ASYMPTOTIC FORM OF THE AMPLITUDE OF THE INELASTIC SCATTERING OF FAST ELECTRONS BY HYDROGEN ATOMS

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Submitted June 1, 1972

Zh. Eksp. Teor. Fiz. **63**, 2094–2104 (December, 1972)

An angle-uniform asymptotic expression for the differential cross section for scattering with excitation and also for the exchange scattering of fast electrons by hydrogen atoms is obtained in the second Born approximation for the transition amplitude. The formulas obtained are in good agreement with the available experimental data for the 1s → 2s, 2p transitions in the hydrogen atom. An asymptotic expression is also obtained for the amplitude derived in the framework of the distorted-wave Born approximation.

1. INTRODUCTION

EXPERIMENTS performed on the measurement of the differential cross sections for scattering of fast electrons by atoms[1-3] indicate that for sufficiently large scattering angles in the case of scattering with excitation there is a significant disagreement between the measured angular dependences and the theoretical computations carried out in the framework of the first Born approximation. Thus, for example, according to Williams[1], for the scattering of 200-eV electrons through an angle of 50° with a transition of the hydrogen atom from the ground to the first excited state, the theoretical cross section turns out to be approximately one hundred times less than the observed value. At the same time the differential cross section for elastic scattering at energies higher than 100 eV is in good agreement with experiment in the entire angle range[4]. As is well known, the Born expression for the differential cross section for elastic scattering through sufficiently large angles decreases with increase of the incident-electron velocity v as $1/v^4$, the dominant contribution to the asymptotic expression being made by the matrix element containing the interaction $\hat{V}_{pi}$ of the impinging electron e_i with the nucleus. In the case of scattering with excitation, because of the orthogonality of the wave functions of the initial and final bound states, the coefficient in front of the term that decreases as $1/v^4$ vanishes identically, in consequence of which the Born expression for the cross section contains only the interelectronic interaction $\hat{V}_{if}$ and decreases as $1/v^{12}$.

The physical interpretation of these results is well known (see, for example,[5]). It is clear that on account of the pair interaction $\hat{V}_{ip}$ alone, only the state of the incident electron can change: the state of the bound electron remains unchanged. The small value of the matrix element containing the interaction $\hat{V}_{if}$ is connected with the fact that as the momentum of the incident electron changes from the initial $\mathbf{k}_i$ to the final $\mathbf{k}_{i'}$, the electron e_f acquires, owing to the momentum conservation law, a sufficiently large momentum $\sim \mathbf{k}_i - \mathbf{k}_{i'}$, and the probability that it will remain in the bound state is extremely small for large v.

From the above-presented interpretation of the processes of first order in the interaction we can infer that for sufficiently large v processes in which the incident electron participates in at least two pair interactions become important, the pair interactions involving the following: in one of them the incident electron imparts to the bound electron a small part of its momentum—just enough to effect a transition—and, in the other, it is scattered by the nucleus, such that its momentum changes from the initial $\mathbf{k}_i$ to $\mathbf{k}_{i'}$. An adequate quantum mechanical description of the indicated processes is the use of the second Born approximation for the transition amplitude, and this is adopted in the present paper. The asymptotic form of the differential cross section for scattering with excitation, as well as for exchange scattering, for $v \to \infty$ is computed in the framework of the second Born approximation.

It should be noted that the second Born approximation for the problem under consideration has been computed by a number of authors (see, for example, the review[6]). In computing the differentiating cross section, however, these authors considered only the real part of the second-order terms, whereas, as the present calculation shows, the leading part of the asymptotic form of the second-order terms is purely imaginary and, despite the fact that it contains the second powers of the interaction, it is, for scattering through sufficiently large angles, the dominant term in comparison with the first-order terms. In this case the asymptotic form of the terms of the first Born approximation virtually contains the second powers of the interaction also. The purely imaginary value of the asymptotic form of the amplitude is connected with the possibility of fulfilling the conservation law for the kinetic energy in the intermediate states in the above-indicated successive collisions.

Note that this limit was considered in[7] in one of the modifications of the first distorted-wave Born approximation. It is shown in Sec. 4 of the present paper that the asymptotic form obtained for the amplitude by the distorted-wave method when account is taken only of the first-order terms essentially depends on the form of the distorted potentials, and is not, in consequence, well defined. This ambiguity disappears only when the second-order terms of the distorted-wave method are taken into account, so that the asymptotic expression for the sum of the first- and second-order terms coincides with the asymptotic expression for the second Born approximation. Furthermore, we formulate for the distorted potentials conditions upon fulfillment of which the amplitude obtained in the first approximation of the distorted-wave method will nevertheless have the correct asymptotic form for $v \to \infty$. It should be noted that the distorted potentials chosen in[7] do not satisfy these conditions. In Sec. 5 the results of the present calculation are also compared with the experimental data[1]; a good agreement is found between the computed angular dependence of the differential cross section and the experimentally observed dependence. Thus, the expressions obtained in this paper for the differential cross sections can be used to normalize experimental results.

2. COMPUTATION OF THE ASYMPTOTIC FORM OF THE AMPLITUDE FOR SCATTERING WITH EXCITATION

The expression for the amplitude of the process under consideration has the form

$$T_{i'i} = \lim_{\varepsilon \to +0} \langle i' | \hat{v}_i + \hat{v}_i \hat{G}(E + i\varepsilon) \hat{v}_i | i \rangle, \qquad (1)$$

where $|i\rangle \equiv |\mathbf{k}_i n_i\rangle$ is the initial-state vector of the system, $\mathbf{k}_i$ is the momentum of the incident electron e_i, $n_i = \{1s\}$ is the set of quantum numbers of the bound electron e_f in the ground state of the hydrogen atom, $\langle i'| \equiv \langle k_{i'}, n_{i'}|$ is the final-state vector, $\mathbf{k}_{i'}$ is the final momentum of e_i, $n_{i'}$ are the quantum numbers which describe the final bound state of e_f, $\hat{v}_i = \hat{V}_{ip} + \hat{V}_{if}$ is the interaction operator, which vanishes as e_i moves away, $\hat{G} = [E + i\epsilon - \hat{H}]^{-1}$ is the resolvent of the total Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}_{pi} + \hat{V}_{pf} + \hat{V}_{if}$, and $\hat{H}_0$ is the electron kinetic-energy operator. Then, on the surface, where energy is conserved, we have

$$E = {}^1\!/_2 k_i^2 - E_i = {}^1\!/_2 k_{i'}^2 - E_{i'}.$$

Here E_i and $E_{i'}$ are the energies of the initial and final states of the hydrogen atom; we shall henceforth use the Coulomb system of units. In conformity with our discussion in the Introduction, we apply the second Born approximation to (1), i.e., we set

$$T_{i'i} \approx T_{i'i}^{\mathrm{IIB}} = \lim_{\varepsilon \to +0} \langle i' | \hat{v}_i + \hat{v}_i \hat{G}_i (E + i\varepsilon) \hat{v}_i | i \rangle,$$
$$\hat{G}_i = [E + i\varepsilon - \hat{H}_0 - \hat{V}_{pf}]^{-1}. \qquad (2)$$

The expression (2) is obtained from (1) by the substitution $\hat{G} \approx \hat{G}_i$, which is the first term of the iterational expansion of the corresponding integral equation of the Lippmann-Schwinger type.

In the basis $|q_i q_f\rangle$, consisting of the eigenvectors of the momentum operators $\hat{q}_i$ and $\hat{q}_f$ of the individual electrons, the resolvent $\hat{G}_i$ is connected with the Coulomb Green function $G_i(q_f, q_f'; s)$ in the momentum representation by the relation

$$\langle q_i q_f | \hat{G}_i (E + i\varepsilon) | q_i' q_f' \rangle = \delta^3 (\mathbf{q}_i - \mathbf{q}_i') G_i (\mathbf{q}_f, \mathbf{q}_f'; E + i\varepsilon - {}^1\!/_2 q_i^2). \qquad (3)$$

Let us now proceed to compute the asymptotic forms of the individual matrix elements in (2). The sole first-order term has the form

$$T_{i'i}^{\mathrm{I}} = \langle i' | \hat{V}_{if} | i \rangle = V_{if}(\Delta)\, \varepsilon_{i'i}(\Delta), \qquad (4)$$

where $V_{if}(\Delta) = 1/2\pi^2\Delta^2$, $\boldsymbol{\Delta} = \mathbf{k}_i - \mathbf{k}_{i'}$, and

$$\varepsilon_{\alpha\beta}(\Delta) = \int d\mathbf{q}\, \psi_\alpha(\mathbf{q})\, \psi_\beta(\mathbf{q} + \boldsymbol{\Delta}) = \int d\mathbf{r}\, e^{i\boldsymbol{\Delta}\mathbf{r}} \tilde{\psi}_\alpha(\mathbf{r})\, \tilde{\psi}_\beta(\mathbf{r}),$$
$$\psi_\alpha(\mathbf{q}) \equiv \langle \mathbf{q} | n_\alpha \rangle, \quad \tilde{\psi}_\alpha(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{q}\, e^{i\mathbf{q}\mathbf{r}} \psi_\alpha(\mathbf{q}). \qquad (5)$$

Henceforth each of the indices α and β in (5) independently takes on values from the set of indices $\{i, i', f\}$. The explicit expression for (5) for arbitrary final and initial ground states of the bound states is given in[6]. As a function of Δ, the integral $\epsilon_{i'i}(\Delta) \equiv \epsilon_{nlm,1s}(\Delta)$ is localized in the neighborhood of $\Delta \approx 1$, and for $\Delta \to \infty$

$$\varepsilon_{nlm,1s}(\Delta) \propto 1/\Delta^{l+4},$$

while for $\Delta \to 0$, $\epsilon_{nlm,1s}(\Delta) \propto \Delta$ for "optically allowed" transitions and $\propto \Delta^2$ for the rest[5]. Thus, for $\Delta \to \infty$ we have for the dominant part of the asymptotic form of (4)

$$T_{i'i}^{\mathrm{I}} = \frac{1}{2\pi^2} \frac{\tilde{\psi}_i(0)\tilde{\psi}_{i'}(0)}{\Delta^4}. \qquad (6)$$

Let us consider further the second-order terms in (2):

$$T_{i'i}^{\mathrm{II}} = \langle i' | \hat{V}_{if}\hat{G}_i\hat{V}_{if} + \hat{V}_{if}\hat{G}_i\hat{V}_{ip} + \hat{V}_{ip}\hat{G}_i\hat{V}_{if} + \hat{V}_{ip}\hat{G}_i\hat{V}_{ip} | i \rangle, \qquad (7)$$

For $v \to \infty$ the contribution of the matrix element $\langle i' | \hat{V}_{if}\hat{G}_i\hat{V}_{if} | i \rangle$ is small compared to the corresponding first Born term $\langle i' | \hat{V}_{if} | i \rangle$. Furthermore, because of the orthogonality of the initial and final bound states, the matrix element $\langle i' | \hat{V}_{ip}\hat{G}_i\hat{V}_{ip} | i \rangle$ vanishes identically. The two remaining matrix elements in (7)

$$P_{i'i} = \langle i' | \hat{V}_{ip}\hat{G}_i\hat{V}_{if} | i \rangle, \quad Q_{i'i} = \langle i' | \hat{V}_{if}\hat{G}_i\hat{V}_{ip} | i \rangle$$

are connected by the relation $Q_{i'i} = P_{ii'}$, so that it is sufficient to consider only one of them.

The corresponding integral has the form

$$P_{i'i} = \iiint d\mathbf{q}_1\, d\mathbf{q}_2\, d\mathbf{q}_3 V_{if}(\mathbf{q}_3 - \mathbf{k}_i) V_{ip}(\mathbf{q}_3 - \mathbf{k}_{i'})$$
$$\times\, \psi_i(\mathbf{q}_1) G_i(\mathbf{q}_1 + \mathbf{k}_i - \mathbf{q}_3, \mathbf{q}_2;\ E + i\varepsilon - {}^1\!/_2\, q_3^2) \psi_{i'}(\mathbf{q}_2),$$

$$V_{ip}(q) = V_{fp}(q) = -1/2\pi^2 q^2. \qquad (8)$$

The integral over $d\mathbf{q}_2$ can be evaluated taking account of the fact that $G_i(\mathbf{q}, \mathbf{q}'; s)$ is the Green function of the Hamiltonian whose eigenfunction is $\psi_{i'}(\mathbf{q}_2)$. We obtain as a result

$$P_{i'i} = \int d\mathbf{q}_3 \frac{V_{if}(\mathbf{q}_3 - \mathbf{k}_i) V_{ip}(\mathbf{q}_3 - \mathbf{k}_{i'})\, \varepsilon_{i'i}(\mathbf{q}_3 - \mathbf{k}_i)}{E + i\varepsilon + E_{i'} - q_3^2/2}. \qquad (9)$$

To find the asymptotic form of (9), we note that the main contribution to the integral are made by the regions of localization of $\epsilon_{i'i}$ and V_{if}, i.e., by the neighborhood of the point $\mathbf{q}_3 = \mathbf{k}_i$. Furthermore, the denominator of the Green function also vanishes in this region. Expanding the potential V_{ip} around $\mathbf{q}_3 \approx \mathbf{k}_i$ and dropping the leading (with respect to $1/v$) terms in the denominator of the Green function, we have

$$P_{i'i} \approx -V_{pi}(\Delta) \int d\mathbf{q} \frac{V_{if}(\mathbf{q})\, \varepsilon_{i'i}(\mathbf{q})}{\mathbf{q}\mathbf{k}_i - i\varepsilon}. \qquad (10)$$

After evaluating the integral in (10) with respect to the angular variables, we find that the asymptotic form of

(8) for $\Delta \to \infty$ has the form

$$P_{i'i} \approx -V_{pi}(\Delta)\frac{i}{v}\int_0^\infty \frac{dq}{q}\varepsilon_{i'i}(q) \tag{11}$$

and that it decreases as $1/v^3$ as $v \to \infty$. Comparing (11) with (6), we find that the dominant contribution to the asymptotic form of $T^{II}_{i'i}$ are made by the second-order terms, so that for $v \to \infty$

$$T^{II}_{i'i} = \frac{i}{\pi^2 v\Delta^2}\int_0^\infty \frac{dq}{q}\varepsilon_{i'i}(q). \tag{12}$$

This expression is valid in the region of sufficiently large scattering angles, where $\Delta \gg 1$. To find the asymptotic form of (7) in the region $\Delta \lesssim 1$, it is necessary to consider all the cofactors in the integral (9) together. Then, for forward scattering the integral for the leading term of the expansion of (9) becomes divergent. The singularity of the integrand at the point $\mathbf{q}_3 = \mathbf{k}_i$ is connected with the long-range nature of the Coulomb interaction[1)]. However, in view of the fact that the atom as a whole is electrically neutral, this singularity vanishes when the matrix element $R = \langle i'|\hat{V}_{if}\hat{G}_i\hat{V}_{if}|i\rangle$ in (7) is taken into account. Let us use the spectral representation for $\hat{G}_i$ in R and separate out the two polar terms:

$$R = \int d\mathbf{q}\frac{\langle i'|\hat{V}_{if}|n_i\mathbf{q}\rangle\langle n_i\mathbf{q}|\hat{V}_{if}|i\rangle}{E+i\varepsilon+E_i-{}^1/_2 q^2} + \int d\mathbf{q}\frac{\langle i'|\hat{V}_{if}|n_{i'}\mathbf{q}\rangle\langle n_{i'}\mathbf{q}|\hat{V}_{if}|i\rangle}{E+i\varepsilon+E_{i'}-{}^1/_2 q^2} + \tilde{R}. \tag{13}$$

The integrand in the matrix element $\tilde{R}$ is a well defined quantity for all scattering angles, and the contribution of $\tilde{R}$ is asymptotically small compared to the corresponding first-order term (4).

As for the first two integrals in (13), the computation of the leading parts of their asymptotic forms meets with the same difficulty encountered in the computation of $P_{i'i}$. Let us denote the first integral in (13) by R_{ii} and the second by $R_{i'i'}$. Taking account of the fact that R_{ii} and $R_{i'i'}$ have signs opposite to those of $P_{i'i}$ and $Q_{i'i}$, we consider the combination

$$I^{(1)}_{i'i} = P_{i'i} + R_{i'i'} \approx \int d\mathbf{q}\frac{\varepsilon_{i'i}(q)V_{if}(q)V_{ip}(\mathbf{q}+\Delta)}{\mathbf{q}\mathbf{k}_i - i\varepsilon}[1-\varepsilon_{i'i'}(|\mathbf{q}+\Delta|)], \tag{14}$$

which also determines the sum of the other pair: $I^{(2)}_{i'i} \equiv Q_{i'i} + R_{ii} = I^{(1)}_{ii'}$. It is not difficult to show that $1-\epsilon_{i'i'}(q) \propto q^2$ for $q \to 0$, and, as a result of this, the integral (14) is well defined. As can be seen from (14), in the region of small scattering angles, $\Delta \lesssim 1$, the second-order terms decrease as $1/v$ and are asymptotically small compared to the first-order term (4), which has in this angle region the asymptotic form $T^I_{i'i} \sim v$ for optically allowed transitions and $T^I_{i'i} \sim$ const for the rest of the transitions. Matching now the asymptotic expressions found for the second-order terms for $\Delta \ll 1$ and $\Delta \gg 1$, we thus find that the angle-uniform leading part of the asymptotic form of the amplitude (2) for $v \to \infty$ has the form

$$T_{i'i} = \frac{1}{8\pi^2 v^2}\left\{\varepsilon_{i'i}(\Delta)\left(\sin^2\frac{\theta}{2}+\frac{(\Delta E)^2}{4v^4}\right)^{-1} + \frac{i}{v}\left[\left(\sin^2\frac{\theta}{2}+\frac{E^{(1)}_{i'i}}{v^2}\right)^{-1} + \left(\sin^2\frac{\theta}{2}+\frac{1}{v^2}E^{(2)}_{i'i}\right)^{-1}\right]\int_0^\infty \frac{dq}{q}\varepsilon_{i'i}(q)\right\}, \tag{15}$$

where $\Delta E = E_i - E_{i'}$, and the constants $E^{(1)}_{i'i}$ and $E^{(2)}_{i'i}$, which do not depend on v and $\cos\theta = \mathbf{k}_i\cdot\mathbf{k}_{i'}/k_i k_{i'}$, are determined by the expressions

$$E^{(1)}_{i'i} = \frac{1}{4}\int_0^\infty \frac{dq}{q}\varepsilon_{i'i}(q)\left\{\int_0^\infty \frac{dq}{q^3}\varepsilon_{i'i}(q)[1-\varepsilon_{i'i'}(q)]\right\}^{-1}, \tag{16}$$

$$E^{(2)}_{i'i} = E^{(1)}_{ii'}.$$

As regards the total cross section

$$\sigma_{i'i} = (2\pi)^5\int_0^\pi |T_{i'i}|^2\sin\theta\, d\theta,$$

since the main contribution to the integral is made by the region of small scattering angles, where the first-order term predominates, the asymptotic form of $\sigma_{i'i}$ coincides with the well-known asymptotic form of the first Born approximation[4]: $\sigma_{i'i} \propto v^{-1}\ln v$ for the $1s \to np$ transitions and $\sigma_{i'i} \propto 1/v^2$ for transitions to the remaining final states.

3. ASYMPTOTIC FORM OF THE EXCHANGE-SCATTERING AMPLITUDE

The general expression for the amplitude of the three-particle scattering with rearrangement in the case of the exchange scattering of an electron by a hydrogen atom has the form

$$T_{fi} = \langle f|\hat{V}_{if} + \hat{V}_{if}\hat{G}\hat{V}_{ip} + \hat{V}_{fp}\hat{G}\hat{V}_{if} + \hat{V}_{if}\hat{G}\hat{V}_{if}|i\rangle, \tag{17}$$

since, according to[9],

$$\langle f|\hat{V}_{fp} + \hat{V}_{fp}\hat{G}V_{ip}|i\rangle = 0.$$

Here $\langle f| \equiv \langle \mathbf{k}_f n_f|$ is the final-state vector of the system, $\mathbf{k}_f$ is the final momentum of the initially bound electron e_f, n_f is the set of quantum numbers describing the final bound state of e_i. We shall compute the asymptotic form of (17) using the first Born approximation for the total Green function $\hat{G}$; this is equivalent to the second Born approximation for T_{fi}. It is then sufficient to limit ourselves to only the first term in the Born series for $\hat{G}$:

$$\hat{G} = \hat{G}_0 + \hat{G}_0\hat{V}\hat{G}_0 + \ldots \tag{18}$$

(here $\hat{G}_0 = [E + i\epsilon - \hat{H}_0]^{-1}$ and $\hat{V}$ is the total interaction). However, the computation of the asymptotic form of (17) becomes simpler if we partially sum up the series (18); this, of course, does not change the form of the asymptotic expression. In this connection we assume

$$T_{fi} \approx T^{IIB}_{fi} = T^I_{fi} + U^{(1)}_{fi} + U^{(2)}_{fi} + U_{fi}, \tag{19}$$

where

$$U^{(1)}_{fi} = \langle f|\hat{V}_{if}\hat{G}_i\hat{V}_{ip}|i\rangle, \quad U^{(2)}_{fi} = \langle f|\hat{V}_{fp}\hat{G}_f\hat{V}_{if}|i\rangle,$$
$$U_{fi} = \langle f|\hat{V}_{if}(\hat{G}_f + \hat{G}_i - \hat{G}_0)\hat{V}_{if}|i\rangle.$$

The first-order matrix element T^I_{fi} in (19) has the form

$$T^I_{fi} = \int d\mathbf{q}\,\psi_i(\mathbf{q})\psi_f(\mathbf{q}+\Delta')V_{if}(\mathbf{q}-\mathbf{k}_f), \quad \Delta' = \mathbf{k}_i - \mathbf{k}_f. \tag{20}$$

The main contribution to the integral is made by the regions of localization of the wave functions ψ_i and ψ_f in momentum space, i.e., by the neighborhoods of the points $\mathbf{q} = 0$ and $\mathbf{q} = -\Delta'$, which lead to the asymptotic form

$$T^I_{fi} \cong V_{if}(v)\varepsilon_{fi}(\Delta'), \tag{21}$$

[1)]An analogous divergence of the matrix element in the p-H charge-transfer problem was previously noted in [8].

which was previously obtained in[10]. The quantity $\epsilon_{fi}(\Delta')$ in (21) is determined by the formula (5). For large v (21) decreases as $1/v^{6+l}$ in the region $\Delta' \gg 1$ and as $1/v^2$ for $\Delta' \lesssim 1$.

Let us consider further the second-order matrix element

$$U_{fi}^{(2)} = \iint \frac{\psi_i(q_1) V_{if}(q_1 - q_3) V_{fp}(q_3 - k_f) \psi_f(q_1 + k_i - q_3)}{E + i\varepsilon + E_f - \frac{1}{2} q_3^2} dq_1 dq_3. \quad (22)$$

Here E_f is the final energy of the hydrogen atom. The main contribution to the integral (22) for $v \to \infty$ is made by the regions of localization of the wave functions ψ_i and ψ_f, i.e., by the neighborhoods of the points $q_1 = 0$ and $q_3 = k_i$. Expanding the potentials V_{if} and V_{fp}, which are nonsingular in these regions, in a series and dropping the leading (with respect to 1/v) terms in the denominator of the Green function, we obtain for the leading part of the asymptotic form of (22) the expression

$$U_{fi}^{(2)} \approx -\frac{i}{v^3} V_{fp}(\Delta') \int_0^\infty q \varepsilon_{fi}(q) dq, \quad (23)$$

which decreases as $1/v^5$. In view of the fact that $U_{fi}^{(1)} = U_{if}^{(2)}$ and the contribution of the matrix element U_{fi} containing the iterated interactions is asymptotically small compared to the corresponding first Born term (20), we find that for $\Delta' \gg 1$ the asymptotic form of (19) coincides with the expression (23) multiplied by 2:

$$T_{fi}^{IIB} = \frac{i}{\pi^2 v^3 \Delta'^2} \int_0^\infty q \varepsilon_{fi}(q) dq. \quad (24)$$

To find the asymptotic form of (22) in the region $\Delta' \lesssim 1$, we must consider the integral

$$U_{fi}^{(2)} \approx -V_{if}(v) \int \frac{\varepsilon_{fi}(q) V_{fp}(q - \Delta') dq}{q k_f - i\varepsilon}, \quad (25)$$

which diverges logarithmically at $\Delta' = 0$ for the 1s → 1s transitions and is anomalously large for the other transitions. The same difficulty encountered in the analysis of the integral (9) arises here. Proceeding in similar fashion, we consider the matrix element $\langle f|\hat{V}_{if}\hat{G}_i\hat{V}_{if}|i\rangle$ together with (25), first separating out from the former the following polar term:

$$\langle f|\hat{V}_{if}\hat{G}_f\hat{V}_{if}|i\rangle = \int \frac{\langle f|\hat{V}_{if}|qn_f\rangle\langle qn_f|\hat{V}_{if}|i\rangle}{E + i\varepsilon + E_f - \frac{1}{2}q^2} dq + \ldots \quad (26)$$

The expression for the main contribution of the sum of the integrals (26) and (25) then has the form

$$-V_{if}(v) \int \frac{dq\, V_{fp}(q - \Delta') \varepsilon_{fi}(q)[1 - \varepsilon_{ff}(|q - \Delta'|)]}{q k_f - i\varepsilon}. \quad (27)$$

In the region $\Delta' \lesssim 1$, (27) decreases as $1/v^3$ and is thus small compared to the first Born term (21). The corresponding asymptotic expression for the sum of $U_{fi}^{(1)}$ and $\langle f|\hat{V}_{if}\hat{G}_i\hat{V}_{if}|i\rangle$ is obtained from (27) by interchanging i and f.

The matching of the asymptotic expressions found for the second-order terms for $\Delta' \ll 1$ and $\Delta' \gg 1$ leads to the following angle-uniform expression for the dominant part of the asymptotic form of (19):

$$T_{fi}^{IIB} = \frac{1}{2\pi^2 v^2}\left\{ \varepsilon_{fi}(\Delta') + \frac{i}{4v^3}\left[\left(\sin^2\frac{\theta}{2} + \frac{E_{fi}^{(1)}}{v^2}\right)^{-1} + \left(\sin^2\frac{\theta}{2} + \frac{E_{fi}^{(2)}}{v^2}\right)^{-1}\right] \int_0^\infty \varepsilon_{fi}(q) q\, dq \right\}, \quad (28)$$

where

$$E_{fi}^{(2)} = \frac{1}{4}\int_0^\infty \varepsilon_{fi}(q) q\, dq \left\{ \int_0^\infty \frac{dq}{q} \varepsilon_{fi}(q)[1 - \varepsilon_{ff}(q)] \right\}^{-1},$$

$$E_{fi}^{(1)} = E_{if}^{(2)}. \quad (29)$$

The asymptotic expression for the total exchange-scattering cross section σ_{fi} coincides, as in the case of scattering with excitation, with the asymptotic form of the first Born approximation, so that $\sigma_{fi} \propto 1/v^4$ for $v \to \infty$. At the same time the differential scattering cross section for $\Delta' \gg 1$ is determined by the second-order terms. The scattering process responsible for each of the matrix elements $U_{fi}^{(1)}$ and $U_{fi}^{(2)}$ can be interpreted as two successive pair encounters. $U_{fi}^{(2)}$ then corresponds to the process in which the incident electron e_i imparts through any collision its momentum $\mathbf{k}_i$ to the bound electron e_f, after which, being in a small-momentum state, it is captured into a final bound state. In its turn, having gained the momentum $\mathbf{k}_i$, e_f undergoes elastic scattering by the nucleus, changing its momentum in the process by $\mathbf{k}_f$. Similarly, in the process described by $U_{fi}^{(1)}$, e_i is first scattered by the nucleus, the change in its momentum $\mathbf{k}_i$ as a result of the scattering being close to $\mathbf{k}_f$. In the second encounter, e_i imparts a momentum $\mathbf{k}_f$ to e_f through any collision mechanism, after which it is captured into a bound state. Thus, despite the fact that the probability for multiple scattering at high velocities decreases with the growth of their number, in order for e_f to acquire a finite momentum $\mathbf{k}_f$, at least two pair collisions should occur.

4. ON THE NECESSITY TO TAKE INTO ACCOUNT THE SECOND-ORDER TERMS OF THE DISTORTED-WAVE METHOD FOR THE PROBLEM OF SCATTERING WITH EXCITATION

Let us show that the correct asymptotic form of the amplitudes $T_{i'i}$ computed in the framework of the distorted-wave method[11]:

$$T_{i'i} = \langle \Phi_{i'}^{(-)}|\hat{v}_i - \hat{w}^{(2)} + (\hat{v}_i - \hat{w}^{(2)})\hat{G}(\hat{v}_i - \hat{w}^{(1)})|\Phi_i^{(+)}\rangle. \quad (30)$$

is, generally speaking, obtained only when the terms of second order in the interaction are taken into account together with the first-order terms. Setting in (30) $\hat{G} \approx \hat{G}_i$, we obtain in the case of scattering with excitation being considered the following expression for the second distorted-wave Born approximation:

$$T_{i'i}^{II\,DW} = \langle \Phi_{i'}^{(-)}|\hat{V}_{if}|\Phi_i^{(+)}\rangle + \langle \Phi_{i'}^{(-)}|\hat{v}_i\hat{G}_i\hat{v}_i - \hat{w}^{(2)}\hat{G}_i\hat{V}_{if} - \hat{V}_{if}\hat{G}_i\hat{w}^{(1)}|\Phi_i^{(+)}\rangle, \quad (31)$$

since in the present case the matrix elements of the operators $\hat{w}^{(1)}$, $\hat{w}^{(2)}$, $\hat{V}_{ip}\hat{G}_i\hat{w}^{(1)}$, and $\hat{w}^{(2)}\hat{G}_i\hat{V}_{ip}$, taken between the states $|\Phi_i^{(+)}\rangle$ and $\langle\Phi_{i'}^{(-)}|$, are identically equal to zero. In (30) and (31) $\hat{w}^{(1)}$ and $\hat{w}^{(2)}$ are distorted potentials which do not induce transitions and depend in the coordinate representation only on the distance of the incoming electron from the nucleus; $|\Phi_i^{(+)}\rangle \equiv |n_i, \chi_{\mathbf{k}_i,1}^{(+)}\rangle$, $\langle\Phi_i^{(-)}| \equiv \langle n_{i'}, \chi_{\mathbf{k}_{i'},2}^{(-)}|$; finally, $\langle q|\chi_{\mathbf{k},1}^{(+)}\rangle$ and $\langle\chi_{\mathbf{k},2}^{(-)}|q\rangle = \langle q|\chi_{\mathbf{k},2}^{(+)}\rangle$ are respectively the wave functions of the scattering problem with the potentials $\hat{w}^{(1)}$ and $\hat{w}^{(2)}$. The wave functions are connected with the scattering amplitudes

$$t_{w^{(\alpha)}}(q, k; \tfrac{1}{2}k^2 + i\varepsilon) = \int w^{(\alpha)}(q - q')\chi_{k,\alpha}^{(+)}(q')dq' \quad (\alpha = 1, 2), \quad (32)$$

by the relations

$$\chi_{\mathbf{k},\alpha}^{(+)}(\mathbf{q}) = \delta^3(\mathbf{q}-\mathbf{k}) + 2\lim_{\varepsilon\to+0}\frac{t_{w(\alpha)}(\mathbf{q},\mathbf{k};\,{}^1/_2\,k^2+i\varepsilon)}{k^2+i\varepsilon-q^2}, \tag{33}$$

continued with respect to $\mathbf{q}$ outside the energy surface. In (33) $w^{(\alpha)}(\mathbf{q}-\mathbf{q}') = \langle\mathbf{q}|\hat{w}^{(\alpha)}|\mathbf{q}'\rangle$.

We shall assume that the potentials $\hat{w}^{(\alpha)}$ are such that at large k we can use the Born approximation for the amplitudes in (33). This yields

$$\chi_{\mathbf{k},\alpha}^{(+)}(\mathbf{q}) \approx \delta^3(\mathbf{q}-\mathbf{k}) + 2\frac{w^{(\alpha)}(\mathbf{q}-\mathbf{k})}{k^2-q^2+i0}. \tag{34}$$

The expression for the first-order term in (31) arising upon the substitution of (34) has the form

$$T_{i'i}^{\mathrm{IDW}} \approx T_{i'i}^{\mathrm{I}} + T_1 + T_2 + T_{12}, \tag{35}$$

where $T^{\mathrm{I}}_{i'i}$ is given by (4),

$$T_1 = \int \frac{w^{(1)}(\mathbf{q}-\mathbf{k}_{i'})\,V_{if}(\mathbf{q}-\mathbf{k}_i)\,\varepsilon_{i'i}(\mathbf{q}-\mathbf{k}_i)\,d^3\mathbf{q}}{E+i\varepsilon-{}^1/_2\,q^2}, \tag{36}$$

and T_2 is obtained from (36) by making the interchanges $i \rightleftarrows i'$ and $1 \rightleftarrows 2$. For $v\to\infty$ the matrix element T_{12}, which contains the product of $w^{(1)}$ and $w^{(2)}$, is asymptotically small compared to T_1 and T_2. Concerning the potentials $w^{(\alpha)}$, we shall assume that in the momentum representation they decrease more slowly than $1/q^6$ as $q\to\infty$. The dominant contribution to (36) will then be made by the neighborhood of the point $\mathbf{q} = \mathbf{k}_i$, so that

$$T_1 \approx -\frac{i}{v}\,w^{(1)}(\Delta)\int_0^\infty \frac{dq}{q}\,\varepsilon_{i'i}(q) \tag{37}$$

and, consequently,

$$T_{i'i}^{\mathrm{IDW}} \approx \frac{\Phi_i(0)\Phi_{i'}(0)}{\Delta^6} - \frac{i}{v}\left[w^{(1)}(\Delta)+w^{(2)}(\Delta)\right]\int_0^\infty \frac{dq}{q}\,\varepsilon_{i'i}(q). \tag{38}$$

As can be seen from (38), the asymptotic form of the first distorted-wave Born approximation essentially depends on the form of the distorted potentials, and this makes it nonunique. This nonuniqueness, however, vanishes when the second-order terms in (31) are taken into account. In fact, the dominant part of the asymptotic form of the matrix element

$$\langle\Phi_{i'}^{(-)}|\hat{V}_{if}\hat{G}_i\hat{w}^{(1)}|\Phi_i^{(+)}\rangle = 2\int \frac{w^{(1)}(\mathbf{q}-\mathbf{k}_i)\,V_{if}(\mathbf{q}-\mathbf{k}_{i'})\,\varepsilon_{i'i}(\mathbf{q}-\mathbf{k}_{i'})}{k_i^2+i\varepsilon-q^2}\,d\mathbf{q} \tag{39}$$

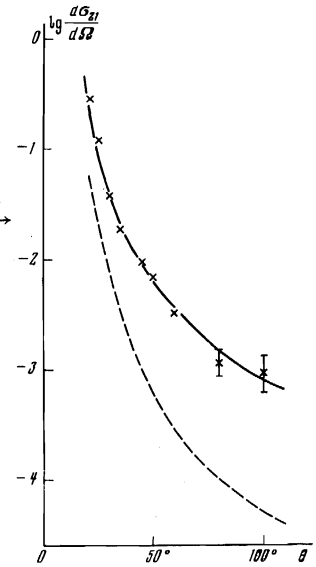
is equal to

$$-\frac{i}{v}\,w^{(1)}(\Delta)\int_0^\infty \frac{dq}{q}\,\varepsilon_{i'i}(q), \tag{40}$$

and, correspondingly,

$$\langle\Phi_{i'}^{(-)}|\hat{w}^{(2)}\hat{G}_i\hat{V}_{if}|\Phi_i^{(+)}\rangle \approx -\frac{i}{v}\,w^{(2)}(\Delta)\int_0^\infty \frac{dq}{q}\,\varepsilon_{i'i}(q). \tag{41}$$

Comparing (37) and (38) with (40) and (41) and taking into account the fact that these matrix elements enter into (31) with opposite signs, we find that the dominant parts of the asymptotic forms of the first- and second-order terms containing the distorted potentials cancel each other. As for the asymptotic form of the matrix element $\langle\Phi_{i'}^{(-)}|\hat{v}_i\hat{G}_i\hat{v}_i|\Phi_i^{(+)}\rangle$ in (31), it coincides with the asymptotic form (12) of the above-computed second-order terms $\langle i'|\hat{v}_i\hat{G}_i\hat{v}_i|i\rangle$ and is the dominant part of



The differential cross section (in units of the Born radius) for the 1s → 2s, 2p excitation of the hydrogen atom by electron impact at 200 eV. Continuous curve, the result of the present calculation; broken curve, cross section obtained in [7] in the first distorted-wave Born approximation; points, experimental data from [1].

the asymptotic form. Thus, we find that as $v\to\infty$

$$T_{i'i}^{\mathrm{IIDW}} \to T_{i'i}^{\mathrm{IIB}},$$

where $T_{i'i}^{\mathrm{IIB}}$ is given by (12).

Notice that in spite of the ambiguous nature of the first distorted-wave Born approximation, we can, by imposing definite conditions on the distorted potentials, make the amplitude $T_{i'i}^{\mathrm{IDW}}$ have the correct asymptotic form. Comparing (38) and (12), we find that for this to happen the distorted potentials should satisfy the condition

$$\lim_{\Delta\to\infty}\frac{w^{(1)}(\Delta)+w^{(2)}(\Delta)}{2V_{pi}(\Delta)} = -\pi^2\lim_{\Delta\to\infty}\Delta^2\left(w^{(1)}(\Delta)+w^{(2)}(\Delta)\right) = 1, \tag{42}$$

which can serve as one of the criteria to be used when selecting the potentials.

5. COMPARISON WITH THE EXPERIMENTAL DATA

The experimental data on the differential cross section for the scattering of 200-eV electrons by the hydrogen atom with a transition of the latter from the ground to the first excited state in the scattering-angle range from 20 to 100° are cited in[1]. These data are compared in the figure with the results of the present computation. Since, as follows from (28), the contribution of the exchange-scattering amplitude at large v is small compared to that of the amplitude of the scattering with excitation, the leading part of the asymptotic form of the differential cross section $d\sigma_{21}/d\Omega$ for the 1s → 2s, 2p transitions has the form

$$\frac{d\sigma_{21}}{d\Omega} = (2\pi)^4\left(|T_{2s,1s}|^2 + 3|T_{2p,1s}|^2\right), \tag{43}$$

where the $T_{i'i}$'s are determined by the expressions (15). The computation of the constants (16) entering into (15) with the appropriate Coulomb functions leads to the following values:

$$E^{(1)}_{2s\,1s} = 6.3\cdot10^{-2},\quad E^{(2)}_{2s\,1s} = 7.3\cdot10^{-1},\quad E^{(1)}_{2p\,1s} = 1.0\cdot10^{-3},\quad E^{(2)}_{2p\,1s} = 5.2. \tag{44}$$

The differential cross section computed from (43) and (44) taken into account is represented in the figure by the continuous curve. Also shown in the figure are the results of the computation carried out by Geltman and Hidalgo[7] in the framework of the first distorted-wave Born approximation. It was assumed in the calculation in[7] that $w^{(1)}(\Delta) \equiv 0$ and $w^{(2)}(\Delta) = -1/2\pi^2\Delta^2$. Such a choice for the distorted potentials does not, as follows from (42), yield the correct asymptotic form of the differential cross section.

The absolute values of the experimental cross sections in the figure have been chosen such that they coincide with the results of the present calculation for $\theta = 30°$. The observed angular dependence of the cross section is then reproduced within the limits of experimental error by the cross section computed on the basis of the angle-uniform asymptotic form of the second Born approximation (15). As the computation shows, the dominant contribution to the $d\sigma_{21}/d\Omega$ is made by the transition to the final 2p state, whereas the contribution of the transitions to the 2s state constitutes only a few per cent. Notice also that in the range of angles $\theta \lesssim 30°$, comparable contributions to the cross section are made by the first- and second-order terms, whereas for $\theta > 30°$ the contribution of the second-order terms to (15) is overwhelming.

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Translated by A. K. Agyei
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