

Nonrelativistic Compton effect on a bound electron

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The photon energy region $E_b \ll E_{ph} \ll m$ is considered (E_b is the electron binding energy). Expressions for the pA terms in the cross section for Compton scattering in the K shell are presented in finite algebraic form. An analytic estimate is obtained for the contributions of the pA and AA terms to the cross section. According to this estimate, in the region considered the main contribution to the cross section is from the AA terms. It is shown that for validity of the plane-wave approximation, in addition to the condition $E_{e1} \gg E_b$, it is necessary also that momentum be approximately conserved in the scattering process, which occurs only in the region of the Compton line peak. For light elements we obtain for the scattered photons angular distributions that are the nonrelativistic equivalents of the Klein–Nishina distribution for scattering by bound K electrons. It is shown that the ratio of the cross section for scattering in the K shell to the Klein–Nishina cross section is a universal function of the parameter $\gamma = \bar{p}_{free}/\bar{p}_{bound}$, where \bar{p}_{free} is the momentum of the ejected electron at the peak of the Compton line and \bar{p}_{bound} is the average momentum of an electron in the K shell. In the plane-wave approximation an expression is obtained for the cross section for Compton scattering by a molecular electron cloud, and an analysis is made of the influence of nuclear vibrations on the cross section. Calculation of Compton scattering in the H_2 molecule shows that the line shape depends substantially on the state in which the H_2^+ molecular ion is formed.

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1. INTRODUCTION. FEATURES OF SCATTERING BY A BOUND ELECTRON

In scattering of a photon by a bound electron, in contrast to the case of scattering by a free electron, three processes are distinguished: 1) Rayleigh or coherent scattering, in which the state of the electron is not changed, 2) Raman scattering, as a result of which the scattering system goes over to another bound state, and 3) Compton scattering, which is accompanied by ionization.

In the nonrelativistic approximation in second-order perturbation theory in the interaction of the electron with the electromagnetic field, the scattering amplitude in relativistic units has the following form (see for example ref. 1):

$$M = M_{AA} + M_{pA}, \quad (1)$$

$$M_{AA} = e_1 e_2 \langle 2 | \exp\{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{r}\} | 1 \rangle, \quad (2)$$

$$M_{pA} = \sum_n \frac{\langle 2 | e_2 \hat{\mathbf{p}} e^{-i\mathbf{k}_2 \cdot \mathbf{r}} | n \rangle \langle n | e_1 \hat{\mathbf{p}} e^{i\mathbf{k}_1 \cdot \mathbf{r}} | 1 \rangle}{m(E_1 - E_n + \omega_1)} + \left\{ \begin{matrix} \mathbf{k}_1 \neq -\mathbf{k}_2 \\ \omega_1 \neq -\omega_2 \\ e_1 \neq e_2 \end{matrix} \right\}. \quad (3)$$

The subscripts 1 and 2 refer to the initial and final states, \mathbf{e} is the polarization of a photon with wave vector \mathbf{k} and energy ω , E_1 is the energy of the electron in the initial state, m is its mass, and E_n is the energy of the intermediate states.

The term M_{AA} is obtained by summation over the intermediate states with negative energies of the exact expression for the amplitude of the scattering matrix for the following two conditions:

$$|E - m| \ll m, \quad \omega \ll m, \quad (4)$$

where E is the total energy of the electron. Expression (3) for the terms M_{pA} was obtained with inclusion of only the first of the conditions (4), and it is not possible to simplify it by means of the second inequality in the general case. This leads to the result that terms of order ω/m appear in calculation of M_{pA} . As pointed out in the papers of Gorshkov and co-workers, [2–4] the relativistic correction is also of order ω/m , and consequently expression (3) is written with excessive accuracy.

Summation over the intermediate states in Eq. (3) is equivalent to finding the Green's function of the scattering system. Use of closed expressions for the Coulomb Green's function [5,6] permits calculation of the amplitude M_{pA} for hydrogen-like systems. Expressions have been obtained for M_{pA} for scattering by K electrons in the dipole approximation [7–11] and with inclusion of retardation. [12–16] In the case of Rayleigh and combination scattering, the exact expressions for the amplitude (3) contain hypergeometric functions of the two variables, [14,15] and in the case of Compton scattering they contain hypergeometric functions of four variables [16] (Lauricella functions [17]).

Gorshkov et al. [2,4] showed that the contribution to the cross section of the dispersion terms in the case of Rayleigh and Raman scattering is $\sim E_b/\omega$, where E_b is the binding energy of the ejected electron. In the case of Compton scattering, the qualitative estimates of the contribution of the pA terms are ambiguous. For example, the estimates made by Eisenberger and Platzman [18] lead to an incorrect result: $M_{pA}/M_{AA} \sim (E_b/m)^{1/2}$. In the present work for photon energies $\omega \gg E_b$ the Compton scattering cross section obtained by Gavrilin [16] is presented in finite algebraic form. This has made it possible, in particular, to obtain an analytic estimate of the contribution of the pA terms; it is shown that $M_{pA}/M_{AA} \sim (E_b/\omega)(E_b/E_{e1})$, i.e., the cross section is determined with high accuracy by the AA terms of the scattering amplitude. Inclusion in the cross section of only the AA terms we will designate in what follows as the AA approximation.

In Compton scattering by a bound electron, the energy of the scattered photon, which for a free electron and for a given scattering angle is completely determined by the conservation of momentum, varies within the range from zero to a maximum value $\omega_1 - E_b$. As a result the δ -function Compton line of a free electron is broadened, and its peak is shifted somewhat to higher frequencies. For incident electron energies $E_{e1} \gg E_b$ its wave function is usually approximated by a plane wave. As shown in the present work, this approximation is valid only in

the region of the Compton line peak. A similar conclusion follows from analysis of the contributions of the corresponding Feynman diagrams to the scattering amplitude.^[3]

In the nonrelativistic photon-energy region the half-width of the Compton line for K electrons has been found in the AA approximation.^[19, 20] It is of interest to obtain an estimate of the half-width of the line over the entire region of photon energies. For this purpose it is sufficient to consider Compton scattering by a free electron but with a distribution of velocities as for a bound electron. In the case $E_b \ll m$ in the generalized Compton formula we can limit ourselves to terms of first order in v :

$$\omega_2 = \frac{\omega_1}{1 + \omega_1(1 - \cos \theta)/m} \left(1 - v \cos \theta_1 + \frac{v \cos \theta_2}{1 + \omega_1(1 - \cos \theta)/m} \right), \quad (5)$$

where v is the initial velocity of the electron, θ is the scattering angle, $\theta_{1,2}$ are the angles between the initial momentum of the electron and the photon wave vectors before and after scattering. The uncertainty in the velocity of the bound electron is of the order $(2E_b/m)^{1/2} = \alpha Z_{\text{eff}}$, and therefore it follows from Eq. (5) that for any photon energies the width of the Compton line is proportional to the square root of the binding energy.

If the inequality $\omega_1(1 - \cos \theta) \ll m$ is satisfied (this is always true in the nonrelativistic region), we obtain from (5) the estimate

$$\Delta\omega \sim \omega_1 \alpha Z_{\text{eff}} \sin(\theta/2), \quad (6)$$

i.e., the Compton line width is proportional to the photon energy and the square root of the binding energy, which is in agreement with the results of calculations of the cross section for scattering by the K shell in the AA approximation.^[19, 20] With increasing photon energy the dependence of the half-width on the photon energy ceases to be linear. In the ultrarelativistic case, if the inequality $\omega_1(1 - \cos \theta) \gg m$ is satisfied, the broadening is determined by the expression

$$\Delta\omega \sim \alpha m Z_{\text{eff}} (1 - \cos \theta)^{-1} \quad (7)$$

and the line width ceases to depend on the energy of the incident photon.

The well known formula for the angular distribution of scattered photons in the Compton effect was obtained for scattering by a free, stationary electron.^[1] Significant departures from the Klein-Nishina distribution should be expected in the small-angle region for scattering by a weakly bound electron. While the Klein-Nishina cross section is maximal for a scattering angle $\theta = 0$, the Compton effect cross section for a bound electron should drop with decrease of θ , since the energy transferred to the atom for small scattering angles becomes insufficient for ionization.

In the present work we have obtained in terms of the AA approximation the angular distribution of scattered photons for the Compton effect in the K shell of the lightest elements and have found the region of scattering parameters in which departures from the Klein-Nishina distribution are important. It is shown that the ratio of the cross section for scattering in the K shell to the Klein-Nishina cross section is determined by a universal function of the parameter $\gamma = \bar{p}_{\text{free}}/\alpha m Z_{\text{eff}}$, where

$$\bar{p}_{\text{free}} = 2\omega_1 \sin \frac{\theta}{2} \left[1 + \frac{\omega_1}{m} (1 - \cos \theta) \right]^{-1/2}$$

is the average value of the momentum of the emitted

electrons in the Compton line peak and $\alpha m Z_{\text{eff}}$ is the average value of the electron momentum in the K shell.

We have also considered Compton scattering by a molecular electron cloud. The specific nature of the scattering in the case of molecules is the many-centered nature of the distribution of electron density and the necessity of taking into account the vibrational and rotational motion of the nuclei. As a consequence of the many-centered distribution, an oscillating factor appears in the cross section. However, its influence falls off as the role of vibrations increases. Calculations of the cross sections for scattering in an H_2 molecule have shown that the Compton line shape depends substantially on the state in which the H_2^+ molecular ion is formed.

2. CROSS SECTION FOR SCATTERING BY K ELECTRONS

Let the unit vectors ν_1 , ν_2 , and \mathbf{n} be directed respectively along \mathbf{k}_1 , \mathbf{k}_2 , and \mathbf{p} (\mathbf{p} is the momentum of the emitted electron). As the unit of energy for the K-shell electrons it is natural to take Ry. The matrix element of the scattering cross section can conveniently be made dimensionless: $M \rightarrow (\eta^2 Z^2 p / 16\pi^3)^{1/2} M$, $\eta = \alpha m$. In these units

$$d^2\sigma = \frac{r_0^2 \omega_2}{Z^2 \omega_1} |M|^2 d\omega_2 d\omega_1, \quad (8)$$

where $d\omega_e$ is the element of solid angle in which the momentum of the ejected electron lies.

The term corresponding to the AA term in the complete matrix element of the cross section (8) has been calculated by Schnaidt^[19]:

$$M_{AA} = 4e_1 e_2 (2/\pi)^{1/2} \eta^4 Z^4 [1 - \exp\{-2\pi\eta Z/p\}]^{-1/2} \cdot [\eta^2 Z^2 + (k-p)^2]^{-1/2} [k^2 + (\eta Z - ip)^2]^{-1/2} [k^2 + (\xi - 1)kp], \quad (9)$$

where $\xi = \eta Z/ip$, $\mathbf{k} = \mathbf{k}_1 - \mathbf{k}_2$. Expressions for the terms M_{pA} were found in the work of Gavrilu^[16] and are a superposition of the hypergeometric functions of Lauricella. The expressions for M_{pA} are substantially simplified if we consider processes with a large momentum transfer to the electron, $E_b \ll E_1$. Here the Lauricella functions are expressed in terms of the Appell hypergeometric functions F_1 , and Eq. (9) is transformed to

$$\tilde{M}_{AA} = e_1 e_2 \frac{4}{\pi} \left(\frac{p}{\eta Z} \right)^{1/2} \left[1 + \left(\frac{p-k}{\eta Z} \right)^2 \right]^{-1/2} \left[\frac{k^2 + (\xi - 1)kp}{k^2 + (\eta Z - ip)^2} \right]. \quad (10)$$

The complete matrix element of the cross section will have the form

$$\tilde{M} = e_1 e_2 \tilde{M}_{AA} + e_2 \mathbf{n} \left(\mathbf{e}_1 \mathbf{n} + \frac{\omega_2}{p} \mathbf{e}_1 \nu_2 \right) \tilde{M}_1 + e_1 \mathbf{n} \left(\mathbf{e}_2 \mathbf{n} - \frac{\omega_1}{p} \mathbf{e}_2 \nu_1 \right) \tilde{M}_2. \quad (11)$$

The quantity \tilde{M}_1 in Eq. (11) represents the following combination of F_1 functions:

$$\tilde{M}_1 = 2^7 \pi^{-1/2} \tau_1^{1/2} \rho_1^{1/2} [(1 + \tau_1)^2 + \delta_1^2]^{-3/2} [1 + (\rho_1 + \delta_2)^2]^{-1/2} \{ [(1 - \tau_1)^2 + \delta_1^2] \cdot (4 - \tau_1)^{-1} F_1(4 - \tau_1; 3, 3; 5 - \tau_1; x_1, x_2) - [(1 + \tau_1)^2 + \delta_1^2] \cdot (2 - \tau_1)^{-1} F_1(2 - \tau_1; 3, 3; 3 - \tau_1; x_1, x_2) \} \quad (12)$$

and can in principle be calculated numerically by the method of Gavrilu.^[11] The expression for \tilde{M}_2 differs from (12) by the following substitution:

$$\tau_1 \rightarrow \tau_2, \quad \rho_1 \rightarrow \rho_2, \quad \delta_{1,2} \rightarrow -\delta_{2,1}, \quad (13)$$

where

$$\tau_{1,2} = \eta Z [\mp 2m(\omega_{1,2} \mp E_b)]^{-1/2}, \quad \delta_{1,2} = -ik_{1,2} (2m(\omega_{1,2} - E_b))^{-1/2}, \\ \rho_{1,2} = k_{1,2} [2m(\omega_{1,2} + E_b)]^{-1/2}, \quad \nu_{1,2} = \mathbf{p} [\mp 2m(\omega_{1,2} \mp E_b)]^{-1/2},$$

and the parameters $x_{1,2}$ are found from Eqs. (44) and

(45) of ref. 16 by substituting in them the corresponding quantities from (13).

In the energy region $E_b \ll \omega \ll m$ the scattering cross section can be represented in finite algebraic form by expansion of the Appell function occurring in Eq. (12) in the small parameters $(E_b/\omega)^{1/2}$, $(E_{el}/\omega)^{1/2}$, and $(\omega/m)^{1/2}$. By means of Eq. (49) we obtain to fifth order in the indicated parameters instead of Eq. (12)

$$\tilde{M}_1 \approx 2^2 \pi^{-1} \tau_i^{-1/2} \rho_i^{-1/2} [(1+\tau_i)^2 + \delta_i^2]^{-3} [1 + (\rho_i + \delta_i)^2]^{-2} A_1^{-1} B_1^{-2} P_1, \quad (14)$$

where

$$\begin{aligned} P_1 = & -4\tau_i(1-A_1^2)^{-2} [5A_1^2 - 3 + 3C_1(1-A_1^2)^2] + B_1(1-A_1^2)^{-1} [3-A_1^2 \\ & - 3C_1(1-A_1^2)] \{ (1+\tau_i) [(1-\tau_i)^2 + \delta_i^2] - (3+\tau_i) [(1+\tau_i)^2 + \delta_i^2] \} \\ & + 1/2 B_1^2 (3C_1 - 3 - A_1^2) \{ \tau_i(1+\tau_i) [(1-\tau_i)^2 + \delta_i^2] \\ & - (3+\tau_i)(2+\tau_i) [(1+\tau_i)^2 + \delta_i^2] \} - \\ & - 1/2 B_1^2 [3 - 2A_1^2 - 3C_1(1-A_1^2)] \{ \tau_i(1-\tau_i)^2 [(1-\tau_i)^2 + \delta_i^2] \\ & + (3+\tau_i)(2+\tau_i)(1+\tau_i) [(1+\tau_i)^2 + \delta_i^2] \} \\ & + 1/2 B_1^2 [5A_1^2 + 3C_1(1-A_1^2) - 3] \{ \tau_i(1-\tau_i)^2 (2-\tau_i) [(1-\tau_i)^2 + \delta_i^2] \\ & - (3+\tau_i)(2+\tau_i)(1+\tau_i) \tau_i [(1+\tau_i)^2 + \delta_i^2] \}. \end{aligned} \quad (15)$$

The quantities A_1 , B_1 , and C_1 are found from the formulas

$$\begin{aligned} A_1 = & -(a_1^2 - b_1)^{1/2} B_1^{-1}, \quad B_1 = 1 - a_1, \quad C_1 = \frac{1}{2A_1} \ln \left(\frac{1+A_1}{1-A_1} \right), \\ a_1 = & \frac{4\delta_i(\rho_i + \delta_i) + (1-\tau_i)^2 - \delta_i^2 [1 - (\rho_i + \delta_i)^2]}{[(1+\tau_i)^2 + \delta_i^2] [1 + (\rho_i + \delta_i)^2]}, \\ b_1 = & [(1-\tau_i)^2 + \delta_i^2] [(1+\tau_i)^2 + \delta_i^2]^{-1}, \end{aligned}$$

and for calculation of \tilde{M}_2 in Eqs. (14) and (15) it is necessary to make the substitution (13).

The expressions obtained for the matrix element of the scattering cross section permit an estimate to be made of the contribution of the dispersion terms. For $\omega \sim \eta Z$ the main contribution to the cross section is from electrons emitted with energy $E_{el} \sim E_b$. In this case from Eq. (14) it follows that $M_{pA} \sim E_b/\omega$. In the energy region $\omega \gg \eta Z$ the greater part of the electrons are emitted with $E_{el} \gg E_b$ and the relative contribution of the pA terms is determined by the value of the cross section at the peak of the Compton line. As a result we obtain

$$\frac{M_{pA}}{M_{AA}} \sim \frac{E_b}{\omega} \frac{E_b}{E_{el}} \sim \frac{E_b}{\omega} \left(\frac{\eta Z}{\omega \sin(\theta/2)} \right)^2. \quad (16)$$

It is interesting to compare the results obtained here with those obtained by the traditional method for such estimates. We will assume that in Eq. (3) the main contribution is from terms with $|E_1 - E_\eta| \ll \omega$. Without considering polarization vectors, and introducing average values of the momenta in the initial and final states $\hat{p}|1\rangle \sim \eta Z|1\rangle$, $\hat{p}|2\rangle \sim p_f|2\rangle$, it is easy to obtain from (3)

$$M_{pA} \sim \eta Z p_i M_{AA} / m \omega. \quad (17)$$

In the case of Rayleigh and Raman scattering (or Compton scattering with $\omega \lesssim \eta Z$) the main contribution is from $p_f \sim \eta Z$, and therefore Eq. (17) for these processes leads to $M_{pA}/M_{AA} \sim E_b/\omega$. In the case of the Compton effect for energies $\omega \gg \eta Z$, the estimate (17) leads to an incorrect result. In this region $p_f \sim \omega$ and from (17) we obtain immediately the result of Eisenberger and Platzman^[18]: $M_{pA}/M_{AA} \sim \alpha Z$, i.e., the relative contribution of the dispersion terms is independent of the incident photon energy.

3. COMPTON SCATTERING IN THE AA APPROXIMATION

In the region of applicability of the AA approximation it follows from Eq. (8) that

$$d^2\sigma_{AA} = \frac{r_0^2}{2Z^2} (1 + \cos^2\theta) \frac{\omega_2}{\omega_1} |M_{AA}|^2 d \left(\frac{\omega_2}{Ry} \right) d\omega_2 d\omega_1, \quad (18)$$

where we have extracted the polarization terms from the matrix element M_{AA} . In the case of a hydrogen-like atom the matrix element M_{AA} is calculated exactly (see Eq. (9)). The scattering cross section (18) integrated over the direction of the emitted electron is

$$d^2\sigma_{AA} = \frac{r_0^2}{Z^2} (1 + \cos^2\theta) I_{AA} d \left(\frac{\omega_2}{Ry} \right) d\omega_2, \quad (19)$$

$$\begin{aligned} I_{AA} = & 2^2 \left[1 - \exp \left\{ -\frac{2\pi\eta Z}{p} \right\} \right]^{-1} \\ & \times \exp \left\{ -\frac{2\eta Z}{p} \text{Arctg} \left(\frac{2p/\eta Z}{1 + k^2/\eta^2 Z^2 - p^2/\eta^2 Z^2} \right) \right\} \left[\frac{k^4}{\eta^4 Z^4} \right. \\ & \left. + \frac{k^2}{3\eta^2 Z^2} \left(1 + \frac{p^2}{\eta^2 Z^2} \right) \right] \left[\left(\frac{k^2 + \eta^2 Z^2 - p^2}{\eta^2 Z^2} \right)^2 + 4 \frac{p^2}{\eta^2 Z^2} \right]^{-1}, \end{aligned} \quad (20)$$

where the principal value of the arc tangent is chosen to be $\tan^{-1} x$ if $x \geq 0$ and $\pi + \tan^{-1}(x)$ if $x < 0$.

Let us investigate the influence of the choice of the wave function of the system in the final state on the scattering cross section. The ordinarily used plane-wave approximation assumes replacement in the exact wave function

$$\psi_p = e^{i\eta Z r} \Gamma(1-i\xi) \Phi(\xi, 1, -i(\mathbf{pr} + \mathbf{pr})) e^{i\mathbf{p}\mathbf{r}} \quad (21)$$

of the degenerate hypergeometric function Φ , with the factor in front of it, by unity, which corresponds to the formal substitution $\xi \equiv 0$ (we have used the designation $\xi = \eta Z/ip$). This procedure, however, is not at all obvious. In order to clarify it, we will consider the behavior of the function Φ from Eq. (21):

$$\Phi(\xi, 1, -i(\mathbf{pr} + \mathbf{pr})) = 1 - i\xi(\mathbf{pr} + \mathbf{pr}) - \frac{\xi(\xi+1)}{2 \cdot 2!} (\mathbf{pr} + \mathbf{pr})^2 + \dots \quad (22)$$

for small values of $|\xi|$. Going to the limit $|\xi| \ll 1$, it is important to take into account that the parameter $\xi p = i\eta Z$ is not small and the hypergeometric function (22) in this case goes over to

$$\Phi(\xi, 1, -i(\mathbf{pr} + \mathbf{pr})) \approx 1 - \eta Z(\mathbf{nr} + \mathbf{r}) \left\{ \sum_{l=0}^{\infty} \frac{(-i)^l (\mathbf{pr} + \mathbf{pr})^l}{(l+1)(l+1)!} \right\}, \quad (23)$$

from which it is evident that it can differ substantially from unity.

The possibility of replacing the function (23) by unity is due not to the small value of $|\xi|$, but to the oscillating nature of the sum in the right-hand side of Eq. (23). Let us determine the region of scattering parameters in which the contribution of this sum to the cross section is small. The behavior of the Compton effect cross section is determined by the integral

$$\int d^3r \exp\{-\eta Z r + i(\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{p})\mathbf{r}\} \Phi(\xi, 1, -i(\mathbf{pr} + \mathbf{pr})). \quad (24)$$

In order that the function Φ in Eq. (24) can be approximated by unity, the exponential in the integrand must be a slowly varying function in distances of the order of several periods of oscillation of the sum in (23). This is equivalent to the following two conditions:

$$|\xi| = \eta Z/p \ll 1, \quad |\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{p}|/p \ll 1. \quad (25)$$

The vector

$$\mathbf{g} = (\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{p})/p \quad (26)$$

occurring in Eq. (25) characterizes the degree of non-conservation of momentum in the process of scattering by a bound electron. Thus, in addition to the condition $E_b \ll E_{el}$, for validity of the plane-wave approximation

it is necessary also that the condition $g \ll 1$ be satisfied. The latter is true only in the region of the maximum of the cross section.

In the case of scattering by K electrons the necessity of the conditions (25) can be obtained if we start from the exact expression (9) for M_{AA} . Introducing the parameters ξ and g in explicit form, we will write it

$$M_{AA} = 4e_1 e_2 \left(\frac{2}{\pi} \right)^{1/2} [1 - \exp\{-2\pi|\xi|\}]^{-1/2} \left[1 + \left(\frac{k-p}{\eta Z} \right)^2 \right]^{-1/2} \cdot \left(\frac{\xi + ng + g^2 + ng\xi}{2\xi + 2ng + g^2 - \xi^2} \right) \left(\frac{2\xi + 2ng + g^2 - \xi^2}{g^2 + \xi^2} \right)^{1/2}. \quad (27)$$

Hence to zero order in ξ we obtain

$$M_{AA} \approx e_1 e_2 \frac{4}{\pi} |\xi|^{-1/2} \left[1 + \left(\frac{k-p}{\eta Z} \right)^2 \right]^{-1/2} \left(\frac{\xi + ng + g^2}{2\xi + 2ng + g^2} \right). \quad (28)$$

In the case of the calculation with a plane wave we have the expression

$$M_{AA}^{pl} = \frac{2}{\pi} \left(\frac{p}{\eta Z} \right)^{1/2} \left[1 + \left(\frac{k-p}{\eta Z} \right)^2 \right]^{-1/2}, \quad (29)$$

which is obtained from (28) only for the condition $g \ll 1$. The necessity of this condition for applicability of the plane-wave approximation follows also from consideration of the cross sections integrated over the direction of the emitted electrons. Comparison of Eq. (20) with its analog in the plane-wave approximation

$$I_{AA}^{pl} = \frac{2^4}{\pi} \frac{p}{\eta Z} \left(\frac{kp}{\eta^2 Z^2} + \frac{2}{3} \frac{k^2 p^2}{\eta^4 Z^4} + \frac{k^2 p + kp^2}{\eta^4 Z^4} \right) \left[\left(\frac{k^2 - p^2 + \eta^2 Z^2}{\eta^2 Z^2} \right)^2 + 4 \frac{p^2}{\eta^2 Z^2} \right]^{-3/2} \quad (30)$$

shows that Eqs. (20) and (30) agree only if, in addition to the condition $|\xi| \ll 1$, we impose the requirement $k \sim p$ (which is equivalent to $g \ll 1$).

In Fig. 1 we have shown the Compton lines for scattering by K electrons in hydrogen and lithium. For convenience the curves have been plotted in units $\sim Z^2$ for the ordinate. The dependence of the half-width of the lines on photon energy and nuclear charge agrees with the estimate (6) obtained in the Introduction.¹¹ We can also see from Fig. 1 that the relative error produced by the plane-wave approximation increases on the wings of the line, which corresponds to deviation from the momentum conservation law (thus, for $Z = 1$ on the long-wavelength wing of the line we have $\sigma^{pl}/\sigma^{exact} \approx 1.8$ for $E_{e1} \approx 4$ keV, while near the maximum of the peak where $E_{e1} \approx 2.4$ keV we have $\sigma^{pl}/\sigma^{exact} \approx 0.99$).

Integration of the cross section (19) and (20) over the energy of the emitted photon gives the nonrelativistic equivalent of the Klein-Nishina formula for scattering by K electrons. The early experimental results on the angular distribution of hard x rays in light elements have been analyzed in Heitler's book.^[22] He concluded that the Klein-Nishina formula was in complete agreement with the experimental data. However, in the small-angle region there were no reliable measurements at that time, as a result of difficulties in separation of the elastic component. As noted in ref. 4, according to Wentzel's rule^[23] the sum of the cross sections for the elastic process and all inelastic processes must be equal to the cross section for scattering by a free electron. If the cross sections of only inelastic processes are measured, we should expect significant deviations from the Klein-Nishina distribution in the small-angle region. Measurements of the inelastic scattering of γ rays ($\omega_1 = 662$ keV) on the K shell have shown^[24-26] that for small scattering angles the experimental values of the cross section are significantly lower than those given by

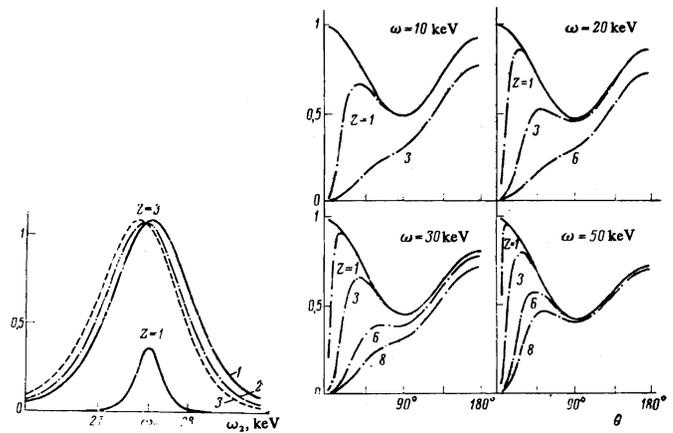


FIG. 1

FIG. 2

FIG. 1. Compton line in the case of scattering of a 30-keV photon at 120° by a K electron in H and Li atoms. The calculation was carried out in the AA approximation: 1—with the exact expression (27) for the matrix element M_{AA} , 2—with expression (28), 3—in the plane-wave approximation. As the ordinate we have plotted the quantity

$$\frac{10}{r_0^2} \frac{d^2 \sigma_{AA}}{d(\omega_2/Z^2 \text{ Ry}) d\omega_2}$$

(ω_C is the Compton frequency).

FIG. 2. Angular distribution of scattered photons in the Compton effect on K electrons. The solid line corresponds to scattering by a free electron (the Klein-Nishina cross section).

the Klein-Nishina formula, and for large angles for heavy elements they are even higher.

In Fig. 2 we have shown the results of calculations of the angular distribution of the cross section on K electrons of light elements. For comparison we have everywhere shown also the Klein-Nishina cross section. It is evident that the departure from the angular distribution given by the Klein-Nishina formula is greater, the higher Z and the smaller ω_1 or θ . In the formulas for the cross section (19) and (20), k and p enter only in the form of the ratios $k/\eta Z$ and $p/\eta Z$. Since the greatest contribution to the cross section is from the region $g \ll 1$, where $k \approx p$, the behavior of the cross section can be characterized by the value of the parameter $\gamma = \bar{p}_{free}/\eta Z$ in the peak of the Compton line, where

$$\gamma = \frac{2\omega_1 \sin(\theta/2)}{\alpha m Z [1 + \omega_1(1 - \cos \theta)/m]} \quad (31)$$

Calculation shows that for all values of θ , ω_1 , and Z in the AA approximation the ratio of the cross section for scattering by K electrons to the Klein-Nishina cross section can be represented as a universal function of the parameter γ . This function is shown in Fig. 3.

4. COMPTON SCATTERING BY MOLECULES

In the photon energy region discussed by us ($\omega \gg E_b$) the matrix element of the Compton scattering cross section can be taken with sufficient accuracy in the AA approximation. The specific feature of scattering by molecules (in comparison with atoms) lies in the many-centered nature of the electron cloud and in the need of taking into account nuclear motion. The wave function of a molecule is described with good accuracy in the adiabatic approximation²¹:

$$\Psi = \phi(r, R) \Lambda(Q) \Theta(\theta), \quad (32)$$

where $\phi(r, R)$, $\Lambda(Q)$, and $\Theta(\theta)$ are respectively the electronic, vibrational, and rotational wave functions; r and R are the sets of electron and nuclear coordinates, Q

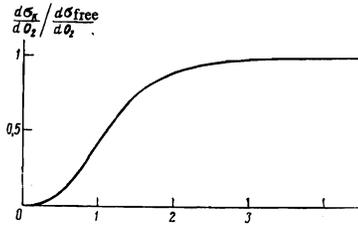


FIG. 3. Ratio of the cross section for Compton scattering on K electrons to the Klein-Nishina cross section, as a function of the parameter $\gamma = \bar{p}_{\text{free}}/\bar{p}_{\text{bound}}$; see Eq. (31).

are the coordinates of the normal vibrations, and ϑ are the Euler angles characterizing the orientation of the molecule.

The scattering cross section, summed over all final vibrational-rotational states of the ion, is given by the following expression (cf. ref. 28):

$$\frac{d^2\sigma_{AA}}{d\omega_2 d\Omega_2 d\Omega_e} = \frac{r_0^2}{2} (1 + \cos^2 \theta) \frac{\omega_2}{\omega_1} \langle \Lambda_2(Q) \Theta_2(\theta) | | \mathfrak{M}_{AA} |^2 | \Lambda_1(Q) \Theta_1(\theta) \rangle, \quad (33)$$

where

$$\mathfrak{M}_{AA}(R) = \left\langle \phi_2(r, R) \left| \sum_j e^{ikr_j} \right| \phi_1(r, R) \right\rangle. \quad (34)$$

The main features of scattering in molecules appear distinctly already in the case of diatomic molecules. Let us consider the simplest of them—the molecule H_2 .

As the electron coordinate function of the ground state of H_2 we will take the Weinbaum function, which satisfactorily describes the electron density distribution^[29]:

$$\phi_1 = N_1 \{ \varphi_a(r_1) \varphi_b(r_2) + \varphi_b(r_1) \varphi_a(r_2) + \mu [\varphi_a(r_1) \varphi_a(r_2) + \varphi_b(r_1) \varphi_b(r_2)] \}. \quad (35)$$

The functions φ_a and φ_b are Slater 1s orbitals centered on the corresponding nuclei, and N_1 is a normalization factor. The optimum value of μ is 0.2644 for an equilibrium distance $R_0 = 1.431$ atomic units and an effective Slater charge $Z^* = \kappa/\eta = 1.1937$ (ref. 29). For $\mu = 0$ the function (35) goes over to the Heitler-London function, and for $\mu = 1$, to the function of the molecular orbital method.

For the lowest vibrational levels it is sufficient to limit ourselves to the harmonic approximation. Then the vibrational-rotational function of the H_2 molecule takes the form

$$\Lambda_1(Q) \Theta_1(\theta) = \left(\frac{a}{\pi^{3/2} \nu! 2^{2\nu+1}} \right)^{1/2} \exp \left\{ -\frac{a^2 (R-R_0)^2}{2} \right\} H_\nu [a(R-R_0)] Y_{JM}(\theta', \varphi'), \quad (36)$$

where H_ν are Hermite polynomials, Y_{JM} are spherical functions, $a = \sqrt{M_p \omega_0/2}$, M_p is the proton mass, ω_0 is the frequency of zero-point oscillations, and θ' and φ' are the angles between \mathbf{k} and \mathbf{R} in the spherical coordinate system with z axis along \mathbf{k} .

We will construct the electron coordinate function of the final state of the system, which corresponds to a singlet state, in the form

$$\phi_2 = N_2 \{ \phi_{H_1^+}(r_1) V_p(r_2) + V_p(r_1) \phi_{H_1^+}(r_2) \}. \quad (37)$$

We will take the coordinate function of the H_2^+ ion in the ground state and in the first excited electronic state in the form of a linear combination of the atomic orbitals

$$\phi_{H_2^+}^{s,u} = N_{s,u} (\phi_a \pm \phi_b), \quad (38)$$

where g refers to the ground state of the ion (Σ_g^+) and u

to the excited state (Σ_u^+); the functions ϕ_a and ϕ_b are centered on the corresponding nuclei and in the simplest case are atomic 1s orbitals.^[30] Inclusion of the polarization of the electron cloud by the neighboring proton can be carried out most simply by replacing $\exp\{-\kappa r_a\}$ by $\exp\{-\kappa_a r_a - \kappa_b r_b\}$ (ref. 31) (for more detail see ref. 32).

We will approximate the wave function of the ejected electron by a plane wave normalized to unit volume:

$$V_p(\mathbf{r}) = e^{i\mathbf{p}\mathbf{r}}. \quad (39)$$

As was shown in the preceding section, for validity of the plane-wave approximation, in addition to the condition $E_{e1} \gg E_b$, it is necessary that the condition of momentum conservation $g \ll 1$ (25) be satisfied. This means that our results will be invalid on the wings of the Compton line.

Calculation of the matrix element (34) with the functions (35), (37) and (38) leads to the following expression:

$$\begin{aligned} \mathfrak{M}_{AA}(R_{ab}) = & 2N_1 N_2 N_{s,u} \{ \langle \phi_a \pm \phi_b | e^{ikr} | \varphi_a \rangle \langle V_p | \varphi_b + \mu \varphi_a \rangle \\ & + \langle \phi_a \pm \phi_b | e^{ikr} | \varphi_b \rangle \langle V_p | \varphi_a + \mu \varphi_b \rangle \\ & + (1 \pm \mu) (s_{aa} \pm s_{ab}) \langle V_p | e^{ikr} | \varphi_a \pm \varphi_b \rangle \}. \end{aligned} \quad (40)$$

where s_{aa} and s_{ab} are overlap intervals between the one-electron wave functions in the ion and in the molecule: $s_{aa} = \langle \phi_a | \varphi_a \rangle$, $s_{ab} = \langle \phi_a | \varphi_b \rangle$. It is not difficult to show that

$$\frac{\langle V_p | \varphi_a \rangle}{\langle V_p | e^{ikr} | \varphi_a \rangle} = \left\{ \frac{\kappa^2 + (\mathbf{k}-\mathbf{p})^2}{\kappa^2 + p^2} \right\}^2 \sim \left\{ \frac{E_b}{E_{e1}} + g^2 \right\}^2. \quad (41)$$

From the conditions (25) it follows that ratios of the type of (41) are small, and therefore in (40) it is sufficient to limit ourselves to the last terms:

$$\mathfrak{M}_{AA}(R_{ab}) \approx 2N_1 N_2 N_{s,u} (1 \pm \mu) (s_{aa} \pm s_{ab}) \langle V_p | e^{ikr} | \varphi_a \pm \varphi_b \rangle. \quad (42)$$

This not only considerably simplifies the form of the matrix element of the cross section, but in addition it permits avoiding calculations of complicated two-centered integrals of the type $\langle \phi_b | e^{ikr} | \varphi_a \rangle$.

We finally obtain the following expression for the cross section for scattering by an H_2 molecule in its ν -th vibrational level:

$$\begin{aligned} d^2\sigma_{s,u} = & \frac{2^2 r_0^2}{\pi^2} (1 + \cos^2 \theta) \frac{\omega_2 p m}{\omega_1 \kappa^2} W_{s,u} \left[1 + \left(\frac{\mathbf{k}-\mathbf{p}}{\kappa} \right)^2 \right]^{-1} \\ & \times \{ 1 \pm e^{-\delta} L_\nu(2\delta) \cos[(\mathbf{k}-\mathbf{p})\mathbf{R}_0] \} d\omega_2 d\Omega_2 d\Omega_e, \end{aligned} \quad (43)$$

$\delta = [(\mathbf{k}-\mathbf{p})\mathbf{R}_0/2aR_0]^2$, $W_{s,u} = [N_1 N_2 N_{s,u} (1 \pm \mu) (s_{aa} \pm s_{ab})]^2$, where L_ν is a Laguerre polynomial. The cross section (43) contains an oscillating factor (in the curly bracket). The presence of this factor is specific for the molecule, and it does not appear in the case of atoms. The factor $e^{-\delta} L_\nu(2\delta)$ appears as a consequence of taking into account nuclear vibrations and is determined by the value of the parameter δ . In the vicinity of the maximum in the cross section this parameter is small, and hence it follows that inclusion of vibrations need not change the scattering picture substantially. As can be seen from Eq. (43), the entire dependence of the cross section on the parameters of the wave function of the ion produced (38) occurs in the factor $W_{s,u}$. As these parameters are varied, the angular and energy characteristics of the cross section remain as before.

Equation (43) represents the cross section for scattering by an oriented molecule. In view of the weak influence of nuclear vibrations on the cross section, we will carry out averaging over the orientations of the molecule in space, taking expression (43) without inclu-

sion of vibrations ($\delta \ll 1$). This gives

$$d^3\bar{\sigma}_{e,u} = \frac{2^2 r_0^2}{\pi^2} (1 + \cos^2 \theta) \frac{\omega_2 p m}{\omega_1 z^3} \times W_{e,u} \left[1 + \left(\frac{\mathbf{k} - \mathbf{p}}{z} \right)^2 \right]^{-1} \times \left\{ 1 \pm \frac{\sin(|\mathbf{k} - \mathbf{p}| R_0)}{|\mathbf{k} - \mathbf{p}| R_0} \right\} d\omega_2 d\omega_1 d\theta. \quad (44)$$

On the basis of Eq. (44) we have calculated the Compton line for scattering by an H_2 molecule with formation of the H_2^+ ion in its ground and excited electronic states. As the wave function for H_2^+ we took the function from the work of Finkelstein and Horowitz^[30] with the optimal effective charge at $R_0 = 1.431$ atomic units. In this case the factors depending on the electronic states of the ion and the molecule are respectively $W_g \approx 0.146$ and $W_u \approx 8.88 \times 10^{-3}$. The results of the calculation are shown in Fig. 4. As follows from the figure, the line shape depends substantially on the final state of the system. This permits information to be obtained on the distribution of electron density not only in the molecule but in the ion formed.^[3]

We are grateful to V. G. Gorshkov for helpful discussion and for sending a preprint, and also to A. V. Kireeva, who carried out the numerical calculations by computer.

APPENDIX

CALCULATION OF APPELL FUNCTIONS

For the Appell hypergeometric function

$$F_1(\alpha; \beta, \beta'; \gamma; x, y) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\gamma-\alpha)} \int_0^1 dt t^{\alpha-1} (1-t)^{\gamma-\alpha-1} (1-tx)^{-\beta} (1-ty)^{-\beta'}$$

the following expansion^[17] is valid:

$$F_1(\alpha; \beta, \beta'; \gamma; x, y) = \sum_{m=0}^{\infty} \frac{(a)_m (\beta')_m}{(\gamma)_m m!} (y-x)^m F(\alpha+m, \beta+\beta'+m; \gamma+m; x), \quad (45)$$

where $(a)_m = \Gamma(a+m)/\Gamma(a)$, $\Gamma(a)$ is the Euler gamma function. In the particular case $x = y$ the function F_1 reduces to the ordinary hypergeometric function by means of the relation

$$F_1(\alpha; \beta, \beta'; \gamma; x, x) = F(\alpha, \beta+\beta'; \gamma; x). \quad (46)$$

We will be interested in the expression for the function F_1 when the values of $|x|$ and $|y|$ are close to unity, in the so-called logarithmic case—for the condition that $\beta + \beta' - \gamma + \alpha = p > 0$ is an integer. Using the analytic representations for the hypergeometric functions occurring in the right-hand side of Eq. (45), we obtain with accuracy to order $p-1$ in $|1-x|$ and $|1-y|$ the following expansion:

$$F_1(\alpha; \beta, \beta'; \gamma; x, y) \approx \sum_{n=0}^{p-1} (-1)^n (1-x)^{-\beta-n} \frac{\Gamma(\gamma)\Gamma(p-n)}{\Gamma(\alpha)n!} (\gamma-\beta-\beta')_n (\gamma-\alpha)_n F\left(\beta+\beta'+\alpha-\gamma-n, \beta'; \beta+\beta'; \frac{y-x}{1-x}\right). \quad (47)$$

If the parameter $|z| = |y-x|/|1-x|$ here is small or large, the functions in the right-hand side are calculated by direct expansion in z or, with use of analytic continuations, in z^{-1} .

In the special case $\beta = \beta'$ we use for the function F in the right-hand side of (47) the relation

$$F(\alpha, \beta; 2\beta; x) = \left(1 - \frac{x}{2}\right)^{-\alpha} F\left(\frac{\alpha}{2}, \frac{\alpha+1}{2}; \beta + \frac{1}{2}; \left(\frac{x}{2-x}\right)^2\right).$$

From Eq. (47) we then obtain

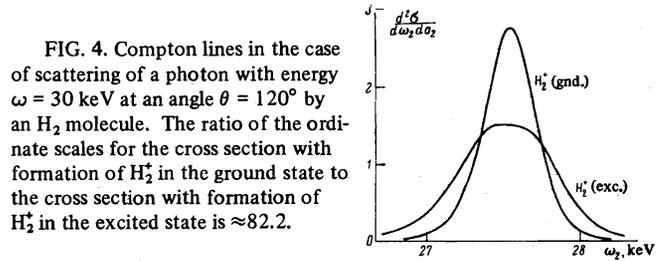


FIG. 4. Compton lines in the case of scattering of a photon with energy $\omega = 30$ keV at an angle $\theta = 120^\circ$ by an H_2 molecule. The ratio of the ordinate scales for the cross section with formation of H_2^+ in the ground state to the cross section with formation of H_2^+ in the excited state is ≈ 82.2 .

$$F_1(\alpha; \beta, \beta'; \gamma; x, y) \approx \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(2\beta)} \left(\frac{2-x-y}{2}\right)^{-\beta} \sum_n^{p-1} (-1)^n \left(\frac{2-x-y}{2}\right)^n \frac{\Gamma(p-n)\Gamma(\gamma-2\beta)_n(\gamma-\alpha)_n}{n!} F\left(\frac{2\beta+\alpha-\gamma-n}{2}, \frac{2\beta+\alpha-\gamma-n+1}{2}; \beta + \frac{1}{2}; \left(\frac{y-x}{2-x-y}\right)^2\right). \quad (48)$$

If the parameter β is an integer, then after a number of transformations with use of recurrence relations for the ordinary hypergeometric functions, all F in the right-hand side of (48) can be reduced to elementary functions.

For example, with accuracy to fourth order in $|1-x|$ and $|1-y|$ we have

$$F_1(\alpha; 3, 3; \alpha+1; x, y) \approx \frac{1}{6} \alpha A^{-4} C^{-3} \{ (1-A^2)^{-2} [5A^2 - 3 + 3B(1-A^2)^2] - C(\alpha-5)(1-A^2)^{-1} [3 - 2A^2 - 3B(1-A^2)] + \frac{1}{3}(\alpha-5)(\alpha-4)C^2 [3B - 3 - A^2] - \frac{1}{6}(\alpha-5)(\alpha-4)(\alpha-3)C^3 [3 - 2A^2 - 3B(1-A^2)] + \frac{1}{24}(\alpha-5)(\alpha-4)(\alpha-3)(\alpha-2)C^4 [5A^2 - 3 + 3B(1-A^2)^2] \}, \quad (49)$$

where

$$A = \frac{y-x}{2-x-y}, \quad B = \frac{1}{2A} \ln \frac{1+A}{1-A}, \quad C = \frac{2-x-y}{2}.$$

¹The same agreement exists also in the relativistic energy region. Thus, the dependence of the half-width of the Compton line on the scattering parameters, as obtained from Eq. (5), is in good agreement with the Compton lines calculated by Gorshkov, Mikhaïlov, and Sherman^[21] for $Z = 1, 13, 26$ and $\omega = 412$ keV.

²For the H_2 molecule, as has been shown by the precision calculations of Kolos and Vol'nevich^[27], the accuracy of the adiabatic approximation is $\sim 10^{-3}\%$.

³In this connection we note that the method of constructing Compton profiles^[18,33-35] which has been widely used in recent years permits analysis of the distribution of electron density only in the initial state of the system.

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