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Time-Dependent Scattering Theory for Highly Singular Potentials

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Abstract. Asymptotic completeness of the wave operators is proved for scattering of a particle by a wide class of highly singular short-range potentials, which may be either attractive or repulsive.

Introduction

We consider scattering of a particle by a spherically symmetric potential $V(|\mathbf{r}|)$ which is short range and highly singular at the origin (i.e. more singular than $1/r^2$).

The *existence* of the wave operators $\Omega_\pm = s - \lim e^{iHt} e^{-iH_0 t}$ for such potentials has been proved by Kupsch and Sandhas [1] provided $V(r)$ is locally square integrable for $r > 0$. This condition of local square integrability means that for every $r > 0$ there is a neighbourhood in which V is square integrable; no restriction is imposed on the nature of the singularity at $r = 0$.

However, *completeness* of the wave operators for such potentials has not previously been proved, except in the repulsive case [2, 3]. (See, however, Ref. [4], where completeness is proved for a class of potentials almost identical to that of the present paper, and Ref. [5], where application of some of the methods presented here is made to a rather smaller class of attractive potentials.) By completeness we mean the requirement that the range of $\Omega_\pm$ equal $M_{\text{a.c.}}(H)$, the absolutely continuous subspace of the total Hamiltonian $H = H_0 + V$. This is equivalent to the existence on $M_{\text{a.c.}}(H)$ of the limits $\Omega_\pm^* = s - \lim_{t \to \mp\infty} e^{iH_0 t} e^{-iHt}$.

The proof in Ref. [3] of existence and completeness for repulsive potentials and potentials for which H is semi-bounded relied on the existence in each partial wave subspace of a projection operator P having finite dimensional range such that $V(H_0 - \lambda)^{-N}(1 - P)$ is bounded for N sufficiently large. We shall say in that case that V is bounded relatively to $(H_0 - \lambda)^N$ on a subspace of finite codimension. This property holds for potentials satisfying the condition $\int_0^1 r^k |V(r)|^2 dr < \infty$ for some $k > 0$. In the present paper, by deriving analogous relative bounds with H_0 replaced by H, we extend the proof of completeness to a wider class of repulsive potentials and to a large class of highly singular attractive potentials.

We find that

i) For highly singular attractive potentials V is bounded relatively to $(H - \lambda)^N$ on a subspace of finite codimension (in each partial wave subspace).

ii) For highly singular repulsive potentials V is bounded relatively to $(H-\lambda)^N$ (on the entire partial wave subspace).
iii) In both i) and ii) the wave operators are complete.

Remark 1: In most cases of interest one may take $N = 2$; this is so even for potentials such as $V(r) = \pm \exp(r^{-1})$ which are more singular than any inverse power of r.

Remark 2: In the case $V(r) = -g/r^2$ with strong coupling (i.e. $g > \frac{1}{4}$) one may show that the relative bound obtains on a subspace of finite codimension with $N = 1$. This potential, for which H is not semi-bounded, may be regarded as a borderline between the highly singular and non-singular attractive potentials.

For attractive potentials as singular as $1/r^2$, a classical particle may reach the origin in a finite time. Quantum mechanically, absorption at the origin may be introduced [6] by allowing a *non-unitary* evolution given by a contractive semi-group. However, in the present paper we take a *unitary* evolution generated by a self-adjoint extension of $-\Delta + V$. Since $-\Delta + V$ is not essentially self-adjoint, there is a one-parameter family of self-adjoint extensions in each partial wave subspace. For any two such extensions the resolvents differ by an operator of finite rank, so that completeness for one extension is equivalent to completeness for any other (see Ref. [7], pp. 532 and 548). To choose one of these extensions one must impose a boundary condition at $r = 0$, which physically is perhaps analogous to placing a reflecting barrier at the origin. There seems in general to be no clear mathematical or physical reason to prefer any one boundary condition to any other.

Since presumably completeness is not valid independently of any assumptions whatever on the behaviour of the potential at the origin, one may enquire for what class of potentials completeness is violated. We expect completeness to break down for certain spherically symmetric potentials which are highly oscillatory near the origin, and in other cases where H is not spherically symmetric. Some consequences of such a breakdown of completeness and the connection with the problem of the description of bound states [8] will be discussed in some generality in a subsequent paper.

An outline of the present paper is as follows: In Sections 1 and 2 we investigate the behaviour near $r = 0$ of solutions $u(r)$ of the partial wave eigenvalue equation, respectively for an attractive and repulsive singular potential. We consider first a potential which satisfies conditions implying local differentiability, but the estimates for $u(r)$ obtained in Lemmas 2 and 3 do not demand the local regularity of $V(r)$.

In Section 3 we use the estimates of Sections 1 and 2 to derive relative bounds satisfied by V in each partial wave subspace.

Finally, in Theorem 3 of Section 4 we prove completeness of the wave operators, using the trace criteria of Refs. [3] and [9].

1. Behaviour Near $r = 0$: Attractive Case

We wish to investigate the behaviour, near $r = 0$, of solutions of the equation

$$\left(-\frac{d^2}{dr^2} + V(r) + \frac{l(l+1)}{r^2} - \lambda\right) u(r) = 0 \tag{1}$$

where $V(r)$ is a singular potential. We consider first the case of an attractive singular potential $V(r) = -q(r)$, where $q(r)$ satisfies, for some $\epsilon > 0$, the folowing conditions:

$$q(r) > 0 \quad \text{for} \quad 0 < r \leqslant \epsilon, \quad \text{and} \quad \lim_{r\to 0+} q(r) = \infty, \tag{2}$$

$$\int_0^\varepsilon \left[\frac{d}{dr}\{(q(r))^{-1/4}\}\right]^2 dr < \infty \tag{3}$$

$$\frac{d}{dr}\{(q(r))^{-1/2}\} \text{ is of bounded variation for } 0 < r \leqslant \epsilon. \tag{3$'$}$$

In the repulsive case we shall impose the same conditions on $q(r)$, with $V(r) = +q(r)$.

Here and subsequently, the notation $(d/dr)\,F(r)$ is taken to imply that $F(r)$ is locally absolutely continuous. We shall later consider more general singular potentials which are not necessarily differentiable.

Now letting $I_\alpha = \int_\alpha^\epsilon r^{-2}(q(r))^{-1/2}\,dr$, we have

$$I_\alpha = [-r^{-1}(q(r))^{-1/2}]_\alpha^\varepsilon + \int_\alpha^\varepsilon r^{-1}\frac{d}{dr}\{(q(r))^{-1/2}\}\,dr. \tag{4}$$

Using (3)$'$, we see that $(d/dr)\{(q(r))^{-1/2}\}$ tends to a limit as $r \to 0$, so that $\lim_{r\to 0} r^{-1}(q(r))^{-1/2}$ is finite. Hence the first term on the right-hand side of (4) is bounded as $\alpha \to 0$. The second term may be written

$$\int_\alpha^\varepsilon 2r^{-1}(q(r))^{-1/4}\frac{d}{dr}\{(q(r))^{-1/4}\})\,dr,$$

and by the Cauchy–Schwarz inequality this integral is bounded in absolute value by

$$2\left[\left(\int_\alpha^\varepsilon r^{-2}(q(r))^{-1/2}\,dr\right)\left(\int_\alpha^\varepsilon \left(\frac{d}{dr}\{(q(r))^{-1/4}\}\right)^2 dr\right)\right]^{1/2}.$$

Hence (3) implies that, for some contants a, b, we have

$$I_\alpha \leqslant a + bI_\alpha^{1/2},$$

so that I_α remains bounded as $\alpha \to 0$.

Thus we have shown that

$$\int_0^\varepsilon r^{-2}(q(r))^{-1/2}\,dr < \infty. \tag{5}$$

Also we have $\lim_{r\to 0} r^{-1}(q(r))^{-1/2} = 0$, since a positive limit would make the integral in (5) diverge at least logarithmically. So we have

$$\lim_{r\to 0} r^2 q(r) = \infty. \tag{6}$$

Equation (6) tells us that $q(r)$ must be more singular than $1/r^2$ at the origin. Conditions (2), (3) and (3)$'$ are satisfied, for example, by $q(r) = 1/r^{2+c}$ $(c > 0)$, or for more singular potentials such as $q(r) = \exp(1/r)$.

Lemma 1: Let $u(r)$ satisfy, for $0 < r \leqslant \epsilon$,

$$\left(\frac{d^2}{dr^2} + q(r) - \frac{l(l+1)}{r^2} + \lambda\right) u(r) = 0, \tag{7}$$

where $q(r)$ satisfies (2), (3) and (3)′. Then for $0 < r \leqslant \epsilon$ we have

$$|u(r)| \leqslant \text{const. } (q(r))^{-1/4}. \tag{8}$$

Proof: Let us first suppose that, in $(0, \epsilon]$, $q(r)$ is twice continuously differentiable. We introduce, for $r \in (0, \epsilon]$, the new variable

$$z = \int_r^\varepsilon (q(\rho))^{1/2}\, d\rho, \quad \frac{dz}{dr} = -(q(r))^{1/2}. \tag{9}$$

Equation (6) shows that $z \to \infty$ as $r \to 0$, so that (9) defines a bijection from $(0, \epsilon]$ onto $[0, \infty)$.

We substitute $u(r) = (q(r))^{-1/4} v(r)$, and write $w(z)$ for the function $v(r)$ expressed in terms of $z : w(z) = v(r)$. A simple calculation now shows that equation (7) is transformed into

$$\frac{d^2 w(z)}{dz^2} + (1 + P(z))\, w(z) = 0 \tag{10}$$

where

$$P(z) = (q(r))^{-3/4} \frac{d^2}{dr^2}\{(q(r))^{-1/4}\} + \left[\lambda - \frac{l(l+1)}{r^2}\right](q(r))^{-1},$$

expressed in terms of z by change of variable.

Now

$$\int_0^\infty |P(z)|\, dz = -\int_0^\varepsilon |P(z)| \frac{dz}{dr}\, dr$$

$$\leqslant \int_0^\varepsilon dr (q(r))^{-1/4} \left|\frac{d^2}{dr^2}\{(q(r))^{-1/4}\}\right| + \int_0^\varepsilon dr (q(r))^{-1/2} + l(l+1) \int_0^\varepsilon dr r^{-2} (q(r))^{-1/2}.$$

The first integral on the right-hand side converges, using (3) and (3)′, since

$$(q(r))^{-1/4} \frac{d^2}{dr^2}\{(q(r))^{-1/4}\} = \frac{1}{2}\frac{d}{dr}\left[\frac{d}{dr}\{q(r))^{-1/2}\}\right] - \left[\frac{d}{dr}\{(q(r))^{-1/4}\}\right]^2.$$

The second integral converges since the integrand is bounded, and the third integral converges as we have shown in equation (5).

Hence $P(z) \in L^1(0, \infty)$. Equation (10) is equivalent to the Volterra integral equation

$$w(z) = \alpha \cos z + \beta \sin z + \int_z^\infty dt \sin(z - t)\, P(t)\, w(t). \tag{10$'$}$$

Equation (10)′ may be iterated, and if we choose $M \geqslant 0$ such that $\int_M^\infty |P(z)|dz < 1$ we may deduce from standard estimates that the iteration converges uniformly on $[M, \infty)$, and that the solution $w(z)$ is bounded on $[M, \infty)$. $w(z)$ is also locally bounded, so that $w(z)$ is bounded on $[0, \infty)$.

Hence $|u(r)| \leqslant (q(r))^{-1/4}|w(z)|$ implies (8). The proof of (8) is similar if we do not assume $q(r)$ to be twice continuously differentiable. In that case equation (10) is replaced by

$$\frac{d}{dz}\left\{\frac{dw(z)}{dz} + w(z)\, I(z)\right\} - I(z)\frac{dw(z)}{dz} + w(z) = 0,$$

where

$$I(z) = -(q(r))^{-1/4}\frac{d}{dr}\{q(r))^{-1/4}\} + \int_0^r \left[\frac{d}{d\rho}\{(q(\rho))^{-1/4}\}\right]^2 d\rho$$

$$-\int_0^r \left[\lambda - \frac{l(l+1)}{\rho^2}\right](q(\rho))^{-1/2}\, d\rho \quad \text{(as a function of } z\text{).}$$

[Formally, $P(z) = dI(z)/dz$ and equation (10) follows, but in fact $dI(z)/dz$ is defined only as a distribution. However, one may show that $(dw(z)/dz) + w(z)\, I(z)$ is locally absolutely continuous].

The integral equation (10)′ becomes

$$w(z) = \alpha\cos z + \beta\sin z + \int_z^\infty dt \sin(z-t)\, w(t)\, dI(t).$$

$I(t)$ defines a signed measure such that $\int_0^\infty |dI(t)| < \infty$, so that again the integral equation may be iterated to show that $w(z)$ is bounded, and this completes the proof of the lemma.

The conclusion of Lemma 1 remains valid for potentials which are increasing relatively to $q(r)$ and for potentials which include a perturbation of $q(r)$, satisfying an integral condition. Thus we have

Lemma 2: Let $q(r)$ satisfy (2), (3) and (3)′, and suppose that, for $0 < r \leqslant \epsilon$,

$$V(r) = -a(r)\, q(r) + b(r)\, q(r))^{1/2} \tag{11}$$

where $a(r) \geqslant 1$ and is non-increasing and

$$\int_0^\varepsilon |b(r)|dr < \infty. \tag{12}$$

Then any solution $u(r)$ of equation (1) for $0 < r \leqslant \epsilon$ satisfies $|u(r)| \leqslant \text{const.}\ (q(r))^{-1/4}$.

Proof: We consider only the case where $q(r)$ is twice continuously differentiable; as for Lemma 1 there is an analogous proof in the more general case.

We again make the change of variable (9), and write $u(r) = (q(r))^{-1/4} v(r)$, with $w(z) = v(r)$. In terms of z, equation (1) becomes

$$\frac{d^2 w(z)}{dz^2} + (A(z) + (Q(z))\, w(z) = 0 \tag{13}$$

where $A(z) = a(r)$ and $Q(z) = P(z) - b(r)(q(r))^{-1/2}$.

We have already shown that $\int_0^\infty |P(z)|\, dz < \infty$. Hence it follows that from (12) that $\int_0^\infty |Q(z)|\, dz < \infty$.

As for Lemma 1, we can write down a Volterra integral equation for $w(z)$, the kernel and inhomogeneous term being given in terms of the solution of

$$\frac{d^2 w}{dz^2} + A(z)\, w(z) = 0. \tag{14}$$

As for Lemma 1, we can prove that the solutions of equation (13) are bounded if we can prove that the solutions of equation (14) are bounded. But this follows from the fact that $A(z) \geqslant 1$ and is non-decreasing. The proof that, under these conditions, every solution of equation (14) is bounded on $[0, \infty)$ is based on Ref. [10], p. 1417 et seq. The real solutions of equation (14) are oscillating, since $A(z) \geqslant 1$, and one shows that the amplitude of successive oscillations cannot increase. (It is not necessary to suppose $A(z)$ to be continuous.)

The conclusion of Lemma 2 now follows. Further, each real solution of equation (14) may be bounded in absolute value by a non-increasing function. From the Volterra integral equation we may deduce that the solutions $w(z)$ of equation (13) have the same property. Hence we have the following

Corollary to Lemma 2: Under the same hypotheses as for Lemma 2, any solution $u(r)$ of equation (1) satisfies, for some $U(r)$

$$|u(r)| \leqslant |U(r)|, \quad 0 < r \leqslant \epsilon,$$

where

$$|U(r)| \leqslant \text{const.} \quad (q(r))^{-1/4},$$

and

$$|U(r)| \text{ is non-decreasing.}$$

Example: Let $V(r) = (-1/r^N) + U(r)$, where

$$N > 2 \quad \text{and} \quad \int_0^\varepsilon |U(r)|\, r^{(1/2)N}\, dr < \infty.$$

Then as $r \to 0$ every solution of equation (1) satisfies, for some α, β,

$$u(r) = r^{N/4} \left\{ \alpha(1 + o(1)) \cos\left(\frac{1}{(\frac{1}{2}N - 1)\, r^{(1/2)N-1}} \right) + \beta(1 + o(1)) \sin\left(\frac{1}{(\frac{1}{2}N - 1)\, r^{(1/2)N-1}} \right) \right\}.$$

2. Behaviour Near $r = 0$: Repulsive Case

We consider now the behaviour, near $r = 0$, of solutions of equation (1) where $V(r)$ is a repulsive singular potential. To facilitate the more detailed estimates which we shall need in this case, we first prove a proposition:

Proposition 1: Let $A(z) \geqslant 1$ be any locally integrable real function on $[0, \infty)$, and let $R(z)$ be any function satisfying $\int_0^\infty |R(z)| dz < \infty$.

Then the equation

$$\frac{d^2 w(z)}{dz^2} - A(z) w(z) = 0; \quad (0 \leqslant z < \infty) \tag{15}$$

has two solutions $w_1(z)$, $w_2(z)$ having the following peoperties:

i) $w_1(z) > 0$; $w_2(z) > 0$; $\lim_{z\to\infty} w_1(z) = \infty$; $\lim_{z\to\infty} w_2(z) = 0$.

$$\frac{d}{dz} w_1(z) \geqslant w_1(z); \quad \frac{d}{dz} w_2(z) \leqslant -w_2(z).$$

ii) $w_1(z) w_2(z)$ is bounded.

iii) Every solution of the equation

$$\frac{d^2 w(z)}{dz^2} - (A(z) + R(z)) w(z) = 0 \quad (0 \leqslant z < \infty) \tag{15$'$}$$

satisfies $|w(z)| \leqslant$ const. $w_1(z)$.

Moreover, every *bounded* solution satisfies $|w(z)| \leqslant$ const. $w_2(z)$.

Proof: We define $w_1(z)$ to be the solution of equation (15) with the boundary condition $w_1(0) = 1$, $w_1'(0) = 1$.

Define

$$P_1(z) = (w_1(z)^{-1} \frac{d}{dz} w_1(z).$$

Then

$$\frac{d}{dz} P_1(z) = A(z) - (P_1(z))^2 \geqslant 1 - (P_1(z))^2.$$

Now $P_1(0) = 1$. Since for any $z > 0$ such that $0 < P_1(z) < 1$ one would have (d/dz) $P_1(z) > 0$, one may deduce that in fact $P_1(z) \geqslant 1$ for *all* $z > 0$.

That is, we have $(d/dz) w_1(z) \geqslant w_1(z)$; hence $w_1(z) \geqslant \exp(z)$. We define the second solution of equation (15) by

$$w_2(z) = w_1(z) \int_z^\infty [w_1(t)]^{-2} dt.$$

Then

$$w_1(z)\,w_2(z) = (w_1(z))^2 \int\limits_z^\infty \left(\frac{w_1(t)}{w_1'(t)}\right) \frac{w_1'(t)}{(w_1(t))^3}\,dt$$

$$\leqslant (w_1(z))^2 \int\limits_z^\infty \frac{w_1'(t)}{(w_1(t))^3}\,dt = \tfrac{1}{2}.$$

Hence $w_1(z)\,w_2(z)$ is bounded, so that $\lim\limits_{z\to\infty} w_2(z) = 0$. Now define

$$P_2(z) = (w_2(z))^{-1} \frac{d}{dz} w_2(z).$$

Then $(d/dz)\,P_2(z) \geqslant 1 - (P_2(z))^2$, from which we may deduce that $P_2(z) \leqslant -1$ for $z \geqslant 0$. (Note that $P_2(z) > -1$ for some z would imply $\liminf\limits_{z\to\infty} P_2(z) \geqslant 1$, in which case $w_2(z)$ would increase at least exponentially.) That is we have $(d/dz)\,w_2(z) \leqslant -w_2(z)$. This completes the proof of i) and ii).

We may construct a solution of equation (15)$'$ by iterating the integral equation

$$w(z) = w_2(z) - w_1(z) \int\limits_z^\infty w_2(t)\,R(t)\,w(t)\,dt + w_2(z) \int\limits_z^\infty w_1(t)\,R(t)\,w(t)\,dt.$$

Writing $w(t) = W(t)\,w_2(t)$, and using the fact that $w_1(t)\,w_2(t) \leqslant$ const., and that w_2 is decreasing, we find that the iterated solution for W converges uniformly in some interval $[R, \infty)$, and that $W(z)$ is bounded. In fact this solution of equation (15)$'$ satisfies $w(z) = w_2(z)\,(1 + o(1))$ as $z \to \infty$, and any bounded solution of equation (15)$'$ is a constant multiple of this solution.

For a second solution, we iterate the equation

$$w(z) = w_1(z) - w_1(z) \int\limits_z^\infty w_2(t)\,R(t)\,w(t)\,dt - w_2(z) \int\limits_\alpha^\infty w_1(t)\,R(t)\,w(t)\,dt.$$

Writing $w(t) = w_1(t)\,W(t)$, the iterated solution for W converges uniformly in $[\alpha, \infty)$, for sufficiently large α. If α is suitably chosen, we have, for $z > \alpha$,

$$\tfrac{1}{2} w_1(z) < |w(z)| < 2 w_1(z).$$

Since every solution of equation (15)$'$ is locally bounded, the proof of iii) now follows immediately.

This completes the proof of the proposition. With the aid of Proposition 1, we can now obtain an analogue of Lemma 2 for repulsive potentials. We omit the proof, which is essentially the same as for Lemma 2.

Lemma 3: Let $q(r)$ satisfy (2), (3) and (3)$'$ and suppose that, for $0 < r \leqslant \epsilon$,

$$V(r) = a(r)\,q(r) + b(r)\,(q(r))^{1/2} \tag{16}$$

where $a(r) \geqslant 1$ and

$$\int_0^\varepsilon |b(r)|dr < \infty. \tag{17}$$

Let $z(r)$ be defined by equation (9), and let $w_1(z)$, $w_2(z)$ be the two solutions of equation (15) satisfying the conditions of Proposition 1, where $A(z) = a(r)$.

Then any solution $u(r)$ of equation (1) for $0 < r \leqslant \epsilon$ satisfies

Either (a) $(q(r))^{1/4}|u(r)|$ is bounded, in which case

$$|u(r)| \leqslant \text{const. } (q(r))^{-1/4} w_2(z), \tag{18}$$

or (b) $(q(r))^{1/4}|u(r)|$ is unbounded, in which case

$$|u(r)| \leqslant \text{const. } (q(r))^{-1/4} w_1(z), \tag{18$'$}$$

and for r sufficiently small

$$|u(r)| \geqslant \beta(q(r))^{-1/4} w_1(z) \quad \text{for some } \beta > 0.$$

There is just one linearly independent solution of type (a), and this solution is in $L^2(0,\epsilon)$. Solutions of type (b) do not belong to $L^2(0,\epsilon)$.

3. Bounds for $(H - \lambda)^{-N}$

We denote by $\hat{H}$ the symmetric operator

$$\frac{-d^2}{dr^2} + V(r) + \frac{l(l+1)}{r^2}$$

acting on C^∞ functions having compact support in $(0,\infty)$. (We assume $V(r)$ to be locally L^2 in $(0,\infty)$). We denote by H a self-adjoint extension of $\hat{H}$ in the Hilbert space $L^2(0,\infty)$.

H_0 is the self-adjoint extension of the differential operator

$$\frac{-d^2}{dr^2} + \frac{l(l+1)}{r^2}.$$

In the case $l = 0$, this differential operator is not essentially self-adjoint, and we impose the boundary condition $f(0) = 0$ on elements f in the domain of H_0.

In order to obtain an integral representation for $(H - \lambda)^{-1}$, it remains to estimate the behaviour at infinity of solutions of equation (1). We make the assumption

$$V(r) \in L^2(a,\infty) + L^\infty(a,\infty),$$

for any $a > 0$. Hence

$$V(r) \in L^1(a,\infty) + L^\infty(a,\infty).$$

It follows that, for $r > a$ and $\mathrm{Re}\,\lambda$ sufficiently large negative, equation (1) is of the form

$$\frac{d^2 u(r)}{dr^2} - (M(r) + N(r))\, u(r) = 0 \tag{19}$$

where

$$2\,\mathrm{Re}\,M(r) \geqslant 1 \quad \text{and} \quad \int_a^\infty |N(r)|\,dr < \infty.$$

Defining now

$$p(r) = (u(r)\,\bar{u}(r))^{-1}\frac{d}{dr}(u(r)\,\bar{u}(r)),$$

we have, in the case $N(r) \equiv 0$,

$$\frac{d}{dr}p(r) \geqslant 2\,\mathrm{Re}\,M(r) - (p(r))^2 \geqslant 1 - (p(r))^2.$$

Following arguments which closely follow those by which we determined the behaviour of solutions of equations (15) and (15)′ we may derive bounds for the solutions of equation (19) which are analogous to the conclusions of Proposition 1. We choose two particular linearly independent solutions of equation (1).

First we take a solution $\phi(r)$ which belongs to $L^2(a,\infty)$. $\phi(r)$ is determined up to a multiplicative constant. The second solution $\psi(r)$ is chosen to be a solution independent of $\phi(r)$, and satisfying $\psi(r) \in L^2(0,a)$. (If $V(r)$ is such that one is in the limit point case at the origin than $\psi(r)$ is determined up to a multiplicative constant.) We also choose $\phi(r)$ and $\psi(r)$ to satisfy

$$\psi'(r)\,\phi(r) - \phi'(r)\,\psi(r) = 1. \tag{20}$$

The analogue for equation (19) of Proposition 1 implies that there exist two functions $\Phi(r)$, $\overline{\Psi}(r)$, $r \geqslant a$, such that

$$\left.\begin{aligned} &|\phi(r)| \leqslant \text{const. } |\Phi(r)| \\ &|\psi(r)| \leqslant \text{const. } |\overline{\Psi}(r)| \\ &\frac{d}{dr}(\Phi(r)\,\bar{\Phi}(r)) \leqslant -\Phi(r)\,\bar{\Phi}(r) \\ &\frac{d}{dr}(\Psi(r)\,\overline{\Psi}(r)) \geqslant \Psi(r)\,\overline{\Psi}(r) \end{aligned}\right\} \tag{21}$$

and

$$|\Phi(r)\,\overline{\Psi}(r)| \leqslant \text{const.} \tag{21$'$}$$

For $g \in L^2(0,\infty)$, define the function

$$(Tg)(r) = \phi(r)\int_0^r \psi(t)\,g(t)\,dt + \psi(r)\int_r^\infty \phi(t)\,g(t)\,dt. \tag{22}$$

We first note that $(Tg)(r)$ is uniformly bounded for $r \in [a,\infty)$.

We have, for example,

$$\left|\int_r^\infty \phi(t)\, g(t)\, dt\right| \leqslant \int_r^\infty |\Phi(t)|\,|g(t)|\,dt \leqslant \|g\| \left(\int_r^\infty \Phi(t)\,\bar{\Phi}(t)\,dt\right)^{1/2}$$

$$\leqslant \|g\| \left(-\int_r^\infty \frac{d}{dt}(\Phi(t)\,\bar{\Phi}(t))\,dt\right)^{1/2} = \|g\|\,|\Phi(r)|.$$

Hence

$$\left|\psi(r)\int_r^\infty \phi(t)\, g(t)\, dt\right| \leqslant \|g\|\,|\Phi(r)\,\Psi(r)|$$

and is uniformly bounded in $[a,\infty)$ according to (21)$'$. Similarly the first term on the right-hand side of (22) is uniformly bounded for $r \in [a,\infty)$.

Since $(Tg)(r)$ is bounded locally for $r \in (0,\infty)$, it follows that $(Tg)(r)$ is bounded in $[a,\infty)$ for each $a > 0$.

Now let $h = (H-\lambda)^{-1}g$; we take $\operatorname{Im}\lambda \neq 0$. Then h satisfies $(\hat{H}^* - \lambda)\,h = g$. That is, for $r > 0$ we have

$$\left(\frac{-d^2}{dr^2} + V(r) + \frac{l(l+1)}{r^2} - \lambda\right) h(r) = g(r). \tag{23}$$

As a consequence of the normalization (20), a particular solution of this equation is $h(r) = (Tg)(r)$. Hence

$$((H-\lambda)^{-1}g)(r) = (Tg)(r) + B_1\,\phi(r) + B_2\,\psi(r).$$

Since $(Tg)(r)$ is bounded for $r \geqslant a$, and both $(H-\lambda)^{-1}g$ and ϕ belong to $L^2(a,\infty)$, whereas $\psi(r)$ increases at least exponentially as $r \to \infty$, we must have $B_2 = 0$. Hence

$$((H-\lambda)^{-1}g)(r) = (Tg)(r) + B_1(g)\,\phi(r). \tag{24}$$

We now consider separately the case of an attractive and a repulsive singular potential.

i) Attractive singular potential

If $V(r)$ satisfies the conditions of Lemma 2 or, more generally, if we have the limit circle case at the origin, then $\phi(r) \in L^2(0,\infty)$ and we have

$$(H-\lambda)^{-1}g = Tg + B_1(g)\,\phi \tag{24$'$}$$

where T is a linear operator defined on $L^2(0,\infty)$. One readily checks from equation (22) that T is closed. Hence T is a bounded linear operator.

Suppose now that $V(r)$ satisfies the conditions of Lemma 2, and that in addition we have, for some integer $N > 0$,

$$\int_0^\varepsilon (V(r))^2\,(q(r))^{-N}\,dr < \infty. \tag{25}$$

Suppose that $g(r)$ is orthogonal to $\bar{\phi}(r)$ and to $[T^* - (H - \bar{\lambda})^{-1}]\phi$. Then equation (22) becomes

$$(Tg)(r) = \phi(r) \int_0^r \psi(t) g(t)\, dt - \psi(r) \int_0^r \phi(t)\, g(t)\, dt, \tag{26}$$

and we also have, from equation (24)′,

$$B_1\|\phi\|^2 = \langle \phi, B_1 \phi \rangle = \langle (H - \bar{\lambda})^{-1} \phi - T^* \phi, g \rangle = 0.$$

so that $B_1 = 0$. Hence in this case $Tg = (H - \lambda)^{-1} g$.

If we further assume that $(H - \lambda)^{-1} g$ is also orthogonal to $\bar{\phi}(r)$ and to $[T^* - (H - \bar{\lambda})^{-1}]\phi$ then we have $T^2 g = (H - \lambda)^{-2} g$, and $T^2 g$ is given in terms of Tg by an equation similar to (26), in which both integrals are over the interval $[0, r]$. For this to hold, then, we impose the condition that g be orthogonal to $(H - \bar{\lambda})^{-1}\bar{\phi}$ and to $(H - \bar{\lambda})^{-1}[T^* - (H - \bar{\lambda})^{-1}]\phi$.

More generally, by taking g to be orthogonal to a space of dimension $2N$, we have

$$(H - \lambda)^{-n} g = T^n g, \quad n = 1, 2, \dots N,$$

and $T^n g$ is related to $T^{n-1} g$ by an equation in which only integrals over $[0, r]$ appear.

We now use Lemma 2 to estimate $((H - \lambda)^{-N} g)(r)$ near the origin. According to the corollary to Lemma 2, for $0 < r \leqslant \epsilon$ we can find functions $\Phi(r)$, $\Psi(r)$ such that

$$|\phi(r)| \leqslant |\Phi(r)|; \quad |\psi(r)| < |\Psi(r)|,$$

$$|\Phi(r)|, |\Psi(r)| \quad \text{are non-decreasing, and}$$

$$|\Phi(r)| \leqslant \text{const. } (q(r))^{-1/4}, \quad |\Psi(r)| \leqslant \text{const. } (q(r))^{-1/4}.$$

Hence for the first term on the right-hand side of equation (26) we have the estimate

$$\left| \phi(r) \int_0^r \psi(t)\, g(t)\, dt \right| \leqslant \|g\|\, |\Phi(r)| \left(\int_0^r |\Psi(t)|^2\, dt \right)^{1/2}$$

$$\leqslant r^{1/2} \|g\|\, |\Phi(r)|\, |\Psi(r)|; \quad 0 < r \leqslant \epsilon.$$

A similar estimate holds for the second term, so that we have

$$|(Tg)(r)| \leqslant \text{const. } |\Phi(r)\, \Psi(r)|; \quad 0 < r \leqslant \epsilon.$$

Using this estimate for Tg, we find

$$|(T^2 g)(r)| \leqslant \text{const. } |\Phi(r)\, \Psi(r)|^2; \quad 0 < r \leqslant \epsilon,$$

and successive estimates lead finally to the inequality

$$|((H - \lambda)^{-N} g)(r)| = |(T^N g)(r)| \leqslant \text{const. } |\Phi(r)\, \Psi(r)|^N$$

$$\leqslant \text{const. } (q(r))^{(-1/2)N}; \quad 0 < r \leqslant \epsilon.$$

Hence from (25) we have

$$V(H - \lambda)^{-N} g \in L^2(0, \epsilon).$$

Since $((H-\lambda)^{-N}g)(r)$ is bounded for $r \geqslant \epsilon$, and $V(r) \in L^{\infty}(\epsilon, \infty) + L^2(\epsilon, \infty)$, it follows that

$$V(H-\lambda)^{-N} g \in L^2(0, \infty).$$

Further, $(H-\lambda)^{-N}g \in D(\hat{H}^*)$, from which we may deduce that $H_0(H-\lambda)^{-N}g \in L^2(0,\infty)$. (We have $H_0(H-\lambda)^{-N}g = \hat{H}^*(H-\lambda)^{-N}g - V(H-\lambda)^{-N}g$; we also notice that in the case $l=0$ the boundary condition at the origin is satisfied.)

The estimates which we have obtained hold for all g orthogonal to a subspace of dimension $2N$, and we shall denote by P the orthogonal projection onto this subspace.

$V(H-\lambda)^{-N}\,(1-P)$ is closed, and hence bounded. We state our conclusions as a

Theorem 1: Let $q(r)$ satisfy (2), (3) and (3)′, and suppose that, for $0 < r \leqslant \epsilon$,

i) $V(r) = -a(r)\,q(r) + b(r)(q(r))^{1/2}$,

where $a(r) \geqslant 1$ and is non-increasing and

$$\int_0^{\epsilon} |b(r)|\,dr < \infty.$$

Suppose further that

ii) $$\int_0^{\epsilon} (V(r))^2\,(q(r))^{-N}\,dr < \infty,$$

for some positive integer N and

iii) $V(r) \in L^{\infty}(a,\infty) + L^2(a,\infty)$

for all $a > 0$.

Then $\exists$ a projection operator P onto a subspace of dimension $2N$ such that, for all non-real λ,

$$V(H-\lambda)^{-N}(1-P) \quad \text{and} \quad H_0(H-\lambda)^{-N}(1-P)$$

are bounded operators defined on the entire Hilbert space.

Remark: In estimating the behaviour for large r, we found it convenient to take $\operatorname{Im}\lambda$ to be large negative; however, one easily verifies that the conclusion of Theorem 1 holds for all λ such that $\operatorname{Im}\lambda \neq 0$, provided the conclusion is valid for a single such value of λ.

ii) Repulsive singular potential

If $V(r)$ satisfies the conditions of Lemma 3, or more generally if we have the limit point case at the origin, then $B_1 = 0$ in equation (24), and $Tg = (H-\lambda)^{-1}g$ for *all* g in the Hilbert space, where equation (22) defines the integral representation for T [see, for example, Ref (10), p. 1329].

Suppose now that $V(r)$ satisfies the conditions of Lemma 3, and that in addition equation (25) holds for some positive integer N. We use Lemma 3 to estimate $((H-\lambda)^{-N}g)(r)$ near the origin. According to Lemma 3, and defining $z(r)$ by (9), we can find functions $w_1(z)$, $w_2(z)$ satisfying conditions i), ii), iii) of Proposition 1 such that, for $0 < r \leqslant \epsilon$,

$$|\phi(r)| \leqslant \text{const.}\,(q(r))^{-1/4}\,w_1(z),$$

$$|\psi(r)| \leqslant \text{const.}\,(q(r))^{-1/4}\,w_2(z).$$

Now, for any real k, we have

$$\frac{d}{dr}\{(q(r))^{-k}\,w_1(z)\} = \frac{d}{dr}\{[(q(r))^{-1/2}]^{2k}\,w_1(z)\}$$

$$= (q(r))^{-k+1/2}\left\{\frac{-d}{dz}\,w_1(z) + 2kw_1(z)\,\frac{d}{dr}[(q(r))^{-1/2}]\right\}.$$

In Section 1 we showed that $\lim_{r\to 0}(d/dr)[(q(r))^{-1/2}]$ exists, and that $\lim_{r\to 0} r^{-1}(q(r))^{-1/2} = 0$. Hence $\lim_{r\to 0}(d/dr)[(q(r))^{-1/2}] = 0$, so that using i) of Proposition 1, we see that for r sufficiently close to zero we have $(d/dr)\{(q(r))^{-k}w_1(z)\} < 0$.

Similarly, $(d/dr)\{(q(r))^{-k}w_2(z)\} > 0$ for r sufficiently small. (In particular, we have $w_2(z) \leqslant \text{const.}\,(q(r))^{-n}$ for any $n > 0$.)

For the first term on the right-hand side of equation (22) we have the estimate

$$\left|\phi(r)\int_0^r \psi(t)\,g(t)\,dt\right| \leqslant \text{const.}\,(q(r))^{-1/4}\,w_1(z)\left(\int_0^r (q(t))^{-1/2}\,[w_2(z(t))]^2\,dt\right)^{1/2}$$

$$\leqslant \text{const.}\,r^{1/2}\,(q(r))^{-1/2}\,w_1(z)\,w_2(z) \leqslant \text{const.}\,(q(r))^{-1/2},$$

since $w_1(z)\,w_2(z)$ is bounded.

A similar bound holds for the second term, so that

$$|(Tg)(r)| \leqslant \text{const.}\,|(q(r)|^{-1/2} \quad \text{for } 0 < r \leqslant \epsilon.$$

Successive estimates lead finally to the inequality

$$|((H-\lambda)^{-N}g)(r)| \leqslant \text{const}\,(q(r))^{(-1/2)N},$$

and repeating the arguments of Theorem 1 we have

Theorem 2: Let $q(r)$ satisfy (2), (3) and (3)$'$, and suppose that, for $0 < r \leqslant \epsilon$,

i) $V(r) = a(r)q(r) + b(r)(q(r))^{1/2}$,

where $a(r) \geqslant 1$ and $\int_0^\epsilon |b(r)|\,dr < \infty$. Suppose further that

ii) $\displaystyle\int_0^\epsilon (V(r))^2\,(q(r))^{-N}\,dr < \infty$,

for some positive integer N, and

iii) $V(r) \in L^\infty(a,\infty) + L^2(a,\infty)$

for all $a > 0$. Then, for all non-real λ, $V(H-\lambda)^{-N}$ and $H_0(H-\lambda)^{-N}$ are bounded operators defined on the entire Hilbert space.

4. Proof of Completeness

Suppose $V(r)$ satisfies either the conditions of Theorem 1 or those of Theorem 2, and that in addition

$$V(r) \in L^1(a, \infty) \cap L^2(a, \infty) \quad \text{for all } a > 0.$$

Then $s - \lim\limits_{t \to \pm\infty} e^{iH_0 t} e^{-iHt}$ exist in $M_{a.c.} H)$.

Proof: Let $E_0(\Delta)$ be the spectral projection for H_0 associated with a finite interval Δ, and let $E_1(\Delta)$ be the corresponding spectral projection for H. We have in the first case when the conditions of Theorem 1 are satisfied

$$\begin{aligned}(E_0(\Delta) H - H_0 E_0(\Delta))(H-\lambda)^{-N}(1-P) \\ = E_0(\Delta) V (H-\lambda)^{-N}(1-P) \\ = E_0(\Delta) \chi V (H-\lambda)^{-N}(1-P) + E_0(\Delta)(1-\chi) V (H-\lambda)^{-N}(1-P),\end{aligned}$$

where in position space χ is the operator of multiplication by the characteristic function of the interval $[0,1]$.

Now $E_0(\Delta)\chi$ is of trace class, and $V(H-\lambda)^{-N}(1-P)$ is bounded; hence the first term on the right-hand side is of trace class. For the second term we may make the factorization $(1-\chi)V = V_1 V_2$, where both V_1 and V_2 belong to $L^2(0,\infty)$. Further $V_1 E_0(\Delta)$ is Hilbert-Schmidt, and $V_2(H-\lambda)^{-N}(1-P) = V_2(H_0-\lambda)^{-1}(H_0-\lambda)(H-\lambda)^{-N}(1-P)$ is Hilbert–Schmidt, since $V_2(H_0-\lambda)^{-1}$ is Hilbert–Schmidt. Hence the second term is of trace class. That is $(E_0(\Delta)H - H_0 E_0(\Delta))(H-\lambda)^{-N}(1-P)$ is of trace class. But P is of finite rank.

Hence $(E_0(\Delta)H - H_0E_0(\Delta))(H-\lambda)^{-N}$ is of trace class, from which it follows that

$$E_0(\Delta) H E_1(\Delta) - H_0 E_0(\Delta) E_1(\Delta) \in T$$

(trace class), since $(H-\lambda)^N E_1(\Delta)$ is bounded.

From Lemma 1 of Ref. [3], in order to prove the existence of $s - \lim\limits_{t\to\infty} e^{iH_0 t} e^{-iHt} f$ for any $f \in M_{a.c.}(H)$, it remains only to show that, with $\Delta = [0, \alpha]$, and given any $\epsilon > 0$,

$$\|(1 - E_0(\Delta)) e^{-iHt} f\| < \epsilon$$

for sufficiently large α and t.

Now if $f = (H-\lambda)^{-N} g$, we have

$$\begin{aligned}&\|(1-E_0(\Delta))(H-\lambda)^{-N}(1-P) e^{-iHt} g\| \\ &\leqslant \|(1-E_0(\Delta))(H_0+c)^{-1}\| \cdot \|(H_0+c)(H-\lambda)^{-N}(1-P) e^{-iHt} g\| \\ &\leqslant \text{const.} (\alpha + c)^{-1} < \tfrac{1}{2}\epsilon\end{aligned}$$

for sufficiently large α, where c is any positive constant.

Also P is compact, so that $\lim\limits_{t\to\infty} \|Pe^{-iHt} g\| = 0$. Therefore $\|(1-E_0(\Delta)) e^{-iHt} f\| < \epsilon$ for sufficiently large α and t. It follows that $s - \lim\limits_{t\to\infty} e^{iH_0 t} e^{-iHt} f$ exists for all $f \in M_{a.c.}(H)$, since elements in the domain of $(H-\lambda)^N$ are dense in the Hilbert space.

The case where the conditions of Theorem 2 are satisfied follows immediately, since it corresponds to setting $P = 0$. This concludes the proof of Theorem 3.

Remark: According to Ref [1], the *existence* of the wave operators $\Omega\pm = s-\lim_{t\to\mp\infty} e^{iHt}e^{-iH_0t}$ follows from the assumption $\int_a^\infty r^{1+\varepsilon}V^2(r)\,dr < \infty$ for some $\epsilon > 0$ and for all $a > 0$. This assumption implies $V(r) \in L^1(a,\infty) \cap L^2(a,\infty)$. Hence for potentials satisfying the conditions of Theorems 1 or 2, together with the assumption of Ref. [1] (which relates only to the behaviour of $V(r)$ away from the origin) we have

$$R(\Omega_+) = R(\Omega_-) = M_{\text{a.c.}}(H).$$

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