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Compton Scattering of Two Photons by an Atomic Ion

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The analytical structure and absolute values of the doubly differential cross section of the Compton scattering of two X-ray photons by a multicharged neon-like atomic ion are theoretically predicted.

Keywords: Compton scattering, neon-like atomic ion, X-ray photon, scattering probability amplitude, double differential cross section.

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1. Introduction

A large number of experimental [1–4] and theoretical [5–7] papers are devoted to the study of the fundamental process in the microworld of nonlinear (the number of absorbed photons $n \geq 2$) Compton scattering by a free electron. The first theoretical studies of Compton scattering of two photons by an atom were carried out in the papers of the authors [8,9]. The main result of these papers is the prediction of the area of anomalous Compton scattering (ACS) with the energy of the scattered photon $\eta\omega_c \in (\eta\omega; 2\eta\omega - I_{1s})$ ($\eta\omega$ — energy of the incident photon, I_{1s} — ionization threshold energy $1s^2$- atomic shell). The ACS effect of two X-ray free-electron laser (XFEL) photons was experimentally discovered for metallic beryllium [10] and polycrystalline diamond [11]. We understand that, similar experiments for atoms (atomic ions) in the gas phase have not yet been carried out. The physical interpretation of the experimental results [10] remains the subject of theoretical discussions [12,13]. In this paper, we carry out the first theoretical study of Compton scattering of two X-ray photons by a multiply charged atomic ion. The theory of papers [8,9] is generalized, first of all, by taking into account (a) the following orders of the Tamm-Dankov approximation [14] for the probability amplitudes of the process and (b) non-zero widths of the decay of the $1s$-vacancy of the atomic ion and spectral resolution of the proposed experiment. Such studies are in great demand, in particular, for the interpretation of the background (continuum) structures of the observed X-ray emission spectra of multiply charged atomic ions in laboratory and astrophysical plasma [15,16]. The neon-like ion of the argon atom (Ar^{8+}, nuclear charge of the $Z = 18$ ion, configuration and ground state term $[0] = 1s^2 2s^2 2p^6 [^1S_0]$) was taken as the object of study. The choice is due to (a) the spherical symmetry of the ground state of the Ar^{8+} ion, (b) its availability in the gas phase for conducting high-precision experiments, for example, on the absorption of synchrotron radiation by an ion captured in a „trap“ [17], and (c) the pronounced presence of its lines in the observed spectra of X-ray emission from hot astrophysical objects [18,19].

2. Method theory

Let us review the processes of Compton scattering of two photons by a neon-like atomic ion:

$$2\omega + [0] \to [x, \omega] \to [\varepsilon, \omega_c], \tag{1}$$

$$[x, \omega] = 1sxp(^1P_1) + \omega], \tag{2}$$

$$[\varepsilon, \omega_c] = 1s\varepsilon p(^1P_1) + \omega_c, \tag{3}$$

$$2\omega + [0] \to [x, \omega] \to \begin{Bmatrix} L_s \\ L_d \end{Bmatrix} \to [\varepsilon, \omega_c], \tag{4}$$

$$L_s = 1sys(^1S_0), \quad L_d = 1syd(^1D_2). \tag{5}$$

In (1)– (4) and further the atomic system of units ($e = \eta = m_e = 1$) is adopted, $\omega(\omega_c)$ — energy of the incident (scattered) photon, x, y, ε — energy of electrons of the continuous spectrum, $x, y \in [0; \infty)$, $\varepsilon = 2\omega - I_{1s} - \omega_c$, I_{1s} — energy ionization threshold $1s^2$-shell of the ion. The scattering along the channel (1) corresponds (Fig. 1, *a*) to the absorption of one ω photon (at time instant t_1) by the radiative transition operator:

$$\hat{R} = -\frac{1}{c}\sum_{n-1}^{N}(\hat{p}_n\hat{A}_n), \tag{6}$$

and local (at one spatially-temporal point) re-emission of another ω photon into ω_c photon ($t_2 > t_1$) according to the contact interaction operator:

$$\hat{C} = \frac{1}{2c^2}\sum_{n=1}^{N}(\hat{A}_n\hat{A}_n). \tag{7}$$

In (6) and (7) I$\hat{p}_n$ — momentum operator n -electron ion, $\hat{A}_n$ — electromagnetic field operator in the representation

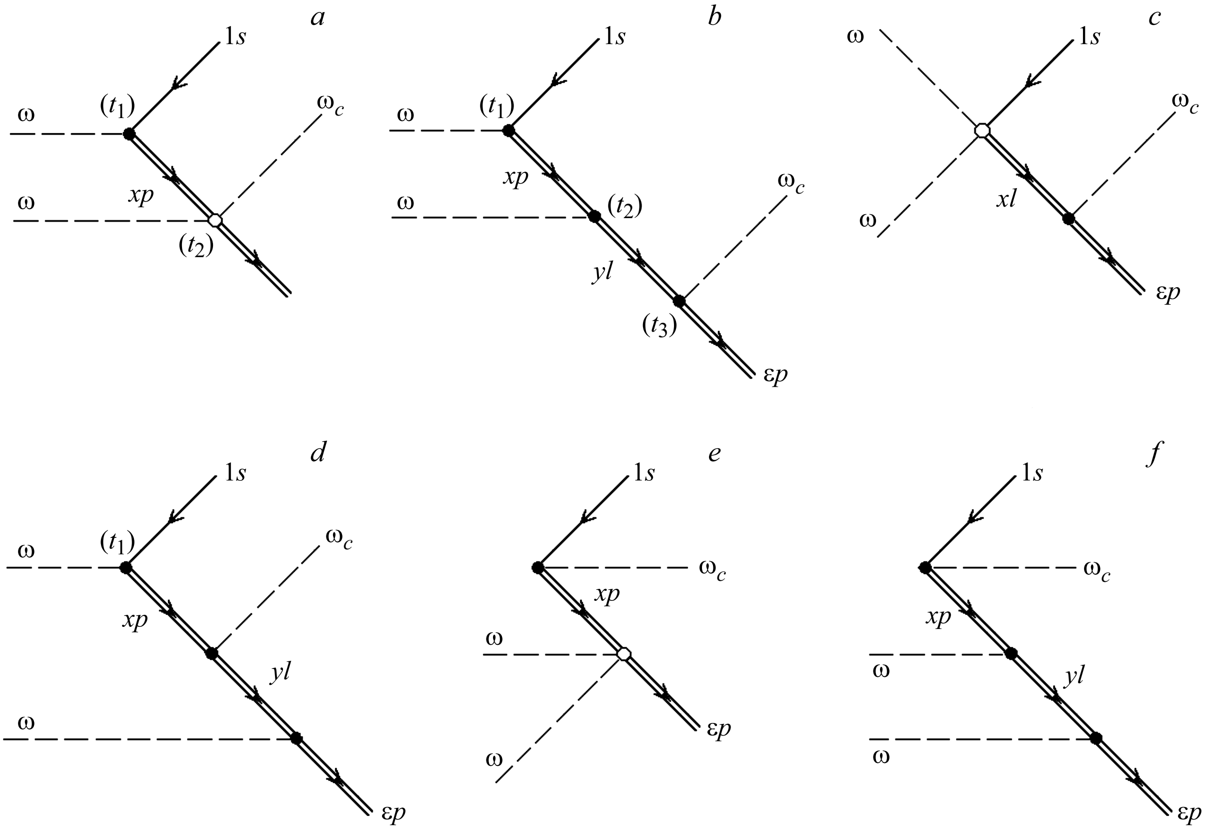

Figure 1. Amplitudes of the probability of Compton scattering of two photons by a neon-like atomic ion (Ar^{8+}) in the representation of Feynman diagrams: (a) amplitude of the probability of local re-emission, (b) amplitude of the probability of absorption with subsequent emission, (c) amplitude of the probability of local absorption of two photons, (d) amplitude of the probability of emission followed by absorption, (e,f) amplitude of spontaneous excitation of the ground state of an atomic ion. Right arrow — electron ($l = s, d$), left arrow — vacancy. Double line — the state was obtained in the Hartree-Fock field of the1s-vacancy. Black (light) circle — top of radiative (contact) transition, $\omega(\omega_c)$ — incident (scattered) photon. Time direction — left to right ($t_1 = t_2 = t_3$).

of secondary quantization, c — speed of light in vacuum, N — number of electrons in ion. Scattering along channel (4) corresponds (Fig. 1, b) to sequential absorption ($t_1 < t_2$) of incident photons and emission ($t_3 > t_2$) of ω_c- photon according to the $\hat{R}$ radiative transition operator.

When constructing scattering probability amplitudes, (a) third (in terms of the fine structure constant) order of quantum mechanical perturbation theory, (b) dipole approximation ($\exp[i(\mathbf{k}\cdot\mathbf{r}_n)] \cong 1$, $\mathbf{k}$ — photon wave vector, $\mathbf{r}_n$ — radius vector n-electron of the ion) for$\hat{R}$- and $\hat{C}$-operators, (c) Tamm.Dankov approximation [14] with the maximum number of „particles" (electrons, vacancies and photons) in the cuts of Feynman diagrams $\mathrm{I}m_{\max} = 4$, (d) approximation of ignoring (at $\omega \geq I_{1s}$; see below) the contributions of the probability amplitudes of transitions from the subvalent $2s^2$- and valence $2p^6$-shells due to their strong spatial and energetic distance from the deep $1s^2$-shell [20]. As a result, for example, the amplitude of the scattering probability in Fig. 1, c in the dipole approximation for the $\hat{C}$-operator vanishes ($\langle 1s|\hat{j}_{0,2}|x(s,d)\rangle \to \langle 1s|xs\rangle = 0$, where $\hat{j}_l$ — spherical Bessel function of the first kind of l-order). The probability amplitude in Fig. 1, d is discarded, since for it $m = 5 > m_{\max} = 4$. The amplitudes of the probability of spontaneous birth of „particles" before the moment of photon absorption (see, for example, Fig. 1, e,f) in the Tamm-Dankov approximation are discarded.

The analytical structure of the doubly differential scattering cross section along channels (1) and (4) was obtained by the methods of the algebra of photon creation (annihilation) operators, the theory of irreducible tensor operators and the theory of non-orthogonal orbitals [21] and has the form:

$$\frac{d^2\sigma_\perp}{d\omega_c d\Omega_c} \equiv \sigma_\perp^{(2)} = r_0^2\mu\,\frac{\xi\omega_c D Q^2}{(\omega-\omega_c)^2 + (\gamma_{1s}\xi)^2}, \qquad (8)$$

$$D = \theta_1 + \frac{\eta_m(2\theta_1 + \eta_m)}{1 + (\gamma_{1s}/\omega)^2}, \qquad (9)$$

$$Q = (2 - \omega_c/\omega) N_{1s} G_m, \qquad (10)$$

$$N_{1s} = \langle 1s_0|1s_+\rangle\langle 2s_0|2s_+\rangle^2\langle 2p_0|2p_+\rangle^6, \qquad (11)$$

$$G_m = \langle 1s_0|\hat{r}|\varepsilon_m p_+\rangle - \frac{\langle 1s_0|\hat{r}|2p_+\rangle\langle 2p_0|\varepsilon_m p_+\rangle}{\langle 2p_0|2p_+}. \qquad (12)$$

In (8)−(12) Ω_c — spatial angle of departure of a scattered photon, r_0 — classical electron

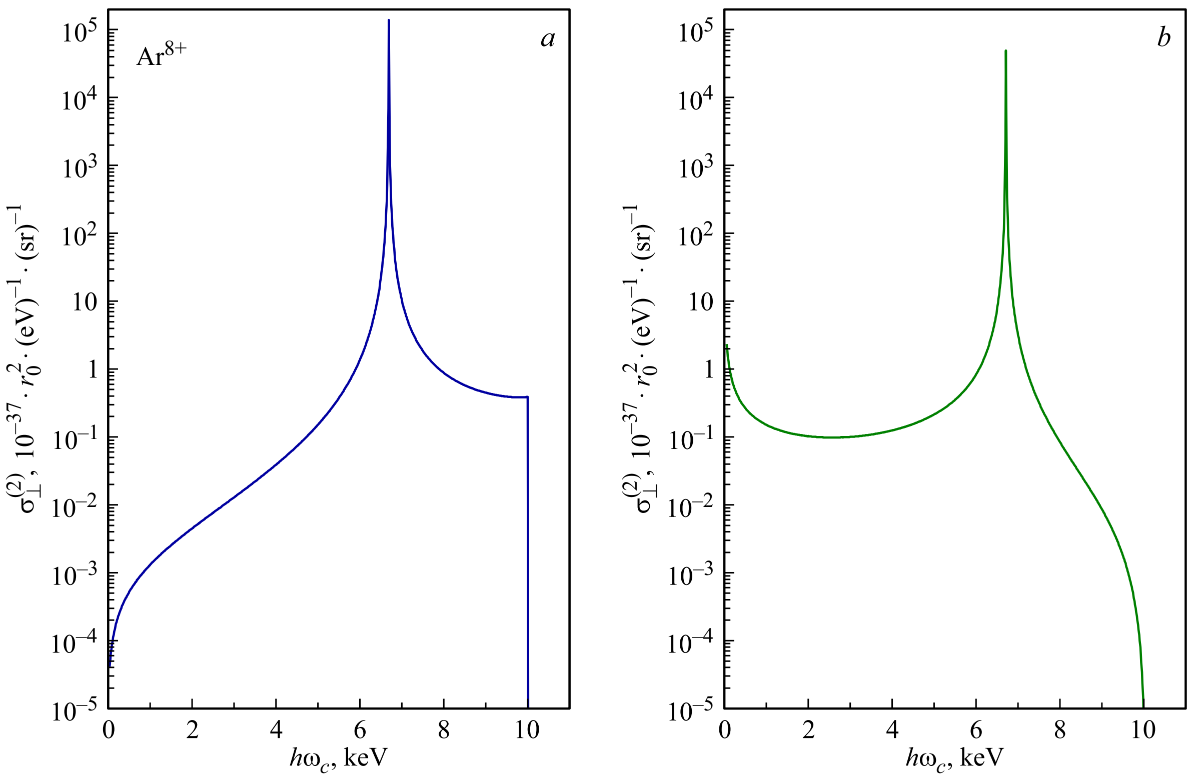

Figure 2. Partial double-differential cross sections for Compton scattering of two photons by the Ar^{8+} ion for $\perp$ — experimental schemes: (*a*) — cross section by probability amplitude in Fig. 1, *a* (see (8) for $\theta_1 = 1$, $\theta_2 = 0$), (*b*) — cross section by probability amplitude in Fig. 1, *b* (see (8) for$\theta_1 = 0$, $\theta_2 = 1$). Incident photon energy $\eta\omega = 6.70$ keV, $\eta\omega_c$ — scattered photon energy, $\Gamma_{1s} = 0.59$ eV, $\Gamma_{beam} = 0.50$ eV.

radius,$\mu = (4/3)\pi\alpha r_0(c\eta)^3/(a_0\epsilon_0 V)$, α — fine structure constant, a_0 — Bohr radius, $\epsilon_0 = 27.21$, V — electromagnetic field quantization volume, $\xi = 1 + (\gamma_b/\gamma_{1s}$, $\gamma_{b,1s} = \Gamma_{beam,1s}/2$, Γ_{beam} — spectral resolution width of the proposed experiment, Γ_{1s} — natural decay width $1s$-ion vacancy, $\eta_m = (6/5)\theta_2(1 - \omega_m/\omega_c)$, $\omega_m = 2\omega - I_{1s}$, $\varepsilon_m = \omega_m - \omega_c$, θ_1, θ_2 — „control“ parameters (Fig. 2, 3). Let us note that the analytical structure of the section (8) reproduces the well-known Weisskopf-Wigner result [22]:

$$(\gamma_b/\pi)\int_{-\infty}^{+\infty}\frac{dx}{\Psi(x)} = \frac{\xi}{\Delta^2 + (\gamma_{1s}\xi)^2}, \qquad (13)$$

$$\Psi(x) = (x^2 + \gamma_{1s}^2)[(x - \Delta)^2 + \gamma_b^2]. \qquad (14)$$

In (13) $\Delta = \omega - \omega_c$ and the second factor in (14) is determined by replacing the Dirac delta function δ with the Cauchy-Lorentz spectral function in the Golden Rule:

$$\delta(\varepsilon - \varepsilon_0) \to (\gamma_b)/\pi,\ [(\varepsilon - \varepsilon_0)^2 + \gamma_b^2]^{-1}, \qquad (15)$$

when integrated over the ε electron energy of the continuous spectrum of the final scattering state, $\varepsilon_0 = 2\omega - I_{1s} - \omega_c$.

The index „$\perp$“ in (8) corresponds to the choice of the most simple mathematically $\perp$-scheme of the assumed coplanar ($\mathbf{k}$, $\mathbf{k}_c \in P$; $\mathbf{k}(k_c)$ — wave vector of the incident (scattered) photon, P — scattering plane) and axially symmetric (relative to the vector $\mathbf{k}$) experiment — photon polarization vectors are perpendicular to the scattering plane: $\mathbf{e}, \mathbf{e}_c \perp P$. The indices „0“ and „+“ in (11) and (12) correspond to the radial parts of the electron wave functions obtained by solving the self-consistent Hartree-Fock field equations for the initial ([0]) and final ($[1s_+2s_+^2 2p_+^6]$) states of the ion. Thus, the factor $N_{1s}G_m$ in (10) describes the many-particle effect of radial relaxation of one-electron wave functions of the excited state of the ion in the field of the $1s$ vacancy. Singular one-electron amplitudes of the probability of absorption (bremsstrahlung absorption) of the ω photon and emission (bremsstrahlung radiation) of the ω_c photon during the transition from continuum to continuum (Fig. 1, *b*) are obtained in the form of velocity in the plane wave approximation for radial parts of the wave functions of the continuous spectrum:

$$(x - y)\langle xp_+|\hat{r}|yl_+\rangle \cong i\sqrt{2x}\delta(x - y), \qquad (16)$$

$$(y - \varepsilon)\langle yl_+|\hat{r}|\varepsilon p_+ \cong i\sqrt{2y}\delta(y - \varepsilon), \qquad (17)$$

$$|x\rangle \cong \left(\frac{2}{\pi^2 x}\right)^{1/4}\sin(r\sqrt{2x}), \qquad (18)$$

$$\langle xl_+|yl'_+\rangle = \delta_{ll'}\delta(x - y), \qquad (19)$$

where $\delta_{ll'}$ — Kronecker-Weierstrass symbol and δ — Dirac delta function. Taking into account$\gamma_{1s} > 0$ in (9) leads to

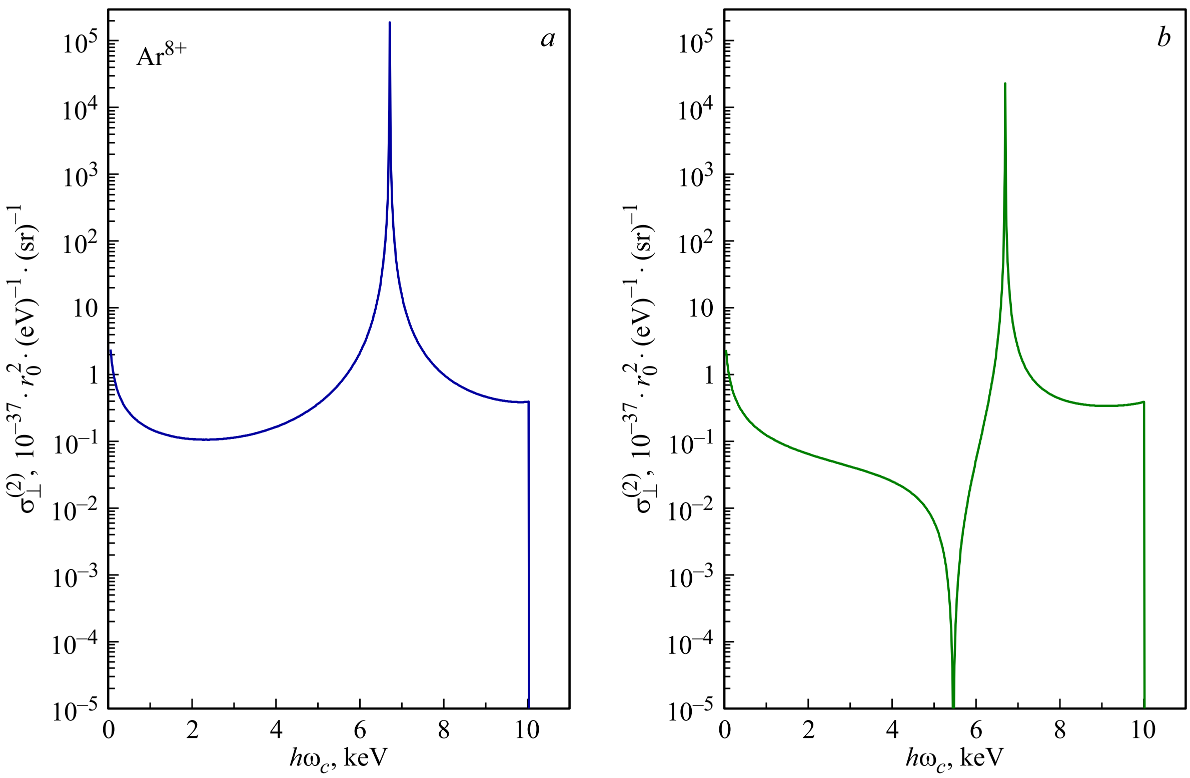

Figure 3. Total double-differential cross sections for Compton scattering of two photons by an Ar^{8+} ion for the $\perp$ experimental scheme: (a) without taking into account (see the sum of cross sections in Fig. 2, *a, b*) and (b) taking into account (see (8) for $\theta_1 = \theta_2 = 1$) quantum interference of probability amplitudes in Fig. 1, *a, b*. Incident photon energy $\eta\omega = 6.70$ keV, $\eta\omega_c$ — scattered photon energy,$\Gamma_{1s} = 0.59$ eV, $\Gamma_{beam} = 0.50$ eV.

the fact that the „infrared divergence“ of cross section (8) formally mathematically arising at $\gamma_{1s} = 0$ ($\sigma_\perp^{(2)} \to \infty$ at $\omega_c \to 0$) disappears. At $\omega \to \infty$, section (8) satisfies the asymptotic condition:

$$\lim_{\omega \to \infty} \sigma_\perp^{(2)} = 0. \tag{20}$$

At $\varepsilon_m \to 0$ ($\omega_c \to \omega_m$) the partial scattering cross section according to the probability amplitude in Fig. 1, *b* (see. (8) at $\theta_1 = 0$, $\theta_2 = 1$) goes to zero. This result reproduces that for single Compton scattering [23] and bremsstrahlung [24]. For the partial scattering cross section by probability amplitude in Fig. 1, *a* (see (8) for $\theta_1 = 1$, $\theta_2 = 0$) there is no „infrared divergence“ and at $\varepsilon_m \to 0$ a break of the cross-section occurs .

3. Results and discussion

The calculation results are presented in Fig. 2, 3. For the cross-section parameters (8), the following values are taken: $I_{1s} = 3380.83$ eV [25], $\Gamma_{1s} = 0.59$ eV [26] and $\omega = 6700$ eV (energy $K\alpha$ - ion emission line Fe^{24+} [27]). Notice, that $I_{1s} \gg I_{2s}(I_{2p}) = 500.68(425.33)$ eV [28]. For the width of the spectral resolution of the proposed experiment, the value $\Gamma_{beam} = 0.50$ eV, achieved in a series of XFEL experiments [29,30], was adopted. The energy value of the incident photon implements the criterion for the applicability of the dipole approximation for the $\hat{R}$- and $\hat{C}$- operators: $\lambda_\omega / r_{1s} \gg 1$, where $\lambda_\omega = 1.852$ Å is the wavelength of the radiation incident on the ion and the average radius $1s^2$ of the Ar^{8+} $t_{1s} = 0.046$ Åion shell. Notice, that $r_{1s} \ll r_{2s}(r_{2p}) = 0.216(0.196)$ Å. (calculation of this paper).

The result in Fig. 2, *a* demonstrates the leading role of the scattering probability amplitude in Fig. 1, *a* when a wide area of anomalous Compton scattering occurs for $\omega_c \in (\omega; 2\omega - I_{1s})$ in the short-wavelength region from the giant Thomson scattering ($\omega_c = \omega$) resonance. The result in Fig. 2, *b* demonstrates the leading role of the scattering probability amplitude in Fig. 1, *b* at $\omega_c \to 0$ (a tendency towards „infrared divergence“ at $\gamma_{1s} \to 0$). Meanwhile, taking into account the quantum interference of the L_s- and L_d scattering channels from (5) almost doubles the theoretical values of the cross section, obtained taking into account only the channel L_s. Comparison of the results in Fig. 3, *a* and Fig. 3, *b* demonstrates the effect of destructive (quenching) quantum interference of the probability amplitudes of processes (1) and (4), entering with different signs into the full amplitude of the scattering probability. Meanwhile (a) there is a redistribution of the scattering probability into the energy region $\omega_c \to 0$ and (b) at $\omega_c \cong 5.3$ keV the total scattering cross section practically goes to zero. No doubt, the analysis of the contributions of partial amplitudes of the scattering probability is of a relative nature, while only the total amplitude of the scattering probability acquires physical meaning (including gauge invariance). The birth of a photon with maximum energy $\omega_c^{\max} = 2\omega - I_{1s}$ in the area of anomalous Compton scattering can be physically interpreted as the effect of inelastic (the ion goes into an excited state) merger of two incident ω photons in the field of an atomic ion.

4. Conclusion

A nonrelativistic version of the quantum theory of the process of Compton scattering of two X-ray photons by a multiply charged atomic ion has been constructed. Dominance areas and the effect of destructive quantum interference of partial scattering probability amplitudes have been established. The main result of the theory (Fig. $3, b$) qualitatively reproduces the result of the authors' work [8,9] for atom and XFEL experiments [10,11] for solids on the occurrence of a region of anomalous Compton scattering with a local maximum of the scattering cross section at $\omega_c \to 2\omega - I_{1s}$ (inelastic fusion of photons in the atomic ion field). In the long-wavelength region from the Thomson resonance ($\omega_c = \omega$), the theory predicts a deep local minimum of the cross section at $\omega_c \cong 5.3\,\text{keV}$ and a tendency for the „infrared divergence" of the cross section at $\omega_c \to 0$ in the $\gamma_{1s} \to 0$ approximation. Going beyond the dipole approximation for the $\hat{C}$ operator and moving to the next orders of the Tamm-Dankov approximation and other schemes of the proposed experiment is the subject of future development of the theory. It can be assumed that experimental detection of the process of Compton scattering of two X-ray photons by an atomic ion is possible, in particular, by methods of scattering synchrotron [32] or XFEL radiation [33] by an atomic ion captured in a „trap". Finally, let us estimate the observed scattering cross section (Fig. $3, b$) for the vicinity of the local maximum at $\omega_c^{\max} = 2\omega - I_{1s}$ ($\cong 10\,\text{keV}$) in the XFEL experiment. For example, for the average brightness of laser radiation (the number of photons in a laser pulse) $N = 10^{20}$([34], EuropeanXFEL) we have:

$$\frac{N!}{2!(N-2)!}\,\sigma_\perp^{(2)} \cong 140\left(\frac{\text{barn}}{\text{eV}\cdot\text{sr}}\right).$$

The resulting value is quite measurable. For the maximum (peak) brightness of laser radiation $N = 10^{35}$, achieved in the paper [35] (PAL-XFEL, Republic of Korea), this estimate increases by 30 orders of magnitude.

Conflict of interest

The authors declare that they have no conflict of interest.

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