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Merging of photons in the atomic ion field

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The analytical structure, absolute values, and angular anisotropy of the differential cross section of the fusion of X-ray photons in the atomic ion field are theoretically predicted. The absolute value of the maximum of the „observed" fusion cross section in the proposed experiment with an X-ray laser on free electrons is estimated.

Keywords: Merging of X-ray photons, neon-like atomic ion, scattering probability amplitude, differential cross section.

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1. Introduction

The effect of photon merging through the creation of virtual electron-positron pairs of the quantum electrodynamics (QED) vacuum is the subject of extensive theoretical study [1–15]. The proposed schemes of experimental observation of photon merging are still waiting for implementation. Within QED in the weak field approximation (the incident photon energy $\hbar\omega \ll m_e c^2$, m_e is the electron mass, c is the speed of light in vacuum) at the leading order in perturbation theory, the merging probability amplitude is described by the Feynman loop diagram with three incident photons in the initial state and one photon in the final state of the process (Figure 1, *a*). Parity of the number of photons on the loop reproduces Furry's QED theory [16]. In [17–19], the first theoretical studies were performed to investigate the equivalent QED photon fusion effect in atomic physics — merging of the photons of the soft ($\hbar\omega \sim I_{1s}/2$, I_{1s} — ionization threshold energy of the deep $1s^2$-shell) X-ray energy band in the atom field (atomic ion). A research brief [20] provides generalization of the theory and results of these studies for the hard ($\hbar\omega \sim I_{1s}$) X-ray energy band of an incident photon: This study provides a more detailed description of the theory and physical results of [20] are supplemented. In this case, the leading amplitude of the merging probability corresponds to the Feynman loop diagram in Figure 1, *b*. Such investigations are needed, in particular, for interpretation of the hard ($\hbar\omega_R \sim 20-30\,\text{keV}$) X-ray emission spectra from galactic clusters [21] and black holes of active galactic nuclei [22]. A Ne-like ion of the Fe atom (Fe^{16+}, the ion nucleus charge $Z = 26$, the configuration and ground state term $[0] = 1s^2 2s^2 2p^6 [^1S_0]$) was chosen as the subject of research. The choice is driven by the spherical symmetry of the ground state of the Fe^{16+} ion and its availability in the gas phase [23] in the experiments for merging X-ray free-electron laser (XFEL) photons in the trapped ion field [24].

2. Theory

Merging probability amplitude and differential cross-section were obtained in the leading third (by the number interaction vertices) order of nonrelativistic perturbation theory. In the radiative ($\hat{R}$) and contact ($\hat{Q}$) transition structure,

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

$$\hat{Q} = \frac{1}{2c^2}\sum_{n=1}^{N}(\hat{A}_n \hat{A}_n), \tag{2}$$

the dipole approximation is taken for the electromagnetic field operator (in the second quantization representa-

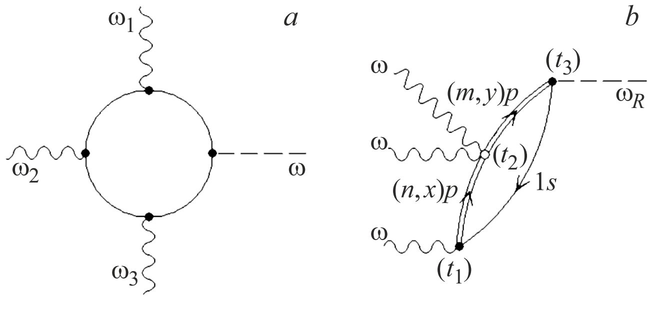

Figure 1. Photon merging probability amplitudes in the Feynman diagram representation: (*a*) through creation of a QED-vacuum virtual electron-positron pair [12] ($\omega_{i=1,2,3}$ — laser photon energies, ω — „signal" photon energy); (*b*) through virtual states of discrete (n, m) and continuous (x, y) spectra electrons. Arrow of time — left to right ($t_1 < t_2 < t_3$). Right arrow — electron, left arrow — vacancy. Double line — the state was obtained in the Hartree-Fock field of the (*b*) $1s$-vacancy. Black (light) circle in Figure 1, *b* — vertex of radiative (contact) transition. $\omega(\omega_R)$ — incident (scattered) photon. $\omega_R = 3\omega$.

tion) [25]:

$$\hat{A}_n = \sum_{\mathbf{k}} \sum_{\rho=1,2} \mathbf{e}_{\mathbf{k}\rho} (\hat{a}^{+}_{\mathbf{k}\rho} + \hat{a}^{-}_{\mathbf{k}\rho}). \quad (3)$$

This is the dipole approximation applicability criterion ($\rho = \lambda / r_{1s} \gg 1$, λ is the „signal" photon wavelength, r_{1s} is the mean radius of the 1s-shell of an ion) that defines the limits of applicability of the discussed theory. For the given case of the Fe^{16+} ion, at the maximum energy of the „signal" photon $\hbar\omega_R = 24.57\,\text{keV}$ and $r_{1s} = 0.031\,\text{Å}$ we have $\rho \approx 16$. However, at $\hbar\omega_R = 400\,\text{keV}$, we have $\rho \approx 1$, and the dipole approximation loses its meaning. In equations (1)−(3), N is the number of electrons in an ion, $\mathbf{p}_n$ is the pulse operator of the n-electron of an ion, $\mathbf{e}_{\mathbf{k}\rho}(\mathbf{k})$ is the photon polarization vector (wave vector), $\hat{a}^{+}_{\mathbf{k}\rho}(\hat{a}^{-}_{\mathbf{k}\rho})$ is the photon creation (annihilation) operator. Large spatial and energy remoteness of the subvalence ($2s^2$) and valence ($2p^6$) shells from the deep $1s^2$-shell of the Fe^{16+} ion [25] makes it possible to ignore their contribution to the probability of merging process in the energy region $\hbar\omega \sim I_{1s}$.

Besides the dipole approximation for the electromagnetic field operator, the Tamm−Dancoff approximation [26] is accepted for the merging probability amplitudes with the maximum number of „particles" (photons, electrons, vacancies) in the Feynman diagram dissections $N_0 = 5$. Then, only the amplitudes shown in Figure 1,b remain from the full set of merging probability amplitudes (sum of 128 Feynman diagrams). Actually [25], the amplitudes involving the wave function of the 1s-electron and j_l — spherical Bessel function disappear in the dipole approximation. Whereby in the Tamm−Dancoff approximation, the „particle" creation probability amplitudes are dropped until the photon falling on the ion is absorbed.

Amplitude of the merging probability through the virtual continuous spectrum states according to the Feynman diagram in Figure 1,b in the atomic system of units ($e = \hbar = m_e = 1$) is written as

$$A = \sum_{M'} \sum_{M''} \int_0^\infty \int_0^\infty \frac{dx\,dy}{\Delta(x,y)} M(x,y), \quad (4)$$

$$\Delta(x,y) = (\omega - I_{1s} - x + i\gamma_{1s})(3\omega - I_{1s} - y + i\gamma_{1s}), \quad (5)$$

$$M(x,y) = \langle 0|\hat{R}|X\rangle \langle X|\hat{Q}|Y\rangle \langle Y|\hat{R}|\overline{0}\rangle, \quad (6)$$

$$|0\rangle = [0] \otimes (\hat{a}^{+}_{\omega})^3 |0_{\text{ph}}\rangle, \quad (7)$$

$$|X\rangle = |1s\,xp(^1P_1), M'\rangle \otimes (\hat{a}^{+}_{\omega})^2 |0_{\text{ph}}\rangle, \quad (8)$$

$$|Y\rangle = |1s\,yp(^1P_1), M''\rangle \otimes |0_{\text{ph}}\rangle, \quad (9)$$

$$|\overline{0}\rangle = [0] \otimes \hat{a}^{+}_{\omega_R} |0_{\text{ph}}\rangle. \quad (10)$$

Equations (4)−(10) define the full wave functions of the initial ($|0\rangle$), intermediate ($|X\rangle, |Y\rangle$) and final ($|\overline{0}\rangle$) merging states, total angular momentum projections of the „ion $\otimes$ electron" $M', M'' = -1, 0, 1$ systems, $|0_{\text{ph}}\rangle$ — wave function of the photon QED-vacuum, $\gamma_{1s} = \Gamma_{1s}/2$, where Γ_{1s} is the natural decay width of the1s-vacancy of the ion, the occupied ion shell are not specified. Using the methods of the photon creation (annihilation) operator algebra, irreducible tensor operator theory and non-orthogonal orbital theory [27], for (4) we obtain

$$A = \xi \int_0^\infty \frac{dx}{\Delta(x,y)} [(x + I_{1s}) J_x]^2, \quad (11)$$

$$\xi = -\frac{1}{3} \left(\frac{2\pi}{V\omega} \right)^2 (\mathbf{e} \cdot \mathbf{e}_R), \quad (12)$$

$$J_x = N_{1s} \big(\langle 1s_0 | \hat{r} | xp_+ \rangle - \Psi_x \big), \quad (13)$$

$$N_{1s} = \langle 1s_0 | 1s_+ \rangle \langle 2s_0 | 2s_+ \rangle^2 \langle 2p_0 | 2p_+ \rangle^6, \quad (14)$$

$$\Psi_x = \frac{\langle 1s_0 | \hat{r} | 2p_+ \rangle \langle 2p_0 | xp_+ \rangle}{\langle 2p_0 | 2p_+ \rangle}. \quad (15)$$

Equation (12) defines: $V(\text{cm}^3) = c$ the electromagnetic field quantization volume [28] and $\mathbf{e}(\mathbf{e}_R)$ the incident (scattered) photon polarization vector. In equations (13)−(15) , the indices „0" and „+" correspond to the radial parts of the electron wave functions obtained through solution of the Hartree−Fock self-consistent field equations for the [0]- and $1s_+(n,x)p_+$-configurations of the ion states. The result for the merging probability amplitude through the virtual states of the discrete spectrum is equivalent to that for A (11) with replacements $xp \to np$, $I_{1s} \to I_{1snp}$ (I_{1snp} is the photoexcitation energy of $1s \to np$), $J_x \to J_n$ and integration over $x \in [0;\infty)$ with summation over $n \in [3;\infty)$.

Considering the quantum interference of the merging probability amplitudes through the virtual states of the continuous and discrete spectra and following the Fermi „golden rule" [29], we obtain for the differential merging cross-section

$$\frac{d\sigma}{d\Omega_R} = r_0^2 \eta \mu (C^2 + D^2), \quad (16)$$

$$C = \int_0^\infty dx (x - x_0) f(x) - \sum_{n=3}^{\infty} \Delta_n \varphi_n, \quad (17)$$

$$D = \gamma_{1s} \left(\int_0^\infty dx\, f(x) + \sum_{n=3}^{\infty} \Delta_n \varphi_n \right), \quad (18)$$

$$f(x) = \frac{[(x + I_{1s}) J_x / \omega]^2}{(x - x_0)^2 + \gamma_{1s}^2}, \quad (19)$$

$$\varphi_n = \frac{(I_{1snp} J_n / \omega]^2}{\Delta_n^2 + \gamma_{1s}^2}. \quad (20)$$

Note that structures (17) and (18) consider the full set of virtual states of the discrete and continuous spectra. However, the mathematically infinite sums in (17) and (18) over virtual (intermediate) states of the discrete spectrum formally inevitably require the approximate computation methods. This study uses the approximation method proposed in [25] for calculation of I_{1snp} and J_n with the principal quantum number $n \gg 3$. Equations (16)−(20)

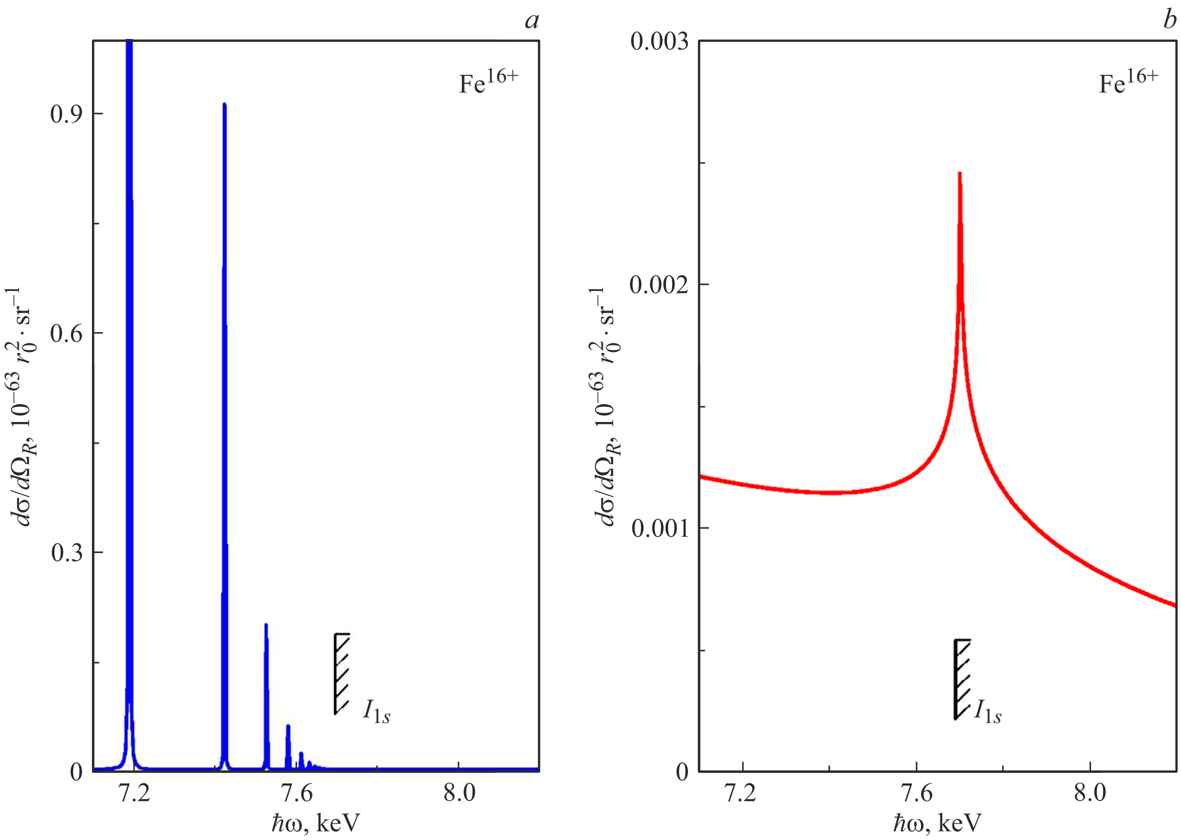

Figure 2. Partial differential cross-sections of photon merging in the Fe^{16+} ion field for the $\perp$ experiment scheme ($\mu^{\perp} = 1$): (*a*) only virtual states of the discrete spectrum are considered (Table); (*b*) only virtual states of the continuous spectrum are considered. $\hbar\omega$ is the incident photon energy.

determine: Ω_R — spatial angle of scattered photon escape, r_0 — classical electron radius,

$$\eta = \frac{1}{3}\left(\frac{\pi r_0}{\in V}\right)^2 \frac{\alpha}{a_0} (c\hbar)^5,$$

α — is the fine structure constant, $\in = 27.21$, a_0 is the Bohr radius, $x_0 = \omega - I_{1s}$ and $\Delta_n = \omega - I_{1snp}$. The axially symmetric (with respect to the incident photon wave vector) parameter $\mu = (\mathbf{e} \cdot \mathbf{e}_R)^3$ in (16) defines the angular anisotropy effect of the merging cross-section. It is specified for three XFEL-experiment schemes. The first scheme — photon polarization vectors are perpendicular to the scattering plane ($\mathbf{e}, \mathbf{e}_R \perp P$). The second scheme — photon polarization vectors are parallel to the scattering plane ($\mathbf{e}, \mathbf{e}_R \parallel P$). The third scheme — the scheme with nonpolarized (UP) photons. P — the scattering plane goes through the wave vectors of the incident ($\mathbf{k}$) and scattered ($\mathbf{k}_R$) photons. As a result we have

$$\mu^{\perp} = 1, \tag{21}$$

$$\mu^{\parallel} = \cos^2\theta, \tag{22}$$

$$\mu_{UP} = \frac{1}{2}(\mu^{\perp} + \mu^{\parallel}), \tag{23}$$

where θ is the angle between the vectors $\mathbf{k}$ and $\mathbf{k}_R$.

As could be expected, cross-section (16) satisfies the asymptotic condition: $d\sigma/d\Omega_g \to 0$ at $\omega \to \infty$. In the formally mathematical limit ($\omega > 0$ in the experiment) $\omega \to 0$, „infrared divergence" of the merging cross-section occurs: $d\sigma/d\Omega_R \to \infty$. This result reproduces that obtained in [17].

3. Findings and discussion

The calculation results are shown in Figure 2, 3, 4 and in the table. For the cross-section parameters in (16), $I_{1s} = 7699.23$ eV (relativistic calculation in this study), $\Gamma_{1s} = 1.046$ eV [30] and $\omega \in (7.15; 8.19)$ keV ([31], Linac Coherent Light Source XFEL, USA) are assumed. Thus, the probability of creation of a „signal" photon with $\omega_R \in (21.45; 24.57)$ keV is investigated.

The results in Figure 2, *a* and in the table demonstrate the leading role of the $1s \to np$-resonances of photoexcitation in the merging cross-section (the principal quantum number values $n \in [3; 500]$ are considered). The result in Figure 2, *b* in the energy region $\omega \in (7.1; 7.5)$ keV demonstrates the trend to the „infrared divergence" of the merging cross-section. Whereby a merging resonance through virtual states of the continuous spectrum occurs at the ionization limit

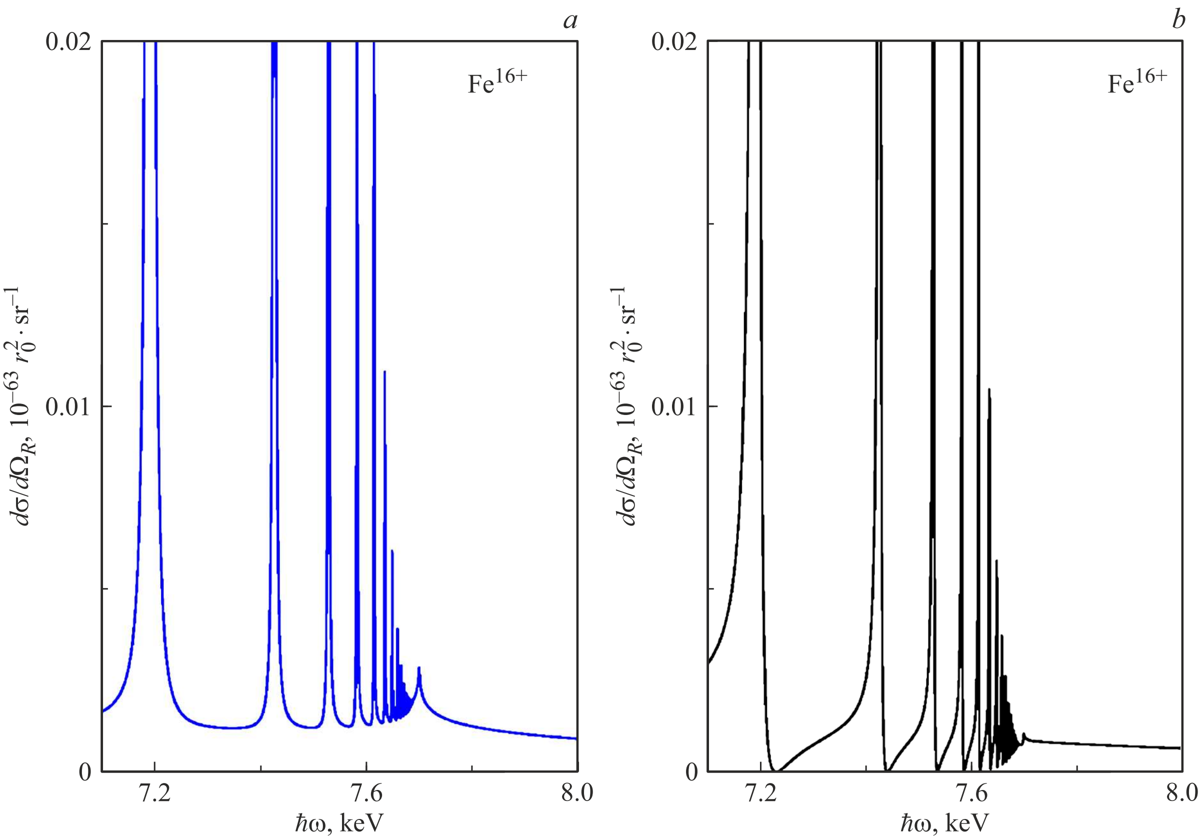

Figure 3. Full differential cross-sections of photon merging in the Fe^{16+} ion field for the $\perp$ experiment scheme ($\mu^{\perp} = 1$): (a) without considering (sum of cross-sections in Figure 2, a, b); (b) considering the quantum interference of summands in the amplitude C from (17). $\hbar\omega$ is the incident photon energy.

Spectral characteristics of the leading resonances of the differential photon merging cross-section in the Fe^{16+} ion field in the $\perp$ experiment scheme

np_+	I_{1snp}, keV	$d\sigma/d\Omega_R$ $(10^{-63} r_0^2 \cdot \mathrm{sr}^{-1})$
$3p_+$	7.1937	7.9768
$4p_+$	7.4272	0.9104
$5p_+$	7.5293	0.1985
$6p_+$	7.5832	0.0607
$7p_+$	7.6150	0.0232
$8p_+$	7.6354	0.0105
$9p_+$	7.6489	0.0058
$10p_+$	7.6587	0.0037

($\omega \cong I_{1s}$). The structures in Figure 2 are identical to those in [17–19], but the corresponding merging cross-sections exceed them by ~ 12 orders of magnitude. Actually, in the region of high energies of photons falling on the ion, the merging probability amplitudes involving the wave function of the $1s$-electron and j_l — spherical Bessel function [17–19] are almost suppressed and vanish in the dipole approximation for the contact transition operator. Thus, transition to the hard X-ray range of incident photon energies considerably increases the probability of detection of merging in the XFEL experiment. Comparison of the results in Figure 3, a and Figure 3, b demonstrates the effect of destructive (quenching) quantum interference of the probability amplitudes for virtual states of the discrete and continuous spectra included with unlike signs into the amplitude C from (17). The merging resonance in Figure 2, b „shrinks“ dramatically and spectral windows (sharp drop of the merging probability) appear at $\omega \in (7.2; 7.6)$ keV. The result in Figure 4 for $\perp$- and UP experiment schemes demonstrates a clearly pronounced angular merging anisotropy — predominant and symmetric merging in the direction of angles $\theta = 0°$, $180°$. Here, a qualitative difference from the results obtained in [17,18] is found, where the angle $\theta = 180°$ („signal“ photon is „reflected“ from the ion) is the prevailing merging direction. Thus, transition to the hard X-ray range of incident photon energies considerably expands the spatial domain of the probability of detection of merging in the XFEL experiment. Note that the result shown in Figure 4 qualitatively reproduces that for elastic photon-photon scattering in the atomic ion field [25] and through the QED vacuum [32,33].

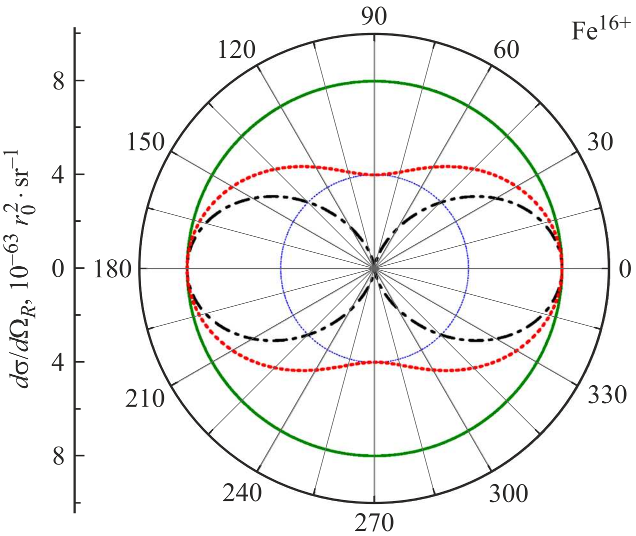

Figure 4. Indicatrices of photon merging in the Fe^{16+} ion field with the polar radius $d\sigma/d\Omega_R$ and polar angle θ at the incident photon energy $\hbar\omega = 7.1937$ keV ($1s \to 3p$-photoexcitation resonance energy). Experiment schemes: $\perp$ (solid curve), $\|$ (dash-dotted curve), nonpolarized curve (dashed curve).

4. Conclusion

The nonrelativistic version of the quantum theory of elastic merging of hard X-ray energy photons in the multicharged Ne-like atomic ion filed has been constructed. It has been found that giant resonances of the differential merging cross-section and angle anisotropy occur in the corresponding schemes of the suggested XFEL experiment. Exceeding the dipole approximation limits for the $\hat{R}$- and $\hat{Q}$-operators of the transition and consideration of the next orders of perturbation theory are the objective of the future development of the theory. Theory generalization for atoms and atomic ions of other type, defining the role of their nucleus charge and relativistic effects that are not considered in this study is the subject of future investigations. Finally, let's evaluate the maximum value of the „observed" merging cross-section ($1s \to 3p$-resonance in the tasble) in the suggested XFEL−experiment. At the mean laser brightness (the number of photons in the laser pulse)$N = 10^{21}$ ([34], European XFEL, Germany), by virtue of the theorem of the sum of incompatible events (selection of three of N photons falling onto the atomic ion) we have

$$\frac{N!}{3!(N-3)!}\left(\frac{d\sigma}{d\Omega_R}\right) \cong 0.106\left[\frac{\text{barn}}{\text{sr}}\right].$$

The resulting value is quite measurable.

Conflict of interest

The authors declare that they have no conflict of interest.

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