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Time-Dependent Scattering Theory for Singular Potentials

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Abstract. Scattering states are constructed for nonrelativistic multiparticle systems with singular potentials. The case of hard-core potentials provides a simple example of a system whose Hilbertspace is not simply defined by the kinematical structure, but also by the interactions. This leads to a modification of the usual scattering formalism and of the notion of asymptotic observables: quantities like the momenta of single particles are not observables of the system, but still defined as asymptotic observables.

1. Introduction

Recently, J. Kupsch and W. Sandhas [1] have proved the existence of scattering states for two-particle systems with potentials which may have strong singularities on a compact set of measure zero, so that the Hilbertspace of the interacting system is still the same as for the free particles. Regardless of the sign of the singularities, the Hamiltonian can then always be taken as a (generally not unique) selfadjoint extension of a real, symmetric operator, and the asymptotic condition is proved for any such extension. This generalizes easily to a multiparticle system for the channel in which all particles are asymptotically free. For channels containing bound states, however, we need not only the selfadjointness of H, but also that the momentum operators of single particles are defined on $D(H)$ and can be estimated in terms of H. Therefore, we shall assume that the (strong) singularities of the potentials are repulsive and then construct the Hamiltonian by the method of Friedrichs-extension.

If the potentials are singular on a set of non-zero measure, as in the example of hard spheres, then the situation is complicated by the fact that the Hilbertspace of the system is not simply defined by the kinematical structure, but also by the interactions. Therefore, if we decompose the system by dropping all interactions between certain subsystems, the Hamiltonian *and* the Hilbertspace are altered. This requires a modification of the usual scattering formalism, which will be discussed first.

2. A Suitably Generalized Scattering Formalism

Let H be the Hamiltonian of the system, acting on a Hilbertspace $\mathcal{H}$. A channel, α, of the system is a triple

$$\alpha = (\mathcal{H}_\alpha, H_\alpha, P_\alpha),$$

where $\mathcal{H}_\alpha$ is a Hilbertspace (space of channel states), H_α a selfadjoint operator on $\mathcal{H}_\alpha$

(channel Hamiltonian) and P_α a bounded operator from $\mathcal{H}_\alpha$ to $\mathcal{H}$ with the property

$$\lim_{|t|\to\infty} \| P_\alpha \, e^{-iH_\alpha t} \, \psi_\alpha \| = \| \psi_\alpha \| \tag{1}$$

for all $\psi_\alpha \in \mathcal{H}_\alpha$, and such that

$$\lim_{t\to\pm\infty} e^{-iHt} \, P_\alpha \, e^{-iH_\alpha t} \, \psi_\alpha = \Omega_\alpha^\pm \, \psi_\alpha \tag{2}$$

exists for any $\psi_\alpha \in \mathcal{H}_\alpha$. By virtue of (1), the wave-operators $\Omega_\alpha^\pm$ are isometric from $\mathcal{H}_\alpha$ into $\mathcal{H}$ and satisfy

$$e^{-iHt} \, \Omega_\alpha^\pm = \Omega_\alpha^\pm \, e^{-iH_\alpha t}. \tag{3}$$

Therefore, the ranges $R_\alpha^\pm$ of $\Omega_\alpha^\pm$ reduce H and the parts of H in $R_\alpha^\pm$ are unitarily equivalent to H_α. Note also that two operators P_α and P_α are equivalent if for all $\psi_\alpha \in \mathcal{H}_\alpha$

$$\lim_{|t|\to\infty} \| (P_\alpha - P_\alpha') \, e^{-iH_\alpha t} \, \psi_\alpha \| = 0 \,, \tag{4}$$

in the sense that they give rise to the same wave-operators.

For a multichannel system we require a set of mutually orthogonal channels, i.e.

$$R_\alpha^\pm \perp R_\beta^\pm \quad (\alpha \neq \beta) \tag{5}$$

or, equivalently,

$$\lim_{|t|\to\infty} (P_\alpha \, e^{-iH_\alpha t} \, \psi_\alpha, P_\beta \, e^{-iH_\beta t} \, \psi_\beta) = 0 \tag{6}$$

for all $\psi_\alpha \in \mathcal{H}_\alpha$, $\psi_\beta \in \mathcal{H}_\beta$. If the set of channels is denumerable, the S-operators can be constructed as usual: Let

$$\mathcal{H}' = \bigoplus_\alpha \mathcal{H}_\alpha \,,$$

and define two isometric operators $\Omega^\pm$ from $\mathcal{H}'$ into $\mathcal{H}$ by

$$\Omega^\pm \, \psi = \sum_\alpha \Omega_\alpha^\pm \, \psi_\alpha \,,$$

where $\psi \in \mathcal{H}'$ and ψ_α denotes the component of ψ in $\mathcal{H}_\alpha$. In view of (5), the ranges in $\mathcal{H}$ of $\Omega^\pm$ are

$$R^\pm = \bigoplus_\alpha R_\alpha^\pm \,.$$

Defining $\Omega^{\pm *}$ by $(\varphi, \Omega^\pm \psi)_{\mathcal{H}} = (\Omega^{\pm *} \varphi, \psi)_{\mathcal{H}'}$ for all $\varphi \in \mathcal{H}$ and $\psi \in \mathcal{H}'$, we find that $\Omega^{\pm *} \varphi = (\Omega^\pm)^{-1} \varphi$ if $\varphi \in R^\pm$ and $\Omega^{\pm *} \varphi = 0$ if $\varphi \perp R^\pm$. The S-operators are then

$$S' = \Omega^{+*} \, \Omega^- = \text{operator on } \mathcal{H}', \text{ unitary if and only if } R^+ = R^-,$$

$$S \;= \Omega^+ \, \Omega^{-*} = \text{operator on } \mathcal{H}, \text{ unitary if and only if } R^+ = R^- = \mathcal{H}.$$

S is the S-operator defined by JAUCH [2], while $\mathcal{H}'$ and S' have first been introduced by BEREZIN, FADDEEV and MINLOS [3]. S' has a simple physical interpretation: let $\psi = \{\psi_\alpha\} \in \mathcal{H}'$. By [2], there exists a motion of the system, with initial state $\varphi = \Omega^- \psi$, such that

$$e^{-iHt} \, \varphi \to \sum_\alpha P_\alpha \, e^{-iH_\alpha t} \, \psi_\alpha \quad (t \to -\infty) \,.$$

If $\varphi \in R^+$ (which is the case if $R^- = R^+$), this motion has a similar asymptotic behaviour for $t \to +\infty$:

$$e^{-iHt}\,\varphi \to \sum_{\alpha} P_\alpha\, e^{-iH_\alpha t}\,\psi'_\alpha \quad (t \to +\infty)\,,$$

where ψ'_α is the component in $\mathcal{H}_\alpha$ of the asymptotic state

$$\psi' = S'\,\psi$$

in $\mathcal{H}'$. The operator S', therefore, gives the asymptotic behaviour in the future in terms of the asymptotic behaviour in the past. From the point of view of S-matrix theory, $\mathcal{H}'$ is the Hilbertspace of the system and S' the operator characterizing the system.

The scattering formalism presented here is suitable for the multiparticle systems treated in this paper. However, it can be extended to include other systems as well. For example, we could allow that $P = P(t)$, uniformly bounded in t for sufficiently large $|t|$, and such that (1) (2) (6) hold. To preserve (3), it is sufficient to require that

$$\lim_{|t|\to\infty} \left\| \left(P\,(t+s) - P(t)\right) e^{-iHt}\,\psi_\alpha \right\| = 0$$

for any real s and any $\psi_\alpha \in \mathcal{H}_\alpha$. Precisely this generalization is necessary in the presence of Coulomb interactions, where $P(t)$ is a phase-factor in momentum space, with a phase proportional to $\log|t|$ [4].

3. Construction of Hamiltonians

Formally, the N-particle systems under consideration are characterized by a Hamiltonian

$$H = \sum_{k=1}^{N} \frac{p_k^2}{2\,m_k} + \sum_{l} V_l(x_l) = H_0 + V\,,$$

where l labels the pairs of particles and x_l is the relative coordinate of the pair l. The potentials satisfy the following conditions: $V_l(x)$ is a real-valued function on the set

$$E_l = \{x \mid x \notin K_l\}\,,$$

where $K_l \subset R^3$ is compact (hard core, possibly empty). On E_l, $V_l(x)$ is of the form

$$V_l(x) = V_{l,R}(x) + V_{l,S}(x)\,,$$

where the 'regular' part $V_{l,R}$ satisfies the usual conditions of time-dependent scattering theory for non-singular potentials,

$$V_{l,R}(\,.\,) \in L^2(E_l) + L^p(E_l)\,, \qquad (2 \leqslant p < 3)$$

meaning that $V_{l,R}(x)$ is the sum of an L^2-function and an L^p-function almost everywhere. For the singular part we assume:

$a \leqslant V_{l,S}(x)$ a. e. for some real a, supp $V_{l,S}$ is compact, and $V_{l,S}(x)$ is locally square integrable on an open set whose complement in E_l has measure zero.

The Hilbertspace of the N-particle system is $\mathcal{H} = L^2(E)$, where E is the subset of R^{3N} defined by

$$E = \{(x_1 \ldots x_N) \mid x_l \notin K_l \text{ for all pairs } l\}\,.$$

By our assumption on the potentials,

$$V(x_1 \ldots x_N) = \sum_l V_{l,R}(x) + \sum_l V_{l,S}(x) = V_R(x_1 \ldots x_N) + V_S(x_1 \ldots x_N)$$

is (term by term) locally square-integrable on an open set $M \subset E$, whose complement in E has measure zero. Therefore, we can define

$$H' = \sum_{k=1}^{N} \frac{p_k^2}{2\, m_k} + V = H_0' + V$$

in the usual way on the dense set $\Delta = C_0^\infty(M)$ (infinitely differentiable functions with compact supports contained in M), where it is symmetric. Since V_R is a Kato-potential [5] with respect to H_0', $^1/_2\, H_0' + V_R$ is bounded below on Δ, which implies

$$\frac{1}{2}\,(\psi, (H_0' + 1)\,\psi) \leqslant (\psi, (H_0' + V_R + b)\,\psi)$$

for some real b and all $\psi \in \Delta$. Adding the non-negative form $(\psi, V_S\,\psi) - a(\psi, \psi)$ on the right, we obtain

$$(4\, m_i)^{-1}\, \| p_i\, \psi \|^2 + \frac{1}{2}\, \| \psi \|^2 \leqslant (\psi, (H' + c)\,\psi) \tag{7}$$

for all i, all $\psi \in \Delta$ and $c = b - a$, where the p_i are the usual differential operators. Therefore, we can define:

$$H + c = \text{Friedrichs-extension of } H' + c\,.$$

The momentum operators of single particles are defined in the usual way on $C_0^\infty(E)$, where they are symmetric. They will not have selfadjoint extensions, since the corresponding translation groups are forbidden by the geometry of E (hard cores). They have, however, symmetric closures, which will be denoted by $p_1 \ldots p_N$.

Lemma 1

$$D\left((H + c)^{1/2}\right) \subset D(p_i) \text{ and } \| p_i\, \psi \| \leqslant 2\, m_i^{1/2}\, \| (H + c)^{1/2}\, \psi \|$$

$$\text{for all } i \text{ and all } \psi \in D\left((H + c)^{1/2}\right).$$

Proof

By construction of the Friedrichs-extension, $D(H) \subset \mathcal{H}_1 =$ completion of Δ in the Friedrichs-norm $\| \psi \|_1^2 = (\psi, \psi)_1 = (\psi, (H + c)\,\psi)$. Therefore, if $\psi \in D(H)$, there exists a sequence $\psi_n \in \Delta$ with $\| \psi_n - \psi \|_1 \to 0$, which, by (7) implies that $p_i\, \psi_n$ is a Cauchy-sequence and that $\psi_n \to \psi$. Since p_i is closed, it follows that $\psi \in D(p_i)$ and $p_i\, \psi_n \to p_i\, \psi$, and the inequality (7) is preserved in the limit. Since $(H + c)^{1/2}$ is the closure of its restriction to $D(H)$, this extends, again by continuity, to all $\psi \in D\,((H + c)^{1/2})$.

4. Scattering Theory

Let $D = (C_1 \ldots C_n)$ be a partition of the set $(1 \ldots N)$ into n subsets C_k, and let $\mathcal{H}(D)$ and $H(D)$ be the Hilbertspace and the Hamiltonian of the decomposed system (formally obtained by dropping in H all interactions linking different subsets C_k), which are constructed in the same way as $\mathcal{H}$ and H in Section 3. In particular, $\mathcal{H}(D) = L^2(E(D))$, where

$$E(D) = \{(x_1 \dots x_N) \mid x_l \notin K_l \text{ for all pairs } l \text{ not linking different subsets } C_k\} .$$

Next, we define a mapping $P(D)$ of $\mathcal{H}(D)$ into $\mathcal{H}$. Let R be such that the hard cores K_l, as subsets of R^3, are all contained in the sphere $|x| < R$. Then we choose a cut-off function $F(r)$ with the properties:

$$\begin{gathered} F \in C^\infty[0, \infty) , \\ 0 \leqslant F(r) \leqslant 1 \text{ for } 0 \leqslant r < \infty , \\ F(r) = 0 \text{ for } r \leqslant R \text{ and } F(r) = 1 \text{ for } r \geqslant R + 1 . \end{gathered} \tag{8}$$

For any $\psi \in \mathcal{H}(D)$, we define $P(D)\,\psi \in \mathcal{H}$ by

$$(P(D)\,\psi)\,(x_1 \dots x_N) = \prod_l F(|\,x_l\,|)\,\psi(x_1 \dots x_N) \tag{9}$$

where l runs over all pairs linking different subsets C_k.

The results of this section are collected in the following two theorems:

Theorem 1

For any decomposition D, $[\mathcal{H}(D),\, H(D),\, P(D)]$ is a channel of the system; i.e. $P(D)$ is asymptotically in the sense of (1), and the strong limits

$$\Omega_D^\pm = \lim_{t \to \pm\infty} e^{iHt}\, P(D)\, e^{-iH(D)t}$$

exist on $\mathcal{H}(D)$. Moreover, they are independent of the particular choice of the cut-off function $F(r)$: if $F'(r)$ is a second cut-off satisfying (8), then the corresponding operator $P(D)'$ is equivalent to $P(D)$ in the sense of (4).

The channels mentioned in Theorem 1 are not orthogonal as required by (5). In order to get a set of orthogonal channels, we restrict D by the condition that each composite subsystem C_k possesses at least one bound state, and we choose a complete set of orthogonal bound states for each of these C_k. A channel, α, then specifies such a decomposition into fragments and, in addition, one of the bound states, φ_k, for each composite fragment C_k:

$$\alpha = \begin{vmatrix} C_1 \dots C_n \\ \varphi_1 \dots \varphi_n \end{vmatrix}$$

($\varphi_k = 1$ if C_k is a single particle). $\mathcal{H}_\alpha \subset \mathcal{H}(D)$ is then the set of states of the form

$$\psi_\alpha(x_1 \dots x_N) = \phi_\alpha(y_1 \dots y_n) \sum_{k=1}^{n} \varphi_k(z_k) ,$$

where $\phi_\alpha \in L^2(R^{3n})$ and where y_k, z_k are the coordinates of the center-of-mass of C_k and internal coordinates of C_k, respectively. On $\mathcal{H}_\alpha$, $H(D)$ reduces to

$$H_\alpha = \sum_{k=1}^{n} \left(\frac{P_k^2}{2\,M_k} + \varepsilon_k \right), \tag{10}$$

P_k, M_k, ε_k being the total momentum, the total mass and the bound state energy of C_k. If we denote the restriction of $P(D)$ to $\mathcal{H}_\alpha$ by P_α, Theorem 1 implies that $\alpha = (\mathcal{H}_\alpha, H_\alpha, P_\alpha)$ is a channel of the system, and the wave-operators $\Omega_\alpha^\pm$ are simply the restrictions of $\Omega_D^\pm$ to $\mathcal{H}_\alpha$.

Theorem 2

The channels defined above are orthogonal in the sense of (5).

Proof of Theorem 1

Since $E \subset E(D)$, we have $\mathcal{H} \subset \mathcal{H}(D)$, and the identity map $\mathcal{H} \to \mathcal{H}(D)$ is isometric. Therefore, $P(D)$ may also be viewed as a bounded operator mapping $\mathcal{H}(D)$ into itself. In this sense,

$$\lim_{|t|\to\infty} \| (1 - P(D))\, e^{-iH(D)t}\, \psi \| = 0 \tag{11}$$

for all $\psi \in \mathcal{H}(D)$. Since $P(D)$ is bounded, it suffices to prove this on the dense set used in Appendix 3. Writing F_l for $F(|x_l|)$, the inequality of Appendix 1 yields

$$1 - \prod_l F_l \leqslant \sum_l (1 - F_l)$$

and therefore

$$\| (1 - P(D))\, e^{-iH(D)t}\, \psi \| \leqslant \sum_l \| (1 - F_l)\, e^{-iH(D)t}\, \psi \| .$$

Since $1 - F_l \in L^2(R^3)$, each term in this sum vanishes like $|t|^{-3/2}$ as $|t| \to \infty$, by the estimate of Appendix 3. This proves (11), and as a consequence, $P(D)$ is asymptotically isometric in the sense of (1). Also, if $P(D)'$ is defined by a second cut-off $F'(r)$ with the properties (8), we have

$$\| (P(D) - P(D')\,)\, e^{-iH(D)t}\, \psi \| \leqslant \| (1 - P(D))\, e^{-iH(D)t} \psi \| + \| (1 - P(D)')\, e^{-iH(D)t} \psi \| ,$$

which vanishes as $|t| \to \infty$, by (11).

Finally, we establish the asymptotic condition (2) for ψ in the dense set of Appendix 3. Using our freedom in the choice of F, we choose R in (8) so large that $V_{l,S}(x) = 0$ for $|x| > R$ and all l. Since $\psi \in D(H(D))$, we can apply the result of Appendix 2 and obtain

$$e^{iHt}\, P(D)\, e^{-iH(D)t}\, \psi = P(D)\, \psi + i \int_0^t d\tau\, e^{iH\tau} \left(H\, P(D) - P(D)\, H(D)\right) e^{-iH(D)\tau}\, \psi ,$$

where the integral is bounded in norm by

$$\int_0^t d\tau\, \| ([H_0, P(D)] + I(D)\, P(D))\, e^{-iH(D)\tau}\, \psi \| , \tag{12}$$

provided that $P(D) \exp(-\, i\, H(D)\, t)\, \psi \in D(I(D))$. But this follows from our choice of the cut-off, by which

$$I(D)\, P(D) = \sum_l V_{l,R} \prod_{l'} F_{l'} ,$$

and since the 'potentials' $V_{l,R}(x)\, F_l(x)$ satisfy the assumptions of Appendix 3,

$$\| I(D)\, P(D)\, e^{-tH(D)\tau}\, \psi \| \leqslant \sum_l \| V_{l,R}\, F_l\, e^{-iH(D)\tau}\, \psi \| \leqslant \text{const.}\ (1 + |\tau|)^{-s} \text{ for some } s > 1\,.$$

Therefore, the contribution of the term $I(D)\, P(D)$ to the integrand in (12) is well-defined and integrable over $-\infty < \tau < +\infty$.

To show the same for the term $[H_0, P(D)]$, we consider a typical part

$$\prod_{l'} G_{l'}(x_{l'})\, A\,, \tag{13}$$

where one of the functions $G_{l'}$, say G_l, has compact support. If A is 1 or the total momentum of one of the subsystems C_k, it commutes with $\exp(-i\, H(D)\, \tau)$ and the contribution of (13) to the integrand in (12) is estimated by

$$\text{const.}\ \| G_l\, e^{-iH(D)\tau}\, A\, \psi \|\,. \tag{14}$$

But A maps the dense set of ψ's of Appendix 3 into itself, therefore (14) is bounded by const. $(1 + |\tau|)^{-3/2}$. It remains to consider the case where A is an internal momentum of one of the subsystems C_k, say of C_1. Then the contribution of (13) is bounded by

$$\text{const.}\ \| G_l\, A\, e^{-iH(D)\tau}\, \psi \| \leqslant \text{const.}\ (1 + |\tau|)^{-3/2}\, \| A\, e^{-ih_1\tau}\, \varphi_1 \|\,,$$

by the estimate of Appendix 3. Applying Lemma 1 (to the internal Hamiltonian h_1 of C_1, which is also a Friedrichs-extension), we see that the last norm is bounded uniformly in τ:

$$\| A\, e^{-ih_1\tau}\, \varphi_1 \| \leqslant a\, \| (h_1 + c)^{1/2}\, e^{-ih_1}\, \varphi_1 \| = a\, \| (h_1 + c)^{1/2}\, \varphi_1 \|\,,$$

for some constant a.

Proof of Theorem 2

First, consider the case where the set $D = (C_1 \ldots C_n)$ of fragments in the channels α and β is the same, so that the two channels differ only in the assignment of bound states to these fragments. Due to the orthogonality of bound states, we then have $\mathcal{H}_\alpha \perp \mathcal{H}_\beta$ (as subspaces of $\mathcal{H}(D)$). Since $\Omega_\alpha^\pm$ and $\Omega_\beta^\pm$ are the restrictions of the isometric operators $\Omega_D^\pm$ to $\mathcal{H}_\alpha$ and $\mathcal{H}_\beta$, the orthogonality of their ranges follows from the orthogonality of the domains.

In the case where the decompositions specified by α and β are not the same, it is actually simpler to prove a statement more general than (6), namely

$$\lim_{|t| \to \infty} (P_\alpha\, e^{-iH_\alpha t}\, \psi_\alpha, P_\beta\, e^{-iH_\beta t}\, \psi_\beta) = 0$$

for any $\psi_\alpha, \psi_\beta \in L^2(R^{3N})$, where H_α, H_β, P_α, P_β are defined by (10) and (9) in an obvious way as operators on $L^2(R^{3N})$. From

$$\begin{aligned}(P_\alpha\, e^{-iH_\alpha t}\, \psi_\alpha, P_\beta\, e^{-iH_\beta t}\, \psi_\beta) &= (e^{-iH_\alpha t}\, \psi_\alpha, e^{-iH_\beta t}\, \psi_\beta) \\ &\quad - ((1 - P_\alpha)\, e^{-iH_\alpha t}\, \psi_\alpha, e^{-iH_\beta t}\, \psi_\beta) - (P_\alpha\, e^{-iH_\alpha t}\, \psi_\alpha, (1 - P_\beta)\, e^{-iH_\beta t}\, \psi_\beta)\,,\end{aligned}$$

we see that, by (11), it suffices to show that the first term on the right vanishes as $|t| \to \infty$ for $\psi_\alpha, \psi_\beta \in S(R^{3N})$. Up to a constant, $H_\alpha - H_\beta$ is a quadratic form of $p_1 \dots p_N$, which can be diagonalized by introducing new momentum variables $\pi_1 \dots \pi_N$:

$$(H_\alpha - H_\beta)(p_1 \dots p_N) = \sum_{i=1}^{N} \lambda_i \pi_i^2 + \text{const.},$$

where we can assume $\lambda_1 \neq 0$ since the quadratic form $(H_\alpha - H_\beta)(p_1 \dots p_N)$ does not vanish identically. For states ψ_α, ψ_β of the form

$$\psi(\pi_1 \dots \pi_N) = \prod_{k=1}^{N} \psi^k(\pi_k), \quad \psi^k \in S(R^3),$$

which still span a dense set in $L^2(R^{3N})$, we then obtain

$$|(\psi_\alpha, e^{i(H_\alpha - H_\beta)t} \psi_\beta)| \leqslant \text{const.} \left| \int d\pi_1 \, e^{-i\lambda_1 \pi_1^2 t} \, \overline{\psi_\alpha^1(\pi_1)} \, \psi_\beta^1(\pi_1) \right|,$$

which vanishes as $|t| \to \infty$.

5. Asymptotic Observables

In the framework of Section 1, an asymptotic observable in channel α is represented by a selfadjoint operator on $\mathcal{H}_\alpha$. It is immaterial whether or not the same quantity is an observable of the system, i.e. whether or not it is also represented by a selfadjoint operator on $\mathcal{H}$.

For example: In the channel $[\mathcal{H}(D), H(D), P(D)]$, the total momenta of the subsystems $C_1 \dots C_n$ are observables: they generate an n-parameter unitary group $U(a_1 \dots a_n)$ on $\mathcal{H}(D)$, representing a translation of each subsystem C_k by a_k. As mentioned before, these momentum operators can also be defined in $\mathcal{H} = L^2(E)$ on the dense set $C_0^\infty(E)$, where they are symmetric. However, they will not have selfadjoint extensions, since the corresponding translations are forbidden by the hard cores. Therefore, these momenta are not observables of the system. Nevertheless, they are well-defined asymptotic observables, so that it is perfectly meaningful to specify the momenta of ingoing and outgoing fragments in a collision. If the pair-potentials are spherically symmetric, similar statements hold for the other observables associated with the Galilei-group: energy, angular momentum and parity.

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Appendix 1

Let $0 \leqslant a_i \leqslant 1$, $i = 1 \dots n$. Then

$$1 - \prod_{i=1}^{n} a_i \leqslant \sum_{i=1}^{n} (1 - a_i). \tag{15}$$

Proof

(15) holds for $n = 1$, and if it holds for $n - 1$, it also holds for n if $a_n = 1$. Since both sides are linear in a_n, it therefore suffices to compare the derivatives with respect to a_n:

$$\frac{\partial}{\partial a_n}\left(1 - \prod_{i=1}^{n} a_i\right) = - \prod_{i=1}^{n-1} a_i \geqslant - 1 = \frac{\partial}{\partial a_n} \sum_{i=1}^{n} (1 - a_i)\,,$$

which implies (15).

Appendix 2

For any decomposition D, we define the operator $I(D)$ on $\mathcal{H}$ by

$$I(D) = \sum_l V_l\,,$$

where l runs over all pairs linking different subsets C_k. As in the proof of the asymptotic condition, we choose the cut-off $F(r)$ such that

$$I(D)\ P(D) = \sum_l V_{l,R}\ P(D)\,.$$

Lemma

If $\psi \in D(H(D))$ and $P(D)\,\psi \in D(I(D))$, then $P(D)\,\psi \in D(H)$ and

$$H\ P(D)\ \psi = P(D)\ H(D)\ \psi + [H_0,\ P(D)]\ \psi + I(D)\ P(D)\ \psi\,,$$

where $[H_0, P(D)]$ is formally the commutator, on $L^2(R^{3N})$, of the usual differential operator H_0 with the multiplication operator $\Pi_l\, F_l$, i.e. a sum of terms of the form

$$\prod_l G_l(x_l)\ A\,, \tag{16}$$

where the G_l are bounded C^∞-functions on R^{3N} of which at least one has compact support (being a derivative of F_l), and where A is either the identity or one of the momentum operators $p_1 \ldots p_N$. The precise meaning of (16) is then the following: A is an operator on $\mathcal{H}(D)$, either 1 or one of the closed, symmetric $p_1 \ldots p_N$, so that $D(H(D)) \subset D(A)$, by Lemma 1. $\Pi_l\, G_l$ is a (bounded) multiplication operator mapping $\mathcal{H}(D)$ into $\mathcal{H}$, so that $[H_0, P(D)]$ is defined as an operator from $D(H(D))$ into $\mathcal{H}$.

Proof

Let $\Delta(D) \subset \mathcal{H}(D)$ be defined in the same way as $\Delta \subset \mathcal{H}$ in Section 3. Then $P(D)\,\Delta(D) \subset \Delta \subset \Delta(D)$ so that $P(D)$ has an obvious meaning as a mapping of $\Delta(D)$ into itself. By virtue of Lemma 1, it is easily seen that this mapping is also bounded with respect to the Friedrichs-norm $\|\psi\|_1^D = (\psi, (H(D) + c)\,\psi)^{1/2}$ on $\Delta(D)$. Since $I(D)\ P(D)$ is a Kato-potential [5], $H(D) - I(D)$ is bounded below on $P(D)\,\Delta(D)$, which implies

$$(\varphi,\ I(D)\ \varphi) \leqslant (\varphi,\ H(D)\ \varphi) + a(\varphi, \varphi)\,,$$

for any $\varphi = P(D)\,\psi$, $\psi \in \Delta(D)$, and some real a. Since for these φ, $H\,\varphi = H(D)\,\varphi + I(D)\,\varphi$, we have

$$(\varphi,\ H\ \varphi) \leqslant 2\ (\varphi,\ H(D)\ \varphi) + a(\varphi, \varphi)\,. \tag{17}$$

Now, let $\psi \in D(H(D))$. Since $H(D)$ is the Friedrichs-extension of its restriction to $\Delta(D)$, there exists a sequence $\psi_n \in \Delta(D)$ with $\| \psi_n - \psi \|_1^D \to 0$. Since $P(D)$ is bounded in the norm $\| \ \|_1^D$, $\varphi_n = P(D)\, \psi_n$ is also a Cauchy-sequence in this norm. By (17), φ_n is then a Cauchy-sequence in the Friedrichs-norm associated with H, and it follows that $\lim P(D)\, \psi \in \mathcal{H}_1$ (Notation as in proof of Lemma 1). For any $\varphi \in \Delta$, we have now

$$(\varphi, P(D)\, \psi)_1 - c(\varphi, P(D)\, \psi) = (H\, \varphi, P(D)\, \psi) = (P(D)\, H\, \varphi, \psi)$$
$$= (H(D)\, P(D)\, \varphi, \psi) + ([P(D), H_0]\, \varphi, \psi) + (P(D)\, I(D)\, \varphi, \psi),$$

where $[P(D), H_0]$ is a sum of terms of the form $A \prod_l G_l(x_l)$ as described in (16). By Lemma 1, $\psi \in D(A)$ and, since A is symmetric, we obtain

$$(\varphi, P(D)\, \psi)_1 = (\varphi, P(D)\, H(D)\, \psi) + (\varphi, [H_0, P(D)]\, \psi) + (\varphi, I(D)\, P(D)\, \psi) + c(\varphi, P(D)\, \psi), \tag{18}$$

provided that $P(D)\, \psi \in D(I(D))$, which is assumed in the Lemma. If follows that $|(\varphi, P(D)\, \psi)_1| \leqslant \text{const.}\ \| \varphi \|$ for all $\varphi \in \Delta$, hence $P(D)\, \psi \in D(H)$ and $(\varphi, P(D)\, \psi)_1 = (\varphi, (H + c)\, P(D)\, \psi)$. Comparison with (18) now yields the expression for $H\, P(D)\, \psi$ stated in the Lemma.

Appendix 3

For convenience, we collect here the usual estimates of time-dependent scattering theory which were derived, in one form or another, by various people.

For any decomposition $D = (C_1 \ldots C_n)$ of the system, consider the set of states of the form

$$\psi(x_1 \ldots x_N) = \prod_{k=1}^{n} \phi_k(y_k)\, \varphi_k(z_k),$$

with $\phi_k \in C_0^\infty(R^3)$, $\varphi_k \in D(h_k)$ (y_k = center-of-mass of C_k, h_k = internal Hamiltonian of C_k, z_k = internal coordinates in C_k). These states span a dense set in $\mathcal{H}(D)$. Let V be a pair-potential linking two of the subsystems C_k, say C_1 and C_2, and suppose that $V(.) \in L^s(R^3)$, $2 \leqslant s \leqslant \infty$. Then we have:

$N(t) = \| V \exp(-i\, H(D)\, t)\, \psi \|$ is uniformly bounded in $-\infty < t < +\infty$ and satisfies the estimate

$$N(t) \leqslant C(\phi_1, \phi_2, s)\, |t|^{-3/s}\, \| V(.) \|_s\, \| e^{-i h_1 t}\, \varphi_1 \|\, \| e^{-i h_2 t}\, \varphi_2 \| .$$

The last two factors are independent of t. They are exhibited only to show how the internal motion in the subsystem C_1, C_2 enters in the estimate. (This is important in the last step of the proof of Theorem 1.)

Proof

Obviously, $N(t) = \| V \exp(-i\, H_{12}\, t)\, \psi_{12} \|$, where H_{12} is the internal energy of the (decomposed) subsystem (C_1, C_2) and $\psi_{12} = \Pi_{k=1}^2\, \phi_k(y_k)\, \varphi_k(z_k)$. Now

$$e^{-i H_{12} t}\, \psi_{12} = e^{-i H_{12}^0 t}\, \phi_1\, \phi_2 \otimes e^{-i h_1 t}\, \varphi_1 \otimes e^{-i h_2 t}\, \varphi_2,$$

where H_{12}^0 is the kinetic energy of the relative motion of C_1, C_2. To estimate the first factor on the right, let η be the coordinate of the CM (center-of-mass) of (C_1, C_2), and ξ the relative coordinate of the CM of C_1 with respect to the CM of C_2. Then

$$\left| e^{-iH_{12}^0 t} \phi_1 \phi_2(\xi, \eta, t) \right| = \left| -i \left(\frac{\mu}{2\pi t}\right)^{3/2} \int d\xi' \, e^{i\mu(\xi-\xi')^2/2t} (\phi_1 \phi_2)(\xi', \eta) \right|$$
$$\leqslant \left(\frac{\mu}{2\pi |t|}\right)^{3/2} \left| \int d\xi' \, e^{-2\pi i(\mu\xi/2\pi t)\xi'} e^{i\mu\xi'^2/2t} (\phi_1 \phi_2)(\xi', \eta) \right|,$$

μ being the reduced mass of C_1, C_2.

Applying the Hausdorff-Young inequality to this Fourier-integral, we obtain

$$\| (e^{-iH_{12}^0 t} \phi_1 \phi_2)(., \eta, t) \|_p \leqslant \left(\frac{\mu}{2\pi |t|}\right)^{(3/2-3/p)} \| (\phi_1 \phi_2)(., \eta) \|_q \tag{19}$$

where $2 \leqslant p \leqslant \infty$ and $p^{-1} + q^{-1} = 1$.

Since supp ϕ_k is contained in a sphere of radius R, one easily sees that $\| \phi_1 \phi_2(., \eta) \|_q = 0$ for $|\eta| > 3R$, so that

$$M^2(q) = \int d\eta \, \| (\phi_1 \phi_2)(., \eta) \|_q < \infty .$$

Now we have

$$N^2(t) \leqslant \| e^{-ih_1 t} \varphi_1 \|^2 \, \| e^{-ih_2 t} \varphi_2 \|^2$$
$$\times \sup_{z_1, z_2} \int d\eta \int d\xi \, | V(\xi + \alpha_1 z_1 + \alpha_2 z_2) |^2 \, | (e^{-iH_{12}^0 t} \phi_1 \phi_2)(\xi, \eta, t) |^2 , \tag{20}$$

where $\alpha_k z_k$ is some linear combination of the internal coordinates of C_k. Hoelder's inequality and (19) imply

$$\int d\eta \int d\xi \ldots \leqslant \| V(.) \|_s^2 \left(\frac{\mu}{2\pi |t|}\right)^{6/s} M^2 \left(\frac{s+2}{2s}\right)$$

or, finally,

$$N(t) \leqslant \left(\frac{\mu}{2\pi |t|}\right)^{3/s} M \left(\frac{s+2}{2s}\right) \| V(.) \|_s \, \| e^{-ih_1 t} \varphi_1 \| \, \| e^{-ih_2 t} \varphi_2 \|$$

for $2 \leqslant s \leqslant \infty$.

On the other hand, $N(t)$ is bounded uniformly in t – even if $V \in L^2 + L^\infty$. For $V \in L^\infty$ this is trivial. For $V \in L^2$ this follows from (20) and from the fact that $\| \exp(-i H_{12}^0 t) \phi_1 \phi_2(\xi, .) \|_2$ is bounded by $\| \phi_1 \|_2 \, \| \phi_2 \|_2$ uniformly in ξ and t.

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