Exchange excitation of an atom by electrons with high angular momenta

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A parameter is found which governs the exponential decrease at large angular momenta of the partial amplitudes for exchange scattering of an electron on an atom (in general with excitation of the atom). This decrease becomes slower as the energy of the collision increases. The contribution of these partial amplitudes to the differential cross section has a peak for forward scattering. The effective parameters which describe this peak are discussed, and we also consider the dependence of the shape of the peak on the properties of the wave functions of the initial and final states of the atom.

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1. In the present note we consider the exchange scattering of an electron on a one-electron atom for large values of the total angular momentum L; in general the state of the atom is changed in the scattering. The case of large orbital angular momenta, i.e., distant passages, is investigated in the asymptotic theory of atomic collisions (see, e.g., [1–3]). So far only such collisions of heavy atomic particles have been considered, accompanied by the exchange of electrons between them. For not too small velocities the motion of the atomic nuclei can be regarded as classical, with given trajectories. For electron-atom collisions the motion of the incident electron must be treated quantum mechanically, and this greatly complicates the problem.

For large angular momenta L the partial amplitudes F_L for exchange scattering show a characteristic exponential decrease

$$F_L=c(L+{}^1/_2)^\nu A^{L+{}^1/_2}=c(L+{}^1/_2)^\nu \exp\left[(L+{}^1/_2)\ln A\right],\quad A<1, \tag{1}$$

which corresponds to the tunnel nature of the process in this case, brought about by the necessity of penetrating the centrifugal barrier. The exponential index $(L+\frac{1}{2})|\ln A|$ is an extremely important parameter, being a generalization of the Massey parameter well known in atomic physics. The problem of the asymptotic theory is to calculate the parameters c, ν, and A. The treatment of the charge-transfer process in collisions of heavy atomic particles[1–3] shows that the parameter A is determined excatly even in the first Born approximation, whereas the finding of the factor preceding the exponential in Eq. (1) requires the use of much more refined methods.

In the present paper we determine the argument of the main exponential in the asymptotic formula for the partial amplitudes of exchange scattering. The differential cross sections considered are for scattering at small angles, which is mainly given by the contributions from large angular momenta.

In the more general case of scattering with redistribution in a system of three particles with comparable masses the exponential index has been investigated in[4] by a different method. A technique of calculations like those of the present paper can also be used to find the asymptotic behavior of the widths for exchange autoionization decay of doubly excited states of a two-electron atom for large values of the total angular momentum.[5]

2. We shall confine ourselves here to the determination of the argument of the exponential for the exchange scattering of an electron on a one-electron atom; This allows us to use the Born approximation (which when applied to problems of exchange scattering is called the Born-Oppenheimer approximation):

$$F_L=-2\iint d\mathbf{r}_1 d\mathbf{r}_2 \Phi_i(\mathbf{r}_1,\mathbf{r}_2)\left(\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}-\frac{1}{r_1}\right)\Phi_f(\mathbf{r}_1,\mathbf{r}_2). \tag{2}$$

We use the atomic system of units and treat the nucleus of the atom as infinitely heavy. The initial and final states of the electron+atom system are, respectively,

$$\Phi_i(\mathbf{r}_1,\mathbf{r}_2)=\varphi_i(r_1)(\pi/2k_2r_2)^{1/2}J_{L+1/2}(k_2r_2)Y_{LM}(\mathbf{n}_2), \tag{3}$$

$$\Phi_f(\mathbf{r}_1,\mathbf{r}_2)=\varphi_f(r_2)(\pi/2k_1r_1)^{1/2}J_{L+1/2}(k_1r_1)Y_{LM}(\mathbf{n}_1),\quad \mathbf{n}_j=\mathbf{r}_j/r_j. \tag{4}$$

The free motion of the incident (second) electron with coordinate r_2 and momentum k_2 and of the emerging (first) electron with coordinate r_1 and momentum k_1, both with angular momentum L, are described in Eqs. (3) and (4) by spherical Bessel functions of the respective radial coordinates and spherical functions Y_{LM} of the respective angular variables. We assume that in the initial and final states the atom has zero orbital angular momentum, and that the respective normalized wave functions and energies are

$$\varphi_i(r_1)=\frac{\alpha_1^{3/2}}{\pi^{1/2}}e^{-\alpha_1 r_1},\quad E_1=-\alpha_1^2/2, \tag{5}$$

$$\varphi_f(r_2)=\frac{\alpha_2^{3/2}}{\pi^{1/2}}e^{-\alpha_2 r_2},\quad E_2=-\alpha_2^2/2. \tag{6}$$

The polynomial factors in the atomic radial wave functions can be taken into account by differentiating the final expressions for F_L with respect to the parameters α_1 and α_2.

Using the multipole expansion of the electron interaction $1/|\mathbf{r}_1-\mathbf{r}_2|$,[1)] we carry out the integration in Eq. (2)

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over the angular coordinates of both electrons;

$$F_L=-\frac{(\alpha_1\alpha_2)^{3/2}}{(k_1k_2)^{1/2}}\frac{4\pi}{2L+1}\int_0^\infty\int_0^\infty dr_1\,dr_2\,(r_1r_2)^{3/2}e^{-\alpha_1r_1}J_{L+1/2}(k_2r_2)\,e^{-\alpha_2r_2}J_{L+1/2}(k_1r_1)\frac{r_<^L}{r_>^{L+1}},$$

$$r_<=\min(r_1,\ r_2),\qquad r_>=\max(r_1,\ r_2). \tag{7}$$

Using the integral respresentation[6]

$$\left(\frac{r_<}{r_>}\right)^{L+1/2}=(2L+1)\int_0^\infty J_{L+1/2}(\xi r_1)J_{L+1/2}(\xi r_2)\frac{d\xi}{\xi}, \tag{8}$$

we then integrate the expression (7) over the radial coordinates

$$F_L=-\frac{4}{\pi}\frac{(\alpha_1\alpha_2)^{1/2}}{k_1k_2}\frac{\partial^2}{\partial\alpha_1\partial\alpha_2}\int_0^\infty\frac{d\xi}{\xi}Q_L\left(\frac{\alpha_1^2+k_1^2+\xi^2}{2\xi k_1}\right)Q_L\left(\frac{\alpha_2^2+k_2^2+\xi^2}{2\xi k_2}\right), \tag{9}$$

where Q_L is the Legendre function of the second kind. The representation (9) for the Born amplitude is exact, and is convenient for studying the asymptotic behavior for $L\to\infty$.

For large L we use the asymptotic formula[7]

$$Q_L(z)=\left(\frac{\pi}{2}\right)^{1/2}(z^2-1)^{-1/4}[z-(z^2-1)^{1/2}]^{L+1/2}(1+O(L^{-1})) \tag{10}$$

and calculate the integral (9) by the method of steepest descents. It is interesting that the functions $z_1(\xi)$ and $z_2(\xi)$

$$z_j(\xi)=(\alpha_j^2+k_j^2+\xi^2)/2\xi k_j \tag{11}$$

take their minimum values at the same point $\xi=q$, with

$$q=(\alpha_1^2+k_1^2)^{1/2}=(\alpha_2^2+k_2^2)^{1/2}, \tag{12}$$

which is also the saddle point. The second equality in (12) follows from the conservation of energy; i.e., it holds on the energy surface. The quantity $q^2/2$, which is extremely characteristic for the exchange-scattering process, is the energy transferred from one electron to the other. It is to be noted that when the problem is generalized to the case of "electrons" of different masses the maxima of the functions $z_1(\xi)$ and $z_2(\xi)$ no longer coincide in position, and the finding of the saddle point is a complicated matter. Thus the case of exchange of indistinguishable particles is mathematically a special one.

The final asymptotic form of the amplitude F_L is

$$F_L=-2(2\pi)^{1/2}\frac{(\alpha_1\alpha_2)^{3/2}}{(k_1k_2)^{1/2}}\frac{1}{q^{7/2}(\alpha_1+\alpha_2)^{1/2}}\left(L+\frac{1}{2}\right)^{1/2}\left\{\frac{(q-\alpha_1)(q-\alpha_2)}{k_1k_2}\right\}^{L+1/2}, \tag{13}$$

and is thus of the form (1). The coefficient of the exponential is here found only approximately. However, the factor A in Eq. (1) as found here

$$A=\frac{(q-\alpha_1)(q-\alpha_2)}{k_1k_2}=\left[\frac{(q-\alpha_1)(q-\alpha_2)}{(q+\alpha_1)(q+\alpha_2)}\right]^{1/2} \tag{14}$$

is exact and is determined only by the energies of the bound states and of the incident and emergent electrons. For a small collision energy ($k_1/\alpha_1,\ k_2/\alpha_2\to0$) the parameter A is small:

$$A\approx k_1k_2/4\alpha_1\alpha_2, \tag{15}$$

and for fast collisions ($k_1\approx k_2\equiv k\gg\alpha_1,\ \alpha_2$) it approaches unity from below:

$$A\approx1-(\alpha_1+\alpha_2)/k. \tag{16}$$

3. Inclusion of large angular momenta is important for the description of scattering through small angles θ. In the case of exponential decrease of the partial amplitudes, such as occurs in exchange processes, see Eq. (1), the contribution of large values of L becomes important if the parameter approaches unity. It follows from Eq. (1) that this occurs at large collision energies.

To determine the angular dependence of the cross section $\sigma(\theta)=|F(\theta)|^2$ it is necessary to calculate the series for the scattering amplitude:

$$F(\theta)=\sum_{L=0}^\infty(2L+1)F_LP_L(\cos\theta). \tag{17}$$

In a case in which the dependence of the partial amplitudes on L is given by Eq. (1) with integer values of ν, we can use the well known generating function for the Legendre polynomials.[7] By successive differentiations with respect to the parameter we get for $\nu=0$

$$F(\theta)=\frac{2c(z^2-1)^{1/2}}{(z-\cos\theta)^{3/2}},\quad z=\frac{A+A^{-1}}{2}=\frac{q^2+\alpha_1\alpha_2}{k_1k_2}, \tag{18}$$

and for $\nu=1$

$$F(\theta)=\frac{2c[3(z^2-1)-2z(z-\cos\theta)]}{(z-\cos\theta)^{5/2}} \tag{19}$$

and so on. As A approaches unity the expressions for the amplitude have an increasingly sharp peak for forward scattering ($z\approx1+(\alpha_1+\alpha_2)^2/2k^2$). The peak also becomes sharper at ν increases. Of course the expression (1) which we have used here does not hold for small L, and in particular may not satisfy the unitarity condition, but the contribution from this region gives a smooth angular dependence and can be replaced by a constant for small θ.

If we use the expression (1) for the partial amplitudes, a closed expression for $F(\theta)$ cannot be obtained for noninteger ν. It perhaps can be found if instead of Eq. (1) we take a different functional dependence whose main term agrees asymptotically with Eq. (1). Such a procedure is permissible in asymptotic theory. For example, for $\nu=\frac{1}{2}$ we can take

$$F_L=\frac{4(\alpha_1\alpha_2)^{1/2}(\alpha_1+\alpha_2)}{(qk_1k_2)^2}Q_L'(z). \tag{20}$$

With the use of this equation it can be easily verified that the asymptotic form (20) is identical with (13). On the other hand, with the partial amplitudes (20) the series (17) can be summed exactly:

$$F(\theta)=-\frac{4(\alpha_1\alpha_2)^{1/2}(\alpha_1+\alpha_2)}{(qk_1k_2)^2}\frac{1}{(z-\cos\theta)^2}. \tag{21}$$

This expression also has a peak for forward scattering. Examining Eqs. (18), (19), and (21), we can find the nature of the dependence of the amplitude on the scattering angle for small θ:

$$F(\theta)\sim(z-\cos\theta)^{-\nu-3/2}. \tag{22}$$

4. These small-angle maxima of the differential cross section for exchange scattering, with sharpness increasing with the energy, may give the explanation for similar maxima observed in experiments on exchange excitation[8,9]

$$e+\mathrm{He}(1\,{}^1S)\rightarrow e+\mathrm{He}(2\,{}^3S). \tag{23}$$

For a detailed comparison with experiment there is a need for more accuracy both in the experimental data, which at present provide only a point or two in the region of the maximum of the differential cross section, and in the theory—the calculation of an accurate coefficient of the exponential, which is a rather complicated problem. Nevertheless the results of the present paper reveal a qualitative agreement with the available experimental data, enable us to identify the characteristic parameter describing the process, and are a natural extension of the results found previously in the case of charge transfer, in which the two particles between which the exchange took place could be treated classically.

1)The interaction $1/r_1$ with the nucleus does not contribute to the partial amplitude F_L for $L \neq 0$ because of the orthogonality of the angular functions.

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Anisotropy of the polarization of hot photoluminescence in gallium arsenide crystals

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The theoretically predicted strong angular dependence of the degree of linear polarization ρ_L of hot photoluminescence in GaAs crystals, due to undulation of the equal-energy surfaces in the valence band, has been observed experimentally. The measurements were performed for samples cut parallel to the planes (100), (110), and (111) at an energy in the luminescence-spectrum 1.93 eV, which is close to the excitation energy (1.96 eV) when the relaxation effects can be neglected. The obtained dependences of ρ_L on the angles between the polarization vector of the exciting radiation and the crystallographic directions are in good agreement with the results of the theoretical calculation. The temperature dependence of ρ_L at different excitation polarizations is discussed.

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The spectrum of the hot photoluminescence of cubic p-GaAs crystals excited by linearly polarized light has revealed a noticeable linear polarization of the recombination radiation.[1] At frequencies close to the frequency $\hbar\omega_{ex}=1.96$ eV of the exciting line, the degree of linear polarization ρ_L^0 obtained in[1] was 0.14–0.18 and decreased to zero with energy relaxation of the photoexcited electrons. At the same time, anomalously large values of the degree of circular polarization were observed when the excitation was with circularly polarized light. The polarization dependences in the spectrum of hot luminescence in GaAs are described in greater detail in[2]. Dymnikov, D'yakonov, and Perel'[3] have shown that these singularities of hot photoluminescence are due to the fact that the momentum distribution of the photoexcited electrons is anisotropic in the case of interband absorption of light in semiconductors having the band structure of GaAs. Thus, in