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- ²A more exact estimate of the angular dimension of one mode is given in Ref. 24.
- ³This particular case of the solution of the system (21) was considered in Ref. 16.
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Calculations of inelastic electron scattering from atoms in the second Born approximation

L. A. Burkova and V. I. Ochkur

A. A. Zhdanov Leningrad State University

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The high-energy asymptotic behavior of the second Born approximation is examined. The formulas obtained are used to calculate differential and total cross sections for inelastic scattering of electrons from hydrogen and helium atoms. The results of the calculations are compared with experiment.

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1. INTRODUCTION

Until recently the second Born approximation, unlike the first one, had not been much used in the theory of collisions of electrons with atoms. This is evidently due to the simplicity and efficacy of the first approximation and the complexity of the second, together with the fact that the early studies seemed to indicate that the second approximation was not very efficacious.

Of course problems involving two-electron transitions cannot be treated consistently without going beyond the limitations of first-order perturbation theory. But such problems are complex and have not been worked out well so far. In most of the studies total cross sections for single-electron transitions were calculated and compared with experiment, and various attempts were made to improve the results of the first Born approximation in the region of low collision energies where it usually gives values some 50-100% higher than the experimen-

tal values. In particular, attempts were made to improve these results by taking the higher-order (mainly the second-order) perturbation-theory contributions into account.

Difficulties involved in calculating the integrals that arose hindered the use of the second Born approximation for a long time. But when Dalitz,¹ Lewis,² and others had developed a technique for calculating these integrals, the calculation of the contributions from individual intermediate states ceased to present any difficulties in principle, although the calculations remained rather laborious.

The proposed technique was used in a series of studies by Moiseevich and collaborators³⁻⁶ and by Wollings and McDowell⁷ to calculate the total elastic scattering cross sections of hydrogen and helium as well as the total cross sections for excitation of the 2s and 2p levels of hydrogen and the 2¹S and 2¹P levels of helium.

However, the cross sections obtained by taking into account a number of what would seem to be the most important intermediate states were close to the cross sections given by the first Born approximation, and the attempt to improve these cross sections in the low-energy region was not successful. Not only was an attempt made in these studies to take precisely into account the contribution from individual levels, but an attempt was also made to take approximately into account the contribution from all other levels, including those of the continuous spectrum, by using the so-called closure formula. Although this method of summing over the intermediate states does lead to results that are fairly reasonable as well as simple, we feel that it cannot be justified for the purposes for which it was used in the present case (to reduce the error below 50%), and the fact that it did not lead to very good results does not seem surprising. Moreover, only the real part of the scattering amplitude was calculated in these studies. In any case, more recent studies^{8,9} have shown that the accurate calculation of the cross sections for the $1s-2s$ and $1s-2p$ transitions and similar ones is a delicate problem for which the second-order corrections do not suffice.

At the same time one may suppose (and the available experience with calculations confirms this) that the second-Born-approximation formulas can give a qualitatively correct description of many second-order effects, just as the first Born approximation has led to many useful results in the case of one-electron transitions. On adopting such a qualitative approach it is natural to think of performing the calculation without using the correct matrix elements themselves, but to examine their asymptotic behavior at high collision energies and use only the asymptotic form of the matrix elements in the calculation. Such a procedure would be analogous to that used to describe the effect of electron exchange in first order perturbation theory.¹⁰ It is essentially the same as the usual method of employing the Born approximation itself, the only difference being that the Born formula is so simple that the question of extracting its asymptotic behavior simply does not arise.

We shall see below that using the asymptotic behavior instead of calculating the integrals exactly makes it possible to obtain many useful results and leads to formulas that are quite comparable as regards simplicity to the first-Born-approximation formulas. Such simple asymptotic behavior arises in two cases; when the momentum transfer is small, and when it is large. Moreover, more complete calculations in which the integrals are evaluated accurately show that the amplitude is a monotonic and fairly smooth function of the momentum transfer even at medium collision energies, and the more so at high energies. It is therefore reasonable to fit the resulting asymptotic formulas together somehow and thereby obtain the scattering amplitude as a function of angle for all angles.

We have already noted that the second Born approximation is most naturally used to calculate essentially two-particle processes. However, there are at least three problems that seem at first glance to be single-

particle problems, but in which second-order effects actually play a predominant part. These are the problems of large-angle electron inelastic scattering, the problem of calculating the cross sections for transitions involving a change of more than unity in the orbital quantum number, and the problem of calculating the exchange-scattering differential cross section at small and large angles. We shall examine these three problems in this paper.

All three problems have been treated before. The first one was treated by Potapov,¹¹ who proposed an elegant method for extracting the asymptotic behavior of the scattering amplitude for small and large momentum transfers, as well as a procedure for joining the asymptotic formulas together. Unfortunately certain features of the structure of the matrix elements occurring in the integral over the intermediate momentum were not taken into account in this paper, and the final formulas turned out to be valid only for $s-s$ transitions.

The second problem was treated by Vainshtein and Presnyakov,¹² but on the basis of an oversimplified modification of the second-Born-approximation formulas. It was also treated on the basis of the complete formulas by Wollings and McDowell.¹³ However, these authors calculated only the real part of the scattering amplitude; such a treatment cannot be regarded as valid, and indeed it led to poor final results.

The third problem was treated, but only for forward (zero-angle) scattering, by Bonham,¹⁴ using the $1S-2^3S$ and $1S-2^3P$ transitions in helium as examples. These calculations were compared with Lassette's experiment¹⁵ for the 2^3S level, which gave a cross section some 10^4 times larger than a first-order perturbation theory calculation at a collision energy of 500 eV. Both these papers appeared soon after that of Vriens *et al.*¹⁶ in which it was first shown that the first-order formula does not correctly describe the behavior of the exchange-scattering cross section at small angles and that the calculated cross sections are much smaller than the experimental values. The experiment¹⁶ was performed at collision energies from 100 to 225 eV, and the authors suggested that these energies may be too low for perturbation theory to be applicable. Lassette's experiment showed that that view is incorrect. Bonham was able to show that using the second-order formulas would increase the calculated forward-scattering cross section with excitation of the 2^3S state by almost 100 times, although the calculated cross section still remained far below the experimental value. Bonham therefore concluded that even the second-Born-approximation formalism does not give a satisfactory description of experiment.

The present work also arose from an attempt to understand the behavior of exchange-scattering differential cross sections. Below we shall show that, contrary to Bonham's conclusion, the second Born approximation can provide a reasonable basis for the description of exchange processes at fairly high energies. Bonham's conclusion turns out to be based on an accidental coincidence of circumstances. Precisely the case of exchange excitation of the 2^3S level of helium at energies

above 300 eV and scattering angles below 10° is an exception to the general rule and requires additional study.

In the calculations presented below we follow Potapov's method¹¹ to obtain the principle terms in the asymptotic behavior of the Born approximation, which are valid for all transitions. Our procedure for fitting together the asymptotic results differs from Potapov's, being both simpler and more accurate. Using these formulas we calculate the differential cross sections for excitation of the 2s and 2p hydrogen levels and the 2¹S, 2¹P, 2³S, and 2³P helium levels, as well as the total cross sections for excitation of the 3¹D and 4¹D helium levels. The results of the calculations are compared with experiment and with the results of other investigators.

We use the hydrogen atom to illustrate the method for extracting the leading terms in the asymptotic scattering amplitude. No difficulties will be encountered in extending the results to more complex atoms.

2. THE SCATTERING AMPLITUDE IN THE FIRST BORN APPROXIMATION

In the first Born approximation, the scattering amplitude has the form

$$f_{\beta\alpha}^{(1)}(\Delta) = \frac{2}{\Delta^2} \int \bar{\psi}_\beta(\mathbf{r}) \exp(i\Delta\mathbf{r}) \psi_\alpha(\mathbf{r}) d\mathbf{r} = \frac{2}{\Delta^2} F_{\beta\alpha}(\Delta), \quad (1)$$

where ψ_α and ψ_β are the wave functions for the initial and final states of the atom and $\Delta = \mathbf{k} - \mathbf{k}'$ is the momentum transfer, \mathbf{k} and \mathbf{k}' being the momenta of the incident and scattered electrons. In the subsequent calculations it will be convenient to choose the quantization axis in the direction of \mathbf{k} . We therefore rewrite Eq. (1) in a coordinate system having its z axis in the direction of \mathbf{k} and explicitly exhibit the dependence of $F_{\beta\alpha}$ on the angles defining the direction of Δ . On inserting the atomic wave functions in the form of products of radial and angular functions and making use of the expansion of a plane wave in a series of spherical functions, we obtain

$$f_{\beta\alpha}^{(1)}(\Delta) = \frac{2}{\Delta^2} \sum_{l=|l_\alpha-l_\beta|}^{l_\alpha+l_\beta} Y_{l, m_\beta - m_\alpha}^*(\hat{\Delta}) F_{\beta\alpha}^l(\Delta), \quad (2)$$

where $\Delta = |\Delta|$, $\hat{\Delta} = \Delta/\Delta$, and

$$F_{\beta\alpha}^l(\Delta) = (-1)^{l+m_\beta} i^{l_\alpha-l_\beta} \begin{pmatrix} l_\beta & l & l_\alpha \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_\beta & l & l_\alpha \\ -m_\beta & m & m_\alpha \end{pmatrix} \times [4\pi(2l_\alpha+1)(2l_\beta+1)(2l+1)]^{1/2} \int_0^\infty R_{\alpha}(r) R_{\beta}(r) j_l(\Delta r) r^2 dr, \quad (3)$$

$j_l(\Delta r)$ being a spherical Bessel function.

If the initial state is an s state ($l_\alpha=0$), as will be the case in all the examples examined below, Eq. (2) simplifies to

$$f_{\beta\alpha}^{(1)}(\Delta) = \frac{2}{\Delta^2} Y_{l, m_\beta}^*(\hat{\Delta}) F_{\beta\alpha}^l(\Delta). \quad (4)$$

The exchange scattering amplitude is

$$g_{\beta\alpha}^{(1)}(\mathbf{k}, \mathbf{k}') = \frac{1}{2\pi} \int \exp(-ik'r_1) \psi_\beta(\mathbf{r}_2) \frac{1}{r_{12}} \exp(ikr_2) \psi_\alpha(\mathbf{r}_1) d\mathbf{r}_1 d\mathbf{r}_2. \quad (5)$$

It is not difficult to show¹⁷ that the expansion of $g_{\beta\alpha}^{(1)}$ in

powers of the reciprocal velocity has the form

$$g_{\beta\alpha}^{(1)}(\mathbf{k}, \mathbf{k}') = \frac{2}{k^2} F_{\beta\alpha}^{(1)}(\Delta) + \frac{4i}{k'^3} \int d^3r \psi_\beta(\mathbf{r}) \exp(i\Delta\mathbf{r}) \frac{\partial}{\partial z} \psi_\alpha(\mathbf{r}). \quad (6)$$

For $\Delta \sim 1$, the first term is the leading term in the asymptotic exchange-scattering amplitude. It has been repeatedly used. Sometimes, however, the second term, which is proportional to k^{-3} , must also be retained since, as we shall see below, the principal second-order terms in the interaction are also proportional to k^{-3} . Moreover, $F_{\beta\alpha}^{(1)}(\Delta)$ is proportional to k^{-1} or k^{-2} when $\Delta \ll 1$, and then the first term turns out to be proportional to k^{-3} or k^{-4} , respectively.

3. THE SCATTERING AMPLITUDE IN THE SECOND BORN APPROXIMATION

The contribution of the second-order terms to the scattering amplitude has the form

$$f_{\beta\alpha}^{(2)}(\mathbf{k}, \mathbf{k}') = -(2\pi)^2 \sum_{\gamma} \int d^3q \frac{\langle \mathbf{k}'\beta | V | \mathbf{q}\gamma \rangle \langle \mathbf{q}\gamma | V | \mathbf{k}\alpha \rangle}{E_{k\alpha} - E_{q\gamma} + i\eta}. \quad (7)$$

In our case

$$V(r_1, r_2) = 1/r_{12} - 1/r_1, \quad (8)$$

and $E_{k\alpha} = E_\alpha + k^2/2$, where E_α is the energy of the atom in state α . The summation is taken over all intermediate states γ . For the Coulomb interaction, Eq. (7) reduces immediately to the form

$$f_{\beta\alpha}^{(2)}(\mathbf{k}, \mathbf{k}') = -\frac{1}{\pi^2} \sum_{\gamma} \int d^3q \frac{[F_{\beta\gamma}(\mathbf{q}-\mathbf{k}') - \delta_{\beta\gamma}] [F_{\gamma\alpha}(\mathbf{k}-\mathbf{q}) - \delta_{\gamma\alpha}]}{|\mathbf{k}-\mathbf{q}|^2 |\mathbf{q}-\mathbf{k}'|^2 (E_{k\alpha} - E_{q\gamma} + i\eta)}, \quad (9)$$

in which $F_{\beta\alpha}(\mathbf{q})$ is defined as in Eq. (1).

It will be convenient in the subsequent calculations to separate out the terms with $\gamma = \alpha$ and $\gamma = \beta$ in the summation over γ :

$$\begin{aligned} \pi^2 f_{\beta\alpha}^{(2)}(\mathbf{k}, \mathbf{k}') &= \int d^3q \frac{\delta_{\alpha\beta}}{|\mathbf{k}-\mathbf{q}|^2 |\mathbf{q}-\mathbf{k}'|^2 (E_{k\alpha} - E_{q\alpha} + i\eta)} \\ &+ \int d^3q \frac{F_{\beta\alpha}(\mathbf{q}-\mathbf{k}') [F_{\alpha\alpha}(\mathbf{k}-\mathbf{q}) - 1]}{|\mathbf{k}-\mathbf{q}|^2 |\mathbf{q}-\mathbf{k}'|^2 (E_{k\alpha} - E_{q\alpha} + i\eta)} \\ &+ \int d^3q \frac{[F_{\beta\beta}(\mathbf{q}-\mathbf{k}') - 1] F_{\beta\alpha}(\mathbf{k}-\mathbf{q})}{|\mathbf{k}-\mathbf{q}|^2 |\mathbf{q}-\mathbf{k}'|^2 (E_{k\alpha} - E_{q\beta} + i\eta)} \\ &+ \sum_{\gamma} \int d^3q \frac{F_{\beta\gamma}(\mathbf{q}-\mathbf{k}') F_{\gamma\alpha}(\mathbf{k}-\mathbf{q})}{|\mathbf{k}-\mathbf{q}|^2 |\mathbf{q}-\mathbf{k}'|^2 (E_{k\alpha} - E_{q\gamma} + i\eta)}. \end{aligned} \quad (10)$$

The first of the integrals in Eq. (10) can be evaluated without much difficulty,² but, since it contributes only to the elastic scattering, it is of no interest to us here and we shall drop it.

The remaining integrals can also be calculated accurately but, as we noted in the Introduction, we shall not undertake that task but shall examine their behavior only in the limiting case of high scattering energies ($k \gg 1$). Then the two limiting cases of large and small momentum transfers naturally arise.

The scattering amplitude for $\Delta \gg 1$

In view of the behavior of the matrix elements $F_{\mu\nu}(\kappa)$ at small and large κ :

$$\begin{aligned} F_{\mu\nu}(\kappa) &\sim \kappa, & l_\mu = l_\nu \pm 1 \\ F_{\mu\nu}(\kappa) &\sim \kappa^2, & l_\mu \neq l_\nu \pm 1 \end{aligned} \quad \kappa \ll 1, \quad (11)$$

$$F_{\mu\nu}(\kappa) \sim \kappa^{-l_\mu - l_\nu}, \quad \kappa \gg 1,$$

it is not difficult to see that the main contribution to the integrals of interest to us comes from values of κ close to unity. It can be seen in an obvious way that the second and third integrals in (10) are proportional to Δ^{-2} . The last integral, however, is proportional to $\Delta^{-6-l\beta-l\gamma}$ and should be dropped for the case $\Delta \gg 1$. Thus, for the case $k \gg 1$ and $\Delta \gg 1$ we reach the following simple result¹¹:

$$f_{\beta\alpha}^{(2)}(\Delta) = \frac{2}{\pi^2 \Delta^2} \left\{ \int \frac{F_{\beta\alpha}(\kappa)}{2k\kappa + i\eta} \frac{d^3\kappa}{\kappa^2} + (-1)^l \int \frac{F_{\beta\alpha}(\kappa)}{2k'\kappa + i\eta} \frac{d^3\kappa}{\kappa^2} \right\}. \quad (12)$$

Here, in accordance with the condition $k \gg 1$, we have retained only the leading terms in the Green's function. The angular integration in the first of these integrals can be performed at once. Recalling that, in accordance with (4), we have $F_{\beta\alpha}(\kappa) = F_{\beta\alpha}^l(\kappa) Y_{l\beta m_\beta}(\hat{\kappa})$, we obtain

$$f_{\beta\alpha}^{(2)}(\Delta) = \frac{2\delta_{m_\beta 0} C_{l\beta}}{\pi k \Delta^2} \int F_{\beta\alpha}^l(\kappa) \frac{d\kappa}{\kappa}, \quad (13)$$

in which

$$C_l = \left(\frac{2l+1}{\pi} \right)^{1/2} \left\{ \text{v.p.} \int P_l(x) \frac{dx}{x} - i\pi P_l(0) \right\}, \quad (14)$$

where the $P_l(x)$ are Legendre polynomials and the sign "v.p." indicates that the principal value of the integral is to be taken. Thus, the contribution comes from either the first or the second term in the braces, depending on the parity of l .

In the second integral we must take account of the fact that we have chosen the quantization axis in the direction of \mathbf{k} , whereas it is convenient to use a coordinate system with the z axis in the direction of \mathbf{k}' when calculating the integrals; the wave functions occurring in $F_{\beta\alpha}$ must therefore be subjected to the appropriate preliminary transformation. We finally obtain

$$f_{\beta\alpha}^{(2)}(\Delta) = \frac{2C_{l\beta}}{\pi k \Delta^2} \Phi_{l\beta m_\beta}(\vartheta) \int F_{\beta\alpha}^l(\kappa) \frac{d\kappa}{\kappa}, \quad (15)$$

in which

$$\Phi_{lm}(\vartheta) = \delta_{m,0} + (-1)^l \left(\frac{(l-m)!}{(l+m)!} \right)^{1/2} P_l^m(\cos \vartheta), \quad (16)$$

where the $P_l^m(x)$ are associated Legendre polynomials. In accordance with (14), the coefficients C_l for $l=0, 1, 2$ have the following values:

$$C_0 = -i\pi^{1/2}, \quad C_1 = 2(3/\pi)^{1/2}, \quad C_2 = i(5\pi)^{1/2}.$$

For the case of exchange scattering we must return to Eq. (7) and, in analogy with Eq. (5), interchange the arguments of the final-state wave function. By performing calculations similar to the preceding ones we can easily show that the following expression, in which the coefficients $C_{l\beta}$ are the same as in (14), is obtained for the exchange amplitude:

$$g_{\beta\alpha}^{(2)}(\Delta) = \frac{2C_{l\beta}}{\pi k^2 \Delta^2} \Phi_{l\beta m_\beta}(\vartheta) \int F_{\beta\alpha}^l(\kappa) \kappa d\kappa. \quad (17)$$

We note that the dependence of $F_{\beta\alpha}$ on the direction of the vector κ was not taken into account in Ref. 11, so that the results obtained there are valid only for $s-s$ transitions.

The scattering amplitude for $\Delta \ll 1$

For small-angle scattering we have $\Delta \approx (E_\beta - E_\alpha)/h\nu$ with $\mathbf{k} \sim \mathbf{k}'$ and $k \gg 1$. Hence it is not necessary here to transform the coordinate system as we did in the case $\Delta \gg 1$. In view of (11), all the integrals are well defined, and for the term involving electron-electron interaction, for example, we obtain

$$\begin{aligned} & \sum_{\gamma} \int d^3\kappa \frac{F_{\beta\gamma}(\Delta - \kappa) F_{\gamma\alpha}(\kappa)}{\kappa^2 |\Delta - \kappa|^2 (k\kappa + i\eta)} \\ &= \frac{1}{k\pi} \sum_{\gamma} \int \frac{d\kappa}{\kappa^2} F_{\gamma\alpha}^l(\kappa) \sum_{l=|\beta-\gamma|}^{l\beta+l\gamma} F_{\beta\gamma}^l(\kappa) C_{l\gamma m_\gamma}^l, \end{aligned} \quad (18)$$

where

$$C_{l\gamma m_\gamma}^l = \int Y_{l\gamma m_\gamma}^*(\hat{\kappa}) Y_{lm}(\hat{\kappa}) \frac{d\Omega_{\kappa}}{\cos(k, \kappa) + i\eta}. \quad (19)$$

Cancellation of terms arising from the electron-electron and electron-nucleus interactions, which assures the electrical neutrality of the atom as a whole when Δ is small, plays an important part in the integrals containing $\gamma = \alpha$ and $\gamma = \beta$. Finally, as Potapov pointed out,¹¹ it is useful to bear in mind that in the case $\Delta \ll 1$ the second-order terms will be of the order of $1/k$, while the second order terms in the scattering amplitude for dipole transitions will be of the order of k , and in the other cases, of the order of unity. Hence for direct scattering in the small-angle region there is no reason to expect the second-order terms to alter the cross sections greatly.

For exchange transitions the situation is different. An expression for a typical integral occurring in the scattering amplitude can be written down directly by analogy with (18); it has the form

$$\frac{1}{k^2} \int \frac{d\kappa}{\kappa} F_{\gamma\alpha}^l(\kappa) \sum_{l=|\beta-\gamma|}^{l\beta+l\gamma} F_{\beta\gamma}^l(\kappa) C_{l\gamma m_\gamma}^l, \quad (20)$$

the $C_{l\gamma m_\gamma}^l$ being defined by formula (19) as before.

It is not difficult to see, however, that in the case of small-angle exchange scattering the first-order term is of the order of k^{-3} for dipole transitions and of the order of k^{-4} in the other cases. Thus, for small-angle scattering the second-order terms in many cases turn out to be the principal ones, as was first shown by Bonham.¹⁴ For large scattering angles the first-order scattering amplitude falls off even faster (as $\Delta^{-6-l\alpha-l\beta}$) and the second-order terms are always the governing ones.¹⁸

Thus, formulas (15) and (18) solve the problem of finding the asymptotic behavior of the scattering amplitude for large and small scattering angles. As we noted before, analysis of more complete calculations in which the assumptions $k \gg 1$ and $\Delta \gg 1$ were not made^{8, 9, 19} shows that the imaginary part of the scattering amplitude varies rather smoothly on going from large to small scattering angles. The preceding analysis [and indeed the very structure of formulas (10)] suggests a procedure for smoothly fitting together the two asymptotic expressions. It is obvious that we shall correctly write both limiting cases if we replace $|\Delta + \kappa|^2$ in the denominators of the integrals in (10) by $Q^2 = \kappa^2 + \Delta^2$. It is also obvious that that substitution corresponds simply to employing the theorem of the mean in

calculating the integrals over the angles specifying the direction of the vector κ . In this manner we finally obtain the following formulas, useful at all scattering angles, for the scattering amplitude in the second order:

$$f_{\beta\alpha}^{(2)} = \frac{1}{\pi k} \left\{ C_i \Phi_{i_\beta m_\beta}(\theta) \int_0^\infty F_{\beta\alpha}^i(\kappa) \frac{d\kappa}{\kappa Q^2} - (-1)^{i\beta} C_{\alpha\beta}^0 \int_0^\infty \frac{F_{\beta\alpha}^i(\kappa) F_{\alpha\alpha}^0(Q)}{\kappa Q^2} d\kappa \right. \\ \left. - \sum_{m_\beta} \int_0^\infty \left[F_{\beta\alpha}^i(\kappa) \sum_{\gamma} C_{i_\beta m_\beta}^i F_{\beta\beta}^i(Q) \right] \frac{d\kappa}{\kappa Q^2} \right. \\ \left. - \sum_{\gamma \neq \alpha} \int_0^\infty \left[F_{\gamma\alpha}^i(\kappa) \sum_{\gamma} F_{\beta\gamma}^i(Q) C_{i_\gamma m_\gamma}^i \right] \frac{d\kappa}{\kappa Q^2} \right\}, \quad (21)$$

where $Q^2 = \Delta^2 + \kappa^2$, the C_{i_β} and $C_{i_\gamma m_\gamma}^i$ are defined by formulas (14) and (19), and $\Phi_{i_\beta m_\beta}$ is defined by formula (16).

For the exchange-scattering amplitude we obtain the same formula (21) but with κ^2 replaced by k^2 in the denominators:

$$g_{\beta\alpha}^{(2)} = \frac{1}{\pi k^2} \left\{ C_i \Phi_{i_\beta m_\beta}(\theta) \int_0^\infty \frac{F_{\beta\alpha}^i(\kappa) \kappa d\kappa}{Q^2} - (-1)^{i\beta} C_{\alpha\beta}^0 \int_0^\infty \frac{F_{\beta\alpha}^i(\kappa) F_{\alpha\alpha}^0(Q) \kappa d\kappa}{Q^2} \right. \\ \left. - \sum_{m_\beta} \int_0^\infty \left[F_{\beta\alpha}^i(\kappa) \sum_{\gamma} C_{i_\beta m_\beta}^i F_{\beta\beta}^i(Q) \right] \frac{\kappa d\kappa}{Q^2} \right. \\ \left. - \sum_{\gamma \neq \alpha} \int_0^\infty \left[F_{\gamma\alpha}^i(\kappa) \sum_{\gamma} F_{\beta\gamma}^i(Q) C_{i_\gamma m_\gamma}^i \right] \frac{\kappa d\kappa}{Q^2} \right\}. \quad (22)$$

The total direct- and exchange-scattering amplitudes are of course

$$f = f^{(1)} + f^{(2)}, \quad g = g^{(1)} + g^{(2)}. \quad (23)$$

It will be useful to discuss once again the orders of magnitude of the individual terms in these formulas. The preceding analysis shows that it is useful not only to discuss the limiting cases of large and small scattering angles ($\Delta \gg 1$ and $\Delta \ll 1$, respectively), but also to examine the case $\Delta \sim 1$. From formulas (1), (21), and (22) we obtain the estimates listed in Table I. Here we use the notation $g^{(1)} = g_1^{(1)} + g_2^{(1)}$ in accordance with the separation of $g^{(1)}(\Delta)$ into two terms in Eq. (6). It is especially clearly evident from the Table that the main contribution to the direct scattering comes from the first-order terms when $\Delta \ll 1$ or $\Delta \sim 1$, and from the second-order terms when $\Delta \gg 1$.

For exchange scattering the situation is more complicated. Here the second-order terms always contribute to the principal terms in the asymptotic expansion of the scattering amplitude for both small and large angles. For medium angles ($\Delta \sim 1$) the first order term $g_1^{(1)}$ turns out to be the principal one. Since it is just this angular region that makes the main contribution to the total exchange-scattering cross sections, we can understand why earlier calculations in which only this term was considered led to poor agreement with experiment.

TABLE I.

	Δ	$f^{(1)}$	$f^{(2)}$	$g_1^{(1)}$	$g_2^{(1)}$	$g^{(2)}$
$l_\beta = l_\alpha \pm 1$	$\Delta \ll 1$	$k\Delta^{-1}$	k^{-1}	$k^{-2}\Delta$	k^{-3}	k^{-3}
	$\Delta \sim 1$	1	k^{-1}	k^{-2}	k^{-3}	k^{-3}
	$\Delta \gg 1$	Δ^{-7}	$k^{-1}\Delta^{-3}$	$k^{-2}\Delta^{-5}$	$k^{-3}\Delta^{-4}$	$k^{-3}\Delta^{-2}$
$l_\beta \neq l_\alpha \pm 1$	$\Delta \ll 1$	1	k^{-1}	$k^{-2}\Delta^2$	$k^{-3}\Delta$	k^{-3}
	$\Delta \sim 1$	1	k^{-1}	k^{-2}	k^{-3}	k^{-3}
	$\Delta \gg 1$	Δ^{-6}	$k^{-1}\Delta^{-2}$	$k^{-2}\Delta^{-4}$	$k^{-3}\Delta^{-3}$	$k^{-3}\Delta^{-2}$

Finally, for optically allowed transitions at small scattering angles one must take into account the contribution from the first-order terms $g_1^{(1)}$ and $g_2^{(1)}$, both of which are proportional to k^{-3} , while g_1 becomes the principal term when $\Delta \sim 1$.

4. CALCULATIONS AND DISCUSSION

Using formulas of the type of Eqs. (1), (6), (21), and (22), we made calculations for many transitions in hydrogen and helium, since it is just for these atoms that a fairly large mass of experimental data has now been accumulated and calculations have been made in various alternative approximations. We shall consider the several problems in the order in which they were listed in the Introduction.

1. Excitation with large-angle scattering

The simplest problem in which it is necessary to take into account the contribution to the scattering amplitude from second-order terms in the interaction in order to obtain a correct description of the process is that of calculating the excitation of an atom with deviation of the scattered electron through a large angle. Actually, an electron cannot be scattered through an angle greater than $\pi/2$ by an electron at rest. Since an atomic electron is not at rest, however, such large-angle scattering is indeed possible, but its probability is very low in the case of fast incident electrons since in addition to the usual Rutherford factor Δ^{-4} , it is also proportional to the probability that the atomic electron have a velocity comparable to that of the incident electron. This probability, in turn, is proportional to k^{-2} ; hence if only the electron-electron interaction is taken into account the cross section falls off as $\Delta^{-4}k^{-2}$, and this is already in sharp contradiction with experiment for scattering angles above 40° and collision energies above 50 eV.

These simple considerations have been noted by a number of authors^{11, 20, 21} and quite obviously make it necessary to take at least two interactions into account in the calculation; the interaction with the atomic electron, and with the nucleus. In that case, as is evident from Eq. (13), the cross section turns out to be proportional only to $k^{-2}\Delta^{-4}$. Of course a similar result can be obtained by using the Glauber approximation or some modification of the distorted-wave method.

Figure 1 shows the combined differential cross sections for excitation of the 2s and 2p levels of hydrogen over the wide range of incident-electron energies from 54 to 680 eV (curves 2). The scattering amplitudes were calculated with formulas (1) and (21), using the initial (1s) and final (2s or 2p) states as intermediate states. The contribution from other states was considerably smaller. The experimental cross sections obtained by Williams and Willis²² are also shown on the figure, as well as the cross sections calculated in the first Born approximation (curves 1) and a cross section calculated by Byron and Latour,⁹ using a more accurate method than ours for calculating the second-Born-approximation integrals (curve 3).

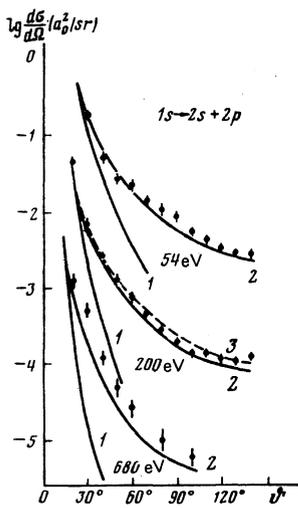


FIG. 1. Cross section for excitation of the 2s and 2p states of hydrogen. Curves: 1—first Born approximation, 2—scattering amplitude calculated with formulas (1) and (21) of the present paper, 3—second Born approximation (Ref. 8). The experimental points are from Ref. 22.

Figures 2 and 3 show the differential cross sections for excitation of the 2^1S and 2^1P states of helium. The calculations show that in these cases the main contribution to the scattering amplitude comes from the $1S$, 2^1S , and 2^1P intermediate states. In our calculations for these and all other transitions we used the wave functions from Refs. 23 and 24 for the ground and excited states of helium; these wave functions are fairly simple but are quite accurate enough for our purposes.

To illustrate the difference between our results and those that can be obtained with Potapov's formulas we show cross sections calculated in accordance with Ref. 11 in Figs. 2 and 3 (curves 3). We recall that for $s-s$ transitions our formulas differ from Potapov's only in the method for matching the cross sections for large and small momentum transfers, while for $s-p$ transitions they differ also by a numerical coefficient. As is evident from the figures, this difference is clearly seen on comparing the calculations with experiment.

Finally, the calculations of Geltman and Hidalgo,²⁰ in which Coulomb wave functions were used instead of plane waves for the final state, are also shown in the

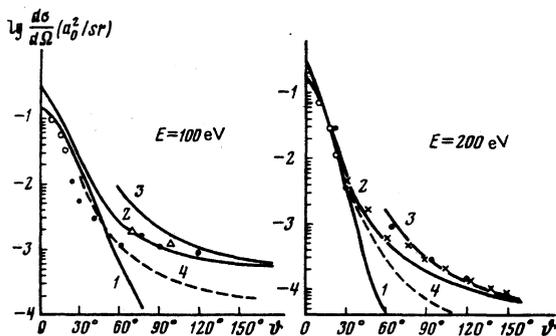


FIG. 2. Cross section for excitation of the 2^1S state of helium. Curves: 1—first Born approximation, 2—calculated with formulas (1) and (21) of the present paper, 3—second Born approximation (Ref. 11), 4—calculated²⁰ using Coulomb wave functions. Experimental points: ○—Ref. 16, ●—Ref. 25, △—Ref. 26, ×—Ref. 32.

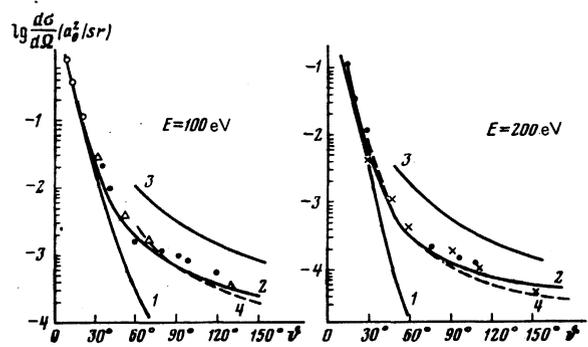


FIG. 3. Cross section for excitation of the 2^1P state of helium. The notation is the same as in Fig. 2.

figures (curves 4). Critical remarks regarding these calculations will be found in Ref. 11.

On the whole, we can evidently say with some confidence that the simple second-Born-approximation asymptotic formulas (1) and (21) reproduce the experimental data for problems of this type fairly well at collision energies above 100 eV and for all scattering angles.

2. The total cross sections for excitation of the 3^1D and 4^1D He levels

First-Born-approximation calculations give cross sections for transitions of the type $1s - ns$ or $1s - np$ that are 50–100% larger than the experimental values. That situation is standard. For $1s - nd$ transitions, however, whose probabilities are considerably lower, the first-Born-approximation cross sections turn out to be smaller than the experimental values and only approach the latter at high collision energies. Vainshtein and Presnyakov¹² suggested an explanation for this situation, pointing out that in this case the direct transition might be less intense than the two-stage cascade consisting of two intense dipole transitions. Essentially the same possibility was noted even earlier²⁷ in connection with a discussion of the Coulomb excitation of nuclei. Formulas (21) and (22) provide a simple and natural means for calculating such processes.

The results of a calculation for the $1S-3^1D$ transition in He are shown in Fig. 4 as an example. As before, curve 1 shows the contribution of the first-order terms to the cross section, and curve 2 was calculated with

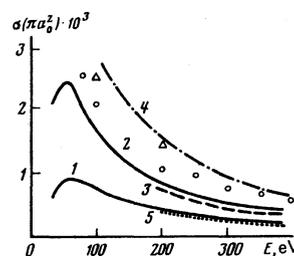


FIG. 4. Cross section for excitation of the 3^1D state of helium. Curves: 1—first Born approximation, 2—calculated with formulas (1) and (21) of the present paper, 3 and 4—calculated²⁸ by the method of second-order potentials with and without allowing for the 2^1P level, 5—calculated¹³ in the second Born approximation taking only Ref. (2) into account. Experimental points: ○—Ref. 29, △—Ref. 30.

formulas (1) and (21) with the 1^1S , 2^1P , 3^1P , and 3^1D states included as intermediate states. These results can be compared not only with experiment, but also with the second-Born-approximation calculations of Wollings and McDowell,¹³ in which, however, only the real part of the scattering amplitude was taken into account, and with a calculation by Bransden and Issa²⁸ using the so-called method of second-order potentials, which is essentially a variant of the strong coupling method. The latter calculation was performed twice; once with the $1S$, 3^1P , and 3^1D states included as intermediate states (curve 3) and once with the $1S$, 2^1P , 3^1P , and 3^1D states so included (curve 4).

Figure 5 shows the parts played by different intermediate states in the excitation of the 3^1D level of He. It is evident from the figure that the main contribution to this process actually comes from two successive dipole transitions that go via the 2^1P or 3^1P level. Scattering from the nucleus as well as the contribution from the first-order amplitude play a much less important part here than in the preceding problem. Taking the higher n^1P states into account also makes little difference. Thus the difference between curves 3 and 4 in Fig. 4 also becomes quite understandable.

Similar results can be obtained for the 4^1D level.

3. Differential cross sections for exchange scattering with excitation of the 2^3S and 2^3P He levels

In the Introduction we noted that experiment clearly indicates that the exchange-scattering differential cross section has a peak at small scattering angles. Recent experiments (see Ref. 15, and especially Ref. 25) show that at energies of 100–200 eV the peak in the differential cross section for excitation of the 2^3P He level lies in the angular range 10 – 20° , whereas the differential cross section for excitation of the 2^3S level increases clear down to 5° —the smallest angle at which it was measured. Such behavior is in obvious conflict with the first-order perturbation-theory predictions, especially for the 2^3S level.

Taking the second-order terms into account improves the situation considerably, as will be seen from the calculation results shown in Figs. 6 and 7. In both cases all states with $n=1$ and $n=2$ were taken into account as intermediate states; states with $n=3$ give a considerably smaller contribution.

Contributions from individual states to the amplitude

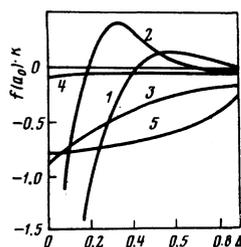


FIG. 5. First-order amplitude and contributions of various intermediate states to the second-order amplitude for the $1S$ – 3^1D transition in helium. Curves: 1— $f^{(2)}(2^1P)$, 2— $f^{(2)}(3^1P)$, 3— $f^{(2)}(3^1D) \cdot 10$, 4— $f^{(2)}(1S) \cdot 10$, 5— $f^{(1)} \cdot 10$.

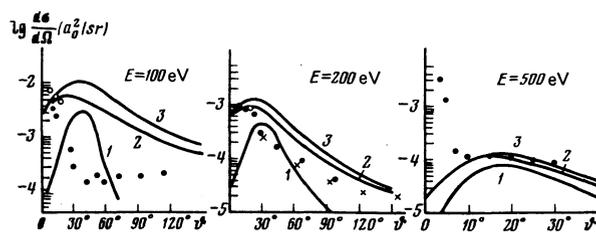


FIG. 6. Cross section for excitation of the 2^3S state of helium. Curves: 1—first Born approximation, 2—calculated with formula (22), 3—calculated with formulas (6) and (22). Experimental points: \circ —Ref. 16, \bullet —Ref. 25, \times —Ref. 32.

for excitation of the 2^3S and 2^3P levels are shown in Fig. 8. It is quite evident how the total amplitudes for these processes are made up. In particular, it is evident that for the $1S$ – 2^3P transition the term $g_2^{(1)}$, the second term in formula (6), plays an important part in forward scattering, whereas for the $1S$ – 2^3S transition $g_2^{(1)}(0) = 0$ and the amplitude is due almost entirely to the second-order terms. Moreover, the main contribution comes from terms describing the interaction with the nucleus in the initial or final state, i.e., from the distortion of the incident plane wave by the nuclear field. In the case of excitation of the 2^3P level, the density of atomic electrons in the final state near the nucleus is smaller than in the case of excitation of the 2^3S level, and the part played by terms corresponding to two-electron transitions is accordingly more important. The part played by the 2^1P intermediate state is especially large.

Returning to Figs. 6 and 7 for the differential cross sections, we see that the calculations agree less well with experiment for exchange scattering than for direct scattering. This is especially the case for excitation of the 2^3S level. At 100 eV our calculations reproduce the cross section more or less well only for the smallest and largest scattering angles, the calculated cross sections being much too large at intermediate angles. The calculation agrees considerably better with experiment, however, even at the collision energy $E = 200$ eV, and at $E = 500$ eV the calculated cross sections practically agree with experiment for scattering angles larger than 10° .

At high energies, however, the differential cross sections for this transition exhibit a new feature; they develop a sharp peak at scattering angles below 10° . Our formulas do not reproduce this peak, and that is what led Bonham¹⁴ to conclude that second-Born-approximation calculations are inadequate. It is rather to be concluded from our results, however, that the theory employed merely cannot explain the sharp forward peak in

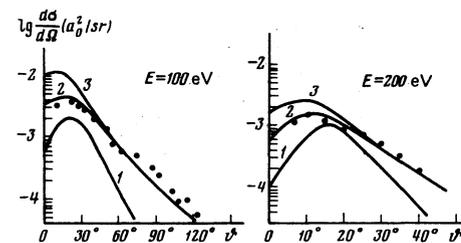


FIG. 7. Cross section for excitation of the 2^3P state of helium. The notation is the same as for Fig. 6.

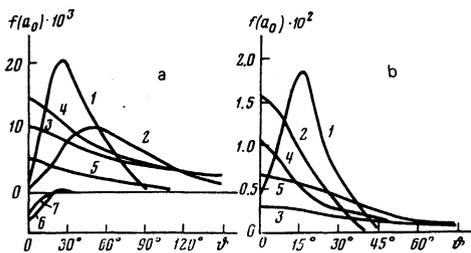


FIG. 8. First-order amplitude and contributions of various intermediate states to the second-order amplitude for the $1S-2^3S$ and $1S-2^3P$ transitions in helium at $E=200$ eV. a—The $1S-2^3S$ transition; curves: 1— $g_1^{(1)}$, 2— $g_2^{(1)}$, 3— $g^{(2)}(1S)$, 4— $g^{(2)}(2^3S)$, 5— $g^{(2)}(2^1S)$, 6— $g^{(2)}(2^1P)$, 7— $g^{(2)}(2^3P)$. b—The $1S-2^3P$ transition; curves: 1— $g_1^{(1)} \cdot 1/2$, 2— $g_2^{(1)}$, 3— $g^{(2)}(1S)$, 4— $g^{(2)}(2^3P)$, 5— $g^{(2)}(2^1P)$.

the scattering with excitation of the 2^3S level and that the asymptotic cross sections approach the experimental values less rapidly in this case than in other cases.

Huo³¹ attempted to explain the sharp peak in the excitation cross section for the 2^3S level and found that intermediate P states of the continuous spectrum make a large contribution to this transition. She was able to obtain the correct order of magnitude for the cross section and even to show that, as a function of energy, the cross section has a minimum at $E \sim 200$ eV and falls off slowly at energies above 300 eV in accordance with the experimental data then available. More recent experiments²⁵ showed, however, that the cross section actually falls off considerably faster than Huo's calculations predicted. Moreover, in Ref. 31 the cross section was obtained only for zero scattering angle, and it is not clear how sharp a peak this theory predicts. Finally, the relation between this theory and Bonham's theory is not clear. The closure formula was used in Bonham's theory, i.e., it is supposed that the entire continuous spectrum (including the P states) is included in the treatment in some reasonable approximation. We therefore feel that this problem requires further study.

The cross section for excitation of the 2^3P level does not exhibit any special features and agrees fairly well with our calculations in the energy region $50 \leq E \leq 200$ eV in which measurements have been made. One can only see a certain enhancement of the cross section at the smallest scattering angles. This enhancement is due to the term $g_2^{(1)}$ in the amplitude. In general we may stress that although we did include this term in the calculations since it behaves as k^{-3} and is therefore not to be dropped on formal grounds, it actually always leads

to a certain discrepancy with experiment. This is illustrated by Figs. 6 and 7, which show the cross sections calculated with (curves 3) and without (curves 2) using this term.

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