J. Math. Kyoto Univ. (JMKYAZ)
32-3 (1992) 533-555

Semi-classical asymptotics for total scattering cross sections of 3-body systems

Dedicated to Professor Teruo Ikebe on his sixtieth birthday

By

Hiroshi T. ITO and Hideo TAMURA

Introduction

The scattering cross section is directly related to experimental observations in laboratories and is one of the most important quantities in scattering theory. There are many works on the semi-classical analysis for scattering matrices of 2-body systems. For example, such a problem has been studied for scattering amplitudes in the works [14, 18, 21] and for total scattering cross sections in the works [7, 13, 16, 19, 20]. In the present work, we study the semi-classical asymptotic behavior of total scattering cross sections with 2-body initial states for 3-body systems. Such an initial state is of most practical interest. In fact, for many-body scattering systems, k-body initial states with $k \geq 3$ are not easy to realize through actual physical experiments. There seems to be only a few works on the analysis for scattering matrices of many-body systems. In a series of works [3, 4, 5], the following properties of total scattering cross sections have been studied in detail: (1) finiteness of total scattering cross sections; (2) continuity as a function of energy; (3) behavior at high and low energies. The asymptotic behavior in the semi-classical limit has not been discussed in detail in these works.

Throughout the entire discussion, the constant h, $0 < h \ll 1$, denotes a small parameter corresponding to the Planck constant. We require several basic notations and definitions in many-body scattering theory to define precisely the total scattering cross section in question. We here state our main theorem somewhat loosely. The precise formulation of the main result is given as Theorem 1.1 in section 1.

Consider a system consisting of three particles moving in the 3-dimensional space R^3 through real pair potentials V_{jk}, $1 \leq j < k \leq 3$. We denote by m_j, $1 \leq j \leq 3$, the mass of the j-th particle and by $r_j \in R^3$ its position vector. A partition of $\{1, 2, 3\}$ into nonempty disjoint subsets is called a cluster decomposition. We use the letter a or b to denote such a cluster decomposition. The Jacobi coordinates $(y_a, z_a) \in R^{3\times 2}$ associated with given 2-cluster decomposition $a = \{l, (j, k)\}$ with $j < k$ are defined as

Received October 19, 1990

$$y_a = r_j - r_k\,, \qquad z_a = r_l - \frac{m_j r_j + m_k r_k}{m_j + m_k} \tag{0.1}$$

and also, after separating the center of mass motion, the free Hamiltonian $H_0(h)$ is represented in terms of these coordinates as follows:

$$H_0(h) = -\frac{1}{2N_a} h^2 \Delta_y - \frac{1}{2n_a} h^2 \Delta_z\,, \tag{0.2}$$

where the reduced masses N_a and n_a are defined through the relations

$$\frac{1}{N_a} = \frac{1}{m_j} + \frac{1}{m_k}\,, \qquad \frac{1}{n_a} = \frac{1}{m_j + m_k} + \frac{1}{m_l}\,, \tag{0.3}$$

while Δ_y and Δ_z denote the Laplace operator with respect to the variables y_a and z_a, respectively. The total Hamiltonian $H(h)$ is defined by adding to $H_0(h)$ the sum of pair potentials;

$$H(h) = H_0(h) + \sum_{1 \le j < k \le 3} V_{jk}(r_j - r_k)\,. \tag{0.4}$$

All the relative coordinates $r_j - r_k$ are represented as a linear combination of the Jacobi coordinates (y_a, z_a) and hence the Hamiltonian $H(h)$ can be regarded as an operator acting on the space $L^2(R^6)$. We assume all the pair potentials $V_{jk}(r)$, $r \in R^3$, to decay like $O(|r|^{-\rho})$ as $|r| \to \infty$ for some $\rho > 5/2$.

Let $a = \{l, (j, k)\}$ be again a 2-cluster decomposition. As a 2-body initial state, we now consider the state in which at time $t = -\infty$, the j-th and k-th particles form a bound state at energy $\lambda_\alpha(h)$ and the 3rd particle labelled by l comes into the scatterer from the long distance at relative energy $\lambda - \lambda_\alpha(h)$ and at incident direction $\omega \in S^2$, S^2 being the 2-dimensional unit sphere. We also assume that the total energy $\lambda > 0$ is restricted to a positive energy range and that the binding energy $\lambda_\alpha(h) < 0$ is strictly negative uniformly in h. Then, for such a 2-body initial state, the total scattering cross section $\sigma_\alpha(\lambda, \omega; h)$ can be defined for *a.e.* $(\lambda, \omega) \in (0, \infty) \times S^2$. It should be noted that the exceptional set of (λ, ω) for which $\sigma_\alpha(\lambda, \omega; h)$ is not finite may depend on the parameter h. Such an exceptional set is expected to be empty, but it seems that this fact has not yet proved even for the class of finite-range interactions. Thus we consider the total scattering cross secion $\sigma_\alpha(\lambda, \omega; h)$ as a function of (λ, ω) in $D'((0, \infty) \times S^2)$ (in the distributional sense) and study its asymptotic behavior as $h \to 0$. The main result is, somewhat loosely speaking, that under the assumptions above, $\sigma_\alpha(\lambda, \omega; h)$ behaves like

$$\sigma_\alpha(\lambda, \omega; h) \sim h^{-2/(\rho - 1)}$$

as $h \to 0$ in $D'((0, \infty) \times S^2)$. Here we should note that the above decaying assumption is rather strong to deal with total scattering cross sections. In fact, we can show that $\sigma_\alpha(\lambda, \omega; h)$ is finite for *a.e.* $(\lambda, \omega) \in (0, \infty) \times S^2$ under the weak decaying assumption with $\rho > 2$.

For 2-body scattering systems, a similar result has been already obtained by several authors [13, 16, 19, 20] under the weak decaying assumption with $\rho > 2$. If, in particular, the total energy $\lambda > 0$ is restricted to a non-trapping energy range, then the above result has been also proved for $(\lambda, \omega) \in (0, \infty)$ fixed in the 2-body case ([13, 19]).

During the last decade, the many-body scattering theory has made a major progress by the remarkable works [6, 10, 11, 15]. The proof of the result above is based on the two fundamental facts in the spectral theory for many-body Schrödinger operators. One is the principle of limiting absorption proved by Mourre [10] and the other is the asymptotic completeness of wave operators proved by Enss [6]. These results have been extended to N-body systems by [11] (limiting absorption principle) and by [15] (asymptotic completeness). The principle of limiting absorption guarantees, without assuming the absence of zero resonance energy, that the limits as $\kappa \to 0$ of the resolvents

$$R(\lambda \pm i0; H(h)) = \lim_{\kappa \to 0} R(\lambda \pm i\kappa; H(h))$$

with $R(\lambda \pm i\kappa; H(h)) = (H(h) - \lambda \mp i\kappa)^{-1}$ exist in an appropriate weighted L^2 space topology. This enables us to represent scattering amplitudes with 2-body initial states in terms of $R(\lambda \pm i0; H(h))$. On the other hand, the asymptotic completeness enables us to relate total scattering cross sections to forward scattering amplitudes. This relation is called the optical theorem. The proof of the main theorem is done by approximating the resolvents $R(\lambda \pm i0; H(h))$ through the time-dependent representation formula of resolvents.

§ 1. Total scattering cross sections

In this section we define the total scattering cross section and formulate the main theorem precisely.

We start by making the assumption on the pair potentials V_{jk}, $1 \le j < k \le 3$. We assume $V_{jk}(r)$, $r \in R^3$, to have the following decaying property:
$(V)_\rho$ $V_{jk}(r)$ is a real C^2-smooth function and

$$|\partial_r^\alpha V_{jk}(r)| \le C_\alpha \langle r \rangle^{-(\rho + d|\alpha|)}, \qquad 0 \le |\alpha| \le 2$$

for some $\rho > 5/2$ and d, $0 < d \le 1$, where

$$\langle r \rangle = (1 + |r|^2)^{1/2} .$$

This assumption can be somewhat relaxed. For details, see Remark 1.2 after Theorem 1.1. The constants ρ and d are used throughout with the meanings ascribed above. Under assumption $(V)_\rho$, the Hamiltonian $H(h)$ formally defined by (0.4) admits a unique self-adjoint realization in $L^2(R^6)$ and we denote by the same notation $H(h)$ this self-adjoint realization.

Let $a = \{l, (j, k)\}$ be a 2-cluster decomposition and let $(y_a, z_a) \in R^{3 \times 2}$ be the Jacobi coordinates associated with a. In addition to $H_0(h)$ and $H(h)$, we use the cluster Hamiltonian $H_a(h)$ defined by

$$H_a(h) = H_0(h) + V_{jk}(y_a)\,. \tag{1.1}$$

The operator $H_a(h)$ acts on the space $L^2(R^6)$. This space can be viewed as the tensor product

$$L^2(R^6) = L^2(R^3; dy_a) \otimes L^2(R^3; dz_a)$$

and hence $H_a(h)$ has the following decomposition:

$$H_a(h) = H^a(h) \otimes Id + Id \otimes T_a(h)\,,$$

Id being the identity operator, where

$$H^a(h) = -\frac{1}{2N_a} h^2 \Delta_y + V_{jk}(y_a) \tag{1.2}$$

is the 2-body subsystem Hamiltonian for the pair (j, k) acting on $L^2(R^3; dy_a)$ and

$$T_a(h) = -\frac{1}{2n_a} h^2 \Delta_z$$

acting on $L^2(R^3; dz_a)$ is the kinetic operator of the center of mass motion of the clusters in a. We further define the intercluster potential I_a as

$$I_a(y_a, z_a) = H(h) - H_a(h)\,. \tag{1.3}$$

Let $H^a(h)$ be as above. Under assumption $(V)_\rho$, this operator has only a finite number of (non-positive) bound state energies. We denote by $d^a(h)$ the number of such bound state energies with repetition according to the multiplicities. A pair $\alpha = (a, j)$ with $1 \le j \le d^a(h)$ is called a 2-body channel associated with a. For such a channel α, we here introduce the following notations: (0) the j-th eigenvalue $\lambda_\alpha(h) \le 0$ of $H^a(h)$; (1) the normalized eigenstate $\psi_\alpha = \psi_\alpha(y_a: h) \in L^2(R^3; dy_a)$ associated with $\lambda_\alpha = \lambda_\alpha(h)$, $H^a(h)\psi_\alpha = \lambda_\alpha \psi_\alpha$; (2) the channel Hamiltonian

$$H_\alpha(h) = T_a(h) + \lambda_\alpha \tag{1.4}$$

acting on $L^2(R^3; dz_a)$; (3) the channel identification operator $J_\alpha: L^2(R^3; dz_a) \to L^2(R^6)$ defined by $J_\alpha u = \psi_\alpha \otimes u$; (4) the channel wave operator $W_\alpha^\pm(h)$: $L^2(R^3; dz_a) \to L^2(R^6)$ defined by

$$W_\alpha^\pm(h) = s - \lim_{t \to \pm\infty} \exp(ih^{-1}tH(h)) J_\alpha \exp(-ih^{-1}tH_\alpha(h))\,. \tag{1.5}$$

If $a = \{1, 2, 3\}$ is a 3-cluster decomposition, then a has only one channel. We call such a single channel a 3-body channel. For the 3-body channel α, we define the channel Hamiltonian $H_\alpha(h)$ as the free Hamiltonian $H_0(h)$ and the channel wave operator $W_\alpha^\pm(h)$: $L^2(R^6) \to L^2(R^6)$ by (1.5) with $J_\alpha = Id$.

We know (for example, see [12]) that under assumption $(V)_\rho$, the channel wave operators, including a 3-body channel case, really exist and that their ranges are mutually orthogonal;

$$Range\ W_\alpha^\pm(h) \perp Range\ W_\beta^\pm(h)\,, \qquad \alpha \neq \beta\,.$$

The channel wave operators are said to be asymptotically complete, if

$$\sum_\alpha \oplus Range\ W_\alpha^-(h) = \sum_\alpha \oplus Range\ W_\alpha^+(h)\,,$$

where the summation is taken over all the channels α. It is also known ([6]) that under assumption $(V)_\rho$, the channel wave operators are asymptotically complete. In fact, this result holds true under the weaker decaying assumption with $\rho > 1$.

We now proceed to the spectral representation for channel Hamiltonians. Let α be a 2-body channel associated with a and let $H_\alpha(h)$ be the channel Hamiltonian defined by (1.4). We define the generalized eigenfunction φ_α of $H_\alpha(h)$ by

$$(1.6) \qquad \varphi_\alpha(z_a; \lambda, \omega, h) = \exp\left(ih^{-1}(2n_a(\lambda - \lambda_\alpha(h)))^{1/2}\langle z_a, \omega\rangle\right)$$

for $(\lambda, \omega) \in (\lambda_\alpha(h), \infty) \times S^2$, where $\langle\ ,\ \rangle$ denotes the scalar product in R^3. Let

$$X_\alpha = L^2((\lambda_\alpha(h), \infty); L^2(S^2))\,.$$

We also define the unitary operator $F_\alpha(h)$: $L^2(R^3; dz_a) \to X_\alpha$ by

$$(1.7) \qquad (F_\alpha(h)f)(\lambda, \omega) = c_\alpha(\lambda, h)\int \bar{\varphi}_\alpha(z_a; \lambda, \omega, h) f(z_a)dz_a$$

with the normalization constant

$$c_\alpha = (2\pi h)^{-3/2} n_a^{1/2}(2n_a(\lambda - \lambda_\alpha(h)))^{1/4}\,,$$

where the integration with no domain attached is taken over the whole space. This abbreviation is used throughout. The mapping $F_\alpha(h)$ defined above yields the spectral representation for $H_\alpha(h)$ in the sense that $H_\alpha(h)$ is transformed into the multiplication by λ in the space X_α. In the case of 3-body channel α, we can also construct a similar representation for $H_\alpha(h) = H_0(h)$ in the space

$$X_0 = L^2((0, \infty); L^2(E^5))\,,$$

where E^5 is the 5-dimensional ellipsoid defined by

$$(1.8) \qquad E^5 = \left\{(p, q) \in R^{3\times 2}: \frac{1}{2N_a}|p|^2 + \frac{1}{2n_a}|q|^2 = 1\right\}$$

with the reduced masses N_a and n_a defined by (0.3) and also the space $L^2(E^5)$ is defined with respect to the Lebesgue measure with a suitably chosen normalization constant. We do not require the explicit expression for such a constant in the discussion below.

From now on, we fix a 2-cluster decomposition $a = \{l, (j, k)\}$ with $j < k$ and consider, as an initial state, a 2-body channel α associated with a. The initial

2-body channel α may change with parameter h. Let β be a 2-body channel associated with 2-cluster decomposition b. Then we define the scattering operator $S_{\alpha\to\beta}(h)$: $L^2(R^3; dz_a) \to L^2(R^3; dz_b)$ for scattering from the initial state α to the final one β as follows:

$$S_{\alpha\to\beta}(h) = W_\beta^+(h)^* W_\alpha^-(h)\,.$$

If β is a 3-body channel, then $S_{\alpha\to\beta}(h)$ is defined as an operator from $L^2(R^3; dz_a)$ into $L^2(R^6)$. By definition, it follows immediately that the scattering operator $S_{\alpha\to\beta}(h)$ intertwines the channel Hamiltonians $H_\alpha(h)$ and $H_\beta(h)$ in the sense that

$$\exp(-ih^{-1}tH_\beta(h))S_{\alpha\to\beta}(h) = S_{\alpha\to\beta}(h)\exp(-ih^{-1}tH_\alpha(h)) \tag{1.9}$$

and also, by the asymptotic completeness of channel wave operators, we obtain the relation

$$\sum_\beta S_{\alpha\to\beta}(h)^* S_{\alpha\to\beta}(h) = Id \tag{1.10}$$

as an operator acting on $L^2(R^3; dz_a)$. This relation plays an important role in the study on the semi-classical behavior of total scattering cross sections.

We proceed to the definition of total scattering cross sections with 2-body initial states. As an initial state, we again consider the 2-body channel α as above which is associated with a. We define the operator $T_{\alpha\to\beta}(h)$ by

$$T_{\alpha\to\beta}(h) = S_{\alpha\to\beta}(h) - \delta_{\alpha\beta} Id\,, \tag{1.11}$$

$\delta_{\alpha\beta}$ being the Kronecker delta notation. As is easily seen, this operator also has the same intertwining property as in (1.9). Hence, by the spectral representation constructed above, we can represent $T_{\alpha\to\beta}(h)$ as a decomposable operator

$$T_{\alpha\to\beta}(h) = \{T_{\alpha\to\beta}(\lambda; h)\} \tag{1.12}$$

for $\lambda \in (\lambda_{\alpha\beta}(h), \infty)$, $\lambda_{\alpha\beta} = \max(\lambda_\alpha(h), \lambda_\beta(h))$. The operator $T_{\alpha\to\beta}(\lambda; h)$ is defined as an operator from $L^2(S^2)$ into $L^2(S^2)$ or $L^2(E^5)$, E^5 being defined by (1.8), according as β is a 2-body channel or a 3-body channel. For example, $T_{\alpha\to\alpha}(\lambda; h)$: $L^2(S^2) \to L^2(S^2)$ is defined through the relation

$$(F_\alpha(h)T_{\alpha\to\alpha}(h)f)(\lambda, \omega) = (T_{\alpha\to\alpha}(\lambda; h)(F_\alpha(h)f)(\lambda, \cdot))(\omega)\,.$$

We will show in the next section that $T_{\alpha\to\beta}(\lambda; h)$ is of Hilbert-Schmidt class for *a.e.* $\lambda > 0$.

We denote by $T_{\alpha\to\beta}(\theta, \omega; \lambda, h)$, $(\lambda, \omega) \in (0, \infty) \times S^2$, the integral kernel of $T_{\alpha\to\beta}(\lambda; h)$, where θ ranges over S^2 or E^5, according as β is a 2-body channel or a 3-body channel. Then the scattering amplitude $f_{\alpha\to\beta}(\omega\to\theta; \lambda, h)$ for scattering from the initial state α to the final one β at energy λ is represented as

$$f_{\alpha\to\beta}(\omega\to\theta; \lambda, h) = -2\pi ih(2n_a(\lambda - \lambda_\alpha(h)))^{-1/2} T_{\alpha\to\beta}(\theta, \omega; \lambda, h)\,. \tag{1.13}$$

For the representation formula above, see the book [2] (p. 627). We now define the total scattering cross section $\sigma_\alpha(\lambda, \omega; h)$ for scattering initiated in the 2-body channel α at energy λ and at incident direction ω by

(1.14) $$\sigma_\alpha(\lambda, \omega; h) = \sum_\beta \int |f_{\alpha\to\beta}(\omega \to \theta; \lambda, h)|^2 d\theta$$

for *a.e.* $(\lambda, \omega) \in (0, \infty) \times S^2$. As stated in Introduction, it should be noted that $\sigma_\alpha(\lambda, \omega; h)$ is defined only for *a.e.* (λ, ω) and that the exceptional set may depend on the parameter h.

Before formulating the main theorem, we further introduce a new notation. Let Π_ω denote the 2-dimensional hyperplane (impact plane) orthogonal to the direction ω. We write $z_a \in R^3$ as $z_a = u + x\omega$ with $u \in \Pi_\omega$ and $x = \langle z_a, \omega\rangle \in R^1$. The variables $u \in \Pi_\omega$ are called the impact parameters.

Theorem 1.1. *Let the notations be as above. In addition to* $(V)_\rho$ *with* $\rho > 5/2$, *assume that the binding energy* $\lambda_\alpha(h)$ *associated with the 2-body initial channel* α *satisfies*

$$\lambda_\alpha(h) < -\lambda_0$$

for some $\lambda_0 > 0$ *uniformly in* h. *Then, as a function of* $(\lambda, \omega) \in (0, \infty) \times S^2$, *the total scattering cross section* $\sigma_\alpha(\lambda, \omega; h)$ *obeys the following asymptotic formula as* $h \to 0$ *in* $D'((0, \infty) \times S^2)$:

$$\sigma_\alpha = 4 \int_{\Pi_\omega} \sin^2 \left\{ \frac{1}{2\mu_\alpha(\lambda) h} \int I_a(0, u + x\omega)dx \right\} du + o(h^{-2/(\rho-1)}),$$

where

(1.15) $$\mu_\alpha(\lambda) = \sqrt{\frac{2(\lambda - \lambda_\alpha(h))}{n_a}}$$

is the relative velocity along the incident direction ω *of the incoming particle and* $I_a(y_a, z_a)$ *is the intercluster potential defined by* (1.3) *for the 2-body cluster decomposition* a *with which the initial state* α *is associated.*

We here make some comments on the theorem above.

Remark 1.2. In assumption $(V)_\rho$, the pair potential $V_{jk}(r)$, $r \in R^3$, is assumed to be a C^2-smooth function over the whole space R^3. In proving the theorem, it suffices to assume that V_{jk} is a C^2-smooth function in $\{r \in R^3: |r| > R\}$ for some $R \gg 1$ large enough and also the theorem can be extended to an appropriate class of pair potentials with local singularities. We do not discuss about such an extension in detail here.

Remark 1.3. The leading term in the asymptotic formula above has the order comparable to $O(h^{-m})$ with $m = 2/(\rho - 1)$. In fact, if $I_a(0, z_a)$, $z \in R^3$, behaves like

$$I_a(0, z) = \Phi(z/|z|)|z|^{-\rho} + o(|z|^{-\rho}), \qquad |z| \to \infty,$$

with $\Phi(\neq 0) \in C^2(S^2)$, then we can see by taking the spherical coordinates in Π_ω that

$$\sigma_\alpha = \sigma_0 \mu_\alpha(\lambda)^{-m} h^{-m}(1 + o(1)), \qquad h \to 0,$$

with some $\sigma_0 > 0$ ([19]).

§ 2. Optical theorem

Throughout the entire discussion below, we always assume all the assumptions of Theorem 1.1 to be satisfied, although all the results obtained in the present section can be proved to hold true under the weaker decaying assumption with $\rho > 2$. It seems to be difficult to treat directly the total scattering cross section defined by (1.14). The first step toward the proof of the main theorem is to rewrite this quantity by use of the representation formula called the optical theorem. The aim here is to formulate this relation.

As is well-known, the principle of limiting absorption plays a basic role in the stationary scattering theory. We begin by making a brief review of some important spectral properties of the 3-body Schrödinger operator $H(h)$, which are required to formulate the optical theorem. Let $L^2_\nu(R^6)$ be the weighted L^2 space defined by

$$L^2_\nu(R^6) = L^2(R^6; \langle y_a, z_a \rangle^{2\nu} dy_a dz_a)$$

with

$$\langle y_a, z_a \rangle = (1 + |y_a|^2 + |z_a|^2)^{1/2}.$$

Then $H(h)$ has the following spectral properties: (1) $H(h)$ has no positive eigenvalues; (2) The limits $R(\lambda \pm i0; H(h))$, $\lambda > 0$, of $R(\lambda \pm i\kappa; H(h))$ as $\kappa \to 0$ exist as an operator from $L^2_\nu(R^6)$ into $L^2_{-\nu}(R^6)$ for any $\nu > 1/2$ and have the local Hölder continuity as a function of λ in the uniform operator topology. Property (1) has been proved by [8] and (2) by [1, 10, 11, 17]. Indeed, these properties have been verified under much weaker decaying assumptions of pair potentials, including the N-body systems.

We keep the same notations as in the previous sections. Let $\lambda_\alpha(h)$ be the binding energy of the 2-body initial state α associated with $a = \{l, (j, k)\}$. This is defined as a non-positive eigenvalue of the 2-body subsystem Hamiltonian

$$H^a(h) = -\frac{1}{2N_a} h^2 \Delta_y + V_{jk}(y_a)$$

acting on $L^2(R^3; dy_a)$. By assumption, $\lambda_\alpha(h) < -\lambda_0 < 0$ uniformly in h and hence we can easily see that the normalized eigenstate $\psi_\alpha = \psi_\alpha(y_a; h)$ associated with the eigenvalue $\lambda_\alpha(h)$ satisfies

$$\int (1 + |y_a|)^{2N} |\psi_\alpha(y_a; h)|^2 dy_a \leq C_N \tag{2.1}$$

for any $N \gg 1$ uniformly in h.

The analysis in this section is based on the following proposition on the representation formula of scattering amplitudes. The proof can be done in almost the same way as in the 2-body case. For a proof, see, for example, Ito [9] (Proposition 2.4).

Proposition 2.1. *Assume all the assumptions of Theorem* 1.1. *Denote by* $(\, , \,)_0$ *the* L^2 *scalar product in* $L^2(R^6)$. *Let* $\varphi_\alpha(z_a; \lambda, \omega, h)$ *be the generalized eigenfunction defined by* (1.6) *and write*

$$e_\alpha(\omega) = \psi_\alpha(y_a; h) \otimes \varphi_\alpha(z_a; \lambda, \omega, h) . \tag{2.2}$$

Then the operator $T_{\alpha\to\alpha}(\lambda; h)$: $L^2(S^2) \to L^2(S^2)$ *is of Hilbert-Schmidt class for all* $\lambda > 0$ *and it has the integral kernel*

$$T_{\alpha\to\alpha}(\theta, \omega; \lambda, h) = c_{0\alpha} G_\alpha(\theta, \omega; \lambda, h) \tag{2.3}$$

with

$$c_{0\alpha} = (2\pi)^{-2} i n_a (2n_a(\lambda - \lambda_\alpha(h)))^{1/2} h^{-3} ,$$

where

$$G_\alpha = ((-I_a + I_a R(\lambda + i0; H(h)) I_a) e_\alpha(\omega), e_\alpha(\theta))_0$$

with the intercluster potential $I_a(y_a, z_a)$ *defined by* (1.3). *In particular, the scattering amplitude* $f_{\alpha\to\alpha}(\omega \to \theta; \lambda, h)$ *for scattering from the initial direction* ω *to the final one* θ *at energy* λ *is represented as*

$$f_{\alpha\to\alpha}(\omega \to \theta; \lambda, h) = (2\pi)^{-1} n_a h^{-2} G_\alpha(\theta, \omega; \lambda, h) \tag{2.4}$$

We here make some comments on the proposition above. If β is a 2-body channel with strictly negative binding energy, then we can prove that $T_{\alpha\to\beta}(\lambda; h)$: $L^2(S^2) \to L^2(S^2)$ is also of Hilbert-Schmidt class for all $\lambda > 0$ and that it has the integral kernel represented by a formula similar to (2.3). However, it seems that such a nice representation formula has not yet obtained if β is a 2-body channel with zero binding energy or a 3-body channel. We know that $H(h)$ has no positive eigenvalues and that $R(\lambda + i0; H(h))$: $L^2_\nu(R^6) \to L^2_{-\nu}(R^6)$, $\nu > 1/2$, is well-defined for all $\lambda > 0$, but it does not immediately from these facts that for such a channel β, $T_{\alpha\to\beta}(\lambda; h)$ is of Hilbert-Schmidt class for all $\lambda > 0$. To prove this, we have to study in detail the limits as $\kappa \to 0$ of such operators as $V_a R(\lambda \pm i\kappa; H(h)) V_b$ with pair potentials V_a and V_b. This study has been done by use of the Faddeev equation method ([2, 5]) and we require the additional assumption that all 2-body subsystem Hamiltonians have no zero resonance energies. Thus this method does not directly apply to the semi-classical problems with parameter h and also this makes difficult the semi-classical analysis for scattering matrices with energy and incident direction fixed in many-body scattering systems.

By making use of the above proposition, we first show that $T_{\alpha\to\beta}(\lambda; h)$ is of Hilbert-Schmidt class for *a.e.* $\lambda > 0$, even if β is a 2-body channel with zero binding energy or a 3-body channel.

Proposition 2.2. *Under the same assumptions as in Theorem* 1.1, *the operator* $T_{\alpha\to\beta}(\lambda; h)$ *is of Hilbert-Schmidt class for a.e.* $\lambda > 0$.

Proof. We denote by $\langle\ ,\ \rangle_\beta$ the L^2 scalar product in $L^2(S^2)$ or $L^2(E^5)$, E^5 being defined by (1.8), according as β is a 2-body or a 3-body channel. Let $\{e_k\}_{k=1}^{\infty}$ be a complete orthonormal system in $L^2(S^2)$ and let $g(\lambda)$ be a real smooth function with compact support in $(0, \infty)$. We first note that by Proposition 2.1, the operator

$$Re\ T_{\alpha\to\alpha}(\lambda; h) = \tfrac{1}{2}(T_{\alpha\to\alpha}(\lambda; h) + T_{\alpha\to\alpha}(\lambda; h)^*)$$

is of trace class for all $\lambda > 0$ as an operator acting on $L^2(S^2)$.

Now, recall the relation (1.10), which follows from the asymptotic completeness of channel wave operators. Then, by definition (1.11), we obtain

$$\sum_\beta T_{\alpha\to\beta}(\lambda; h)^* T_{\alpha\to\beta}(\lambda; h) = -2\ \mathrm{Re}\ \mathrm{T}_{\alpha\to\alpha}(\lambda; h) \tag{2.5}$$

for *a.e.* $\lambda > 0$. This relation yields that

$$\sum_\beta \sum_{k=1}^{\infty} \int g(\lambda)^2 \langle T_{\alpha\to\beta}(\lambda; h)e_k, T_{\alpha\to\beta}(\lambda; h)e_k\rangle_\beta d\lambda$$
$$= -2 \sum_{k=1}^{\infty} \int g(\lambda)^2 \langle Re\ T_{\alpha\to\alpha}(\lambda; h)e_k, e_k\rangle_\alpha d\lambda\ ,$$

which proves the proposition. □

The goal here is to prove the following proposition called the optical theorem which is obtained as a consequence of the asymptotic completeness of channel wave operators.

Proposition 2.3. *Under the same assumptions as in Theorem* 1.1, *one has*

$$\sigma_\alpha(\lambda, \omega; h) = 4\pi(2n_\alpha(\lambda - \lambda_\alpha(h)))^{-1/2} h\ Im\ f_{\alpha\to\alpha}(\omega \to \omega; \lambda, h) \tag{2.6}$$

in $D'((0, \infty) \times S^2)$ *as a function of* (λ, ω), *where*

$$Im\ f_{\alpha\to\alpha}(\omega \to \omega; \lambda, h) = (2\pi)^{-1} n_\alpha h^{-2}\ Im\ (R(\lambda + i0; H(h)) I_a e_\alpha(\omega), I_a e_\alpha(\omega))_0\ .$$

Proof. Let $g(\lambda, \omega)$ be a real smooth function with compact support in $(0, \infty) \times S^2$. We denote by g_λ the multiplication operator by $g(\lambda, \omega)$ acting on $L^2(S^2)$. Then, by (2.5), we have

$$\int\int g(\lambda, \omega)^2 \sigma_\alpha(\lambda, \omega; h) d\omega d\lambda$$
$$= -2(2\pi)^2 h^2 \int (2n_\alpha(\lambda - \lambda_\alpha(h)))^{-1}\ Trace\ (g_\lambda\ Re\ T_{\alpha\to\alpha}(\lambda; h) g_\lambda) d\lambda$$
$$= 4\pi h \int\int g(\lambda, \omega)^2 (2n_\alpha(\lambda - \lambda_\alpha(h)))^{-1/2}\ Im\ f_{\alpha\to\alpha}(\omega \to \omega; \lambda, h) d\omega d\lambda\ .$$

This proves the proposition. □

§ 3. Basic representation formula

For notational brevity, we fix the 2-cluster decomposition $a = \{1, (2, 3)\}$ with which the 2-body initial channel α is associated and write the Jacobi coordinates as

$$y = y_a = r_2 - r_3 , \qquad z = z_a = r_1 - \frac{m_2 r_2 + m_3 r_3}{m_2 + m_3} .$$

We further write

$$e_\alpha = e_\alpha(y, z; \lambda, \omega, h) = \psi_\alpha(y; h) \otimes \varphi_\alpha(z; \lambda, \omega, h) .$$

The quantity which we analyze in the present section is

$$Q = Im\,(R(\lambda + i0; H(h)) I_a e_\alpha, I_a e_\alpha)_0 ,$$

which goes into the representation formula (2.6). The second step toward the proof of the main theorem is to write this quantity in a more convenient form.

Throughout the proof, we fix the constant γ as

$$\gamma = \frac{1}{\rho - 1} \tag{3.1}$$

and take β as

$$\beta = \gamma(1 + \delta) > \gamma \tag{3.2}$$

for some $\delta > 0$, δ being chosen small enough in the discussion below. We now introduce a non-negative smooth partition of unity $\{\chi_j\}_{j=1}^3$, $\chi_j = \chi_j(z; h)$, over R^3 with the following properties: $(\chi.0)$ $\sum_{j=1}^3 \chi_j = 1$; $(\chi.1)$ χ_1 has support in $\{z \in R^3: |z| < 2h^{-\gamma}\}$ and $\chi_1 = 1$ on $\{z \in R^3: |z| \le h^{-\gamma}\}$; $(\chi.2)$ χ_2 has support in

$$B_{\gamma\beta} = \{z \in R^3: h^{-\gamma} < |z| < 2h^{-\beta}\} \tag{3.3}$$

and $\chi_2 = 1$ on $\{z \in R^3: 2h^{-\gamma} \le |z| \le h^{-\beta}\}$; $(\chi.3)$ χ_3 has support in $\{z \in R^3: |z| > h^{-\beta}\}$ and $\chi_3 = 1$ on $\{z \in R^3: |z| \ge 2h^{-\beta}\}$; $(\chi.4)$ For any multi-index α,

$$|\partial_z^\alpha \chi_j(z; h)| \le C_\alpha \langle z \rangle^{-|\alpha|} , \qquad 1 \le j \le 3 ,$$

uniformly in h.

Let $H_a(h)$ be the cluster Hamiltonian defined by (1.1). Then we have $H_a(h) e_\alpha = \lambda e_\alpha$. We now write

$$R(\lambda + i0; H(h)) I_a e_\alpha = \chi_1 e_\alpha + v .$$

As is easily seen, the remainder term v above must satisfy the equation

$$(H(h) - \lambda) v = [\chi_1, H_0(h)] e_\alpha + (\chi_2 + \chi_3) I_a e_\alpha ,$$

where [,] denotes the commutator relation. Define $\theta_j = \theta_j(y, z; \lambda, \omega, h)$, $1 \le j \le 2$, by

$$\begin{aligned} \theta_1 &= [\chi_1, H_0(h)] e_\alpha + \chi_2 I_a^0 e_\alpha , \\ \theta_2 &= \chi_2 (I_a - I_a^0) e_\alpha + \chi_3 I_a e_\alpha , \end{aligned} \tag{3.4}$$

where

$$I_a^0(z) = I_a(y, z)|_{y=0} \,. \tag{3.5}$$

Then

$$R(\lambda + i0; H(h))I_a e_\alpha = \chi_1 e_\alpha + \sum_{j=1}^{2} R(\lambda + i0; H(h))\theta_j \,.$$

A similar representation is obtained for $R(\lambda - i0; H(h))I_a e_\alpha$ also. Hence the quantity Q under consideration is written as

$$Q = \sum_{j=1}^{2} Im\,(\theta_j, \chi_1 e_\alpha)_0 + \sum_{j,k=1}^{2} Im\,(R(\lambda + i0; H(h))\theta_j, \theta_k)_0 \,.$$

By partial integration, the first term on the right side vanishes and hence it follows from Proposition 2.3 that

$$\sigma_\alpha(\lambda, \omega; h) = 2\mu_\alpha(\lambda)^{-1}h^{-1} \sum_{j,k=1}^{2} Im\,(R(\lambda + i0; H(h))\theta_j, \theta_k)_0 \,, \tag{3.6}$$

where $\mu_\alpha(\lambda)$ is defined by (1.15). This representation formula plays an important role in proving the main theorem.

By relation (3.6), the proof is now reduced to evaluating the terms $(R(\lambda + i0; H(h))\theta_j, \theta_k)_0$, $1 \le j, k \le 2$. The remaining sections are devoted to evaluating these terms. Roughly speaking, the leading term of the asymptotic formula in Theorem 1.1 comes from the term $(R(\lambda + i0; H(h))\theta_1, \theta_1)_0$.

§ 4. Remainder estimate

In this section we evaluate the above remainder terms with pairs $(j, k) = (1, 2)$, $(2, 1)$ and $(2, 2)$.

Lemma 4.1. *Let γ be as in* (3.1). *Then one has*

(1) $Im\,\{(R(\lambda + i0; H(h))\theta_1, \theta_2)_0 + (R(\lambda + i0; H(h))\theta_2, \theta_1)_0\} = o(h^{1-2\gamma})$,

(2) $Im\,(R(\lambda + i0; H(h))\theta_2, \theta_2)_0 = o(h^{1-2\gamma})$,

as $h \to 0$ in $D'((0, \infty) \times S^2)$.

Proof. We prove the statement (1) only. The same argument applies to (2) also. The proof is based on the formula

$$\frac{d}{d\lambda}E(\lambda; H(h)) = \frac{1}{2i\pi}(R(\lambda + i0; H(h)) - R(\lambda - i0; H(h)))\,, \qquad \lambda > 0\,, \tag{4.1}$$

where $E(\lambda; H(h))$ denotes the spectral resolution associated with $H(h)$.

Let $g(\lambda, \omega)$ be a real smooth function with compact support in $(0, \infty) \times S^2$ and define the integral $J_1(\omega; h)$ by

$$J_1 = \int_0^\infty g(\lambda, \omega)\, Im\,\{(R(\lambda + i0; H(h))\theta_1, \theta_2)_0 + (R(\lambda + i0; H(h))\theta_2, \theta_1)_0\}d\lambda \,.$$

To prove (1), it suffices to show that

$$J_1(\omega; h) = o(h^{1-2\gamma}), \qquad h \to 0, \tag{4.2}$$

uniformly in $\omega \in S^2$. By formula (4.1), this integral is rewritten as

$$J_1 = \pi \int_0^\infty g(\lambda, \omega)\{(E'(\lambda; H(h))\theta_1, \theta_2)_0 + (E'(\lambda; H(h))\theta_2, \theta_1)_0\}d\lambda$$

with $E'(\lambda; H(h)) = (d/d\lambda)E(\lambda; H(h))$. Let $\|\cdot\|_0$ denote the L^2 norm in $L^2(R^6)$. Then we integrate by parts in λ to obtain that

$$J_1 = O(1)(\|\theta_1\|_0\|\theta_2\|_0 + \|\theta_1\|_0\|\partial_\lambda\theta_2\|_0 + \|\theta_2\|_0\|\partial_\lambda\theta_1\|_0).$$

We evaluate the L^2 norm of the terms θ_1 and $\partial_\lambda\theta_1$. Let $B_{\gamma\beta}$ be defined by (3.3). Recall the notation $z = u + x\omega$ with $u \in \Pi_\omega$ and $x = \langle z, \omega\rangle \in R^1$. Since θ_1 has support in $B_{\gamma\beta}$ as a function of z, we have

$$|\theta_1| \le C(|z| + h^{-\gamma})^{-\rho}|\psi_\alpha(y; h)|.$$

Therefore it follows that

$$\|\theta_1\|_0 = O(h^{\gamma(\rho-3/2)}) = O(h^{1-\gamma/2}), \tag{4.3}$$

$$\|\partial_\lambda\theta_1\|_0 = O(h^{-1})\|x\theta_1\|_0 = O(h^{-3\gamma/2}). \tag{4.4}$$

Next we evaluate the L^2 norm of the terms θ_2 and $\partial_\lambda\theta_2$. By assumption $(V)_\rho$ and (2.1), we have

$$\|\theta_2\|_0 = O(h^{\gamma(\mu-3/2)}) + O(h^{\beta(\rho-3/2)}) = o(h^{1-\gamma/2}) \tag{4.5}$$

for any μ, $\rho < \mu < \rho + d$, d being as in $(V)_\rho$. Similarly we obtain

$$\|\partial_\lambda\theta_2\|_0 = o(h^{-3\gamma/2}). \tag{4.6}$$

The strong decaying assumption with $\rho > 5/2$ is used to evaluate the L^2 norm of the terms $\partial_\lambda\theta_1$ and $\partial_\lambda\theta_2$. The estimates (4.3) ~ (4.6) prove (4.2) and the proof is complete. □

§5. Term with small impact parameter

We decompose the term θ_1 into two terms with small and large impact parameters $u \in \Pi_\omega$. In this section we analyze the term with small impact parameter.

The term θ_1 defined by (3.4) takes the form

$$\theta_1 = f(z; h)e_\alpha,$$

where f has support in $B_{\gamma\beta}$ and satisfies the estimate

$$|\partial_z^\alpha f| \le C_\alpha(|z| + h^{-\gamma})^{-\rho}, \qquad 0 \le |\alpha| \le 2, \tag{5.1}$$

uniformly in h. The explicit representation for $f(z; h)$ is not required throughout the discussion in the present section. In addition to the constants γ and β, we here introduce another constant κ as

$$\kappa = \gamma(1 - \delta) < \gamma \tag{5.2}$$

for the same $\delta > 0$ as in (3.2). As is stated above, we decompose θ_1 as

$$\theta_1 = \theta_{1s} + \theta_{1l} = f_s(z; h)e_\alpha + f_l(z; h)e_\alpha\,, \tag{5.3}$$

where f_s and f_l have the following properties: (1) As a function of $u \in \Pi_\omega$, f_s has support in $\{u \in \Pi_\omega: |u| < 2h^{-\kappa}\}$ and f_l has support in $\{u \in \Pi_\omega: |u| > h^{-\kappa}\}$; (2) Both the functions f_s and f_l are supported in $B_{\gamma\beta}$ and satisfy the estimate (5.1).

The aim here is to prove the following

Lemma 5.1. *Let γ be as in (3.1) and let θ_{1s} and θ_{1l} be as above. Then one has*

(1) $Im\,\{(R(\lambda + i0; H(h))\theta_{1s}, \theta_{1l})_0 + (R(\lambda + i0; H(h))\theta_{1l}, \theta_{1s})_0\} = o(h^{1-2\gamma})$,

(2) $Im\,(R(\lambda + i0; H(h))\theta_{1s}, \theta_{1s})_0 = o(h^{1-2\gamma})$,

as $h \to 0$ in $D'((0, \infty) \times S^2)$.

Proof. The lemma is proved in the same way as in the proof of Lemma 4.1. We prove the statement (1) only.

Let $g(\lambda, \omega)$ be again a real smooth function with compact support in $(0, \infty) \times S^2$. We define the integral $J_2(\omega; h)$ as in the proof of Lemma 4.1. Then we have

$$J_2 = O(1)(\|\theta_{1s}\|_0\|\theta_{1l}\|_0 + \|\theta_{1s}\|_0\|\partial_\lambda\theta_{1l}\|_0 + \|\theta_{1l}\|_0\|\partial_\lambda\theta_{1s}\|_0)$$

where $\|\cdot\|_0$ again denotes the L^2 norm in $L^2(R^6)$.

We now evaluate the L^2 norm of the above terms. We first note that as a function of $x = \langle z, \omega\rangle \in R^1$, θ_{1s} and θ_{1l} are supported in

$$\Gamma = \{x \in R^1: |x| < 2h^{-\beta}\}\,.$$

Since θ_{1s} has support in $\{u \in \Pi_\omega: |u| < 2h^{-\kappa}\}$, we have

$$\|\theta_{1s}\|_0^2 = O(h^{-2\kappa})\int_\Gamma (|x| + h^{-\gamma})^{-2\rho}dx\,,$$

which shows that

$$\|\theta_{1s}\|_0 = O(h^{\gamma(\rho-1/2)-\kappa})\,. \tag{5.4}$$

Similarly we have

$$\|\partial_\lambda\theta_{1s}\|_0^2 = O(h^{-2-2\kappa})\int_\Gamma \langle x\rangle^2(|x| + h^{-\gamma})^{-2\rho}dx$$

and hence

$$\|\partial_\lambda\theta_{1s}\|_0 = O(h^{\gamma(\rho-3/2)-1-\kappa})\,. \tag{5.5}$$

We also have

$$(5.6)\qquad \|\theta_{1l}\|_0 = O(h^{\gamma(\rho-3/2)})$$

and

$$\|\partial_\lambda \theta_{1l}\|_0^2 = O(h^{-2}) \int_\Gamma \langle x \rangle^2 (|x| + h^{-\gamma})^{-2\rho+2} dx$$

which yields that

$$(5.7)\qquad \|\partial_\lambda \theta_{1l}\|_0 = O(h^{\gamma(\rho-2)-1-\beta/2}).$$

It follows immediately from (5.4) and (5.6) that

$$\|\theta_{1s}\|_0 \|\theta_{1l}\|_0 = o(h^{1-2\gamma}).$$

By (5.4) and (5.7), we have

$$\|\theta_{1s}\|_0 \|\partial_\lambda \theta_{1l}\|_0 = h^{1-2\gamma} O(h^\nu)$$

with

$$\nu = \gamma(2\rho - 1/2) - 2 - \kappa - \beta/2 = \delta\gamma/2 > 0$$

and also, by (5.5) and (5.6), we have

$$\|\theta_{1l}\|_0 \|\partial_\lambda \theta_{1s}\|_0 = h^{1-2\gamma} O(h^\nu)$$

with

$$\nu = \gamma(2\rho - 1) - 2 - \kappa = \delta\gamma > 0.$$

These estimates prove that

$$J_2(\omega; h) = o(h^{1-2\gamma}), \qquad h \to 0,$$

uniformly in $\omega \in S^2$ and the proof is complete. □

§6. Term with large impact parameter

By Lemmas 4.1 and 5.1, only the term $(R(\lambda + i0; H(h))\theta_{1l}, \theta_{1l})_0$ makes a contribution to the leading term of the semi-classical asymptotic formula for the total scattering cross secton $\sigma_\alpha(\lambda, \omega; h)$. The aim of this section is to analyze this term with large impact parameter $u \in \Pi_\omega$. The analysis is based on the time-dependent representation formula of resolvent;

$$(6.1)\qquad R(\lambda + i0; H(h)) = ih^{-1} \int_0^\infty \exp(ih^{-1}t\lambda) \exp(-ih^{-1}tH(h)) dt.$$

More precisely, we have to write

$$ih^{-1} \lim_{\varepsilon \downarrow 0} \int_0^\infty \exp(-h^{-1}t\varepsilon) \exp(ih^{-1}t\lambda) \exp(-ih^{-1}tH(h)) dt.$$

For notational brevity, we proceed with the formal representation formula (6.1), because the rigorous justification can be easily done.

Let $g(\lambda, \omega)$ be a real smooth function with compact support in $(0, \infty) \times S^2$ and define the integral $J_0(\omega; h)$ as

$$J_0 = \int_0^\infty g(\lambda, \omega)(R(\lambda + i0; H(h))\theta_{1l}, \theta_{1l})_0 d\lambda \tag{6.2}$$

By (6.1), this is rewritten as

$$J_0 = ih^{-1} \int_0^\infty g(\lambda, \omega) d\lambda \int_0^\infty \exp(ih^{-1}t\lambda)(\exp(-ih^{-1}tH(h))\theta_{1l}, \theta_{1l})_0 dt\,.$$

Let β be as in (3.2). We now fix τ as

$$\tau = Nh^{-\beta} \tag{6.3}$$

for $N \gg 1$ large enough and decompose the integral above into two parts;

$$J_0 = ih^{-1} \int_0^\infty g(\lambda, \omega) d\lambda \left\{ \int_0^\tau \dots dt + \int_\tau^\infty \dots dt \right\}.$$

We denote by $J_0^1(\omega; h)$ and $J_0^2(\omega; h)$ the first and second integrals on the right side, respectively.

Lemma 6.1.

$$J_0^2(\omega; h) = o(h^{1-2\gamma})\,, \qquad h \to 0\,,$$

uniformly in $\omega \in S^2$.

Proof. Recall the form of θ_{1l}; $\theta_{1l} = f_l(z; h)e_\alpha$. By use of the relation

$$\exp(ih^{-1}t\lambda) = -h^2t^{-2}\partial_\lambda^2 \exp(ih^{-1}t\lambda)\,,$$

we integrate by parts in λ, so that the integral J_0^2 under consideration is represented as a linear combination of such integrals as

$$h \int_0^\infty \partial_\lambda^k g d\lambda \int_\tau^\infty t^{-2} \exp(ih^{-1}t\lambda)(\exp(-ih^{-1}tH(h))f_l\partial_\lambda^m e_\alpha, f_l\partial_\lambda^n e_\alpha)_0 dt$$

with $k + m + n = 2$. We evaluate the L^2 norm of $x^m f_l e_\alpha$ with $0 \le m \le 2$. Since f_l has support in $B_{\gamma\beta}$ and satisfies (5.1), these terms obey the following estimates: If $\rho > m + 3/2$, then

$$\|x^m f_l e_\alpha\|_0 = O(h^{\gamma(\rho - m - 3/2)})$$

and if $\rho \le m + 3/2$, then we can take ε, $1 > \varepsilon > -\rho + m + 3/2$, so that

$$\|x^m f_l e_\alpha\|_0 = O(h^{-\beta\varepsilon})\|x^m\langle z\rangle^{-\varepsilon} f_l e_\alpha\|_0 = O(h^\nu)$$

with

$$\nu = -\varepsilon(\beta - \gamma) + \gamma(\rho - m - 3/2).$$

This proves the lemma. □

Next we consider the integral $J_0^1(\omega; h)$. We study this integral by constructing an approximate representation for $\exp(-ih^{-1}tH(h))\theta_{1l}$ with t, $0 \le t \le \tau$.

Let $\mu_\alpha = \mu_\alpha(\lambda)$ be defined by (1.15). Then we define $v = v(t, z; \lambda, \omega, h)$ by

$$v = f_l(z - \mu_\alpha \omega t; h) \exp\left(-ih^{-1}\int_0^t I_\alpha^0(z - \mu_\alpha\omega(t-s))ds\right). \tag{6.4}$$

After an elementary but somewhat tedious computation, we see that ve_α satisfies the equation

$$(ih\partial_t - H(h) + \lambda)ve_\alpha = r,$$

where $r(t) = r(t, y, z; \lambda, \omega, h)$ is written as $r = r_1 + r_2$ with

$$\begin{aligned} r_1 &= \frac{1}{2n_\alpha}h^2(\Delta_z v)e_\alpha, \\ r_2 &= (I_\alpha^0(z) - I_\alpha(y, z))ve_\alpha. \end{aligned} \tag{6.5}$$

Therefore, by Duhamel's principle, we have

$$\begin{aligned} &\exp(ih^{-1}t\lambda)\exp(-ih^{-1}tH(h))\theta_{1l} \\ &= ve_\alpha + ih^{-1}\int_0^t \exp(ih^{-1}(t-s)\lambda)\exp(-ih^{-1}(t-s)H(h))r(s)ds. \end{aligned}$$

Thus the integral $J_0^1(\omega; h)$ under consideration behaves like

$$J_0^1 = ih^{-1}\int_0^\infty g(\lambda, \omega)d\lambda \int_0^\tau (v, f_l)_z dt + O(h^{-2})\|\theta_{1l}\|_0 \int_0^\tau\int_0^t \|r(s)\|_0 ds dt \tag{6.6}$$

as $h \to 0$, where $(\ ,\ )_z$ denotes the L^2 scalar product in $L^2(R^3; dz)$.

Lemma 6.2.

$$J_0^1(\omega, h) = ih^{-1}\int_0^\infty g(\lambda, \omega)d\lambda \int_0^\tau (v, f_l)_z dt + o(h^{1-2\gamma}), \qquad h \to 0,$$

uniformly in $\omega \in S^2$.

Proof. We evaluate the L^2 norm of the remainder term $r(s)$ with $0 \le s \le \tau$. Since f_l is supported in

$$\Lambda = \{u \in \Pi_\omega : |u| > h^{-\kappa}\},$$

$r_1(s)$ and $r_2(s)$ defined by (6.5) have also support in Λ as a function of $u \in \Pi_\omega$.

Therefore we obtain

$$\|r_1(s)\|_0^2 = O(h^4)\int_A \langle u\rangle^{-2\rho+1}du + O(h^2)\int_A \langle u\rangle^{-4\rho+3}du + O(1)\int_A \langle u\rangle^{-6\rho+5}du .$$

This yields that

$$\|r_1(s)\|_0 = O(h^{\kappa(3\rho-7/2)})$$

uniformly in $s \geq 0$. Similarly, we use the assumption $(V)_\rho$ to obtain that

$$\|r_2(s)\|_0 = O(h^{\kappa(\rho+\mu-3/2)})$$

for any μ, $\rho < \mu < \rho + d$. Since

$$\|\theta_{1l}\|_0 = O(h^{\gamma(\rho-3/2)}),$$

the second term on the right side of (6.6) is of order $(O(h^\nu) + O(h^{\nu'}))h^{1-2\gamma}$, where

$$\nu = 2\gamma - 3 - 2\beta + \gamma(\rho - 3/2) + \kappa(3\rho - 7/2) = \{(\rho - 2) - 3\delta(\rho - 1/2)\}\gamma$$

and

$$\nu' = 2\gamma - 3 - 2\beta + \gamma(\rho - 3/2) + \kappa(\rho + \mu - 3/2) = \{(\mu - \rho) - \delta(\rho + \mu + 1/2)\}\gamma .$$

Thus we can take δ in (3.2) so small that $\nu > 0$ and $\nu' > 0$. This proves the lemma. □

By assumption, $\lambda_\alpha(h) < -\lambda_0$ uniformly in h and hence it follows by definition (1.15) that

$$\mu_\alpha = \mu_\alpha(\lambda) > \sqrt{2\lambda_0/n_\alpha} .$$

Since f_l is supported in $\{x = \langle z, \omega\rangle \in R^1 : |x| < 2h^{-\beta}\}$ as a function of x, we can take N in (6.3) so large that $(v, f_l)_z = 0$ for $t > \tau$. Hence we have by Lemmas 6.1 and 6.2 that

$$J_0(\omega; h) = ih^{-1}\int_0^\infty g(\lambda, \omega)d\lambda \int_0^\infty (v, f_l)_z dt + o(h^{1-2\gamma}), \qquad h \to 0, \tag{6.7}$$

uniformly in $\omega \in S^2$.

§ 7. Calculation of leading term

In this section we calculate explicitly the leading term of the semi-classical asymptotic formula for the total scattering cross section $\sigma_\alpha(\lambda, \omega; h)$ and complete the proof of the main theorem.

The next lemma, together with relation (3.6), completes the proof of Theorem 1.1.

Lemma 7.1.

$$Im\,(R(\lambda + i0; H(h))\theta_{1l}, \theta_{1l})_0 = k_0(\lambda, \omega; h) + o(h^{1-2\gamma}), \qquad h \to 0,$$

in $D'((0, \infty) \times S^2)$, *where*

$$k_0 = 2\mu_\alpha(\lambda)h \int_{\Pi_\omega} \sin^2 \left\{ \frac{1}{2\mu_\alpha(\lambda)h} \int I_a^0(u + x\omega)dx \right\} du \tag{7.1}$$

with $\mu_\alpha(\lambda)$ *defined by* (1.15).

Proof. The proof is divided into several steps.

(1) Let $J_0(\omega; h)$ be defined by (6.2). To prove the lemma, it suffices to show that

$$Im\, J_0 = \int_0^\infty g(\lambda, \omega)k_0(\lambda, \omega; h)d\lambda + o(h^{1-2\gamma}) \tag{7.2}$$

uniformly in $\omega \in S^2$. Note that $g(\lambda, \omega)$ is real-valued. By (6.7), $Im\, J_0(\omega; h)$ behaves like

$$Im\, J_0 = h^{-1} \int_0^\infty g(\lambda, \omega)d\lambda \int_0^\infty Re\,(v, f_l)_z dt + o(h^{1-2\gamma})\,. \tag{7.3}$$

Thus the proof is reduced to calculating the term on the right side.

(2) Define the differential operator

$$A(h) = \mu_\alpha \left\langle \omega, \frac{1}{i}\nabla_z \right\rangle + h^{-1}I_a^0$$

with $\mu_\alpha = \mu_\alpha(\lambda)$. The operator $A(h)$ admits a unique self-adjoint realization in $L^2(R^3; dz)$. We denote by the same notation $A(h)$ this self-adjoint realization and by

$$G_t = \exp\,(-itA(h))\,, \qquad t \in R^1\,,$$

the unitary group generated by $A(h)$. Then the solution $w(t, z; h) = (G_t w_0)(z; h)$ to the evolution equation

$$i\partial_t w - A(h)w = 0\,, \qquad w(0, z) = w_0 \in L^2(R^3; dz)$$

is explicitly represented by formula (6.4) with $f_l = w_0$;

$$G_t w_0 = w_0(z - \mu_\alpha \omega t) \exp\left(-ih^{-1} \int_0^t I_a^0(z - \mu_\alpha\omega(t - s))ds \right).$$

According to this notation, we may write v as $v = G_t f_l$.

Now, recall the decomposition

$$\theta_1 = f(z; h)e_\alpha = f_s(z; h)e_\alpha + f_l(z; h)e_\alpha\,,$$

where f_s is supported in $\{u \in \Pi_\omega\colon |u| < 2h^{-\kappa}\}$ as a function of u. As is easily seen,

$$\int_0^\infty (G_t f_s, f)_z dt = o(h^{2-2\gamma})$$

and

$$\int_0^\infty (G_t f_l, f_s)_z dt = o(h^{2-2\gamma}).$$

Therefore it follows from (7.3) that

$$Im\, J_0 = h^{-1} \int_0^\infty g(\lambda, \omega) d\lambda \int_0^\infty Re\,(G_t f, f)_z dt + o(h^{1-2\gamma}). \tag{7.4}$$

(3) We are now in a position to require the explicit representation for $\theta_1 = f(z; h) e_\alpha$. Define $f_0 = f_0(z; h)$ as

$$f_0 = ih\mu_\alpha \langle \omega, \nabla_z \rangle \chi_1$$

and $f_j = f_j(z; h)$, $1 \le j \le 3$, as

$$f_j = \chi_j(z; h) I_a^0(z).$$

Then, by definition,

$$I_a^0(z) = \sum_{j=1}^3 f_j(z; h)$$

and also it follows that

$$f(z; h) = f_0(z; h) + f_2(z; h) + \text{remainder term}.$$

The remainder term above is supported in $\{z \in R^3 : h^{-\gamma} < |z| < 2h^{-\gamma}\}$ and obeys the bound $O(h) \langle z \rangle^{-\rho-1}$. Hence this term can be proved to make no contribution to the leading term.

The next lemma plays a basic role in calculating the leading term.

Lemma 7.2.

(1) $$h^{-1} \int_0^\infty G_t f_0 dt = i\chi_1 + h^{-1} \int_0^\infty G_t f_1 dt.$$

(2) $$h^{-1} \int_0^\infty G_{-t} f_0 dt = -i\chi_1 + h^{-1} \int_0^\infty G_{-t} f_1 dt.$$

Proof. We prove (1) only. By definition,

$$f_0 - f_1 = -hA(h)\chi_1$$

and hence

$$G_t(f_0 - f_1) = -ih \frac{d}{dt} G_t \chi_1.$$

This proves the relation (1) immediately. □

Since $(i\chi_1, f_0)_z = 0$ by partial integration, Lemma 7.2, together with (7.4), implies that

$$(7.5)\quad Im\, J_0 = h^{-1}\int_0^\infty g(\lambda, \omega)d\lambda \int_0^\infty Re\,(G_t(f_1 + f_2), f_1 + f_2)_z dt + o(h^{1-2\gamma}).$$

(4) The next lemma is easy to prove.

Lemma 7.3.

$$(1)\qquad \int_0^\infty Re\,(G_t f_3, f_j)_z dt = o(h^{2-2\gamma}),\ 1 \le j \le 3.$$

$$(2)\qquad \int_0^\infty Re\,(G_t f_j, f_3)dt = o(h^{2-2\gamma}),\ 1 \le j \le 3.$$

Proof. Since $|f_2| \le C(|z| + h^{-\gamma})^{-\rho}$ and $|f_3| \le C(|z| + h^{-\beta})^{-\rho}$ by definition, relations (1) and (2) can be easily proved for the cases $j = 2$ and $j = 3$. In the case $j = 1$, we use Lemma 7.2. If we take account of the bound $|f_0| \le C(|z| + h^{-\gamma})^{-\rho}$, relations (1) and (2) can be similarly proved for the case $j = 1$ also. □

The lemma above, together with relation (7.5), yields that

$$Im\, J_0 = h^{-1}\int_0^\infty g(\lambda, \omega)d\lambda \int_0^\infty Re\,(G_t I_a^0, I_a^0)_z dt + o(h^{1-2\gamma}).$$

(5) The proof of the lemma is completed in this step. We calculate the integral

$$L_0 = h^{-1}\, Re(\int_0^\infty G_t I_a^0 dt, I_a^0)_z = Im(ih^{-1}\int_0^\infty G_t I_a^0 dt, I_a^0)_z .$$

Lemma 7.4. *Write $z \in R^3$ as $z = u + x\omega$ with $u \in \Pi_\omega$ and $x = \langle z, \omega\rangle \in R^1$. Then one has*

$$ih^{-1}\int_0^\infty G_t I_a^0 dt = 1 - \exp\left(-i\frac{1}{\mu_a h}\int_{-\infty}^x I_a^0(u + s\omega)ds\right).$$

Proof. Define

$$F(t, z; h) = \exp\left(-ih^{-1}\int_0^t I_a^0(z - \mu_a\omega(t - s))ds\right).$$

Then we have

$$\frac{d}{dt}F = -ih^{-1}G_t I_a^0$$

and also

$$F(\infty, z; h) = \exp\left(-i\frac{1}{\mu_\alpha h}\int_{-\infty}^{x} I_a^0(u + s\omega)ds\right)$$

by making a simple change of variables. Hence the lemma follows at once. □

By Lemma 7.4, we obtain that

$$L_0 = \int_{\Pi_\omega}\int I_a^0(u + x\omega)\sin\left\{\frac{1}{\mu_\alpha h}\int_{-\infty}^{x} I_a^0(u + s\omega)ds\right\}dxdu$$

$$= -\mu_\alpha h\int_{\Pi_\omega}\int \frac{d}{dx}\left[\cos\left\{\frac{1}{\mu_\alpha h}\int_{-\infty}^{x} I_a^0(u + s\omega)ds\right\}\right]dxdu\,.$$

This shows that $L_0 = k_0(\lambda, \omega; h)$, k_0 being defined by (7.1), and completes the proof of Lemma 7.1. □

The proof of the main theorem is now complete.

DEPARTMENT OF MATHEMATICS,
KYOTO UNIVERSITY
DEPARTMENT OF MATHEMATICS,
IBARAKI UNIVERSITY

References

[1] W. Amrein, A. M. Berthier and V. Georgescu, On Mourre's approach to spectral theory, Helv. Phys. Acta., **62** (1989), 1–20.

[2] W. Amrein, J. Jauch and K. Sinha, Scattering Theory in Quantum Mechanics, W. A. Benjamin, 1977.

[3] W. Amrein and D. Pearson, A time-dependent approach to the total scattering cross section, J. Phys. A: Math. Gen., **12** (1979), 1469–1492.

[4] W. Amrein, D. Pearson and K. Sinha, Bounds on the total scattering cross-section for N-body systems, Nuovo Cimento, **52** (1979), 115–131.

[5] W. Amrein and K. Sinha, On three-body scattering cross sections, J. Phys. A: Math. Gen., **15** (1982), 1567–1586.

[6] V. Enss, Quantum scattering theory of two- and three-body systems with potentials of short and long range, Schrödinger operators, Lect. Notes in Math. **1159** (1985).

[7] V. Enss and B. Simon, Finite total cross sections in non-relativistic quantum mechanics, Commun. Math. Phys., **76** (1980), 177–209.

[8] R. Froese and I. Herbst, Exponential bounds and absence of positive eigenvalues of N-body Schrödinger operators, Commun. Math. Phys., **87** (1982), 429–447.

[9] H. T. Ito, Charge transfer model and (2-cluster) → (2-cluster) three-body scattering, to appear in J. Math. Kyoto Univ.

[10] E. Mourre, Absence of singular continuous spectrum of certain self-adjoint operators, Commun. Math. Phys., **78** (1981), 391–408.

[11] P. Perry, I. M. Sigal and B. Simon, Spectral analysis of N-body Schrödinger operators, Ann. of Math., **114** (1981), 519–567.

[12] M. Reed and B. Simon, Methods of Modern Mathematical Physics, III, Scattering Theory, Academic Press, 1979.

[13] D. Robert and H. Tamura, Semi-classical estimates for resolvents and asymptotics for total scattering cross-sections, Ann. Inst. H. Poincaré, **46** (1987), 415–442.

[14] D. Robert and H. Tamura, Asymptotic behavior of scattering amplitudes in semi-classical and low energy limits, Ann. Inst. Fourier Grenoble, **39** (1989), 155–192.

[15] I. M. Sigal and A. Soffer, The N-particle scattering problem: asymptotic completeness for short-range systems, Ann. of Math., **126** (1987), 35–108.

[16] A. V. Sobolev and D. R. Yafaev, On the quasi-classical limit of the total scattering cross-section in non-relativistic quantum mechanics, Ann. Inst H. Poincaré, **44** (1986),195–210.

[17] H. Tamura, Principle of limiting absorption for N-body Schrödinger operators, a remark on the commutator method, Lett. Math. Phys., **17** (1989), 31–36.

[18] B. R. Vainberg, Ouasi-classical approximation in stationary scattering problems, Func. Anal. Appl., **11** (1977), 6–18.

[19] D. R. Yafaev, The eikonal approximation and the asymptotics of the total cross-section for the Schrödinger equation, Ann. Inst. H. Poincaré, **44** (1986), 397–425.

[20] D. R. Yafaev, Ouasiclassical asymptotics of the scattering cross-section for the Schrödinger equation, Math. USSR Izvestiya, **32** (1989), 141–165.

[21] K. Yajima, The quasi-classical limit of scattering amplitude—L^2-approach for short-range potentials—, Japan J. Math., **13** (1987), 77–126.