Intershell correlations in Compton photon scattering by an atom

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The role of the intershell correlation effect is theoretically investigated using the example of the Ne atom in nonresonance Compton high-energy x-ray photon scattering by a free atom. The calculation results qualitatively reproduce the same results in the formalism of the generalized oscillator strength and the random phase approximation with exchange for the Compton photon and electron scattering by an atom; when the incident photon energy is 11 keV and the scattering angle is 90°, they correspond well with the results of the synchrotron experiment presented in the work by Jung *et al.* [Phys. Rev. Lett. **81**, 1596 (1998)].

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I. INTRODUCTION

Theoretical and experimental study of the nonersonance Compton x-ray photon scattering by a free atom (Kane [1], Pratt *et al.* [2]) in the soft and hard energy range (from 300 eV to 1.5 MeV) allow one to receive fundamental information on the scattering object, specifically on the nature and role of many-particle effects and their quantum interference. Such studies are widely required in modern physics. They appear to be important especially in such fields as laser thermonuclear fusion, creation and use of x-ray free electron laser, plasma physics, surface physics, ionization radiation, and astrophysics.

The program of studies of correlation, nonlocal-exchange, and dynamic effects in the states of nonresonance Compton photon scattering by an atom are represented by Carney and Pratt [3] and Suri [4] in the context of modifications of incoherent scattering function approximation and impulse approximation which are widely used in scientific literature. In Ref. [5] the theory of nonresonance Compton x-ray photon scattering by a many-electron atom is developed beyond the limits of the mentioned approximations. Incidentally, this theory does not contain the limitation $\eta = qa_0/Z \gg 1$ peculiar to the impulse approximation (Eisenberger and Platzmann [6]). Here, q is the impulse given to the atom, a_0 is the Bohr radius, and Z is the atomic nucleus charge. So, if the energy of the incident photon studied in the present work is 11 keV and the scattering angle is 90°, we have $\eta \approx 0.42$ and the impulse approximation turns out to be formally ill-posed. The theory and analysis technique in Ref. [5] lets us realize the indicated program. In the work [5], the role of radial relaxation effects of atomic core electron shells in the deep vacancy field for incident photon energies ($\hbar\omega_1$) in the $1s$ shell ionization threshold region (I_{1s}) is studied. In the present work we study the absolute values and form of the doubly differential cross section of the nonresonance Compton scattering in the far postthreshold ($\hbar\omega_1 \gg I_{1s}$) scattering region. In such energies of the incident photon, the valence and subvalence atomic shells make the main contribution to the scattering cross section (Biggs *et al.* [7], Jaiswal and Shukla [8]). It is known, that if we deal with an excitation-ionization of the few-electron subvalent atomic shell, the effect of correlation appears between this shell and the adjoined many-electron shells (Amusia and Ivanov [9]). This effect has been examined in detail for the Compton photon and electron (and other charged particles) scattering by atoms in the context of the generalized oscillator strength (GOS) formalism and the random phase approximation with exchange (RPAE) (Amusia *et al.* [9,10]). In this work we are not investigating any new physics beyond the intershell correlations effect already studied in the GOS formalism and the RPAE. Our goal is to investigate the degree to which this effect occurs in the nonresonance Compton scattering of a hard x-ray photon by a light atom. The neon atom [Ne; ground-state configuration $[0] = 1s^2 2s^2 2p^6(^1S_0)$] is taken as a subject of inquiry.

II. THEORY

We shall examine the nonresonance Compton unpolarized photon scattering by the atomic $n_1 l_1$ shell with $^1S_0$ term of the ground state:

$$\hbar\omega_1 + [0] \to n_1 l_1^{4l_1+1} \varepsilon l(^1L_J) + \hbar\omega_2, \qquad (1)$$

where $n_1 l_1 \leqslant f$, $\varepsilon l > f$, $\hbar$ is the Planck constant, $\omega_1(\omega_2)$ is the cyclic frequency of the incident (scattered) photon, f is the Fermi level (quantum number population of atom valence shell), and the resultant ^1L_J term ($J = L$) of the open core $n_1 l_1$ shell and of the luminous εl electron of continuous spectrum is determined in the LS coupling scheme. In Eq. (1) and further we do not record closed shells.

The $2s$ subvalence and $2p$ valence shells in the Ne atom are significantly separated in energy from the $1s$ deep shell (for example, $I_{1s} - I_{2s} \cong 822$ eV). This fact enables one to neglect the correlation influence of $2s$ and $2p$ shells on the $1s$ shell. As a result, we examine the wave function of the final state of $1s\varepsilon l$ scattering in the Hartree-Fock one-configurational approximation. Then, the doubly differential cross section of the nonresonance Compton unpolarized photon scattering by the $1s$ shell of the Ne atom takes the following form in the atomic units system ($e = \hbar = m_e = 1$, e is the electron charge, and m_e is its mass) [5]:

$$\sigma_{1s} = \alpha\beta \int_0^\infty M(\varepsilon) G_{1s}(\varepsilon)\, d\varepsilon, \qquad (2)$$

$$M(\varepsilon) = \sum_{l=0}^{\infty} [l] R_l^2(1s,\varepsilon l), \qquad (3)$$

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$$R_l(1s,\varepsilon l) = \int_0^\infty P_{1s}(r) j_l(qr) P_{\varepsilon l}(r)\, dr, \tag{4}$$

$$G_{1s}(\varepsilon) = \frac{1}{\gamma_b\sqrt{\pi}} \exp\left[-\left(\frac{\varepsilon - \Delta_{1s}}{\gamma_b}\right)^2\right], \tag{5}$$

$$q = \frac{\omega_1}{c}\sqrt{1+\beta^2 - 2\beta\cos\theta}. \tag{6}$$

In Eqs. (2)–(6) the following values are determined: $d^2\sigma^{(1s)}/d\omega_2 d\Omega \equiv \sigma_{1s}$, $\alpha = r_0^2(1+\cos^2\theta)$, r_0 is the classical electron radius, Ω is the spatial escape angle of scattered photon, θ is the scattering angle, $\beta = \omega_2/\omega_1$, $[l] = 2l+1$, $P_{\varepsilon l}$ is the radial part of the wave function of εl electron, $\gamma_b = \Gamma_{\text{beam}}/2\sqrt{\ln 2}$, Γ_{beam} is the width at half maximum of the instrumental Gaussian function G, $\Delta_{1s} = \omega_1 - \omega_2 - I_{1s}$, j_l is the spherical Bessel function of the first type of l order, q is the module of the scattering vector (impulse given to atom), and c is the speed of light in vacuum.

To take into account the radial relaxation effect in the $1s$ vacancy field we have to substitute in Eq. (3) when $l = 0,1$ the probability amplitude of R_l transition for the following expression:

$$B_l(1s,\varepsilon l) = N_{1s}\left[R_l(1s_0,\varepsilon l_+) - R_l(1s_0,2l_+)\frac{\langle 2l_0 \mid \varepsilon l_+\rangle}{\langle 2l_0 \mid 2l_+\rangle}\right], \tag{7}$$

$$N_{1s} = \langle 1s_0 \mid 1s_+\rangle\langle 2s_0 \mid 2s_+\rangle^2\langle 2p_0 \mid 2p_+\rangle^6, \tag{8}$$

$$\langle 2l_0 \mid \varepsilon l_+\rangle = \int_0^\infty P_{2l_0}(r) P_{\varepsilon l_+}(r)\, dr. \tag{9}$$

In Eqs. (7)–(9) the radial parts of the wave functions of the $1s_0, 2s_0, 2p_0$ electrons are obtained by solving the Hartree-Fock equations for configuration of the atom ground state. The radial parts of the wave functions of the $1s_+, 2s_+, 2p_+, \varepsilon l_+$ electrons are obtained by solving the Hartree-Fock equation averaged over ${}^{1,3}l$ terms for configuration of the $1s_+\varepsilon l_+$ scattering final state.

When the incident photon energy examined in the present work is $\omega_1 = 11$ keV, the probability of direct transition into the final state of $2p^5\varepsilon l$ scattering is three times as much as the probability of transition into the intermediate virtual state of $2s\varepsilon l'$ scattering. Due to this fact we can neglect the correlation influence of $2s$ shell on $2p$ shell. Then, the doubly differential cross section of the nonresonance Compton unpolarized photon scattering by the $2p$ shell of the Ne atom takes the following form [5]:

$$\sigma_{2p} = 3\alpha\beta\int_0^\infty L(\varepsilon) G_{2p}(\varepsilon)\, d\varepsilon, \tag{10}$$

$$L(\varepsilon) = \sum_{l=0}^{\infty}(l+1)\left[R_l^2\big(2p,\varepsilon(l+1)\big) + R_{l+1}^2(2p,\varepsilon l)\right]. \tag{11}$$

We shall consider the inverse correlation influence of the many-electron $2p$ shell on the few-electron $2s$ shell in the first order of quantum mechanical perturbation theory and build the wave function of the $2s\varepsilon l$ scattering final state in the well-known (see, e.g., the works by Jucys [11] and Froese-Fischer [12]) configurations mixing presentation:

$$\phi_l = |2s\varepsilon l\rangle + \int_0^\infty Q_l \frac{dx}{z + i\lambda}, \tag{12}$$

$$Q_l = (-1)^l \sum_{l'=l\pm 1} V_{ll'}|2p^5 x l'\rangle, \tag{13}$$

$$\lim_{\lambda\to 0}\frac{1}{z+i\lambda} = P\frac{1}{z} - i\pi\delta(z). \tag{14}$$

In Eqs. (12) and (14) the following values are defined: $z = x_0 - x$, the wandering pole of the integrand function $x_0 = \omega_1 - \omega_2 - I_{2p}$, P is the symbol of the Cauchy principal value integral and δ is the Dirac delta function. In Eq. (13) the matrix element of the $\hat{H}$ operator of electrostatic configurations mixing ($T_i \equiv L_i S_i$)

$$C_1 = l_1^{N_1-1} l_2^{N_2}\big(l_3^{N_3}, T_3\big), T, \tag{15}$$

$$C_2 = \big(l_1^{N_1} l_2^{N_2-1}\big(l_3^{N_3-1}, T_3'\big), T_0\big) x l', T, \tag{16}$$

is determined in the LS coupling scheme by specification of the general result (Karazija [13]) for $V = \langle C_1|\hat{H}|C_2\rangle$. Exactly, for $l_1 = 0$, $l_2 = 1$, $l_3 = l$, $N_1 = 2$, $N_2 = 6$, $N_3 = 1$, $T = {}^1l$ in Eqs. (15) and (16), we obtain

$$V_{ll'} = a_{ll'}F_1(2p\varepsilon l; 2sxl') + b_{ll'}G_l(2p\varepsilon l; xl'2s), \tag{17}$$

$$a_{ll'} = (-1)^g\sqrt{\frac{\max(l,l')}{3[l]}}, \tag{18}$$

$$b_{ll'} = \frac{2}{[l]}(1\|C^{(l)}\|l'). \tag{19}$$

In Eqs. (17)–(19) F_1 and G_l are direct and exchange integrals of electrostatic mixing and $l + l' + 1 = 2g$ is a whole number. Then, the doubly differential cross section of the nonresonance Compton unpolarized photon scattering by the $2s$ shell of the Ne atom (modified in comparison with the expression from Ref. [5]) takes the form:

$$\sigma_{2s} = \alpha\beta\int_0^\infty A(\varepsilon) G_{2s}(\varepsilon)\, d\varepsilon, \tag{20}$$

$$A(\varepsilon) = \sum_{l=0}^{\infty}[l]|R_l(2s,\varepsilon l) + D_l|^2, \tag{21}$$

$$D_l = \int_0^\infty \psi_l \frac{dx}{z+i\lambda}, \tag{22}$$

$$\psi_l = \sum_{l'=l\pm 1}(1\|C^{(l)}\|l')V_{ll'}R_l(2p,xl'). \tag{23}$$

The physical interpretation of scattering probability amplitude in Eq. (21) can be represented in the form of Feynman diagrams in the context of nonrelativistic quantum theory of many bodies (March *et al.* [14], Amusia [15]). Figure 1 represents the diagrams for interfering partial amplitudes of scattering probabilities $R_l(2s,\varepsilon l)$ [Fig. 1(a)] and D_l [Fig. 1(b) for the direct part and Fig. 1(c) for the exchange part of the matrix element $V_{ll'}$]. The symbols are as follows: $\omega_1(\omega_2)$ is an incident (scattered) photon; $i(j) = 2p(2s)$ is a vacancy; x is an electron of intermediate scattering state; ε is an electron of final scattering state; the right (left) arrow indicates the state coming into being above (below) Fermi level; the

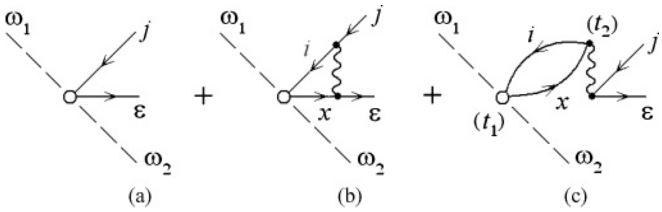

FIG. 1. Presentation of Feynman diagrams for the probability amplitude of the nonresonance Compton photon scattering by $2s$ shell of the Ne atom with provision for intershell correlations. The symbols are given in the text.

wavy line indicates the Coulomb interaction; time direction is from left to right ($t_1 < t_2$); the light circle agrees with the matrix element of the $j_l(qr)$ operator of contact interaction. For example, the diagram given in Fig. 1(a) describes the probability amplitude of four events in one spatial-temporal point: ω_1 photon absorption by atomic j shell, j vacancy production, and production of ω_2 photon and ε electron in vacuum as well. In the present work we do not deal with the mathematical techniques of Feynman diagrams. They are given just to illustrate the quantum dynamic of intershell correlations in nonresonance Compton photon scattering by an atom on the one-particle level.

III. RESULTS AND DISCUSSION

The calculations are made at the fixed value of the incident photon energy $\omega_1 = 11$ keV as in the experiment in the work by Jung *et al.* [16]. Variation of the ω_1 value is the subject of separate study. For the width of instrumental function the value $\Gamma_{\text{beam}} = 5$ eV is taken. This value is much less than characteristic widths of calculated (see Figs. 4 and 5) Compton scattering cross-section profiles ($\sim$200 eV). In this case, the information on the role of intershell correlations is not distorted by the value of the instrumental resolution. On the other side, the adopted value Γ_{beam} exceeds the region widths ($\Delta\omega$, eV) of the resonance line appearance of L_1 ($\Delta\omega \sim 1$; Wilhelmi *et al.* [17]) and L_{23} ($\Delta\omega \sim 10^{-16}$; Zinner *et al.* [18]) spectra of Ne atom photoabsorption. This fact enables one to consider in Eqs. (3), (11), and (21) only the continuous spectrum of scattering final states. We also neglect the spin-orbit splitting of the $2p_{1/2,3/2}$ core shell (splitting constant $\delta_{\text{SO}} \sim 0.1$ eV; Deslattes *et al.* [19]).

In computing the principal value of the integral in Eq. (22) we use the parabolic interpolation of the integrand function numerator on the interval $[a,b], a = x_0 - \mu, b = x_0 + \mu, \mu \sim (I_{2s} - I_{2p}) \times 10^{-2}$. Then, we obtain

$$P\int_0^\infty \varphi dx \to f(a) - f(b) + \left(\int_0^a + \int_b^\infty\right)\varphi dx, \quad (24)$$

$$\varphi = f(x)(x_0 - x)^{-1}. \quad (25)$$

Due to the singular structure of the function from Eqs. (24) and (25), the effect of electrostatic configurations mixing $2s\varepsilon l$ and $2p^5xl'$ becomes apparent at the small energy values of the εl and xl' electrons of the continuous spectrum. This statement is illustrated in Fig. 2 by the calculation results of integrals F_1 and G_1 for the partial $2s\varepsilon p$ scattering channel in the cross section from Eq. (20): if $\varepsilon, x \sim (0; 500)$ eV, the values of these integrals change grossly.

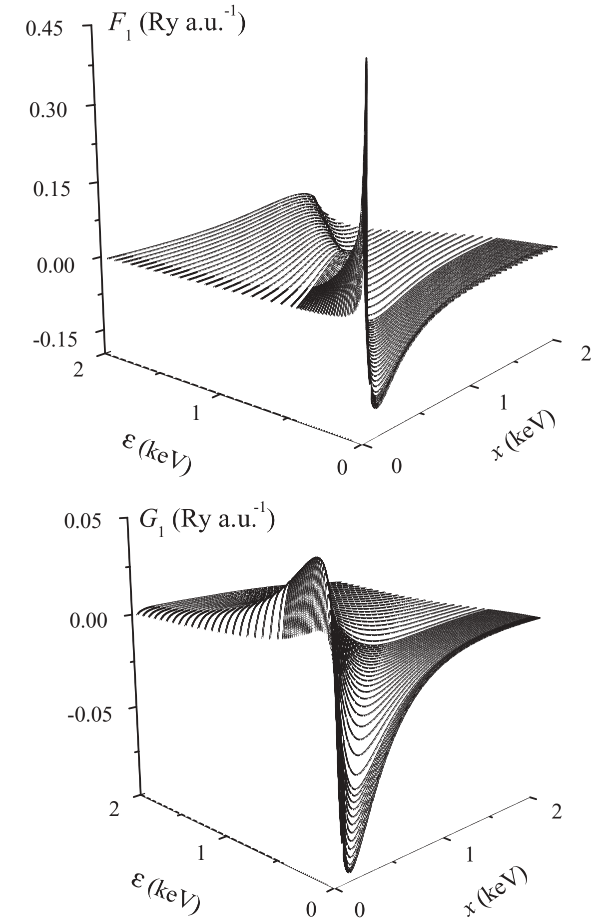

FIG. 2. Values of electrostatic mixing integrals $F_1(2p\varepsilon p; 2sxd)$ and $G_1(2p\varepsilon p; xd2s)$ for the partial $2s\varepsilon p$ channel of the nonresonance Compton photon scattering by the Ne atom.

When calculating the scattering cross sections from Eqs. (2), (10), and (20) we consider the harmonics l from 0 to 25. Considering the higher harmonics ($l > 25$), we change the results not more than for 0.1%. This statement is illustrated by data given in Table I, where the relative contributions of l harmonics in the $2s\varepsilon l$ and $2p^5\varepsilon l$ scattering channels are shown in relation to the incident photon energy. It can be seen, if ω_1 increases, that the nonresonance Compton scattering process becomes more and more multipolar: increasingly higher harmonics are involved in the scattering process. So, if there is the one leading harmonic $l = l_1 + 1$ for $\omega_1 = 1$ keV in scattering channels $2l_1^{4l_1+1}\varepsilon l$, there are several leading harmonics when $\omega_1 = 11$ keV. This result qualitatively reproduces the same in the formalism of GOS and RPAE in the case of increasing the impulse given to the atom in the Compton photon and electron scattering by an atom [9,10]. Thus, the harmonics having $l > 10$ are practically depressed in the sum from Eq. (21) for the $2s\varepsilon l$ scattering channel compared with harmonics having $l \leqslant 10$. For this reason, the correlation integral D_l is calculated only for l values from 0 to 10 (for $l > 10$ the value is accepted $D_l = 0$). Figure 3

TABLE I. Relative contributions of l harmonics to the doubly differential cross section of the nonresonance Compton x-ray photon scattering by the Ne atom in scattering $2s\varepsilon l$ and $2p^5\varepsilon l$ channels. The scattering angle $\theta = 90^\circ$. The calculation is made in one-configurational Hartree-Fock approximation with provision for radial relaxation effects.

$\hbar\omega_1$ (keV)	l	$\eta_{sl}(\%)$[a]	$\eta_{pl}(\%)$
	0	15	14
1	1	70	10
	2	14	74
Σ		99	98
	0	8	5
	1	12	15
11	2	36	32
	3	24	25
	4	15	19
Σ		95	96

[a] $\eta_{sl} = (\sigma_{2s}^{(l)}/\sigma_{2s}) \times 100\%$, σ_{2s} is the maximum value of the cross section from Eq. (20), and $\sigma_{2s}^{(l)}$ is the maximum value of the cross section from Eq. (20) for the fixed l harmonic from Eq. (21).

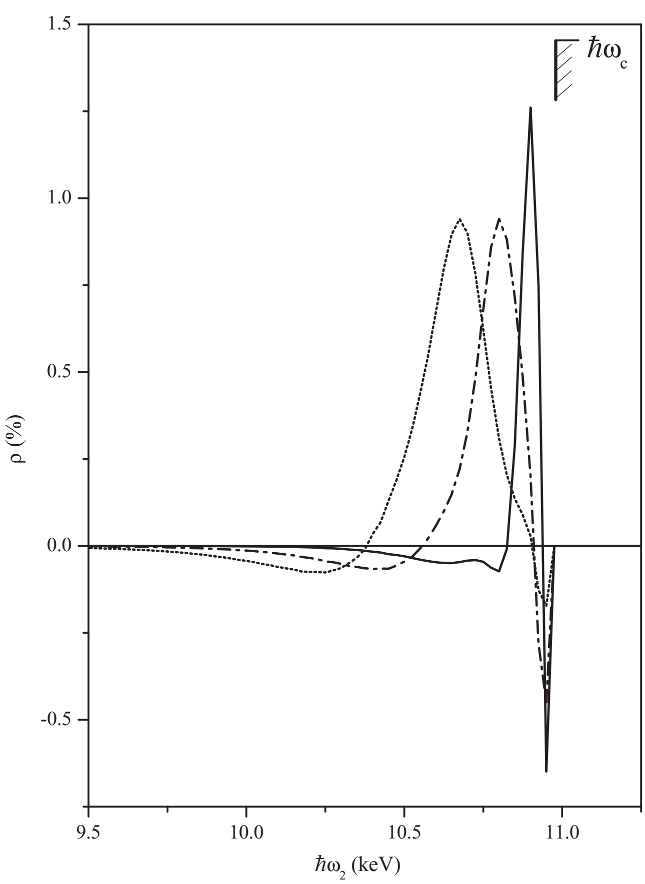

FIG. 3. Intershell correlations function from Eq. (26) for the Ne atom. The incident photon energy $\hbar\omega_1 = 11$ keV; the width of spectral resolution $\Gamma_{\mathrm{beam}} = 5$ eV. Scattering angles are as follows: continuous curve, 60°; chain-dotted curve, 90°; broken curve, 120°. The Compton profile break threshold $\hbar\omega_c = \hbar\omega_1 - I_{2p}$, $I_{2p} = 19.84$ eV (our nonrelativistic calculation).

shows the calculation results for the intershell correlations function:

$$\rho = \left[(\sigma^{IC} - \sigma^{\mathrm{HF}})/\sigma_m^{\mathrm{HF}}\right] \times 100\%, \tag{26}$$

$$\sigma = \sum_{nl\leqslant f} \sigma_{nl}. \tag{27}$$

The following indexes are determined here: *HF* is the calculation of the Compton scattering full cross section from Eq. (27) in the Hartree-Fock (*HF*) one-configurational approximation with provision for the radial relaxation effect, m is the maximal (fixed for every scattering angle) value of the scattering full *HF* cross section, and *IC* indicates that the intershell correlations (*IC*) are considered by Eqs. (22) and (23) in the scattering full cross-section $2s\varepsilon l$ channel. Figure 3 shows two effects: (1) Intershell correlations result in redistribution of scattering intensity in the maximum region of the Compton profiles. When $\omega_1 = 11$ keV and θ is from 60° to 120° the value of this redistribution turns out to be ∼0.9%–1.3%. (2) The more the scattering angle is, the wider the influence region of intershell correlations. This result confirms the well-known fact (Kane [1], Karazija [13]) that the more the scattering angles are, the wider the Compton profiles. We shall notice that the determined insignificant value of the intershell correlation influence on the full cross section from Eq. (27) is primarily conditioned by two circumstances. First, when $\omega_1 = 11$ keV, the influence of this effect in the $2s\varepsilon l$ scattering channel is efficiently extinguished by high values of the scattering cross section in the $2p^5\varepsilon l$ scattering channel. Second, in l-partial channels of $2s\varepsilon l$ scattering the intershell correlations affect amounts practically to magnitudes of greater order. Indeed, considering this effect enlarges the *HF* cross section in ∼9% for $l = 0$, lessens the *HF* cross section in ∼30% for $l = 1$, enlarges the *HF* cross section in ∼3% for $l = 2$, and lessens the *HF* cross section in ∼7% for $l = 3$ (Fig. 4). In addition, the intershell correlations affect results in the redistribution of scattering intensity both for the fixed l harmonic and between harmonics. However (see Table I), the role of the dipole ($l = 1$) harmonic significantly sinks if compared with the quadrupole harmonic ($l = 2$). In addition, the role of the intershell correlation is insignificant in the quadrupole harmonic scattering (∼3%). This result qualitatively reproduces the same in the formalism of GOS and RPAE in the case of the Compton photon and electron scattering by an atom [9,10].

In Fig. 5, the calculation results of the scattering full cross section from Eq. (27) are compared with the results of the synchrotron experiment in the work by Jung *et al.* [16]. Here, we did not include the final $1s\varepsilon l$ state of the nonresonant Compton scattering since its contribution to the cross section at $\omega_2 \geqslant \omega_1 - I_{1s} \cong 10.13$ keV turned out to be $\sigma_{1s}(10^3 r_0^2\,\mathrm{eV}^{-1}\ \mathrm{sr}^{-1}) \sim 10^{-2}$. The doubly differential cross section of Rayleigh elastic scattering by atom electrons with provision for a wide hierarchy of many-particle effects is calculated by using the techniques of the authors of Ref. [20].

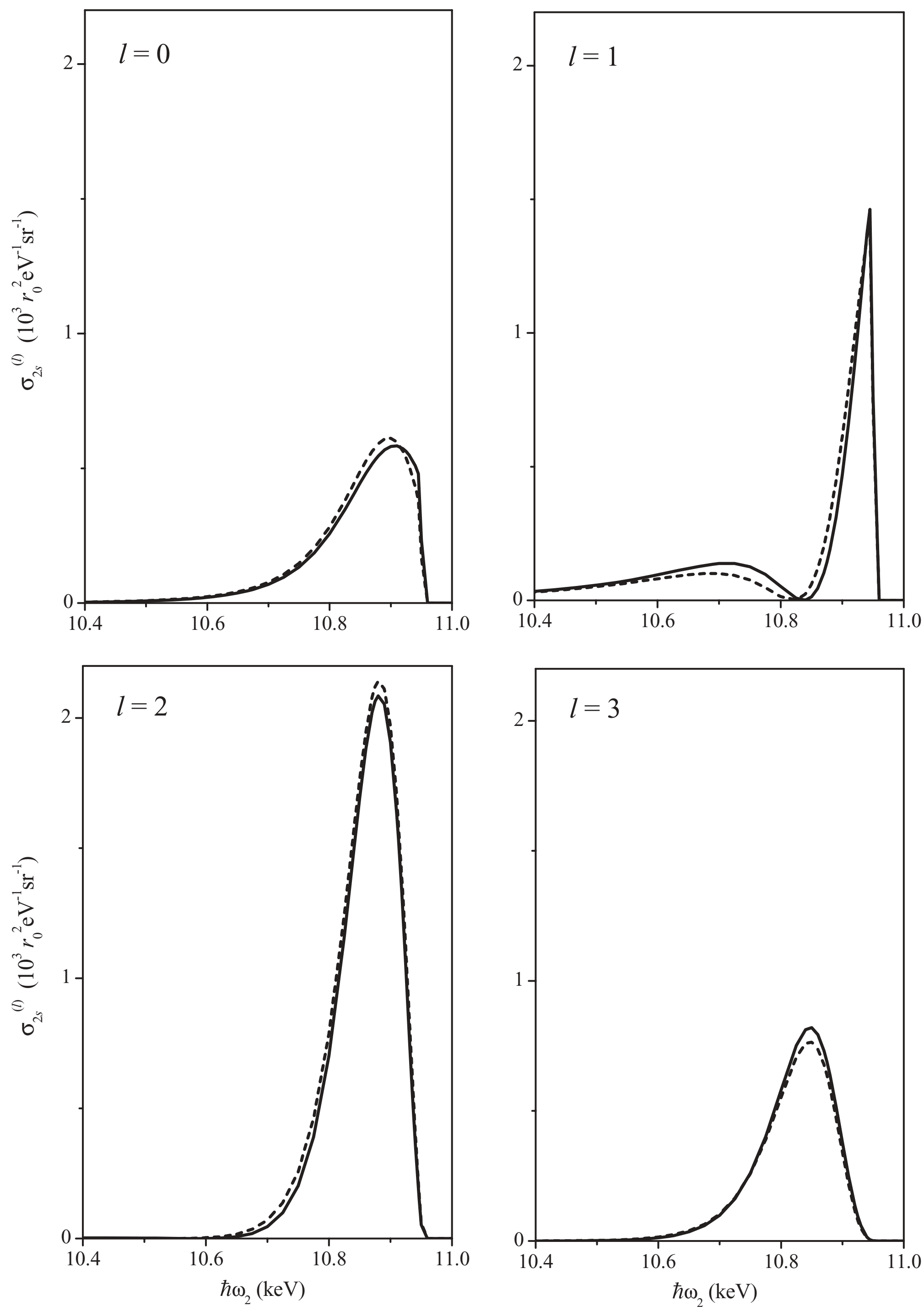

FIG. 4. Doubly differential cross sections of the nonresonance Compton unpolarized x-ray photon scattering from Eq. (20) by the Ne atom in fixed l harmonics in the scattering partial $2s\varepsilon l$ channel. Theory of the present work is as follows: continuous curve indicates one-configurational Hartree-Fock approximation with provision for the radial relaxation effect; broken curve indicates the considered intershell correlations. $\hbar\omega_1 = 11$ keV, $\theta = 60^\circ$, $\Gamma_{\mathrm{beam}} = 5$ eV.

The experimental profile of the scattering cross section is obtained in relative units. Thereby we tied the results of our calculation to the maximum of the experimental spectrum when $\omega_2 \cong 10.97$ keV. The theory of our work agrees well with the experiment. But the high precision of the experiment (inaccuracy of the measurements is $\sim$2%) does not allow one to see the intershell correlations effect, whose magnitude does not exceed $\sim$0.5%–1.0% at the experimental spectral resolution $\Gamma_{\mathrm{beam}} = 250$ eV. Therefore, from a methodological standpoint the one-configurational Hartree-Fock approximation (with provision for the radial relaxation effect) remains at 2% inaccuracy and the spectral resolution is the quite reliable

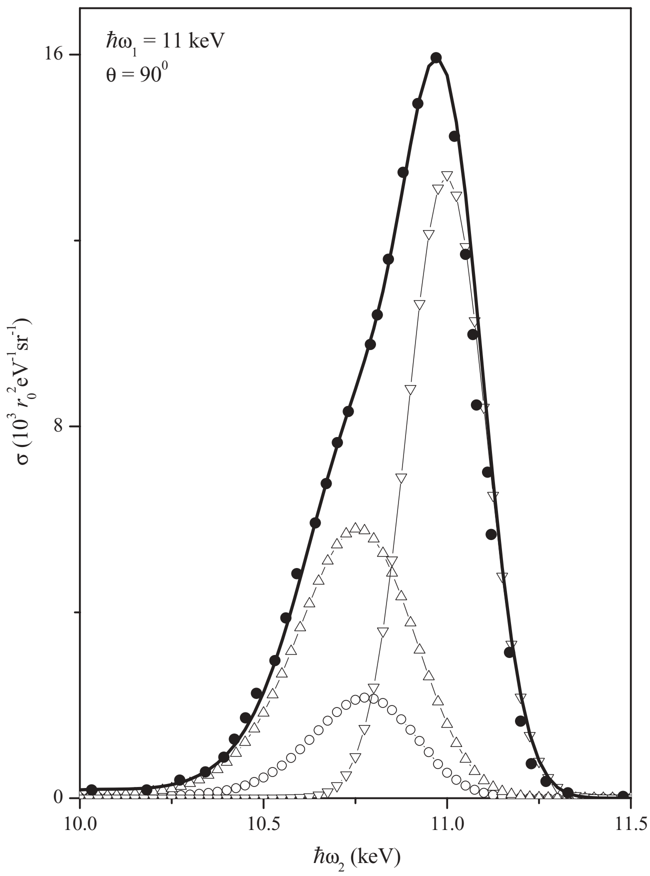

FIG. 5. Doubly differential cross section of the unpolarized x-ray photon scattering by the Ne atom at $\hbar\omega_1 \gg I_{1s}$. Theory of the present work is as follows: light circles and up-triangles indicate contributions of $2s \to \varepsilon l$ and $2p \to \varepsilon l$ transitions to nonresonance Compton scattering accordingly; down-triangles indicate the contribution of Rayleigh scattering (Hopersky *et al.* [20]); the continuous curve indicates the full theoretical scattering cross section with provision for radial relaxation effects and intershell correlations. Dark circles indicate the synchrotron experiment (in relative units) by Jung *et al.* [16]. $\Gamma_{\text{beam}} = 250$ eV (from Ref. [16]).

method for calculation of absolute values and forms of the doubly differential cross section of the nonresonance Compton high-energy x-ray photon scattering by a free atom.

IV. CONCLUSION

Using the example of the Ne atom, it is stated that the intershell correlations effect changes the full, doubly differential scattering cross section of the one-configurational Hartree-Fock approximation in ~0.9%–1.3%, when the incident photon energy is 11 keV (it is much more than the energy of the core shell ionization thresholds) and the studied range of the scattering angles is from 60° to 120°. It is stated that the change of incident photon energy results in changing the participating degree of partial l symmetries of continuous spectrum electrons in the scattering process. It is also determined that the intershell correlations effect has a different influence on the scattering partial l cross sections in the scattering $2s\varepsilon l$ channel. These two facts qualitatively reproduce the physical results obtained in the formalism of GOS and RPAE in studies of Compton photon and electron scattering by an atom (Amusia *et al.* [9,10]) and give the theoretical description of the intershell correlation dynamics a complicated character. It should be noted that the role of this effect in studied scattering spectra can significantly increase according to the decrease of incident photon energy. It should also be expected that the creation of the x-ray free electron laser (Plönjes *et al.* [21]), which can generate the photons with energy to 12.4 keV (the wave length is ~1.0 Å), enables a detailed and high-sensitivity experimental observation of the intershell correlations effect in the nonresonance Compton high-energy x-ray photon scattering by a free atom.

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