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Scattering theory with singular potentials.

I. The two-body problem

by

Derek W. ROBINSON (*)

ABSTRACT. — Firstly we consider the definition of a self-adjoint Hamiltonian for a two-body system interacting with a positive singular potential. For highly singular potentials we obtain a result of essential self-adjointness, for less singular potentials we prove equality of the Friederichs extension and the form sum extension. Secondly we introduce an approximation scheme for singular potentials and demonstrate that if the potentials are approximated from below by bounded potentials then the corresponding Hamiltonians converge in the strong resolvent sense. Thirdly we extend Lavine's results on scattering with positive, decreasing, H_0 -relatively bounded potentials to positive, decreasing potentials with an arbitrary singularity at the origin. In particular we establish absolute continuity of the spectrum and strong asymptotic completeness. Finally we develop monotonicity criteria for the application of perturbation theory to systems with a residual repulsive interaction. We obtain results on the negative spectrum, by linear bounds, and weak asymptotic completeness, by quadratic bounds. These results are illustrated by a discussion of the Lennard-Jones interaction. Most of our results are valid in all but two dimensions.

INTRODUCTION

Scattering theory has developed over the last two decades to become a well established branch of perturbation theory. Typically this latter theory

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allows one to obtain informations about interacting systems of particles whenever the interaction energy is small, in a suitable sense, with respect to the kinetic energy, *i. e.* whenever the interacting system is a small perturbation of the non-interacting system. Unfortunately this is seldom the situation encountered in molecular and nuclear physics; in such contexts potentials of the Lennard-Jones type

$$v(x) = \frac{a}{|x|^{12}} - \frac{b}{|x|^6}, \quad a > 0,$$

frequently occur. This potential is far from being small, in the usual senses, with respect to the kinetic energy and hence perturbation theory is not directly applicable.

One way to circumvent this difficulty is to view the potential as the sum of two components

$$v(x) = v_1(x) + v_2(x)$$

where v_1 , is chosen to be positive, decreasing, and highly singular, and v_2 is chosen to be bounded. Such a decomposition is obviously possible in many ways. Thus it is natural to regard the problems posed by such potentials as perturbations of problems with positive, singular, decreasing potentials. This raises the question whether it is possible to understand systems with decreasing potentials sufficiently well to be able to fruitfully apply perturbation theory. This is the question which will be the object of the sequel.

Scattering theory with repulsive potentials has already been highly developed by Lavine [1] [2]. In these two papers a large number of useful estimates have been obtained and applied to the demonstration of spectral properties and strong asymptotic completeness. Although the basic method of Lavine, a variation of the virial theorem, is non-perturbative his results are only valid for potentials which are perturbations of the non-interacting system. Thus the potentials are only allowed to have a weak singularity at the origin. One of our principal purposes is to extend Lavine's work to cover repulsive potentials of an arbitrary singularity in all dimensions but two, by eliminating all traces of perturbation theory.

The assumption that the potential is a perturbation enters Lavine's theory for three separate reasons:

1. To ensure self-adjointness of the total Hamiltonian.
2. To control domain problems occurring in the basic commutator estimates.
3. To provide *a priori* estimates on asymptotic observables which are sufficient to control potentials of slow decrease.

We avoid the first of these problems by appealing to recent results of Kato [3] and Simon [4] for positive highly singular potentials and by deriving a quadratic form result for less singular potentials. The second is circumvented by a monotone approximation scheme which allows us to work

almost entirely with bounded potentials. Finally we show that, at least for the two-body problem, the *a priori* estimates are not necessary but can be replaced by another monotonicity argument.

After this discussion of repulsive systems we then consider perturbations of such systems. One might well think that the application of perturbation theory would be difficult because of inability to make detailed calculations for the unperturbed system. This is not the case, however, and we demonstrate that by monotonicity arguments one can obtain results on bound states and weak asymptotic completeness in an essentially effortless manner; it is only necessary to apply the known results for perturbations of non-interacting systems. We finish by applying the theory we develop to the Lennard-Jones potential and demonstrate that it is possible to obtain an almost complete understanding of such systems.

In the present paper we limit our attention to the problem of two particles without hard-cores. In subsequent publications we will consider the hard-core and multi-particle problems.

1. THE HAMILTONIAN

In this section we discuss the definition of the Hamiltonian as a self-adjoint operator and derive approximation theorems which will be of practical use in the sequel. We will be interested in positive potentials with possible local singularities. In low dimensions and with weak singularities there will be a definite ambiguity in the definition of the Hamiltonian. Not surprisingly this ambiguity disappears in higher dimensions or for strong singularities, *i. e.* highly repulsive forces. Even in the ambiguous cases we will show that the two natural definitions of the Hamiltonian by quadratic forms coincide; thus physically the ambiguity plays no direct role. This conclusion, together with others obtained in subsequent sections, is unfortunately not obtained in two dimensions; our techniques of estimation fail in this case.

We consider two particles in the configuration space \mathbb{R}^v . The Hilbert space appropriate to the description of the relative motion is $L^2(\mathbb{R}^v)$; the kinetic energy operator of this motion is H_0 , the unique self-adjoint extension of the symmetric operator T_0 ,

$$(T_0\psi)(x) = -\nabla^2\psi(x) \quad , \quad D(T_0) = C_0^\infty(\mathbb{R}^v)$$

The interaction between the particles will be mediated by a real potential v that determines an interaction operator V as follows:

$$(V\psi)(x) = v(x)\psi(x)$$

$$D(V) = \left\{ \psi ; \psi \in L^2(\mathbb{R}^v), \int dx |v(x)|^2 |\psi(x)|^2 < \infty \right\}$$

At the moment we will not specify any further conditions on v , these will appear in the theorems, but it will always be the case that V is densely defined and, by definition, closed.

The principal problem is to give a precise meaning to the Hamiltonian $H_0 + V$ when v has a singularity at the origin. We are interested in lower semi-bounded potentials but, by addition of a constant, these can be made positive; we will only consider the positive case.

THEOREM 1.1. — *Let the potential $x \in \mathbb{R}^n \mapsto v(x) \in \mathbb{R}$ satisfy the following two conditions*

- (1) $v \in L^2(K)$ for all compacts $K \subset \mathbb{R}^n \setminus \{0\}$
 (2) $v(x) \geq A_v / |x|^2$

where

$$A_v = \max(0, 1 - (v - 2)^2/4)$$

It follows that $-\nabla^2 + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n \setminus \{0\})$.

In the original version of this manuscript we gave a detailed proof of a weaker form of this proposition; condition (2) was replaced by

$$v(x) > 2A_v / |x|^2 \quad \text{for } v \leq 3.$$

It has since been pointed out to the author, by A. Grossmann, that a proof of the stronger result has recently been given by Simon [4]. Thus we omit the full proof and refer to [4] for details. Nevertheless we would like to comment on the proof of the weaker version of the theorem as its proof is technically simpler and uses techniques which we will be forced to introduce in the later discussion.

Both Simon's proof, and that of the author, are applications of a new technique due to Kato [3]. The basis of this technique is an inequality which allows one to straightforwardly deduce that if $\psi \in L^2(\mathbb{R}^n)$ is real and orthogonal to the range of $-\nabla^2 + V + 1$ then it follows that

$$(|\psi|, (-\nabla^2 + A_v / |x|^2 + 1)\varphi) \leq 0$$

for all $\varphi \geq 0$, $\varphi \in C_0^\infty(\mathbb{R}^n \setminus \{0\})$. Next, by passing to spherical coordinates and using a simple result from the theory of differential operators (see, for example [5], p. 225), one deduces that $-\nabla^2 + c / |x|^2 + 1$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n \setminus \{0\})$ if $c \geq A_v$. If $S_c + 1$ denotes the self-adjoint extension of this operator it is also well known that for $\varphi \geq 0$ the vector $(S_c + 1)^{-1}\varphi \geq 0$. Thus we are tempted to extend the above inequality by weak closure to the positive elements of $D(S_c + 1)$ and then claim that if $\varphi \geq 0$, then

$$(|\psi|, (-\nabla^2 + A_v / |x|^2 + 1)(S_{A_v} + 1)^{-1}\varphi) = (|\psi|, \varphi) \leq 0$$

This would imply $\psi = 0$, and hence $-\nabla^2 + V$ is essentially self-adjoint. The argument as it stands is, however, fallacious. The difficulty is to establish

that if $\varphi \in D(S_c)$, and $\varphi \geq 0$, then there is a sequence of $\varphi_n \in C_0^\infty(\mathbb{R}^v \setminus \{0\})$, with $\varphi_n \geq 0$ such that

$$\lim_{n \rightarrow \infty} (\chi, (-\nabla^2 + A_v/|x|^2 + 1)\varphi_n) = (\chi, (S_{A_v} + 1)\varphi) \quad , \quad \chi \in L^2(\mathbb{R}^v).$$

This does not follow from the essential self-adjointness because of the positivity restrictions. If φ is zero in a neighbourhood of the origin then this property can be easily established because $1/|x|^2$ is bounded away from the origin, but if φ is non-zero near the origin the argument is trickier. In the case of $-\nabla^2 + c/|x|^2$ with $c > 2A_v$, if $v \leq 3$, it is, however, relatively easy to construct $\varphi_n \geq 0$, $\varphi_n \in D(S_c)$ such that the φ_n vanish near the origin and also approximate an arbitrary positive $\varphi \in D(S)$ in the above sense. This is done in the manner of [6], p. 300-301 (Simon uses a similar argument in [4]). Introduce a sequence of $f_n \in C_0^\infty(\mathbb{R}^v \setminus \{0\})$ such that $0 \leq f_n \leq 1$, and $f_n(x) = 1$ for $|x| > 1/n$. With $\varphi_n = f_n\varphi$ we then have

$$(S_c + 1)\varphi_n = f_n(S + 1)\varphi - 2\nabla f_n \cdot \nabla \varphi - (\nabla^2 f_n)\varphi$$

The first term converges weakly to the desired result and it remains to show that the other terms converge weakly to zero for a suitable choice of f_n . But f_n can be chosen such that $|\nabla^2 f_n(x)| < a|x|^{-2}$ for $|x| < 1/n$ and then

$$|(\chi, (\nabla^2 f_n)\varphi)| \leq a \|\chi\| \|\varphi\| \left[\int_{|x| < 1/n} dx |\chi(x)|^2 \right]^{1/2}$$

and this tends to zero if $\varphi \in D(|x|^{-2})$.

Although $\varphi \in D(S_c)$ and $S_c = (H_0 + c/|x|^2)^*$ it does not follow that $\varphi \in D(|x|^{-2})$. If, however, $c > 2A_v$ it can be established (see the remarks after Theorem 5.5 of section 5) that

$$H_0 + c/|x|^2 = (H_0 + c/|x|^2)^*$$

Thus, for $c > 2A_v$, $\varphi \in D(|x|^{-2})$ and the proof is complete. For $v \geq 4$ and $c = 0$, a similar approximation scheme works for all $\varphi \in C_0^\infty(\mathbb{R}^v)$ and this is sufficient to draw the desired conclusion.

If the potentials we consider are less singular than $A_v/|x|^2$ at the origin then there is a genuine ambiguity in defining a self-adjoint extension of $H_0 + V$; it is known that $H_0 + c/|x|^2$ is not essentially self-adjoint if $0 < c < A_v$. Nevertheless there is a uniqueness result concerning the form extensions of $H_0 + V$, at least in the case $v \neq 2$.

We will need a certain amount of quadratic form terminology. If A is a positive, densely defined, symmetric operator we introduce the quadratic form a associated with it by the definition

$$a(\psi) = (\psi, A\psi) \quad , \quad D(a) = D(A)$$

Such a form is closable (for details see [6], chapter 6) and we denote its

closure by \tilde{a} . This form determines a positive self-adjoint extension \tilde{A} of A such that

$$\tilde{a}(\psi) = \|\tilde{A}^{\frac{1}{2}}\psi\|^2, \quad D(\tilde{a}) = D(\tilde{A}^{\frac{1}{2}})$$

If A and B are two such operators and $A + B$ is densely defined then we can use forms to define at least two self-adjoint extensions of $A + B$.

We denote these extensions by $\widetilde{A + B}$, and $\tilde{A} + \tilde{B}$ and call them the Friedrichs extension and form sum extension, respectively. The first is associated with the closure $\widetilde{a + b}$ of the form $a + b$ where

$$(a + b)(\psi) = a(\psi) + b(\psi), \quad D(a + b) = D(A) \cap D(B)$$

the second is associated with the closed form $\tilde{a} + \tilde{b}$ where

$$(\tilde{a} + \tilde{b})(\psi) = \tilde{a}(\psi) + \tilde{b}(\psi), \quad D(\tilde{a} + \tilde{b}) = D(\tilde{a}) \cap D(\tilde{b}).$$

In general addition and closure, are not interchangeable and hence these extensions are distinct. Nevertheless one easily checks that

$$\widetilde{a + b} \subseteq \tilde{a} + \tilde{b}$$

THEOREM 1.2 (*). — *Let the potential $x \in \mathbb{R}^{\nu} \mapsto v(x) \in \mathbb{R}$ be positive and such that $v \in L^{\infty}(\mathbb{K})$ for all compacts $\mathbb{K} \subset \mathbb{R}^{\nu} \setminus \{0\}$.*

It follows that if $\nu \neq 2$ the Friedrichs extension and the form sum extension of $H_0 + V$ coincide.

Remark. — We expect this result to also be true for $\nu = 2$ but our proof is not valid. Further it follows from Theorem 1.1 that the result is true if $\nu \geq 4$ under the weaker assumption $v \in L^2(\mathbb{K})$. This stronger result can also be obtained if $\nu = 1$, as we will indicate after the proof of the theorem. Thus it seems reasonable to conjecture that Theorem 1.2 is valid for all ν under the assumption $v \in L^2_{\text{loc}}(\mathbb{R}^{\nu} \setminus \{0\})$.

Proof. — Let h_0 , and v , denote the forms associated with H_0 , and V , respectively, we have

$$\widetilde{h_0 + v} \subseteq \tilde{h}_0 + \tilde{v}$$

and to establish equality it suffices to construct, for every $\varphi \in D(\tilde{h}_0 + \tilde{v})$, a sequence $\{\varphi_n\}_{n \geq 0}$ such that $\varphi_n \in D(H_0) \cap D(V)$ and

$$\begin{aligned} \lim_{n \rightarrow \infty} \|\varphi_n - \varphi\| &= 0 \\ \lim_{n \rightarrow \infty} (\tilde{h}_0 + \tilde{v})(\varphi_n - \varphi) &= 0 \end{aligned}$$

(*) If $\nu = 1$ the free Hamiltonian H_0 occurring in this theorem and the sequel must be defined in a slightly different manner. We take H_0 to be the self-adjoint extension of $-\Delta^2$ such that $\psi(0) = 0$ for $\psi \in D(H_0)$.

The construction of an approximating sequence of this kind is achieved in the same manner as above.

Firstly note that if $\varphi \in D(\tilde{h}_0 + \tilde{v})$ has compact support K in $\mathbb{R}^n \setminus \{0\}$ then the construction is straightforward because

$$\tilde{v}(\varphi) \leq \sup_{x \in K} |v(x)| \|\varphi\|^2$$

Thus it suffices to construct a sequence $\varphi_n \in D(H_0)$ such that each φ_n has compact support in $\mathbb{R}^n \setminus \{0\}$ and

$$\begin{aligned} \lim_{n \rightarrow \infty} \|\varphi_n - \varphi\| &= 0 \\ \lim_{n \rightarrow \infty} \tilde{h}_0(\varphi_n - \varphi) &= 0. \end{aligned}$$

This presents no problem and we omit the details.

Secondly let f_n be the sequence of functions introduced above but assume that they have compact support. Explicitly we take $f_n \in C_0^\infty(\mathbb{R}^n \setminus \{0\})$; $0 \leq f_n \leq 1$; $f_n(x) = 1$ if $1/n < |x| < n$; and $f_n(x) = 0$ if $|x| > 2n$ or $|x| < 1/2n$. Now if $\varphi \in D(\tilde{h}_0 + \tilde{v})$ then $\varphi_n = f_n\varphi$ is also in this domain and it has compact support in $\mathbb{R}^n \setminus \{0\}$. Thus the φ_n can be approximated in the desired manner by $\varphi_{m,n} \in D(H_0)$ by the discussion of the previous paragraph. Thus it now suffices to prove that

$$\begin{aligned} \lim_{n \rightarrow \infty} \|f_n\varphi - \varphi\| &= 0 \\ \lim_{n \rightarrow \infty} \tilde{h}_0(f_n\varphi - \varphi) &= 0 \end{aligned}$$

and

$$\lim_{n \rightarrow \infty} \tilde{v}(f_n\varphi - \varphi) = 0.$$

The first of these conditions is readily verified. Consider the third

$$\tilde{v}(f_n\varphi - \varphi) = \int dx v(x) |\varphi(x)|^2 (1 - f_n(x))^2.$$

By assumption $\varphi \in D(\tilde{v})$ and hence

$$\tilde{v}(\varphi) = \int dx v(x) |\varphi(x)|^2 < +\infty.$$

Therefore the desired convergence follows from the dominated convergence theorem.

Finally consider the condition involving \tilde{h}_0 . As $\varphi \in D(\tilde{h}_0)$ it is once-differentiable in the sense of distributions, $\nabla\varphi \in L^2(\mathbb{R}^n)$, and

$$\tilde{h}_0(\psi) = \|\nabla\psi\|^2, \quad \psi \in D(\tilde{h}_0).$$

Therefore

$$\tilde{h}_0(f_n\varphi - \varphi) = \|(\nabla f_n)\varphi - (1 - f_n)\nabla\varphi\|^2 \leq 2\|(\nabla f_n)\varphi\|^2 + 2\|(1 - f_n)\varphi\|^2.$$

The second term in this expression again converges to zero by the dominated convergence theorem. Consider the first term. The f_n can be chosen such that

$$\begin{aligned} |\nabla f_n(x)| &< a/|x| \quad , \quad |x| < 1/n \\ |\nabla f_n(x)| &< 1 \quad , \quad |x| > n \end{aligned}$$

and hence if $\varphi \in D(|x|^{-1})$ one has

$$\|(\nabla f_n)\varphi\|^2 \leq a^2 \int_{|x| < 1/n} dx | |x|^{-1}\varphi(x) |^2 + \int_{|x| > n} dx |\varphi(x)|^2$$

But noting that

$$H_0 \geq (v - 2)^2/4 |x|^2$$

(for a proof, see the proof of Lemma 2.5 in section 2) we conclude that $D(|x|^{-1}) \subset D(\tilde{h}_0)$ if $v \neq 2$. Therefore

$$\lim_{n \rightarrow \infty} \|(\nabla f_n)\varphi\|^2 = 0$$

and the proof is complete.

Remark. — If $v = 1$ it suffices to have $v \in L^2_{loc}(\mathbb{R}^v \setminus \{0\})$. The proof then uses the fact that every $\varphi \in D(\tilde{h}_0)$ is a bounded, uniformly continuous function. This is proved in the same manner as analogous results for $\varphi \in D(H_0)$ if $v \leq 3$ (see [6], p. 302-303). Thus if $\varphi \in D(\tilde{h}_0)$ has compact support $K \subset \mathbb{R}^v \setminus \{0\}$ one has

$$\tilde{v}(\varphi) \leq \|\varphi\|_\infty \|\varphi\|_2 \left[\int_K dx |v(x)|^2 \right]^{1/2}$$

The first argument in the proof now uses this estimate in a straightforward way. The second part of the proof is unchanged.

Although the singular potentials we are considering are nice as far as self-adjointness properties are concerned they are very inconvenient for calculations because of domain problems. The point of the next theorem is to introduce an approximation scheme in terms of bounded potentials. Applications of this scheme will be given in the succeeding sections. Firstly we discuss the situation when the form extensions coincide and secondly the case of essential self-adjointness. Actually the first discussion is sufficient for the sequel but the essential self-adjointness does give us more information which is worth noting.

THEOREM 1.3. — *Let V be a densely defined interaction operator associated with a positive potential v . Assume $H_0 + V$ is densely defined and that its*

Friederichs extension and form sum extension are equal. Denote this extension by H .

Let $\{V_n\}_{n \geq 0}$ be a sequence of interactions associated with bounded potentials v_n such that

- (1) $0 = v_0(x) \leq v_1(x) \leq \dots \leq v_n(x) \leq \dots \leq v(x)$
- (2) $\lim_{n \rightarrow \infty} v_n(x) = v(x)$

It follows that $H_n = H_0 + V_n$ is self-adjoint on $D(H_0)$ and H_n converges to H in the strong resolvent sense, i. e.

$$\lim_{n \rightarrow \infty} \|((H_n + E)^{-1} - (H + E)^{-1})\psi\| = 0$$

for all $\psi \in L^2(\mathbb{R}^v)$ and $\text{Re}E > 0$. Consequently one has

$$\lim_{n \rightarrow \infty} \|(e^{iH_n t} - e^{iH t})\psi\| = 0$$

for all $\psi \in L^2(\mathbb{R}^v)$, uniformly for t in any finite interval of \mathbb{R} .

Proof. — The self-adjointness of H_n is a well-known consequence of the boundedness of the v_n , and consequently the V_n . Next let \tilde{h}_n denote the closed quadratic form associated with H_n . These forms satisfy

$$0 \leq \tilde{h}_0 \leq \tilde{h}_1 \leq \dots \leq \tilde{h}_n \leq \dots \leq \widetilde{h_0 + V}$$

by property (1) of the potentials. This is sufficient to demonstrate the strong convergence of the resolvents $(H_n + E)^{-1}$ (see [6], p. 459-460 for details). The basis of the proof is the observation that

$$(H_0 + E)^{-1} \geq (H_1 + E)^{-1} \geq \dots \geq (H_n + E)^{-1} \geq \dots \geq \widetilde{(H_0 + V + E)^{-1}} \geq 0$$

for $E > 0$. This allows one to conclude that the resolvents converge strongly to the resolvent of a positive self-adjoint operator H_∞ and

$$(H_\infty + E)^{-1} \geq \widetilde{(H_0 + V + E)^{-1}}$$

for $E > 0$. We now argue that $H_\infty = H$.

Let \tilde{h}_∞ denote the closed form associated with H_∞ then the ordering of the resolvents implies that

$$\tilde{h}_\infty \leq \widetilde{h_0 + V}$$

and in particular $D(\tilde{h}_\infty) \supseteq D(\widetilde{h_0 + v})$. But from the argument given in [6] one has

$$\lim_{n \rightarrow \infty} \tilde{h}_n(\psi) = \tilde{h}_\infty(\psi)$$

for all $\psi \in D(\tilde{h}_\infty)$.

Next introduce the form

$$h'(\psi) = \sup_n \tilde{h}_n(\psi)$$

with $D(h')$ the set of ψ such that the supremum is finite. As the supremum is a monotonic limit h' is a quadratic form and

$$h' \supseteq \tilde{h}_\infty.$$

But as $\tilde{h}_n = \tilde{h}_0 + \tilde{v}_n$ one deduces immediately that

$$h' = \tilde{h}_0 + \tilde{v}$$

Thus $\tilde{h}_0 + \tilde{v}$ is an extension of \tilde{h}_∞ . However as the Friederichs extension is assumed equal to the form sum extension

$$D(\tilde{h}_0 + \tilde{v}) = D(\widetilde{h_0 + v}) \subseteq D(\tilde{h}_\infty), \quad \text{i. e. } \tilde{h}_0 + \tilde{v} \supseteq \tilde{h}_\infty \supseteq \widetilde{h_0 + v}.$$

This concludes the proof because the convergence of the exponentials is a standard consequence of strong resolvent convergence. We have included this statement because it will be the information of importance in our applications.

We conclude this section by discussing the extra information obtained in this approximation procedure if one assumes $H_0 + V$ to be essentially self-adjoint.

THEOREM 1.4. — *Adopt the assumptions and notations of Theorem 1.3 but further assume $H_0 + V$ to be essentially self-adjoint, i. e. $H = (H_0 + V)^*$. The graph $G(H)$ of H is given by the pairs (φ, ψ) such that there exists a sequence $\varphi_n \in D(H_n) = D(H_0)$ with the properties that*

$$\begin{aligned} \lim_{n \rightarrow \infty} \|\varphi - \varphi_n\| &= 0 \\ \lim_{n \rightarrow \infty} \|\psi - H_n \varphi_n\| &= 0. \end{aligned}$$

Proof. — Let G denote the graph introduced in the theorem. The proof consists of two parts which we give in two lemmas.

LEMMA 1.4.

$$G \subseteq G(H)$$

Proof. — First note that if $\chi \in D(V)$ we have

$$\lim_{n \rightarrow \infty} \|(V_n - V)\chi\| = 0.$$

This follows from the positivity of the $\{v_n\}$ and v by the dominated convergence theorem once one notes that

$$\|(V_n - V)\chi\|^2 = \int dx |\chi(x)|^2 (v_n(x)^2 - v(x)^2) + 2 \int dx |\chi(x)|^2 v(x)(v(x) - v_n(x)),$$

Next take $(\varphi, \psi) \in G$ and $\chi \in D(H_0) \cap D(V)$ then

$$(\varphi, (H_0 + V)\chi) = \lim_{n \rightarrow \infty} (\varphi_n, (H_0 + V_n)\chi)$$

because of the above convergence and the assumed strong convergence of φ_n to φ . But H_n is self-adjoint and $\varphi_n \in D(H_n)$. Therefore

$$(\varphi, (H_0 + V)\chi) = \lim_{n \rightarrow \infty} (H_n \varphi_n, \chi) = (\psi, \chi)$$

by the definition of ψ . Hence by the definition of the adjoint one has $\varphi \in D((H_0 + V)^*)$ and $\psi \in (H_0 + V)^* \varphi$, *i. e.* $(\varphi, \psi) \in G((H_0 + V)^*)$, or $G \subseteq G((H_0 + V)^*)$. But $H = (H_0 + V)^*$ and the proof is complete.

LEMMA 1.5. — *Let H_∞ denote the self-adjoint operator obtained from the strong resolvent convergence of H_n . It follows that*

$$G(H_\infty) \subseteq G$$

Proof. — Consider $(\varphi, \psi) = (\varphi, H_\infty \varphi) \in G(H_\infty)$. Then one has for some $\chi \in \mathcal{H}$ and $E > 0$

$$\begin{aligned} \varphi &= (H_\infty + E)^{-1} \chi \\ &= \lim_{n \rightarrow \infty} (H_n + E)^{-1} \chi \\ &= \lim_{n \rightarrow \infty} \varphi_n \end{aligned}$$

where we have defined φ_n by

$$\varphi_n = (H_n + E)^{-1} \chi$$

and the limits are in the sense of strong convergence. But

$$H_n \varphi_n = \chi - E \varphi_n$$

and hence the strong limit of $H_n \varphi_n$ exists and

$$\lim_{n \rightarrow \infty} H_n \varphi_n = \chi - E \varphi = H_\infty \varphi = \psi$$

Thus $(\varphi, \psi) \in G$, *i. e.* $G(H_\infty) \subseteq G$.

Combining these two results proves the theorem and in fact gives an independent proof that $H = H_\infty$ because we have

$$G(H_\infty) \subseteq G \subseteq G(H)$$

This implies that H is an extension of H_∞ . As both operators are self-adjoint the only possible extension is the trivial extension, *i. e.* $H = H_\infty$.

2. SMOOTHNESS ESTIMATES

In this section we derive smoothness estimates for systems with decreasing interaction potentials. These estimates are the basic ingredient for the

subsequent discussion of asymptotic completeness. The estimates we derive are very similar to those of Lavine [I] and the material presented in this section is to a large extent a repetition of the calculations of [I]. We feel that this repetition is justified, firstly because we do need different estimates, secondly we have the additional problem of establishing that our estimates are uniform with respect to a sequence of approximating potentials, and thirdly we extend the method of Lavine to one-dimension.

We begin by deriving a basic estimate for the progress operator of Lavine. We will denote by q_i the operator of multiplication by the i -th component of x on $L^2(\mathbb{R}^v)$, *i. e.*

$$(q_i\psi)(x) = x_i\psi(x)$$

and use the notation $p_i = -i\partial/\partial x_i$. Lavine's progress operator A_g is initially defined as a symmetric operator by

$$A_g = g(|q|) \frac{q}{|q|} \cdot p + p \cdot \frac{q}{|q|} g(|q|)$$

$$D(A_g) = C_0^\infty(\mathbb{R}^v)$$

where the function $x \in \mathbb{R}^v \mapsto g(x) \in \mathbb{R}$ is defined by

$$g(r) = \int_0^r d\rho h(\rho)^2$$

and

$$h(\rho) = \frac{1}{(1 + \rho^2)^{\frac{1}{2} + \delta}}$$

We will always choose δ such that $0 < \delta < 1/6$. Lavine has shown that A_g is relatively bounded by H_0 . We will use a quadratic form estimate of this kind.

LEMMA 2.1. — *Let a_g denote the quadratic form defined by*

$$a_g(\psi) = (\psi, A_g\psi) \quad , \quad D(a_g) = D(A_g).$$

It follows that a_g is relatively bounded by the quadratic form $h_0(\psi) = \|H_0^{\frac{1}{2}}\psi\|^2$, $D(h_0) = D(H_0^{\frac{1}{2}})$ associated with H_0 . In particular

$$|a_g(\psi)| \leq h_0(\psi) + \left(1 + \frac{1}{2\delta}\right)^2 \|\psi\|^2 \quad , \quad \psi \in D(A_g),$$

and a_g can be extended by continuity to $D(h_0)$. One has

$$|a_g((H_0 + 1)^{-\frac{1}{2}}\psi)| \leq \left[\left(1 + \frac{1}{2\delta}\right)^2 + 1\right] \|\psi\|^2 \quad , \quad \psi \in L^2(\mathbb{R}^v).$$

Proof. — For $\psi \in D(A_g)$ one has

$$\left| \left(\psi, g(|q|) \frac{q}{|q|} \cdot p + p \cdot \frac{q}{|q|} g(|q|) \psi \right) \right| \leq \|p\psi\|^2 + \|g(|q|)\psi\|^2.$$

But it is easily checked that

$$|g(r)| \leq 1 + \frac{1}{2\delta}$$

and hence we obtain the first estimate. The second follows immediately because

$$\begin{aligned} |a_g((H_0 + 1)^{-\frac{1}{2}}\psi)| &\leq \|H_0^{\frac{1}{2}}(H_0 + 1)^{-\frac{1}{2}}\psi\|^2 + \left(1 + \frac{1}{2\delta}\right)^2 \|\psi\|^2 \\ &= \left[\left(1 + \frac{1}{2\delta}\right)^2 + 1\right] \|\psi\|^2 - \|(H_0 + 1)^{-\frac{1}{2}}\psi\|^2 \end{aligned}$$

COROLLARY 2.2. — *Let V be a positive bounded interaction and H = H₀ + V the associated self-adjoint Hamiltonian. One has*

$$|a_g(H + 1)^{-\frac{1}{2}}\psi| \leq \left[\left(1 + \frac{1}{2\delta}\right)^2 + 1\right] \|\psi\|^2, \quad \psi \in L^2(\mathbb{R}^v).$$

This conclusion is a consequence of the positivity of V which implies $(H + 1)^{-1} \leq (H_0 + 1)^{-1}$ which in turn gives

$$\|(H + 1)^{-\frac{1}{2}}(H_0 + 1)^{\frac{1}{2}}\| \leq 1.$$

Next we calculate the commutator $i[H, A_g]$ where H is a Hamiltonian defined via a potential v which is bounded, once differentiable in the sense of distributions, and decreasing *i. e.*

$$-x \cdot \underline{\nabla} v(x) \geq 0.$$

One immediately establishes that

$$i(\varphi, [V, A_g]\varphi) = -2 \int dx |\varphi(x)|^2 g(x) \frac{x}{|x|} \cdot \underline{\nabla} v(x) \geq 0$$

for all $\varphi \in C_0^\infty(\mathbb{R}^v)$. Next we calculate $i[H_0, A_g]$ in the manner of [7] (*). All calculations and statements are to be understood as results between vectors of $C_0^\infty(\mathbb{R}^v)$.

LEMMA 2.3. — *Let H = H₀ + V be a Hamiltonian defined with a bounded interaction V whose associated potential is bounded, once differentiable and decreasing. It follows that*

$$\begin{aligned} i[H, A_g] &\geq i[H_0, A_g] = 4 \sum_{ij=1}^v p_i \frac{1}{|q|} (g - |q| g' \left(\delta_{ij} - \frac{q_i q_j}{|q|^2} \right) p_j \\ &+ 4 \sum_{i=1}^v p_i g' p_i - g''' - 2(v-1)|q|^{-1} g'' + 2(v-1)(v-3)|q|^{-3} (g - |q| g'). \end{aligned}$$

(*) We thank M. Reed and B. Simon for making this reference available to us in advance of publication.

Proof. — Introduce $g_i(x) = x_i g(|x|)/|x|$ and then

$$\begin{aligned} i[H_0, g_i p_i] &= i \sum_{j=1}^{\nu} [p_j^2, g_i p_i] \\ &= 2 \sum_{j=1}^{\nu} p_j \frac{\partial g_i}{\partial q_j} p_i + i \sum_{j=1}^{\nu} \frac{\partial^2 g_i}{\partial q_j^2} p_i. \end{aligned}$$

Adding the complex conjugate of this expression and summing over i we then find

$$i[H_0, A_g] = 2 \sum_{i,j=1}^{\nu} p_i \left(\frac{\partial g_i}{\partial q_j} + \frac{\partial g_j}{\partial q_i} \right) p_j - \nabla^2 \left(\sum_{i=1}^{\nu} \frac{\partial g_i}{\partial q_i} \right).$$

But one has

$$\frac{\partial g_j}{\partial q_i} = \frac{g}{|q|} \left(\delta_{ij} - \frac{q_i q_j}{|q|^2} \right) + g' \frac{q_i q_j}{|q|^2}$$

and hence

$$\sum_{i=1}^{\nu} \frac{\partial g_i}{\partial q_i} = (\nu - 1) |q|^{-1} g + g'.$$

The result then follows by noting that for a spherically symmetric function f

$$\nabla^2 f = |q|^{-1} (|q| f)'' + (\nu - 3) |q|^{-1} f'.$$

To fully exploit this result we also need the following.

LEMMA 2.4. — *Let $x \in \mathbb{R}^{\nu} \mapsto f(x) \in \mathbb{R}$ be twice differentiable. It follows that*

$$\sum_{i=1}^{\nu} p_i f^2 p_i = f p^2 f + f f'' + (\nu - 1) f f' / |q|$$

Proof. — The proof follows from the identity

$$\begin{aligned} p_i f^2 p_i &= f p_i^2 f + [[p_i, f], f p_i] \\ &= f p_i^2 f - i f [f' q_i / |q|, p_i] \\ &= f p_i^2 f + f f'' q_i^2 / |q|^2 + f f' (1 - q^2 / |q|^2) |q|^{-1} \end{aligned}$$

The foregoing lemmas now lead to the following result.

LEMMA 2.5. — *Let $H_n = H_0 + V_n$ be a sequence of Hamiltonians defined by bounded, differentiable, and decreasing potentials v_n . If $\nu \neq 2$, there are constants $C_{1\nu}, C_{2\nu}, C_{3\nu}$ independent of n such that*

$$h^6 \leq i C_{1\nu} [H_0, A_g] \leq i C_{1\nu} [H_n, A_g]$$

$$h p^2 h \leq ic_{2\nu}[H_0, A_g] \leq ic_{2\nu}[H_n, A_g]$$

$$\sum_{i=1}^{\nu} p_i h^2 p_i \leq ic_{3\nu}[H_0, A_g] \leq ic_{3\nu}[H_n, A_g]$$

where

$$h = (g')^{1/2} = (1 + x^2)^{-1-\delta}$$

Proof. — Lavine has established a similar result for $\nu \geq 3$; the proof for $\nu = 1$ needs a slight modification of his argument.

First note that $g \geq |q|g'$. Further

$$M_{ij}(x) = \delta_{ij} - x_i x_j / |x|^2$$

is a matrix of positive type. Hence from Lemma 2.3 we have

$$i[H_0, A_g] \geq 4 \sum_{i=1}^{\nu} p_i g' p_i - g''' - 2(\nu - 1)g'' / |q|.$$

But then from Lemma 3.3 and the observation that

$$g' = h^2, \quad g'' = 2hh', \quad g''' = 2hh'' + 2h'^2$$

we have that

$$i[H_0, A_g] \geq 4hH_0h + 2hh'' - 2h'^2$$

Next note that

$$\sum_{i=1}^{\nu} \left(-ip_i + \frac{|v-2|}{2} q_i / |q| \right) \left(ip_i + \frac{(v-2)}{2} q_i / |q| \right) \geq 0$$

and therefore

$$H_0 = p^2 = \sum_{i=1}^{\nu} p_i^2 \geq (v-2)^2 / 4 |q|^2.$$

Thus if $0 < \alpha < 1$ we have

$$i[H_0, A_g] \geq 4(1-\alpha)hH_0h + \alpha(v-2)^2 h^2 / |q|^2 + 2hh'' - 2h'^2$$

$$= 4(1-\alpha)hH_0h + \frac{\alpha(v-2)^2}{|q|^2(1+|q|^2)^{1+2\delta}} + \frac{(1+4\delta)(|q|^2-1)}{(1+|q|^2)^{5/2+2\delta}}$$

Finally with the choice $2\alpha(v-2)^2 = 1 + 4\delta$ we find

$$i[H_0, A_g] \geq 4(1-\alpha)hH_0h + \frac{3(1+4\delta)}{(1+|q|^2)^{3/2+2\delta}}.$$

As both terms have positive coefficients the first two statements of the

lemma are established. The third statement follows because $h' \leq 0$ and hence from Lemma 2.4 one has

$$\begin{aligned} \sum_{i=1}^{\nu} p_i h^2 p_i &\leq h H_0 h + h h'' \\ &\leq h H_0 h + \frac{1}{4} (5 + 4\delta)(1 + 4\delta) / (1 + |q|^2)^{3/2 + 2\delta}. \end{aligned}$$

But we have just established that the two terms on the right hand side are bounded by multiples of $i[H_0, A_g]$.

The foregoing lemma is the essential step in establishing the desired smoothness results. Let us introduce the following appropriate notation.

Let B be a bounded operator and $\{H_n\}$ a sequence of self-adjoint operators, Hamiltonians. Following Kato, B is defined to be H_n -smooth if

$$\| \| B \| \|_n^2 = \sup_{\| \psi \| = 1} \int_{-\infty}^{\infty} dt \| B e^{-iH_n t} \psi \|^2 < + \infty.$$

We use a similar notation for a Hamiltonian H ; we simply drop the suffix n .

THEOREM 2.6. — *Let $\{H_n\}_{n \geq 0}$ be a sequence of Hamiltonians $H_n = H_0 + V_n$ on $L^2(\mathbb{R}^\nu)$ where the interaction V_n is given by a positive, bounded, decreasing, differentiable potential v_n .*

If $\nu \neq 2$, the following three operators on $L^2(\mathbb{R}^\nu)$ are H_n -smooth uniformly in n

$$1. \quad h^3(H_n + 1)^{-\frac{1}{2}}, \quad 2. \quad \sqrt{H_0} h (H_n + 1)^{-\frac{1}{2}}, \quad 3. \quad h p (H_n + 1)^{-\frac{1}{2}}$$

If, further, the sequence $\{H_n\}_{n \geq 0}$ converges in the strong resolvent sense to a self-adjoint Hamiltonian H then the operators

$$1. \quad h^3(H + 1)^{-\frac{1}{2}}, \quad 2. \quad \sqrt{H_0} h (H + 1)^{-\frac{1}{2}}, \quad 3. \quad h p (H + 1)^{-\frac{1}{2}}$$

are H -smooth.

Proof. — The proof follows, by an argument similar to Lavine's, from Lemmas 2.1 and 2.5, and Corollary 2.2.

One has

$$\begin{aligned} &\int_{t_1}^{t_2} ds ((H_n + 1)^{-\frac{1}{2}} \psi, e^{iH_n s} h^3 e^{-iH_n s} (H_n + 1)^{-\frac{1}{2}} \psi) \\ &\leq C_{1\nu} \int_{t_1}^{t_2} ds ((H_n + 1)^{-\frac{1}{2}} \psi, e^{iH_n s} i[H_n, A_g] e^{-iH_n s} (H_n + 1)^{-\frac{1}{2}} \psi) \\ &= C_{1\nu} \int_{t_1}^{t_2} ds \frac{d}{ds} a_g((H_n + 1)^{-\frac{1}{2}} e^{-iH_n s} \psi) \\ &= C_{1\nu} [a_g((H_n + 1)^{-\frac{1}{2}} e^{-iH_n s} \psi)]_{t_1}^{t_2} \\ &\leq 2C_{1\nu} \left[\left(1 + \frac{1}{2\delta}\right)^2 + 1 \right] \| \psi \|^2 \end{aligned}$$

A certain care has to be exercised in this estimate as the intermediate steps are only valid for a suitably chosen dense set of ψ , e. g. $\psi \in D(H_0^2)$. But the conclusion

$$\int_{t_1}^{t_2} ds \|h^3(H_n + 1)^{-\frac{1}{2}} e^{-iH_n s} \psi\|^2 \leq 2c_{1v} \left[\left(1 + \frac{1}{2\delta}\right)^2 + 1 \right] \|\psi\|^2$$

extends by continuity to all $\psi \in L^2(\mathbb{R}^v)$. Note that if H_n converges to H in the strong resolvent sense then $(H_{n+1})^{-\frac{1}{2}} e^{-iH_n s}$ converges strongly to $(H + 1)^{-\frac{1}{2}} e^{-iH s}$ uniformly for $S \in [t_1, t_2]$. Hence as C_{1v} is independent of n we also conclude that

$$\| \| h^3(H + 1)^{-\frac{1}{2}} \| \|^2 \leq 2 \left[\left(1 + \frac{1}{2\delta}\right)^2 + 1 \right]$$

The derivation of smoothness for the other operators is identical.

The conclusion of this theorem can now be combined with the results of Section 1 to derive smoothness results for singular decreasing potentials, or for H_0 -bounded potentials. The latter choice extends the results of Lavine to one dimension.

THEOREM 2.7. — *Let V be an interaction operator determined by a positive potential $x \in \mathbb{R}^v \mapsto v(x) \in \mathbb{R}$ which is decreasing in the sense that*

$$v(\lambda x) \leq v(x) \quad , \quad \lambda \geq 1 \quad , \quad x \in \mathbb{R}^v.$$

Assume that v satisfies the assumptions of either Theorem 1.1 or Theorem 1.2. In the first case define a self-adjoint Hamiltonian as the closure of $H_0 + V$. In the second case define H as the Friederichs extension of $H_0 + V$.

If $v = 1$, or $v \geq 3$, it follows that the operators

$$1. \quad h^3(H + 1)^{-\frac{1}{2}} \quad 2. \quad \sqrt{H_0} h(H + 1)^{-\frac{1}{2}} \quad 3. \quad h_{\mathcal{P}}(H + 1)^{-\frac{1}{2}}$$

are H -smooth. Consequently the spectrum of H is absolutely continuous.

Proof. — Note that in neither case is it necessary that v is differentiable. The proof is essentially a consequence of the foregoing results. We can always approximate v , in the manner of Theorem 1.3 or Theorem 1.4, by a monotonically increasing sequence of bounded, once-differentiable, potentials $\{v_n\}_{n \geq 0}$ and be assured that the corresponding sequence of Hamiltonians $\{H_n\}_{n \geq 0}$ converge in the strong resolvent sense to H . The smoothness results then follow from Theorem 2.6. The spectral property follows from Kato's smoothness theory [8] which states, in particular, that if B is H -smooth then the range of B^* is contained in the subspace of absolute continuity of H . But taking

$$B = h^3(H + 1)^{-\frac{1}{2}}$$

we see that the range of B^* is dense.

3. ASYMPTOTIC COMPLETENESS I

In this section, and the following one, we will concentrate on proving asymptotic completeness for a large class of repulsive interactions. In this first part we will concentrate on interactions which decrease like $|x|^{-3-\varepsilon}$ at infinity and return to the discussion of slowly decreasing interactions, *i. e.* $O(|x|^{-1-\varepsilon})$ in the following section. This division of the problem follows Lavine [2], although our methods will differ somewhat from his.

We will first prove that the Møller matrix

$$\Omega_{\pm}(H, H_0) = \text{str. lim}_{t \rightarrow \pm\infty} e^{iHt} e^{-iH_0 t}$$

exists by using an old method due to Kupsch and Sandhas [9]. This proof will be valid for both long and short range interactions. Secondly we will use the methods of Lavine, combined with the existence of $\Omega_{\pm}(H, H_0)$ to conclude that the Møller matrices

$$\Omega_{\pm}(H_0, H) = \text{str. lim}_{t \rightarrow \pm\infty} e^{iH_0 t} e^{-iHt}$$

exist, and hence are unitary. This pattern of reasoning generalizes to the n -body case, at least when the interactions are of $O(|x|^{-3-\varepsilon})$ at infinity.

LEMMA 3.1. — *Let H be the self-adjoint Hamiltonian defined in Theorem 2.7 with a decreasing potential v .*

Further assume that

$$\limsup_{|x| \rightarrow \infty} |x| |v(x)| = 0$$

It follows for all $v \geq 1$ that the strong limits

$$\Omega_{\pm}(H, H_0) = \lim_{t \rightarrow \pm\infty} e^{iHt} e^{-iH_0 t}$$

exist.

Proof. — This proof is well-known; the existence of $\Omega_{\pm}(H, H_0)$ is the easy part of the discussion of asymptotic completeness. Nevertheless we outline the argument as it serves as a model for the proof of the existence of $\Omega_{\pm}(H_0, H)$.

The first step is to introduce a positive C_0^∞ function χ_R with the properties

$$\chi_R(x) = 1 \quad , \quad |x| < R \quad ; \quad \chi_R(x) = 0 \quad , \quad |x| > R + 1$$

One then notes that

$$\|e^{iHt} \chi_R e^{-iH_0 t} \psi\| = \|\chi_R e^{-iH_0 t} \psi\| \xrightarrow{|t| \rightarrow \infty} 0 \quad , \quad \psi \in \mathcal{H}$$

This follows for example by taking ψ to be a Gaussian and explicitly calcu-

lating $\|\chi_R e^{-iH_0 t} \psi\|$. This tends to zero and then one can use the fact the finite sums of Gaussians are dense.

Secondly for $\varphi \in D(H_0)$ one establishes that

$$\begin{aligned} & \|e^{iHt}(1 - \chi_R)e^{-iH_0 t} \varphi - e^{iHs}(1 - \chi_R)e^{-iH_0 s} \varphi\| \\ & \leq \int_s^t dr \| [H_0, \chi_R] e^{-iH_0 r} \varphi \| + \int_s^t dr \| (1 - \chi_R) V e^{-iH_0 r} \varphi \|. \end{aligned}$$

Note that to avoid domain problems in the derivation of this inequality one can first obtain similar inequalities for H_n , where $\{H_n\}_{n \geq 0}$ approximates H in the manner of Theorem 1.3. One then takes the limit over n noting that $(1 - \chi_R)V_n$ and $(1 - \chi_R)V$ are bounded operators. Again by explicit calculations with Gaussians, if $\nu \geq 3$, or by using well-known properties of wave-packets, if $\nu < 3$, one establishes that the two functions appearing as integrands in the above inequality are indeed integrable. Hence

$$\Omega_{\pm}(H, H_0)\psi = \lim_{t \rightarrow \pm\infty} e^{iHt} e^{-iH_0 t} \psi = \lim_{t \rightarrow \pm\infty} e^{iHt} (1 - \chi_R) e^{-iH_0 t} \psi$$

exists for all $\psi \in L^2(\mathbb{R}^\nu)$.

The proof of the existence of $\Omega_+(H_0, H)$ follows roughly the same lines as the above argument but replaces the explicit calculations by smoothness estimates.

LEMMA 3.2. — *Let H satisfy the conditions of Lemma 3.1 and let χ_R be the « characteristic function » introduced above. It follows that if $\nu = 1$, or $\nu \geq 3$, then*

$$\text{str. lim}_{t \rightarrow \pm\infty} e^{iH_0 t} \chi_R e^{-iHt} \psi = 0 \quad , \quad \psi \in L^2(\mathbb{R}^\nu)$$

Proof. — One has

$$\|e^{iH_0 t} \chi_R e^{-iHt} (H + 1)^{-1} \psi\|^2 = \|(H + 1)^{-1} \psi, e^{iHt} \chi_R^2 e^{-iHt} (H + 1)^{-1} \psi\|.$$

But χ_R^2 is dominated by a suitable multiple of h^6 , e. g.

$$\chi_R^2 \leq (1 + (R + 1)^2)^{3/2 + 6\delta} h^6$$

and hence

$$\|e^{iH_0 t} \chi_R e^{-iHt} (H + 1)^{-1} \psi\|^2 \leq C \|h^3 e^{-iHt} (H + 1)^{-1} \psi\|^2.$$

The smoothness estimates of Theorem 2.7 establish that the right hand side of this inequality is a positive integrable function of t . Further its first derivative is uniformly bounded. Therefore it tends to zero as $t \rightarrow \pm \infty$ and

$$\text{str. lim}_{t \rightarrow \pm\infty} e^{iH_0 t} \chi_R e^{-iHt} \varphi = 0$$

for all $\varphi \in D(H)$. But this latter set is dense and hence the statement of the lemma is established.

LEMMA 3.3. — Let H satisfy the conditions of Lemma 3.1 but assume further that

$$\limsup_{|x| \rightarrow \infty} |x|^3 v(x) = 0$$

It follows that if $v = 1$, or $v \geq 3$, that

$$\widehat{\Omega}_{\pm}(H_0, H)\psi = \text{str. lim}_{t \rightarrow \pm\infty} (H_0 + 1)^{-\frac{1}{2}} e^{iH_0 t} e^{-iHt} \psi, \quad \psi \in L^2(\mathbb{R}^v)$$

exists.

Proof. — Let $\{H_n\}_{n \geq 0}$ approximate H in the sense of Theorem 1.3 and assume the v_n are bounded, differentiable, and decreasing. Define

$$D_n(t, s) = e^{iH_0 t} (1 - \chi_R) e^{-iH_n t} - e^{iH_0 s} (1 - \chi_R) e^{-iH_n s}$$

then for $\psi \in D(H_0) = D(H_n)$ one has

$$|(\varphi, D_n(t, s)\psi)| \leq E_{1n}(\varphi, \psi) + E_{2n}(\varphi, \psi) + E_{3n}(\varphi, \psi)$$

where

$$\begin{aligned} E_{1n}(\varphi, \psi) &= \left| \int_s^t dr (\varphi, e^{iH_0 r} \nabla^2 \chi_R e^{-iH_n r} \psi) \right| \\ E_{2n}(\varphi, \psi) &= \left| \int_s^t dr (\varphi, e^{iH_0 r} \underline{\nabla} \chi_R \cdot \mathcal{P} e^{-iH_n r} \psi) \right| \\ E_{3n}(\varphi, \psi) &= \left| \int_s^t dr (\varphi, e^{iH_0 r} (1 - \chi_R) \mathbb{V}_n e^{-iH_n r} \psi) \right|. \end{aligned}$$

We estimate each of these terms separately using the smoothness estimates of the foregoing section.

Note first that

$$\nabla^2 \chi_R = (\nabla^2 \chi_R) \chi_{R+1}$$

and hence by the Schwartz inequality

$$\begin{aligned} &|E_{1n}((H_0 + 1)^{-\frac{1}{2}} \varphi, (H_n + 1)^{-\frac{1}{2}} \psi)|^2 \\ &\leq \int_s^t dr ((H_0 + 1)^{-\frac{1}{2}} \varphi, e^{iH_0 r} |\nabla^2 \chi_R| e^{-iH_0 r} (H_0 + 1)^{-\frac{1}{2}} \varphi) \\ &\quad \cdot \int_s^t dr ((H_n + 1)^{-\frac{1}{2}} \psi, e^{iH_n r} \chi_{R+1} e^{-iH_n r} (H_n + 1)^{-\frac{1}{2}} \psi) \end{aligned}$$

But both $|\nabla^2 \chi_R|$ and χ_{R+1} are dominated by multiples of h^6 and thus we conclude from Theorem 2.6 that

$$|E_{1n}((H_0 + 1)^{-\frac{1}{2}} \varphi, (H_n + 1)^{-\frac{1}{2}} \psi)|^2 \leq C_{1R} \|\varphi\|^2 \int_s^t dr \|h^3 (H_n + 1)^{-\frac{1}{2}} e^{-iH_n r} \psi\|^2$$

where $C_{1R} > 0$ is independent of n .

By an identical argument one finds E_{2n} has a bound of the form

$$\|E_{2n}((H_0 + 1)^{-\frac{1}{2}}\varphi, (H_n + 1)^{-\frac{1}{2}}\psi)\|^2 \leq C_{2R} \|\varphi\|^2 \int_s^t dr \|h p e^{-iH_n r} (H_n + 1)^{-\frac{1}{2}}\psi\|^2$$

and using $v(x) = O(|x|^{-3-\epsilon})$ at infinity one also finds

$$\|E_{3n}((H_0 + 1)^{-\frac{1}{2}}\varphi, (H_n + 1)^{-\frac{1}{2}}\psi)\|^2 \leq C_{3R} \|\varphi\|^2 \int_s^t dr \|h^3 e^{-iH_n r} (H_n + 1)^{-\frac{1}{2}}\psi\|^2$$

with C_{2R} and C_{3R} independent of n . Taking the limit of n to infinity and using the strong resolvent convergence of H_n to H one concludes that

$$\begin{aligned} \| (H_0 + 1)^{-\frac{1}{2}}(e^{iH_0 t}(1 - \chi_R)e^{-iHt} - e^{iH_0 s}(1 - \chi_R)e^{-iHs})(H + 1)^{-\frac{1}{2}}\psi \| \\ \leq C_{1R}^{\frac{1}{2}} \left[\int_s^t dr \|h^3 e^{-iHr}(H + 1)^{-\frac{1}{2}}\psi\|^2 \right]^{\frac{1}{2}} \\ + C_{2R}^{\frac{1}{2}} \left[\int_s^t dr \|h p e^{-iHr}(H + 1)^{-\frac{1}{2}}\psi\|^2 \right]^{\frac{1}{2}} \\ + C_{3R}^{\frac{1}{2}} \left[\int_s^t dr \|h^3 e^{-iHr}(H + 1)^{-\frac{1}{2}}\psi\|^2 \right]^{\frac{1}{2}}. \end{aligned}$$

But the integrability of the right hand side is established in Theorems 2.6 and 2.7. Therefore one concludes with the aid of Lemma 3.2 that

$$\text{str. lim}_{t \rightarrow \pm\infty} (H_0 + 1)^{-\frac{1}{2}} e^{iH_0 t} e^{-iHt} (H + 1)^{-\frac{1}{2}} \psi$$

exists. Finally note that $D((H + 1)^{\frac{1}{2}})$ is dense and hence the desired result is established.

LEMMA 3.4. — *With the assumptions of Lemma 3.3 the following limits exist*

$$\text{str. lim}_{t \rightarrow \pm\infty} e^{iHt} (H_0 + 1)^{-\frac{1}{2}} e^{-iHt} = f_{\pm} ((H_0 + 1)^{-\frac{1}{2}})$$

and define bounded, invertible, self-adjoint operators f_{\pm} . Consequently the ranges of f_{\pm} are dense.

Proof. — First note that

$$e^{iHt} (H_0 + 1)^{-\frac{1}{2}} e^{-iHt} = (e^{iHt} e^{-iH_0 t}) ((H_0 + 1)^{-\frac{1}{2}} e^{-iH_0 t} e^{-iHt}).$$

But the two expressions on the right hand side converge strongly by Lemmas 3.1 and 3.3. Hence the product converges strongly, *i. e.* the f_{\pm} of the lemma exist. These operators are clearly bounded and self-adjoint. To deduce the invertibility note that as H is constructed with a positive potential

$$(H_0 + 1)^{-\frac{1}{2}} \geq (H + 1)^{-\frac{1}{2}}.$$

Therefore we conclude that

$$f_{\pm}((H_0 + 1)^{-\frac{1}{2}}) \geq (H + 1)^{-\frac{1}{2}}.$$

This implies the invertibility of f_{\pm} because $(H + 1)^{-\frac{1}{2}}$ is invertible.

Remark that after we have concluded that the $\Omega_{\pm}(H_0, H)$ exist it is possible to conclude that

$$f_{\pm}((H_0 + 1)^{-\frac{1}{2}}) = (H + 1)^{-\frac{1}{2}}$$

but at this stage we can only derive the lower bound. This bound allows us to conclude the existence of the $\Omega_{\pm}(H_0, H)$ when combined with the foregoing results.

THEOREM 3.5. — *Let H be a self-adjoint Hamiltonian defined with a positive potential v satisfying the conditions of Theorem 2.7.*

Further assume that

$$\lim_{|x| \rightarrow \infty} |x|^3 v(x) = 0$$

If $v = 1$, or $v \geq 3$, it follows that the Møller matrices

$$\Omega_{\pm}(H, H_0) = \text{str. lim}_{t \rightarrow \pm \infty} e^{iHt} e^{-iH_0 t}$$

$$\Omega_{\pm}(H_0, H) = \text{str. lim}_{t \rightarrow \pm \infty} e^{iH_0 t} e^{-iHt}$$

exist and are unitary.

Proof. — The only thing that remains to be proved is the existence of $\Omega_{\pm}(H_0, H)$. Consider

$$\begin{aligned} & \| e^{iH_0 t} e^{-iHt} f_{\pm}((H_0 + 1)^{-\frac{1}{2}}) \psi - (H_0 + 1)^{-\frac{1}{2}} e^{iH_0 t} e^{-iHt} \psi \| \\ &= \| (f_{\pm}((H_0 + 1)^{-\frac{1}{2}}) - e^{iHt} (H_0 + 1)^{-\frac{1}{2}} e^{-iHt}) \psi \|. \end{aligned}$$

We conclude from Lemmas 3.3 and 3.4 that the limits

$$\text{str. lim}_{t \rightarrow \pm \infty} e^{iH_0 t} e^{-iHt} f_{\pm}((H_0 + 1)^{-\frac{1}{2}})$$

exist. But the range of f_{\pm} is dense, Lemma 3.4, and hence $\Omega_{\pm}(H_0, H)$ exist.

We conclude this section with a remark concerning the Hamiltonians $\{H_n\}_{n \geq 0}$ that we have used throughout the proofs to approximate H . As a by-product of the above argument it is evident that the Møller matrices $\Omega_{\pm}(H_n, H_0)$ and $\Omega_{\pm}(H_0, H_n)$ exist but it is also possible to deduce that

$$\text{str. lim}_{n \rightarrow \infty} \Omega_{\pm}(H_n, H_0) = \Omega_{\pm}(H, H_0)$$

It suffices to deduce that $\Omega_{\pm}(H_n, H)$ tends to the identity and this is possible because the estimates for $\Omega_{\pm}(H_n, H_m)$ are uniform in n and m .

4. ASYMPTOTIC COMPLETENESS II

The proof of asymptotic completeness given in the previous section is only valid if the potential is $O(|x|^{-3-\varepsilon})$, $\varepsilon > 0$, at infinity. In this section we give a proof which covers the situation of potentials which are $O(|x|^{-1-\varepsilon})$, $\varepsilon > 0$, at infinity. The proof is a little less satisfactory as one must further assume that the potential is once differentiable at infinity.

We begin by remarking that Lemmas 3.1 and 3.2 are valid for long range potentials but we need an alternative proof for the conclusion of Lemma 3.3. Once this is established one can again use Lemma 3.4, which is independent of a short range assumption for the potential, to draw the desired conclusion by repetition of the same arguments.

LEMMA 4.1. — *Let H be the self-adjoint Hamiltonian defined in Theorem 2.7. Further assume that the potential is positive, decreasing, once-differentiable at infinity, and*

$$\limsup_{|x| \rightarrow \infty} |x| |v(x)| = 0$$

It follows for $v = 1$, or $v \geq 3$, that

$$\widehat{\Omega}_{\pm}(H_0, H) = \text{str.} \lim_{t \rightarrow \pm \infty} (H_0 + 1)^{-\frac{1}{2}} e^{iH_0 t} e^{-iHt}$$

exists.

Proof. — We use the notation introduced in the proof of Lemma 3.3 and consider

$$E_{3n}(\varphi, H_n^2(H_n + 1)^{-2}\psi) \leq F_{1n}(\varphi, H_n(H_n + 1)^{-2}\psi) + F_{2n}(\varphi, H_n(H_n + 1)^{-2}\psi)$$

where

$$F_{1n}(\varphi, \psi) = \left| \int_s^t dr (\varphi, e^{iH_0 r} (1 - \chi_R) V_n H_0 e^{-iH_n r} \psi) \right|$$

$$F_{2n}(\varphi, \psi) = \left| \int_s^t dr (\varphi, e^{iH_0 r} (1 - \chi_R) V_n^2 e^{-iH_n r} \psi) \right|$$

We estimate F_{1n} following Lavine. With $v_{nR} = (1 - \chi_R)v_n$ one has

$$\begin{aligned} v_{nR} H_0 &= (v_{nR}/h)(h p^2) \\ &= (v_{nR}/h)(p^2 h) + (v_{nR}/h)[h, p^2] \\ &= [(v_{nR}/h \sqrt{H_0})][\sqrt{H_0} h] + [h v_{nR}] \left[4i p \cdot \frac{q}{|q|} \frac{h'}{h^2} \right] \\ &\quad - [h v_{nR}][4h''/h^2 + (v-1)h'/|q|h^2]. \end{aligned}$$

Now each of the terms included in square brackets is H_0 -smooth and H_n -smooth uniformly in n when multiplied by an appropriate factor

$(H_0 + 1)^{-\frac{1}{2}}$ at the left or $(H_n + 1)^{-\frac{1}{2}}$ at the right. Notice that the proof of smoothness of $(v_{nR}/h)\sqrt{H_0}$ assumes v_{nR}/h once-differentiable because to bound an expression of the form $f_n H_0 f_n$ one must use

$$f_n H_0 f_n = p f_n^2 p + f_n'^2 - i p \cdot \frac{q}{|q|} f_n f_n' + i f_n' f_n \frac{q}{|q|} \cdot p.$$

The identity allows one to introduce uniform bounds on the $f_n = v_{nR}/h$ but without using this rearrangement it is not possible to uniformly bound $(v_{nR}/h)H_0(v_{nR}/h)$ in terms of bounds of v_n . The identity uses the differentiability of the v_{nR} and to have uniform bounds it is necessary to have a bound on the limit potential $v_R = (1 - \chi_R)v$. Thus the potential has to be once differentiable outside some sphere $|x| \leq R$.

Next consider

$$F_{2n}(\varphi, H_n(H_n + 1)^{-2}\psi) \leq G_{1n}(\varphi_1(H_n + 1)^{-2}\psi) + G_{2n}(\varphi_1(H_n + 1)^{-2}\psi)$$

where

$$G_{1n}(\varphi, \chi) = \left| \int_s^t dr(\varphi, e^{iH_0 r}(1 - \chi_R)V_n^2 H_0 e^{-iH_n r}\chi) \right|$$

$$G_{2n}(\varphi, \chi) = \left| \int_s^t dr(\varphi, e^{iH_0 r}(1 - \chi_R)V_n^3 e^{-iH_n r}\chi) \right|.$$

G_{1n} can again be separated into a sum of terms containing H_0 - and H_n -smooth factors in an identical manner to the treatment of F_{1n} . G_{2n} is already in the desired form because

$$(1 - \chi_R)V_n^3 \leq C_R h^6$$

for $C_R > 0$ independent of n .

By this process of division and using the Schwartz inequality, the standard smoothness arguments, and the strong resolvent convergence of the $\{H_n\}_{n \geq 0}$ to H we conclude that the strong limits

$$\text{str. lim}_{t \rightarrow \pm\infty} (H_0 + 1)^{-\frac{1}{2}} e^{iH_0 t} e^{-iHt} H^2 (H + 1)^{-5/2} \psi$$

exist. But the range of $H^2(H + 1)^{-5/2}$ is dense and hence the conclusion of the lemma is established.

THEOREM 4.2. — *The conclusions of Theorem 3.5, asymptotic completeness, are valid for an Hamiltonian H satisfying the assumptions of Lemma 4.1.*

The proof is identical to that of 3.5.

5. PERTURBATION THEORY

In the introduction we mentioned that one of our motivations in studying positive singular potentials was to provide a starting point for a perturbation-

theoretic discussion of general singular potentials. In this section we consider some aspects of perturbation theory when the unperturbed system has a positive interaction. To apply perturbation theory successfully it is necessary to make various estimates of the perturbation in terms of the unperturbed Hamiltonian. If the unperturbed system is non-interacting such estimates can usually be explicitly calculated. This is not necessarily the case when the basic system includes a repulsive interaction but we will demonstrate that monotonicity arguments can often be used to make estimates.

We will consider perturbations V arising from potentials v in the Rollnik class \mathbf{R} in $L^2(\mathbb{R}^3)$. The two-particle perturbation theory of such potentials has been thoroughly analysed when the unperturbed system has Hamiltonian H_0 (see for example [10]). We will use the notation and results of [10] extensively.

First note that for $V \in \mathbf{R}$ one has $|V|^{\frac{1}{2}}$ is relatively bounded by $(H_0 + E)^{\frac{1}{2}}$, $E > 0$, with a relative bound which can be chosen arbitrarily small if E is chosen large.

It then follows that

$$A_E^0 = |V|^{\frac{1}{2}}(H_0 + E)^{-1} |V|^{\frac{1}{2}}$$

and

$$B_E^0 = (H_0 + E)^{-\frac{1}{2}} |V| (H_0 + E)^{-\frac{1}{2}}$$

are bounded. The first principal estimates, concerning the negative spectrum of the form of $H_0 + V$, use the fact that A_E^0 and B_E^0 are in fact Hilbert-Schmidt for all $E \geq 0$. The Hilbert-Schmidt norms satisfy

$$\|A_E^0\|_{\text{H.S.}}^2 = \|B_E^0\|_{\text{H.S.}}^2 = (4\pi)^{-2} \int dx^3 dy^3 \frac{|v(x)| |v(y)|}{|x - y|^2} e^{-\sqrt{E}|x-y|}.$$

If H is a general Hamiltonian which is larger than H_0 we have the following.

THEOREM 5.1. — *Let H be a self-adjoint operator on $L^2(\mathbb{R}^3)$ such that*

$$H \geq H_0$$

in the sense of quadratic forms. It follows that the operators

$$\begin{aligned} A_E &= |V|^{\frac{1}{2}}(H + E)^{-1} |V|^{\frac{1}{2}} \\ B_E &= (H + E)^{-\frac{1}{2}} |V| (H + E)^{-\frac{1}{2}} \end{aligned}$$

where $V \in \mathbf{R}$, are Hilbert-Schmidt, for all $E \geq 0$, and

$$\begin{aligned} \|A_E\|_{\text{H.S.}} &\leq \|A_E^0\|_{\text{H.S.}} \\ \|B_E\|_{\text{H.S.}} &\leq \|B_E^0\|_{\text{H.S.}} \end{aligned}$$

Proof. — As $H + E \geq H_0 + E$ for $E \in \mathbb{R}$ it follows that

$$(H + E)^{-1} \leq (H_0 + E)^{-1} \quad \text{for } E \geq 0.$$

Hence $0 \leq A_E \leq A_E^0$. As A_E^0 is compact it follows from the mini-max principle that A_E is compact. Further if λ_n, λ_n^0 , denote the eigenvalues of A_E , and A_E^0 , arranged in decreasing order and repeated according to multiplicity, the mini-max principle gives

$$0 \leq \lambda_n \leq \lambda_n^0$$

Hence

$$\|A_E\|_{\text{H.S.}}^2 = \sum_{n \geq 1} \lambda_n^2 \leq \sum_{n \geq 1} (\lambda_n^0)^2 = \|A_E^0\|_{\text{H.S.}}^2.$$

Next consider B_E . One has

$$B_E = (H + E)^{-\frac{1}{2}}(H_0 + E)^{\frac{1}{2}}B_E^0(H_0 + E)^{\frac{1}{2}}(H + E)^{-\frac{1}{2}}.$$

But we now have

$$1 \geq (H + E)^{-\frac{1}{2}}(H_0 + E)(H + E)^{-\frac{1}{2}}$$

and hence $\|(H + E)^{-\frac{1}{2}}(H_0 + E)^{\frac{1}{2}}\| \leq 1$. Thus B_E is the product of two bounded operators and a Hilbert-Schmidt operator B_E^0 . Hence B_E is Hilbert-Schmidt and the norm estimate follows from the usual inequalities for such operators.

COROLLARY 5.2. — *Under the assumptions of the theorem the form sum $H_p = H + V$ defines a lower-semi-bounded, self-adjoint operator. The negative spectrum of H_p consists of a finite number of discrete eigenvalues in $[-\infty, 0]$, each with finite multiplicity. The total number of eigenstates, counting multiplicity, is bounded by $\|A_0\|_{\text{H.S.}}^2 \leq \|A_0^0\|_{\text{H.S.}}^2$.*

The corollary follows by the arguments of [10], see especially p. 79-87. The derivations given there depend only on the Hilbert-Schmidt properties obtained in the theorem.

The foregoing estimates are linear, comparing $|V|^{\frac{1}{2}}$ to $(H + E)^{\frac{1}{2}}$. There are also quadratic estimates, comparing $|V|^{\frac{1}{2}}$ to $(H + E)$, which are used in scattering theory to obtain weak properties of asymptotic completeness, called Kato completeness in [10]. To obtain these properties it is sufficient to have quadratic bounds connecting H and H_0 .

THEOREM 5.3. — *Let H be a positive self-adjoint operator on $L^2(\mathbb{R}^3)$ such that*

$$(H + E_0)^2 \geq H_0^2$$

in the sense of quadratic forms, for some $E_0 \geq 0$. Let V be a Rollnik interaction such that

$$C_E^0 = |V|^{\frac{1}{2}}(H_0 + E)^{-1}$$

is Hilbert-Schmidt for $E > 0$. It follows that

$$C_E = |V|^{\frac{1}{2}}(H + E)^{-1}$$

is Hilbert-Schmidt for $E > E_0$ and

$$\|C_{E+E_0}\|_{\text{H.S.}}^2 \leq \|C_E^0\|_{\text{H.S.}}^2.$$

If these conditions are satisfied it follows that

$$D_E = (H + V + E)^{-1} - (H + E)^{-1}$$

is trace-class for E sufficiently large, where $H + V$ denotes the form sum.

Proof. — First note that $(H + E_0)^2 \geq H_0^2$ implies $H + E_0 \geq H_0$ and hence $(H + E + E_0)^2 \geq (H_0 + E)^2$ for all $E \geq 0$. Hence we have

$$(H + E + E_0)^{-2} \leq (H_0 + E)^{-2}$$

for all $E \geq 0$ and therefore

$$(C_{E+E_0})(C_{E+E_0})^* \leq (C_E^0)(C_E^0)^*$$

The first implication is immediate.

Next we refer to [10], p. 72-74. The representation obtained for $(H + E)^{-1} - (H_0 + E)^{-1}$ in Theorem II.34 can now be rederived for D_E as its derivation relies only on the fact that A_E and C_E have norms much smaller than one for E sufficiently large. But this is true because

$$\begin{aligned} \|A_{E+E_0}\|_{\text{H.S.}} &\leq \|A_E^0\|_{\text{H.S.}} \\ \|C_{E+E_0}\|_{\text{H.S.}} &\leq \|C_E^0\|_{\text{H.S.}} \end{aligned}$$

The conclusion of the theorem then follows directly from the representation as it expresses D_E as a product of two Hilbert-Schmidt operators and a bounded operator.

COROLLARY 5.4. — *Let H and V satisfy the assumptions of Theorem 5.3. Further let \mathcal{H}_{ac}^0 and \mathcal{H}_{ac}^p denote the subspaces of absolute continuity of the Hamiltonians H , and $H + V$, respectively.*

It follows that

$$\begin{aligned} \Omega_{\pm}(H + V, H)\psi &= \text{str. lim}_{t \rightarrow \pm\infty} e^{i(H+V)t} e^{-iHt} \psi, \quad \psi \in \mathcal{H}_{ac}^0, \\ \Omega_{\pm}(H, H + V)\varphi &= \text{str. lim}_{t \rightarrow \pm\infty} e^{iHt} e^{-i(H+V)t} \varphi, \quad \varphi \in \mathcal{H}_{ac}^p, \end{aligned}$$

exist as unitary mappings between \mathcal{H}_{ac}^0 and \mathcal{H}_{ac}^p .

This conclusion follows from the results of Birman and Kato, see [6], p. 545; its proof depends on the trace class property of D_E derived in Theorem 5.3.

Note that if we also know that $\Omega_{\pm}(H, H_0)$, $\Omega_{\pm}(H_0, H)$ exist, *e. g.* if H satisfies the assumptions of Theorem 3.5, it then follows by the chain rule that $\Omega_{\pm}(H + V, H_0)$, $\Omega_{\pm}(H_0, H + V)$ exist as unitary mappings between $L^2(\mathbb{R}^3)$ and \mathcal{H}_{ac}^p .

If H is obtained from H_0 by the addition of a positive interaction then $H \geq H_0$. It is, however, more difficult to ensure that $H^2 \geq H_0^2$ so that it is useful to have criteria on the potentials such that this latter property is assured.

THEOREM 5.5. — *Let V be an interaction derived from a positive potential v which is once differentiable on $\mathbb{R}^n \setminus \{0\}$. Assume $H_0 + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n \setminus \{0\})$ and denote its closure by H .*

It follows that if

$$(v + E_0)^2 + \frac{(v - 2)^2}{2|\varphi|^2}(v + E_0) - 2|\underline{\nabla}\sqrt{v + E_0}|^2 \geq 0$$

then

$$(H + E_0)^2 \geq H_0^2$$

In particular if v satisfies

$$\inf_{x \in \mathbb{R}^n} \left\{ v(x)^2 + \frac{(v - 2)^2}{2|x|^2}v(x) - 2|\underline{\nabla}\sqrt{v(x)}|^2 \right\} > -\infty$$

then there is an E_0 such that

$$(H + E_0)^2 \geq H_0^2$$

Proof. — Take $\varphi \in C_0^\infty(\mathbb{R}^n \setminus \{0\})$ and then one has

$$\|(H_0 + V + E_0)\varphi\|^2 = \|H_0\varphi\|^2 + (\varphi, R\varphi)$$

where

$$\begin{aligned} R &= (V + E_0)^2 + (V + E_0)H_0 + H_0(V + E_0) \\ &= (V + E_0)^2 + [\sqrt{V + E_0}, [\sqrt{V + E_0}, H_0]] + 2\sqrt{V + E_0}H_0\sqrt{V + E_0} \\ &\geq (V + E_0)^2 + \frac{(v - 2)^2}{2|\varphi|^2}(V + E_0) - 2|\underline{\nabla}\sqrt{V + E_0}|^2. \end{aligned}$$

The lower bound is obtained by explicit calculation of the double commutator and the estimate given for H_0 in the proof of Lemma 2.5. Next note that as V is positive

$$\begin{aligned} R &\geq V^2 + \frac{(v - 2)^2}{2|\varphi|^2}V - \frac{1}{2} \frac{|\underline{\nabla}V|^2}{V + E_0} + E_0^2 \\ &\geq V^2 + \frac{(v - 2)^2}{2|\varphi|^2}V - 2|\underline{\nabla}\sqrt{V}|^2 + E_0^2 \end{aligned}$$

The last statement of the theorem follows immediately.

The criterion of this theorem is particularly simple to apply and its validity is easily checked for $v(x) = c/|x|^n$, $n > 2$ and $c \geq 0$. If $n = 2$, we find from this bound that

$$\|(\mathbf{H}_0 + c/|q|^2)\varphi\|^2 \geq \|\mathbf{H}_0\varphi\|^2 + (c^2 - 2cA_v) \| |q|^{-2}\varphi \|^2$$

where A_v is the constant introduced in Theorem 1.1. Thus if $c > 2A_v$, we see that $\mathbf{H}^2 \geq \mathbf{H}_0^2$ but we can also conclude that $\mathbf{H}_0 + c/|q|^2$ is closed (cf. the remarks after Theorem 1.1). Thus for repulsive potentials of this kind all the conclusions of this section are valid; of course the results of the foregoing sections also apply because the potentials are positive and decreasing.

Thus we have shown that the standard results of perturbation theory can be extended to a large class of singular potentials by use of the results for decreasing potentials and simple monotonicity arguments. The only feature which we have not touched upon is the detailed analysis of the positive spectrum of Hamiltonians obtained by perturbations of positive Hamiltonians. There are two aspects to this analysis locating, or more habitually proving the absence of, positive eigenvalues and singular continuous spectrum. The known methods of handling these problems are quite detailed and it appears difficult to give generic statements for the kinds of systems we have been studying. In particular cases this is, however, possible.

We conclude by applying the foregoing analysis to the interaction which motivated our interest in this subject, the Lennard-Jones potential. The following theorem establishes almost all desirable properties for this potential.

THEOREM 5.6. — *Let V denote the Lennard-Jones interaction in three-dimensions, i. e. V is multiplication on $L^2(\mathbb{R}^3)$ by*

$$v(x) = \frac{a}{|x|^{12}} - \frac{b}{|x|^6}$$

where $a > 0$, $b \geq 0$. It follows that $\mathbf{H}_0 + V$ is essentially self-adjoint. We denote its closure by \mathbf{H} . The following properties are valid.

1. The spectrum of \mathbf{H} consists of a finite number of eigenvalues, with finite multiplicity, on the interval $[b^2/4a, 0]$ and a continuous part on $[0, +\infty)$.
2. The Møller matrices

$$\Omega_{\pm}(\mathbf{H}, \mathbf{H}_0)\psi = \lim_{t \rightarrow \pm\infty} e^{i\mathbf{H}t} e^{-i\mathbf{H}_0 t} \psi, \quad \psi \in L^2(\mathbb{R}^3),$$

$$\Omega_{\pm}(\mathbf{H}_0, \mathbf{H})\varphi = \lim_{t \rightarrow \pm\infty} e^{i\mathbf{H}_0 t} e^{-i\mathbf{H}t} \varphi, \quad \varphi \in \mathcal{H}_{ac}$$

exist, where \mathcal{H}_{ac} is the subspace of absolute continuity of \mathbf{H} .

Proof. — $\mathbf{H}_0 + V + b^2/4a$, and hence $\mathbf{H}_0 + V$ is essentially self-adjoint by Theorem I.1.

Next write

$$v = v_+ + v_-$$

where

$$v_+(x) = \begin{cases} \frac{a}{|x|^{12}} - \frac{b}{|x|^6} & , \quad |x|^6 \leq a/b \\ 0 & , \quad |x|^6 > a/b \end{cases}$$

and note that $v_- = v - v_+$ is bounded and $v_+ \in L^{3/2}(\mathbb{R}^3) \subset R$. Further, the operator $H_0 + V_+$ is essentially self-adjoint by Proposition 1.1 and its closure H_+ satisfies $H_+ \geq H_0$. Thus Theorem 5.1 and Corollary 5.2 are applicable. But as $H_0 + V$ is essentially self-adjoint the form sum of $H_+ + V_-$ is equal to H . Thus the stated property of the negative spectrum is established.

Let $f \in C_0^\infty$ have the following properties: $1 \geq f \geq 0$, $f(x) = 0$, if $|x|^6 \geq a/b$, $f(x) = 1$ for all x in an open neighbourhood of the origin. Define

$$v_{+f} = v_+ f \quad , \quad v_{-f} = v - v_{+f}$$

and note that $H_0 + V_{+f}$ is again essentially self-adjoint. But it follows from Theorem 5.5 that its closure H_{+f} satisfies

$$(H_{+f} + E_0)^2 \geq H_0^2$$

for E_0 sufficiently large. To verify this note that v and hence v_{+f} satisfies

$$|v(x)|^2 - 2|\nabla\sqrt{v(x)}|^2 \geq 0$$

for all x in an open neighbourhood of the origin. Outside of this neighbourhood v_{+f} together with its first derivative are bounded, Hence the criterion of Theorem 5.5 is satisfied. With this division $v_{-f} \in L^2 \cap L^1 \subset R \cap L^1$ and hence $|V_{-f}|^{\frac{1}{2}}(H_0 + E)^{-1}$ is Hilbert-Schmidt for $E \geq 0$. Thus the conclusions of Theorem 5.3 and Corollary 5.4 apply. Again the form sum of H_{+f} and V_{-f} is equal to H . But as v_{+f} is positive and decreasing, Theorem 3.5 applies. Applying the chain rule to $\Omega_\pm(H, H_{+f})$ and $\Omega_\pm(H_{+f}, H_0)$ we obtain the existence of $\Omega_\pm(H, H_0)$. The existence of $\Omega_\pm(H_0, H)$ follows in a similar manner.

The absence of positive discrete spectrum can be inferred from [II]; the proof given there does not rely on V being a perturbation of H_0 and it can be readily adapted to the present situation.

Thus we have derived all desirable properties of the Lennard-Jones potential except the absence of positive singular continuous spectrum.

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