ASYMPTOTIC BEHAVIOR OF THE CROSS SECTION FOR CHARGE EXCHANGE

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The asymptotic behavior of the individual terms of an iterative expansion of the transition amplitude for reaction (1a) is studied in the limit of high relative velocities of the colliding particles. Asymptotic expressions are obtained for the total and differential cross sections. Also a number of properties, which the Born approximation possesses in connection with its utilization in problems involving rearrangement collisions, are mentioned.

1. INTRODUCTION

IN this article the behavior of the cross sections for inelastic atomic collisions of the form

$$H(1s) + H^+ \to H^+ + H(n, l), \tag{1a}$$

$$He(1s^2) + H^+ \to He^+(n, l) + H(n', l') \tag{1b}$$

and so forth is studied in the limit of high relative velocities of the colliding particles. In this connection primary attention is focused on reaction (1a) for $n = 1$ and $l = s$. The particular theoretical interest in reaction (1a) is associated with the fact that it is the simplest example of nonrelativistic three-particle scattering involving rearrangement associated with known potentials. In connection with this, the cross sections for (1a) obtained upon calculation enable us to reach important conclusions about the behavior of the cross sections for many-particle scattering in the general case. On the other hand, at the present time processes of the form (1) are being intensively investigated experimentally.[1]

Definite progress in the treatment of the problem of three-particle nonrelativistic scattering has recently been achieved. In the first place it is associated with the discovery of "nonsingular" integral equations of the type of the Faddeev equations,[2,3] which possess a number of advantages in comparison with the essentially singular Lippmann-Schwinger equation. However, solution of the indicated "nonsingular" equations remains extremely difficult.[4] Up to now only model calculations in the approximation of a separable interaction have been carried out on electronic computing machines; however, the validity and limits of applicability of this approximation actually remain undetermined.[5]

In such a situation calculations in which one is able to obtain an explicit expression for the transition amplitude in some limiting case take on special importance. As the simplest real example we analyzed, in the light of the latest results,[2,3] the possibility of using perturbation theory for calculations of the amplitude for charge transfer (1a) as $\nu = v_0/v \to 0$, where v denotes the relative velocity of the incident proton and $v_0 = e^2/\hbar$, i.e., for reaction (1a) at still nonrelativistic energies larger or of the order of 25 keV. As is well-known, the Green's function of the three-particle Schrödinger equation

$$G(E) = [E + i\varepsilon - H]^{-1}, \quad H = H_0 + \sum_{\alpha=1}^{3} V_\alpha,$$

(where H_0 is the operator for the kinetic energy of the system of three particles, and V_α are the operators of the pair interaction in the subsystem of particles with indices different from α) satisfies the Lippmann-Schwinger equation, which upon iteration yields the following expansion in a perturbation theory series (the δ-function corresponding to conservation of total momentum is omitted):

$$G = G_0 + G_0\Big(\sum_{\alpha=1}^{3} V_\alpha\Big)G_0 + G_0\Big(\sum_{\alpha=1}^{3} V_\alpha\Big)G_0\Big(\sum_{\alpha=1}^{3} V_\alpha\Big)G_0 + \dots \tag{2}$$

The shortcomings of this operator expansion in the three-particle problem are rather well known.[2,3] They appear, for example, in the fact that the matrix elements of the individual terms in the series (2), taken between states with definite momenta, contain singularities of the form $\nu^3(q_\alpha - q'_\alpha)\varphi(p_\alpha, p'_\alpha, q^2_\alpha)$ (q_α is the momentum of particles α, p_α is the relative momentum of the particles in the two-particle subsystem α, φ is a certain function which is nonsingular for $q_\alpha = q'_\alpha$) owing to the singular nature (noncompactness) of the kernel of the Lippmann-Schwinger equation. An attempt to take account of the contributions of possible intermediate bound states of the two-particle subsystems leads[2] to a conclusion about the necessity to rearrange the series (2) in such a way that, instead of the two-particle potentials V_α, it would only contain the two-particle amplitudes T_α off the energy shell.[1)] In this connection, instead of Eq. (2) expansions of the form

$$G = G_0 + G_0\Big(\sum_{\alpha=1}^{3} T_\alpha\Big)G_0 + \sum_{\substack{\alpha=1\\ \alpha\neq\beta}}^{3}\sum_{\beta=1}^{3} G_0 T_\alpha G_0 T_\beta G_0 + \dots, \tag{3}$$

are obtained, where the singularities indicated above have obviously been isolated in the second term.

The specific properties of the problem of scattering on a bound state with rearrangement lead to the result that in the matrix element required for calculation of the cross section, the operator G does not operate on arbitrary generalized functions in general, but only acts on quadratically integrable functions. As a result in

[1)] The operators T_α are defined in the space of three-particle states and are related to the corresponding two-particle amplitudes t_α by relation (8).

the perturbation theory expansion for the transition amplitude, the higher-order terms may all turn out to be small in comparison with the first terms, even if the operator series (2) by itself is formally unsatisfactory. In the present article it is shown that as $\nu \to 0$ the utilization of expansion (2) in expression (5) actually gives for reaction (1a) the same asymptotic expression for the leading terms of T_{fi} as the utilization of expansion (3) would give. In this connection, an important property of the three-particle Born expansion of T_{fi}, which has not been taken into account earlier and which consists in the fact that the terms of second-order in the interaction corresponding to "connected diagrams"[2] give the same contribution to the asymptotic behavior of T_{fi} in the common range of variation of the scattering angle $\theta(0 \ll \theta \ll \pi)$ as the terms of first order whereas the terms of second-order corresponding to "disconnected" diagrams, and all terms of third-order, and also terms of higher order give smaller contributions, is properly explained. Also a generalization of the present result to the case of the inelastic scattering of two fragments, consisting in all of N particles, into two other fragments is indicated.

In Sec. 5 the regions of angles and energies, in which one can anticipate experimentally observable deviations from the calculations carried out earlier, are specifically examined.

2. BASIC FORMULAS AND METHOD OF CALCULATION

The differential cross section for the reaction (1a) is connected with the matrix element of the transition matrix in the center of mass system by the relation

$$\frac{dQ_{fi}}{d\Omega} = (2\pi)^4 \hbar^2 \mu_p^2 |T_{fi}|^2, \tag{4}$$

$$T_{fi} = \langle n_f \mathbf{k}_f | V_2 + V_3 + (V_1 + V_3) G(E + i\varepsilon)(V_2 + V_3) | n_i \mathbf{k}_i \rangle. \tag{5}$$

Particles 1 and 2 are protons with masses $m_1 = m_2 = m_p$; particle 3 is an electron with mass $m_3 = m_e$; $\mathbf{k}_i$ denotes the momentum of the incident proton 1 relative to the center of mass of the particles (2, 3) which are in a bound state with quantum numbers n_i; $\mathbf{k}_f$ denotes the center-of-mass momentum of particles (1, 3) which are in the state n_f after scattering; V_1, V_2, and V_3 denote the Coulomb potentials of the interactions between particles (2, 3), (3, 1), and (1, 2), respectively; $G(E + i\epsilon)$ is the Green's function of the three-particle Schrödinger equation corresponding to asymptotic behavior with diverging waves as $\epsilon \to 0$:

$$E = \frac{k_i^2}{2\mu_p} - E_0 = \frac{k_f^2}{2\mu_p} - E_0, \quad \mu_p = \frac{m_p(m_p + m_e)}{2m_p + m_e}$$

E_0 denotes the ground state energy of the hydrogen atom.

In order to estimate the contributions of the disconnected graphs, and also in order to estimate the contributions of intermediate bound states to expression (5), it is convenient to make the following transformation. We introduce the operators

$$T^{(1)} = V_1 G(V_2 + V_3), \; T^{(3)} = V_3 + V_3 G(V_2 + V_3), \tag{6}$$

satisfying the equations

$$\begin{aligned} T^{(1)} &= T_1 G_0 T_2 + T_1 G_0 T^{(3)} + T_1 G_0 T_2 G_0 (T^{(1)} + T^{(3)}), \\ T^{(3)} &= T_3 + T_3 G_0 T_2 + T_3 G_0 T^{(1)} + T_3 G_0 T_2 G_0 (T^{(1)} + T^{(3)}), \end{aligned} \tag{7}$$

where the T_α ($\alpha = 1, 2, 3$) denote the two-particle amplitudes defined in the space of three-particle states:[3]

$$\langle \mathbf{p}_\alpha \mathbf{q}_\alpha | T_\alpha(E) | \mathbf{p}_\alpha' \mathbf{q}_\alpha' \rangle = \delta^3(\mathbf{q}_\alpha - \mathbf{q}_\alpha') t_\alpha(\mathbf{p}_\alpha, \mathbf{p}_\alpha'; E - q_\alpha^2/2\mu_\alpha)$$

$$\mu_\alpha = \frac{m_\alpha m_{\beta\gamma}}{m_\alpha + m_{\beta\gamma}}, \quad m_{\beta\gamma} = m_\beta + m_\gamma, \quad \alpha \neq \beta \neq \gamma, \quad (\alpha, \beta, \gamma) = (1, 2, 3). \tag{8}$$

For the amplitude T_{fi} we have the expression

$$T_{fi} = \langle n_f \mathbf{k}_f | V_1 | n_i \mathbf{k}_i \rangle + \langle n_f \mathbf{k}_f | T^{(3)} + T^{(1)} | n_i \mathbf{k}_i \rangle. \tag{9}$$

Let us investigate the asymptotic behavior of T_{fi} as $\nu \to 0$ using an iterative expansion of Eqs. (7) for $T^{(1)}$ and $T^{(3)}$:

$$T_{fi} = \langle n_f \mathbf{k}_f | V_1 + T_3 + (T_1 + T_3) G_0 T_2 + T_1 G_0 T_3 + \ldots | n_i \mathbf{k}_i \rangle. \tag{10}$$

The accepted general method of calculating the asymptotic behavior of the individual matrix elements consists in the fact that in the integral over intermediate momenta the region, where the contribution from the discrete spectrum and from the spectrum of small energies of the two-particle amplitude is important, is separated from the region where its Born expansion is satisfactory. In order to estimate the contributions from the indicated regions, we shall use spectral representations for $t_\alpha(E')$.

In the region $|E'| \lesssim q_{0\alpha}^2/2\mu_{\beta\gamma}$ we set

$$t_\alpha(E') = \sum_n \frac{|g_n^{(\alpha)}\rangle \langle g_n^{(\alpha)}|}{E' - E_n} + \int_{\Omega_{cq_{0\alpha}}} \frac{|g_k^{(\alpha)}\rangle \langle g_k^{(\alpha)}|}{E' - k^2/2\mu_{\beta\gamma} + i\varepsilon} d\mathbf{k}, \tag{11}$$

(here $\Omega_{cq_{0\alpha}}$ denotes a region of spherical shape of radius $cq_{0\alpha}$ with center at zero, $c > 1$, $q_{0\alpha} = \mu_{\beta\gamma} v_0$, $\mu_{\beta\gamma} = m_\beta m_\gamma / m_{\beta\gamma}$; $|g_n^{(\alpha)}\rangle = V_\alpha |n_\alpha\rangle$, where the summation runs over the entire discrete spectrum).

In the region $|E'| > q_{0\alpha}^2/2\mu_{\beta\gamma}$ we confine our attention to the Born approximation:

$$t_\alpha \approx V_\alpha. \tag{12}$$

Here the following estimates are required for the Coulomb functions in the momentum representation[6] (here the momenta are expressed in atomic units):

$$\Psi_k^+(p) \approx \frac{e^{-\pi/2k}\,\Gamma(1 + i/k)}{p^4} \quad \text{for } |p| \gg k \tag{13a}$$

for a continuous spectrum in a repulsive field (in an attractive field $\kappa \to -k$) and

$$\Psi_{nl}(p) \approx \left[\frac{2(n+l)!}{(n-l-1)!}\right]^{1/2} \frac{2}{\Gamma(l + 3/2)} \frac{1}{n^{l+2}} \frac{1}{p^{l+4}} \quad \text{for } |p|^2 \gg E_n \tag{13b}$$

for the radial functions of the discrete spectrum. Estimates for $g_n^{(\alpha)}(p) = \langle p | V_\alpha | n_\alpha \rangle$ are obtained from (13), taking the relation $g_n^{(\alpha)}(p) = (-p^2/2\mu_{\beta\gamma} + E_{n\alpha})\psi_{n\alpha}(p)$ into account so that $g_n^{(\alpha)}(p) \approx -(p^2/2\mu_{\beta\gamma})\psi_{n\alpha}(p)$ for $p^2/2\mu_{\beta\gamma} \gg |E_{n\alpha}|$.

As an example of the use of the adopted method, first let us consider the asymptotic behavior of the

[2] We have in mind the graphical representation proposed in [3] for the individual terms of the series (2).

[3] It is not difficult to obtain Eq. (7) by using the definition (6), resolvent identities of the type $G = G_\alpha + G_\alpha v_\alpha G$, where $G_\alpha = [E + i\epsilon - H_0 - V_\alpha]^{-1}$, $v_\alpha = \sum_{\beta=1}^{3} V_\beta - V_\alpha$, and the relation $V_\alpha G_\alpha = T_\alpha G_0$.

terms of first order in the expansion (10) as $\nu \to 0$:

$$T_{fi}^{I} = \langle \mathbf{k}_f n_f | V_1 | \mathbf{k}_i n_i \rangle + \langle \mathbf{k}_f n_f | T_3 | \mathbf{k}_i n_i \rangle \equiv U_1 + U_3. \quad (14)$$

We introduce the following notation for the momentum transfers:

$$\mathbf{q}_i = \frac{M}{M+1}\mathbf{k}_f - \mathbf{k}_i, \quad \mathbf{q}_f = \frac{M}{M+1}\mathbf{k}_i - \mathbf{k}_f; \quad \mathbf{q}_e = \mathbf{q}_i + \mathbf{q}_f$$

and let $M = m_p/m_e$ where $|\mathbf{k}_i| = |\mathbf{k}_f| = k_0$, $q_{0i} = q_{0f} = q_0$, and $q_i^2 = q_f^2$ in the problem under consideration. Then let

$$\Psi_i(p_1) \equiv \langle \mathbf{p}_1 | n_i \rangle = \frac{2\sqrt{2}}{\pi} \frac{q_0^{5/2}}{[p_1^2 + q_0^2]^2},$$

$$\Psi_f(p_2) \equiv \langle \mathbf{p}_2 | n_f \rangle = \frac{2\sqrt{2}}{\pi} \frac{q_0^{5/2}}{[p_2^2 + q_0^2]^2}$$

denote the wave functions of the initial and final bound states, respectively. For the second term in Eq. (14) we have the expression

$$U_3 = \int \Psi_i\left(\mathbf{q}_3 + \frac{m_3}{m_{23}}\mathbf{k}_i\right) \times t_3\left(\mathbf{k}_i + \frac{m_1}{m_{12}}\mathbf{q}_3, \mathbf{k}_f - \frac{m_2}{m_{12}}\mathbf{q}_3; E - \frac{q_3^2}{2\mu_3}\right)\Psi_f'\left(\mathbf{q}_3 - \frac{m_3}{m_{13}}\mathbf{k}_f\right) d\mathbf{q}_3. \quad (15)$$

In order to determine the contribution to the asymptotic behavior of U_3 coming from the region where the expansion of t_3 in a Born series is not valid, we isolate from the entire region of integration over $\mathbf{q}_3$ a subregion Ω_3, which is a spherical shell of thickness $\sim K_3 q_{03}^2/k_0$ next to the sphere $q_3^2/2\mu_3 = E$, where K_3 is a certain constant, $K_3 > 1$. Let us denote the complement of Ω_3 with respect to the whole space by $\bar{\Omega}_3$; in it one can use the Born expansion for t_3. In this connection U_3 is divided into two integrals which we denote, respectively, by I(3) and I($\bar{3}$):

$$U_3 = \int_{\Omega_3} \{\ldots\} d\mathbf{q}_3 + \int_{\bar{\Omega}_3} \{\ldots\} d\mathbf{q}_3 = I(3) + I(\bar{3}). \quad (16)$$

In I(3) we use expression (11) for t_3:

$$I(3) \approx \int_{\Omega_3} \Psi_i\left(\mathbf{q}_3 + \frac{m_3}{m_{23}}\mathbf{k}_i\right) \times \left[\int_{\Omega_{cq_{03}}} d\mathbf{k} \frac{g_{\mathbf{k}}^{(3)}\,(\mathbf{k}_i + m_1\mathbf{q}_3/m_{12})\, g_{\mathbf{k}}^{(3)*}\,(-\mathbf{k}_f + \mathbf{q}_3 m_2/m_{12})}{k^2/2\mu_{12} + q_3^2/2\mu_3 - E - i\varepsilon}\right] \times \Psi_f(\mathbf{q}_3 - \mathbf{k}_f m_3/m_{13})\, d\mathbf{q}_3. \quad (17)$$

Since in the integral over $\mathbf{k}$ the integration is performed over the region $0 \leq |\mathbf{k}| \lesssim cq_{03}$, but for $\mathbf{q}_3 \in \Omega_3$ the arguments of $g_{\mathbf{k}}^{(3)}$, $g_{\mathbf{k}}^{(3)*}$, ψ_i, and ψ_f are of the order of k_0, then in order to estimate the integrand in (17) one can apply formulas (13). Having made in addition the replacement $\mathbf{q}_3 = k_0\mathbf{q}$ in the integral over $\mathbf{q}_3$, upon which the region Ω_3 goes over into the region Ω_3', and having omitted the leading terms in ν, we obtain

$$I(3) \approx \frac{2N\mu_{ep}}{k_0^{11}} \times \int_{\Omega_3'} d\mathbf{q}\left(\mathbf{q} + \frac{m_3}{m_{23}}\mathbf{u}_i\right)^{-4}\left(\mathbf{q} - \frac{m_3}{m_{13}}\mathbf{u}_f\right)^{-4}\left(\mathbf{u}_i + \frac{m_1}{m_{12}}\mathbf{q}\right)^{-2}\left(-\mathbf{u}_f + \frac{m_2}{m_{12}}\mathbf{q}\right)^{-2} \times \left(\frac{q^2}{2\mu_3} - \frac{1}{2\mu_1} - i\varepsilon\right)^{-1} \int_{\Omega_{cq_{03}}} e^{-\pi/k}\Gamma\left(1 + \frac{i}{k}\right)\Gamma\left(1 - \frac{i}{k}\right) d\mathbf{k}, \quad (18)$$

where $\mathbf{u}_i = \mathbf{k}_i/k_0$ and $\mathbf{u}_f = \mathbf{k}_f/k_0$ are unit vectors; $N = 4\pi^{-2}q_0^4 v_0$.

Changing to spherical coordinates in the integral over $\mathbf{q}$ and integrating the singular denominator with respect to the radial variable, we obtain the following estimate for I(3):

$$I(3) \sim 1/v^{11}. \quad (19)$$

We find, then, an expression for the leading term of I($\bar{3}$). For $\mathbf{q}_3 \in \bar{\Omega}_3$ the Born approximation may be used for t_3 in Eq. (15), which gives

$$I(\bar{3}) \approx \int_{\bar{\Omega}_3} d\mathbf{q}_3 \Psi_i\left(\mathbf{q}_3 + \frac{m_3}{m_{23}}\mathbf{k}_i\right) V_3(\mathbf{q}_3 + \mathbf{k}_i - \mathbf{k}_f)\Psi_f\left(\mathbf{q}_3 - \frac{m_3}{m_{13}}\mathbf{k}_f\right). \quad (20)$$

An analysis of this expression shows that the regions of localization of the wave functions ψ_i and ψ_f give the major contribution to the asymptotic behavior as $\nu \to 0$, i.e., the major contribution comes from the neighborhoods of the points $\mathbf{q}_3 = -\mathbf{k}_i m_3/m_{23}$, $\mathbf{q}_3 = \mathbf{k}_f m_3/m_{13}$, where if $[(\mathbf{k}_i + \mathbf{k}_f)m_3/m_{23}]^2 \approx q_0^2$, then the contributions from these regions should be taken into account simultaneously. The following expression is obtained for the leading term of I($\bar{3}$):

$$I(\bar{3}) = \frac{2N}{q_i^2[q_e^2 + 4q_0^2]^2} \quad (21)$$

Comparing (21) and (19) we find that the regions of localization of the wave functions of the initial and final bound states, i.e., the regions where t_3 may be expanded in a Born series, give the most important contribution to the asymptotic form of U_3, namely, a contribution $\sim 1/v^6$ for $q_e^2 \gg q_0^2$ and $\sim 1/v^2$ for $q_e^2 \approx q_0^2$.

The first term in (14) represents the well-known Brinkman-Kramers approximation[7] for the problem of charge transfer: $U_1 = \psi_f(q_i)g_i(q_f) \approx -N/q_i^6$ and falls off like $1/v^6$ as $\nu \to 0$. Thus, the asymptotic behavior of T_{fi}^{I} is determined by the following expression:

$$T_{fi}^{I} = N\left[\frac{2}{q_i^2 q_e^4} - \frac{1}{q_i^6}\right] \quad \text{for } q_e^2 \gg q_0^2, \quad (22)$$

$$T_{fi}^{I} = \frac{2N}{q_i^2[q_e^2 + 4q_0^2]^2} \quad \text{for } q_e^2 \approx q_0^2. \quad (23)$$

3. TERMS OF SECOND ORDER IN THE EXPANSION (10)

Let us go on to a discussion of the results of an investigation of the asymptotic behavior of the terms of second order in (10):

$$T_{fi}^{II} = \langle n_f \mathbf{k}_f | T_1 G_0 T_3 + T_3 G_0 T_2 + T_1 G_0 T_2 | n_i \mathbf{k}_i \rangle \equiv U_{13} + U_{32} + U_{12},$$

$$U_{\alpha\beta} = \int\int \Psi_f\left(\mathbf{q}_\alpha - \frac{m_\alpha}{m_{13}}\mathbf{k}_f\right) t_\alpha\left(E - \frac{q_\alpha^2}{2\mu_\alpha}\right) t_\beta\left(E - \frac{q_\beta^2}{2\mu_\beta}\right)\Psi_i\left(\mathbf{q}_\beta + \frac{m_\beta}{m_{23}}\mathbf{k}_i\right) \times \left(\frac{q_\alpha^2}{2m_\alpha} + \frac{q_\beta^2}{2m_\beta} + \frac{(\mathbf{q}_\alpha + \mathbf{q}_\beta)^2}{2m_\gamma} - E - i\varepsilon\right)^{-1} d\mathbf{q}_\alpha\, d\mathbf{q}_\beta, \quad (24)$$

$$\alpha = 1,3; \quad \beta = 2,3; \quad \alpha \neq \beta.$$

In order to simplify the discussion, here only the energy dependence of the amplitudes t_α and t_β is explicitly singled out. The two-particle amplitudes $t_\alpha(E - q_\alpha^2/2\mu_\alpha)$ cannot be expanded in a Born series in the regions $|E - q_\alpha^2/2\mu_\alpha| \lesssim K_\alpha q_{0\alpha}^2/2\mu_\beta\gamma$, where the K_α are certain constants, $K_\alpha > 1$. Let us single out the corresponding regions in the integral over the intermediate momenta $\mathbf{q}_\alpha$; let us denote these regions by Ω_α—a spherical shell of thickness $\sim K_\alpha q_{0\alpha}^2/k_0$ next to the sphere $q_\alpha^2/2\mu_\alpha = E$; we denote the complement of Ω_α with respect to the entire region of integration

over q_α (the region where the Born expansion is valid for t_α) by $\overline{\Omega}_\alpha$. In this connection the expression for $U_{\alpha\beta}$ decomposes into the following sum:

$$U_{\alpha\beta} = \int\limits_{\Omega_\alpha\otimes\Omega_\beta}\int \{\ldots\}\, d\mathbf{q}_\alpha\, d\mathbf{q}_\beta + \int\limits_{\overline{\Omega}_\alpha\otimes\overline{\Omega}_\beta}\int \{\ldots\}\, d\mathbf{q}_\alpha d\mathbf{q}_\beta + \int\limits_{\Omega_\alpha\otimes\overline{\Omega}_\beta}\int \{\ldots\}\, d\mathbf{q}_\alpha d\mathbf{q}_\beta + \int\limits_{\overline{\Omega}_\alpha\otimes\overline{\Omega}_\beta}\int \{\ldots\}\, d\mathbf{q}_\alpha d\mathbf{q}_\beta \equiv \equiv I(\alpha,\beta) + I(\bar{\alpha},\beta) + I(\alpha,\bar{\beta}) + I(\bar{\alpha},\bar{\beta}). \quad (25)$$

In order to find the leading asymptotic behavior of the individual terms in (25), we use expression (11) for t_α in the region Ω_α and expression (12) in the region $\overline{\Omega}_\alpha$. The regions $\Omega_\alpha \otimes \Omega_\beta$, in which one should use expression (11) for both amplitudes, give a contribution

$$I(\alpha,\beta) \sim 1/v^{16}, \quad (26)$$

where the corresponding estimate is carried out in analogy to the one carried out in Sec. 2 for I(3).

For the contributions from the regions $\overline{\Omega}_\alpha \otimes \Omega_\beta$ and $\Omega_\alpha \otimes \overline{\Omega}_\beta$, in which one can limit one's attention to the Born approximation for one of the two-particle amplitudes, the following expressions are derived in the Appendix:

$$I(\bar{1},2) + I(\bar{3},2) \sim 1/v^7,\ I(1,\bar{3}) + I(1,\bar{2}) \sim 1/v^7, \quad (27a)$$

$$I(\bar{1},3) \sim 1/v^{11},\ I(3,\bar{2}) \sim 1/v^{11}. \quad (27b)$$

The regions $\Omega_\alpha \otimes \Omega_\beta$, in which the Born expansion is valid for each two-particle amplitude, give substantially larger contributions to the asymptotic behavior of the terms of second order than (26) and (27). A method of calculating the asymptotic form of the corresponding matrix elements and evaluations of the integrals which arise are given in[8]. Upon its utilization (see also[9]) the following asymptotic expressions are obtained for the leading terms of $I(\overline{\alpha},\overline{\beta})$:

$$I(\bar{1},\bar{3}) + I(\bar{3},\bar{2}) \approx \langle n_f\mathbf{k}_f | V_1G_0V_3 + V_3G_0V_2 | n_i\mathbf{k}_i\rangle \approx \sim \frac{2N(1+1/M)}{q_i^2 q_e^4} \quad \text{for } q_e^2 \gg q_0^2, \quad (28)$$

$$I(\bar{1},\bar{2}) \approx \langle n_f\mathbf{k}_f | V_1G_0V_2 | n_1\mathbf{k}_i\rangle \approx$$

$$\approx N\left(1+\frac{1}{M}\right)^2 \Big/ q_i^4\left[q_i^2 - \left(\frac{m_3}{\mu_1}k_0\right)^2 - 4iv\left(\frac{m_3}{\mu_1}k_0\right)^2\right]. \quad (29)$$

The regions of localization of the wave functions ψ_i and ψ_f give the major contributions $\sim 1/v^6$ to the asymptotic form of the indicated matrix elements in the common range of variation of the scattering angles.

As follows from Eq. (28), the region of scattering angles $q_e^2 \approx 0$, that is, $\theta \approx \pi$, requires special investigation for $I(\bar{1},\bar{3})$ and $I(\bar{3},\bar{2})$. For definiteness let us consider $I(\bar{3},\bar{2})$, the diagram for which is represented in Fig. 1 a ($I(\bar{1},\bar{3})$ is considered in similar fashion). In the regions of localization of the wave functions ψ_i and ψ_f, i.e., $q_2 \approx -k_i m_2/m_{23}$ and $q_3 \approx k_f m_3/m_{13}$, the denominator of the Green's function G_0 also tends to zero for $\theta \approx \pi$. In this connection, however, the two-particle subsystem (2, 3) in the intermediate state possesses an energy

$$E - \frac{1}{2\mu_1}\left(\frac{m_3}{m_{13}}\mathbf{k}_f - \frac{m_2}{m_{23}}\mathbf{k}_i\right)^2 \approx E_0 \quad \text{for } \theta \approx \pi,$$

so that for this subsystem we cannot use the "free propagator" G_0. In order to correctly take account of the contribution from the range of angles under consideration, it is necessary to sum all diagrams of the form shown in Fig. 1b, where the discrete spectrum and the spectrum of small energies of the function G_1 which thus arises (Fig. 1c) will give the most important contribution.

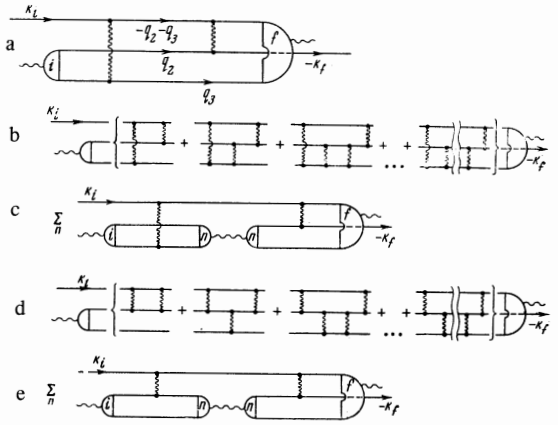

FIG. 1. Graphs of the matrix elements: a represents the graph of second order which corresponds to the matrix element $\langle n_f\mathbf{k}_f | V_3G_0V_2 | n_i\mathbf{k}_i\rangle$; b and d are sums of graphs giving an identical contribution to the charge exchange amplitude in the region of scattering angles $\theta \approx \pi$; c and e are a graphical representation of the contribution from the discrete spectrum of the two-particle Green's function G_1.

It is necessary to also carry out a similar procedure in the region of angles $\theta \approx \pi$ with the matrix elements represented in Fig. 1d, as a result of which the graphs (1e) will give the leading contribution to this sum. It is not difficult to obtain an expression for the contribution of the graphs (1c) and (1e) $\sim 1/v^3$ by using the method set forth in the Appendix. Comparing the present result with expression (23), we find that in the angular region $\theta \approx \pi$ the contribution of the first-order term is dominant.

A special feature of the matrix element $I(\bar{1},\bar{2})$ consists in the fact that for certain values of the scattering angle, namely, for $q_i^2 \approx (k_0 m_3/\mu_1)^2$ in the regions of localization of the wave functions ψ_i and ψ_f giving the largest contribution to the asymptotic behavior, the denominator of the Green's function G_0 also vanishes, which corresponds to the possibility of fulfilling the law of energy conservation in intermediate states of the Weinberg diagrams. The scattering angle, $q_i^2 = (k_0 m_3/\mu_1)^2$, at which $|I(\bar{1},\bar{2})|$ reaches its maximum, corresponds to such a scattering process with fulfilment of the law of energy conservation in the intermediate states, for which the electron is scattered first by the incoming proton 1, and then by proton 2, whereupon as a result of these successive collisions the velocity of the electron relative to the incident proton 1 becomes equal to zero.[4)]

[4)]It is not difficult to verify this by solving the equations for the laws of energy and momentum conservation for each successive collision under the following additional conditions: 1) prior to the first scattering process the relative velocity of the electron and proton 2 is equal to zero, which corresponds to a region of localization of the wave function ψ_i in momentum space, and 2) after the second scattering process the relative velocity of the electron and proton 1 is also equal to zero, which corresponds to a region of localization of ψ_f.

4. CONTRIBUTIONS OF THE HIGHER-ORDER TERMS

As indicated, in order to determine the leading terms of the asymptotic form of T_{fi} to first and second orders, one can use the Born approximation for each two-particle amplitude and, consequently, the substitution $G \approx G_0$ in Eq. (5) is valid. In this connection it is essential that the "facings" in the expression for the transition amplitude play a twofold role. On one hand, in view of their presence the entire energy spectrum of each two-particle amplitude is affected. On the other hand, in the region of sufficiently high energies where one can only anticipate the applicability of the perturbation theory under consideration, the wave functions ψ_i and ψ_f are sufficiently strongly localized so that the regions of localization of the hydrogen-atom wave functions in momentum space give the major contribution to each of the integrals representing the individual terms of the series, and in these regions one can expand the two-particle amplitudes in a Born series; the regions where the Born approximation for the two-particle amplitudes is not valid give appreciably an smaller contribution as $\nu \to 0$. The other special property of the first- and second-order expressions consists in the fact that in the common range of angular variation the terms of second order give the same contribution $\sim 1/v^6$ to the asymptotic behavior as the terms of first order. As follows from what was set forth above, this result is related to the structure of the initial formula for T_{fi}, namely, with the presence of "disconnected graphs."

Let us explain this once more by the following example: let us consider the term of first order written in the form

$$I(\bar{3}) = \int\int \Psi_f\left(\mathbf{q}_3 - \frac{m_3}{m_{13}}\mathbf{k}_f\right) V_3(\mathbf{q}_3 + \mathbf{k}_i - \mathbf{k}_f) \times \Psi_i\left(\mathbf{q}_3' + \frac{m_3}{m_{23}}\mathbf{k}_i\right)\delta^3(\mathbf{q}_3 - \mathbf{q}_3')\, d\mathbf{q}_3\, d\mathbf{q}_3', \tag{30}$$

and any of the second-order terms, for example,

$$I(\bar{1},\bar{3}) = \int\int \Psi_f\left(\mathbf{q}_1 - \frac{m_1}{m_{13}}\mathbf{k}_f\right) V_1(\mathbf{q}_1 + \mathbf{q}_3 - \mathbf{k}_f)\, V_3(\mathbf{q}_1 - \mathbf{k}_i)\, \Psi_i\left(\mathbf{q}_3 + \frac{m_3}{m_{23}}\mathbf{k}_i\right) \times \left(\frac{q_1^2}{2m_1} + \frac{(\mathbf{q}_1 + \mathbf{q}_3)^2}{2m_2} + \frac{q_3^2}{2m_3} - E - i\varepsilon\right)^{-1} d\mathbf{q}_1\, d\mathbf{q}_3. \tag{31}$$

The regions of localization of the wave functions ψ_i and ψ_f give the major contribution to the integrals (30) and (31). However, the leading contribution of the term of first order $\sim 1/v^5$ vanishes identically because of the presence of the δ-function corresponding to conservation of the third particle's momentum, which is a consequence of the "disconnected nature" of the diagram for $I(\bar{3})$. Therefore, only the contribution to the asymptotic behavior $\sim 1/v^6$ is left.

The situation is different in the case of the terms of second order. Although one more power of v is added in the denominator upon going from first to second order, however, in this connection a restriction is removed, the imposed δ-function corresponding to conservation of the third particle's momentum to first order in the intermediate momenta, thanks to which the leading contribution from the terms of second order, arising from the regions of localization of the wave functions ψ_i and ψ_f, becomes of the same order $\sim 1/v^6$ as the contribution from the terms of first order.[5)]

This fact, that the terms of first and second orders in the problem of charge transfer for hydrogen give the same contribution to the asymptotic behavior of the amplitude, is obviously a consequence of a certain general principle which can be formulated in the following way. In connection with the scattering of two fragments, consisting in all of N particles, into two fragments (with rearrangement or without it), the terms of the Born series up to the (N – 1)-st order in the interaction, inclusively, give a comparable contribution to the asymptotic behavior of the transition amplitude at high energies. In this connection in each order it is necessary to take into account only the "most connected graphs" of Weinberg, and the regions of localization of the wave functions of the initial and final bound states in momentum space will give the major contribution to the corresponding matrix element. By "most connected graph" of the m-th order is to be understood a graph connecting at least m + 1 particles. It is important to note that terms of the N-th order and higher give a smaller contribution than the terms mentioned above. We shall investigate the assertion which has been made in general form in a separate article.[6)] Here we confine our attention to the results of an analysis of the principal asymptotes of the terms of N-th order (N > 2) for reaction (1a) (n = 1), which confirms that the contribution from these terms is small in comparison with the contribution from the terms of first and second order.

First of all we note that the regions in the space of integration variables, in which the two-particle amplitudes cannot be expanded in a Born series, form a set

$$\left|\frac{q_\alpha^2}{2\mu_\alpha} - \frac{1}{2\mu_p}\right| \sim \frac{q_{0\alpha}^2}{2k_0^2\mu_{\beta\gamma}},$$

whose measure $\Omega_\alpha \sim \nu^2 \to 0$ as $\nu \to 0$. Therefore, in order to find the leading terms of the asymptotes of the amplitudes T_{fi}^N to N-th order, we attempt to confine ourselves to the Born approximation $t_\alpha \approx V_\alpha$ for each two-particle amplitude, where for $\nu \to 0$ we extend the range of integration with respect to the intermediate momenta to the entire space ($\Omega_\alpha \to 0$). Let us consider the general form of the term of N-th order which is thus obtained, whose diagram is shown in Fig. 2a. Substitution of the variables $\mathbf{q}_\alpha^{(s)} = k_0\tilde{\mathbf{q}}_\alpha^{(s)}$ leads to the result

$$T_{fi}^N \approx \frac{N_i N_f}{k_0^{3N+6}} \int J_N(\tilde{\mathbf{q}}_1^{(3)}, \tilde{\mathbf{q}}_N^{(3)})\, d\tilde{\mathbf{q}}_1^{(3)} d\tilde{\mathbf{q}}_N^{(3)}.$$

[5)] This is obviously associated with the fact that it is impossible to change the momenta of all three particles by means of a single "pair collision." But then this can be realized as the result of two collisions. For certain values of the scattering angle the terms of second order may give an even larger contribution than the terms of first order. This is possible when the momenta of the particles in intermediate states of the Weinberg diagrams belong to the regions of localization of the wave functions ψ_i and ψ_f and simultaneously satisfy the law of energy conservation.

[6)] The formulated principle can be directly verified for reaction (1a), for inelastic scattering of a proton by hydrogen without rearrangement, and also for reaction (1b). As the calculation which has been carried out indicates, for reaction (1b) it is still necessary to take terms up to third order, inclusively, into account.

$$\times\left[\left(\tilde{q}_1^{(3)}+\frac{m_3}{m_{23}}u_i\right)^2+\eta^2\right]^{-2}\left[\left(\tilde{q}_N^{(3)}-\frac{m_3}{m_{23}}u_f\right)^2+\eta^2\right]^{-2}, \quad (32)$$

$$J_N(\tilde{q}_1^{(3)},\tilde{q}_N^{(3)})=\int V_3^{(1)}(\tilde{q}_2^{(1)}-u_i)V_1^{(2)}(\tilde{q}_1^{(3)}+\tilde{q}_3^{(1)}+\tilde{q}_3^{(2)})\dots$$
$$\times V_3^{(N)}(\tilde{q}_{N-1}^{(2)}+u_f)\cdot\left[\frac{\tilde{q}_1^{(3)2}}{2m_3}+\frac{\tilde{q}_2^{(1)2}}{2m_1}+\frac{(\tilde{q}_1^{(3)}+\tilde{q}_2^{(1)})^2}{2m_2}-\frac{1}{2\mu_p}-i\varepsilon\right]^{-1}\dots$$
$$\dots\left[\frac{\tilde{q}_{N-1}^{(2)2}}{2m_2}+\frac{\tilde{q}_N^{(3)2}}{2m_3}+\frac{(\tilde{q}_N^{(3)}+\tilde{q}_{N-1}^{(2)})^2}{2m_1}-\frac{1}{2\mu_p}-i\varepsilon\right]^{-1}\cdot d\tilde{q}_2^{(1)}\dots d\tilde{q}_{N-1}^{(2)}, \quad (33)$$

where N_i and N_f are normalization constants and $\eta = q_0/k_0$. The neighborhoods of the points $q_1(3) = -u_i m_3/m_{23}$, $\tilde{q}_N^{(3)} = u_f m_3/m_{13}$ at which the wave functions ψ_i and ψ_f became singular as $\eta \to 0$ give the major contribution to the asymptotic form of the integral (32) over $\tilde{q}_1$ and $\tilde{q}_N$. As to the integral (33), it does not depend on v at all; however, J_N may be singular at certain values of $\tilde{q}_1$ and $\tilde{q}_N$, and upon integration over $d\tilde{q}_1$ and $d\tilde{q}_N$ these singularities will give a contribution to the asymptotic form (32). We note that the singularities of (33), which are important for elucidation of the analytic properties of the three-particle amplitude and arise in connection with "pinching" of the denominators of the Green's functions, and which correspond to successive collisions with fulfilment of the law of energy conservation in the intermediate states,[10] do not, however, give the major contribution to (33) as $\nu \to 0$ since the amplitude of each such scattering process at a nonvanishing angle, determined from the solution of the Landau-Bjorken equations, becomes small: $\sim 1/v^2$ as $\nu \to 0$. By using the method proposed in[11] one can obtain an estimate for the contribution to (32) coming from the indicated singularities, which gives a value $\sim v^{-2N-1}\ln v$ for values (u_i, u_f) which satisfy the Landau-Bjorken equations. The singularities of (33) which arise from regions in which together with the vanishing of the denominators of the Green's functions the denominators of the potentials also vanish, which corresponds to scattering at angles close to zero for each successive collision, give essentially the largest contribution to the asymptotic expression (32). It is precisely these singularities which are the leading terms as $\nu \to 0$.

Here, however, it is necessary to note the following. An analysis of expression (32) indicates that not more than N − 1 denominators of the potentials and not more than N − 1 denominators of the Green's functions can simultaneously vanish. In order to be definite, let us consider the contribution from a region in which the denominators of the potentials from the first to the m-th and from the (m +3)-rd to the N-th and, respectively, the denominators of the Green's functions G_0 from the first to the m-th and from the (m +2)-nd to the N-th vanish. In this region the intermediate momenta $q_\alpha^{(s)}$ ($\alpha = 1, \dots, m+1$) are localized in the neighborhoods of the points $q^{(1)} = k_i$, $q_\alpha^{(2)} = -k_i m_2/m_{23}$, $q_\alpha^{(3)} = -k_i m_3/m_{23}$, but the momenta $q_\beta^{(s)}$ ($\beta = m+2, \dots, N$) are localized in the neighborhoods of $q_\beta^{(1)} = k_f m_1/m_{13}$, $q_\beta^{(2)} = -k_f$, and $q_\beta^{(3)} = k_f m_3/m_{13}$.

In this connection we have the expression $E - q_\alpha^{(1)2}/2\mu_1 \approx E_0$ for the energy of the subsystem (2, 3) in the intermediate states of the part of the graph which contains the interaction from the first to the m-th, and similarly the energy of the subsystem (1. 3) in the intermediate states of the part of the graph containing the interactions from the (m +3)-rd to the N-th will be a quantity of the order of $E - q_\beta^{(2)2}/2\mu_2 \approx E_0$, so that for these subsystems we cannot use the "free propagator" G_0 in the intermediate states of the corresponding parts of the graphs. In order to take proper account of the contributions from the region under consideration, instead of G_0 one should use the appropriate two-particle Green's function, namely, G_1 in the part of the graph which contains the interaction from the first to the m-th and G_2 should be used in the part containing the interaction from the m +3-rd to the N-th, which actually reduces to a summation of certain graphs. Thus, instead of the diagrams of Fig. 2a, one should consider the graphs of Fig. 2b. In this connection the following estimate is obtained for the contribution from the term of N-th order in the expansion (10) in the common range of angular variations:

$$T_{fi}^{(N)} \sim \begin{cases} v^{-6}v^{-(N-1)/2} & \text{for N odd,} \\ v^{-6}v^{-(N-2)/2} & \text{for N even.} \end{cases}$$

5. EXPRESSION FOR THE CROSS SECTION

Since the terms of third and higher orders give a smaller contribution to the asymptotic form of T_{fi} than the terms of first and second order, by using Eqs. (22), (23), (28), and (29) we obtain the following expression for the leading asymptotic behavior as $\nu \to 0$:

$$T_{fi} \approx T_{fi}^{I} + T_{fi}^{II} =$$
$$= N\left[\frac{2}{Mq_e^4 q_i^2}-\frac{1}{q_i^4[q_i^2-(k_0 m_e/\mu_p)^2-4i\nu(k_0 m_e/\mu_p)^2]}-\frac{1}{q_i^6}\right] \quad (34)$$
$$\text{for } q_e^2 \gg q_0^2,$$
$$T_{fi} \approx \frac{2N}{q_i^2[q_e^2+4q_0^2]^2} \quad \text{for } q_e^2 \approx q_0^2. \quad (35)$$

It should be stressed that in the angular range $q_e^2 \gg q_0^2$ ($\theta \ll \pi$) only a partial cancellation of the leading terms of expression (28) for $I(\bar{1}, \bar{3}) + I(\bar{3}, \bar{2})$ and expression (21) for $I(\bar{3})$ occurs, but not the exact cancellation indicated, for example, in[7,12,13]. In this connection the contribution from the sum of these terms remains very important. In fact, in terms of the angular variables we have

$$I(\bar{3}) + I(\bar{1}, \bar{3}) + I(\bar{3}, \bar{2}) \approx M^3/4k_0^6(1-\cos\theta)(1+\cos\theta)^2, \quad (36)$$

whereas the remaining terms in (34) give the following contribution for $\theta \gg 0$:

$$U_1 + I(\bar{1}, \bar{2}) \approx 1/4k_0^6(1-\cos\theta)^3, \quad (37)$$

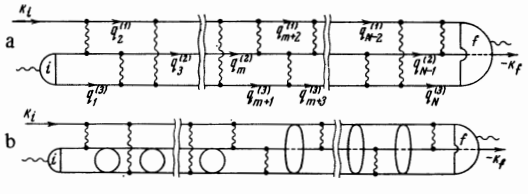

FIG. 2. Diagrams considered in connection with the investigation of the asymptotic behavior of the term of N-th order in the expansion (10): a indicates the general form of an N-th order diagram in which the Born approximation is used for each two-particle amplitude; b is a representation of one of the matrix elements which give the largest contribution to the term of N-th order. A circle enclosed between two vertical lines represents the corresponding two-particle Green's function.

so that expression (36) is dominant in the region $0 \ll \theta \ll \pi$.

From Eqs. (34) and (35) it follows that the differential cross section of the reaction (1a), together with a maximum at small scattering angles, also has a maximum at $\theta = \pi$. The origin of this maximum is associated with the possibility of scattering which satisfies the law of energy conservation in the intermediate states, in which the incident proton 1 undergoes a head-on collision with the proton of the hydrogen atom and occupies its position, forming a new bound state. Taking the contributions to the differential cross section coming from the regions $\theta \approx \pi$, $\theta \approx 0$ into consideration leads to the following final asymptotic expression for the total cross section of reaction (1a):

$$Q_{fi} = \left[\frac{5}{12\cdot 2^6}\frac{1}{M^2}\left(\frac{v}{v_0}\right)^6 + \frac{5\pi}{2^{12}}\left(\frac{v}{v_0}\right) + 0{,}295\right] Q_{BK}, \qquad (38)$$

$$Q_{BK} = \frac{2^{18}}{5}\left(\frac{v_0}{v}\right)^{12}\pi r_0^2,$$

where r_0 denotes the Bohr radius.

An analysis of expression (38) indicates that the contribution from the region $\theta \approx \pi$ (the first term in (38)), which also determines the asymptotic behavior of Q_{fi} as $\nu \to 0$, becomes significant starting with energies of 3 MeV, already giving 30% of the contribution to (38) at 10 MeV, whereas the fraction of relativistic corrections at 10 MeV amounts to a contribution of less than 3%.[14] Thus, an energy range exists where one can directly compare the results of the nonrelativistic calculation which has been carried out with an experiment, associated with the variation of both the total cross section as well as, especially, the differential cross section. In this connection, together with a maximum at small scattering angles, at sufficiently high energies the differential cross section should also have a maximum at $\theta \approx \pi$; in the region $\theta > 0$ the differential cross section, as follows from Eqs. (36) and (37), should be approximately M^6 times larger than the result which follows from the calculations[12,13] made earlier, in which an erroneous exact cancellation of the terms in (36) occurred.

APPENDIX

Let us estimate the contribution to $U_{\alpha\beta}$, defined by expression (24), which comes from a region of the type $\Omega_\alpha \otimes \Omega_\beta$. In order to be definite let us consider

$$I(1,\bar{3}) + I(1,\bar{2}) = \int\limits_{\bar{\Omega}_3\otimes\Omega_1}\int d\mathbf{q}_3 d\mathbf{q}_1 \Psi_i\left(\mathbf{q}_3 - \frac{m_3}{m_{23}}\mathbf{k}_i\right) V_3(\mathbf{q}_1 - \mathbf{k}_i)$$
$$\times\left(\sum_n + \int\limits_{\Omega_{cq_0}} d\mathbf{k}\right)\frac{\Psi_n^{(1)}(\mathbf{q}_3 - \mathbf{q}_1 m_3/m_{23})}{E + i\varepsilon - E_n - q_1^2/2\mu_1}$$
$$\times g_n^{(1)*}\left(-\mathbf{k}_f + \frac{m_2}{m_{23}}\mathbf{q}_1\right)\Psi_f\left(\mathbf{q}_1 - \frac{m_1}{m_{13}}\mathbf{k}_f\right)$$
$$+ \int\limits_{\bar{\Omega}_2\otimes\Omega_1}\int d\mathbf{q}_2 d\mathbf{q}_1 \Psi_i\left(\mathbf{q}_2 + \frac{m_2}{m_{23}}\mathbf{k}_i\right) V_2(\mathbf{q}_1 - \mathbf{k}_i)$$
$$\times\left(\sum_n + \int\limits_{\Omega_{cq_0}} d\mathbf{k}\right)\frac{\Psi_n^{(1)}(\mathbf{q}_2 + \mathbf{q}_1 m_2/m_{23})\, g_n^{(1)*}(-\mathbf{k}_f + \mathbf{q}_1 m_2/m_{23})}{E + i\varepsilon - E_n - q_1^2/2\mu_1}$$
$$\times \Psi_f\left(\mathbf{q}_1 - \frac{m_1}{m_{13}}\mathbf{k}_f\right). \qquad (A.1)$$

Here expression (11) is used for t_1, where the relation $G_0 T_\alpha = G_\alpha V_\alpha$ is taken into consideration. For $\mathbf{q}_1 \otimes \Omega_1$ we have the following result for the argument of $g_n^{(1)}$: $|\mathbf{k}_f - \mathbf{q}_1 m_2/m_{23}| \geq k_0 m_3/m_{23} \gg q_0$ for $v \gg v_0$ so that in order to estimate $g_n^{(1)}$ in Eq. (A.1) expression (13) is valid where the s-states ($l = 0$) give the leading contribution out of the entire sum over the discrete spectrum, as follows from Eq. (13): $g_{nl}(k_0) \approx 1/k_0^{2+l}$. The major contribution to the first integral (over q_3 and q_1) in Eq. (A.1) originates from the neighborhood of the points $\mathbf{q}_1 = \mathbf{k}_i$, $\mathbf{q}_3 = \mathbf{k}_i m_3/m_{23}$, at which the singularities of ψ_i, V_3, and $\psi_n^{(1)}$ coincide and also the denominator of the Green's function vanishes. In the second integral (over q_1 and q_2) in Eq. (A.1) the corresponding regions are the neighborhoods of the points $\mathbf{q}_1 = \mathbf{k}_i$ and $\mathbf{q}_2 = -\mathbf{k}_i m_2/m_{23}$. In both of the integrals in (A.1), the remaining regions give an appreciably smaller contribution.

In the integral over q_1 in both terms in Eq. (A.1) we distinguish the neighborhood of the point $\mathbf{q}_1 = \mathbf{k}_i$, which we choose in the form of the intersection of a spherical shell of thickness $\sim q_0 \nu^{1+\kappa}$ ($\kappa \ll 1$) next to the sphere $|\mathbf{q}_1| = k_0$ and a cone with vertex at zero, vertex angle 2R, and axis directed along $\mathbf{k}_i$, where $\nu \ll R \ll 1$. Let us denote this region by $\Omega_{\mathbf{k}_i}$. Let us expand the functions $g_n^{(1)}$ and ψ_f in the neighborhood of $\Omega_{\mathbf{k}_i}$ with retention of the major terms, where it follows from Eq. (13) that

$$g_{n0}^{(1)}\left(\mathbf{k}_f - \frac{m_2}{m_{23}}\mathbf{k}_i\right) \cong \frac{\text{const}}{n^{3/2}}\frac{1}{(\mathbf{k}_f - \mathbf{k}_i m_2/m_{23})^2};$$

then for the leading asymptotic behavior of (A.1) we obtain the expression

$$I(1,\bar{3}) + I(1,\bar{2}) \approx$$
$$\approx \frac{\text{const}_1}{q_i^4 q_f^2}\int\limits_{\Omega_{k_i}} dq_1 V(\mathbf{q}_1 - \mathbf{k}_i)\left\{\sum_{n=1}^{\infty}\frac{1}{n^{3/2}}\left[\frac{1}{2\mu_1}q_1^2 - \frac{1}{2\mu_1}k_0^2 - E_n + E_0 - i\varepsilon\right]^{-1}\right.$$
$$\left.\times\int d\mathbf{q}\left[\Psi_i\left(\mathbf{q} + \frac{m_3}{m_{23}}(\mathbf{q}_1 - \mathbf{k}_i)\right) - \Psi_i\left(\mathbf{q} - \frac{m_2}{m_{23}}(\mathbf{q}_1 - \mathbf{k}_i)\right)\right]\Psi_n(\mathbf{q})\right\}$$
$$+ \frac{\text{const}_2}{q_i^4 q_f^2}\int\limits_{\Omega_{k_i}} dq_1 V(\mathbf{q}_1 - \mathbf{k}_i)\int\limits_{\Omega_{cq_0}} d\mathbf{k} e^{+\pi i/2k}\Gamma\left(1 + \frac{i}{k}\right)$$
$$\times\left[\frac{1}{2\mu_1}q_1^2 - \frac{1}{2\mu_1}k_0^2 + \frac{k^2}{2\mu_{23}} + E_0 - i\varepsilon\right]^{-1}$$
$$\times\int\left[\Psi_i\left(\mathbf{q} + \frac{m_3}{m_{23}}(\mathbf{q}_1 - \mathbf{k}_i)\right) - \Psi_i\left(\mathbf{q} - \frac{m_2}{m_{23}}(\mathbf{q}_1 - \mathbf{k}_i)\right)\right]\Psi_k(\mathbf{q})\, d\mathbf{q}. \qquad (A.2)$$

Here it is taken into consideration that $V_2 = -|V_3|$ and the sum over the discrete spectrum (over all s-states, which give the largest contribution) is separated from the integral over the part of the continuous spectrum; $V(q) = 1/q^2$. In the integral over q_1 in (A.2) let us change to spherical coordinates with the z axis directed along $\mathbf{k}_i$. The integration over the polar angle is trivial. In the integral over the azimuthal angle θ[$\cos\theta = \mathbf{n}_{q_1}\cdot\mathbf{n}_{k_i} = t$] we distinguish the following regions: 1) $0 \leq (\mathbf{n}_{q_1} - \mathbf{n}_{k_i})^2 \leq \eta^2$ and 2) $\eta^2 \leq (\mathbf{n}_{q_1} - \mathbf{n}_{k_i})^2 \leq R^2$, but in the integral over the radial variable we set $q_1 = k_0 + q_0 \nu^{1+\kappa} q'$, ($\kappa \ll 1$); having carried out the indicated procedure and having omitted the higher terms in ν, we obtain:

$$I(1,\bar{3}) + I(1,\bar{2}) \approx \frac{4i\pi^2}{v q_i^4 q_f^2}\left[\int\limits_{1-R^2/2}^{1-\eta^2} + \int\limits_{1-\eta^2}^{1}\right]\frac{dt}{(\mathbf{n}_{q_1} - \mathbf{n}_{k_i})^2}\int d\mathbf{q}$$
$$\times\left[\Psi_i\left(\mathbf{q} + \frac{m_3 k_0}{m_{23}}(\mathbf{n}_{q_1} - \mathbf{n}_{k_i})\right) - \Psi_i\left(\mathbf{q} - \frac{m_2 k_0}{m_{23}}(\mathbf{n}_{q_1} - \mathbf{n}_{k_i})\right)\right]. \qquad (A.3)$$

In order to find the contribution to (A.3) coming

$$\times\Big[\sum_{n=1}^{\infty}\frac{\text{const}_1}{n^{3/2}}\Psi_n(q)+\text{const}_2\int\limits_{\Omega_{cq_0}}d\mathbf{k}\Psi_{\mathbf{k}}(q)\,e^{+\pi/2k}\,\Gamma\Big(1+\frac{i}{k}\Big)\Big]=J_1+J_2.$$

from the region 1) which was singled out (the integral over this region is denoted by J_1), we note that

$$\begin{aligned}&\int[\Psi_i(\mathbf{q}+\alpha_1\Delta)-\Psi_i(\mathbf{q}-\alpha_2\Delta)]\,\Psi_n(\mathbf{q})\,d\mathbf{q}\\&=\int\widetilde{\Psi}_{\mathbf{i}}(\mathbf{r})\,\widetilde{\Psi}_n(\mathbf{r})\,[e^{i\alpha_1\Delta\mathbf{r}}-e^{-i\alpha_2\Delta\mathbf{r}}]\,d\mathbf{r}\approx\\&\approx\int\widetilde{\Psi}_i(\mathbf{r})\,\widetilde{\Psi}_n(\mathbf{r})\,[i\,|\,\Delta\,|\,(\alpha_1+\alpha_2)\,r\cos(\mathbf{n}_r\mathbf{n}_\Delta)\\&\quad+\frac{\alpha_2^2-\alpha_1^2}{2}r^2\Delta^2\cos^2(\mathbf{n}_r\mathbf{n}_\Delta)+\ldots\Big]\,d\mathbf{r}\end{aligned}\qquad(A.4)$$

as $|\Delta|\to 0$ where $\widetilde{\psi}_{\mathbf{i}}(\mathbf{r})$ and $\psi_{\mathbf{n}}(\mathbf{r})$ are the corresponding wave functions in the coordinate representation. For the s-states of the discrete spectrum this expansion begins with terms which are quadratic in $|\Delta|$, but for wave functions of the continuous spectrum the expansion begins with linear terms. Taking the mentioned remark into account, for the leading contribution from region 1) we have

$$\begin{aligned}J_1\approx\frac{4i\pi^2}{vq_i^4q_f^2}\int\limits_{1-\nu^2}^{1}\frac{dt}{(\mathbf{n}_{q_1}-\mathbf{n}_{k_i})^2}\Big[&\frac{\text{const}_1k_0^2(\mathbf{n}_{q_1}-\mathbf{n}_{k_i})^2}{2}\sum_{n=1}^{\infty}\frac{f_{in}}{n^{3/2}}\\&+i\,\text{const}_2\,k_0\,|\,\mathbf{n}_{q_1}-\mathbf{n}_{k_i}|\int\limits_{\Omega_{cq_0}}d\mathbf{k}e^{+\pi/2k}\Gamma\Big(1+\frac{i}{k}\Big)f_{ik}\Big]\\&=\frac{4i\pi^2}{vq_i^4q_f^2}\Phi(q_0)\sim\frac{1}{v^7},\end{aligned}\qquad(A.5)$$

where $f_{ik}=\int\widetilde{\psi}_{\mathbf{i}}(\mathbf{r})\widetilde{\psi}_{\mathbf{k}}(\mathbf{r})r\cos(\mathbf{n}_r\mathbf{n}_\Delta)d\mathbf{r}$, and $\Phi(q_0)$ is a convergent integral over t in (A.5) which does not depend on v.

Then let us estimate the contribution to (A.3) from region 2) which was singled out above:

$$\begin{aligned}J_2=\frac{4i\pi^2}{vq_i^4q_f^2}\Big\{\Big[&-\int\limits_{1-R^2/2}^{1-\eta^2}\frac{dt}{2(1-t)}\int d\mathbf{q}\Psi_i\Big(\mathbf{q}-\frac{m_2k_0}{m_{23}}(\mathbf{n}_{q_1}-\mathbf{n}_{k_i})\Big)\\&+\int\limits_{1-R^2/2}^{1-\nu^2}\frac{dt}{2(1-t)}\int d\mathbf{q}\Psi_i\Big(\mathbf{q}+\frac{m_3k_0}{m_{23}}(\mathbf{n}_{q_1}-\mathbf{n}_{k_i})\Big)\\&+\int\limits_{1-\nu^2}^{1-\eta^2}\frac{dt}{2(1-t)}\int d\mathbf{q}\Psi_i\Big(\mathbf{q}+\frac{m_3k_0}{m_{23}}(\mathbf{n}_{q_1}-\mathbf{n}_{k_i})\Big)\Big]\\\times\Big(&\sum_{n=1}^{\infty}\frac{\text{const}_1}{n^{3/2}}\Psi_n(\mathbf{q})+\text{const}_2\int\limits_{\Omega_{cq_0}}\Psi_{\mathbf{k}}(q)\,e^{+\pi/2k}\Gamma\Big(1+\frac{i}{k}\Big)d\mathbf{k}\Big)\Big\}\\&=\frac{4i\pi^2}{vq_i^4q_f^2}\{-A_1+A_2+A_3\},\end{aligned}\qquad(A.6)$$

where the integrals inside the curly brackets in (A.6) are denoted by A_1, A_2, and A_3, respectively, with respect to the regions

$$1-\frac{R^2}{2}\leqslant t\leqslant 1-\eta^2;\quad 1-\frac{R^2}{2}\leqslant t\leqslant 1-\nu^2,\quad 1-\nu^2\leqslant t\leqslant 1-\eta^2.$$

In the integrals A_1 and A_2 the regions of localization of the functions $\psi_{\mathbf{i}}$ and $\psi_{\mathbf{n}}$ in the integral over q will be well separated, and one can take their contributions into account separately; for $|\Delta|\gg q_0^2$ we shall have

$$\begin{aligned}\int\Psi_i(\mathbf{q}+\Delta)\Psi_n(\mathbf{q})\,d\mathbf{q}&\approx\frac{\text{const}'}{n^{3/2}\Delta^4},\\\int\Psi_i(\mathbf{q}+\Delta)\Psi_{\mathbf{k}}(\mathbf{q})\,d\mathbf{q}&\approx\frac{\text{const}''}{\Delta^4}e^{+\pi/2k}\Gamma\Big(1-\frac{i}{k}\Big).\end{aligned}\qquad(A.7)$$

In view of the smallness of $m_3/m_{23}\approx m_e/m_p$, we have the following result for the integral A_3 in the region $1-\nu^2\leq t\leq 1-\eta^2$:

$$\int\Psi_i\Big(\mathbf{q}+\frac{m_3}{m_{23}}(\mathbf{n}_{q_1}-\mathbf{n}_{k_i})\Big)\Psi_n(\mathbf{q})\,d\mathbf{q}\approx\delta_{i,n}\qquad(A.8)$$

as a consequence of the orthogonality of the wave functions. Taking relations (A.7) and (A.8) into consideration, we obtain the following estimate for the major contribution to (A.6):

$$\begin{aligned}J_2\approx\frac{4i\pi^2}{vq_i^4q_f^2}\Big\{&\frac{1}{k_0^4}\Big[\int\limits_{1-R^2/2}\frac{dt}{8(1-t)^3}\Big(\frac{m_{23}}{m_3}\Big)^4-\int\limits_{1-R^2/2}^{1-\eta^2}\frac{dt}{8(1-t)^3}\Big(\frac{m_{23}}{m_2}\Big)^4\Big]\\&\times\Big[\text{const}_1'\sum_{n=1}^{\infty}\frac{1}{n^3}+\text{const}_2'\int\limits_{\Omega_{cq_0}}e^{+\pi/k}\Gamma\Big(1-\frac{i}{k}\Big)\Gamma\Big(1+\frac{i}{k}\Big)d\mathbf{k}\Big]\\&+\int\limits_{1-\nu^2}^{1-\eta^2}\frac{dt\,\text{const}_1}{2(1-t)}\Big\}=\frac{4i\pi^2}{vq_i^4q_f^2}F(q_0)\sim\frac{1}{v^7},\end{aligned}\qquad(A.9)$$

where $F(q_0)$ is the integral, independent of v, inside the curly brackets in Eq. (A.9). Comparing expressions (A.5) and (A.9) we find $|I(1,\bar{2})+I(1,\bar{3})|\sim 1/v^7$, which corresponds to the estimate (27a) cited in the text. An estimate of the contributions of $|I(\bar{1},2)+I(\bar{3},2)|\sim 1/v^7$ is carried out in similar fashion.

Out of the contributions from regions of the type $\bar{\Omega}_\alpha\otimes\Omega_\beta$ we still have to consider $I(\bar{1},3)I(3,\bar{2})$. The expressions for these contributions have the same structure. For example, let us consider

$$\begin{aligned}I(\bar{1},3)=\int\limits_{\Omega_3\otimes\bar{\Omega}_1}&d\mathbf{q}_3d\mathbf{q}_1\Psi_i\Big(\mathbf{q}_3+\frac{m_3}{m_{23}}\mathbf{k}_i\Big)\cdot\\&\times\int\limits_{\Omega_{cq_0}}d\mathbf{k}g_{\mathbf{k}}^{(3)*}\Big(\mathbf{k}_i+\frac{m_1}{m_{12}}\mathbf{q}_3\Big)\Big(\frac{k^2}{2\mu_{12}}+\frac{q_3^2}{2\mu_3}-E-i\varepsilon\Big)^{-1}\\&\times\Psi_{\mathbf{k}}^{(3)}\Big(\mathbf{q}_1+\frac{m_1}{m_{12}}\mathbf{q}_3\Big)V_1(\mathbf{q}_1+\mathbf{q}_3-\mathbf{k}_f)\,\Psi_f\Big(\mathbf{q}_1-\frac{m_1}{m_{13}}\mathbf{k}_f\Big).\end{aligned}\qquad(A.10)$$

For $\mathbf{q}_3\in\Omega_3$ estimate (13) is valid for $g_{\mathbf{k}}^{(3)}(\mathbf{k}_i+\mathbf{q}_3m_1/m_{12})$. The neighborhoods of the points $\mathbf{q}_1=\mathbf{k}_fm_1/m_{13}$ and $\mathbf{q}_1=-\mathbf{q}_3m_1/m_{12}$ give the leading contribution to the integral over $\mathbf{q}_1$, where for $\mathbf{q}_3\in\Omega_3$ these regions, in contrast to the case analyzed above, do not overlap and one can take their contributions into account separately. Having made the substitution $\mathbf{q}_1=k_0\mathbf{q}_1$ and $\mathbf{q}_3=k_0\widetilde{\mathbf{q}}_3$, and having omitted higher-order terms in q_0/k_0 in the denominator of the Green's function, it is not difficult to verify that $I(\bar{1},3)\sim 1/v^{11}$ and $I(3,\bar{2})\sim 1/v^{11}$.

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