

Asymptotic behavior of charge-transfer cross sections

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Explicit asymptotic expressions are derived for the terms of the perturbation theory series for the T matrix of the process (1) in the case of arbitrary quantum numbers of the compound particles. The cross sections for charge transfer into arbitrary ns and np states in a collision of a "heavy" charged particle (a proton, an atomic nucleus with $Z \sim 1$) with hydrogen atoms at high energies are computed. A simple method of deriving the asymptotic wave functions of two-particle systems in the momentum representation as $p \rightarrow \infty$ directly in terms of the asymptotic form of the Fourier transform $\tilde{U}(p)$ of the potential is presented.

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In the present paper we consider within the framework of nonrelativistic quantum mechanics high-energy collisions in a system of three "elementary"¹ particles, of which two in both the initial and final states are bound, i.e., form a "compound" particle:

$$1+(2+3) \rightarrow (1+2)+3, \quad (1)$$

where 1, 2, and 3 number the particles of the system and (1+2) and (2+3) denote the corresponding compound particles.

To the type of collisions in question pertain such processes of atomic physics as charge transfer in the collisions of a proton (or some other charged "elementary" particle: the positron, a nucleus, etc., but not an ion) with the hydrogen atom. The cross sections for such processes occurring at high energies have been computed in quite a large number of papers (see Refs. 1 and 2 for reviews) in various approximations (and for different quantum numbers of the compound particles—the hydrogen-like atoms). It has been established that the asymptotic form of the amplitude for $V \rightarrow \infty$ is given by the first two terms of the perturbation theory series, but a consistent calculation of the asymptotic form of the cross section has been performed only for the reaction $H^+ + H(1s) \rightarrow H(1s) + H^+$ in the case in which the atoms are in the ground $1s$ states.¹⁻⁴ Let us note that the highly developed asymptotic—in terms of the impact parameter—methods of the theory of atomic collisions^{5,6} cannot be used to compute the cross sections for charge transfer at high energies, since the small impact parameters are, on the contrary, important in this case.

In the present paper we develop a method for the computation of the asymptotic forms of the terms of the perturbation theory series for the T matrix of the process (1) in the case of arbitrary quantum numbers, n_r and l , of the compound particles. This method allows us to derive explicit expressions for the amplitudes for high energies under conditions when the changes in the momenta of all the three particles participating in the collision are also large. On the basis of these expressions, we consider charge transfer to arbitrary ns and np states during the collision of a "heavy" particle (a proton, nucleus) of charge Ze with a hydrogen atom in the s state:

$$Ze + (e^- + p) \rightarrow (Ze + e^-) + p. \quad (2)$$

We derive explicit expressions for the cross sections for charge transfer to the indicated states in first-order perturbation theory and the exact asymptotic expressions by considering the amplitude in the first two orders of perturbation theory (the cross sections for charge transfer to states with higher orbital angular momenta can be computed in similar fashion). We also present below a simple method of deriving the asymptotic form of the wave function of a two-particle system in the momentum representation for $p \rightarrow \infty$ and quite arbitrary potentials.

ASYMPTOTIC FORM OF THE WAVE FUNCTION OF A TWO-PARTICLE SYSTEM IN THE MOMENTUM REPRESENTATION AS $p \rightarrow \infty$

Let us set forth the principal notations and assumptions used in the paper. The mass of the a -th particle is denoted by m_a and the reduced masses are denoted by

$$\mu_{ab} = \frac{m_a m_b}{m_a + m_b}, \quad \mu_{ab,c} = \frac{(m_a + m_b) m_c}{m_a + m_b + m_c}.$$

The interaction potential $U = \sum_{a < b} U_{ab}$ for the particles in the system is given by central pair potentials $U_{ab}(|\mathbf{r}_a - \mathbf{r}_b|)$, where

$$U_{ab}(r) = \frac{1}{(2\pi)^3} \int e^{i\Delta r} \tilde{U}_{ab}(\Delta) d^3\Delta.$$

According to the general theory of many-channel scattering,⁷ the expression for the T matrix of the process (1) in perturbation theory has the form

$$T = U_{12} + U_{13} + (U_{13} + U_{23}) \frac{1}{E - H_0 + i0} (U_{12} + U_{13}) + \dots$$

The differential cross section for the process is given by

$$\frac{d\sigma}{d\Omega} = (2\pi)^4 \mu_{23,1} \mu_{12,3} \frac{p_2}{p_1} |T_{ij}|^2, \quad (3)$$

where p_1 is the momentum of the first particle in the c.m. system before the collision and p_2 , with $p_2^2 \approx \mu_{12,3} p_1^2 / \mu_{23,1}$, is the momentum of the compound particle (1+2).

Of importance for the analysis below are the following limitations on the behavior of the Fourier transforms of the potentials as $q \rightarrow \infty$ and arbitrarily small $\varepsilon > 0$:

$$1) \tilde{U}_{ab}(q) q^{1+\varepsilon} \rightarrow 0, \quad 2) \tilde{U}_{ab}(q) \exp(\alpha q^{1-\varepsilon}) \rightarrow \infty, \quad (4)$$

3) $\tilde{U}_{ab}(q)$ does not contain a rapidly oscillating factor of the type $\sin(\alpha q^n)$ with $n \geq 1$. Remembering the relation

$$U(q) = \frac{2\pi}{iq} \int_{-\infty}^{\infty} e^{iqr} U(|r|) dr$$

and the general ideas about the character of the law governing the decrease of the Fourier transform as $q \rightarrow \infty$, we note that the indicated limitations 2) and 3) imply that the function $U(|r|)$, the even continuation into the region $r < 0$ of the function $U(r)$ regarded as an analytic function of the variable r , has a singularity at $r=0$. It is precisely this singularity which determines the asymptotic form of $\tilde{U}(q)$ as $q \rightarrow \infty$; in particular, the "weaker" the singularity of the function $U(|r|)$ is, the more rapidly $\tilde{U}(q)$ decreases. The condition 1), on the other hand, limits the nature of the singularity by the requirement that

$$U(r)r^{2-\varepsilon} \rightarrow 0 \text{ as } r \rightarrow 0 \quad (5)$$

($\varepsilon > 0$ is arbitrarily small; for the function $U = \alpha/r^2$ we have $\tilde{U} = 2\pi^2 \alpha/q$).

As is well known,⁸ for a particle in a central field satisfying the condition (5), the bound-state wave function

$$\psi_{n_r l m}(r) = r^l Y_{lm}(r/r) R_{n_r l}(r) \quad (6)$$

possesses as $r \rightarrow 0$ the properties $R_{n_r l}(0) = \text{const} \neq 0$ and $R_{n_r l}(0) < \infty$. Above we noted the prospective singular behavior of the even continuation of the potential at the point $r=0$. In this case the even continuation of the radial function $R_{n_r l}$ also has a singularity at $r=0$. It is, however, significant that the singularity of the function $R_{n_r l}$ is weaker than that of the potential U . This assertion is a direct consequence of the Schrödinger equation. In particular, if the singular part of $U(r)$ has the form $U^{(s)}(r) \approx \alpha r^\nu$,²⁾ then the singular part of the radial function is

$$R_{n_r l}^{(s)}(r) \approx \frac{2m\alpha}{(\nu+2)^2(\nu+2l+3)} R_{n_r l}(0) r^{\nu+2},$$

and vanishes as $r \rightarrow 0$, in contrast to $R_{n_r l}(0)$.

For the subsequent calculations, it is convenient to write the spherical function in the form

$$r^l Y_{lm}(r/r) = \varepsilon_{i_1 \dots i_n}(m) x_{i_1} \dots x_{i_n}, \quad (7)$$

where $\varepsilon_{i_1 \dots i_n}$ is symmetric in any two of the indices of the traceless tensor of rank l : $\varepsilon_{i_1 \dots i_n} = 0$. We shall also need the asymptotic forms of the wave functions in the momentum representation of the two-particle system, or, bearing in mind the general approach to the two-body problem, of one particle in an external field. This asymptotic form can be found as follows. Multiplying both sides of the Schrödinger equation

$$\left(-\frac{\Delta}{2m} - E_{n_r l}\right) \psi_{n_r l m}(r) = -U(r) \psi_{n_r l m}(r)$$

by $(2\pi)^{-3/2} \exp(-ipr)$, and integrating over the coordinates, we effect the following transformation:

$$\begin{aligned} \left(\frac{p^2}{2m} - E_{n_r l}\right) \varphi_{n_r l m}(p) &= -\frac{\varepsilon_{i_1 \dots i_n}}{(2\pi)^{3/2}} \int e^{-ipr} x_{i_1} \dots x_{i_n} U(r) R_{n_r l}(r) d^3r \\ &= -\frac{i^l}{(2\pi)^{3/2}} \varepsilon_{i_1 \dots i_n} \frac{\partial}{\partial p_{i_1}} \dots \frac{\partial}{\partial p_{i_n}} \int e^{-ipr} U(r) R_{n_r l}(r) d^3r. \end{aligned}$$

As $p \rightarrow \infty$ we can take out from under the integral sign $R_{n_r l}(r)$ at the point $r=0$ (in so doing we nevertheless retain the most singular part of the integrand at the point $r=0$, i.e., the part that determines the asymptotic form of the integral in question!). Using also the relation

$$\partial U(p) / \partial p_i = 2p_i \partial U(p) / \partial p^2$$

and the fact that the tensor $\varepsilon_{i_1 \dots i_n}$ is traceless, we obtain the sought asymptotic form

$$\varphi_{n_r l m}(p) \approx -\frac{2m}{(2\pi)^{3/2}} (2i)^l p^{l-2} R_{n_r l}(0) Y_{lm}(p/p) \frac{\partial^l}{\partial p^{2l}} U(p). \quad (8)$$

From (8) it follows that $\varphi(p)$ decreases more rapidly than $\tilde{U}(p)$, which reflects the above-noted fact that the radial function behaves less singularly than the potential at the point $r=0$.

Bearing in mind the above calculations, we can easily see that the result (8) can be generalized in an obvious manner to the case in which the points $r = \pm a$ on the real axis are the only singular points of the even continuation of the potential (various kinds of model potentials with sharply marked boundaries or kinks): to do this we must replace $R_{n_r l}(0)$ in (8) by $R_{n_r l}(a)$. But despite the fact that the asymptotic forms in these cases are outwardly similar, they differ significantly from each other. This difference is due to the fact that, in the case of the singular points $r = \pm a \neq 0$, the Fourier transform $\tilde{U}(p)$ contains the rapidly oscillating factor $\sin(pa)$, whose presence gives rise to a situation in which all the derivatives of $\tilde{U}(p)$ decrease in the same fashion as $\tilde{U}(p)$. Accordingly, the wave functions of states with different values of l also decrease in the same manner as $p \rightarrow \infty$. But in the case of the singular point $r=0$ the higher the value of the angular momentum l is, the faster the wave function of the state with l decreases.

Let us make two other observations in regard to the notation. Below we shall often drop the quantum numbers n_r , l , and m of the states of the compound particles, denoting the corresponding wave functions in the coordinate and momentum representations as $\psi_{1,2}(\mathbf{r})$ and $\varphi_{1,2}(p)$ respectively [the subscript 1 pertains to the compound particle (2+3); the subscript 2, to (1+2)]. Finally, we introduce the following notation for the combinations of the momenta $\mathbf{p}_{1,2}$:

$$\mathbf{f}_1 = \mathbf{p}_1 - \frac{m_1}{m_1+m_2} \mathbf{p}_2, \quad \mathbf{f}_2 = \mathbf{p}_2 - \frac{m_2}{m_2+m_3} \mathbf{p}_1, \quad \mathbf{g} = \mathbf{f}_1 + \mathbf{f}_2.$$

The analysis performed below presupposes the fulfillment of the conditions

$$f_1 a \gg 1, \quad f_2 a \gg 1, \quad g a \gg 1, \quad (9)$$

where a is the characteristic range of the pair interaction potentials; $-f_1$, \mathbf{g} , and $-f_2$ then actually determine the changes that occur in the momenta of the 1st, 2nd, and 3rd particles respectively in the process (1).

ASYMPTOTIC BEHAVIOR OF THE TERMS OF THE PERTURBATION-THEORY SERIES

Before proceeding to derive the asymptotic expressions for the amplitude T_{if} of the process (1), let us

demonstrate the main idea of the calculation of such asymptotic forms with a simpler example.

Let us consider the asymptotic form, as $q \rightarrow \infty$, of the integral

$$I(q) = \int \varphi_2^*(q-\Delta) \varphi_1(\Delta) d^3\Delta \quad (10)$$

in the case in which the angular momentum has the value $l_1 = 0$ in the state 1 and an arbitrary value l_2 in the state 2. In the integrand the functions $\varphi_{1,2}$ are localized in regions of dimension of the order of $1/a$ around the points $\Delta = 0$ and $\Delta = q$. Furthermore, the entire integrand is localized in the indicated regions [here it is essential that $\varphi(q)$, like $\tilde{U}(q)$, decrease more slowly than an exponential function; in the opposite case, e.g., when $\varphi_{1,2} \propto \exp(-\alpha q^2)$ the region of localization is completely different]. Accordingly,

$$I(q) \approx \int_{|\Delta| \leq 1/a} \varphi_2^*(q-\Delta) \varphi_1(\Delta) d^3\Delta + \int_{|\Delta| \leq 1/a} \varphi_2^*(\Delta) \varphi_1(q-\Delta) d^3\Delta = I_1 + I_2 \quad (11)$$

[since, on account of (4) and (8), $\varphi(q)$ decreases faster than $1/q^3$, the contribution of the rest of the region $\Delta \sim q$ to the value of the integral (10) is asymptotically negligible in comparison with the contribution of the regions indicated in (11)].

In the expression for I_1 in (11) we can drop the Δ in $\varphi_2^*(q-\Delta)$ [it is then essential that φ , like \tilde{U} , satisfy the conditions (2) and (3) (see (4) and below)] and extend the integration over Δ to cover the entire space. We then obtain

$$I_1(q) \approx (2\pi)^{3/2} \psi_1(0) \varphi_2^*(q). \quad (12)$$

The asymptotic form of I_2 in the $l_2 = 0$ case is derived in an entirely similar fashion. But we cannot thus proceed when $l_2 \equiv l \neq 0$ [$\psi_{l \neq 0}(0) = 0$]. In this case we must first expand $\varphi_1(q-\Delta)$ in powers of Δ right up to the terms of the l -th order in the Δ_i inclusively:

$$I_2 \approx \int d^3\Delta \varphi_2^*(\Delta) \sum_{n=0}^l \frac{(-1)^n}{n!} \frac{\partial^n}{\partial q_1 \dots \partial q_n} \varphi_1(q) \Delta_1 \dots \Delta_n. \quad (13)$$

The first l terms of the sum vanish, and the asymptotic form of (13) is given by the last term (with $n=l$; the subsequent terms of the expansion in Δ give corrections to the asymptotic form). The vanishing of the first l terms follows from the orthogonality of the spherical functions, since the n -th rank tensor $\Delta_1 \dots \Delta_n$ can be represented in the form of combinations of the spherical functions $Y_{l',m}(\Delta/\Delta)$ (multiplied by Δ^n) with $l' \leq n \leq l-1$ and $\varphi_2^*(\Delta)$ contains $Y_{l,m}(\Delta/\Delta)$. To compute in (13) the integral corresponding to the term with $n=l$, we proceed in the following manner. Let us take the $(\partial/\partial x_1 \dots \partial/\partial x_n)$ -type l -th derivatives of both sides of the equality

$$\psi_{n,l,m}(r) = \frac{1}{(2\pi)^{3/2}} \int e^{i\mathbf{r}\cdot\Delta} \varphi_{n,l,m}(\Delta) d^3\Delta.$$

Taking (6) and (7) and the symmetry and tracelessness of $\varepsilon_{i\dots k}$ into account, and letting $\mathbf{r} \rightarrow 0$ in the expression obtained after the differentiation, we find that

$$(ll) R_{n,l}(0) \varepsilon_{i\dots k}(m) = \frac{i^l}{(2\pi)^{3/2}} \int \Delta_1 \dots \Delta_n \varphi_{n,l,m}(\Delta) d^3\Delta.$$

Accordingly, the asymptotic expression for I_2 assumes the form

$$\begin{aligned} I_2(q) &\approx (2\pi)^{3/2} (-i)^l R_{n,l}^{(2)*}(0) \varepsilon_{i\dots k}(m) \frac{\partial^l}{\partial q_1 \dots \partial q_n} \varphi_1(q) \\ &= (2\pi)^{3/2} (-2i)^l R_{n,l}^{(2)*}(0) Y_{lm} \left(\frac{\mathbf{q}}{q} \right) q^l \frac{\partial^l}{\partial q^{2l}} \varphi_1(q). \end{aligned} \quad (14)$$

The sum of the expressions (12) and (14) with allowance for (8) completely determines the explicit asymptotic form of the integral (10):

$$\begin{aligned} I(q) &\approx -2(-2i)^l \psi_1(0) R_{n,l}^{(2)*}(0) Y_{lm} \left(\frac{\mathbf{q}}{q} \right) q^l \\ &\times \left[\mu_{23} \frac{\partial^l}{\partial q^{2l}} \frac{U_{23}(q)}{q^2} + \mu_{12} q^{-2} \frac{\partial^l}{\partial q^{2l}} U_{12}(q) \right]. \end{aligned}$$

Let us proceed to derive the asymptotic expressions for the amplitude. In first order perturbation theory $T_{if}^{(1)} = \langle f | U_{12} + U_{13} | i \rangle$, the amplitude of the process is given by the relations

$$\langle f | U_{12} | i \rangle = -[f_1^2 / 2\mu_{12} - \varepsilon_2] \varphi_2^*(\mathbf{f}_1) \varphi_1(\mathbf{f}_2), \quad (15)$$

$$\langle f | U_{13} | i \rangle = \frac{1}{(2\pi)^3} \int U_{13}(\Delta) \varphi_2^*(\mathbf{f}_1 + \Delta) \varphi_1(\mathbf{f}_2 - \Delta) d^3\Delta. \quad (16)$$

The asymptotic form of the expression (15) is found directly with the aid of the formula (8), and has in the case $l_1 = 0$, $l_2 \equiv l$ (which is the only one we shall consider below) the form

$$\langle f | U_{12} | i \rangle \approx \mu_{23} B_{i\dots k}(m) f_{i\dots k} \frac{U_{23}(f_2)}{f_2^2} \frac{\partial^l}{\partial f_1^{2l}} U_{12}(f_1), \quad (17)$$

where

$$B_{i\dots k}(m) = -\frac{(-2i)^l}{4\pi^3} \psi_1(0) R_{n,l}^{(2)*}(0) \varepsilon_{i\dots k}(m). \quad (18)$$

The asymptotic form of the expression (16) is found in much the same way as used to derive the integral (10) above. The integrand in (16) is localized in three regions of the space of the momenta Δ :

$$|\mathbf{f}_2 - \Delta| \leq 1/a, \quad |\mathbf{f}_1 + \Delta| \leq 1/a, \quad |\Delta| \leq 1/a, \quad (19)$$

and these regions, under the conditions (9), clearly do not overlap. Since $\varphi(p)$ decreases faster than $\tilde{U}(p)$, it is easy to understand that the contribution to the asymptotic form of the expression (16) from the third of the regions in (19) (where the potential is localized) is asymptotically negligible, and the asymptotic form of the expression is given by the contribution of only the first and second regions in (19). Consequently, we can write

$$\langle f | U_{13} | i \rangle \approx \langle f | U_{13} | i \rangle_1 + \langle f | U_{13} | i \rangle_2$$

[cf. (11)]. The asymptotic form of $\langle f | U_{13} | i \rangle_1$ can then be found in much the same way as (12) was found, and has the form

$$\langle f | U_{13} | i \rangle_1 \approx \mu_{12} B_{i\dots k}(m) g_1 \dots g_k \frac{U_{13}(f_2)}{g^2} \frac{\partial^l}{\partial g^{2l}} U_{12}(g). \quad (20)$$

The asymptotic form of $\langle f | U_{13} | i \rangle_2$, on the other hand, is computed in much the same way as expression (14):

$$\langle f | U_{13} | i \rangle_2 \approx \frac{\mu_{23}}{2^l} B_{i\dots k}(m) \frac{\partial^l}{\partial f_{11} \dots \partial f_{1k}} \frac{U_{13}(f_1) U_{23}(|\mathbf{f}_1 + \mathbf{f}_2|)}{(\mathbf{f}_1 + \mathbf{f}_2)^2}. \quad (21)$$

The described method of deriving asymptotic expressions can be directly applied in the computation of the asymptotic amplitude of the process (1) in second-order perturbation theory:

$$T_{ij}^{(2)} = \left\langle f \left| (U_{13} + U_{23}) \frac{1}{E - H_0 + i0} (U_{12} + U_{13}) \right| i \right\rangle. \quad (22)$$

Let us show how this can be done for one of the terms in (22). For this purpose, let us write it in the momentum representation ($\Delta = \mathbf{g} - \mathbf{q}_1 - \mathbf{q}_2$):

$$\begin{aligned} & \langle f | U_{13} (E - H_0 + i0)^{-1} U_{12} | i \rangle = \\ & = \iint \frac{d^3 q_1 d^3 q_2}{(2\pi)^6} \frac{\varphi_2^*(\mathbf{q}_2) \varphi_1(\mathbf{q}_1) U_{12}(\mathbf{g} - \mathbf{q}_1 - \mathbf{q}_2) U_{13}(\mathbf{f}_2 - \mathbf{q}_1)}{\mathbf{p}_1 \Delta / \mu_{23,1} - \mathbf{q}_1 \Delta / m_2 - \Delta^2 / 2\mu_{12} - \mathbf{q}_1^2 / 2\mu_{13} + i0}. \end{aligned}$$

Arguments similar to those adduced in the analysis of the integrals (10) and (16) allow us to assert that the dominant role in the integral is played by the momentum regions $|\mathbf{q}_{1,2}| \leq 1/a$. We can then neglect the dependence on \mathbf{q}_1 of the expressions for \tilde{U}_{12} , \tilde{U}_{13} , and the energy denominator [in exactly the same way as was done in the derivation of (12)], and allow for the dependence on \mathbf{q}_2 by expanding them in series in powers of q_{2i} right up to the terms of the l -th order inclusive [as was done in the derivation of (14)]. After this, the integration over $\mathbf{q}_{1,2}$ is performed in exactly the same way as in the derivation of (12) and (14). Proceeding in this manner, we find that

$$\langle f | U_{13} (E - H_0 + i0)^{-1} U_{12} | i \rangle \approx - \frac{B_{l...k}(m)}{2^{l+1}} U_{13}(f_2) \frac{\partial^l}{\partial g_{i_1} \dots \partial g_{i_l}} \frac{U_{12}(g)}{\mathbf{p}_1 \mathbf{g} / \mu_{23,1} - g^2 / 2\mu_{12}}. \quad (23)$$

The asymptotic forms of two other terms from (22) can be derived in much the same way:

$$\begin{aligned} & \langle f | U_{23} (E - H_0 + i0)^{-1} U_{12} | i \rangle \approx - \frac{B_{l...k}(m)}{2^{l+1}} U_{23}(f_2) \frac{\partial^l}{\partial f_{i_1} \dots \partial f_{i_l}} \\ & \quad \times \frac{U_{13}(f_1)}{\mathbf{p}_1 \mathbf{f}_1 / \mu_{23,1} - f_1^2 / 2\mu_{12}}, \quad (24) \\ & \langle f | U_{23} (E - H_0 + i0)^{-1} U_{13} | i \rangle \approx - \frac{B_{l...k}(m)}{2^{l+1}} \frac{\partial^l}{\partial f_{i_1} \dots \partial f_{i_l}} \frac{U_{13}(f_1) U_{23}(f_1 + f_2)}{\mathbf{p}_1 \mathbf{f}_1 / \mu_{23,1} - f_1^2 / 2\mu_{12}}. \quad (25) \end{aligned}$$

It is easy to see that the terms (23)–(25) of the amplitude of the second approximation are of the same order of magnitude as the first-order perturbation-theory terms (17), (20), and (21). The fourth term in (22),

$$\langle f | U_{13} (E - H_0 + i0)^{-1} U_{13} | i \rangle,$$

which contains the same pair potential U_{13} on both occasions, is of completely different order of magnitude. An order-of-magnitude estimate shows that this term differs by the factor $U_0 a / V$ (U_0 and a are the characteristic magnitude and range of the potential and V is the relative velocity of the colliding particles) from the magnitude of the $\langle f | U_{13} | i \rangle$ term of the amplitude of the first approximation. Thus, in the case $U_0 a / V \ll 1$, which is the necessary condition of applicability of perturbation theory to fast-particle scattering (see Ref. 8), this amplitude term is asymptotically unimportant, and can be dropped. All the third-order perturbation-theory terms also have negligible asymptotic values, so that the asymptotic form of the amplitude is entirely determined by the considered first- and second-order perturbation-theory terms.

ASYMPTOTIC BEHAVIOR OF THE CHARGE-TRANSFER AMPLITUDES AND CROSS SECTIONS

In this section we compute the cross sections for the charge transfer (2) on the basis of the obtained asymptotic expressions for the amplitude of the process (1).

Here the compound particle (2+3) is a hydrogen atom (2 is an electron and 3 is a proton), while 1 is a heavy "elementary" particle ($m_1 \gg m_2$) of charge Ze , i.e., an atomic nucleus, in particular, a proton; the compound particle (1+2) is consequently a hydrogen-like atom. It is assumed in the calculations below that prior to the collision the hydrogen atom is in the $n_1 s$ state. The state of the hydrogen-like atom after the collision is fixed by the quantum numbers n , l , and m ($n = n_r + l + 1$); the quantization axis for the angular momentum component is chosen in the direction of the vector \mathbf{p}_1 .

For the process (2) we have

$$U_{13}(q) = -U_{12}(q) = 4\pi Z e^2 / q^2, \quad U_{23}(q) = -4\pi e^2 / q^2. \quad (26)$$

Recognizing that $m_2 \equiv m \ll m_1 \sim m_3$ (m is the electron mass), we easily establish the following kinematic relations³:

$$\begin{aligned} \mathbf{f}_{1,2} & \approx \frac{m}{2\mu_{13}} \mathbf{p} \mp \mathbf{q}, \quad \mathbf{g} = \mathbf{f}_1 + \mathbf{f}_2 \approx \frac{m}{\mu_{13}} \mathbf{p}, \quad |\mathbf{q}| \approx p\theta, \\ f_1^2 \approx f_2^2 & \approx \frac{m^2 p^2}{4\mu_{13}^2} \left(1 + \frac{4\mu_{13}^2}{m^2} \theta^2 \right), \quad g^2 \approx m^2 p^2 / \mu_{13}^2, \end{aligned} \quad (27)$$

where \mathbf{q} is that component of the vector \mathbf{p}_2 which is perpendicular to $\mathbf{p}_1 \equiv \mathbf{p}$, and θ is the angle between the vectors \mathbf{p}_1 and \mathbf{p}_2 . The cross section for the process can, according to (3), then be computed with the aid of the formula

$$\sigma(n_1 s \rightarrow n l m) \approx (2\pi)^4 \mu_{13}^2 \int_0^\pi |T(n_1 s \rightarrow n l m)|^2 2\pi \theta d\theta \quad (28)$$

(in view of the rapid convergence, the upper integration limit can be taken to be equal to infinity).

As is well known, the most complete analytical investigation of the asymptotic behavior of charge-transfer cross sections has been performed only in the Oppenheimer–Brinkman–Kramers (OBK) approximation, which is based on the consideration of the amplitude of the process in first order perturbation theory without allowance for the interaction of the nuclei with each other, i.e., $T_{\text{OBK}} = \langle f | U_{12} | i \rangle$. The charge transfer cross section in this approximation is given by the expression

$$\begin{aligned} \sigma_{\text{OBK}}(n_1 s \rightarrow n l) & = \sum_n \Phi_{\text{OBK}}(n_1 s \rightarrow n l m) \\ & = \pi a_0^2 \frac{2^{2l+18} Z^{2l+5} (l!)^2 (2l+1) (n+1)!}{(l+5) ((2l+1)!)^2 (n-l-1)! n^2 n^{2l+4}} V^{-2l-12}, \end{aligned} \quad (29)$$

where $V = m p a_0 / \hbar \mu_{13}$ is the relative velocity of the colliding particles in atomic units and a_0 is the Bohr radius. Notice that this result is very easy to obtain if we take into account the fact that, according to (17) and (26), (27), the asymptotic form of the amplitude in the OBK approximation has the form

$$T_{\text{OBK}}(n_1 s \rightarrow n l m) \approx - \frac{4 (2i)^l Z m e^4 l! \psi_1(0) R_{nl}^{(0)*}(0) Y_{lm}^*(\mathbf{f}_1/f_1)}{\pi p^{l+6} [(m/2\mu_{13})^2 + \theta^2]^{3l/2}},$$

where⁸

$$\psi_1(0) = (\pi n_1^2 a_0^3)^{-1/2}, \quad R_{nl}^{(2)}(0) = \frac{2^{l+1}}{n^{l+2} (2l+1)!} \left[\frac{Z^{2l+3} (n+l)!}{(n-l-1)! a_0^{2l+3}} \right]^{1/2},$$

and in computing $\sigma_{\text{OBK}}(n_1 s \rightarrow n l)$ with the aid of the formula (28) we use the relation

$$\sum_m |Y_{lm}(n)|^2 = (2l+1)/4\pi.$$

The "partial" cross sections $\sigma_{\text{OBK}}(n_1s - nlm)$ then satisfy a relation of the form

$$\sigma_{\text{OBK}}(n_1s \rightarrow nlm) = g(l, m) \sigma_{\text{OBK}}(n_1s \rightarrow nl), \quad (30a)$$

where

$$g(l, m) = \frac{8\pi(l+5)}{2l+1} \int_0^{\pi/2} |Y_{lm}(\theta, \varphi)|^2 \sin \theta \cos^{2l+2} \theta d\theta. \quad (30b)$$

In particular,

$$g(1, 0) = 1/3, \quad g(1, 1) = g(1, -1) = 1/6. \quad (30c)$$

Before proceeding to compute the exact asymptotic expressions for the charge-transfer cross sections, let us consider the energy dependence of the cross sections in first-order perturbation theory. In this approximation the asymptotic form of the amplitude is given by the sum of the expressions (17), (20), and (21), and the cross sections can be computed consistently for different values of the quantum number l (and m) of the atom in the final state. As for the n dependence of the cross sections, which is characteristic of the OBK approximation, it is preserved in first order perturbation theory, since it is entirely determined by the factor $\psi_1(0)R_{n1}^{(2)*}(0)$ in the asymptotic form of the amplitude. Thus, we have in first order perturbation theory the relation

$$\sigma^{(1)}(n_1s \rightarrow nlm) = a^{(1)}(l, m, Z) \sigma_{\text{OBK}}(n_1s \rightarrow nlm), \quad (31)$$

where $a^{(1)}(l, m, Z)$ does not depend on any of the quantities n_1 , n , and V .

In the case of zero orbital angular momentum of the atom in the final state, the amplitude of the process (2) has, according to (17), (20), and (21) with allowance for (26) and (27), the form

$$T^{(1)}(n_1s \rightarrow ns) \approx -2^8 \pi^{-1} Z m e^4 \left(\frac{\mu_{13}}{mp} \right)^2 \psi_1(0) \psi_s^*(0) \left[G^2(\theta) - \frac{Z+1}{16} G(\theta) \right], \quad (32)$$

where

$$G(\theta) = (1 + 4\mu_{13}^2 \theta^2 / m^2)^{-1}, \quad \psi_s(0) = (Z^2 / \pi n^2 a_0^3)^{1/2}$$

(the OBK approximation corresponds to the neglect of the second term in the square brackets). A simple integration in accordance with (28) yields

$$\sigma^{(1)}(n_1s \rightarrow ns) = \frac{Z^2 (623 - 130Z + 15Z^2)}{768 n^2 n_1^2} \sigma_0(V), \quad (33)$$

where $\sigma_0(V) = 2^{16} \pi a_0^2 / 5V^{12}$. In particular, for $Z=1$ and $n_1 = n = 1$ (33) yields the well-known Jackson-Schiff result⁹:

$$\sigma^{(1)}(1s \rightarrow 1s) = (127/192) \sigma_{\text{OBK}}(1s \rightarrow 1s).$$

In the case when the orbital angular momentum of the atom in the final state has the value $l=1$ the asymptotic form of the amplitude in first order perturbation theory has, according to the above-given formulas, the form

$$T^{(1)}(n_1s \rightarrow n p \bar{m}) \approx 8\pi n^{-1} Z m e^4 \psi_1(0) R_{n1}^{(2)*}(0) \varepsilon^*(\bar{m}) \left(\frac{2\mu_{13}}{mp} \right)^2 \times \left\{ q \left[G^2(\theta) - \frac{G^2(\theta)}{16} \right] + \frac{m}{2\mu_{13}} p \left[-G^2(\theta) + \frac{G^2(\theta)}{16} + \frac{Z+2}{32} G(\theta) \right] \right\} \quad (34)$$

[if we retain only the first terms in the two expressions in the square brackets, then (34) reproduces the asymptotic form of the amplitude in the OBK approximation for $l=1$].

Let us note in connection with the computation of the cross sections $\sigma^{(1)}(n_1s \rightarrow n p m)$ from the amplitude (34) that, if we write the amplitude in the form

$$T = \varepsilon^*(m) [qF_1(\theta) + pF_2(\theta)] \quad (35)$$

and take the specific form⁴ of $\varepsilon(m)$ into account, then we can, according to (28), easily arrive at the relations

$$\sigma(n_1s \rightarrow n p 0) = 12\pi^4 \mu_{13}^2 p^2 \int_0^{\pi/2} |F_2(\theta)|^2 d\theta^2, \quad (36)$$

$$\sigma(n_1s \rightarrow n p \pm 1) = 6\pi^4 \mu_{13}^2 p^2 \int_0^{\pi/2} \theta^2 |F_1(\theta)|^2 d\theta^2.$$

The integration yields [see (31)]

$$a^{(1)}(1, 0, Z) = \frac{10292 - 1050Z + 105Z^2}{15360}, \quad a^{(1)}(1, \pm 1, Z) = \frac{979}{1280}, \quad (37)$$

$$\sigma^{(1)}(n_1s \rightarrow n p) = \frac{350 - 30Z + 3Z^2}{512} \sigma_{\text{OBK}}(n_1s \rightarrow n p).$$

In particular, in the case $Z=1$ we have

$$a^{(1)}(1, 0, 1) \approx 0.609, \quad a^{(1)}(1, \pm 1, 1) \approx 0.765, \quad (37a)$$

$$\sigma^{(1)}(n_1s \rightarrow n p) \approx 0.631 \sigma_{\text{OBK}}(n_1s \rightarrow n p).$$

Let us note that the cross sections for charge transfer to excited states with $n \gg 1$ and $l=0, 1$, and 2 are computed in Ref. 10. The n dependence of the cross sections ($\propto n^{-3}$, as in the OBK approximation) obtained in Ref. 10 is correct, but the numerical coefficient is incorrectly determined. The asymptotic form of the term $\langle f | U_{13} | i \rangle$ (in our notation) is computed without allowance for the fact that the dominant role in the matrix element is played by two regions of momentum space [see (20) and (21)], the contribution $\langle f | U_{13} | i \rangle_1$ of only one of them being computed.

Let us proceed to compute the exact asymptotic expressions for the charge transfer cross sections. The asymptotic form of the amplitude is given in this case by the sum of the first and second order perturbation theory terms (17), (20), (21) and (23), (24), (25).

In the case of charge transfer to s states we find from the indicated formulas that

$$T(n_1s \rightarrow ns) \approx -2^8 \pi^{-1} Z m e^4 \psi_s^*(0) \psi_1(0) \left(\frac{\mu_{13}}{mp} \right)^2 \left[G^2(\theta) - \frac{G^2(\theta)}{3 - 4\mu_{13}^2 \theta^2 / m^2} \right]. \quad (38)$$

This expression as a function of θ has a pole at the point $\theta_0 = 3^{1/2} m / 2\mu_{13}$, and is clearly incorrect in the region of angles close to θ_0 . The divergence of the amplitude as $\theta \rightarrow \theta_0$ occurs as a result of the use of the asymptotic expression (24), and is due to the vanishing of the energy denominator

$$\frac{p_1 f_1}{\mu_{23,1}} - \frac{f_1^2}{2\mu_{12}} \approx \frac{mp^2}{8\mu_{13}^2} \left(3 - \frac{4\mu_{13}^2 \theta^2}{m^2} \right). \quad (39)$$

It should, however, be remembered that (39) represents only the asymptotically leading ($\sim V^2$) term in the energy denominator, against whose background we could, generally speaking, neglect the remaining lower order— in V —terms, and it is precisely this circumstance that

led to the simple asymptotic form. But for angles close to θ_0 these terms in the energy denominator are no longer negligible. In this region of angles the expression (24) can be written in the form

$$\langle f | U_{22}(E-H_0+i0)^{-1} U_{12} | i \rangle \approx U_{12}(f_1) U_{22}(f_2) \iint \frac{d^2 q_1 d^2 q_2}{(2\pi)^6} \times \frac{\Psi_2^*(\mathbf{q}_2) \Phi_1(\mathbf{q}_1)}{(mp^2/8\mu_{13}^2)(3-4\mu_{13}^2\theta^2/m^2) - (\mathbf{f}_1\mathbf{q}_1 + \mathbf{f}_2\mathbf{q}_2)/m+i0} \quad (40)$$

(we have retained in the energy denominator the terms of the order of V^2 and V). Taking into account the fact that $q_{1,2} \sim 1/a$ and $f_{1,2} \lesssim mp/\mu_{13}$, we see that the angle region where we cannot use the asymptotic expression (24) for (40) is limited by the condition $|\theta - \theta_0| \lesssim 1/ap$, i.e., this region narrows down as p increases. It is apparently impossible to obtain an explicit expression for the asymptotic form of (40) in the indicated range of scattering angles. But, as will be shown below, we can compute the contribution from this range of scattering angles to the cross section in its explicit form without first computing the amplitude.

Let us write, in accordance with (28), the cross section for the process in the form

$$\sigma = \sigma_1 + \sigma_2 + \sigma_3 = 4\pi^3 m^2 \left[\int_0^{z_1} |T|^2 dz + \int_{z_1}^{z_2} |T|^2 dz + \int_{z_2}^{\infty} |T|^2 dz \right] \quad (41)$$

(we have made the change of variable $z = 4\mu_{13}^2 \theta^2/m^2$). The integration range has been divided into three, with $z_{1,2} = z_0(1 \mp \varepsilon)$, where $z_0 = 3$ and ε is an arbitrary quantity satisfying only the conditions $1/V \ll \varepsilon \ll 1$ (ε does not enter into the final answer). The computation of the contribution to the cross section of the regions $0 \leq z \ll z_1$ and $z \geq z_2$ [the first and third terms in (41)], in which the asymptotic expression (38) obtained above for the amplitude is valid, offers no difficulty: a simple integration yields

$$\sigma_1 + \sigma_3 \approx 2^{10} \pi^3 Z^2 m^4 e^4 |\Psi_2(0) \Psi_1(0)|^2 \left(\frac{\mu_{13}}{mp} \right)^{12} \frac{436 + 15 \ln 3 + 20/\varepsilon}{15 \cdot 2^9} \quad (42)$$

As for the contribution of the region of angles $z_1 \leq z \leq z_2$, it can be computed in the following manner. Let us note first that the dominant term in the amplitude in this region in (40), which determines the asymptotic form of the amplitude, so that

$$\int_{z_1}^{z_2} |T|^2 dz \approx \frac{64\mu_{13}^4}{m^2 p^4} \int_{-3\varepsilon}^{3\varepsilon} d\bar{z} \times \left| \iint \frac{d^2 q_1 d^2 q_2 \Phi_2^*(\mathbf{q}_2) \Phi_1(\mathbf{q}_1) U_{12}(f_1) U_{22}(f_2)}{(2\pi)^6 (\bar{z} + \mathbf{f}_1\mathbf{q}_1 + \mathbf{f}_2\mathbf{q}_2 + i0)} \right|^2, \quad (43)$$

where $\bar{f}_{1,2} = 8\mu_{13}^2 \mathbf{f}_{1,2}/m^2 p^2$. The vectors $\bar{f}_{1,2}$, like the $\mathbf{f}_{1,2}$, depend on θ , but we can neglect this dependence in (43), and take them at $\theta = \theta_0$; then $|\bar{f}_{1,2}| \equiv |\bar{f}_i| = 8\mu_{13}/mp$.

To evaluate (43), we write T^* in the expression $|T|^2 = TT^*$ in the form of integrals over $\mathbf{q}'_{1,2}$, similar to the integrals for T , and first perform the integration over \bar{z} :

$$\int_{-3\varepsilon}^{3\varepsilon} \frac{d\bar{z}}{(\bar{z} + \mathbf{f}_1\mathbf{q}_1 + \mathbf{f}_2\mathbf{q}_2 + i0)(\bar{z} + \mathbf{f}_1\mathbf{q}'_1 + \mathbf{f}_2\mathbf{q}'_2 - i0)} \approx \frac{2}{3\varepsilon} \frac{2\pi i}{\mathbf{f}_1(\mathbf{q}'_1 - \mathbf{q}_1) + \mathbf{f}_2(\mathbf{q}'_2 - \mathbf{q}_2) - i0} \quad (44)$$

[we have taken into account in (44) the fact that $q_{1,2}$

$\sim 1/a$, so that $(\bar{f}_i)_{1,2} \lesssim 8\mu_{13}/mpa \ll 3\varepsilon$]. Using (44), we easily transform the expression (43) into the form

$$\mu_{13}^4 \pi^{-6} m^{-2} p^{-4} U_{12}^2(f_{10}) U_{22}^2(f_{20}) \left\{ -\frac{2}{3\varepsilon} |\Psi_1(0) \Psi_2(0)|^2 + 2\pi i \int \frac{d^2 q_1 d^2 q_2 d^2 q'_1 d^2 q'_2 \Phi_2^*(\mathbf{q}_2) \Phi_1(\mathbf{q}_1) \Phi_2(\mathbf{q}'_2) \Phi_1^*(\mathbf{q}'_1)}{(2\pi)^6 [\mathbf{f}_{10}(\mathbf{q}_1 - \mathbf{q}'_1) + \mathbf{f}_{20}(\mathbf{q}_2 - \mathbf{q}'_2) + i0]} \right\}. \quad (45)$$

It is convenient to write, using the relation

$$\frac{1}{a+i0} = -i \int_0^{\infty} e^{isa} ds,$$

(a is a real quantity), the integral term in the curly brackets of the expression (45) in the coordinate representation:

$$\frac{2\pi}{f_{10}} \int_0^{\infty} dr \left| \Psi_1\left(\frac{\mathbf{f}_{10}}{f_{10}} r\right) \right|^2 \left| \Psi_2\left(\frac{\mathbf{f}_{20}}{f_{20}} r\right) \right|^2. \quad (46)$$

Bearing in mind the above-performed transformations, we easily find σ_2 and, with it, the cross section for the process:

$$\sigma(n_1 s \rightarrow ns) \approx \frac{Z^3}{n_1^3 n^2} \left(0.295 + \frac{5\pi V}{2^{12}} a_{n_1}(n_1, Z) \right) \sigma_0(Z) \quad (47)$$

[we have taken into account the fact that $(436 + 15 \ln 3)/3 \cdot 2^9 \approx 0.295$], where

$$a_{n_1}(n_1, Z) = \frac{4}{a_0} \int_0^{\infty} \left| \frac{\Psi_{n_1 s}^{(1)}(r) \Psi_{n s}^{(2)}(r)}{\Psi_{n_1 s}^{(1)}(0) \Psi_{n s}^{(2)}(0)} \right|^2 dr. \quad (48)$$

In particular, for $n_1 = 1$ we have

$$a_{1s}(1, Z) = 2/(1+Z), \quad a_{2s}(1, Z) = 2(8+4Z+Z^2)/(2+Z)^2.$$

Let also give the values of $a_{ns}(n, Z)$ for the case $Z = 1$, $n_1 = 1$:

$$a_{1s} = 1, \quad a_{2s} = 26/27, \quad a_{3s} = 245/256, \quad a_{ns} \approx 0.953 \text{ for } n \gg 1 \quad (48a)$$

(in computing a_{ns} with $n \gg 1$ we used for the wave function of the ns state of the hydrogen atom the well-known expression for the wave function of the s state with energy $E = 0$ in the Coulomb field⁶).

In the case $Z = 1$, $n = n_1 = 1$ (47) and (48) yield Drisko's well-known result.^{1,2}

The results obtained show that $\sigma(1s - ns) \propto n^{-3}$ virtually for all values of n , and not only for $n \rightarrow \infty$.

Notice that, in the expression (47), because of the numerical smallness of the coefficient $5\pi/2^{12} \approx 0.004$, the term $\propto V^{-11}$ (let us recall that $\sigma_0 \propto V^{-12}$), which predominates for $V \rightarrow \infty$, actually plays the role of a correction to the term $\propto V^{-12}$ at the values of $V \leq 40$, for which it still makes sense to use the nonrelativistic approximation.

In the case of charge transfer to the p states the amplitude of the process has, according to (34) and (23)-(25), the form

$$T(n_1 s \rightarrow np \bar{m}) \approx 8i\pi^{-1} Z m e^4 \Psi_1(0) R_{n_1}^{(2)*}(0) \varepsilon^*(\bar{m}) (2\mu_{13}/mp)^8 \times \left\{ q \left[G^4(\theta) - \frac{G^2(\theta)}{3-z} + \frac{G^2(\theta)}{(3-z)^2} \right] + \frac{m}{2\mu_{13}} p \left[-G^4(\theta) + \frac{G^2(\theta)}{3-z} + \frac{G^2(\theta)}{(3-z)^2} \right] \right\}, \quad (49)$$

where $z = 4m^2 \theta^2/\mu_{13}^2$; this expression, like (38) in the case $l = 0$, is inapplicable when $z = 3$.

The computation of the charge-transfer cross sections

$\sigma(n_1s - npm)$ with the aid of the formulas (35) and (36) can be performed in much the same way as was done above in the $l=0$ case [this computation is more tedious, since, for $l \neq 0$, we cannot, in computing σ_2 in the expression for T , neglect the dependence of $\tilde{f}_{1,2}$ on the scattering angle and limit ourselves to the consideration of only the most singular terms in the expression (43); a simpler method of computing the cross sections will be indicated below]. Let us give the final results:

$$\begin{aligned} \sigma(n_1s \rightarrow np0) &\approx \left[0.197 + \frac{7\pi V^3}{27 \cdot 2^{15}} a_{np}(n_1, Z) \right] \alpha_{\text{OBK}}(n_1s \rightarrow np0), \\ \sigma(n_1s \rightarrow np\pm 1) &\approx \left[0.608 + \frac{7\pi V^3}{3 \cdot 2^{11}} a_{np}(n_1, Z) \right] \alpha_{\text{OBK}}(n_1s \rightarrow np\pm 1), \\ \sigma(n_1s \rightarrow np) &\approx \left[0.256 + \frac{\pi V^2}{9 \cdot 2^{12}} a_{np}(n_1, Z) \right] \alpha_{\text{OBK}}(n_1s \rightarrow np), \end{aligned} \quad (50)$$

where

$$a_{np}(n_1, Z) = \frac{27}{2a_0^3} \int_0^\infty r^2 \left| \frac{\psi_{n_1s}^{(1)}(r) R_{np}^{(2)}(r)}{\psi_{n_1s}^{(1)}(0) R_{np}^{(2)}(0)} \right|^2 dr, \quad (51)$$

and the values of the corresponding cross sections in the OBK approximation are given by the expressions (29) and (30).

The quantity $a_{np}(n_1, Z)$, as in the $l=0$ case, depends weakly on n . Let us give its values for $Z=1$, $n_1=1$:

$$a_{2p}=1; a_{3p} \approx 0.957; a_{4p} \approx 0.942; a_{np} \approx 0.925 \text{ for } n \gg 1. \quad (51a)$$

The expressions obtained above for the charge-transfer cross sections contain terms of different orders in V . Since the perturbation theory parameter in the Coulomb field is Z/V , and the above-performed analysis is based on the consideration of only the asymptotically leading terms in the amplitude, such a form of the expressions needs, as does the question of their accuracy, to be elucidated. With this aim in view, let us discuss the dependence of the differential cross section for the process on the scattering angle. For definiteness, let us limit ourselves to the case $l=1$, $m=0$. Figure 1 shows the qualitative dependence of the quantity $V^{14}d\sigma/d\Omega$ on the scattering angle. The dashed curve corresponds to the case $V \rightarrow \infty$, and was computed in accordance with the expression (49) for the amplitude. As noted above, for finite values of $V \gg 1$ the divergent expression (49) is inapplicable when $z \rightarrow 3$: the true differential cross section is finite in this region of angles, and is depicted by the continuous curve. The dotted curve corresponds to some other V value higher than the value to which the continuous curve corresponds (all the curves differ only in the neighborhood of the point $z_0=3$).

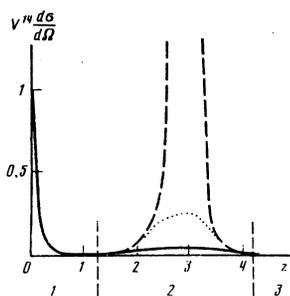


FIG. 1. Differential cross section for the $1s \rightarrow np0$ charge transfer (in relative units); $z = 4m^2\theta^2/\mu_{13}^2$.

The cross section for the process can be represented in accordance with Fig. 1 in the form of a sum of three terms:

$$\sigma = \sigma_1 + \sigma_2 + \sigma_3, \quad (52)$$

where the values of the $\tilde{\sigma}_\alpha$ correspond to the cross sections for scattering at angles in the regions 1, 2, and 3. The energy dependence of these quantities has the form

$$\begin{aligned} \tilde{\sigma}_1 &\approx a_{1,1}(V^{-11} + O(V^{-15})), \\ \tilde{\sigma}_2 &\approx a_{2,1}(V^{-11} + O(V^{-15})). \end{aligned} \quad (52a)$$

It should be emphasized that the second peak in the differential cross section—in the vicinity of the point $z_0=3$ —is distinctly separated from the first: the contribution to the cross section from the region between these peaks is small (as is the contribution to the cross section from the region $z > 4$: $\tilde{\sigma}_1 \gg \tilde{\sigma}_3$). This remark applies also to the differential cross sections for the processes with other quantum numbers.

Thus, the retention of two terms of different orders in V in the asymptotic expressions for the charge-transfer cross sections corresponds to making separate allowances for two scattering-angle regions in the total cross section, and, if we bear in mind the accuracy of such expressions, then they should be written in the form

$$\sigma(n_1s \rightarrow nlm) \approx a_{2nlm}[V^{-11} + O(V^{-15})] + a_{1nlm}[V^{-12-2l} + O(V^{-12-2l})], \quad (53)$$

the validity of the allowance for the term $\propto V^{-12-2l}$ resulting from the numerical smallness of the ratio $a_2/a_1 \ll 1$.

We can, bearing in mind the relations (52) and (53), propose a simpler method of computing the cross section, in which we do not need, as we did above, to "join" the contributions of the terms $(\sigma_1 + \sigma_3)$ and σ_2 to the cross section. For this purpose, let us note that the magnitudes of the cross sections $\tilde{\sigma}_1$ and $\tilde{\sigma}_3$ can be computed directly from the expressions obtained for the asymptotic form of the amplitude, while for the computation of $\tilde{\sigma}_2$ we can use the relation

$$\begin{aligned} \tilde{\sigma}_2 &\approx \sigma_{ac}(n_1l_1m_1 \rightarrow n_2l_2m_2) \\ &= 2^8 \pi^4 Z^2 a_0^7 V^{-11} \int_0^\infty \left| \Psi_{n_1l_1m_1}^{(1)}\left(\frac{f_{10}}{f_{10}}r\right) \Psi_{n_2l_2m_2}^{(2)}\left(\frac{f_{20}}{f_{20}}r\right) \right|^2 dr, \end{aligned} \quad (54)$$

which describes the asymptotically dominant ($\propto V^{-11}$) term in the charge-transfer cross section [this expression follows directly from the formulas (43), (45), and (46); the result (54) is obtained by a different method in Ref. 11]. This less laborious method of computing the cross section leads to practically the same results as above: the difference consists in a change in the first numerical terms in the brackets in the expressions (47), (50) for the cross sections by amounts equal respectively to 0.315, 0.202, 0.635, and 0.264 (the limited indeterminacy in the values of these terms lies within the limits of the errors in the computed expressions for the cross sections).

The values of the quantities $a_{1(2)nlm}$ in (53) are completely determined by the first two terms of the perturbation theory series, whereas the "correction" terms in the square brackets in (53) change, when we

go over to higher orders, in accordance with the fact that the parameter of the perturbation theory is $1/V$. The neglect of this fact can lead to a misunderstanding. In particular, it follows from (53) that

$$\sigma(1s \rightarrow 1s) = a_2 V^{-11} + [a_1 + a_2 O(1)] V^{-12}.$$

According to the foregoing, the third-order perturbation theory term ($\propto V^{-12}$) in this expression should differ somewhat from the second-order perturbation theory result (the difference should be small in accordance with the smallness of $a_2/a_1 \ll 1$; allowance for the fourth-order terms should, however, not change the result). Such a change in the coefficient has been found by Shakeshaft¹²; it corresponds to the replacement of the number 0.295 in the formula (47) for the case of the $1s - 1s$ charge transfer by 0.319. But this natural circumstance is sometimes interpreted incorrectly as an indication of the divergence of the perturbation theory series for reconstructive collision processes (see Ref. 1, as well as Ref. 13, where the question of the convergence of the perturbation theory series at high energies is discussed).

The computation of the cross sections for charge transfer to states with higher angular momenta can be performed in much the same way as the cross sections for charge transfer to the p states were computed above. But we shall, in conclusion, limit ourselves to making the following remark. Comparison of the results obtained for the cross sections for charge transfer to the states with $l=0$ and $l=1$ with the OBK approximation shows that the magnitudes of the terms $\propto V^{-12-2l}$ in the exact asymptotic expressions (47), (50) are 2–5 times smaller than the magnitudes of the corresponding cross sections in the OBK approximation. At the same time, the exact asymptotic expressions contain "additional" terms $\propto V^{-11}$, which increase the cross sections. In view of the slower decrease of these terms, their relative role increases with increasing velocity. The ratio of the magnitude of the term $\propto V^{-11}$ to the term $\propto V^{-12-2l}$ is equal to $1.3 \times 10^{-2} V$ in the case $l=0$ and $3.3 \times 10^{-4} V^3$ for $l=1$ (the indicated quantity pertains to the total cross section for the $1s - np$ charge transfer). Thus, in the case $l=1$ the term $\propto V^{-11}$ in the cross section is more important, its contribution constituting one half of the magnitude of the total cross section even at $V \approx 14$. Further, in the case of charge transfer into states with $l=2$ the contribution, computed in accordance with (54), of the term $\propto V^{-11}$ to the total cross section $\sigma(1s - nd)$ for $n=3$ is equal to

$$\sigma_{as}(1s \rightarrow 3d) = \frac{\pi}{216V^{11}} \pi a_0^2,$$

and its ratio to the analogous cross section in the OBK approximation is equal to $3.7 \times 10^{-6} V^5$. For $V=20$ this ratio is equal to ≈ 12 . Therefore, we can, bearing in mind the exact results for $l=0, 1$, expect that, for $V \geq 20$, the magnitude of the cross section for charge-transfer processes with $l \geq 2$ will be given by the term $\propto V^{-11}$, which can be computed with the aid of the formula (54) without any difficulty.

- ¹By "elementary" particles we mean particles whose interaction with each other is specified by pair potentials; in this sense the nuclei in atomic collisions can be regarded as "elementary" particles.
- ² $\nu > -2$ is not an even number; the nonsingular part is an expansion in integer powers of r^2 .
- ³For the process (2) the amplitude has a sharp peak (actually there are two of them) in the small-angle region $\theta \approx m/\mu_{13} \ll 1$. It is precisely this scattering-angle region that is considered in the paper. Then in the case when the particle 1, like the particle 3, is a proton, the exchange part of the scattering amplitude is negligibly small.
- ⁴ $\epsilon(0) = (0, 0, i(3/4\pi)^{1/2})$ and $\epsilon(\pm 1) = (\mp i(3/8\pi)^{1/2}, (3/8\pi)^{1/2}, 0)$; the phase factor of $Y_{lm}(\mathbf{n})$ has been chosen as in Ref. 8.

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