Ionization of K shells of atoms and ions in collisions with electrons

V. G. Gorshkov, F. F. Karpeshin, and A. I. Mikhaĭlov

Leningrad Institute of Nuclear Physics, USSR Academy of Sciences
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The differential cross section has been obtained for ionization of the K shell of an atom by electron impact for incident-electron energies E much greater than the binding energy and for arbitrary momentum transfers q to the nucleus. In the region of large q the features of the cross section with respect to the momentum transferred to the entire atom have been investigated.

1. INTRODUCTION

Calculation of the ionization of atoms by fast electrons is usually carried out in the Born approximation[1,2] with plane waves as wave functions of all electrons of the continuum (the graph of Fig. 1a). Here the cross section is expressed in the form of a product of the cross section for scattering of the incident particle by a free stationary electron and the square of the Fourier transform of the wave function of the bound electron as a function of the momentum transfer q to the nucleus (the impulse approximation). This factorization gives the possibility of direct measurement of the bound-electron wave function.[3] The bound-electron wave function is maximal for $q \sim \eta$, where η is the average momentum of the bound electron, and therefore the region $q \sim \eta$ gives the main contribution to the total cross section of the process. However, the Born (impulse) approximation is valid only for small momentum transfers to the nucleus, much less than the incident-particle momenta, $q \ll p$, and therefore the bound-electron wave function for $q \sim p$ cannot be measured by this means.

For large momentum transfers to the nucleus $q \gg \eta$ the process becomes essentially three-particle. This region gives a small contribution to the total cross section –of the order $(\alpha Z)^4$ relative to the contribution of small $q \sim \eta$–and has a number of characteristic features.[4] In the lowest approximation in αZ the amplitude for the process is described by the four Feynman diagrams of Fig. 1a–d (minus the corresponding exchange diagrams in the case of electron scattering). For $q \gg \eta$ all diagrams of Fig. 1 turn out to be of the same order of magnitude in the parameter αZ, although at first glance the diagrams of Fig. 1b–d contain the exchange of an addition photon and should maintain a smallness $\sim \alpha Z$ in relation to the diagram of Fig. 1a. This occurs for the reason that in the diagram of Fig. 1a the large momentum is transferred to the nucleus only through the initial-electron wave function, and the latter is small[4] for large q. Furthermore, there is a kinematic region at large q where the diagrams of Fig. 1b–d give a larger contribution than the diagram of Fig. 1a. This region is due to the minimal virtualness of the intermediate electrons. When their propagators become of the order of η, in integration over the intermediate momenta these features do not disappear, and the amplitude acquires a factor $1/\eta$. These features are associated with the higher Coulomb corrections to the wave functions of the continuum and are not contained in the diagrams of Fig. 1a. Their physical meaning has been discussed in detail in ref. 4. On integration over q the main contribution is provided by the diagram of Fig. 1a from the region of small $q \sim \eta$ and the features indicated of diagrams 1b–d disappear. In measurement of cross sections in the region of large q, in addition to smallness of the cross section (of order $(\alpha Z)^4$ in comparison with the cross section for a free electron), difficulties arise in determination of the momentum q. Observation of this region, including the features associated with the intermediate electrons, is possible with measurement of both the energy and the momenta of the two final electrons. Instead of measuring the energy of the two electrons it is possible to measure the energy of one of them and the K x-ray line produced on filling the vacancy in the K shell. Knowledge of the binding energy of the initial electron is necessary, for all of the calculations made here are valid only for deep-lying electrons for which the screening by the atomic shell can be neglected. The experimental possibilities of measuring this process have been discussed in refs. 5 and 6.

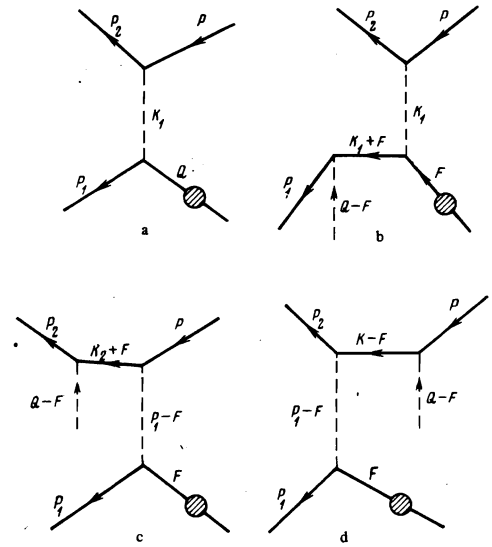

FIG. 1

2. AMPLITUDE AND CROSS SECTION FOR THE PROCESS

The amplitude for the process for any momentum transfer q to the nucleus and for large electron momenta $p_i \gg \eta$ in the lowest order of perturbation theory in αZ is determined by the difference in the sum of the four Feynman diagrams (Fig. 1) and the four exchange diagrams obtained from Fig. 1 by permutation of the final-electron lines. The shaded circle shows the wave

function of the K electron in the Coulomb field of the nucleus. With accuracy to terms of order $\sim\alpha Z$ the wave function of the K electron in the momentum representation has the form

$$\langle \mathbf{f}|\psi_0\rangle = \left(1+\frac{\tilde{f}}{2m}\right) u_0 \langle \mathbf{f}|\varphi_0\rangle, \tag{1}$$

where $\tilde{\mathbf{f}} = \boldsymbol{\alpha}\cdot\mathbf{f}$, $\boldsymbol{\alpha}$ is the Dirac matrix, u_0 is the bispinor of a stationary electron, $\langle \mathbf{f}|\varphi_0\rangle$ is the nonrelativistic Coulomb wavefunction of the K electron,

$$\langle \mathbf{f}|\varphi_0\rangle = N\left(-\frac{\partial}{\partial\eta}\right)\langle \mathbf{f}|V_{i\eta}|0\rangle = \frac{8\pi\eta N}{(f^2+\eta^2)^2},$$
$$N^2=\eta^3/\pi, \quad \eta = m\alpha Z, \quad \alpha = 1/137, \tag{2}$$
$$\int \frac{d^3f}{(2\pi)^3}\langle\varphi_0|\mathbf{f}\rangle\langle\mathbf{f}|\varphi_0\rangle = 1, \quad \langle \mathbf{a}|V_v|\mathbf{b}\rangle \equiv \frac{1}{(\mathbf{a}-\mathbf{b})^2-\nu^2}$$

(here we used the system of units $\hbar = c = 1$).

We will introduce the following designations: $P = (\epsilon, \mathbf{p})$ is the four-momentum of the incident electron; $p_2 = (\epsilon_2, \mathbf{p}_2)$, $P_1 = (\epsilon_1, \mathbf{p}_1)$ are the momenta of the final electrons; $Q = (m, \mathbf{q})$, $-\mathbf{q}$ is the momentum transfer to the nucleus. Then the conservation of energy and momentum can be written in the form

$$P+Q=P_2+P_1. \tag{3}$$

We introduce also the 4-vectors

$$K_1=P_1-Q=P-P_2=(\varepsilon_1-m, \varkappa_1),$$
$$K_2=P_2-Q=P-P_1=(\varepsilon_2-m_1, \varkappa_2), \tag{4}$$
$$K=P+Q=P_1+P_2=(\varepsilon+m, \varkappa).$$

The contribution A_a of the diagram of Fig. 1a to the amplitude of the process is

$$A_a = \frac{4\pi\alpha}{(P-P_2)^2}(\bar{u}_{p_2}\gamma^\mu u_p)\,\bar{u}_{p_1}\gamma_\mu\langle \mathbf{q}|\psi_0\rangle,$$
$$\gamma=(\gamma^0, \boldsymbol{\gamma}), \quad \boldsymbol{\gamma}=\gamma^0\boldsymbol{\alpha}$$

($\gamma^0 = \beta$; β, $\boldsymbol{\alpha}$ are the Dirac matrices). Using Eqs. (1) and (2), we obtain

$$A_a = r_0\frac{(4\pi)^2 N\eta}{a^2 a_1}(\bar{u}_{p_2}\gamma^\mu u_p)\,[\bar{u}_{p_1}\gamma_\mu(2m+\tilde{q})u_0],$$
$$a=q^2+\eta^2, \quad a_1=(P-P_2)^2=K_1^2=(\varepsilon_1-m)^2-\varkappa_1^2, \tag{5}$$

$\tilde{q} = \boldsymbol{\alpha}\cdot\mathbf{q}$, $r_0 = \alpha/m$, u_{p_i} is the bispinor of an electron with momentum p_i, normalized by the condition $\bar{u}_{p_i} u_{p_i} = 2m$.

In the diagram of Fig. 1a the momentum q is transferred to the nucleus through the wave function of the bound electron, and in the diagrams of Figs. 1b–d it is transferred through the Coulomb photon, which leads to an additional integration over the intermediate momentum f. The contribution A_b of the diagram of Fig. 1b can be calculated in the following way:

$$A_b = \frac{4\pi\alpha}{(P-P_2)^2}(\bar{u}_{p_2}\gamma^\mu u_p)\int\frac{d^3f}{(2\pi)^3}\bar{u}_{p_1}\gamma^0\frac{(-4\pi\alpha Z)}{(\mathbf{q}-\mathbf{f})^2}\frac{\hat{K}_1+\hat{F}+m}{(K_1+F)^2-m^2}\gamma_\mu\langle \mathbf{f}|\psi_0\rangle;$$
$$\hat{F}=\gamma^0 m-\boldsymbol{\gamma}\mathbf{f}.$$

Integration over the intermediate momentum f can be carried out easily if we take into account that the main contribution to the integral is from the region of small $f \sim \eta$, since with increasing f the wave function $\langle \mathbf{f}|\psi_0\rangle$ falls off rapidly. Therefore the second term in Eq. (1) gives a contribution $\sim\alpha Z$ relative to the first term and in our approximation can be discarded. Consequently, as the bound-electron wave function $\langle \mathbf{f}|\psi_0\rangle$ we can take the nonrelativistic wave function $\langle \mathbf{f}\ \varphi_0\rangle$. With the same degree of accuracy in the numerator of the electron propagator we can set f = 0. The denominator of the propagator may be small and therefore we must retain the vector f there. For $q \gg \eta$ the integration over f is easily carried out:[4]

$$A_b = \frac{4\pi\alpha}{(P-P_2)^2}(\bar{u}_{p_2}\gamma^\mu u_p)\frac{\alpha Z}{q^2}[\bar{u}_{p_1}\gamma^0(\hat{K}_1+m\gamma^0+m)\gamma_\mu u_0]\langle -\varkappa_1|V_{p_1}|\varphi_0\rangle,$$
$$\langle -\varkappa_1|V_{p_1}|\varphi_0\rangle = N\langle -\varkappa_1|V_{p_1+i\eta}|0\rangle = \frac{4\pi N}{\varkappa_1^2-(p_1+i\eta)^2}$$

For $q \sim \eta$ the integration over f is more complicated but the result differs from the above only in replacement of the second denominator q^2 by $q^2 + \eta^2$.

Using the equality

$$\bar{u}_{p_1}\gamma^0(\hat{K}_1+m\gamma^0+m)=\bar{u}_{p_1}(2\varepsilon_1+\tilde{q}),$$

we obtain for the contribution A_b of the diagram of Fig. 1b

$$A_b = r_0\frac{(4\pi)^2 N\eta}{a a_1 b_1}(\bar{u}_{p_2}\gamma^\mu u_p)\,[\bar{u}_{p_1}(2\varepsilon_1+\tilde{q})\gamma_\mu u_0], \tag{6}$$
$$b_1=\varkappa_1^2-(p_1+i\eta)^2. \tag{6a}$$

The denominator b_1 of Eq. (6) (see Eq. (6a)) arises from the electron propagator and has the form of a Breit-Wigner pole at the point $\kappa_1 = p_1 + i\eta$, which approaches the physical point $\kappa_1 = p_1$ as $\eta \to 0$. In what follows we will call this singularity the Coulomb resonance. The appearance of this pole is due to the structure of the wave function (2), which contains a multiple pole at $f^2 = -\eta^2$, which is the consequence of the long-range nature of the Coulomb interaction. In the short-range case Eq. (2) would contain a unary pole, and Eq. (6) a logarithmic singularity.[4] The appearance of a pole singularity is due to the fact that the diagram of Fig. 1b near the singularity ($\kappa_1 = p_1 + i\eta$) can be represented with accuracy to a normalization factor N in the form of the four-angle Feynman diagram of Fig. 2, where the lower line represents the nucleus, A is the amplitude for scattering of the two free electrons, and B is the amplitude for scattering of the electron by the nucleus; the initial nucleus is at rest. The initial bound electron is taken with an energy $\epsilon_0 = m - \eta^2/2m$ and zero momentum, and the wavy photon line is taken with mass η. The occurrence of a pole singularity in the four-angle diagram is well known.[7] For a large nuclear mass it is possible to close the integral over f_0 to the pole of the nuclear propagator, after which the photon propagator and the electron propagator adjacent to it turn out to be $f^2 + \eta^2$, which also leads to a multiple pole in Eq. (2), and after performing the integration over d^3f to a pole behavior in Eq. (6).

In the diagrams of Figs. 1c and d, the intermediate momentum f enters also in the photon propagator. However, we are discussing the case in which the momenta of all free electrons are significantly greater than η, and therefore in the denominator of the photon propagator we can set f = 0 since this denominator is not small:

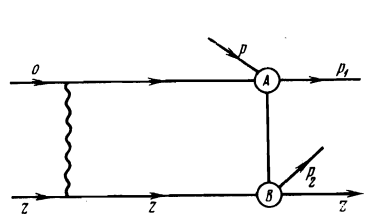

FIG. 2

$$\frac{1}{(P-F)^2}=\frac{1}{(\varepsilon_1-m)^2-(\mathbf{p}_1-\mathbf{f})^2}\approx-\frac{1}{2m(\varepsilon_1-m)}.$$

Here calculation of the contributions A_c and A_d of the diagrams of Figs. 1c and d is similar to that of the contribution A_b:

$$A_c=r_0\frac{(4\pi)^2N\eta}{ab_2c_1}[\bar u_{p_2}(2\varepsilon_2+\tilde q)\gamma^\mu u_p](\bar u_{p_1}\gamma_\mu u_0), \tag{7}$$

$$A_d=r_0\frac{(4\pi)^2N\eta}{abc_1}[\bar u_{p_2}\gamma^\mu(2\varepsilon+\tilde q)u_p](\bar u_{p_1}\gamma_\mu u_0), \tag{8}$$

$$b_2=\varkappa_2^2-(p_2+i\eta)^2,\ b=\varkappa^2-(p+i\eta)^2,\ c_1=-2m(\varepsilon_1-m).$$

The sum of the contributions (5)–(8) with inclusion of the exchange diagrams gives the following expression for the amplitude of the process:

$$A=r_0\frac{(4\pi)^2}{a}N\eta S, \tag{9}$$

$$S=(\bar u_{p_2}\gamma^\mu u_p)\bar u_{p_1}[L_1\gamma_\mu(2m+\tilde q)+L_2(2\varepsilon_1+\tilde q)\gamma_\mu]u_0$$
$$+\bar u_{p_2}[L_3(2\varepsilon_2+\tilde q)\gamma^\mu+L_4\gamma^\mu(2\varepsilon+\tilde q)]u_p(\bar u_{p_1}\gamma_\mu u_0)-(P_1\rightleftarrows P_2): \tag{10}$$

$$L_1=\frac{1}{aa_1},\quad L_2=\frac{1}{a_1b_1},\quad L_3=\frac{1}{b_2c_1},\quad L_4=\frac{1}{bc_1},$$
$$a=q^2+\eta^2,\quad a_1=(\varepsilon_1-m)^2-\varkappa_1^2,\quad c_1=-2m(\varepsilon_1-m), \tag{11}$$
$$b=\varkappa^2-(p+i\eta)^2,\quad b_1=\varkappa_1^2-(p_1+i\eta)^2,\quad b_2=\varkappa_2^2-(p_2+i\eta)^2.$$

The term $(P_1\rightleftarrows P_2)$ in Eq. (10) signifies the contribution from the exchange diagrams, which is obtained from the expression written out by the substitution $P_1\rightleftarrows P_2$.

The denominators of Eq. (10) which contain a correspond to the Coulomb photons, a_1 and c_1 to the propagators of the photons which exchange with the electrons. The denominators b, b_1, and b_2 correspond to electron propagators and for $q\gg\eta$ contain Coulomb resonances respectively in the regions $|\kappa-p|\sim\eta$ and $|\kappa_1-p_1|\sim\eta$. For small q ($p\gg q\gtrsim\eta$), as follows from Eq. (4), b and b_1 are always small: $b\sim b_1\sim qp$. However, in the region $p\gg q\gtrsim\eta$ the principal term in Eq. (10) is the first term, which contains a $\sim q^2$ in the denominator; the remaining terms containing b and b_1 in the denominators are correction terms relative to the first quantity of order q/p. Thus, it is directly evident from Eq. (10) that for large q ~ p all terms of the amplitude corresponding to the diagrams of Figs. 1a–d are of the same order. However, in the region of the Coulomb resonances ($|\kappa-p|\sim\eta$, $|\kappa_1-p_1|\sim\eta$) the main terms are the second, third, or fourth terms, which contain a resonance.

The differential cross section for the process, averaged over the initial polarizations and summed over the final polarizations of the electrons, has the form

$$d\sigma=\frac{1}{2m}\frac{1}{2\varepsilon}\frac{1}{i}\frac{1}{4}\sum_{\text{pol}}|A|^2\frac{d^3p_2}{2\varepsilon_2(2\pi)^3}\frac{d^3p_1}{2\varepsilon_1(2\pi)^3}\cdot2\pi\delta(\varepsilon_1+\varepsilon_2-\varepsilon-m), \tag{12}$$

$j=p/\epsilon$ is the incident-particle flux density. Substituting (9) into (12), we obtain

$$d\sigma=\frac{r_0^2}{2\pi^2}\frac{\eta^5}{a^2}\frac{1}{mp}J\,d\Gamma, \tag{13}$$

$$J=\frac{1}{4}\sum_{\text{pol}}|S|^2,\quad d\Gamma=\frac{1}{\varepsilon_1\varepsilon_2}d^3p_1\,d^3p_2\,\delta(\varepsilon_1+\varepsilon_2-\varepsilon-m). \tag{14}$$

The general expression for the cross section is very cumbersome and we will not give it here. The awkwardness of the general formula is due to the necessity of calculating a large number of turns of the Dirac matrix in squaring the amplitude (10) and averaging over the polarizations. Existing programs for calculation of traces can be used for calculation of the cross section (12) by computer. Below we present a number of simple formulas for the differential cross sections and some integrated distributions in limited regions of variation of the kinematic variables.

3. KINEMATICS

The phase space (14) contains differentials in five independent variables. One of the azimuthal angles after averaging over polarizations corresponds to rotation of a fixed system of vectors and can be replaced by 2π. For investigation of the region of the Coulomb resonances and large momentum transfers to the nucleus, it is convenient to use as the remaining variables q, κ, p_i or q, κ_i, p_1. We will use the following sets of variables below:

$$1)\ q,\varkappa_i,p_i,\varphi_i,\quad d\Gamma=2\pi\frac{p_iq}{\varepsilon_ip}dp_i\,d\varkappa_i\,dq\,d\varphi_i,\quad i=1,2, \tag{15}$$

where φ_i is the angle between the planes formed by the vectors $\mathbf{p}_i$, $\mathbf{q}$ and $\mathbf{p}$, $\mathbf{p}_j$, which intersect along the vector $\boldsymbol{\kappa}_i$ (Fig. 3a).

$$2)\ q,\varkappa,p_i,\varphi,\quad d\Gamma=2\pi\frac{p_iq}{\varepsilon_ip}dp_i\,d\varkappa\,dq\,d\varphi,\quad i=1,2, \tag{15a}$$

where φ is the angle between the planes formed by the vectors p, q and $\mathbf{p}_2$, $\mathbf{p}_1$, which intersect along the vector $\boldsymbol{\kappa}$ (Fig. 3b).

The angles φ_i and φ in Eqs. (15) and (15a) vary from 0 to 2π. The Jacobians of (15) and (15a) are easily obtained by measuring the polar angle of the vector $\boldsymbol{\kappa}_i(\boldsymbol{\kappa})$, which lies in the intersection of the planes, from the fixed vector $\mathbf{p}$, all the remaining polar angles from the vector $\boldsymbol{\kappa}_i(\boldsymbol{\kappa})$, and the azimuthal angles from the plane formed by the vectors $\boldsymbol{\kappa}_i$, $\mathbf{p}(\boldsymbol{\kappa},\mathbf{p})$.

In the diagram of Fig. 4 we have shown the physical region (Dalitz plot) in the variables κ_1 and p_1 for fixed q and $0\le\varphi_1\le2\pi$. The physical region is limited by the conditions:

$$|p_1-q|\le\varkappa_1\le p_1+q,\quad p-p_2\le\varkappa_1\le p+p_2,$$

or by the three straight lines

$$\varkappa_1=p_1+q,\quad \varkappa_1=p_1-q,\quad \varkappa_1=q-p_1 \tag{16}$$

and the two curves

$$\varkappa_1=p-\sqrt{(\varepsilon-\varepsilon_1)(2m+\varepsilon-\varepsilon_1)},\quad \varkappa_1=p+\sqrt{(\varepsilon-\varepsilon_1)(2m+\varepsilon-\varepsilon_1)}. \tag{16a}$$

The curves (16a) in the nonrelativistic limit p, $p_i\ll m$ degenerate into the half circle with center at

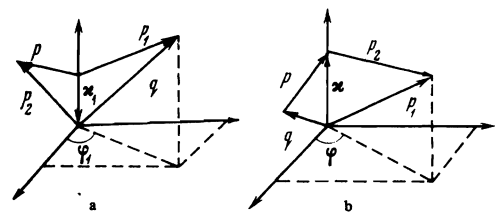

FIG. 3

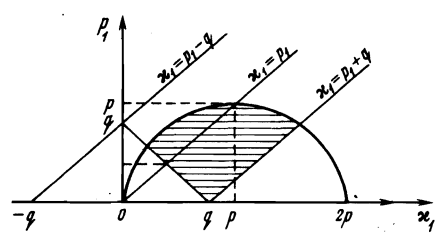

FIG. 4

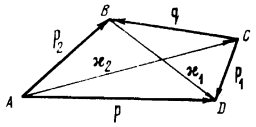

FIG. 5

the point $\kappa_1 = p$ and $p_1 = 0$, and in the extreme relativistic case $p, p_1 \gg m$ into two straight lines: $\kappa_1 = p_1$ and $\kappa_1 = 2p - p_1$.

For small $q \to 0$ the physical region degenerates into the straight line $\kappa_1 = p_1$. The vicinity of this straight line $|\kappa_1 - p_1| \sim \eta$ for large q is the region of the Coulomb resonance of the diagram of Fig. 1b. It can be seen from Fig. 4 that for $p_1 < q/2$ the value of κ_1 cannot equal p_1 and their is no resonance. This is physically obvious, for an electron with momentum p_1 can transfer to the nucleus a maximum momentum $q = 2p_1$. Resonance is impossible also for any p_1 if $2p < q < q_{max} = 2p[1 + 2m/(\epsilon + m)]^{1/2}$.

The curves $\kappa_2 = p_2$ and $\kappa = p$, which correspond to Coulomb resonances in the diagrams of Figs. 1c and d, depend, generally speaking, on the value of the angles φ_2 and φ and have a complicated form. Therefore these curves are conveniently shown on the corresponding diagrams of the physical region in the variables κ_2, p_2 and κ, p. However, the points of intersection of these curves with the straight line $\kappa_1 = p_1$, where resonances arise immediately in the two diagrams, present interest. The regions of overlap of the resonances can be shown more readily in the variables κ_1, κ_2 for fixed p_1 and q. To find the boundary of the physical region on the plane κ_1, κ_2 we will use the vector diagram of Fig. 5. The vector $\mathbf{p}_2$ we will assume lies in the plane of the paper. The triangle formed by the vectors p_1 and q can rotate freely around the vector $\boldsymbol{\kappa}_1$. For fixed κ_1 the minimum and maximum values of κ_2 are obviously obtained when ΔBCD lies in the plane of the paper and respectively $\Delta ADC = \angle ADB \pm \angle BDC$. We therefore have from ΔACD:

$$\kappa_{2\,\substack{min\\max}}^2 = p^2 + p_1^2 - 2pp_1\cos(\angle ADB \mp \angle BDC).$$

The trigometric functions of the angles $\angle ADB$ and $\angle BDC$ are easy to find if we consider the triangles $\angle ADB$ and ΔBDC in which all sides are known. As a result we obtain the desired boundary of the physical region:

$$\kappa_{2\,\substack{min\\max}}^2 = p^2 + p_1^2 - \frac{1}{2\kappa_1^2}\{(p^2+\kappa_1^2-p_2^2)(p_1^2+\kappa_1^2-q^2)$$
$$\pm([4p^2\kappa_1^2-(p^2+\kappa_1^2-p_2^2)^2][4p_1^2\kappa_1^2-(p_1^2+\kappa_1^2-q^2)^2])^{1/2}\}.$$

The resonance regions $|\kappa_2 - p_2| \lesssim \eta$, $|\kappa_1 - p_1| \lesssim \eta$ in the planes κ_1, κ_2 are bands of width $\sim\eta$ parallel to the coordinate axes (see Fig. 6, where we have shown the case $p_1 = q = 40$ keV/c; the physical region is cross-hatched). The region $|\kappa - p| \sim \eta$ has the form of a ring of width $\sim\eta$ and radius $\sqrt{p_1^2 + p_2^2 + q^2}$. The latter is easy to see by setting $|\kappa - p| \sim \eta$ in the relation $q^2 + p^2 + p_1^2 + p_2^2 = \kappa^2 + \kappa_1^2 + \kappa_2^2$, which is easy to check by direct calculation. The location of the straight lines $\kappa_1 = p_1$ and $\kappa_2 = p_2$ does not depend on q; the radius of the ring $\kappa = p$ depends on q in the manner indicated above.

For $q < 2p_0$, where $p_0 = \min\{p_1, p_2\}$, all three points of overlap of resonances will be in the physical region independently of the values of p and p_1.

In the regions of overlap of the resonances it is necessary to take into account not two diagrams as in the case of a solitary resonance but four diagrams of Fig. 1 (including the exchange diagrams). Here there are alternatively two possible reaction mechanisms leading to a large cross section. Their interference produces a rise in the cross section in comparison with an isolated resonance by approximately a factor of four. The interference does not permit the formula for the cross section to be expressed in simple form. In Fig. 7 we have shown the shape of the cross section $d\sigma/do_1 d^3p_2$ for the case $p_1 = p_2 = q = 40$ keV/c, where the straight line $\kappa_1 = p_1$ intersects the resonances $\kappa_2 \sim p_2$ and $\kappa \sim p$, distinct maxima are evident.

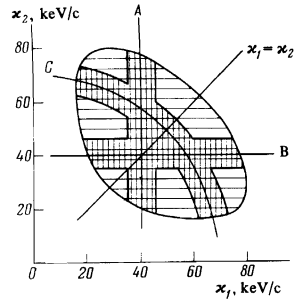

FIG. 6. Physical region of the process in a hydrogen atom (light hatching). A—the straight line $\kappa_1 = p_1$; B—the straight line $\kappa_2 = p_2$; C—the circle $\kappa = p_0$. The resonance region has been heavily hatched. $q = p_1 = p_2 = 40$ keV/c.

Here we have also shown for comparison a plot of the cross section $d\sigma/do_1 d^3p_2$ as a function of κ_2 for fixed $\kappa_1 = 25$ keV/c (the nonresonance straight line). This straight line intersects the resonances at $\kappa_2 \approx 40$ and 64 keV/c; here the cross section is smaller than for the case $\kappa_1 = 40$ keV/c, since here there is no overlap of resonances. However, in comparison with the nonresonance background the cross section in isolated resonances rises roughly by a factor $(p/\eta)^2 \approx 100$.

For overlap of all three resonances, as can be seen from Fig. 6, it is necessary to satisfy the condition

$$\sqrt{p_1^2+p_2^2+q^2} - \sqrt{p_1^2+p_2^2} \lesssim 3\eta. \qquad (17)$$

At the same time with decrease of q the diagram of Fig. 1a increases rapidly, so that it is ncesssary to maintain $q \gg \eta$. Setting $q \approx p_1 \approx p_2 \gg \eta$ in Eq. (17), we obtain the condition for observation of overlap of all three resonances:

$$0.3p_1 \lesssim 3\eta, \quad \text{i.e.,} \quad \eta \ll q \sim p_1 \lesssim 10\eta. \qquad (17a)$$

In Fig. 6 we have shown the physical region for the case of the hydrogen atom where all three resonances overlap in the region $\kappa_1 \sim \kappa_2 \sim 45$ keV/c, and the contribution of the diagram of Fig. 1a is small.

In Fig. 8, we have shown the form of the cross section along the straight line $\kappa_1 = \kappa_2$ shown in Fig. 6. In this case there is no ninefold rise of the cross section, since the overlap is weak in view of the condition (17a).

The calculations for Figs. 7 and 8 were carried out with Eq. (33), which takes into account all four diagrams of Fig. 1.

4. FORMULAS FOR THE CROSS SECTIONS IN PARTICULAR CASES

1. We will consider the region of small momentum transfers to the nucleus, $q \ll p$. In this region, as already pointed out, the first term in Eq. (10) is dominant. The remaining terms of Eq. (10) are corrections of order q/p relative to the first term, and therefore with an accuracy to terms linear in q we can discard quan-

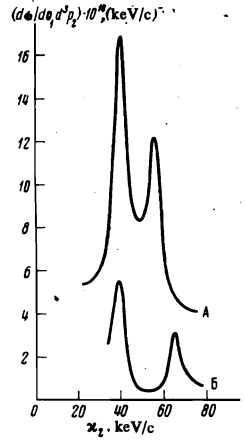

FIG. 7

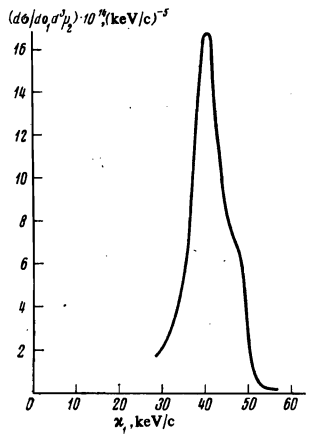

FIG. 8

FIG. 7. A—the cross section $d\sigma/do_1 d^3p_2$ along the straight line $\kappa_1 = 40$ keV/c. B—the same for $\kappa_1 = 25$ keV/c. $q = p_1 = p_2 = 40$ keV/c.

FIG. 8. The cross section $d\sigma/do_1 d^3p_2$ along the straight line $\kappa_1 = \kappa_2$; $q = p_1 = p_2 = 40$ keV/c.

tities of order q/p in the numerators of these terms. Taking into account further the equality

$$(1+\tilde{q}/2m)u_0 = u_q + O(q^2/m^2),$$

the amplitude (10) can be represented in the form

$$S = 2(mL_1 + \varepsilon_1 L_2 + \varepsilon_2 L_3 + \varepsilon L_4)(\bar{u}_{p_2}\gamma^\mu u_p)(\bar{u}_{p_1}\gamma_\mu u_q)$$
$$-(P_1 \rightleftarrows P_2) = \frac{2m}{a}\left[1 + \frac{a}{m}\left(\frac{\varepsilon_1}{b_1} + \frac{\varepsilon_2}{b_2} + \frac{\varepsilon}{b}\right)\right] S_{ee}(q), \qquad (18)$$
$$|S|^2 = \frac{4m^2}{a^2}\left[1 + \frac{2a}{m}\mathrm{Re}\left(\frac{\varepsilon_1}{b_1} + \frac{\varepsilon_2}{b_2} + \frac{\varepsilon}{b}\right)\right] |S_{ee}(q)|^2,$$

where

$$S_{ee}(q) = \frac{1}{(P-P_2)^2}(\bar{u}_{p_2}\gamma^\mu u_p)(\bar{u}_{p_1}\gamma_\mu u_q) - (P_1 \rightleftarrows P_2), \qquad (19)$$

$S_{ee}(q)$ is the amplitude for scattering by a free electron with initial 4-momentum $Q = (m, \mathbf{q})$.

Substituting (18) into (13) and taking into account that (19) depends on the invariant variables

$$QP_1 = m\varepsilon_1 - \mathbf{qp}_1, \quad QP_2 = m\varepsilon_2 - \mathbf{qp}_2,$$

we obtain with accuracy two terms linear in q the following expression for the cross section:

$$d\sigma = |\langle \mathbf{q}|\varphi_0\rangle|^2 r_0^2 \frac{m}{p} f_0 \left\{1 + \frac{2a}{m}\mathrm{Re}\left(\frac{\varepsilon_1}{b_1} + \frac{\varepsilon_2}{b_2} + \frac{\varepsilon}{b}\right) + \frac{f_1}{f_0}\frac{\mathbf{qp}_1}{m\varepsilon_1} + \frac{f_2}{f_0}\frac{\mathbf{qp}_2}{m\varepsilon_2}\right\}\frac{d\Gamma}{(2\pi)^3}, \qquad (20)$$

$$f_0 = f_0(\varepsilon_1, \varepsilon_2) = 1 - \frac{2\varepsilon^2 + 2m\varepsilon - m^2}{(\varepsilon_1 - m)(\varepsilon_2 - m)} + \frac{\varepsilon^2(\varepsilon - m)^2}{(\varepsilon_1 - m)^2(\varepsilon_2 - m)^2}, \qquad (21)$$

$$r_0^2 f_0 = \frac{d\sigma_0}{do_1}\frac{p}{p_1}\frac{\varepsilon + m}{\varepsilon_1 + m} = \frac{d\sigma_0}{d\varepsilon_1}\frac{p^2}{2\pi m}, \qquad (21a)$$

where $d\sigma_0/do_1 (d\sigma_0/d\epsilon_1)$ is the distribution in the laboratory system of reference of the secondary electrons arising in scattering of the primary electrons by free electrons at rest,

$$f_1 = r_0^2 \frac{m\varepsilon_1}{p(\varepsilon_1 - m)}\left\{1 + \frac{2\varepsilon^2}{(\varepsilon_1 - m)^2} + \frac{m^2 - 2m\varepsilon + (\varepsilon_1 - \varepsilon_2)(\varepsilon + m)}{(\varepsilon_1 - m)(\varepsilon_2 - m)} - \frac{\varepsilon - m}{\varepsilon_1 - m} - \frac{(\varepsilon + \varepsilon_1)(\varepsilon_1 - m)}{(\varepsilon_2 - m)^2}\right\}, \quad f_2 = f_1(1 \rightleftarrows 2), \qquad (22)$$

$$2\mathrm{Re}\left(\frac{\varepsilon_1}{b_1} + \frac{\varepsilon_2}{b_2} + \frac{\varepsilon}{b}\right) = \frac{\varepsilon}{p}\frac{\mathbf{nq}}{(\mathbf{nq})^2 + \eta^2} - \frac{\varepsilon_1}{p_1}\frac{\mathbf{n}_1\mathbf{q}}{(\mathbf{n}_1\mathbf{q})^2 + \eta^2} - \frac{\varepsilon_2}{p_2}\frac{\mathbf{n}_2\mathbf{q}}{(\mathbf{n}_2\mathbf{q})^2 + \eta^2},$$
$$\mathbf{n} = \mathbf{p}/p, \quad \mathbf{n}_i = \mathbf{p}_i/p_i.$$

Integrating over φ_1 and q, we obtain the distribution in p_1 and κ_1:

$$\frac{d\sigma}{dp_1 d\varkappa_1} = \frac{16}{3} r_0^2 \eta^5 \frac{mp_1}{p^2\varepsilon_1} f_0 \frac{1 + \gamma x/m}{(x^2 + \eta^2)^3}, \quad x = \varkappa_1 - p_1,$$
$$\gamma = \frac{3}{2}\frac{\varepsilon_1}{p_1} - \frac{p_1}{\varepsilon_1}\frac{f_1}{f_0} - \frac{p_2}{\varepsilon_2}\frac{\varepsilon_2 - m}{\varepsilon_1 + m}\frac{f_2}{f_0} \qquad (23)$$

$$+ \frac{3}{\pi}\int_{|x|}^{\varkappa_1 + p_1} dq \frac{q}{x}\left(\frac{x^2 + \eta^2}{q^2 + \eta^2}\right)^3 \int_0^{2\pi} d\varphi \left(\frac{\varepsilon}{p}\frac{\mathbf{nq}}{(\mathbf{nq})^2 + \eta^2} - \frac{\varepsilon_2}{p_2}\frac{\mathbf{n}_2\mathbf{q}}{(\mathbf{n}_2\mathbf{q})^2 + \eta^2}\right) \qquad (23a)$$

The distribution of the scattered electrons in energy ϵ_2 and scattering angle $\cos\theta_2 = \mathbf{p}\cdot\mathbf{p}_2/pp_2$ can be obtained from the distribution in p_1 and κ_1:

$$\frac{d\sigma}{d\varepsilon_2 do_2} = \frac{pp_2\varepsilon_1}{2\pi\varkappa_1 p_1}\frac{d\sigma}{dp_1 d\varkappa_1}. \qquad (24)$$

The terms linear in x which arise from the terms linear in q in Eq. (20) lead to a shift in the quasielastic peak in the distribution in p_1 for fixed κ_1 (or in the distribution in ϵ_2 for fixed θ_2).

2. The region of Coulomb resonances is due to the existence in the amplitude (10) of the pole terms b_1^{-1} and b^{-1}, which are large for

$$\eta \ll q \sim p, \quad |\varkappa_i - p_i| \sim \eta, \quad |\varkappa - p| \sim \eta,$$

i.e., when the intermediate electron becomes almost real. The physical meaning of these singularities of the cross section has been discussed in detail in ref. 4.

Let us consider the amplitude (9) and (10) for the process in the region of resonance behavior of the diagram of Fig. 1b $|\kappa_1 - p_1| \sim \eta$. In this region only terms proportional to $b_1^{-1} = [\kappa_1^2 - (p_1 + i\eta)^2]^{-1}$ have a resonance behavior. Leaving in the amplitude only resonance terms and setting $\kappa_1 = p_1$ everywhere except in the resonance denominator, we obtain for S the expression

$$S = L_2(\bar{u}_{p_2}\gamma^\mu u_p)[\bar{u}_{p_1}(2\varepsilon_1 + \tilde{q})\gamma_\mu u_0] - M_3[\bar{u}_{p_1}(2\varepsilon_1 + \tilde{q})\gamma^\mu u_p](\bar{u}_{p_2}\gamma_\mu u_0),$$
$$M_i = L_i(1 \rightleftarrows 2), \quad L_2 = 1/a_1 b_1, \quad M_3 = 1/b_1 c_2. \qquad (25)$$

Using the relation

$$\bar{u}_{p_1}(2\varepsilon_1 + \tilde{q}) = \bar{u}_{p_1}\gamma^0(\hat{K}_1 + m) = \sum_\lambda \bar{u}_{p_1}\gamma^0 u_{\varkappa_1}^\lambda \bar{u}_{\varkappa_1}^\lambda,$$

where $K_1 = (\epsilon_1, \kappa_1)$, $u_{K_1}^\lambda$ is a bispinor with 4-momentum K_1 and polarization λ, and the summation is carried out over the polarization of the intermediate electron, the amplitude (9) of the process can be represented in the form of the product of the amplitude A_{ee}^λ for scattering by a free electron with polarization λ and the amplitude A_C^λ for scattering in a Coulomb field (the two amplitudes are related to the total polarization of the intermediate electron):

$$A = \frac{N}{b_1}\sum_\lambda A_C^\lambda A_{ee}^\lambda, \qquad (26)$$

$$A_C^\lambda = \frac{4\pi\alpha Z}{q^2}\bar{u}_{p_1}\gamma^0 u_{\varkappa_1}^\lambda, \quad q = p_1 - \varkappa_1, \qquad (26a)$$

$$A_{ee}^\lambda = 4\pi\alpha\left[\frac{1}{t}(\bar{u}_{p_2}\gamma^\mu u_p)(\bar{u}_{\varkappa_1}^\lambda\gamma_\mu u_0) - \frac{1}{u}(\bar{u}_{\varkappa_1}^\lambda\gamma^\mu u_p)(\bar{u}_{p_2}\gamma_\mu u_0)\right], \qquad (26b)$$
$$t = a_1 = (P - P_2)^2 = -2m(\varepsilon_1 - m),$$
$$u = c_2 = (P - K_1)^2 = -2m(\varepsilon_2 - m).$$

By means of the equality

$$\sum_{\lambda_1}(\bar{u}_{p_1}^{\lambda_1}\gamma^0 u_{\varkappa_1}^{\lambda_1})(\bar{u}_{\varkappa_1}^{\lambda'}\gamma^0 u_{p_1}^{\lambda_1}) = 2(\varepsilon_1^2 + m^2 + p_1\varkappa_1)\delta_{\lambda\lambda'} = 4\varepsilon_1^2\left(1 - \frac{q^2}{4\varepsilon_1^2}\right)\delta_{\lambda\lambda'}, \qquad (27)$$

where the summation is carried out over the polarization of an electron with momentum p_1, it is easy to

carry out the summation over all remaining polarizations for the square of the amplitude:

$$\frac{1}{4}\sum|A|^2=\frac{1}{4}\frac{N^2}{|b_1|^2}\sum|A_C|^2\sum|A_{ee}|^2, \tag{28}$$

$$\sum|A_C|^2=4\frac{(4\pi\alpha Z)^2}{q^4}\varepsilon_1^2\left(1-\frac{q^2}{4\varepsilon_1^2}\right), \tag{28a}$$

$$\frac{1}{4}\sum|A_{ee}|^2=4(4\pi\alpha)^2 f_0 \tag{28b}$$

(f_0 is determined by the equality (21)).

Using the expression for the phase space (15), substituting (28) and (15) into (12) and (13), and taking into account that the cross section does not depend on φ_1, we obtain the following obvious formula:[4]

$$d\sigma(\varkappa_1,p_1)=R(\varkappa_1,p_1)\frac{d\varkappa_1}{2\pi}d\sigma_C\,d\sigma_{ee}, \tag{29}$$

$$R(\varkappa_1,p_1)=\frac{N^2}{(\varkappa_1-p_1)^2+\eta^2},\quad N^2=\frac{\eta^3}{\pi}, \tag{29a}$$

$$d\sigma_C=\pi\left(2\alpha Z\frac{\varepsilon_1}{p_1}\right)^2\left(1-\frac{q^2}{4\varepsilon_1^2}\right)\frac{dq^2}{q^4}, \tag{29b}$$

$$d\sigma_{ee}=2\pi r_0^2 f_0\frac{m d\varepsilon_1}{p^2}. \tag{29c}$$

From Eqs. (29)–(29c) it is evident that the cross section in the region of a resonance is $\sim r_0^2(\alpha Z)^3$. The total contribution to the cross section from the resonance region is found by integration of (29) over κ_1:

$$\frac{d\sigma}{dq^2\,d\varepsilon_1}=\pi r_0^2\alpha^4 Z^4\left(\frac{2m\varepsilon_1}{pp_1}\right)^2\frac{m}{q^4}\left(1-\frac{q^2}{4\varepsilon_1^2}\right)f_0. \tag{30}$$

The contribution from the nonresonance part will be a quantity of the order $r_0^2(\alpha Z)^5$. Thus, for $p_1 \approx q/2$ and any $q \gg \eta$, and also for $q \approx 2p$ and any $p \gg \eta$ the cross section will drop[1)] by a factor αZ.

The expression for the cross section in the vicinity of the resonance behavior of the diagram of Fig. 1c $|\kappa_2 - p_2| \sim \eta$ differs from Eqs. (29) and (30) only by exchange of the subscripts $1 \rightleftarrows 2$. The diagram of Fig. 1d has a resonance behavior in the region $|\kappa - p| \sim \eta$, due to scattering of the incident electron by the Coulomb field of the nucleus with formation of an almost real electron and subsequent scattering of this electron by a free electron at rest. Repeating the same discussion as in derivation of Eq. (29), we obtain

$$d\sigma(\varkappa,p)=R(\varkappa,p)\frac{d\varkappa}{2\pi}d\sigma_{ee}\,d\sigma_C, \tag{31}$$

$$R(\varkappa,p)=N^2/[(\varkappa-p)^2+\eta^2], \tag{31a}$$

$$d\sigma_C=\pi\left(2\alpha Z\frac{\varepsilon}{p}\right)^2\left(1-\frac{q^2}{4\varepsilon^2}\right)\frac{dq^2}{q^4}, \tag{31b}$$

and $d\sigma_{ee}$ is defined in Eq. (29c).

As already mentioned, kinematic regions exist where the pole singularities (resonances) are observed simultaneously in two diagrams. In these regions Eqs. (29)–(31) are inapplicable, and the cross section has a more cumbersome form.

3. We will obtain the cross section for small electron momenta. A momentum p_i will be assumed small if $p_i \ll m$ but the limitation $\eta \ll p_i$ remains in force.

We will consider first the case in which the momentum of the liberated electron is small ($\eta \ll p_1 \ll m$). The expression (10) for the amplitude is significantly simplified:

$$S=L_3[\bar u_{p_2}(2\varepsilon+\tilde q)\gamma^\mu u_p](\bar u_{p_1}\gamma_\mu u_0)+L_4[\bar u_{p_2}\gamma^\mu(2\varepsilon+\tilde q)u_p](\bar u_{p_1}\gamma_\mu u_0)$$
$$(L_3\sim L_4\sim 1/(\varepsilon_1-m),\quad \varepsilon_2=\varepsilon+m-\varepsilon_1\approx\varepsilon).$$

The exchanged terms do not contribute.[1] The differential cross section (13) takes the form

$$\frac{d\sigma}{d\omega_2\,d^3p_1}=r_0^2\frac{8\eta^5\varepsilon^4}{\pi^2m^2q^4(\varepsilon_1-m)^2}\left(1-\frac{q^2}{4\varepsilon^2}\right)\left|\frac{1}{\varkappa^2-(p+i\eta)^2}+\frac{1}{\varkappa_2^2-(p_2+i\eta)^2}\right|^2, \tag{32}$$
$$\eta\ll q,\quad \eta\ll p_1\ll m.$$

The differential cross section in the region $\eta \ll p_2 \ll m$ is obtained from Eq. (32) by the substitution of subscripts $1 \rightleftarrows 2$.

A simple formula for the cross section is obtained also in the case in which the momenta of all particles are small, i.e.,

$$\eta\ll p\sim p_1\sim p_2\ll m.$$

The amplitude S (Eq. (10)) and the differential cross section (13) take the form

$$S=2m\{L(\bar u_{p_2}\gamma^\mu u_p)(\bar u_{p_1}\gamma_\mu u_0)-M(\bar u_{p_1}\gamma^\mu u_p)(\bar u_{p_2}\gamma_\mu u_0)\},$$

where

$$L=L_1+L_2+L_3+L_4,\quad M=M_1+M_2+M_3+M_4,\quad M_i=L_i(1\rightleftarrows 2),$$
$$d\sigma=r_0^2\frac{32\eta^5m^4p_1}{\pi^2p(q^2+\eta^2)^2}\{|L|^2+|M|^2-\mathrm{Re}(L^*M)\}d^3p_2\,d\omega_1. \tag{33}$$

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[1)]The resonance rise of the cross section by a factor $(\alpha Z)^{-1}$ in comparison with background was first noted by Weber, Deck, and Mullin [8] who discussed the scattering of electrons of the K shell of the atom for the condition $\epsilon, \epsilon_2 \gg \epsilon_1$, m in the first approximation in m/ϵ.

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