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Objekttyp: **Article**

Zeitschrift: **Helvetica Physica Acta**

Band (Jahr): **46 (1973)**

Heft 5

PDF erstellt am: **13.09.2024**

Persistenter Link: https://doi.org/10.5169/seals-114499

Helvetica Physica Acta
Vol. 46, 1973.

Birkhäuser Verlag Basel

On the Characterization of Bound States and Scattering States in Quantum Mechanics

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Abstract. Ruelle's definition of bound states and scattering states in quantum mechanics in terms of the position operator is related to the usually accepted definition of these states in terms of the spectral properties of the Hamiltonian H, viz. the states belonging to the point spectrum or the continuous spectrum of H. The equivalence of the two ways of defining these states is established for a large class of n-body Hamiltonians ($n < \infty$) including practically all Schrödinger Hamiltonians of physical interest as well as Dirac Hamiltonians.

I. Introduction

There are two ways of looking at bound states in quantum mechanics, one mathematical and one more intuitive. In the latter a bound state is characterized by the property that it should be essentially localized in a volume of finite size at all times. On the other hand, the mathematical approach is based on spectral theory. One defines $\mathscr{H}_p(H)$ (or in short $\mathscr{H}_p$) to be the closed subspace of the Hilbert space $\mathscr{H}$ spanned by the set of all eigenvectors of the Hamiltonian H, and one easily verifies that every vector of $\mathscr{H}_p$ is a bound state in the sense indicated above (precise mathematical statements will be given later). Furthermore, the Hamiltonians used to describe scattering systems are expected to have the property that the vectors belonging to the continuous subspace $\mathscr{H}_c \equiv \mathscr{H} \ominus \mathscr{H}_p$ will disappear from any fixed bounded region of space in the course of their time evolution. These vectors may then be called *scattering states*.

It is of some interest to know in what circumstances these two definitions coincide. In other words: under what conditions can one assert that the states belonging to $\mathscr{H}_p$ are precisely those that remain essentially concentrated in a bounded region in the course of the evolution? In most presentations of scattering theory, the equivalence of these two definitions is taken for granted. It is the purpose of our paper to give a proof of this equivalence for n-body systems ($n < \infty$) in infinite space under rather general conditions which cover practically all cases of physical interest. The essential point in these conditions is that the Hamiltonian be obtained by perturbing a function of the *momentum* operators.

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[1]) Partially supported by the Swiss National Science Foundation.

It is easy to see that the two definitions will not always coincide by considering the case where H is a (self-adjoint) function of the position operator Q. One then has for any vector $f \in \mathscr{H}$

$$|(e^{-iHt}f)(x)|^2 = |f(x)|^2 \quad (x \in \mathbb{R}^N). \tag{1}$$

Since $f(x)$ is square-integrable, it is essentially localized in a bounded region of $\mathbb{R}^N$; i.e. given $\epsilon > 0$, there exists a subset Δ of $\mathbb{R}^N$ of finite size with

$$\int_{\mathbb{R}^N - \Delta} |f(x)|^2 \, d^N x < \epsilon.$$

This implies, together with (1), that the state f will be essentially concentrated in Δ at all times, i.e. it is a bound state in the physical sense, and this result is independent of any assumption on the spectral type of $H = F(Q)$.

For the Hamiltonians used in standard non-relativistic scattering theory, the equivalence of the two ways of defining bound states and scattering states was established by Ruelle [1] who proved the following result:

Theorem (Ruelle):

In $\mathscr{H} = L^2(\mathbb{R}^N)$, let $H_0 = -\Delta$ and consider one of the following two classes of Hamiltonians:

A) H is the Friedrichs extension of the sum of H_0 and V on $D(H_0) \cap D(V) \cap C_0^\infty(\mathbb{R}^N)$, where V is bounded below and such that there exists $\Delta \subset \mathbb{R}^N$ of Lebesgue measure zero with

$$V \in L^2_{loc}(\mathbb{R}^N - \Delta).$$

B) $H = H_0 + V$, where V is a sum of pair potentials $V_{ij}(x_i - x_j)$ such that $V_{ij} \in L^2(\mathbb{R}^\nu) + L^\infty(\mathbb{R}^\nu)$ with $\nu \leqslant 3$.

Let $f \in \mathscr{H}$. Then

a) $f \in \mathscr{H}_p(H) \Leftrightarrow$ for each $\epsilon > 0$ there exists $R > 0$ such that

$$\sup_{t \in \mathbb{R}} \int_{|x| \geqslant R} d^N x |(e^{-iHt}f)(x)|^2 < \epsilon. \tag{R1}$$

b) $f \in \mathscr{H}_c(H) \Leftrightarrow$ for each $R > 0$:

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T dt \int_{|x| \leqslant R} d^N x |(e^{-iHt}f)(x)|^2 = 0. \tag{R2}$$

Ruelle's proof is based on a characterization of the subspaces $\mathscr{H}_p$ and $\mathscr{H}_c$ obtained in ergodic theory. This characterization is shown to be applicable under the hypothesis of the theorem by means of estimates which may be deduced from the particular form of H_0 and from the assumptions on V. A more detailed analysis of these estimates shows that the same method could be applied for proving (R1) and (R2) under the following hypotheses:

i) $F_R(H_0 + i)^{-1}$ is a compact operator. (F_R denotes the projection operator onto the subspace of states localized in the sphere $|x| \leqslant R$.)
ii) H_0 is bounded below: $H_0 \geqslant b$ with $|b| < \infty$.
iii) $H_0 + V$ defines in a natural way (operator sum, Friedrichs extension) a self-adjoint operator H.
iv) For every finite λ, the operator $(H_0 - b)^{1/2} E(\lambda)$ is bounded and defined everywhere. ($\{E(\lambda)\}$ denotes the spectral family of H.)

Condition i) is not very restrictive. In fact, for free Hamiltonians that are functions of the momenta, i.e. if $H_0 = \phi(P)$, condition i) essentially means that $|\phi(p)| \to \infty$ whenever $|p| \to \infty$ (see Appendix I for details). Condition ii) excludes free Hamiltonians that are not semi-bounded, for instance the free Hamiltonian of the Dirac equation. Condition iv) roughly says that states of finite total energy also have finite kinetic energy. It excludes interactions whose negative part is large.

Since (R1) and (R2) involve only the total Hamiltonian but not H_0, it does not really matter that H was obtained by perturbing a particular free Hamiltonian. Indeed this is not needed and it is possible to prove (R1) and (R2) if in hypothesis i), ii) and iv) one replaces H_0 by an arbitrary self-adjoint operator A. This eliminates in particular the condition that H_0 be semi-bounded. We state this result here in the form of a proposition. In fact, our result is even more general since the operator A which replaces H_0 is not required to satisfy hypothesis ii) and need not be self-adjoint. Moreover A may be a function of the energy λ which appears in iv).

Proposition 1:

Let $\{E(\lambda)\}$ be the spectral family[2] of the self-adjoint operator H in $\mathscr{H} = L^2(\mathbb{R}^N)$. For $K > 0$, denote by $E_K \equiv E(K) - E(-K)$ the spectral projection corresponding to the interval $(-K, K]$, and let E_c be the projection operator onto $\mathscr{H}_c$. Suppose that for each $K < \infty$ there exists an invertible linear operator A_K in $\mathscr{H}$ such that

i) $A_K E_K E_c$ is bounded and defined everywhere.
ii) The closure of $F_R A_K^{-1}$ is compact for every $R < \infty$.

Then (R1) and (R2) hold.

In order to see that this is a generalization of conditions iv) and i) stated before the proposition, it suffices to choose $A_K = (H_0 - b)^{1/2} + i$ and to remark that compactness of $F_R(H_0 + i)^{-1}$ implies compactness of $F_R[(H_0 - b)^{1/2} + i]^{-1}$ (see Appendix I for proof).

Since $(H - z)^M E_K$ is bounded and defined everywhere if $K < \infty$ and $M > 0$, we have the following:

Corollary:

Suppose that there is a number $M > 0$ and a $z \in \rho(H)$ (the resolvent set of H) such that the operator $F_R(H - z)^{-M}$ is compact for every $R < \infty$. Then (R1) and (R2) hold.

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[2]) We refer to the book by Kato [2] for definitions and results from spectral theory.

Our method of proof is different from that used by Ruelle. We first investigate the properties of certain subsets of an abstract Hilbert space which are constructed from a self-adjoint operator H and a family of projection operators in analogy with the right-hand sides of (R1) and (R2). This will allow us to prove a theorem which asserts the validity of relations like (R1) and (R2) under rather general conditions. The proofs are relatively elementary. This is the content of Section II which will be concluded by deducing Proposition 1 from the main theorem.

In Section III we apply the main theorem to establish (R1) and (R2) for a large class of Hamiltonians. The idea is to first prove (R1) and (R2) for functions of the momentum operators (cf. Proposition 2) and then to use perturbation arguments to obtain their validity for other Hamiltonians. The essential point in most of these perturbation arguments is to find an estimate on the domain $D(H)$ of the Hamiltonian under consideration which allows one to compare $D(H)$ with the domain of a suitable function of the momentum operators. The most general result of this type is Proposition 5 which can in particular be used to verify (R1) and (R2) for Schrödinger and Dirac Hamiltonians. For Schrödinger Hamiltonians with two-body interactions V_{ij}, (R1) and (R2) are shown to be true if all V_{ij} belong to $L^2_{loc}(\mathbb{R}^3)$ or to the Rollnik class. Electric and magnetic fields and interactions containing hard cores or highly singular attractive parts will also be treated.

II. The Main Theorem

In this part we give rather general sufficient conditions for the equivalence of the two ways of looking at bound states and scattering states.

Throughout this section we consider a self-adjoint operator H and a family $\{F_r\}$, $r = 1, 2, \ldots$, of orthogonal projections (i.e. $F_r^* = F_r = F_r^2$) acting in a separable Hilbert space $\mathscr{H}$. Let $\mathscr{H} = \mathscr{H}_p \oplus \mathscr{H}_c$ be the decomposition of $\mathscr{H}$ into the subspaces corresponding to the point spectrum and the continuous spectrum of H, and let $V_t = \exp(-iHt)$ be the strongly continuous unitary one-parameter group determined by H. We also assume that

$$s - \lim_{r\to\infty} F_r = I \tag{2}$$

and we shall use the following notation: $F_r' \equiv I - F_r$. (In later applications, H will be the Hamiltonian and F_r the projection operator onto the subspace of states localized in the sphere $|x| < r$. The discreteness of the values of r is assumed only for the sake of convenience of notation.)

In analogy with the right-hand members of (R1) and (R2), we define the following two subsets of $\mathscr{H}$:

$$\mathscr{M}_0 = \{f \in \mathscr{H} \mid \lim_{r\to\infty} \sup_{t\in\mathbb{R}} \|(I - F_r)\, V_t f\|^2 = 0\}$$

$$\mathscr{M}_\infty = \left\{ f \in \mathscr{H} \mid \lim_{T\to\infty} \frac{1}{T} \int_0^T dt \|F_r V_t f\|^2 = 0 \quad \text{for all } r = 1, 2, \ldots \right\}.$$

We first establish some properties of these two subsets:

Lemma 1:

a) $\mathcal{M}_0$ and $\mathcal{M}_\infty$ are closed linear subspaces of $\mathcal{H}$.
b) $\mathcal{M}_0$ is orthogonal to $\mathcal{M}_\infty$.
c) $\mathcal{H}_p \subset \mathcal{M}_0$.
d) $\mathcal{M}_\infty \subset \mathcal{H}_c$.

Before giving the proof, we state the basic inequality which will frequently be used in the sequel: For $f, g \in \mathcal{H}$ one has

$$\|f+g\|^2 \leqslant \|f+g\|^2 + \|f-g\|^2 = 2\|f\|^2 + 2\|g\|^2. \tag{3}$$

Proof:

a) i) Assume $f_1, f_2 \in \mathcal{M}_\infty$ and $\alpha_1, \alpha_2 \in \mathbb{C}$. Using (3) we deduce for fixed but arbitrary r:

$$\frac{1}{T}\int_0^T dt\|F_r V_t(\alpha_1 f_1 + \alpha_2 f_2)\|^2$$

$$\leqslant \frac{2|\alpha_1|^2}{T}\int_0^T dt\|F_r V_t f_1\|^2 + \frac{2|\alpha_2|^2}{T}\int_0^T dt\|F_r V_t f_2\|^2.$$

Each term on the right-hand side converges to zero as $T \to \infty$, which implies that $\alpha_1 f_1 + \alpha_2 f_2 \in \mathcal{M}_\infty$, i.e. $\mathcal{M}_\infty$ is a linear manifold in $\mathcal{H}$.

ii) Assume $f_n \in \mathcal{M}_\infty$ $(n = 1, 2, \ldots)$ and $f = s - \lim\limits_{n\to\infty} f_n$. We use again (3) to deduce that

$$\frac{1}{T}\int_0^T dt\|F_r V_t f\|^2 \leqslant \frac{2}{T}\int_0^T dt\|F_r V_t(f-f_n)\|^2 + \frac{2}{T}\int_0^T dt\|F_r V_t f_n\|^2$$

$$\leqslant \frac{2}{T}\int_0^T dt\|f - f_n\|^2 + \frac{2}{T}\int_0^T dt\|F_r V_t f_n\|^2. \tag{4}$$

Given $\epsilon > 0$, we first choose n such that $\|f - f_n\|^2 < \epsilon/4$. Since $f_n \in \mathcal{M}_\infty$, there exists T_0 such that for $T > T_0$

$$\frac{2}{T}\int_0^T dt\|F_r V_t f_n\|^2 < \epsilon/2.$$

Upon inserting these inequalities into (4), we find

$$\frac{1}{T}\int_0^T dt\|F_r V_t f\|^2 < \epsilon \quad \text{for all } T > T_0.$$

This implies that $f \in \mathcal{M}_\infty$. Hence $\mathcal{M}_\infty$ is closed.

iii) The proof that $\mathcal{M}_0$ is a closed linear subspace is similar and will be omitted.

b) Assume $f \in \mathcal{M}_0$, $g \in \mathcal{M}_\infty$. By using the unitarity of V_t and $F_r^* = F_r$ we deduce

$$|(f,g)|^2 = \frac{1}{T}\int_0^T dt |(f,g)|^2 = \frac{1}{T}\int_0^T dt |(V_t f, V_t g)|^2$$

$$= \frac{1}{T}\int_0^T dt |(F_r' V_t f, V_t g) + (V_t f, F_r V_t, g)|^2$$

We now apply (3) (with $\mathcal{H} = \mathbb{C}$) and then Schwarz's inequality:

$$|(f,g)|^2 \leqslant \frac{2}{T}\int_0^T dt |(F_r' V_t f, V_t g)|^2 + \frac{2}{T}\int_0^T dt |(V_t f, F_r V_t g)|^2$$

$$\leqslant \frac{2}{T}\|g\|^2 \int_0^T dt \|F_r' V_t f\|^2 + \frac{2}{T}\|f\|^2 \int_0^T dt \|F_r V_t g\|^2 \tag{5}$$

Let $\epsilon > 0$ be given. Since $f \in \mathcal{M}_0$, we may choose r such that

$$\|F_r' V_t f\|^2 < \frac{\epsilon}{4\|g\|^2} \quad \text{for } all\ t.$$

Since $g \in \mathcal{M}_\infty$, there exists T such that

$$\frac{1}{T}\int_0^T dt \|F_r V_t g\|^2 < \frac{\epsilon}{4\|f\|^2}.$$

From (5) we can deduce that $|(f,g)|^2 < \epsilon$. Since ϵ was arbitrary, this implies that $f \perp g$ and hence $\mathcal{M}_0 \perp \mathcal{M}_\infty$.

c) Let f be an eigenvector of H: $Hf = Ef$. Then

$$\|F_r' V_t f\|^2 = \|F_r' e^{-iEt} f\|^2 = \|(I - F_r) f\|^2.$$

For $r \to \infty$ this converges to zero as a consequence of the assumption (2). Hence $f \in \mathcal{M}_0$.

By definition, $\mathcal{H}_p$ is the closed subspace spanned by the set of all eigenvectors of H. Since $\mathcal{M}_0$ is a closed linear subspace according to part a), the above argument implies that $\mathcal{H}_p \subset \mathcal{M}_0$.

d) By using first part b) and then part c) of the Lemma, one gets

$$\mathcal{M}_\infty \subset \mathcal{M}_0^\perp \subset \mathcal{H}_p^\perp = \mathcal{H}_c. \qquad \blacksquare$$

Remark:

It is not true in general that $\mathcal{M}_0$ and $\mathcal{M}_\infty$ are orthogonal complements of each other. However this will be true in the cases which interest us here. Indeed it is our purpose to show that $\mathcal{M}_0 = \mathcal{H}_p$ and $\mathcal{M}_\infty = \mathcal{H}_c$ under suitable conditions on H. We remark here that these two identities will be verified as soon as we have shown that $\mathscr{H}_c \subset \mathscr{M}_\infty$. In fact Lemma 1d then implies $\mathscr{H}_c = \mathscr{M}_\infty$, and by combining this with Lemma 1b one deduces

$$\mathscr{M}_0 \subset \mathscr{M}_\infty^\perp = \mathscr{H}_c^\perp = \mathscr{H}_p.$$

This in turn implies, together with Lemma 1c, that $\mathscr{M}_0 = \mathscr{H}_p$.

For the proof of the inclusion $\mathscr{H}_c \subset \mathscr{M}_\infty$ under certain conditions one has to know a suitable characterization of the subspace of continuity $\mathscr{H}_c$. We shall use the following result:

Lemma 2:

If $f \in \mathscr{H}_c$, one has for every $e \in \mathscr{H}$

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T dt |(e, V_t f)|^2 = 0. \tag{6}$$

In fact the implication given in the Lemma also has a converse:

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T dt |(f, V_t f)|^2 = 0 \Rightarrow f \in \mathscr{H}_c.$$

(Cf. [3], Section 5.) However we shall not need this in our later proofs.

Proof:

i) Let $\{E(\lambda)\}$ be the spectral family of H. For $g \in \mathscr{H}$ and $h \in \mathscr{H}_c$, consider the integral

$$J(T) \equiv \frac{1}{T} \int_0^T dt \int_{\mathbb{R}} e^{i\lambda t} d(g, E(\lambda) g) \int_{\mathbb{R}} e^{-i\mu t} d(h, E(\mu) h). \tag{7}$$

This multiple integral is absolutely convergent. In fact

$$|J(T)| \leqslant \int_{\mathbb{R}} d(g, E(\lambda) g) \int_{\mathbb{R}} d(h, E(\mu) h) = \|g\|^2 \|h\|^2.$$

By Fubini's Theorem ([4], p. 25), one may interchange the order of integration:

$$|J(T)| = \left| \int_{\mathbb{R}} d(g, E(\lambda) g) \int_{\mathbb{R}} d(h, E(\mu) h) \frac{e^{i(\lambda-\mu)T} - 1}{i(\lambda-\mu) T} \right|$$

$$\leqslant \int_{\mathbb{R}} d(g, E(\lambda) g) \int_{\mathbb{R}} d(h, E(\mu) h) \left| \frac{2 \sin \frac{(\lambda-\mu) T}{2}}{(\lambda-\mu) T} \right|. \tag{8}$$

We wish to show that

$$\lim_{T\to\infty} |J(T)| = 0 \tag{9}$$

by applying the dominated convergence theorem ([4], p. 24). We first remark that the integrand in the last member of (8) is bounded by 1 for all T and that it converges to zero as $T \to \infty$ at all points $(\lambda, \mu) \in \mathbb{R}^2$ with $\lambda \neq \mu$. Thus it suffices to show that the measure of the line $\lambda = \mu$ is zero.

For this, we use the hypothesis that $h \in \mathscr{H}_c$. This means that the function $\mu \mapsto (h, E(\mu)h)$ is continuous ([2], p. 515). It is even uniformly continuous: given $\epsilon > 0$, choose a so large that $(h, E(-a)h) < \epsilon/2$ and $\|h\|^2 - (h, E(a)h) < \epsilon/2$. $(h, E(\mu)h)$ is uniformly continuous on $[-a, a]$, and since it is also monotone increasing and bounded, it cannot vary by more than $\epsilon/2$ on $(-\infty, -a)$ and on $[a, \infty)$, which implies uniform continuity on $\mathbb{R}$.

It follows that, given any $\epsilon > 0$, we may find $\delta > 0$ such that

$$(h, E(\mu + \delta)h) - (h, E(\mu - \delta)h) < \epsilon/\|g\|^2 \quad \text{for } all \ \mu \in \mathbb{R}.$$

Therefore

$$\int_{\mathbb{R}} d(g, E(\lambda)g) \int_{\lambda-\delta}^{\lambda+\delta} d(h, E(\mu)h) < \epsilon.$$

Thus, given any $\epsilon > 0$, there is a set $D_\delta \equiv \{(\lambda, \mu) \in \mathbb{R} \mid |\lambda - \mu| < \delta\}$ containing the line $\lambda = \mu$ and having measure less than ϵ. This shows that the line $\lambda = \mu$ has measure zero.

ii) Let $f \in \mathscr{H}_c$. If $e \perp \mathscr{H}_c$, one has $(e, V_t f) = 0$ for all t. Hence the Lemma will be proved once we have established (6) for $e \in \mathscr{H}_c$. For this we write

$$\frac{1}{T}\int_0^T dt |(e, V_t f)|^2$$
$$= \frac{1}{T}\int_0^T dt \int_{\mathbb{R}} e^{i\lambda t} d(f, E(\lambda)e) \int_{\mathbb{R}} e^{-i\mu t} d(e, E(\mu)f). \tag{10}$$

In the last integral we replace $(e, E(\mu)f)$ by

$$(e, E(\mu)f) = \tfrac{1}{4}[\|E(\mu)(e+f)\|^2 - \|E(\mu)(e-f)\|^2 - i\|E(\mu)(e+if)\|^2 + i\|E(\mu)(e-if)\|^2$$

and similarly for $(f, E(\lambda)e)$. With these substitutions the right-hand side of (10) is reduced to a sum of integrals of the type (7), and since $\alpha e + \beta f \in \mathscr{H}_c$ for any $\alpha, \beta \in \mathbb{C}$, each of these integrals converges to zero according to (9). ∎

We now state and prove our main theorem:

Theorem:

Let H be a self-adjoint operator and $\{F_r\}$, $r = 1, 2, \ldots$, a family of orthogonal projections such that $s - \lim_{r\to\infty} F_r = I$. Suppose there exists a family $\{S_n\}$, $n = 1, 2, \ldots$, of linear operators acting in $\mathscr{H}$ such that

i) $S_n \in \{H\}'$ [3]) for all n.

[3]) $\{H\}'$ denotes the commutant of H. Thus i) means that each S_n commutes with H and belongs to $\mathscr{B}(\mathscr{H})$, the set of all linear operators on $\mathscr{H}$ that are bounded and defined everywhere.

ii) The sequence $\{S_n\}$ converges strongly to an operator S:

$$s-\lim_{n\to\infty} S_n = S.$$

iii) The range of S is dense in $\mathscr{H}$.

iv) $F_r S_n E_c$ is compact for all $r, n < \infty$.

Then $\mathscr{H}_p = \mathscr{M}_0$ and $\mathscr{H}_c = \mathscr{M}_\infty$.

In the proof we shall use the following characterization of compact operators ([4], p. 200): Every compact operator C is the limit in operator norm of a sequence of operators of finite rank, i.e. given $\epsilon > 0$, there exists an operator T_N of the form

$$T_N f = \sum_{i=1}^{N} (h_i, f)\, g_i \quad \text{with } g_i, h_i \in \mathscr{H} \text{ and } N < \infty \tag{11}$$

such that

$$\|C - T_N\| < \epsilon.$$

Proof:

According to the remark following the proof of Lemma 1, it suffices to show that $\mathscr{H}_c \subset \mathscr{M}_\infty$. Since $\mathscr{M}_\infty$ is closed (Lemma 1a), it is sufficient to verify the inclusion $\mathscr{D} \subset \mathscr{M}_\infty$ for some set $\mathscr{D}$ which is dense in $\mathscr{H}_c$.

Conditions i) and ii) imply that S leaves $\mathscr{H}_p$ and $\mathscr{M}_c$ invariant. Combining this with hypothesis iii), one deduces that $S\mathscr{H}_c$ is dense in $\mathscr{H}_c$. We may therefore choose $\mathscr{D} = S\mathscr{H}_c$.

Let $g \in \mathscr{D}$. Given $r < \infty$, we have to show that

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T dt \|F_r V_t g\|^2 = 0. \tag{12}$$

For this, let $\epsilon > 0$ be given. Choose $f \in \mathscr{H}_c$ such that $g = Sf$ and then n so large that

$$\|(S - S_n) f\|^2 < \epsilon/6. \tag{13}$$

Next, in view of hypothesis iv), we may choose an operator T_N of the form (11) such that

$$\|F_r S_n E_c - T_N\|^2 < \frac{\epsilon}{12\|f\|^2} \tag{14}$$

By writing $g = (S - S_n) f + S_n f$ and using (3), we deduce

$$\frac{1}{T} \int_0^T dt \|F_r V_t g\|^2$$

$$\leqslant \frac{2}{T} \int_0^T dt \|F_r V_t (S - S_n) f\|^2 + \frac{2}{T} \int_0^T dt \|F_r V_t S_n f\|^2. \tag{15}$$

The first term on the right-hand side is less than $\epsilon/3$ as a consequence of (13). Since $f \in \mathscr{H}_c$ and in view of condition i), we have

$$F_r V_t S_n f = F_r S_n E_c V_t f = (F_r S_n E_c - T_N) V_t f + T_N V_t f.$$

We insert this into (15) and apply again (3) and then (14):

$$\frac{1}{T}\int_0^T dt \|F_r V_t g\|^2$$

$$\leqslant (\epsilon/3) + \frac{4}{T}\int_0^T dt \|F_r S_n E_c - T_N\|^2 \, \|V_t f\|^2 + \frac{4}{T}\int_0^T dt \|T_N V_t f\|^2$$

$$\leqslant \tfrac{2}{3}\epsilon + \frac{4}{T}\int_0^T dt \|T_N V_t f\|^2. \tag{16}$$

In order to estimate the remaining integral in (16), we substitute T_N from (11) and then repeatedly apply (3) to the sum over i:

$$\frac{4}{T}\int_0^T dt \|T_N V_t f\|^2 = \frac{4}{T}\int_0^T dt \left\| \sum_{i=1}^{N} (h_i, V_t f)\, g_i \right\|^2$$

$$\leqslant 2^{N-1} \frac{4}{T} \sum_{i=1}^{N} \int_0^T dt |(h_i, V_t f)|^2 \|g_i\|^2. \tag{17}$$

Let $K = \max_{i=1,\dots,N} \|g_i\|^2$. According to Lemma 2, we may choose T_0 such that for $T > T_0$

$$\frac{1}{T}\int_0^T dt |(h_i, V_t f)|^2 < \frac{\epsilon}{3 \cdot 2^{N+1} K N} \quad \text{for all } i = 1, \dots, N.$$

This implies together with (16) and (17) that

$$\frac{1}{T}\int_0^T dt \|F_r V_t g\|^2 < \epsilon \quad \text{for all } T > T_0.$$

Thus we have established (12), which completes the proof. ■

Remark:

Under the hypotheses of the Theorem the time average in (R2) may be omitted if the operator H is known to have no singularly continuous spectrum. More precisely, let $\mathscr{H}_c(H) = \mathscr{H}_{ac} \oplus \mathscr{H}_{sc}$ be the decomposition of $\mathscr{H}_c(H)$ into the subspaces correspon- ding to the absolutely continuous and the singularly continuous spectrum of H. If the hypotheses of the Theorem are verified and $\mathscr{H}_{sc}(H) = \phi$, then $\mathscr{H}_p(H) = \mathscr{M}_0$ and $\mathscr{H}_c(H) = \mathscr{H}_{ac}(H) = \mathscr{M}_\infty$ where $\mathscr{M}_\infty$ is now defined as

$$\mathscr{M}_\infty = \left\{ f \in \mathscr{H} \mid \lim_{t\to\infty} \|F_r V_t f\|^2 = 0 \quad \text{for all } r = 1, 2, \ldots \right\}$$

For the proof one notices that Lemma 1 remains true with the above definition of $\mathscr{M}_\infty$, i.e. in particular $\mathscr{M}_\infty \subset \mathscr{H}_c = \mathscr{H}_{ac}$. For the converse inclusion, let $g = Sf \in \mathscr{D} \subset \mathscr{H}_{ac}$. Then it follows as in (15) that

$$\|F_r V_t g\|^2 \leqslant 2\|F_r V_t (S - S_n) f\|^2 + 2\|F_r V_t S_n f\|^2 \leqslant 2\|(S - S_n) f\|^2 + 2\|F_r S_n E_c V_t f\|^2.$$

The first term on the right-hand side can be made arbitrarily small by choosing n sufficiently large. For the second term one remarks that $f \in \mathscr{H}_{ac}(H)$ implies that $\{V_t f\}$ converges weakly to zero as $t \to \infty$. Since a compact operator maps weakly convergent sequences into strongly convergent ones ([4], Thm. VI. 11), hypothesis iv) of the Theorem implies that $\|F_r S_n E_c V_t f\|^2$ also converges to zero for $t \to \infty$.

Corollary:

Let $E_K \equiv E(K) - E(-K)$ be the spectral projection of H corresponding to the interval $(-K, K]$, and suppose that $F_r E_K E_c$ is compact for all $K < \infty$ and all $r = 1, 2, \ldots$. Then $\mathscr{H}_p = \mathscr{M}_0$ and $\mathscr{H}_c = \mathscr{M}_\infty$.

Proof:

The theorem can be applied with $S_n = E_n$, since $s - \lim_{n\to\infty} E_n = I$. ■

As a typical application of the theorem, we shall now indicate the proof of Proposition *1*:

Proof of Proposition 1:

Let F_r be the projection operator in $L^2(\mathbb{R}^N)$ onto the subspace of functions having support in the sphere $|x| \leqslant r$. We take $S_n = E_n \equiv E(n) - E(-n)$. Then

$$F_r S_n E_c = F_r A_n^{-1} A_n E_n E_c = (F_r A_n^{-1})^{\sim} A_n E_n E_c$$

where $B^{\sim}$ denotes the closure of B. Since $(F_r A_n^{-1})^{\sim}$ was assumed to be compact and $A_n E_n E_c$ bounded and defined everywhere, we have decomposed $F_r S_n E_c$ into a product of a compact operator and an operator belonging to $\mathscr{B}(\mathscr{H})$. This implies that $F_r E_n E_c$ is compact ([2], p. 158). With this, Proposition 1 follows from the above Corollary. ■

III. Applications

In this section we shall consider various classes of n-body Hamiltonians for which the relations (R1) and (R2) can be proved. For the sake of simplicity we shall usually consider only spinless[4]) and non-identical particles.

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[4]) One can easily adapt our propositions to the case where $\mathscr{H} = L^2(\mathbb{R}^N) \otimes \mathbb{C}^s$.

We start with two general remarks about the interpretation of (R1) and (R2) in scattering theory:

i) If we consider the case where $\mathscr{H} = L^2(\mathbb{R}^N)$ and interpret H as the Hamiltonian of an n-body system in the centre-of-mass frame ($N = 3(n-1)$), the vectors $x \in \mathbb{R}^N$ correspond to linearly independent relative positions between the particles. If the particles form an n-body bound state (i.e. if they are *all* bound together), all these relative positions will remain small in the course of time, i.e. the corresponding state will be essentially localized in a bounded volume of $\mathbb{R}^N$. On the other hand, if the n particles do not form an n-body bound state, one expects them to split up into at least two independent fragments which will move apart from each other. Thus *at least one* relative coordinate will become large in the course of time, i.e. the corresponding state is expected to disappear from any bounded region of $\mathbb{R}^N$ as $t \to +\infty$.

ii) $\mathscr{M}_\infty$ was defined by means of an integral over time from $t = 0$ to $t = T$. One could also introduce a similar subspace $\mathscr{M}_\infty^-$ by integrating from $t = -T$ to $t = 0$. It is clear that the hypotheses of the Theorem also imply that $\mathscr{H}_c = \mathscr{M}_\infty^-$, since the replacement of $\mathscr{M}_\infty$ by $\mathscr{M}_\infty^-$ is equivalent to a replacement of H by $-H$, and the conditions i)–iv) of the Theorem as well as the subspaces $\mathscr{H}_p$ and $\mathscr{H}_c$ are invariant under the latter substitution. Hence, under the hypotheses of the Theorem, the scattering states at negative times are the same as those at positive times.

We now look at the case $\mathscr{H} = L^2(\mathbb{R}^N)$. Throughout this section, Q_j ($j = 1, \ldots, N$) will be the self-adjoint multiplication operator by x_j in $L^2(\mathbb{R}^N)$, and P_j the corresponding momentum operator, i.e.

$$[P_j, Q_k] = -i\delta_{jk}, \quad [P_j, P_k] = [Q_j, Q_k] = 0. \tag{18}$$

If ϕ is a real or complex valued function defined on $\mathbb{R}^N$, we shall denote by $\phi(p)$ the value of ϕ at the point $p \in \mathbb{R}^N$ and by $\phi(P)$ the linear operator in $\mathscr{H} = L^2(\mathbb{R}^N)$ defined as multiplication by the function $\phi(p)$ on the Fourier transforms $\tilde{f}$ of the vectors $f \in L^2(\mathbb{R}^N)$. Here

$$\tilde{f}(p) = (2\pi)^{-N/2} \operatorname*{l.i.m.}_{M \to \infty} \int_{|x| \leq M} d^N x \, e^{-ip \cdot x} f(x) \quad (\hbar = 1).$$

Kinematics

As a first application we now show that (R1) and (R2) are verified for *arbitrary kinematics*.

Proposition 2:

Suppose H is a self-adjoint function of the momentum operators $P_1, \ldots, P_N$. Then (R1) and (R2) hold.

Proof:

We verify the hypotheses of the Theorem with $S_n = S = (|P|^N + 1)^{-1}$ where $|P|^2 = \sum_{j=1}^N P_j^2$.

S is the resolvent of the self-adjoint operator $|P|^N$, hence it has dense range. This verifies condition iii). i) and ii) are trivially true.

Let F_r be the projection operator onto the states localized in the sphere $|x| \leqslant r$. $F_r S$ has finite Hilbert–Schmidt norm:

$$\|F_r S\|_{\mathrm{HS}}^2 = \int d^N p \int d^N p' |\tilde{\chi}_r(p - p')|^2 \frac{1}{(|p'|^N + 1)^2} \leqslant V_r \int d^N p' \frac{1}{(|p'|^N + 1)^2} < \infty$$

(see Appendix I for notations and more details). Hence $F_r S$ is compact, which verifies condition iv) of the Theorem. ∎

Hamiltonians satisfying the Asymptotic Condition

The next proposition applies particularly to two-body Hamiltonians for which existence and completeness of wave operators is known. The argument could be generalized to n-body systems, but this is of little interest since our subsequent results are of a much more general nature.

Proposition 3:

Let H_1 and H_2 be self-adjoint on $L^2(\mathbb{R}^N)$ and denote by $E_c^{(i)}$ $(i = 1, 2)$ the projection operator onto the corresponding subspace of continuity. Suppose that H_1 verifies (R1) and (R2), that the wave operator

$$\Omega(H_2, H_1) \equiv \Omega = s - \lim_{t \to +\infty} e^{iH_2 t} e^{-iH_1 t} E_c^{(1)} \tag{19}$$

exists and is complete (i.e. $\Omega\Omega^* = E_c^{(2)}$). Then H_2 also satisfies (R1) and (R2).

Proof:

It suffices to show that $\mathscr{H}_c(H_2) \subset \mathscr{M}_\infty^{(2)}$ (cf. the remark after the proof of Lemma 1). Let $g \in \mathscr{H}_c(H_2)$. $\Omega\Omega^* = E_c^{(2)}$ means that the range of Ω is $\mathscr{H}_c(H_2)$. Hence there exists $f \in \mathscr{H}_c(H_1)$ such that $g = \Omega f$ (in fact $f = \Omega^* g$). Using (3) we find

$$\frac{1}{T}\int_0^T dt \|F_r e^{-iH_2 t} g\|^2 \leqslant \frac{2}{T}\int_0^T dt \|F_r(e^{-iH_2 t}\Omega - e^{-iH_1 t}) f\|^2 + \frac{2}{T}\int_0^T dt \|F_r e^{-iH_1 t} f\|^2$$

$$\leqslant \frac{2}{T}\int_0^T dt \|(\Omega - e^{iH_2 t} e^{-iH_1 t}) f\|^2 + \frac{2}{T}\int_0^T dt \|F_r e^{-iH_1 t} f\|^2.$$

It suffices to show that both of these integrals converge to zero as $T \to \infty$. For the first one, this follows from the hypothesis (19) which states that the integrand and *a fortiori* its time average converge to zero. The second integral converges to zero because $f \in \mathscr{H}_c(H_1)$ and we assumed $\mathscr{H}_c(H_1) = \mathscr{M}_\infty^{(1)}$. ∎

Remark:

It follows that for the case of a simple scattering system ($N = 3$) and H_1 a function of the momentum operators, (R1) and (R2) for H_2 are *necessary* for the wave operator to be complete. Note also that the definition of Ω used above differs from the usual one in which convergence of $\exp(iH_2 t)\exp(-iH_1 t)$ is required only on $E_{ac}^{(1)}\mathscr{H}$ (the subspace of *absolute* continuity of H_1).

Relatively Small Perturbations. Singular Potentials

Proposition 4:

Let $\phi(P)$ be a self-adjoint function of the momentum operators in $L^2(\mathbb{R}^N)$ and suppose that the function ϕ satisfies $\lim_{|p|\to\infty} |\phi(p)| = \infty$. Let V be such that one of the following conditions is verified:

α) $H \equiv \phi(P) + V$ is self-adjoint with domain $D(H) = D(\phi(P)) \cap D(V)$.
β) The sum of the quadratic forms of $\phi(P)$ and V is the quadratic form of a self-adjoint operator H.
γ) $\phi(P) + V$ has a self-adjoint pseudo-Friedrichs extension H.

Then the Hamiltonian H defined by α), β) or γ) satisfies (R1) and (R2).

Proof:

Let $S_n = S = (H + i)^{-1}$. Conditions i), ii) and iii) of the Theorem are verified. The validity of iv) will be established for each of the three cases separately.

α) Since $D(\phi(P)) \supset D(H) =$ range of S, the operator $(\phi(P) + i)S$ is defined on every vector of $\mathscr{H}$. Since $\phi(P)$ and S are closed and $(\phi(P) + i)^{-1}$ is bounded, $(\phi(P) + i)S$ is also closed ([2], page **164**) and hence bounded ([2], page **166**). Therefore $(\phi(P) + i)S \in \mathscr{B}(\mathscr{H})$.

Using the fact that $F_r(\phi(P) + i)^{-1}$ is compact (cf. Appendix I), we may factorize F_rS into a product of a compact operator and an operator belonging to $\mathscr{B}(\mathscr{H})$ by means of the identity

$$F_rS = F_r(\phi(P) + i)^{-1}(\phi(P) + i)S.$$

This shows that F_rS and hence F_rSE_c is compact and verifies iv).

β) The quadratic form of a self-adjoint operator A with spectral family $\{E(\lambda)\}$ is the form $f \mapsto \int \lambda d(f, E(\lambda)f)$ defined for all $f \in Q(A) \equiv D(|A|^{1/2})$ (the form domain of A). Under the hypothesis β), we have $Q(H) \subset Q(\phi(P))$. Since $D(H) \subset D(|H|^{1/2})$, this implies that $D(H) \subset Q(\phi(P)) = D(|\phi(P)|^{1/2})$. Therefore $(|\phi(P)|^{1/2} + i)(H + i)^{-1}$ is defined on every vector of $\mathscr{H}$, and one concludes in the same way as above that

$$(|\phi(P)|^{1/2} + i)(H + i)^{-1} \in \mathscr{B}(\mathscr{H}).$$

We may now write

$$F_rS = F_r(|\phi(P)|^{1/2} + i)^{-1}(|\phi(P)|^{1/2} + i)S.$$

Since $F_r(|\phi(P)|^{1/2} + i)^{-1}$ is also compact (cf. Appendix I), it follows again that F_rS and hence F_rSE_c is compact.

γ) The pseudo-Friedrichs extension H of $\phi(P) + V$ is defined in [2], pp. **341–2**. Its essential property is that $D(H) \subset D(|\phi(P)|^{1/2})$. This permits us to deduce the compactness of F_rSE_c by the same argument as in case β). ■

The essential property of the Hamiltonians treated in the preceding proposition is that their domain $D(H)$ is contained in that of a suitable (unbounded!) function of the momentum operators. In many instances one has such information only about a dense subset $\mathscr{D}$ of $D(H)$. If this subset $\mathscr{D}$ includes all functions of compact support in the spectral representation of H, one can apply Proposition 1 and still conclude that (R1) and (R2) hold. A different situation which one often encounters is that where $\mathscr{D}$ is a domain of essential self-adjointness of H (this occurs whenever the sum of $H_0 \equiv \phi(P)$ and V is only essentially self-adjoint on $D(H_0) \cap D(V)$). In such cases one cannot apply the method of proof of Proposition 4, and in fact it is not difficult to find examples where $\phi(P) + V$ is essentially self-adjoint but the conclusion of Proposition 4 does not hold (e.g. $V = -\phi(P) + W(Q)$ such that the operator W has continuous spectrum). Nevertheless (R1) and (R2) are expected to hold also in such cases if V is 'reasonable'. This question will be handled in Proposition 5 where we shall also treat cases where $H_0 + V$ is only symmetric. It will be seen there that (R1) and (R2) are in fact true for *every* self-adjoint extension H of $H_0 + V$ under suitable conditions on H_0 and V. Before doing this, we indicate some situations where the hypotheses of Proposition 4 are verified.

Condition α) holds for the Hamiltonian describing the relative movement of an n-body system with $H_0 = \sum_{i,j=1}^{n-1} a_{ij} \vec{P}_i \vec{P}_j$ and V a sum of k-body potentials ($k = 2, 3, \ldots, n$) of the form given in Appendix II if the following conditions hold:

i) the matrix a_{ij} is real, symmetric and positive definite,
ii) each k-body potential $V_{i_1 \ldots i_k}$ satisfies

$$V_{i_1 \ldots i_k} \in L^p(\mathbb{R}^{3(k-1)}) + L^\infty(\mathbb{R}^{3(k-1)}) \quad \text{with } p \geqslant 2 \text{ and } p > \frac{3(k-1)}{2} \tag{20}$$

(Nelson [5], pp. 342–3; [2], pp. 302–4). Condition (20) admits in particular two-body potentials which are less singular than const $\cdot r^{-3/2}$ at the origin and which are bounded in the region $|x| \geqslant \rho$ for some finite ρ.

Condition β) is more general than α). It allows stronger local singularities and very large positive parts of V. If $H_0 \equiv \phi(P)$ and V are positive and self-adjoint, β) is verified under the only hypothesis that $Q(H_0) \cap Q(V)$ is dense in $\mathscr{H}$ ([2], Chap. VI, Thms. 1.31, 2.1, 2.6 and Cor. 2.2). This includes highly singular repulsive potentials and potentials that are unbounded and positive at $|x| \to \infty$.

If $H_0 = -\Delta$ in $L^2(\mathbb{R}^3)$, (β) is verified for potentials $V \in R + L^\infty(\mathbb{R}^3)$ (R denotes the Rollnik class; cf. Simon [6], p. 3 and Cor. II.8). The Rollnik class includes $L^{3/2}(\mathbb{R}^3)$ ([6], Thm. I.1), in particular potentials whose singularities are of the form $V(r) =$ const $\cdot r^{-\alpha}$ with $\alpha < 2$. Condition β) can also be used to establish (R1) and (R2) for non-relativistic n-body systems with two-body interactions belonging to $R + L^\infty(\mathbb{R}^3)$ ([6], Thm. VII.1).

Condition γ) is verified for a Dirac particle under the influence of the Coulomb field of a nucleus with atomic number less than 87 ([2], pp. 307–8).

Electric and Magnetic Fields. Singular Potentials at Infinity

The statement of our next proposition involves the notion of a Sobolev space. For details about these spaces, the reader is referred to [7], pp. 52–64. For our purposes it is sufficient to know the definition of $H^s_{\text{loc}}(\mathbb{R}^N) \cap L^2(\mathbb{R}^N)$. If G is a complex valued function defined on $\mathbb{R}^N$, we denote by $G(Q)$ the multiplication operator by $G(x)$ in $L^2(\mathbb{R}^N)$. Then a function $f \in L^2(\mathbb{R}^N)$ belongs to $H^s_{\text{loc}}(\mathbb{R}^N)$ iff $G(Q)f \in D((1 + |P|^2)^{s/2})$ for all $G \in C_0^\infty(\mathbb{R}^N)$.

Proposition 5:

Let $\hat{H}$ be a densely defined symmetric operator in $L^2(\mathbb{R}^N)$ such that the domain of its adjoint $\hat{H}^*$ belongs to $H^s_{\text{loc}}(\mathbb{R}^N)$ for some $s > 0$. Then any self-adjoint extension H of $\hat{H}$ satisfies (R1) and (R2).

Proof:

$\hat{H} \subset H = H^*$ and the fact that $\hat{H}$ is densely defined imply that $H \subset \hat{H}^*$. Thus

$$D(H) \subset D(\hat{H}^*) \subset H^s_{\text{loc}}(\mathbb{R}^N). \tag{21}$$

This implies that $(1 + |P|^2)^{s/2} G(Q)(H + i)^{-1}$ is defined everywhere if $G \in C_0^\infty(\mathbb{R}^N)$. From this one deduces in the same way as in the proof of Proposition 4(α) that

$$(1 + |P|^2)^{s/2} G(Q)(H + i)^{-1} \in \mathscr{B}(\mathscr{H}).$$

Given $R < \infty$, we may choose a $C_0^\infty(\mathbb{R}^N)$ function G_R such that $G_R(x) = 1$ for all x with $|x| \leqslant R$. Then

$$\begin{aligned} F_R(H + i)^{-1} &= F_R G_R(Q) (H + i)^{-1} \\ &= F_R(1 + |P|^2)^{-s/2}(1 + |P|^2)^{s/2} G_R(Q)(H + i)^{-1}. \end{aligned}$$

Since $s > 0$, $F_R(1 + |P|^2)^{-s/2}$ is compact (cf. Appendix I). Hence $F_R(H + i)^{-1}$ is compact, and we may use the Corollary of Proposition 1 to deduce the validity of (R1) and (R2). ■

In order to apply Proposition 5 to n-body systems, we use the following result due to Ikebe and Kato [8]:

Let $\hat{H}$ be the differential operator

$$\hat{H} = \sum_{j,k=1}^{N} \left(i \frac{1}{\partial x_j} + b_j(x) \right) a_{jk}(x) \left(i \frac{1}{\partial x_k} + b_k(x) \right) + V(x)$$

with $D(\hat{H}) = C_0^\infty(\mathbb{R}^N)$ and

i) $a_{jk}(x)$, $b_j(x)$ and $V(x)$ real,
ii) $a_{jk} \in C^2(\mathbb{R}^N)$, $b_j \in C^1(\mathbb{R}^N)$,
iii) there exists $\alpha \in (0, 1]$ such that

$$M(x) \equiv \int_{|x-y| \leqslant 1} d^N y |V(y)|^2 |x - y|^{-N+4-\alpha}$$

is locally bounded,
iv) the matrix $a_{jk}(x)$ is symmetric and positive-definite for all $x \in \mathbb{R}^N$.

Then $D(\hat{H}^*) \subset H^2_{\text{loc}}(\mathbb{R}^N)$ ([8], Lemma 3; cf. also Jörgens [9] and Kalf [10]).

By taking $a_{jk}(x) = \delta_{jk}$, the above conditions are seen to include the case of n non-relativistic particles interacting with external magnetic and electric fields of almost arbitrary nature ($N = 3n$).

The results of Ikebe and Kato can also be applied to n-body systems with the centre-of-mass motion removed (we assume here that there are no external fields). Let $b_j = 0$, a_{jk} independent of x, and suppose for the sake of simplicity that V is a sum of translation invariant two-body interactions: $V = \sum_{1 \leqslant i < j \leqslant n} V_{ij}$. Condition iii) is verified for any set of relative coordinates which are linear combinations of the particle positions if all two-body potentials V_{ij} are locally square-integrable (see Appendix II for proof). This establishes (R1) and (R2) for two-body potentials that are very singular at infinity (positive or negative), since only *local* assumptions are needed.

Of course the conditions i)–iv) given above are by no means sufficient to ensure essential self-adjointness of $\hat{H}$. Sufficient conditions can be found in [8] and [9] and in a recent report by Kato [11] who proves in particular that under his assumptions $D(\hat{H}^*) \subset H^1_{\text{loc}}(\mathbb{R}^N)$ ([11], Props. 5 and 7).

Relativistic Hamiltonians

The results of this section can also be applied to relativistic Hamiltonians as long as the projection operators F_R are the spectral projections (corresponding to the sphere of radius R) of a position operator which satisfies the commutation relations (18). For relativistic elementary systems (with $m > 0$) this means that one has to use the position operator of Newton and Wigner [12] (cf. also Wightman [13]).

In investigations of spectral properties and essential self-adjointness of Dirac Hamiltonians (e.g. in Kato [2], pp. 305–8, and Schmincke [14]) one encounters a different position operator, namely the Dirac position operator $\vec{Q}_D$. It also satisfies the commutation relations (18) but does not commute with the projection operator onto the positive energy states (Jordan and Mukunda [15]). One then considers Hamiltonians which are self-adjoint extensions of operators of the form[5]

$$\hat{H} = \vec{\alpha}\cdot\vec{P} + \beta + V(\vec{Q}_D) \quad D(\hat{H}) = (C_0^\infty(\mathbb{R}^3))^4.$$

In [16] Schmincke showed that under his conditions on the interaction ([16], Thm. 2) one has $D(\hat{H}^*) \subset (H^1_{\text{loc}}(\mathbb{R}^3))^4$ ([16], remark following the proof of Thm. 2). It follows from this and an obvious modification of our Proposition 5 that (R1) and (R2) hold (with respect to the position operator $\vec{Q}_D$) for every self-adjoint extension of $\hat{H}$. The conditions of Schmincke include the case of a Dirac particle in the Coulomb field of a nucleus with atomic number Z less than 137.

Hard Cores

In [17] Hunziker developed the time-dependent scattering theory for the Schrödinger equation with singular two-body interactions the singular part of which is bounded below, and he showed in particular how to define the Hamiltonian if these potentials include hard cores (cf. [17], Section 3). We wish to show that (R1) and (R2), suitably modified, are true for the Hamiltonians considered in that paper.

We consider the relative motion of an n-body system under the following assumptions:

i) $H_0 = \phi(P) \geqslant 0$ in $\mathscr{H} = L^2(\mathbb{R}^N)$ $(N = 3(n-1))$ and $\lim_{|p|\to\infty} \phi(p) = \infty$.

ii) There is a Borel set K in $\mathbb{R}^N$ which is forbidden to the variable $x \in \mathbb{R}^N$ (e.g. hard cores for two-body interactions; cf. [17]). We denote by E the complement of K in $\mathbb{R}^N$.

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[5]) We use the notation of Kato ([2], p. 305).

iii) There is a set Δ in $\tilde{\mathscr{H}} = L^2(E)$ such that
 α) Δ is dense in $\tilde{\mathscr{H}}$;
 β) Δ is contained in $D(H_0) \cap D(V)$;
 γ) $H_0 f \in \tilde{\mathscr{H}}$ for all $f \in \Delta$;
 γ) there exist constants $a \in (0,1)$ and c such that for all $f \in \Delta$:

$$0 \leqslant a\|\sqrt{H_0}f\|^2 + (f, Vf) + c(f,f). \tag{22}$$

(Condition γ) may be viewed as a restriction on the admissible class of functions ϕ. It is satisfied for instance if $\Delta = C_0^\infty(E)$ and ϕ is a polynomial in $P_1, \ldots, P_N$. Condition δ) means that the negative part of V is small relative to H_0; cf. [17].)[6]

We may rewrite (22) in the form

$$(1-a)\|\sqrt{H_0}f\|^2 + \|f\|^2 \leqslant (f, (H_0 + V + c + 1)f) \tag{23}$$

(this is the equivalent of equation (7) in [17]).

The Hamiltonian H acting in $\tilde{\mathscr{H}}$ is defined as follows: $H + c + 1$ is the Friedrichs extension of $H_0 + V + c + 1$ on Δ (cf. [2], pp. 325–6).

Let $\tilde{F}$ be the projection operator in $\mathscr{H} = L^2(\mathbb{R}^N)$ onto the subspace $\tilde{\mathscr{H}} = L^2(E)$, F_R the projection operator in $\mathscr{H}$ onto the states localized in the sphere $|x| \leqslant R$, and $\tilde{F}_R = \tilde{F}F_R$.

By reasoning in the same way as in the proof of Lemma 1 in [17], one deduces from (23) that $D(H) \subset D(\sqrt{H_0}) \cap \tilde{\mathscr{H}}$. This implies that $(\sqrt{H_0} + i)(H+i)^{-1}\tilde{F} \in \mathscr{B}(\mathscr{H})$. Next we may write

$$\tilde{F}_R(H+i)^{-1}\tilde{F} = \tilde{F}F_R(\sqrt{H_0}+i)^{-1}(\sqrt{H_0}+i)(H+i)^{-1}\tilde{F}.$$

Since $F_R(\sqrt{H_0}+i)^{-1}$ is compact in $\mathscr{H}$ (cf. Appendix I), it follows that $\tilde{F}_R(H+i)^{-1}\tilde{F}$ is compact in $\mathscr{H}$ and hence in $\tilde{\mathscr{H}}$.

We may now apply the Theorem with $S_n = S = (H+i)^{-1}$ and the projection operators $\tilde{F}_R$ (interpreted as acting in $\tilde{\mathscr{H}}$). This shows that (R1) and (R2) hold in $\tilde{\mathscr{H}} = L^2(E)$ (i.e. the domains of integration in (R1) and (R2) are restricted to their intersection with E).

Highly Singular Attractive Potentials

By highly singular attractive potentials for the Schrödinger equation we mean two-body interactions which have attractive local singularities that do not satisfy the Rollnik condition. Thus a potential of the form $V(x) = \lambda|x|^{-\alpha}(x \in \mathbb{R}^3)$ is highly singular if $\alpha > 2$ (if $\alpha = 2$ one encounters the same complications for sufficiently large negative values of λ [18]). Such potentials lead to difficulties in classical scattering theory ([19], Chapter 5). In quantum mechanics the Hamiltonian turns out to be unbounded below and not essentially self-adjoint (cf. the precise definition below). Since these potentials are very attractive near the origin, it is intuitively not evident that (R1) and (R2) must hold. One could expect that certain states in the continuous subspace of the Hamiltonian might not escape from the attractive force near the origin and thus be captured by the centre of force. In fact for $\alpha = 2$ Nelson [5] derived a time-evolution which is non-unitary (absorptive) under conditions which reflect exactly the

[6]) δ) could also be formulated in terms of $Q(H_0)$ and $Q(V)$.

classical situation. Our own results indicate that for *self-adjoint* extensions of $H_0 + V$, (R1) and (R2) will nevertheless be true.

In the following we restrict ourselves to the two-body case and assume that the potential is highly singular only at the origin. One can then define a symmetric operator $\hat{H}$ on $C_0^\infty(\mathbb{R}^3 - \{0\})$ by $(\hat{H}f)(x) = -\Delta f(x) + V(x)f(x)$. $\hat{H}$ is in general not essentially self-adjoint. In order to verify (R1) and (R2) for self-adjoint extensions of $\hat{H}$, one could try to derive suitable estimates on the domain of $\hat{H}^*$ which would allow the application of Proposition 5 or a modification of it. Another possibility is to use Proposition 3. For this one has to establish the existence and the completeness of the wave operator $\Omega(H,H_0)$ between a self-adjoint extension H of $\hat{H}$ and $H_0 = |P|^2$. The existence of $\Omega(H,H_0)$ was proved by Kupsch and Sandhas [20] under the assumption that the restriction of $V(x)$ to any region bounded away from the origin is a suitable short-range potential. We have investigated the completeness of $\Omega(H,H_0)$ under the following additional assumptions:

i) V is spherically symmetric: $V(x) = V(r)$ $(r = |x|)$;
ii) one of the following conditions is verified:
 α) $V(r) + r^{-2}|\ln r|$ is an increasing function of r near $r = 0$,
 β) there exists $\epsilon > 0$ such that

$$V(r) < 0 \quad \text{for } r \in (0, \epsilon)$$

$$\int_0^\varepsilon dr r^{-2}|V(r)|^{-1/2} < \infty$$

and

$$\int_0^\varepsilon dr|V(r)|^{1/2}\left|\frac{5}{4}\cdot\frac{[V'(r)]^2}{[V(r)]^3} + \frac{V''(r)}{[V(r)]^2}\right| < \infty;$$

 γ) $V(r) = \alpha r^{-2}$ with $\alpha < 0$.

(Conditions i) and ii) are verified for all potentials of the form $V(r) = \alpha r^{-n}$ with $\alpha < 0$ and $n \geqslant 2$.) Let $\hat{H}_l$ (resp. H_{0l}) be the restriction of $\hat{H}$ (resp. H_0) to the lth partial-wave subspace, and let H_l be a self-adjoint extension of $\hat{H}_l$. One can then prove that H_l has no singularly continuous spectrum and that $\Omega(H_l, H_{0l})$ is complete. (This proof and other results about time-dependent scattering theory and domain properties of Hamiltonians with highly singular potentials will be communicated in a forthcoming separate report.) With this one sees that (R1) and (R2) do hold for every self-adjoint extension H of $\hat{H}$ of the form $H = \bigoplus_{l=0}^{\infty} H_l$, H_l being an arbitrary self-adjoint extension of $\hat{H}_l$.

Acknowledgments

We wish to thank Dr. D. B. Pearson for stimulating discussions and particularly for his contributions to the questions concerning scattering theory for Schrödinger Hamiltonians with highly singular potentials.

Note: We wish to point out a recent paper by C. H. Wilcox [21] in which an abstract scattering theory is developed by requiring convergence of the wave operators on a subspace $\mathscr{H}^s$ of scattering states similar to our $\mathscr{M}_\infty$.

APPENDIX I

In this Appendix we prove two results concerning compactness of operators of the form $F_r\phi(A)$. With the same notation as in Section III we first show that $F_r(\phi(P)+i)^{-1}$ is compact if $|\phi(p)| \to \infty$ for $|p| \to \infty$ with the possible exception of certain directions:

Lemma 3:

Let $\phi: \mathbb{R}^N \to \mathbb{R}$ be Lebesgue measurable and suppose there exists a subset Δ_0 of $\mathbb{R}^N$ with $\mu(\Delta_0) < \infty$ (μ denotes the Lebesgue measure) and such that

$$\lim_{\substack{|p|\to\infty \\ p\notin\Delta_0}} |\phi(p)| = \infty. \tag{24}$$

Then $F_r(\phi(P)+i)^{-1}$ is compact.

Notation:

If Δ is a Borel set of $\mathbb{R}^N$, we denote by χ_Δ its characteristic function (i.e. $\chi_\Delta(x)=1$ if $x \in \Delta$ and $\chi_\Delta(x)=0$ if $x \notin \Delta$) and by $\tilde{\chi}_\Delta$ the Fourier transform of χ_Δ. χ_r denotes the characteristic function of the sphere $|x| \leqslant r$ and $V_r \equiv \mu(|x| \leqslant r)$ its volume. Let D_{OK} be the projection operator onto the states having momentum in the set $\Delta_{OK} \equiv \Delta \cup \{p \mid |p| \leqslant K\}$.

Proof:

Let $K < \infty$ and $r < \infty$. We first show that $F_r(\phi(P)+i)^{-1} D_{OK}$ is a compact operator. In fact it is even a Hilbert–Schmidt operator, since its Hilbert–Schmidt norm ([4], p. 210) can be estimated in the p-representation as follows:

$$\begin{aligned} \|F_r(\phi(P)+i)^{-1} D_{OK}\|_{HS}^2 &= \int d^N p\, d^N p' |\tilde{\chi}_r(p-p')|^2 |(\phi(p')+i)^{-1}|^2 \chi_{\Delta_{OK}}(p') \\ &= \int d^N x |\chi_r(x)|^2 \int d^N p' |(\phi(p')+i)^{-1}|^2 \chi_{\Delta_{OK}}(p') \leqslant V_r \int d^N p' \chi_{\Delta_{OK}}(p') \\ &= V_r \mu(\Delta_{OK}) \leqslant V_r[V_K + \mu(\Delta_0)] < \infty \end{aligned}$$

where we have used the fact that $|(\phi(p')+i)^{-1}| \leqslant 1$.

Next we notice that

$$\begin{aligned} &\|F_r(\phi(P)+i)^{-1} - F_r(\phi(P)+i)^{-1} D_{OK}\| \\ &\quad \leqslant \|(\phi(P)+i)^{-1}(I-D_{OK})\| \leqslant \sup_{p\notin\Delta_{OK}} |(\phi(p)+i)^{-1}|. \end{aligned}$$

By assumption (24), this converges to zero as $K \to \infty$. Hence $F_r(\phi(P)+i)^{-1}$ is the uniform limit of a sequence of compact operators, which means that $F_r(\phi(P)+i)^{-1}$ is itself compact ([4], p. 200). ∎

Lemma 4:

Let $B \in \mathscr{B}(\mathscr{H})$, $A = A^*$ and suppose $B(A-z)^{-M}$ is compact for some $z \in \rho(A)$ and some $M = 1, 2, \ldots$. Let $\phi: \mathbb{R} \to \mathbb{C}$ be bounded and measurable with respect to the spectral family $\{E(\lambda)\}$ of A and suppose $\lim_{\lambda\to\pm\infty} |\phi(\lambda)| = 0$. Then $B\phi(A)$ is compact.

Proof:

Let E_Λ be the spectral projection of A corresponding to the interval

$$(-\Lambda, \Lambda] \quad (0 < \Lambda < \infty).$$

We have

$$BE_\Lambda = B(A-z)^{-M}(A-z)^M E_\Lambda.$$

Since $(A-z)^M E_\Lambda \in \mathscr{B}(\mathscr{H})$, BE_Λ is compact. Since $\phi(A) \in \mathscr{B}(\mathscr{H})$, this implies that $BE_\Lambda \phi(A)$ is compact. Furthermore

$$\|B\phi(A) - BE_\Lambda \phi(A)\| \leqslant \|B\| \, \|(I-E_\Lambda)\,\phi(A)\| \leqslant \|B\| \sup_{|\lambda|>\Lambda} |\phi(\lambda)|.$$

We have assumed that the last member of this inequality converges to zero as $\Lambda \to \infty$. Thus $B\phi(A)$ is the uniform limit of a sequence of compact operators and hence compact.

■

APPENDIX II

In this Appendix we collect some auxiliary facts about non-relativistic n-body Hamiltonians.

For a system of n non-relativistic particles interacting between themselves through translation invariant potentials and such that there are no external fields, the total Hamiltonian $\mathbb{H}$ is known to have absolutely continuous spectrum. The only condition for this is that $\mathbb{H} = (1/2M)\vec{P}^2 \otimes I + I \otimes H$, where $\vec{P}$ is the momentum operator of the centre-of-mass and H is the Hamiltonian of the relative movement. It is not very interesting to apply the main theorem to $\mathbb{H}$. The relative movement is described by a Hamiltonian of the form

$$H = \sum_{i,j=1}^{n-1} a_{ij} \vec{P}_i \cdot \vec{P}_j + \sum_{k=2}^{n} \sum_{1 \leqslant i_1 < \ldots < i_k \leqslant n} V_{i_1 \ldots i_k}.$$

Here $\vec{P}_i = -i\vec{\nabla}_{x_i}$, where $\vec{x}_1, \ldots, \vec{x}_{n-1}$ are linearly independent coordinates describing the relative movement. A convenient choice is

$$\vec{x}_i = \vec{r}_i - \vec{r}_n \tag{25}$$

where $\vec{r}_j$ $(j = 1, \ldots, n)$ denotes the position of the jth particle ([6], pp. 185 and 190 *ff.*) a_{ij} is a real, symmetric and positive definite matrix, and $V_{i_1} \ldots {}_{i_k}$ is the k-body potential corresponding to the set of particles $\{i_1, \ldots, i_k\}$. $V_{i_1} \ldots {}_{i_k}$ is a multiplication operator in the relative coordinates $\vec{x}_1, \ldots, \vec{x}_{n-1}$. We shall indicate its explicit form only for the case $k = 2$ and with the choice (25) for the relative coordinates: If $V(\vec{r}_1, \ldots, \vec{r}_n) = \sum_{1 \leqslant i < j \leqslant n} V_{ij}(\vec{r}_i - \vec{r}_j)$, then in the relative coordinates:

$$\sum_{1 \leqslant i < j \leqslant n} V_{ij} = \sum_{1 \leqslant i \leqslant n-1} V_{in}(\vec{x}_i) + \sum_{1 \leqslant i < j \leqslant n-1} V_{ij}(\vec{x}_i - \vec{x}_j).$$

We now wish to prove the following result which was mentioned in Section III:

Lemma 5:

Suppose V is a sum of translation invariant two-body potentials: $V = \sum_{1 \leqslant i < j \leqslant n} V_{ij}$ and that $V_{ij} \in L^2_{\text{loc}}(\mathbb{R}^3)$ for all $\{i, j\}$. Let $\vec{x}_1, \ldots, \vec{x}_{n-1}$ be linearly independent relative coordinates which are linear combinations of the particle positions $\vec{r}_1, \ldots, \vec{r}_n$. Denote by $\tilde{V} = \sum_{ij} \tilde{V}_{ij}: \mathbb{R}^{3(n-1)} \to \mathbb{R}$ the function V expressed in the coordinates $\vec{x}_1, \ldots, \vec{x}_{n-1}$. Then $\tilde{V} \in Q_{\alpha, \text{loc}}(\mathbb{R}^{3(n-1)})$ for all $\alpha \in (0, 1)$.

We have used the following *definition*: $Q_{\alpha, \text{loc}}(\mathbb{R}^N)$ is the set of all functions $f: \mathbb{R}^N \to \mathbb{C}$ which are such that

$$M_f(x) \equiv \int_{|x-y| \leqslant 1} d^N y |f(y)|^2 |x-y|^{-N+4-\alpha} \quad (x \in \mathbb{R}^N) \tag{26}$$

is locally bounded.

Proof:

It is an immediate consequence of (26) and the inequality (3) that $Q_{\alpha, \text{loc}}(\mathbb{R}^N)$ is a linear vector space. Hence it suffices to show that each $\tilde{V}_{ij}$ belongs to $Q_{\alpha, \text{loc}}(\mathbb{R}^N)$, $N = 3(n-1)$. In order to simplify the notation, we shall write U for V_{ij}.

i) Let $N = 3$. Then for $x \in \mathbb{R}^3$:

$$M(x) = \int_{|x-y| \leqslant 1} d^3 y |U(y)|^2 |x-y|^{-N+4-\alpha} \leqslant \int_{|x-y| \leqslant 1} d^3 y |U(y)|^2$$

since $|x-y| \leqslant 1$ and $-N+4-\alpha > 0$. Since $U \in L^2_{\text{loc}}(\mathbb{R}^3)$, this shows that $M(x)$ is bounded by a continuous function of x, which implies that $M(x)$ is locally bounded.

ii) Let $N > 3$. Then $\tilde{U}(\vec{x}_1, \ldots, \vec{x}_{n-1}) = U(\sum_{i=1}^{n-1} a_i \vec{x}_i)$ with some constants a_i. Let $A = (\sum_{i=1}^{n-1} a_i^2)^{1/2}$.

Let $e_i^{(k)}$ denote the unit vector along the coordinate axis corresponding to the kth component of $\vec{x}_i$ ($i = 1, \ldots, n-1$; $k = 1, 2, 3$). Let $a^{(k)} \in \mathbb{R}^{3(n-1)}$ be as follows:

$$a^{(k)} = \frac{1}{A} \sum_{i=1}^{n-1} a_i e_i^{(k)} \quad (k = 1, 2, 3).$$

Since $a^{(k)} \cdot a^{(k')} = \delta_{kk'}$, we may choose a new coordinate system in $\mathbb{R}^{3(n-1)}$ such that its first three basis vectors are $e_1'^{(k)} = a^{(k)}$ and such that the new basis $\{e_i'^{(k)}\}$ is obtained from $\{e_i^{(k)}\}$ by an orthogonal transformation.

We denote by x' the new coordinates of the point x and we use the abbreviation x_0' for the vector $(\vec{x}_2', \ldots, \vec{x}_{n-1}') \in \mathbb{R}^{3(n-2)}$. In the new coordinate system we have
$\tilde{U}(\vec{x}, \ldots, \vec{x}_{n-1}) = U(A\vec{x}_1')$
and thus

$$M(x) = \int_{|x-y| \leqslant 1} d^N y |\hat{U}(y)|^2 |x-y|^{-N+4-\alpha}$$

$$= \int_{|x'-y'| \leqslant 1} d^N y' |U(A\vec{y}_1')|^2 |x'-y'|^{-N+4-\alpha}. \tag{27}$$

We extend the integration in (27) to the larger domain

$$\{y' \mid y' = (\vec{y}_1', y_0'), |\vec{x}_1' - \vec{y}_1'| \leqslant 1, |x_0' - y_0'| \leqslant 1\}.$$

Thus

$$M(x) \leqslant \int_{|\vec{x}_1' - \vec{y}_1'| \leqslant 1} d^3 y_1' |U(A\vec{y}_1')|^2 \int_{|x_0' - y_0'| \leqslant 1} d^{N-3} y_0' \left| |\vec{x}_1' - \vec{y}_1'|^2 + |x_0' - y_0'|^2 \right|^{(-N+4-\alpha)/2}$$

$$= \frac{1}{A^3} \int_{|A\vec{x}_1' - \vec{z}| \leqslant A} d^3 z |U(\vec{z})|^2 \int_{|x_0' - y_0'| \leqslant 1} d^{N-3} y_0' \left| \vec{x}_1' - \frac{1}{A}\vec{z} |^2 + |x_0' - y_0'|^2 \right|^{(-N+4-\alpha)/2}. \tag{28}$$

Let

$$s = \left| \vec{x}_1' - \frac{1}{A}\vec{z} \right|, \; t = |x_0' - y_0'|.$$

Then, since $-N + 4 - \alpha < 0$:

$$\int_{|x_0' - y_0'| \leqslant 1} d^{N-3} y_0' \left| |\vec{x}_1' - \frac{1}{A}\vec{z}|^2 + |x_0' - y_0'|^2 \right|^{(-N+4-\alpha)/2}$$

$$= \text{const} \int_0^1 dt t^{N-3-1} [s^2 + t^2]^{(-N+4-\alpha)/2}$$

$$\leqslant \text{const} \int_0^1 dt t^{N-4} t^{-N+4-\alpha} = \text{const} \int_0^1 dt t^{-\alpha}.$$

The last integral is finite if $\alpha \in (0,1)$. This implies together with (28) that

$$M(x) \leqslant \text{const} \int_{|A\vec{x}_1' - \vec{z}| \leqslant A} d^3 z |U(\vec{z})|^2.$$

By the same argument as in (i), one sees from this that $M(x)$ is locally bounded. ∎

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