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Asymptotic Observables on Scattering States

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Abstract. In quantum mechanical potential scattering theory we use selected observables to describe the asymptotic properties of scattering states for long times. E.g., we show for the position and momentum operators that for $\Psi \in \mathscr{H}^{\text{cont}}(H)$,

$$\left(m\frac{\mathbf{x}}{t} - p\right)e^{-iHt}\Psi \to 0,$$

and that the set of outgoing states is absorbing. This is obtained easily without any detailed analysis of the interacting time evolution. The class of forces includes highly singular and very long range potentials.

The results may serve as an intermediate step in a proof of asymptotic completeness; as a particular application we present a simple proof of completeness for Coulomb systems.

I. Introduction

In potential scattering theory the states in the continuous spectral subspace of the Hamiltonian are well known to have a simple time evolution asymptotically if the perturbation is suitably localized. If the potential is of short range, then the free time evolution is a good approximation of the interacting one in the far future and in the remote past. Similarly a modified free time evolution can be used if long-range forces are present. This fact, called asymptotic completeness, allows one to deduce various properties of the asymptotic motion since free or modified free time evolutions can be controlled easily. E.g., the position and the momentum vectors become parallel at large times and have been antiparallel in the remote past.

Sometimes one is interested in obtaining partial information about a state without first proving asymptotic completeness, i.e. by studying the interacting time evolution itself. In particular we think of two reasons for doing this. In the case of very long range forces it may be hard to construct and control a modified free time evolution or its existence may be unknown (e.g. if $V(x) \sim [\ln(\ln|x|)]^{-1}$ as $|x| \to \infty$). Nevertheless physical intuition suggests that for the position and momentum of a particle at time t

$$m\frac{\mathbf{x}(t)}{t}\approx p(t) \text{ as } |t|\to\infty, \tag{1.1}$$

as it is true for the free time evolution. We will give a basically simple proof below which does not assume or use any detailed information about the interacting time evolution.

Another application is to use (1.1) as a first step in a proof of asymptotic completeness. That part of the state space where the particle is far from the scatterer and outgoing is absorbing under the full time evolution as a consequence of (1.1). Then one shows by different methods that the (modified) free time evolution is a good approximation of the interacting one on this absorbing subset of the state space. (See e.g. the first version of the completeness proof in Sect. 9 of [8].) For special long range forces like the Coulomb potential this approach allows one to simplify the proof of asymptotic completeness considerably, and it turned out to be a crucial step in the proof for three body systems [9, 11].

It is a very difficult problem to follow the (interacting) time evolution of a scattering state in a good approximation for long times. Therefore we ask more modest questions and study how certain observables evolve on scattering states. The choice of these observables ($\equiv$ self-adjoint operators) has to meet two conflicting requirements. The observables have to provide enough information about the state to be useful. On the other hand they must have a sufficiently simple time evolution which can be controlled even when strong interactions take place. It turns out that there is a simple family which meets both requirements. Denote for an operator A its time translated one by $A(t)$

$$A(t)=e^{iHt}Ae^{-iHt}. \tag{1.2}$$

Then on the continuous spectral subspace $\mathscr{H}^{\mathrm{cont}}(H)$,

$$\frac{m}{2}\frac{x^2(t)}{t^2}\to H; \tag{1.3}$$

$$\frac{D(t)}{t}\to 2H,\ D=\tfrac{1}{2}(\mathbf{x}\cdot\mathbf{p}+\mathbf{p}\cdot\mathbf{x}); \tag{1.4}$$

$$H_0(t)\to H,\ H_0=\frac{1}{2m}\mathbf{p}^2; \tag{1.5}$$

as $|t|\to\infty$ in the sense of strong resolvent convergence.

$$\left(m\frac{\mathbf{x}(t)}{t}-\mathbf{p}(t)\right)^2=2m\left(\frac{m}{2}\frac{x^2(t)}{t^2}-\frac{D(t)}{t}+H_0(t)\right)\to 0, \tag{1.6}$$

thus the desired relation (1.1) follows from (1.3)–(1.5). Moreover there is an intuitive explanation why it should be easy to control the interacting time evolution. For a classical point particle which is reflected elastically at the origin the interacting and free time evolutions are identical for the observables above. Thus the main effect of scattering, the deflection of the trajectory, is not seen by the observables. The other effects which come from the extension of the potential, e.g. time delay, disappear because of the inverse powers of the time t in (1.3) and (1.4).

The assumptions about the potential and the main results are given in the next section. A discussion of domain questions and the proof follow in Sects. III and IV. We conclude with some applications to scattering theory, in particular a simple proof of asymptotic completeness for Coulomb-potentials is given.

In the "algebraic approach" to scattering theory the asymptotics of the time evolution viewed as an automorphism group on suitable algebras of observables have been studied extensively for long-range forces [1]. An equivalent of the modified wave operators was constructed which required detailed knowledge of the interacting dynamics. In contrast to that we restrict the set of observables further such that the effects of the interaction disappear completely. We need not have any detailed knowledge about the interacting time evolution.

While it is clear that eigenvectors of the Hamiltonian are bound states, it requires more work to show that states from the continuous spectral subspace become asymptotically "free" as is suggested by experience from scattering experiments. Various notions have been proposed to describe in which sense a particle becomes free. As the weakest version Ruelle showed that the states will leave any bounded region in the time average [2]. The stronger notion of a particle which "flees the origin with velocity" was proposed by Dollard [3]. This property follows for all continuum states from our Corollary 2.2. Our results state that in addition to the scaled position operator $\mathbf{x}(t)/t$, a few more observables asymptotically behave in the same way as they would do under the free time evolution.

Unless we assume rotational symmetry of the potential, there need not exist an asymptotic angular distribution. Therefore, the results related to "scattering into cones" [4] are generally stronger. Still stronger are the results in the algebraic approach mentioned above and the strongest is asymptotic completeness, where all states are known to have asymptotically a (modified) free time evolution. Clearly at each of these steps stronger assumptions have to be made about the potentials, the methods of proof change and their complexity increases.

Our main results appeared as Sect. 7 in the lecture notes [8]. There the proof was given only under the simplifying condition (3.31) which made the conceptual and mathematical simplicity especially clear. We did not care to state Theorem 2.4 at that time since its applications to long-range scattering and in particular to multiparticle systems came up later. The present paper is worked out technically to include a very wide class of potentials which tend in some sense to zero towards infinity. We regret that the technical generality might hide the basic simplicity of our arguments. For related results see also Sinha and Muthuramalingam [23].

For multiparticle systems the corresponding results were partially announced and proved in [9]. The full results will be given in a forthcoming paper.

After completion of Sect. V of this manuscript we learned about the work of Muthuramalingam [18], where slightly weaker results on completeness for Coulomb potentials are proved with essentially the same method.

II. Assumptions and Results

We consider a quantum mechanical particle moving in ν-dimensional space. The state of a particle is described by a vector in the Hilbert space $\mathscr{H} = L^2(\mathbb{R}^\nu)$. The unitary time evolution is generated by the self-adjoint Hamiltonian

$$H = H_0 + V = H_0 + V_l + V_s, \tag{2.1}$$

which is obtained as a perturbation of the free Hamiltonian

$$H_0 = (2m)^{-1} p^2 = -(2m)^{-1} \Delta. \tag{2.2}$$

The long range part V_l of the potential is a multiplication operator in x-space with a real continuously differentiable function $V_l(\mathbf{x})$ which satisfies

$$V_l(\mathbf{x}) \to 0 \text{ and } \mathbf{x} \cdot (\nabla V_l)(\mathbf{x}) \to 0 \quad \text{as } |\mathbf{x}| \to \infty. \tag{2.3}$$

The symmetric short-range potential

$$V_s = V_1 + V_2 \tag{2.4}$$

may consist of a form-bounded part V_1:

$$|(\Psi, V_1 \Psi)| \leqq a(\Psi, H_0 \Psi) + b \| \Psi \|^2, \; a < 1 \tag{2.5}$$

for all $\Psi \in \mathcal{Q}(H_0)$, the form domain of H_0. The positive self-adjoint part V_2 may be used to describe highly singular positive perturbations. We assume

$$\mathcal{Q}(H_0) \cap \mathcal{Q}(V_2) \cap \mathcal{Q}(x^2) \text{ is dense in } \mathcal{H}. \tag{2.6}$$

Then by standard results [12, 15, 21], H is a closed quadratic form with form domain

$$\mathcal{Q}(H) = \mathcal{Q}(H_0) \cap \mathcal{Q}(V_2), \tag{2.7}$$

corresponding to a unique self-adjoint semibounded operator H with domain $\mathcal{D}(H)$. Let $z \in \mathbb{R}$ be any (sufficiently negative) number which is in the resolvent set of the three operators H, H_0, and

$$H_l = H_0 + V_l. \tag{2.8}$$

All statements below using z are independent of the particular choice. The decay requirements can be expressed as follows.

$$(H_0 - z)^{-1/2} (1 + x^2)^{1/2} V_s (H - z)^{-1} \text{ is compact,} \tag{2.9}$$

or equivalently

$$(1 + x^2)^{1/2} (H_0 - z)^{-1/2} V_s (H - z)^{-1} \text{ is compact.} \tag{2.10}$$

Note that it follows from our assumptions that the operator in (2.10) without the factor $(1 + x^2)^{1/2}$ is bounded. The same proof works if we assume instead that the operator in (2.9) or (2.10) is bounded and

$$\| F(|x| > R) \cdot |x| \cdot (H_0 - z)^{-1/2} V_s (H - z)^{-1} \| \to 0 \text{ as } R \to \infty. \tag{2.11}$$

This slightly weaker assumption will hardly matter in applications. Therefore we use the compactness condition which avoids the necessity to split many terms into two pieces.

These conditions are sufficient if the potential is local, i.e. if it commutes with all bounded functions of x. Otherwise we have to require in addition

$$(H - z)^{-1/2}\{x^2 V_s - V_s x^2\}(H - z)^{-1/2} \text{ is bounded.} \tag{2.12}$$

This may be interpreted by first regularizing $x^2 \to x^2(1 + \lambda x^2)^{-1}$, and then studying the limit $\lambda \to 0$. If the non-local part of V_s is a polynomial in p with x-dependent coefficients of short range, then (2.12) holds since the derivatives of x^2 grow at most linearly. The other non-local potentials of importance are separable ones as used, e.g. in nuclear physics. Typically they have exponential decay and thus satisfy (2.12).

Our decay condition for the short range part is a bit weaker than the integrability conditions often used in scattering theory. E.g. a potential

$$V(x) = [|x| \ln |x|]^{-1} \text{ for } |x| > 2 \tag{2.13}$$

satisfies (2.9) but it gives rise to modified wave operators.

Parts of the proof, in particular domain questions, simplify considerably if the short-range part V_s is a local, Kato-bounded perturbation of H_0 which satisfies

$$(1 + |x|^2)^{1/2} V_s(H_0 - z)^{-1} \text{ is compact.} \tag{2.14}$$

Since this case covers most applications we will give some of the simplifications below.

Denote by P^{cont} the projection onto the continuous spectral subspace $\mathscr{H}^{\text{cont}}$ of the Hamiltonian H. For an operator A the time translated one is

$$A(t) = e^{iHt} A e^{-iHt}.$$

For the notion of strong resolvent convergence, see e.g. [15, 20]. $F(\cdot)$ denotes the spectral projection of the self-adjoint operator to the part of the spectrum as indicated in the parenthesis.

$$D = \tfrac{1}{2}(\mathbf{p} \cdot \mathbf{x} + \mathbf{x} \cdot \mathbf{p}) \tag{2.15}$$

is the generator of the dilations.

Now we are ready to state our main results.

Theorem 2.1. *Let $H = H_0 + V$ satisfy (2.1)–(2.6), (2.9), and (2.12). Then in the sense of strong resolvent convergence*

$$\lim_{|t| \to \infty} \frac{m}{2} \frac{x^2(t)}{t^2} = H P^{\text{cont}}, \tag{2.16}$$

$$\lim_{|t| \to \infty} \frac{D(t)}{t} = 2H P^{\text{cont}}. \tag{2.17}$$

Corollary 2.2 *Let H be as above and $\Psi \in \mathscr{H}^{\text{cont}}$*

a) $\lim_{|t| \to \infty} \| [\mathbb{1} - F(v_1 |t| < |x| < v_2 |t|)] e^{-iHt} \times$

$$F\left(\frac{m}{2} v_1^2 < H < \frac{m}{2} v_2^2\right) \Psi \| = 0 \tag{2.18}$$

for any $0 \leqq v_1 < v_2 \leqq \infty$.

b) $\lim_{|t| \to \infty} \| F(|x| < R) e^{-iHt} \Psi \| = 0$ for all R. (2.19)

c) $\lim_{t \to \infty} \| F(D < 2Et) e^{-iHt} F(H > E) \Psi \| = 0$. (2.20)

d) $\lim_{t \to -\infty} \| F(D > 2Et) e^{-iHt} F(H > E) \Psi \| = 0$. (2.20′)

e) $\lim_{|t| \to \infty} \| F(|D| < d) e^{-iHt} \Psi \| = 0$ for all d. (2.21)

Proof. a)

$$e^{iHt}[\mathbb{1} - F(v_1|t| < |x| < v_2|t|)]e^{-iHt} = \left[\mathbb{1} - F\left(\frac{m}{2}v_1^2 < \frac{m}{2}\frac{x^2(t)}{t^2} < \frac{m}{2}v_2^2\right)\right]$$
$$\to \left[\mathbb{1} - F\left(\frac{m}{2}v_1^2 < H < \frac{m}{2}v_2^2\right)\right]. \tag{2.22}$$

The last convergence is strong convergence on $\mathcal{H}^{\text{cont}}$ which follows from (2.16). Since all operators involved have only continuous spectrum, it is permitted to use discontinuous bounded functions.

b) follows from a) since for any $\Psi \in \mathcal{H}^{\text{cont}}$ and $\varepsilon > 0$ there is a $v_1 > 0$ such that

$$\left\| F\left(H < \frac{m}{2}v_1^2\right)\Psi \right\| < \varepsilon. \tag{2.23}$$

c) $e^{iHt}F(D < 2Et)e^{-iHt} = F(D(t)/t < 2E) \to F(2H < 2E)$ by (2.17).

d) The expression for negative times has the same limit.

e) Analogous to the proof of b). □

We do not know whether our assumptions on the potential exclude the possibility of singular continuous spectrum of H. Nevertheless we could show the local decay (2.19) and exclude recurrence. This is well known for states in the absolutely continuous spectral subspace of H. Moreover (2.18) says that a state propagates into those regions of space where it should be according to its energy support. We will see below that the full energy and the kinetic energy coincide asymptotically.

The sign of the dilation generator D describes whether the angle between $\mathbf{x}$ and $\mathbf{p}$ is acute or obtuse, i.e. whether the velocity of a particle at $\mathbf{x}$ points away from the scatterer or more towards it. The spectral projections of D have been introduced by Mourre [17, Sect. V in 8] to characterize incoming and outgoing states. According to (2.20) and (2.21) any state in $\mathcal{H}^{\text{cont}}$ has been incoming in the remote past and will be outgoing in the far future.

Corollary 2.3. *Let H be as above, $\Psi \in \mathcal{H}^{\text{cont}}$.*

a) $w\text{-}\lim_{|t| \to \infty} e^{-iHt}\Psi = 0$. (2.24)

b) On $\mathscr{H}^{\text{cont}}$ in the sense of strong resolvent convergence

$$\lim_{|t|\to\infty} H_0(t) = H. \tag{2.25}$$

Proof. a) Fix Φ and $\varepsilon > 0$. For any $d \in \mathbb{R}$

$$|(\Phi, e^{-iHt}\Psi)| \leqq \| F(|D| > d)\Phi \| \cdot \| \Psi \| + \| \Phi \| \cdot \| F(|D| < d) e^{-iHt}\Psi \|. \tag{2.26}$$

Choosing d big enough, the first summand is smaller than $\varepsilon/2$. For this d choose T large enough such that the second summand is smaller than $\varepsilon/2$ for all $|t| > T$ by (2.21).

b) $(H_0 - z)^{-1} - (H - z)^{-1}$ is compact. Therefore

$$[(H_0 - z)^{-1} - (H - z)^{-1}] e^{iHt}\Psi \to 0, \tag{2.27}$$

as $|t| \to \infty$ by a) for any $\Psi \in \mathscr{H}^{\text{cont}}$. □

Theorem 2.4. *Let H be as above, $\Psi \in \mathscr{H}^{\text{cont}}$. Let f be the Fourier transform of an integrable function, i.e. $\hat{f} \in L^1(\mathbb{R}^\nu, d^\nu q)$. Then for the operators* $\mathbf{x}$ *and* $\mathbf{p}$

$$\lim_{|t|\to\infty} \left\| \left[f\left(m\frac{\mathbf{x}}{t} \right) - f(\mathbf{p}) \right] e^{-iHt}\Psi \right\| = 0. \tag{2.28}$$

The same holds if $1\text{-}f$ *has integrable Fourier transform.*

This theorem states that the average velocity between time zero and t has a distribution which coincides with the velocity distribution at a large time t. Although we know from (2.25) that the distribution of the modulus of the momentum converges we cannot conclude this for the direction of $\mathbf{p}$. In fact one can imagine a potential which satisfies our assumptions but the momentum direction continues to turn, although slowly.

For smoothed cutoff functions f we conclude from (2.28) a strong correlation between the localization of (a part of) a state at time t and its momentum. This means a localization in classical phase space. A state evolves into a smaller and smaller subset of the outgoing subspace. This behaviour is common to the free time evolution and a very wide class of interacting ones. The basically simple proof of the theorems which we give in the next sections does not use any detailed information about the interacting time evolution, but merely controls that the deviation from the free time evolution is small for these particular observables.

III. Domain Questions

In this section we provide estimates which are necessary to control commutators of unbounded operators and related questions which are used in the next section. The results are trivial if the potential is a continuously differentiable function which satisfies (2.3). They are simple if one adds an operator bounded short range part V_s which satisfies (2.14) (see below). Only our inclusion of perturbations which are form-bounded or highly singular requires more efforts. The reason for the additional problems seems to be the fact that the domain of the Hamiltonian need not be invariant under dilations in this case.

Our first proposition is a slight extension of a result of Radin and Simon [19] to the larger class of potentials which we admit. Part a) also follows from results of Kato [16] which have been rediscovered several times, see e.g. [13, 19] and references given there, also [14] for earlier results.

Proposition 3.1. *Let H satisfy (2.1)–(2.6), (2.9), and (2.12).*

a) $\mathscr{Q}(x^2) \cap \mathscr{Q}(H)$ is dense and invariant under $\exp(-iHt)$.

b) $(\Psi, x^2(t)\Psi) \leqq c^2(\Psi)(1+|t|)^2$ (3.1)

for any $\Psi \in \mathscr{Q}(x^2) \cap \mathscr{Q}(H)$.

Proof. The density is guaranteed by (2.6) and the invariance of $\mathscr{Q}(H)$ is clear. A vector Φ is in $\mathscr{Q}(x^2)$ iff $(\Phi, (1+\lambda x^2)^{-1}x^2\Phi)$ is bounded uniformly as $\lambda \to 0$. Both a) and b) follow if we show that

$$(\Psi, e^{iHt}(1+\lambda x^2)^{-1}x^2 e^{-iHt}\Psi) \leqq c^2(\Psi)(1+|t|)^2 \tag{3.2}$$

for any $\Psi \in \mathscr{Q}(H) \cap \mathscr{Q}(x^2)$ with a constant $c(\Psi)$ which is independent of λ. It follows from (2.9) that

$$H = H_0 + V,$$

as a bounded mapping from $\mathscr{Q}(H)$ into the dual of $\mathscr{Q}(H_0)$ can be written as a sum; moreover

$$\mathscr{Q}(H) \subset \mathscr{Q}(H_0) = (1+\lambda x^2)^{-1}(1+x^2)\mathscr{Q}(H_0) \text{ for } \lambda > 0.$$

Therefore for any $0 < \lambda < 1$ and $\Psi \in \mathscr{Q}(H)$,

$$g(t)^2 := (\Psi, e^{iHt}(1+\lambda x^2)^{-1}(1+x^2)e^{-iHt}\Psi) \geqq 1 \tag{3.3}$$

is continuously differentiable with derivative

$$\begin{aligned}&(\Psi, e^{iHt} i[H_0, (1+\lambda x^2)^{-1}(1+x^2)]e^{-iHt}\Psi) \\ &+ (\Psi, e^{iHt} i[V_s, (1+\lambda x^2)^{-1}(1+x^2)]e^{-iHt}\Psi).\end{aligned} \tag{3.4}$$

The second summand is bounded uniformly in t and λ by

$$c_1(\Psi, (H-z)\Psi), \tag{3.5}$$

where c_1 is simply related to the norm of (2.12). The commutator in the first summand can be calculated as a quadratic form on $\mathscr{Q}(H_0)$ to be

$$i[H_0, (1+\lambda x^2)^{-1}(1+x^2)] = \frac{1}{m}\left(\mathbf{p}\cdot\mathbf{x}\frac{(1-\lambda)}{(1+\lambda x^2)^2} + \frac{(1-\lambda)}{(1+\lambda x^2)^2}\mathbf{x}\cdot\mathbf{p}\right). \tag{3.6}$$

The Schwarz inequality permits us to estimate the expectation value of this by

$$\frac{2}{m}\||p|e^{-iHt}\Psi\| \cdot \left\|\frac{|x|}{(1+\lambda x^2)^{1/2}}e^{-iHt}\Psi\right\| \leqq 2c_2(\Psi, (H-z)\Psi)^{1/2} g(t), \tag{3.7}$$

where we have used that p^2 is bounded by $H-z$ as a quadratic form. Thus we have shown

$$\frac{d}{dt}g(t) \leqq \frac{c_1}{2g(t)}(\Psi,(H-z)\Psi) + c_2(\Psi,(H-z)\Psi)^{1/2} \qquad (3.8)$$
$$\leqq c_3[(\Psi,(H-z)\Psi)+1],$$

with a constant c_3 independent of λ. Integration gives for all λ

$$g(t) \leqq \left\| \left\{ \frac{1+x^2}{1+\lambda x^2} \right\}^{1/2} \Psi \right\| + |t| c_3 [1 + (\Psi,(H-z)\Psi)]. \qquad (3.9)$$

By continuity the estimate extends to all $\Psi \in \mathscr{D}(H)$. If we choose $\Psi \in \mathscr{D}(H) \cap \mathscr{D}(x^2)$ we obtain the uniform estimate in λ

$$(\Psi, e^{iHt}(1+\lambda x^2)^{-1} x^2 e^{-iHt}\Psi) \leqq c^2(\Psi)(1+|t|)^2, \qquad (3.10)$$

where

$$c(\Psi) = \{ \|(1+x^2)^{1/2}\Psi\| + c_3[1+(\Psi,(H-z)\Psi)]\}. \qquad (3.11)$$

□

Corollary 3.2. *Let H be as above. Then for any $\Psi \in \mathscr{D}(H) \cap \mathscr{D}(x^2)$,*

$$e^{-iHt}\Psi \in \mathscr{D}(D), \qquad (3.12)$$

$$|(\Psi, D(t)\Psi)| \leqq c'(\Psi)(1+|t|). \qquad (3.13)$$

Proof.

$$|(\Psi, e^{iHt}\tfrac{1}{2}(\mathbf{x}\cdot\mathbf{p}+\mathbf{p}\cdot\mathbf{x})e^{-iHt}\Psi)| \leqq \| |p| e^{-iHt}\Psi\| \cdot \| |x| e^{-iHt}\Psi\|$$
$$\leqq \text{const} \|(H-z)^{1/2}\Psi\| \cdot c(\Psi)(1+|t|) \,. \qquad (3.14)$$

In the case of an operator bounded perturbation which satisfies (2.14), the domain questions are even simpler [16, 13] and one obtains [19]

Lemma 3.3. *Let H satisfy (2.1)–(2.3), and (2.14). Then $\mathscr{D}(x^2) \cap \mathscr{D}(H_0)$ is dense and invariant under* $\exp(-iHt)$. *Moreover for any $\Psi \in \mathscr{D}(x^2) \cap \mathscr{D}(H_0)$: $e^{-iHt}\Psi \in \mathscr{D}(D)$,*

$$\|De^{-iHt}\Psi\| \leqq c(\Psi)(1+|t|), \qquad (3.15)$$

$$\|x^2 e^{-iHt}\Psi\| \leqq c(\Psi)(1+|t|)^2. \qquad (3.16)$$

In the next section we want to show that

$$\frac{m}{2}\frac{x^2(t)}{t^2} \text{ and } \frac{1}{2t}D(t)$$

are not only bounded but both tend to the Hamiltonian. For that we need better control of the time derivative which is formally

$$\frac{d}{dt}D(t) = e^{iHt} i[H,D] e^{-iHt}. \qquad (3.17)$$

If we still consider the operator bounded case (2.14), then (3.17) is for all t naturally defined as a quadratic form on $\mathscr{D}(H_0) \cap \mathscr{D}(x^2)$ and on these vectors $H = H_0 + V$.

Thus we can calculate

$$\begin{aligned} i[H,D] &= i[H_0,D] + i[V_l,D] + i[V_s,D] \\ &= 2H_0 - \mathbf{x}\cdot(\nabla V_l) + i[V_s,D] \\ &= 2H - \{2V + \mathbf{x}\cdot(\nabla V_l) - i[V_s,D]\}. \end{aligned} \tag{3.18}$$

The operator in curly brackets extends naturally to a compact operator from $\mathscr{D}(H_0)$ to the dual of $\mathscr{Q}(H_0)$ by (2.3) and (2.14). It seems to be difficult to give a meaning to $[V_s, D]$ in the case of singular perturbations. We avoid this problem by using resolvents. Regularizing the operator (3.18) gives

$$\begin{aligned} (H-z)^{-1} i[H,D](H-z)^{-1} &= i[D,(H-z)^{-1}] \\ &= (H-z)^{-2} 2H - K, \end{aligned} \tag{3.19}$$

where K is compact. We will show next that this result holds in the general case as well. By the canonical commutation relations

$$D, \mathbf{p}\cdot\mathbf{x}, \text{ and } \mathbf{x}\cdot\mathbf{p} \tag{3.20}$$

differ only by a bounded operator, $\pm iv/2$. Therefore it is irrelevant in many cases which order of the factors we use. The commutator

$$i[D,(H-z)^{-1}] \tag{3.21}$$

is naturally defined as a quadratic form on $\mathscr{Q}(x^2)$ because e.g. $(H-z)^{-1}\mathbf{p}\cdot\mathbf{x}$ is then bounded. We show in the next proposition that it has an extension to a bounded operator of a particular form.

Proposition 3.4. *Let H satisfy (2.1)–(2.6), (2.9). Then*

$$i[D,(H-z)^{-1}] = 2H(H-z)^{-2} + K, \tag{3.22}$$

where K is compact.

Proof. We split the commutator

$$\begin{aligned} i[D,(H-z)^{-1}] = {} & i[D,(H_l-z)^{-1}] \\ & + iD\{(H-z)^{-1} - (H_l-z)^{-1}\} - i\{(H-z)^{-1} - (H_l-z)^{-1}\}D. \end{aligned} \tag{3.23}$$

The last two terms are adjoints of each other; $H_l = H_0 + V_l = H - V_s$. All three terms are naturally defined as quadratic forms on $\mathscr{Q}(x^2)$. Due to the boundedness of V_l we can calculate

$$\begin{aligned} i[D,(H_l-z)^{-1}] &= (H_l-z)^{-1} i[H_l,D](H_l-z)^{-1} \\ &= (H_l-z)^{-1}\{2H_0 - \mathbf{x}\cdot(\nabla V_l)\}(H_l-z)^{-1} \\ &= (H_l-z)^{-2} 2H_l - K_1 \\ &= (H-z)^{-2} 2H - K_1 - 2K_2. \end{aligned} \tag{3.24}$$

Clearly K_1 is compact as a product of a bounded decaying function of x with the resolvent of H_l

$$K_1 = (H_l-z)^{-1}\{2V_l + \mathbf{x}\cdot(\nabla V_l)\}(H_l-z)^{-1}. \tag{3.25}$$

To show the compactness of K_2 we decompose

$$\begin{aligned}K_2 &= (H-z)^{-2}H - (H_l - z)^{-2}H_l \\ &= (H-z)^{-1} - (H_l - z)^{-1} + z\{(H-z)^{-2} - (H_l - z)^{-2}\}.\end{aligned} \tag{3.26}$$

Since H_0 and H_l are bounded relative to each other,

$$(H_l - z)^{-1} - (H-z)^{-1} = (H_l - z)^{-1} V_s (H-z)^{-1} \tag{3.27}$$

is compact by (2.9). This implies also compactness of the difference of the squares of the resolvents.

Finally

$$\begin{aligned}K_3 &= iD(H_l - z)^{-1} V_s (H-z)^{-1} \\ &= i[D,(H_l - z)^{-1}](H_0 - z)\cdot(H_0 - z)^{-1} V_s (H-z)^{-1} \\ &\quad + (H_l - z)^{-1}(H_0 - z)\{\mathbf{p}(H_0 - z)^{-1/2}\cdot(H_0 - z)^{-1/2}\mathbf{x} V_s (H-z)^{-1} \\ &\quad + \frac{i}{2}v(H_0 - z)^{-1} V_s (H-z)^{-1}\}.\end{aligned} \tag{3.28}$$

The factor $(H_l - z)^{-1}(H_0 - z)$ is bounded and also $i[D,(H_l - z)^{-1}](H_0 - z)$ by the calculations made in (3.24) and (3.25). All other factors are compact by (2.9) which implies compactness of K_3. Consequently

$$-K = K_1 + 2K_2 + K_3 + K_3^*$$

is compact. □

Remark 3.5. The rather technical arguments in this section are caused by the very large class of potentials which we admitted. Equation (3.22) can formally be written for local potentials as

$$\begin{aligned}i[D,(H-z)^{-1}] &= (H-z)^{-1} i[H,D](H-z)^{-1} \\ &= (H-z)^{-1}\{2H_0 - \mathbf{x}\cdot(\nabla V)\}(H-z)^{-1} \\ &= (H-z)^{-1}\{2H - [2V + \mathbf{x}\cdot\nabla V]\}(H-z)^{-1}.\end{aligned} \tag{3.29}$$

The construction in the proof of Proposition 3.4 is needed only to give a rigorous meaning to the formal expression

$$K = -(H-z)^{-1}[2V + \mathbf{x}\cdot(\nabla V)](H-z)^{-1}, \tag{3.30}$$

and to show its compactness. In applications it is often sufficient to treat local potentials which are H_0-compact. If moreover the distributional derivative of $V(x)$ satisfies

$$\mathbf{x}\cdot(\nabla V)(H_0 - z)^{-1} \text{ is compact,} \tag{3.31}$$

then (3.22) is trivially satisfied and one has the stronger

$$(H-z)i[D,(H-z)^{-1}] = 2H(H-z)^{-1} + C, \tag{3.32}$$

where $C = (H-z)K$ is compact. The Coulomb- and Yukawa-potentials belong to this class. If only (2.3) and (2.14) are assumed, the proof of Proposition 3.4 is still very short and simple.

Finally we use Proposition 3.4 to prove a variant of the virial theorem. Denote by D_λ the regularized dilation generator for $\lambda > 0$,

$$D_\lambda = \tfrac{1}{2}\left(\frac{\mathbf{x}}{1+\lambda x^2}\cdot\mathbf{p} + \mathbf{p}\cdot\frac{\mathbf{x}}{1+\lambda x^2}\right). \tag{3.33}$$

For any $\Phi, \Psi \in \mathscr{D}(x^2) \cap \mathscr{D}(H) \subset \mathscr{D}(D)$

$$(\Phi, D_\lambda \Psi) \to (\Phi, D\Psi) \text{ as } \lambda \to 0.$$

Thus, in particular for such Φ, Ψ,

$$(\Phi, [D_\lambda, (H-z)^{-1}]\Psi) \to (\Phi, [D, (H-z)^{-1}]\Psi). \tag{3.34}$$

With the calculation made in the proof of Proposition 3.4 it is easy to check that $i[D_\lambda, (H-z)^{-1}]$ is uniformly bounded as $\lambda \to 0$, therefore the convergence (3.34) holds for any Φ, $\Psi \in \mathscr{H}$. Let now Φ and Ψ be eigenvectors of H for the same eigenvalue E, then

$$(\Phi, [D_\lambda, (H-z)^{-1}]\Psi) = 0 \text{ for all } \lambda. \tag{3.35}$$

This implies

$$P_E\{2H(H-z)^{-2} + K\}P_E = 0, \tag{3.36}$$

where P_E is the projection onto the eigenspace corresponding to some eigenvalue E of the Hamiltonian H. If in particular (3.31) holds, this can be rewritten as

$$P_E\{2H + C(H-z)\}P_E = 0. \tag{3.37}$$

For local potentials of a suitable class, (3.36) can be expressed using (3.30) as

$$P_E\{2H_0 - \mathbf{x}\cdot\nabla V\}P_E = 0. \tag{3.38}$$

This is the traditional way to state the virial theorem. See Chapter 5 of [24] and the Notes for other proofs of (3.38) and detailed references to the literature. Our proof of (3.36) admits stronger singularities and non-locality for the short range part of the potential. We elaborate on this point and give applications in [25].

IV. Proofs of the Theorems

We show Theorem 2.1 first under the simplifying condition (3.31), (3.32) in order to explain the main idea of proof. We begin with (2.17). The following commutator is naturally defined as a quadratic form with domain $\mathscr{D}(x^2) \cap \mathscr{D}(H_0)$:

$$\begin{aligned} i[H, D] &= 2H_0 - \mathbf{x}\cdot(\nabla V) \\ &= 2H - (2V + \mathbf{x}\cdot\nabla V) \\ &= 2H + C\cdot(H-z). \end{aligned} \tag{4.1}$$

It defines uniquely an operator on this domain (recall that C is compact). By Lemma 3.3 the following calculation is justified for $\Psi \in \mathscr{D}(x^2) \cap \mathscr{D}(H_0)$:

$$D(t)\Psi = D(0)\Psi + \int_0^t ds\left[\frac{d}{ds}D(s)\Psi\right]$$

$$= D(0)\Psi + \int_0^t ds\, e^{iHs} i[H, D] e^{-iHs}\Psi$$

$$= D(0)\Psi + t\cdot 2H\Psi + \int_0^t ds\, C(s)(H-z)\Psi. \tag{4.2}$$

Dividing by t we obtain for $\Psi \in \mathscr{D}(x^2) \cap \mathscr{D}(H_0) \cap \mathscr{H}^{\mathrm{cont}}$

$$t^{-1}D(t)\Psi = 2HP^{\mathrm{cont}}\Psi + t^{-1}D\Psi + \frac{1}{t}\int_0^t ds\, C(s)P^{\mathrm{cont}}(H-z)\Psi. \tag{4.3}$$

The first term is the desired limit, the second obviously tends to zero, and the same is true for the last term since

$$\left\| \frac{1}{t}\int_0^t ds\, C(s)P^{\mathrm{cont}} \right\| \to 0 \text{ as } |t| \to \infty \tag{4.4}$$

for any time evolution and any compact operator C (see e.g. Lemma 4.2 in [8]). This is a simple consequence of Wiener's theorem, cf. Appendix to Section XI.17 in [22].

If $\mathscr{D}(x^2) \cap \mathscr{D}(H) \cap \mathscr{H}^{\mathrm{cont}}$ is a core of the limiting operator $H \upharpoonright \mathscr{H}^{\mathrm{cont}}$ (this will typically be the case, otherwise a little extra argument is needed), then we have shown that $t^{-1}D(t)$ converges in strong resolvent sense to HP^{cont} on $\mathscr{H}^{\mathrm{cont}}$. It remains to show convergence to zero on the point spectral subspace. This follows easily from the fact that for any bounded continuous function f and any eigenvector $H\Phi = E\Phi$

$$f[D(t)/t]\Phi = \exp[i(H-E)t] f(D/t)\Phi \to f(0)\Phi. \tag{4.5}$$

If $\Psi \in \mathscr{D}(D) \cap \mathscr{H}^{pp}$ one can give an alternative proof of this result using (4.2) and the special form of the virial theorem (3.37) together with (4.9). A generalization of this latter approach is used below.

This finishes the proof of (2.17) under the condition (3.31). If the weaker assumption (2.14) is used almost the same proof applies. We turn now to the general case.

Let $\Psi \in (H-z)^{-1}[\mathscr{Q}(H) \cap \mathscr{Q}(x^2)] \subset [\mathscr{Q}(H) \cap \mathscr{Q}(x^2)]$, then $(\Psi, D(t)\Psi)$ is well defined for all t by Corollary 3.2 and continuously differentiable:

$$\frac{d}{dt}(\Psi, D(t)\Psi) = ((H-z)\Psi, (H-z)^{-1} e^{iHt} i[H, D] e^{-iHt} (H-z)^{-1}(H-z)\Psi)$$

$$= ((H-z)\Psi, e^{iHt} i[D, (H-z)^{-1}] e^{-iHt}(H-z)\Psi)$$

$$= (\Psi, 2H\Psi) + ((H-z)\Psi, K(t)(H-z)\Psi). \tag{4.6}$$

We have used Proposition 3.4 in the last step. Note that also $(H-z)^{-1}D(t)\Psi$ is well defined and it is strongly differentiable by (4.6):

$$\frac{d}{dt}(H-z)^{-1}D(t)\Psi = (H-z)^{-1}2H\Psi + K(H-z)\Psi.$$

Integration from zero to t yields

$$(H-z)^{-1}D(t)\Psi = (H-z)^{-1}D\Psi + t(H-z)^{-1}2H\Psi$$

$$+ \int_0^t d\tau\, K(\tau)(H-z)\Psi. \tag{4.7}$$

We divide by t and obtain

$$(H-z)^{-1}\frac{D(t)}{t}\Psi=(H-z)^{-1}2H\Psi+\frac{1}{t}\int_0^t d\tau\, K(\tau)(H-z)\Psi+t^{-1}(H-z)^{-1}D\Psi. \tag{4.8}$$

Obviously $t^{-1}(H-z)^{-1}D\Psi$ tends to zero as $|t|\to\infty$. For the remaining terms on the right hand side of (4.8), we split Ψ into its components in the continuous spectral subspace and in the orthogonal complement spanned by the eigenvectors of the Hamiltonian:

$$\Psi=P^{\mathrm{cont}}\Psi+P^{pp}\Psi.$$

Then $(H-z)^{-1}2HP^{\mathrm{cont}}\Psi$ is the desired limit and the second summand vanishes asymptotically by (4.4) since K is compact.

On the point-spectral subspace the first two summands on the right hand side of (4.8) cancel asymptotically by (3.36) and by

$$s\text{-}\lim_{|t|\to\infty}\frac{1}{t}\int_0^t ds\exp[i(H-E)s]=P_E. \tag{4.9}$$

Thus we have shown

$$\lim_{|t|\to\infty}\left\|(H-z)^{-1}\left\{\frac{D(t)}{t}-2HP^{\mathrm{cont}}\right\}\Psi\right\|=0$$

for any $\Psi\in(H-z)^{-1}[\mathscr{D}(H)\cap\mathscr{D}(x^2)]$. This implies

$$\lim_{|t|\to\infty}\left\|F(H<E)\left\{\frac{D(t)}{t}-2HP^{\mathrm{cont}}\right\}\Psi\right\|=0, \tag{4.10}$$

for any $E<\infty$. To eliminate the energy restriction on the left, note that

$$\lim_{E\to\infty}\|F(H>E)2HP^{\mathrm{cont}}\Psi\|=0. \tag{4.11}$$

We will show next that the same applies to the first summand. As used by Davies [6] this is equivalent to finding an increasing function g with $1\leqq g(\omega)\leqq(1+\omega)^{1/2}$ and $g(\omega)\to\infty$ as $\omega\to\infty$ such that

$$\left\|g(H)\frac{D(t)}{t}\Psi\right\| \tag{4.12}$$

is bounded uniformly in t. The formal calculation

$$\begin{aligned}\frac{1}{t}\|g(H)De^{-iHt}\Psi\| &\leqq\frac{1}{t}\|g(H)[D,(H-z)^{-1}]e^{-iHt}(H-z)\Psi\|\\ &\quad+\frac{1}{t}\|g(H)(H-z)^{-1}De^{-iHt}(H-z)\Psi\|\end{aligned} \tag{4.13}$$

is justified for $\Psi\in(H-z)^{-1}[\mathscr{D}(H)\cap\mathscr{D}(x^2)]$, and if g is chosen such that $g(H)[D,(H-z)^{-1}]$ is bounded. The uniform boundedness of the second term in (4.13) follows from the boundedness of

$$g(H)(H-z)^{-1/2}\cdot(H-z)^{-1/2}|p| \tag{4.14}$$

and from Proposition 3.1 which states that

$$t^{-1}\||x|e^{-iHt}(H-z)\Psi\| \leqq \text{const.} \tag{4.15}$$

With Proposition 3.4

$$ig(H)[D,(H-z)^{-1}] = g(H)2H(H-z)^{-2} + g(H)K. \tag{4.16}$$

The first summand is bounded. For any compact operator K and any self-adjoint H there is an increasing function g such that $g(H)K$ is bounded. Using such a function g we have shown

$$\lim_{E\to\infty}\sup_{t\in\mathbb{R}}\left\|F(H>E)\left\{\frac{D(t)}{t}-2HP^{\text{cont}}\right\}\Psi\right\|=0,$$

and consequently

$$\lim_{|t|\to\infty}\left\|\left(\frac{D(t)}{t}-2HP^{\text{cont}}\right)\Psi\right\|=0 \tag{4.17}$$

for any $\Psi\in(H-z)^{-1}[\mathcal{Q}(H)\cap\mathcal{Q}(x^2)]$. In particular we have shown that this set is an invariant domain contained in $\mathcal{D}(D)$. Moreover it is a core for the limiting operator HP^{cont}. This implies [15, 20] the strong resolvent convergence (2.17).

Next we will prove (2.16). The proof for the general case is given below. To show the main idea we first give the very simple proof under the special assumption (2.14). Then the following commutator is naturally defined as a quadratic form on $\mathcal{D}(x^2)\cap\mathcal{D}(H_0)\times\mathcal{D}(x^2)\cap\mathcal{D}(H_0)$:

$$i\left[H,\frac{m}{2}x^2\right]=i\left[H_0,\frac{m}{2}x^2\right]=D. \tag{4.18}$$

It obviously determines uniquely a self-adjoint operator which has $\mathcal{D}(x^2)\cap\mathcal{D}(H_0)$ as a time-invariant core (see Lemma 3.3). This justifies for any $\Psi\in\mathcal{D}(x^2)\cap\mathcal{D}(H_0)$ to write

$$t^{-2}\frac{m}{2}x^2(t)\Psi = t^{-2}\frac{m}{2}x^2(0)\Psi + t^{-2}\int_0^t dt' D(t')\Psi. \tag{4.19}$$

The first summand tends to zero as $|t|\to\infty$. For the second we use the convergence (4.17) of $D(t')$.

$$\begin{aligned} t^{-2}\int_0^t dt'D(t')\Psi &= HP^{\text{cont}}\Psi + t^{-1}\int_0^t dt'\frac{t'}{t}\left(\frac{D(t')}{t'}-2HP^{\text{cont}}\right)\Psi \\ &\to HP^{\text{cont}}\Psi \text{ as } |t|\to\infty. \end{aligned} \tag{4.20}$$

Since $\mathcal{D}(x^2)\cap\mathcal{D}(H_0)$ is a core for HP^{cont}, the strong resolvent convergence (2.16) follows.

In the general case it is difficult to determine a time invariant domain which is included in $\mathcal{D}(x^2)$. We avoid this problem using quadratic forms. Let $\Psi\in(H-z)^{-1}[\mathcal{Q}(x^2)\cap\mathcal{Q}(H)]$. Then $(\Psi,x^2(t)\Psi)$ is continuously differentiable and

$$\left(\Psi,\frac{m}{2}x^2(t)\Psi\right)=\left(\Psi,\frac{m}{2}x^2\Psi\right)+\int_0^t d\tau\left(\Psi,i\left[H,\frac{m}{2}x^2(\tau)\right]\Psi\right). \tag{4.21}$$

Moreover each of these terms can be approximated arbitrarily well by the expressions where x^2 is replaced by $x^2(1+\lambda x^2)^{-1}$ as $\lambda \to 0$. Since multiplication by $x^2(1+\lambda x^2)^{-1}$ maps $\mathscr{D}(H_0)$ into itself, we then can write the Hamiltonian in the commutator term in (4.21) as a sum:

$$\left(\Psi, e^{iH\tau} i\left[H, \frac{m}{2} x^2(1+\lambda x^2)^{-1}\right] e^{-iH\tau}\Psi\right)$$
$$= \left(\Psi, e^{iH\tau} i\left[H_0, \frac{m}{2} x^2(1+\lambda x^2)^{-1}\right] e^{-iH\tau}\Psi\right)$$
$$- i((H-z)\Psi, e^{iH\tau}(H-z)^{-1}\{x^2(1+\lambda x^2)^{-1} V_s$$
$$- V_s x^2(1+\lambda x^2)^{-1}\}(H-z)^{-1} e^{-iH\tau}(H-z)\Psi). \tag{4.22}$$

V_l commutes with functions of x and does not contribute. The second summand in (4.22) vanishes if the potential V_s is local, and it is uniformly bounded if $\lambda \to 0$ for non-local potentials by assumption (2.12). For the given expectation value in the first term of (4.22)

$$i\left[H_0, \frac{m}{2} x^2(1+\lambda x^2)^{-1}\right] = \tfrac{1}{2}\{\mathbf{p}\cdot\mathbf{x}(1+\lambda x^2)^{-2} + \mathbf{x}(1+\lambda x^2)^{-2}\cdot\mathbf{p}\} \to D \quad \text{as} \quad \lambda \to 0. \tag{4.23}$$

Dividing (4.21) by t^2 we thus obtain

$$\left(\Psi, \frac{m}{2}\frac{x^2(t)}{t^2}\Psi\right) \to t^{-2}\int_0^t d\tau\,(\Psi, D(\tau)\Psi). \tag{4.24}$$

Now we can use the limiting behavior of $D(\tau)$.

$$t^{-2}\int_0^t d\tau(\Psi, D(\tau)\Psi)$$
$$= (\Psi, HP^{\text{cont}}\Psi) + t^{-1}\int_0^t d\tau \frac{\tau}{t}\left(\Psi, \left\{\frac{D(\tau)}{\tau} - 2HP^{\text{cont}}\right\}\Psi\right). \tag{4.25}$$

The latter term converges to zero for the given set of vectors Ψ by (4.17). Thus we have shown for any $\Psi \in (H-z)^{-1}[\mathscr{D}(H) \cap \mathscr{D}(x^2)]$,

$$\left(\Psi, \frac{m}{2}\frac{x^2(t)}{t^2}\Psi\right) \to (\Psi, HP^{\text{cont}}\Psi) \quad \text{as} \quad |t| \to \infty. \tag{4.26}$$

Below we will give the proof of Theorem 2.4 using only the results shown so far. We use the statement (2.28) to finish the proof of (2.16). Let $\phi \in C_0^\infty(0,\infty)$, and split the vector $\Psi = \Psi^P + \Psi^{\text{cont}}$ into its spectral components. For any eigenvector $H\Psi_E = E\Psi_E$,

$$\left\|\phi\left(\frac{m}{2}\frac{x^2(t)}{t^2}\right)\Psi_E\right\| = \left\|\phi\left(\frac{m}{2}\frac{x^2}{t^2}\right)\Psi_E\right\| \to \|\phi(0)\Psi_E\| = 0,$$

thus

$$\lim_{|t|\to\infty} \phi\left(\frac{m}{2}\frac{x^2(t)}{t^2}\right)\Psi = \lim_{|t|\to\infty} \phi\left(\frac{m}{2}\frac{x^2(t)}{t^2}\right)\Psi^{\text{cont}}. \tag{4.27}$$

If ϕ is considered as a function on $\mathbb{R}^\nu$ it satisfies the assumptions of Theorem 2.4 and the right hand side of (4.27) equals, by (2.28),

$$\lim_{|t|\to\infty} \phi(H_0(t))\Psi^{\mathrm{cont}} = \phi(H)\Psi^{\mathrm{cont}}. \tag{4.28}$$

The last equality follows from Corollary 2.3b). With $\phi(H)\Psi^{\mathrm{cont}} = \phi(HP^{\mathrm{cont}})\Psi^{\mathrm{cont}} = \phi(HP^{\mathrm{cont}})\Psi$, we have shown for any $\phi \in C_0^\infty(0,\infty)$,

$$\lim_{|t|\to\infty} \phi\left(\frac{m}{2}\frac{x^2(t)}{t^2}\right)\Psi = \phi(HP^{\mathrm{cont}})\Psi,$$

This implies the strong resolvent convergence (2.16). □

Remark 4.1. In the paragraph following (1.6) we pointed out that the interacting time evolution can be controlled since the observables considered here do not "see" the main effects of the interaction. This becomes apparent in the proof, too. In the time evolution of $D(t)/t$, the interactions enter only through the time average of a compact operator C or K which vanishes on the continuous spectral subspace (4.4). The subtle parts in the remainder of the proof are mainly domain questions which are necessary but not essential.

Proof of Theorem 2.4. Note that Eq. (2.17) of Theorem 2.1 and its proof were used alone to show (2.20)–(2.21) and all of Corollary 2.3. We will show Theorem 2.4 using this and Eq. (4.26). In (2.28) we use the Fourier representation for the functions of the operators $\mathbf{x}$ and $\mathbf{p}$, respectively,

$$\begin{aligned} &f\left(m\frac{\mathbf{x}}{t}\right) - f(\mathbf{p}) \\ &= \frac{1}{(2\pi)^{\nu/2}} \int d^\nu q \hat{f}(\mathbf{q})\left\{\exp\left(i\mathbf{q}\cdot m\frac{\mathbf{x}}{t}\right) - \exp(i\mathbf{q}\cdot\mathbf{p})\right\} \\ &= \frac{1}{(2\pi)^{\nu/2}} \int d^\nu q \hat{f}(\mathbf{q}) \exp(i\mathbf{q}\cdot\mathbf{p})\left\{\exp\left[i\mathbf{q}\left(m\frac{\mathbf{x}}{t} - \mathbf{p}\right) - \frac{i}{2}q^2\frac{m}{t}\right] - \mathbb{1}\right\}. \end{aligned} \tag{4.29}$$

We have used the Baker–Campbell–Hausdorff formula in the last step. By the dominated convergence theorem it is sufficient for (2.28) to show that

$$\left\|\left\{\exp\left[i\mathbf{q}\left(m\frac{\mathbf{x}}{t} - \mathbf{p}\right) - \mathbb{1}\right\}e^{-iHt}\Psi\right\| \to 0 \tag{4.30}$$

for (a dense set of) $\Psi \in \mathscr{H}^{\mathrm{cont}}$ and pointwise in $\mathbf{q} \in \mathbb{R}^\nu$. If every eigenvector of H lies in $\mathscr{D}(x^2)$, then $\mathscr{D}(H) \cap \mathscr{D}(x^2) \cap \mathscr{H}^{\mathrm{cont}}$ is dense in $\mathscr{H}^{\mathrm{cont}}$ and one can verify (4.30) for Ψ's in the dense set $(H-z)^{-1}[\mathscr{D}(H) \cap \mathscr{D}(x^2) \cap \mathscr{H}^{\mathrm{cont}}]$. In general we can approximate any $\Psi = (H-z)^{-1}\Phi \in \mathscr{H}^{\mathrm{cont}}$ by $\Psi_\varepsilon = (H-z)^{-1}\Phi_\varepsilon$ such that $\|\Phi - \Phi_\varepsilon\| < \varepsilon/2$ and $\Phi_\varepsilon \in [\mathscr{D}(H) \cap \mathscr{D}(x^2)]$. Then for small enough z

$$\sup_t \|(H - HP^{\mathrm{cont}})e^{-iHt}\Psi_\varepsilon\| < \varepsilon. \tag{4.31}$$

We will show that

$$\lim_{|t|\to\infty} \sup \left\| \left\{ \exp\left[i\mathbf{q}\left(m\frac{\mathbf{x}}{t} - \mathbf{p} \right) \right] - \mathbb{1} \right\} e^{-iHt} \Psi_\varepsilon \right\|^2 < \text{const } \varepsilon \tag{4.32}$$

for any $\varepsilon > 0$ which implies (4.30).
Then

$$\left\| \left\{ \exp\left[i\mathbf{q}\left(m\frac{\mathbf{x}}{t} - p \right) \right] - \mathbb{1} \right\} e^{-iHt} \Psi_\varepsilon \right\|^2$$

$$= \left\| \int_0^1 ds \exp\left[is\mathbf{q}\left(m\frac{\mathbf{x}}{t} - \mathbf{p} \right) \right] \mathbf{q} \cdot \left(m\frac{\mathbf{x}}{t} - \mathbf{p} \right) e^{-iHt} \Psi_\varepsilon \right\|^2$$

$$\leqq |\mathbf{q}|^2 \left\| \left(m\frac{\mathbf{x}}{t} - \mathbf{p} \right) e^{-iHt} \Psi_\varepsilon \right\|^2$$

$$= 2m|q|^2 \left(\Psi_\varepsilon, \left\{ \frac{m}{2} \frac{x^2(t)}{t^2} - \frac{D(t)}{t} + H_0(t) \right\} \Psi_\varepsilon \right). \tag{4.33}$$

The first two summands in the expectation value converge as $|t| \to \infty$ to $(\Psi_\varepsilon, HP^{\text{cont}}\Psi_\varepsilon)$ and $-2(\Psi_\varepsilon, HP^{\text{cont}}\Psi_\varepsilon)$, respectively, by (4.26) and (4.17). Using (4.31) it remains to estimate

$$\lim_{|t|\to\infty} \sup |(\Psi_\varepsilon, [H - H_0(t)]\Psi_\varepsilon)|$$
$$= \lim \sup |(\Phi_\varepsilon, e^{iHt}(H-z)^{-1}(H-H_0)(H-z)^{-1} e^{-iHt}\Phi_\varepsilon)|$$
$$\leqq \text{const} \|\Phi - \Phi_\varepsilon\| + \lim_{|t|\to\infty} \sup \|(H-z)^{-1}(H-H_0)(H-z)^{-1} e^{-iHt}\Phi\| \leqq \varepsilon/2.$$

The last summand vanishes asymptotically by Corollary 2.3a), since $(H-z)^{-1}(H-H_0)(H-z)^{-1}$ is compact and $\Phi \in \mathscr{H}^{\text{cont}}$.

V. Application to Scattering Theory with Coulomb Interaction

Although we do not prove new results here, we want to illustrate how the asymptotic observables can be used as a covenient tool in two-body scattering theory.

A useful dense set of vectors in $\mathscr{H}^{\text{cont}}$ consists of those with strictly positive and finite energies, i.e. for any Ψ, there are $0 < a < b < \infty$ such that

$$\Psi = F(a < H < b)\Psi \in \mathscr{H}^{\text{cont}} \tag{5.1}$$

By Corollary 2.3b),

$$\lim_{|t|\to\infty} \left\| \left[\mathbb{1} - F\left(a < \frac{p^2}{2m} < b \right) \right] e^{-iHt} \Psi \right\| = 0. \tag{5.2}$$

On the spherical shell in momentum space we can find a *finite* decomposition of the identity such that

$$g_i \in C_0^\infty(\mathbb{R}^\nu); 0 \leqq g_i(p) \leqq 1; \tag{5.3}$$

$$\sum_i [g_i(p)]^3 = 1 \text{ if } a \leqq p^2/2m \leqq b; \tag{5.4}$$

there are $\mathbf{v}_i$ such that with $v_i = |\mathbf{v}_i|$,

$$\operatorname{supp} g_i \subset \{\mathbf{p} |\ |\mathbf{p} - m\mathbf{v}_i| < \tfrac{1}{2} v_i\}. \tag{5.5}$$

The precise support condition is not essential. We have chosen it such that $0 \notin \operatorname{supp} g_i$ and that any two vectors in the support of a given g_i include an acute angle. With (5.2) we obtain

$$\lim_{|\tau| \to \infty} \| [\mathbb{1} - \Sigma g_i^3(\mathbf{p})] e^{-iH\tau} \Psi \| = 0. \tag{5.6}$$

Theorem 2.4 implies

$$\lim_{|\tau| \to \infty} \left\| g_i^2(\mathbf{p}) \left[g_i(\mathbf{p}) - g_i\left(m \frac{\mathbf{x}}{\tau} \right) \right] e^{-iH\tau} \Psi \right\| = 0. \tag{5.7}$$

With the canonical commutation relations it is easy to verify that

$$\lim_{|\tau| \to \infty} \left\| \left[g_i(\mathbf{p}), g_i\left(m \frac{\mathbf{x}}{\tau} \right) \right] \right\| = 0. \tag{5.8}$$

Consequently we obtain

$$\lim_{|\tau| \to \infty} \left\| \left[\mathbb{1} - \sum_i g_i(\mathbf{p}) g_i\left(m \frac{\mathbf{x}}{\tau} \right) g_i(\mathbf{p}) \right] e^{-iH\tau} \Psi \right\| = 0. \tag{5.9}$$

Thus for long times a scattering state can be approximated by a sum of terms in the ranges of the finitely many operators

$$P_i = g_i(\mathbf{p}) g_i\left(m \frac{\mathbf{x}}{\tau} \right) g_i(\mathbf{p}), \tag{5.10}$$

with

$$P_i \geqq 0, \quad \| P_i \| \leqq 1.$$

A state in the range of P_i has strictly positive kinetic energy, it is essentially localized far from the origin: $|x| > \frac{1}{2} v_i |\tau|$ up to rapidly decaying tails with decay uniform in τ. For large positive τ it is outgoing and for negative times incoming, the phase space localization is much sharper than those usually applied in geometric time-dependent scattering theory. (see Sect. V of [8] and references therein for various related characterizations.)

On the range of a P_i it is easy to control the localization of the state if it propagates with the free or a modified free time evolution. We will give here a geometric time-dependent proof of asymptotic completeness for short-range and Coulomb forces which is particularly simple. There are geometric time-dependent proofs which cover a wider class of long-range forces [5] and there are many more using time-independent methods. The point of our proof is the following. The information about a scattering state at a late time τ obtained from our asymptotic observables alone is sufficient to show that the further true time evolution is well approximated by Dollard's modified free time evolution. Therefore we neither need an "intermediate" time evolution nor detailed information about the interacting time evolution. For applications to three body scattering this turns out to be useful [11] because it is tedious to control intermediate time evolutions, and detailed information about the interacting time evolution of multiparticle systems is hard to obtain.

Let the long-range potential be

$$V_l(\mathbf{x}) = q(1 + x^2)^{-1/2}, \tag{5.11}$$

which differs from the Coulomb potential of a pointlike charge by a correction of short range. For a weaker condition see Remark 5.2 below. In the proof we will use for the short range part the convenient sufficient condition that it is a local, Kato-bounded potential with decay

$$\| V_s g(H_0) F(|x| > R) \| \in L^1(\mathbb{R}_+, dR) \tag{5.12}$$

for any $g \in C_0^\infty(\mathbb{R})$. This is sufficient for almost all applications of interest in physics. Under these assumptions the proofs in Sects. III and IV are rather simple. It is a standard exercise [8] to include a wider class of short-range potentials such that e.g. the assumptions of Theorem 2.1 are satisfied and the decay assumption is

$$\| g(H) V_s g(H_0) F(|x| > R) \| \in L^1(\mathbb{R}_+, dR). \tag{5.13}$$

In our case the modified free time evolution is as given by Dollard [7]

$$U(t+\tau, \tau) = e^{-iH_0 t} U'(t+\tau, \tau), \tag{5.14}$$

$$U'(t+\tau, \tau) = \exp\left\{ -i \int_\tau^{\tau+t} ds\, V_l\left(\frac{\mathbf{p}}{m} s\right)\right\}. \tag{5.15}$$

Theorem 5.1. *Let $H = H_0 + V_s + V_l$ satisfy (5.11), (5.12) (or as discussed above), then asymptotic completeness holds,* i.e. *for any $\Psi \in \mathscr{H}^{\text{cont}}$*

$$\lim_{\tau \to \infty} \sup_{t \geqq 0} \| [e^{-iHt} - U(t+\tau, \tau)] e^{-iH\tau} \Psi \| = 0. \tag{5.16}$$

Proof. An approximation of V_l is

$$V_R(x) := \begin{cases} q(1+R^2)^{-1/2}\left[1 + \frac{1}{2}\dfrac{R^2 - x^2}{1+R^2}\right] & \text{for } 0 \leqq |x| \leqq R, \\ V_l(x) \text{ for } R \leqq |x| < \infty, \end{cases} \tag{5.17}$$

then

$$[V_l(\mathbf{x}) - V_R(\mathbf{x})] F(|x| > R) \equiv 0, \tag{5.18}$$

$$\| \nabla V_R \| \leqq \frac{\text{const}}{1+R^2}, \quad \| \Delta V_R \| \leqq \frac{\text{const}}{R^\alpha}, \quad \alpha > 2. \tag{5.19}$$

It is sufficient to verify (5.16) for the dense subset of $\mathscr{H}^{\text{cont}}$ which satisfies (5.1). With

(5.9) we thus have to show

$$\lim_{\tau\to\infty}\sup_{t\geqq 0}\left\| [e^{-iHt} - U(t+\tau,\tau)]g_i(\mathbf{p})g_i\left(m\frac{\mathbf{x}}{\tau}\right)g_i(\mathbf{p}) \quad e^{-iH\tau}\Psi\right\| = 0 \tag{5.20}$$

for each of the finitely many terms labelled by i. With $v_0 = \min_i \frac{1}{2}v_i$ we have $g_i(\mathbf{p}) = 0$ if $|p| \leqq mv_0$ for all i. It is an easy consequence of Theorem 2.4 and

$$\left\|\left[\frac{\mathbf{x}}{\tau}, g_i(\mathbf{p})\right]\right\| \to 0, \tag{5.21}$$

that also

$$\left\|\left(m\frac{\mathbf{x}}{\tau} - \mathbf{p}\right)g_i(\mathbf{p})g_i\left(m\frac{\mathbf{x}}{\tau}\right)g_i(\mathbf{p})e^{-iH\tau}\Psi\right\| = : f(\tau) \to 0. \tag{5.22}$$

With

$$\begin{aligned} &[\mathbf{p}, U'(t+\tau,\tau)] = 0, \\ &\left[m\frac{\mathbf{x}}{\tau}, U'(t+\tau,\tau)\right] = \frac{m}{\tau}U'(t+\tau,\tau)\cdot \int_\tau^{t+\tau} ds \frac{s}{m}(\nabla V_l)\left(\frac{\mathbf{p}}{m}s\right), \end{aligned} \tag{5.23}$$

we obtain on the range of $g_i(\mathbf{p})$

$$\left\|\left[\left(m\frac{\mathbf{x}}{\tau} - \mathbf{p}\right), U'(t+\tau,\tau)\right]g_i(\mathbf{p})\right\| \leqq \frac{m}{\tau}\int_\tau^{t+\tau} ds \frac{s\ \mathrm{const}}{m\,(v_0 s)^2} \leqq \mathrm{const}\frac{\ln\left(1+\frac{t}{\tau}\right)}{\tau}. \tag{5.24}$$

This implies

$$\left\|\left(m\frac{\mathbf{x}}{\tau} - \mathbf{p}\right)U'(t+\tau,\tau)g_i(\mathbf{p})g_i\left(m\frac{\mathbf{x}}{\tau}\right)g_i(\mathbf{p})e^{-iH\tau}\Psi\right\| \leqq f(\tau) + \mathrm{const}\frac{\ln(1+t/\tau)}{\tau}. \tag{5.25}$$

Now we are ready to apply the Cook estimate to (5.20)

$$\sup_{t\geqq 0}\| [e^{-iHt} - U(t+\tau,\tau)]g_i(\mathbf{p})g_i\left(m\frac{\mathbf{x}}{\tau}\right)g_i(\mathbf{p})e^{-iH\tau}\Psi \|$$

$$\leqq \int_0^\infty dt \left\|\left\{V_s + V_l(\mathbf{x}) - V_l\left(\frac{\mathbf{p}}{m}(t+\tau)\right)\right\}U(t+\tau,\tau)g_i(\mathbf{p})g_i\left(m\frac{\mathbf{x}}{\tau}\right)\ldots\right\|$$

$$\leqq \int_0^\infty dt\{\| V_s g(H_0)\| + \| V_l \|\} \tag{5.26a}$$

$$\cdot\left\|F(|x| < v_0(t+\tau))U(t+\tau,\tau)g_i(\mathbf{p})g_i\left(m\frac{\mathbf{x}}{\tau}\right)\right\|$$

$$+\int_0^\infty dt \| V_s g(H_0)F(|x| > v_0(t+\tau))\| + \tag{5.26b}$$

$$+\int_0^\infty dt\left\|\left[V_R(\mathbf{x})-V_R\left(\frac{\mathbf{p}}{m}(t+\tau)\right)\right]e^{-iH_0t}U'(t+\tau,\tau)g_i(\mathbf{p})\dots\right\|. \tag{5.26c}$$

Here we have regularized V_s by inserting some $g\in C_0^\infty(\mathbb{R})$ which satisfies $g(H_0)g_i(\mathbf{p})=g_i(\mathbf{p})$ for all i. The parameter R is chosen such that

$$R=v_0(t+\tau), \tag{5.27}$$

then by (5.18) $[V_l(\mathbf{x})-V_R(\mathbf{x})]$ has support in $|x|<v_0(t+\tau)$ and $V_l((t+\tau)\mathbf{p}/m)=V_R((t+\tau)\mathbf{p}/m)$ on the range of all $g_i(\mathbf{p})$. The integral (5.26b) vanishes as $\tau\to\infty$ by (5.12). The same is true for (5.26a) since

$$\left\|F(|x|<v_0(t+\tau))U(t+\tau,\tau)g_i(\mathbf{p})g_i\left(m\frac{\mathbf{x}}{\tau}\right)\right\|\leqq C_n(1+t+\tau)^{-n} \tag{5.28}$$

for any $n\in\mathbb{N}$. This is a simple extension of well known propagation properties under the free time evolution for states well localized in phase space. It is given explicitly as Corollary 2.12 in [10]. It remains to estimate (5.26c). Since by the functional calculus

$$e^{iH_0t}V_R(\mathbf{x})e^{-iH_0t}=V_R\left(\mathbf{x}+\frac{\mathbf{p}}{m}t\right), \tag{5.29}$$

we have to treat

$$\left\|\left[V_R\left(\mathbf{x}+\frac{\mathbf{p}}{m}t\right)-V_R\left(\frac{\mathbf{p}}{m}(t+\tau)\right)\right]U'(t+\tau,\tau)g_i(\mathbf{p})\dots\right\|. \tag{5.30}$$

An elementary calculation with the canonical commutation relations and the Baker Campbell Hausdorff formula gives for suitable functions h

$$\begin{aligned}\frac{d}{ds}h\left[s\left(\mathbf{x}-\frac{\mathbf{p}}{m}\tau\right)+\frac{\mathbf{p}}{m}(t+\tau)\right]&=(\nabla h)\left[s\left(\mathbf{x}-\frac{\mathbf{p}}{m}\tau\right)+\frac{\mathbf{p}}{m}(t+\tau)\right]\cdot\left(\mathbf{x}-\frac{\mathbf{p}}{m}\tau\right)\\&\quad+i\frac{t+\tau}{m}(\Delta h)\left[s\left(\mathbf{x}-\frac{\mathbf{p}}{m}\tau\right)+\frac{\mathbf{p}}{m}(t+\tau)\right].\end{aligned} \tag{5.31}$$

This implies with (5.19)

$$\left\|\left[V_R\left(\mathbf{x}+\frac{\mathbf{p}}{m}t\right)-V_R\left(\frac{\mathbf{p}}{m}(t+\tau)\right)\right]\Phi\right\|\leqq\frac{c_1}{R^2}\frac{\tau}{m}\left\|\left(m\frac{\mathbf{x}}{\tau}-\mathbf{p}\right)\Phi\right\|+c_2\frac{t+\tau}{R^\alpha}\|\Phi\|. \tag{5.32}$$

With (5.25) and the choice (5.27) we obtain for (5.30)

$$\begin{aligned}&\left\|\left[V_R\left(\mathbf{x}+\frac{\mathbf{p}}{m}t\right)-V_R\left(\frac{\mathbf{p}}{m}(t+\tau)\right)\right]U'(t+\tau,\tau)\cdot g_i(\mathbf{p})g_i\left(m\frac{\mathbf{x}}{\tau}\right)g_i(\mathbf{p})e^{-iH\tau}\Psi\right\|\\&\leqq\text{const}\{(t+\tau)^{-2}[\tau f(\tau)+\ln(1+t/\tau)]+(t+\tau)^{1-\alpha}\}.\end{aligned} \tag{5.33}$$

The t-integral over the positive half line exists and vanishes as $\tau\to\infty$. This completes the proof of (5.20) and Theorem 5.1. □

Remark 5.2. The new ingredient of our proof is the combination of the general estimate (5.32) with the bound (5.25). The latter is a direct consequence of our results on asymptotic observables. This is the only place where we have to treat the interacting time evolution. A closely related approach was given independently by Muthuramalingam [18] to show the same results. As assumptions on the long-range force we have used only (5.19) and integrable decay in (5.18). Thus the class of V_l is slightly larger than the typical example (5.11). This shows that the special features of the Coulomb potential, its rotational symmetry and its scaling property, have not been used.

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