The eikonal method in the three-body problem

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Some properties of the first terms of a general eikonal expansion obtained by the authors in the three-body problem are investigated. A numerical calculation of the angular distribution of protons in proton-hydrogen atom charge exchange is performed and agrees with experiment (for the total cross-section) and with the data of other authors.

1. INTRODUCTION

There has been great interest recently in the eikonal approximation, in the form of Glauber[1] or Schiff[2], in the theory of nonrelativistic[3-5] and relativistic[6,7] scattering at high energies. Using the eikonal method, it is possible to obtain good agreement with experiment (compared with the Born, impulse, classical, etc., approximations) in the description of nuclear[8] and atomic[9] scattering, and also to investigate the analytic properties of the high-energy scattering amplitudes[10]. It should be said, however, that the usual derivation of the eikonal formulas from a partial-wave expansion[11] or an integral identity[12] for the scattering amplitude is inapplicable in the case of multi-channel scattering (processes with rearrangement), and also in the determination of the eikonal corrections associated with large momentum transfers in one or several collision events. The different nonrigorous arguments which have often been used by a number of authors in applying the usual eikonal formulas for rearrangement processes lead to errors[13]. A rigorous derivation of the eikonal approximation from the scattering equations is therefore of great interest for the physics of atom-molecule collisions[1)]. The authors[15,16] have previously suggested a general formalism for the eikonal expansion of the Lippmann-Schwinger equations using the technique of eikonal propagators[17] and, in the three-body problem, have obtained explicit analytic expressions for the first three terms of the expansion, suitable for direct calculations of different processes.

In this work, the case of scattering of a particle by a bound state is considered and two terms of the eikonal expansion are given in a form that is more convenient for obtaining numerical estimates and for computer calculations. Certain properties of the eikonal amplitudes, important in the calculation of actual processes, are considered. A concrete calculation is performed of the angular distribution of the resonance charge exchange this calculation is interesting from the point of view of applications, and also, because of the Coulomb divergences of the eikonal phases in the standard approach, from a theoretical point of view.

2. EIKONAL EXPANSION IN THE THREE-BODY PROBLEM

It is well known[12] that the matrix element of the transition operator from channel a to channel b has the form

$$\mathcal{T}_{ab} = (\Psi_b, T_{\bar{b}a}\Psi_a) = (\Psi_b, T_{b\bar{a}}\Psi_a), \tag{1}$$

where Ψ_a and Ψ_b are the asymptotic wavefunctions of the initial and final states, and

$$T_{\bar{b}a} = H_b' + H_b'\mathcal{J}^+(W)H_a', \quad T_{b\bar{a}} = H_a' + H_b\mathcal{J}^+(W)H_a', \qquad W = E + i\varepsilon, \quad \varepsilon \to 0^+. \tag{2}$$

The exact Green function $\mathcal{J}$ of the problem satisfies the equations

$$\mathcal{J} = G_a + \mathcal{J}H_a'G_a = G_b + G_bH_b'\mathcal{J}, \qquad G_a(W) = (W - H_a)^{-1}, \quad G_b(W) = (W - H_b)^{-1}. \tag{3}$$

To obtain the eikonal expansion, we replace the partial Green functions $G_{a,b}$ by the eikonal propagators $G_{i,f}$ describing the free relative motion of the fragments in the initial and final states in specified directions[17]:

$$G_j(\mathbf{p}) = [(\mathbf{k}_j - \mathbf{p})\mathbf{v}_j + i\varepsilon]^{-1}, \quad \varepsilon \to 0^+, \quad j = i, f. \tag{4}$$

Substituting G_i for G_a in (3), we obtain an equation for the exact eikonal Green function $\mathcal{J}_i$. An equation for $\mathcal{J}_f$ is obtained analogously. Expanding the exact Green function in powers of the perturbations

$$N_i = G_i^{-1} - G_a^{-1}, \qquad N_f = G_f^{-1} - G_b^{-1} \tag{5}$$

and substituting into (2), we obtain after the appropriate symmetrization[16]

$$T_{ba} = {}^1/_2(T_i + T_f) + {}^1/_2H_b'\mathcal{J}_f(N_i + N_f)\mathcal{J}_iH_a' + H_b'\mathcal{J}_iN_f\mathcal{J}N_i\mathcal{J}_iH_a', \qquad T_i = H_b' + H_b'\mathcal{J}_iH_a', \quad T_f = H_a' + H_b'\mathcal{J}_fH_a'. \tag{6}$$

We note that the last term in (6) is important only for the description of momentum-transfer processes resulting from repeated collisions, if the interaction of the particles between collisions is important (e.g., excitation to a weakly bound state). Therefore, it is sufficient for the purposes of our work to calculate only the first two terms.

Proceeding as in[16], it is possible to obtain the following approximate expressions, which we write in a "semi-classical" form more convenient for obtaining various estimates and for numerical calculations (see Fig. 1):

a) One-channel scattering (1 + (2, 3) → 1 + (2, 3)*):

$$T_{mn}(\mathbf{p}_f, \mathbf{p}_i) = \int d\mathbf{R}\, d\mathbf{r}\, \varphi_m^*\varphi_n \exp[iS(\Delta, \mathbf{R}, \mathbf{r})] \times \left[W(\mathbf{R}, \mathbf{r})\cos\delta_-(\mathbf{R}, \mathbf{r}) - \frac{\Delta^2}{\mu_i}\sin\frac{\delta_i}{2}\sin\frac{\delta_f}{2}\right]; \tag{7}$$

here, φ_n and φ_m are the functions of the initial and final states of the target,

$$W = V_{13} + V_{12}, \quad \mu_i = m_1(m_2 + m_3)/(m_1 + m_2 + m_3), \quad \Delta = \mathbf{k}_i - \mathbf{k}_f,$$

and S is an approximate expression for the action along

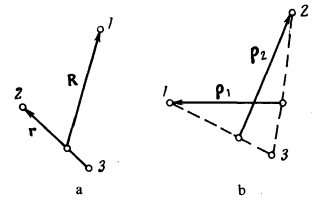

FIG. 1. Coordinate systems for (a) excitation and (b) rearrangement.

a trajectory consisting of two straight lines ($\delta_\pm = \frac{1}{2}(\delta_i \pm \delta_f)$):

$$S = \Delta\mathbf{R} + \delta_+(\mathbf{R}, \mathbf{r}), \quad \delta_{i,f} = -\int_0^\infty W(\mathbf{R} \mp \mathbf{v}_{i,f}t, \mathbf{r})\,dt. \tag{8}$$

Introducing the average potential W_{av} with range R_0, we obtain the estimate

$$\frac{T_1}{T_0} \sim \frac{\Delta^2 W_{av}^2 R_0^2}{W_{av} k^2} \sim \frac{W_{av}}{E}(\Delta R_0)^2. \tag{9}$$

The eikonal parameter W_{av}/E should always be less than unity, and so we obtain that the first correction can be neglected if

$$\Delta R_0 < 1. \tag{10}$$

We note that, since $\Delta_{max} \sim k$, the eikonal formula gives a good description of the scattering at all angles when

$$W_{av} R_0^2 < 1. \tag{11}$$

In this case we may assume, in estimates of the type (9), that

$$V_{av} R_0^2 \sim \int_0^\infty dr\, r |V(r)| e^{i\delta(r)},$$

where $\delta(r)$ is the eikonal phase corresponding to the potential $V(r)$. In this approach, V_{av} is defined even for singular potentials. Thus, (11) serves to strengthen the corresponding result for the Born approximation.

b) Multi-channel scattering ($1 + (2,3) \to 2 + (1,3)$):

$$T_{mn}(\mathbf{p}_f, \mathbf{p}_i) = \iint d\rho_1\, d\rho_2 \exp[iS(\mathbf{k}_i^{(1)}, \mathbf{k}_f^{(2)}, \rho_1, \rho_2)] \frac{\varphi_m^* \varphi_n}{2} \Big\{ V_2 \exp(i\delta_-)$$
$$+ V_1 \exp(-i\delta_-) - \sin\frac{\delta_i}{2} \sin\frac{\delta_f}{2} \Big[\Big(\frac{1}{\mu_1} + \frac{2}{m_{13}} \Big) \mathbf{k}_i^{(1)2} + \Big(\frac{1}{\mu_2} + \frac{2}{m_{23}} \Big) \mathbf{k}_f^{(2)2} \Big] \Big\}; \tag{12}$$

here,

$$V = V_1 + V_{23} = V_2 + V_{13}, \quad m_{ij} = \frac{m_i m_j}{m_i + m_j}, \quad \mu_k = \frac{m_k(m_i + m_j)}{m_k + m_i + m_j},$$

$$\delta_i = -\int_0^\infty dt\, V_1(\rho_1 - \mathbf{v}_i t, \rho_2), \quad \delta_f = -\int_0^\infty dt\, V_2(\rho_1, \rho_2 + \mathbf{v}_f t), \tag{13}$$

where $\delta_\pm = \frac{1}{2}(\delta_i \pm \delta_f)$ and

$$\mathbf{v}_i = \frac{\mathbf{k}_i}{m_1}, \quad \mathbf{v}_f = \frac{\mathbf{k}_f}{m_2} - \frac{\Delta}{m_1 + m_3},$$

$$\mathbf{k}_i^{(1)} = \frac{\mu_1}{m_1}\mathbf{k}_i, \quad \mathbf{k}_f^{(2)} = \frac{\mu_2}{m_2}\Big(\mathbf{k}_f - \frac{m_2}{m_1 + m_3}\Delta\Big),$$

$$S = \mathbf{k}_i^{(1)}\rho_1 - \mathbf{k}_f^{(2)}\rho_2 + \delta_+(\rho_1, \rho_2).$$

If the parameters V_{av} and R_0 are the same for V_1 and V_2, then, as in (9), we obtain

$$\frac{T_1}{T_0} \sim \frac{V_{av}}{E}(kR_0)^2 \sim V_{av} R_0^2. \tag{14}$$

As we shall see, this estimate is too crude. However, it is clear from (14) that, for processes with rearrangement, the first correction is the more important one at all scattering angles.

We now note certain properties of the eikonal approximation that are important for applications. The eikonal approximation is equivalent to an asymptotic summation of the Born series. For potential scattering, this fact is well known[2,18]. For inelastic processes, however, the impression may be gained, in connection with the interpretation of the eikonal expansion as a multiple-scattering series[17], that this is not so. We shall examine this statement using the example of a rearrangement process.

If we perform l iterations of the first Eq. (3) and $n - l$ iterations of the second, then, after substitution into (2), we find that we must consider terms of the form

$$(V_2 G_2)^{n-l} V_i (G_1 V_1)^l, \quad i = 1, 2; \; l = 0, \ldots, n. \tag{15}$$

If the scattering in the $(n + 1)$-st event occurs with small momentum transfer, the matrix elements of all the operators (15) define the same process (the Glauber mechanism); if the scattering occurs in n events with small momentum transfer and in one event with large momentum transfer (the Schiff mechanism), the matrix elements of the operators (15) will be different. In accordance with this,

$$\mathcal{T}_n = \frac{1}{2F_{S,G}} \sum_{l=0}^{n} \langle \mathbf{p}_f, m | (V_2 G_2)^{n-l} (V_1 + V_2)(G_1 V_1)^l | \mathbf{p}_i, n \rangle, \tag{16}$$

where $F_S = 1$ and $F_G = n + 1$.

In the high-energy limit, we can replace the partial Green functions by the eikonal propagators; this corresponds to expanding $G_{1,2}$ in a series and retaining the terms proportional to the momentum $\mathbf{p}_{i,f}$. In this case, the matrix element in the summation, like that for potential scattering[18], can be calculated explicitly. Using the symmetry of this matrix element under permutations of the first l momenta and of the last $n - l$ momenta, and also using the binomial formula, we obtain

$$\mathcal{T}_n \approx \frac{1}{F_{S,G}} \frac{1}{n!} \iint d\rho_1\, d\rho_2 \exp[i\mathbf{k}_i^{(1)}\rho_1 - i\mathbf{k}_f^{(2)}\rho_2] \frac{(V_1 + V_2)}{2} [i\delta_i + i\delta_f]^n \varphi_m^* \varphi_n.$$

Summing all the terms of the iterative series, we shall have

$$\mathcal{T} \approx \iint d\rho_1\, d\rho_2 \exp[i\mathbf{k}_i^{(1)}\rho_1 - i\mathbf{k}_f^{(2)}\rho_2] \varphi_m^* \varphi_n \frac{(V_1 + V_2)}{2} B_{G,S}, \tag{17}$$

where

$$B_{G,S} = \begin{cases} \exp(i2\delta_+), & F = 1 \\ \exp(i\delta_+)\sin\delta_+/\delta_+, & F = n + 1 \end{cases} \tag{18}$$

In the case $F = n + 1$, the expression (17) is equivalent to the first term in (12). To obtain the second term of the eikonal expansion, it is necessary to retain the term proportional to the momentum transfer in the expansion of the partial Green functions. In this way, we obtain the estimate

$$T_1 / T_0 \sim (\varkappa / p)^2 V_{av} R_0^2, \tag{19}$$

where $\varkappa$ is the momentum transfer (concerning the definition of the momentum transfer for processes with rearrangement, see Sec. 3. In the eikonal directions, $\varkappa$ takes small values and so (19) is a refinement of (14).

The eikonal approximation is a high-energy approximation. Therefore, by virtue of the well known fact that the scattering is concentrated about the principal directions as $E \to \infty$[14], in calculating the total cross-section of the different processes we can expand (7) and (12) in a parameter characterizing the deviation from the eikonal direction, assuming this parameter to be small. We shall determine, e.g., the excitation cross-section (the case of multi-channel scattering will differ in that there are several eikonal directions). For the small parameter we can take

$$\beta = \sin(\theta/2) = O(1/p),$$

where θ is the scattering angle. We introduce the polar coordinate system $R(\rho, \varphi, z)$, where the z-axis is along the bisector of θ. Then for $\theta = 0$ ($\delta = \delta_i = \delta_f$),

$$\operatorname{Im} T_{nn}(\mathbf{p}_i, \mathbf{p}_i) = 2\pi \frac{2p}{\mu_1} \int d\mathbf{r}\, d\rho\, \rho \varphi_n^2(\mathbf{r}) \sin^2\delta. \tag{20}$$

For $\theta \neq 0$, in first order in β and 1/p we have

$$\Delta\mathbf{R} = 2p_i\rho\beta\cos\varphi - (p_i - p_f)\rho\beta\cos\varphi + (p_i - p_f)z,$$
$$\delta_+ = \delta + O(\beta^3),\ \delta_- = O(\beta^2),$$
$$(p_i - p_f)/p_i = O(1/p^2).$$

Performing the integration over φ and z, we obtain

$$T_{m,n}(\mathbf{p}_f, \mathbf{p}_i) = 2\pi\frac{2p_i}{\mu_1}\int d\mathbf{r}\,\varphi_m^*\varphi_n\int d\rho\,\rho J_0(2p_i\rho\beta)e^{i\delta}\delta, \qquad (21)$$

which is the three-particle generalization of the Glauber formula[9]. Using the completeness condition on the functions $\{\varphi_n\}$ and an addition theorem for Bessel functions, we obtain

$$\mathrm{Im}\frac{\mu_1}{2\pi}T_{nn}(\mathbf{p}_i, \mathbf{p}_i) = \frac{p_i}{2\pi}\sigma_{tot} + O\left(\frac{1}{p^2}\right), \qquad (22)$$

where σ_{tot} is the total excitation cross-section. The relation (22) is the well known optical theorem. Therefore, in calculating the total cross-section, we can confine ourselves at large E to calculating the differential cross-section only in the region of the eikonal directions. We shall use this fact below in Sec. 3.

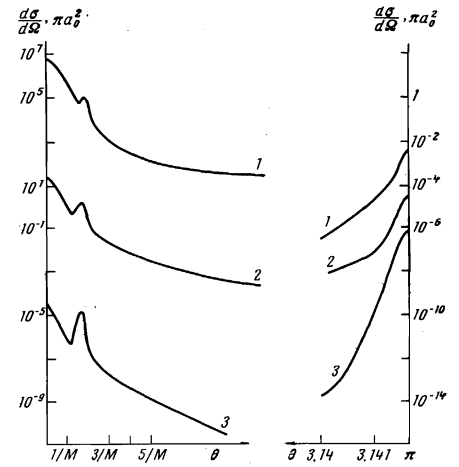

FIG. 2. Differential cross section for resonance charge exchange in the eikonal approximation for E = 100 keV (1), 1 MeV (2) and 10 MeV (3).

3. RESONANCE CHARGE-EXCHANGE CROSS SECTION

The resonance charge-exchange $H^+ + H(1s) \rightarrow H(1s) + H^+$ is one of the most well studied rearrangement processes; for this process, sufficiently good experimental data on the total cross-section at high energies (10^3 eV $< E < 10^5$ eV) exist[19]. However, in spite of the large number of theoretical papers devoted to this process (cf., e.g.,[13,20]), the questions of the choice of the perturbation and coordinate frame, of the role of the two charge-exchange mechanisms (electron capture and proton ejection), etc.,[2)], which are important in the theory of forward reactions with rearrangement, have remained unelucidated up to the present time. It is therefore of interest to calculate the angular distribution for this reaction in the eikonal approximation.

Direct application of the eikonal formula (12) is impossible in the present case, because of the Coulomb divergence of the corresponding expressions for the phases $\delta_{i,f}$; however, this difficulty is easily removed when we change to other coordinates $\mathbf{r}_1$, $\mathbf{r}_2$ and calculate $T_{i,f}$ directly from the formulas (6). We then have

$$T_i = \frac{1}{\pi}\iint d\mathbf{r}_1\,d\mathbf{r}_2\exp\{-i\varkappa_1\mathbf{r}_1 - i\varkappa_2\mathbf{r}_2 - r_1 - r_2\} \times\left(\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} - \frac{1}{r_2}\right)\exp\left\{\frac{i}{v_i}\ln\frac{\mathbf{r}_1\mathbf{v}_i + r_1v_i}{(\mathbf{r}_1 - \mathbf{r}_2)\mathbf{v}_i + |\mathbf{r}_1 - \mathbf{r}_2|v_i}\right\}, \qquad (23)$$

where

$$\mathbf{r}_1 = \mathbf{R}_1 - \mathbf{R}_3,\quad \mathbf{r}_2 = \mathbf{R}_2 - \mathbf{R}_3 \qquad (24)$$

and the transferred momenta are equal to

$$\varkappa_1 = \mathbf{k}_f^{(2)} + \frac{m_2}{m_2 + m_3}\mathbf{k}_i^{(1)},\quad \varkappa_2 = -\mathbf{k}_i^{(1)} - \frac{m_1}{m_1 + m_3}\mathbf{k}_f^{(2)}. \qquad (25)$$

The corresponding expression for T_f is written down analogously. In accordance with the results of Sec. 2, we need not calculate the eikonal corrections.

Elementary estimates by the stationary-phase method show that the differential cross-section for angles differing from the eikonal angles (for the present problem, these are equal to $\sqrt{3/M}$ and π[21]) fall off like E^{-6}; we therefore concentrate our attention on the angular distribution near the eikonal directions. In addition, as shown by the calculations given, the principal contribution to the scattering is made by the eikonal direction $\theta = \sqrt{3/M}$ (the capture mechanism). The integrals (23) for different values of the energies and angles were calculated on a computer by the Monte-Carlo method. It should be noted that the reproduction of the angular distribution in the eikonal approximation by the Monte-Carlo method is unreliable[22], since, even for a large number of draws, the relative variance is extremely great because of the oscillating character of the functions under the integral. We therefore first integrated over r_1 and r_2 by the stationary-phase method, using the fact that the momentum transfers in the energy range of interest are substantially greater than unity.

It is of most interest to calculate the cross-section for $\theta = \sqrt{3/M}$. This is connected with the fact that, in calculations in the first order of iteration of both the Faddeev and the Lippmann-Schwinger equations, the forward direction makes the determining contribution to the cross-section[23], while in the direction $\theta = \sqrt{3/M}$ there is either no maximum or else a minimum. In the calculation of the eikonal cross-section, the forward-scattering peak also gives an important contribution at $\theta = 0$, but it can be seen from the energy dependence of the height and width of the peak that this peak is not an eikonal peak. The eikonal peak at $\theta = \sqrt{3/M}$ is characterized by the fact that its relative height increases and its width decreases with increasing energy (Fig. 2). The height of the forward-scattering maximum is found to be somewhat less in the calculation using formula (23) than in the calculation of Chen and Kramer[23]. We associate this with the presence in the expression (23) of a phase whose oscillations at high energies give rise to a shift of the scattering maximum towards the eikonal direction. The scattering maximum at $\theta = \pi$ is also an eikonal peak; however, as is clear from the calculation, its contribution need only be taken into account when E > 1 MeV. All our conclusions are in agreement with the results of the asymptotic analysis of the paper[21].

Unfortunately, we do not know of any experiments on the measurement of the differential cross-section of the reaction under consideration; comparison with experiment is therefore carried out using the total cross-section[19,20]. For illustration, we also give the corresponding Born cross-section[20]. The comparison shows somewhat better agreement with experiment than in the Born method; the underestimation of the total cross-section at low energies arises from the neglect of the intermediate scattering angles (see the Table).

E, keV	σ, cm²		
	Brinkman-Kramers [24]	Experiment	Eikonal
20	2×0^{-15}	6×0^{-16}	1.25×0^{-16}
100	3.05×0^{-17}	1×0^{-17}	9×0^{-18}
1000	1.1×0^{-21}	$(4-6)\times10^{-22}$	3.7×0^{-22}
10 000	1.12×0^{-27}	—	5.2×0^{-29}

The eikonal formulas obtained are convenient for application in different problems of collision theory (collisions of atoms with diatomic molecules, with a surface, etc.) and can be generalized to the case of a large number of particles. We must also point out the possibilities of using the technique of eikonal propagators in various problems in statistical physics.

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[1)]It was shown in [14] that, in determining the asymptotic form of the high-energy scattering, one can start from either the Fadeev equations or the Lippmann-Schwinger equations.

[2)]The most complete theoretical study of the asymptotic behavior of the charge-exchange cross-section is contained in [21].

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