under suitable circumstances.

As for applications, we note:

THEOREM 3.3 Let $V \in L^1(R^3)$ and suppose that $H = -\Delta + V$ is such that $(H + i)^{-1}(H_o + i)$ is bounded. Then $(H + i)^{-1} - (H_o + i)^{-1}$ is trace class and, in particular, $\Omega^{\pm}(H,H_o)$ exist and are complete.

Proof Writing

$$\begin{aligned}(H + i)^{-1} &- (H_o + i)^{-1} \\ &= [(H + i)^{-1} (H_o + i)]\, [(H_o + i)^{-1}|V|^{\frac12}]\, (\operatorname{sgn} V)[|V|^{\frac12}(H_o + i)^{-1}],\end{aligned}$$

we see that it suffices to prove that $|V|^{\frac12}(H_o + i)^{-1}$ is Hilbert-Schmidt. But this operator has an integral kernel $|V(x)|^{\frac12}(4\pi|x - y|)^{-1}\exp(\alpha|x - y|)$, with $\operatorname{Re}\alpha > 0$, $\alpha^2 = i$, which is clearly in $L^2(R^6)$ Q.E.D.

Roughly speaking, the condition $V \in L^1(R^3)$ requires that $V \sim |x|^{-3-\varepsilon}$ at infinity. If R^3 is replaced by R^ν, then one needs $|x|^{-\nu-\varepsilon}$. Since central potentials are one-dimensional, Kuroda [19] was able to use the trace class theory to prove existence and completeness of wave operators for central potentials obeying

$$\int_0^1 r|V(r)|dr + \int_1^\infty |V(r)|dr < \infty .$$

At first sight, trace class methods appear to be limited to two body problems but Combes [4] had the idea of applying them to N-body problems in the two-cluster regions; i.e. at energies below the lowest three body breakup. Simon [34] has extended this idea, and, in particular has proven:

THEOREM 3.4 Scattering of electrons off neutral atoms is complete below the energy necessary to ionize the atom.

At the present time, this is the only completeness result known for atomic scattering with more than one electron. We also note that Enss [10] has proven Theorem 3.4 with his methods.

4 Kato's Theory of Smooth Perturbations [16]

In this section, we want to say something about a remarkable theory of Kato [16] which has been extended in several ways by Lavine [21]. The basic definition is:

Definition Let A be self-adjoint. B is called A-smooth if and only if

$$\int_{-\infty}^{\infty} \| B e^{-itA} \phi\|^2 \, dt \le c \|\phi\|^2 \tag{4.1}$$

for all ϕ.

Example If $A = -\Delta$ on $L^2(R^3)$ and B is multiplication by a function in L^3, then B is A-smooth. Unfortunately, I know of no simple proof of this fact. The proof can be based on the estimate (2.6').

One use of this notion is seen in

THEOREM 4.1 Let $A = B + \sum_{i=1}^{n} C_i^* D_i$ and suppose that each D_i is A-smooth and each C_i is B-smooth. Then

$$\underset{t\to\mp\infty}{\text{s-lim}}\; e^{itB} e^{-itA} \equiv U_\pm \tag{4.2}$$

exist, are unitary, and

$$U_\pm^{-1} B U_\pm = A \tag{4.3}$$

Proof We show existence of the limit. The fact that the limit is unitary follows from Theorem 3.2, and (4.3) from (1.11). Let ϕ, ψ be in our Hilbert space and write $W(t) = e^{itB} e^{-itA}$.

$$|(\phi,[W(t) - W(s)]\psi)| \le \sum_{i=1}^{n} \int_s^t |(C_i e^{-iuB}\phi, D_i e^{-iuA}\psi)| \, du$$

$$\le \left(\sum_{i=1}^{n} \int_{-\infty}^{\infty} \|C_i e^{-iuB}\phi\|^2 du\right)^{\frac12} \left(\sum_{i=1}^{n} \int_s^t \|D_i e^{-iuA}\psi\|^2 du\right)^{\frac12}$$

by the Schwartz inequality. Using (4.1) and the B-smoothness of C_i we see that

$$\|(W(t) - W(s)\psi\| \le c\left(\sum_{i=1}^{n} \int_s^t \|D_i e^{-iuA}\psi\|^2 du\right)^{\frac12}$$

Using the A-smoothness of D_i, we see that $\|(W(t) - W(s))\psi\| \to 0$ as $s,t \to \infty$. Q.E.D.

In thinking about applications of Theorem 4.1, it is useful to realize the strength of the conclusions. If $A = -\Delta$, B can have no bound states if Theorem 4.2 holds. One case where this is true is small coupling. The following was proven for N = 2 by Kato [26] and for general N by Iorio-O'Carroll [28]:

THEOREM 4.2 For each N, there is a Λ_N so that, if $\|V_{ij}\|_{3/2} < \Lambda_N$ $(1 \le i < j \le N)$, then on $L^2(R^{3N})$

$$H = -\sum_{i=1}^{N} \Delta_i + \sum_{i<j} V_{ij}(r_i - r_j)$$

is unitarily equivalent to $H_o = -\Delta$ under the wave operators $\Omega^\pm(H,H_o)$.

The link between time-dependent and time-independent scattering theory is seen in the fact that the Fourier transform of $\chi_{(0,\infty)}(t)\, e^{-\varepsilon t} B e^{-iAt}\phi$ (with $\chi_{(0,\infty)}(t) = 0$, resp 1 if $t < 0$, resp $t \ge 0$) is $(2\pi)^{-\frac12}(i)^{-1}B(A + \lambda - i\varepsilon)^{-1}$. By the Plancherel relation, (4.1) is equivalent to

$$\lim_{\varepsilon\downarrow 0} \int_{-\infty}^{\infty} [\|B(A + \lambda + i\varepsilon)^{-1}\phi\|^2 + \|B(A + \lambda - i\varepsilon)^{-1}\phi\|^2]$$

$$\le 2\pi c \|\phi\|^2$$

This shows a connection between scattering and boundary values of the resolvent. Since there are also connections between boundary values of the resolvent and the absence of singular spectrum (see Theorem 5.1 below), one has a relation between this problem and smoothness; in fact, one can prove:

THEOREM 4.3 If B is A-smooth then Ran B* is in the absolutely continuous space for A.

A final criteria for smoothness we should mention is the following beautiful result of Kato [16]:

THEOREM 4.4 Let A,B be bounded self-adjoint operators and suppose that $i\,[A,B] \equiv D$ is non-negative. Then $C \equiv \sqrt{D}$ is A-smooth.

Proof. Note that

$$\int_s^t \| Ce^{-iuA}\phi\|^2\, du = \int_s^t i < e^{-iuA}\phi,\ [A,B]\, e^{-iuA}\phi > du$$

$$\equiv \int_s^t \frac{d}{du} < e^{-iuA}\phi,\ B\, e^{-iuA}\phi > du$$

$$\leq 2\, \|B\|\ \|\phi\|^2 \quad \text{Q.E.D.}$$

Lavine [21] noted that if $H = -\Delta + V$ where V is "repulsive" and if D is the generator of dilations, then formally $i[H,D] \geq 0$ so that modulo the technicalities of dealing with unbounded operators, smoothness techniques are available. Indeed, Lavine [21] has used Theorems 4.1 and 4.2 to prove absence of singular spectrum and completeness of wave operators for a large class of (even multiparticle) purely repulsive interactions.

5 The Weighted L^2-Space Method of Agmon and Kuroda [1,20]

Around 1970, Agmon [1] and Kuroda [20] developed what may well be the most powerful method for the study of the basic problems for two-body systems. The method is also useful in the study of multiparticle systems [5, 11, 12]. The method represents the culmination of two developments: the first concerns eigenfunction expansions obtained via Lippmann-Schwinger type equations. This development was initiated by Povzner, Ikebe and Faddeev and developed by a variety of others during the 60's. The second, which we describe below, concerns auxiliary Banach spaces and was developed most especially by Friedrichs, Rejto and Howland. In the late sixties Kuroda and Kato-Kuroda combined the methods and

the main issues concerned the best choice of auxiliary Banach space and a technical problem we mention below solved eventually by the "Agmon bootstrap".

The key to the solution of the completeness and singular spectrum problems by these methods is the control of boundary values of the resolvent. Singular spectrum is eliminated by (see [27]):

THEOREM 5.1 A sufficient condition for an operator, A, to have empty singular continuous spectrum is that there exists $p > 1$, a closed countable set $\mathcal{E}$, in R, and a dense set, X, in $\mathcal{H}$ so that for $[a,b] \subset R\backslash\mathcal{E}$ and $\phi \in X$.

$$\sup_{0 < \varepsilon < 1} \int_a^b |(\phi,\ (A - x - i\varepsilon)^{-1}\phi)|^p\, dx < \infty$$

In particular, if $(\phi, (A - \lambda)^{-1}\phi)$ is bounded as $\lambda \to R\backslash\mathcal{E}$, then A has no singular continuous spectrum.

As we saw in the last section, control of the resolvent also has something to do with completeness; this is most easily seen using Lavine's theory of local smoothness [21]. Now suppose that one tries to choose X to be a Banach space continuously embedded in $\mathcal{H}$. Then any $\phi \in \mathcal{H}$ defines a linear functional via $\chi \to (\phi,\chi)$ (Hilbert space inner product) so $\mathcal{H}$ is imbedded in X*. Of course as λ approaches the spectrum, the norm of $(A - \lambda)^{-1}$ as a map of $\mathcal{H}$ to $\mathcal{H}$ blows up but suppose that as a map of X to X* it does not. Then, so long as $\phi \in X$, $(\phi,(A - \lambda)^{-1}\phi)$ will be bounded as λ approaches the spectrum and we will have the necessary control on spectrum. One natural way of doing this is via a perturbation method. Suppose that $A = H_o + V$ and write

$$(H - \lambda)^{-1} = (H_o - \lambda)^{-1}\,(1 + V(H_o - \lambda)^{-1})^{-1} \tag{5.1}$$

The overall strategy is then the following:

(a) Pick X so that $(H_o - \lambda)^{-1}$ is bounded as a map of X to X*

k V so that V maps X* to X and thus so that $V(H_o - \lambda)^{-1}$
ed from the space X to <u>itself</u>.
w that $(1 + V(H_o - \lambda)^{-1})$ as a map from X to X is
le as λ approaches points not in the point spectrum of H as a
.
ve that the point spectrum as a map on $\mathcal{H}$ lies in a closed
e set.
ice that V must have smoothness or fall-off for (b) to
as X gets smaller, V must get nicer. Thus we want to
as large as possible and compatible with (a). For
, $\mathrm{Im}(H_o - x - i\varepsilon)^{-1}$ gives a $\pi\delta(p^2 - x)$ as $\varepsilon \to 0$, so X
sist of functions which are smooth enough to have meaning
iplied by $\delta(p^2 - x)$. What is important is that
$\delta(p^2 - x)\, d^3p$ make sense for $\phi \in X$. A good choice is

n $L^2_\delta = \{f \in L^2 | (1 + |x|^2)^{2\ \delta/2} f \subset L^2\}$ with the obvious

$\delta >$ 0, $L^2_\delta \subset L^2$ and with the L^2 duality, $(L^2_\delta)^* = L^2_{-\delta}$.

.2 (<u>See [25]</u>). <u>Fix</u> $\delta > \frac{1}{2}$. <u>Then</u> $(-\Delta - \lambda)^{-1}$ <u>extends</u>
<u>of</u> L^2_δ to $L^2_{-\delta}$ <u>from</u> Im $\lambda > 0$ <u>to</u> Im $\lambda \geq 0$, $\lambda \neq 0$.

et (b) to hold, it clearly suffices that

$$< C(1 + |x|)^{-1-\varepsilon} \qquad (5.2)$$

a little more complication, one can accommodate local
ties.

(c) is somewhat trickier. First, one needs some kind of
ss which yields a Fredholm alternative so that non-
lity can only occur if $V(H_o - \lambda)^{-1}\phi = -\phi$ has solutions
en $\psi = (H_o - \lambda)^{-1}\phi$ obeys $H\psi = \lambda\psi$ but $\psi \in X^*$. If one can
L^2, then (c) will be completed. This is accomplished
that if $\psi \in L^2_\alpha$, then the integral equations around
$\psi \in L^2_{\alpha+\frac{1}{2}\varepsilon}$ (the ε of (5.2)). Repeating this (the "Agmon

bootstrap") eventually gets $\psi \in L^2$. Problem (d) is also solved by the Agmon bootstrap and a compactness argument. The net result is (see [1, 20, 27]).

THEOREM 5.3 <u>Suppose that,</u> $(1 + |x|)^{1+\varepsilon}\, V \in L^2(R^3) + L^\infty(R^3)$. <u>Then</u> $H = -\Delta + V$ <u>and</u> $H_o = -\Delta$ <u>obey</u>

(a) $\Omega^\pm(H,H_o)$ <u>exist and are complete</u>

(b) <u>H has empty singular continuous spectrum</u>

6 Phase Space Analysis: The Method of Enss [9]

Within the last six months, a new method has been developed by V. Enss [9] with exciting potentialities. It has recovered Theorem 5.3 using entirely time-dependent methods and it can be extended to accommodate Coulomb potentials [10] and very likely multiparticle systems including atoms! [10]. The first step involves the fact that any state which is not bound is sure to leave the region of the potential at some time although it might return there. The following result is called the RAGE theorem after contributions of Ruelle [28], Amrein-Georgescu [2] and Enss; it is based on Wiener's theorem, (1.12):

THEOREM 6.1 <u>Let</u> F <u>be any bounded operator with</u> $F(H + i)^{-1}$ <u>compact</u>. <u>Suppose that</u> ϕ <u>is orthogonal to</u> $\mathcal{H}_{pp}$, <u>the eigenvectors for</u> H. <u>Then</u>

$$\frac{1}{2T}\int_{-T}^{T} \| F e^{-itH}\phi\|^2\, dt \to 0 \qquad (6.1)$$

Under the hypotheses of Theorem 5.3, one can show that $F(|x| \leq n)\,(H + i)^{-1}$ is compact, so using (6.1) we can choose $\tau_n > \tau_{n-1}$ so that

$$\| F(|x| \leq n)\, e^{-i\tau_n H}\phi\| \leq n^{-1} \qquad (6.2)$$

Suppose that ϕ has energy spectral measure supported in some interval $[a,b]$, $0 < a < b < \infty$. Then, since $\phi_n \equiv e^{-i\tau_n H}\phi$ lives far from the scatterer one expects that the bulk of the momentum in ϕ_n will lie in the region $a < k^2 < b$, since H and H_o look alike near infinity. This can be shown without too much trouble. Now one can make a decomposition $\phi_n = \phi_{n,in} + \phi_{n,out} + \phi_{n,w}$ where $\|\phi_{n,w}\| \to 0$ involves pieces which have momentum or x-space supports in the wrong region and $\phi_{n,out}$ (resp $\phi_{n,in}$) has momenta k so that k (resp - k) is not towards the scatterers. This requires a simultaneous decomposition in x and k space. Using (2.9) and the methods connected with the estimate (2.11), one shows that

$$\|(\Omega^- - 1)\,\phi_{n,out}\| \to 0 \quad ; \quad \|(\Omega^+ - 1)\,\phi_{n,in}\| \to 0$$

and thus

$$\|\phi_n - \Omega^-\,\phi_{n,out} - \Omega^+\,\phi_{n,in}\| \to 0$$

It follows that any ϕ of the above type is automatically in Ran Ω^+ + Ran $\Omega^- \subset \mathcal{H}_{ac}$ so $\mathcal{H}_{sing} = \{0\}$. By a slightly more involved argument one shows that ϕ cannot lie in (Ran $\Omega^+)^\perp$. A density argument then yields the conclusions of Theorem 5.3.

Acknowledgements

The author's research is supported by the U.S. National Science Foundation under Grant GP75-11864.

References

1. Agmon, S.: Ann. Scuola Norm. Sup. Pisa Cl. Sci. II, 151-218 (1975).
2. Amrein, W. and Georgescu, V.: Helv. Phys. Acta 46, 635-658 (1973)
3. Brenig, W, and Haag, R.: Fort. der Phys. 7, 183-242 (1959)
4. Combes, J.: Nuovo Cimento 64A, 111-144 (1969)
5. Combes, J.: Private communication
6. Cook, J.: J. Math and Phys. 36, 82-87 (1957)
7. Deift, P. and Simon, B.: Comm. Pure Appl. Math. 30, 573-583 (1977)

8. Dollard, J.: J. Math. Phys. 5, 729-738 (1964)
9. Enss, V.: Commun. Math. Phys. to appear
10. Enss, V.: Private communication
11. Ginibre, J. and Moulin, M.: Ann. Inst. H. Poincaré, 21, 97-145 (1974)
12. Hagedorn, G.: Princeton preprint
13. Hörmander, L.: Math. Zeit. 146, 69-91 (1976)
14. Iorio, R. and O'Carroll, M.: Commun. Math. Phys. 27, 137-145 (1972)
15. Jauch, J.: Helv. Phys. Acta 31, 127-158; 661-684 (1958)
16. Kato, T.: Math. Ann. 162, 258-279 (1966); Studia Math. 31, 535-546 (1968)
17. Kupsch, J. and Sandhas, W.: Commun. Math. Phys. 2, 147-154 (1966)
18. Kuroda, S.: Nuovo Cimenta 12, 431-454 (1959)
19. Kuroda, S.: J. Math. Phys. 3, 933-935 (1962)
20. Kuroda, S.: J. Math. Soc. Japan, 25, 75-104, 222-234 (1973)
21. Lavine, R.: Commun. Math. Phys. 20, 301-323 (1971); Ind. Univ. Math. J. 21, 543-656 (1972)
22. Pearson, D.: Commun. Math. Phys. 40, 125-146 (1975)
23. Pearson, D.: University of Hull preprint
24. Pearson, D.: J. Func. Anal; to appear
25. Read, M. and Simon, B.: Methods of Modern Mathematical Physics, I. Functional Analysis, 1972, II. Fourier Analysis, Self-Adjointness, Academic Press 1975
26. Read, M. and Simon, B.: Methods of Modern Mathematical Physics, III. Scattering Theory, Academic Press 1979
27. Read, M. and Simon, B.: Methods of Modern Mathematical Physics, IV. Analysis of Operators, Academic Press 1978
28. Ruelle, D.: Nuovo Cimento 61A, 655-662 (1969)
29. Simon, B.: Int. J. Quant. Chem., to appear
30. Simon, B.: Ann. Math. 97, 247-274 (1973), Comm. Math. Phys. 27, 1-9 (1972)
31. Simon, B.: Comm. Math. Phys. 53, 151-153 (1977)
32. Simon, B.: in preparation

33. Simon, B.: Lectures on Trace Ideal Methods, Cambridge University Press, to appear

34. Simon, B.: Commun. Math. Phys. 55, 259-274 (1977), 58, 205-210 (1978)

Barry Simon,
Departments of Mathematics and Physics,
Princeton University,
Princeton, New Jersey, 08540, USA.

TOWARDS DISPERSION RELATIONS FOR ATOMIC SCATTERING

J.M. Combes

This lecture presents some recent applications of complex canonical transformation methods to the investigation of analyticity properties of two-body scattering amplitudes in N-particle systems interacting with Coulomb forces.

1 Introduction

Scattering theory for N-particle systems involving Coulomb forces presents a priori a set of fundamental problems which makes it appear as a very ambitious challenge of Mathematical Physics. In fact it has in addition to the difficulties inherent in many particle systems (such as existence, uniqueness and computation of scattering states) those linked with statistics and with the long range nature of the forces. However such systems also have very nice specific properties (e.g. homogeneity of the interactions, dilation analyticity) and one can expect in this explicit model to derive results on properties of scattering amplitudes not available for general N-particle systems by the methods actually known. The techniques presented here are based on complex canonical transformations; their relevance to analyticity properties of scattering amplitudes in the case of short range forces was stressed originally in [1] and [2]for the one particle problem and further developed in [3] and [4] for two body reactions involving ground state particles in non-relativistic multichannel systems. It appears however that this theory has to be supplemented by other techniques in order to provide complete results for the on-shell amplitudes. In particular local deformation techniques seem to be required for the analysis of excited atoms' amplitudes; unfortunately there does not exist yet a satisfactory operatorial treatment of such transformations for N-particle Hamiltonians, $N > 1$(the $N = 1$