Many-electron effects in anomalous elastic scattering of linearly polarized x-ray radiation by a heavy atom

A. N. Khoperskiĭ and V. A. Yavna

Rostov State University of Communications, 344017 Rostov-on-Don, Russia

We calculate the differential cross section for the elastic scattering of linearly polarized x-radiation by a (heavy) krypton atom in the threshold region of ionization of the $1s$-shell with allowance for the relaxation of atomic shells in the vacancy field and processes of one-photon double excitation/ionization. For the anomalous-dispersion scattering region the theoretical results have predictive value. © *1996 American Institute of Physics.* [S1063-7761(96)00402-8]

1. INTRODUCTION

A large amount of experimental and theoretical work has gone into the study of the fundamental process of elastic scattering of x-ray radiation by a free atom near the thresholds of ionization of the atom's inner electron shells (see the review by Pratt[1]).

However, in the anomalous-dispersion scattering region the existing models of the process, which employ the independent-particle approximation in describing the wave functions of atomic states, lead to considerable deviations from the experimental results. For instance, researchers have discovered[2,3] 20–70 percent discrepancies between the measured values of the differential cross section of the elastic large-angle scattering of an x-ray photon by a number of heavy atoms and the corresponding cross sections calculated in the form-factor approximation (for Zn, Mo, Sn, Ta, and Pb atoms in Ref. 2) and in the second-order S-matrix formalism of quantum electrodynamics (for Pb and Bi atoms in Ref. 3).

The anomalous-dispersion part of the amplitude of the elastic scattering of a photon by an atom is determined by the interference of the squares of the photon absorption amplitudes by all the electron shells of the atom.[4,5] In turn, a theoretical description of the photon absorption amplitudes near the ionization thresholds of the inner electron shells is essentially of a many-electron nature.[6] This suggests that to eliminate the above discrepancy between theory and experiment in the anomalous-dispersion region of the elastic scattering of an x-ray photon by an atom we must first abandon the independent-particle approximation and incorporate a hierarchy of many-electron effects that determine the process of photon absorption by the atom near the thresholds for ionization of the atom's inner electron shells. Studies of the effect of the near[7] (the threshold of ionization of the $1s$-shell of the boron atom in a BN single crystal) and far[8,9] (the threshold of ionization of the $1s$-shell of metallic Al and Cu) fine structures of the x-ray absorption spectra on the atomic scattering factors seem to suggest that the above assumption is true.

This paper is a theoretical study of that assumption, using the (heavy) krypton atom as an example. More precisely, we study the effect of monopole transformation of the electron shells in the field of a virtual vacancy and the virtual processes of one-photon double excitation/ionization on the differential cross section of elastic scattering of polarized x-ray radiation near the ionization threshold of the $1s$-shell of the Kr atom. The reasons for choosing the present object of investigation are twofold:

(a) the structure of the absorption spectrum of an x-ray photon by a Kr atom near the ionization threshold of the $1s$-shell is being intensively studied both theoretically[10,11] and experimentally;[11-13]

(b) experimental and theoretical studies[14] have been carried out of the differential cross section of large-angle elastic scattering of linearly polarized synchrotron x-ray by a Kr atom, with photon energies $\hbar\omega = 21.20 - 43.70$ keV close to the ionization threshold of the $1s$-shell, $\hbar\omega_{1s} = 14.326$ keV.

In our previous paper[15] we analyzed theoretically the differential cross section of zero-angle, or forward, elastic scattering of nonpolarized x-ray radiation by a (light) Ne atom, with photon energies in the vicinity of the ionization threshold of the $1s$-shell. The present work generalizes the methods and results of Ref. 15 to the case of finite-angle elastic scattering of linearly polarized x-ray radiation by a heavy atom (Kr), with photon energies near the ionization threshold of the $1s$-shell. Here, as in Ref. 15, we do not examine Thomson scattering by the nucleus of the atom, Rayleigh scattering by the nucleons in the nucleus, or Delbrück scattering on virtual electron–positron pairs created by the Coulomb field of the nucleus, since their effect on the elastic scattering cross section in the x-ray energy range of the scattered photon is minor.[5,14]

2. THE THEORY OF THE METHOD

Let us examine a quantum system consisting of a heavy atom and photons. Its total Hamiltonian is

$$\hat{H} = \hat{H}_a + \hat{H}_{ph} + \hat{W},$$

where $^4\hat{H}_a$ in the atomic Hamiltonian in the Breit approximation, $\hat{H}_{ph}$ is the free-photon Hamiltonian, and $\hat{W}$ is the operator describing the interaction of the atom with an electromagnetic field in the nonrelativistic approximation:

$$\hat{W} = \sum_{i=1}^{N} \left(\frac{\mathbf{A}_i^2}{2c^2} - \frac{\mathbf{p}_i \cdot \mathbf{A}_i}{c} \right), \quad \mathbf{A}_i \equiv \mathbf{A}(\mathbf{r}_i, 0). \tag{1}$$

The structure of the Breit operator makes it possible to allow for relativistic effects in calculating the energies of the states of atomic configurations as corrections to the nonrelativistic Hamiltonian. Here the wave functions of the core and excited electrons of the atomic configurations are examined not in the Dirac spinor representation but in the nonrelativistic approximation as solutions of the corresponding equation of the Hartree–Fock self-consistent field.

In the second order of the perturbation theory in the interaction operator (1), the differential cross section of elastic scattering of linearly polarized x-ray radiation by the $^1S_0$ term of the ground state can be written as

$$\frac{d\sigma}{d\Omega} = r_0^2 (\mathbf{e}_1 \cdot \mathbf{e}_2)^2 \left| F(\omega; \theta) + \sum_{nl} Q_{nl}(\omega) \right|^2. \tag{2}$$

In (1) the vector potential operator of the free electromagnetic field in the second-quantization representation,

$$\mathbf{A} = \sum_{\mathbf{k}} \sum_{m=1,2} \sqrt{\frac{2\pi}{|\mathbf{k}|}} \mathbf{e}_m (\hat{a}_{\mathbf{k}m} e^{i\mathbf{k}\cdot\mathbf{r}} + \hat{a}_{\mathbf{k}m}^+ e^{-i\mathbf{k}\cdot\mathbf{r}}), \tag{3}$$

is the solution[4] at time $t = 0$ of the wave equation

$$\Box \mathbf{A}(\mathbf{r}, t) = 0. \tag{4}$$

The structure of this equation and of the terms in the interaction operator (1) that are linear in the electromagnetic field is determined by the choice of the Coulomb gauge of the field:

$$\text{div} \mathbf{A}(\mathbf{r}, t) = 0, \quad \varphi(\mathbf{r}) = 0,$$

where $\varphi(\mathbf{r})$ is the scalar potential of the field.

In Eqs. (1)–(3) we used the atomic system of units $\hbar = m = e = 1$, c is the speed of light, N is the number of electrons in the atom, $\mathbf{p}_i$ is the momentum operator and $\mathbf{r}_i$ the position operator of the ith electron, $\hat{a}_{\mathbf{k}m}^+$ and $\hat{a}_{\mathbf{k}m}$ are the operators of creation and annihilation of a photon with a wave vector $\mathbf{k}$ and a polarization vector $\mathbf{e}_m$, r_0 is the classical electron radius, $\mathbf{e}_1$ and $\mathbf{e}_2$ are the unit polarization vectors of the incident and scattered photons, Ω is the solid angle, θ is the scattering angle, $\omega = c|\mathbf{k}_1|$ is the energy of the scattered photon, and summation is over all the electron nl-shells of the atom. The scattering angle is defined as the angle between the wave vectors of the incident ($\mathbf{k}_1$) and scattered ($\mathbf{k}_2$) photons.

The terms in the interaction operator (1) that are quadratic in the electromagnetic field describe the contact interaction of the field with the electrons of the atom and determine the atomic form factor in the nonrelativistic approximation:

$$F(\omega; \theta) = \sum_{nl} (4l+2) \int_0^\infty P_{nl}^2(r) \frac{\sin(qr)}{qr} dr,$$

$$q = |\mathbf{k}_1 - \mathbf{k}_2| = \frac{2\omega}{c} \sin \frac{\theta}{2}, \tag{5}$$

where $P_{nl}(r)$ is the radial part of the wave function of the nlth electron in the ground state of the atom.

The terms in the interaction operator (1) that are linear in the electromagnetic field describe the processes of absorption and emission of a photon by the atom via the atom's virtual excitations/ionization of varying multiplicity and determine the anomalous-dispersion Kramers–Heisenberg elastic scattering amplitudes,

$$Q_{nl}(\omega) = \frac{2}{3} \mathbf{S}_{m>F} \frac{\bar{\omega}_m \omega_m^2}{\omega^2 - \bar{\omega}_m^2} |D_{nl}^{m(l\pm 1)}|^2. \tag{6}$$

Here $\bar{\omega} = \omega_m \mp i\Gamma_{nl}/2$, ω_m is the energy of the virtual transition from the ground state $|0; {}^1S_0>$ of the atom to the intermediate state $|nl^{4l+1}m(m\pm 1); {}^1P_1>$ (the filled shells are not written explicitly) of the system consisting of the atomic "residue" and a virtual photoelectron, F is the Fermi level (the set of the principal quantum numbers of the valence shell of the atom), the symbol S stands for summation (integration) over all the intermediate states of the discrete (continuous) spectrum, and Γ_{nl} is the total decay width of the virtual nl-vacancy, determined by the sum of partial decay widths along channels of the radiative and auto-ionization types.

If the Fourier components of the electromagnetic-field operator (3) are taken in the dipole approximation ($\mathbf{k}_i \cdot \mathbf{r}_i \ll 1$), the matrix element of the transition operator in (6) can be defined either in the form of a length,

$$D_{nl}^{m(l\pm 1)} = \left\langle 0; {}^1S_0 \left| \sum_{i=1}^{N} \mathbf{r}_i \right| nl^{4l+1} m(l\pm 1); {}^1P_1 \right\rangle, \tag{7}$$

or in the form of velocity,

$$D_{nl}^{m(l\pm 1)} = \frac{i}{\omega_m} \left\langle 0; {}^1S_0 \left| \sum_{i=1}^{N} \mathbf{p}_i \right| nl^{4l+1} m(l\pm 1); {}^1P_1 \right\rangle, \tag{8}$$

directly related to the structure of the interaction operator (1). Using (7) or (8) for an arbitrary nl-shell of the atom requires allowing for the effect of correlations of the random-phase approximation with exchange[16] on $Q_{nl}(\omega)$. For atoms with $Z \geqslant 10$ the marked spatial and energy separation of the $1s$-shell from the other shells of the atomic core leads to a situation in which the effect of these correlations on the cross section of photon absorption by the $1s$-shell can be ignored. For instances, Tulkki and Åberg[17] (the Ar atom) and Tulkki[18] (the Xe and Rn atoms) have shown that the discrepancy between the values of cross sections of photon absorption by the $1s$-shell of the atom calculated in forms (7) and (8) is at most 1 or 2 percent. For this reason we use only the length form (7) in building a theoretical model of elastic scattering and in calculations. Here the wave functions of the initial and final states of virtual one-photon single excitation/ionization of the atom are described by the single-configuration Hartree–Fock approximation.

In dealing with elastic scattering of linearly polarized x-ray radiation by an atom, we follow the experimental scheme suggested by Smend et al.,[14] where the unit polarization vectors of the generating (incident) and registered (scat-

tered) photons are either perpendicular ($\perp$) or parallel ($\parallel$) to the scattering plane. For the polarization factor in (1) we then have

$$\mathbf{e}_1\mathbf{e}_2 = \begin{cases} \pm 1, & \perp, \\ \cos\theta, & \parallel. \end{cases}$$

The scattering plane is defined as the plane containing the wave vectors of the incident ($\mathbf{k}_1$) and scattered ($\mathbf{k}_2$) photons.

The presence of a virtual vacancy in an inner shell of the atom leads to a radial monopole transformation (i.e., with no change in the symmetry of the state) of the electron shells of the atomic core in the Hartree–Fock field of the vacancy.[19,20] When the single-configuration Hartree–Fock approximation is used to describe the wave functions of the initial and final photoabsorption states of the atom, the effect of radial transformation can be taken into account by modifying the matrix element (7) by methods of nonorthogonal orbital theory.[21,22] For instance, in the case of photon absorption by the $1s$-shell of the Kr atom, the radial (R) part of the matrix element (7) is expressed, to within first-order terms and with allowance for the requirement that the wave function of the $1s^1mp$ state be orthogonal to the wave functions of the states ns^1mp with the same symmetry but lying below on the energy scale, as follows:

$$D_{1s,R}^{mp} = N_{1s}\left(\langle 1s_0|\hat{r}|mp\rangle - \sum_{n=2,3,4} \frac{\langle 1s_0|\hat{r}|np\rangle\langle np_0|mp\rangle}{\langle np_0|np\rangle} \right). \tag{9}$$

Here the wave function of the $1s_0$-, np_0-, and $(n,m)p$-electrons were obtained by solving the Hartree–Fock equations for the $1s_0^2(^1S_0)$ and $1s^1mp(^1P_1)$ configurations, respectively, N_{1s} is the product of the overlap integrals of the wave functions of the electrons not participating in the transition, and we have introduced the notation

$$\langle np_0|mp\rangle = \int_0^\infty P_{np_0}(r)P_{mp}(r)\,dr,$$

$$\langle 1s_0|\hat{r}|mp\rangle = \int_0^\infty P_{1s_0}(r)P_{mp}(r)r\,dr.$$

Near the ionization threshold of the inner shell, the radial transformation leads to a noticeable decrease in the photoabsorption intensity calculated in the single-configuration Hartree–Fock approximation by using the wave functions of the electrons of the "untransformed" atomic core. The photoabsorption intensity lost in the process is restored primarily in processes of one-photon multiple excitation/ionization of the atom's ground state. For instance, the experimentally observed near fine structure of the spectrum of absorption of a photon by the $1s$-shell of the Kr atom[11–13] is caused primarily by processes of one-photon double $1s^{-1}4p^{-1}$– $n_1l_1n_2l_2$ excitation/ionization of the $1s_0^2(^1S_0)$ state.[10]

To study the near fine structure of the elastic scattering spectrum of an x-ray photon close to the ionization threshold of the $1s$-shell of the Kr atom, the intermediate virtual states of double photoexcitation in (6) are described in the multiconfiguration Hartree–Fock approximation in the following manner:
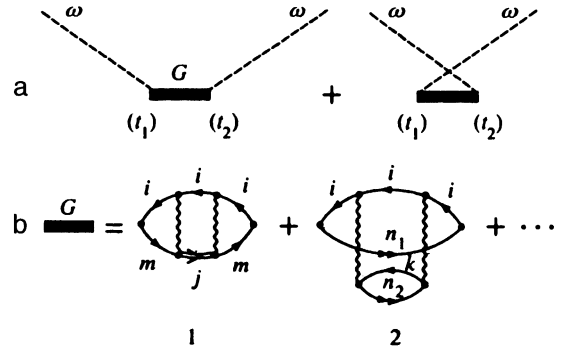

FIG. 1. The Goldstone–Feynman diagrams for the anomalous-dispersion term $Q_{1s}(\omega)$ in the amplitude of elastic scattering of an x-ray photon by a Kr atom near the ionization threshold of the $1s$-shell(see the notation in the text).

$$|i\rangle = \sum_{LS} \sum_{l_{1,2}} \sum_{n_{1,2}>F} a_{12(LS)}^i \psi_{12}^{LS}, \tag{10}$$

where

$$\psi_{12}^{LS} = |1s^14p^5(^{2S+1}P)n_1l_1n_2l_2(LS);{}^1P_1\rangle,$$

$$n_1l_1n_2l_2 = \begin{Bmatrix} 5p & 5p \\ 6p \end{Bmatrix}, \begin{Bmatrix} 4d & 4d \\ 5d \end{Bmatrix}, \begin{Bmatrix} 5s & 4d \\ 5d \end{Bmatrix}, \begin{Bmatrix} 5s & 5s \\ 6s \end{Bmatrix}, \tag{11}$$

and the coefficients $a_{12(LS)}^i$ of configuration mixing are obtained by diagonalizing the energy matrix built on the configurations (11). In (10) we did not include the configurations of the form $1s^14p^5$ ($4f^2$, $4fnf$, $4fnp$), since the $4f$-state proves to be highly delocalized.

The states of one-photon ionization/excitation and double ionization are described in the single-configuration Hartree–Fock approximation by the wave function (11) with

$$n_1l_1n_2l_2 = np\varepsilon p, \quad \varepsilon p\varepsilon'p \quad (n=5,6). \tag{12}$$

A convenient physical interpretation of the anomalous-dispersion terms in the elastic scattering amplitude (6) in the single-configuration Hartree–Fock approximation for photoabsorption states is in the shape of the Goldstone–Feynman diagrams[16] of the many-body theory. Figure 1 diagrammatically represents the term $Q_{1s}(\omega)$ for the case of elastic scattering of an x-ray photon by a Kr atom near the ionization threshold of the $1s$-shell expressed as the sum of the virtual G-block (a) and a fraction of the first (leading) terms in the infinite series of the diagrams for the G-block (b). Here diagrams of type 1 describe the effect of monopole transformation of electron shells in a virtual one-photon single excitation/ionization process, while diagrams of type 2 describe the formation of a virtual near fine structure in the spectrum of photon absorption by the $1s$-shell of the Kr atom. The following notation has been introduced: ω is a scattered photon, $i(k)=1s_0(4p_0)$ is a vacancy, $j=np$ is a photoelectron, an arrow pointing to the right (left) means that the state lies above (below) the Fermi level, a line with a single arrow pointing to the left means that the state was obtained by solving the Hartree–Fock equations for the $1s_0^2(^1S_0)$ configuration, a line with a single arrow pointing to

the right means that the state was obtained by solving the Hartree–Fock equation for the $1s^1mp(^1P_1)$ configuration, a double line means that the state was obtained by solving the Hartree–Fock equation for the $1s^1np(^1P_1)$ configuration, a line with two arrows means that the state was obtained by solving the Hartree–Fock equations for the $1s_0^1 4p_0^5 n_1 l_1 n_2 l_2(^1P_1)$ configuration, a wavy line stands for the Coulomb interaction, and the direction of time is from left to right $(t_1 < t_2)$.

3. RESULTS OF CALCULATIONS

The anomalous-dispersion term $Q_{1s}(\omega)$ in the amplitude (6) of elastic scattering of an x-ray photon by a Kr atom near the ionization threshold of the $1s$-shell has been obtained in three approximations.

Approximation 1 is the single-configuration Hartree–Fock approximation without the effect of monopole transformation of electron shells in the field of the $1s$-vacancy. The wave function of the virtual photoelectron was obtained by solving the Hartree–Fock equation for the $1s_0^1 mp(1P_1)$ configuration. The wave functions of the atomic core electrons were obtained by solving the Hartree–Fock equations for the ground-state configuration $1s_0^2(^1S_0)$. In this approximation the photoabsorption amplitude (9) contains only the first term in the parentheses, $N_{1s}=1$, and the probability of one-photon multiple excitation/ionization processes is nil.

Approximation 2 is the single-configuration Hartree–Fock approximation with the effect of monopole transformation of electron shells in the field of the $1s$-vacancy. The wave function of the virtual photoelectron was obtained by solving the Hartree–Fock equation for the $1s^1mp(1P_1)$ configuration. The wave functions of the atomic core electrons were obtained by solving the Hartree–Fock equations for the $1s^1(^2S_{1/2})$ configuration, i.e., we allow for the relaxation of the atomic core in the field of the $1s$-vacancy. In this approximation the photoabsorption amplitude has the form (9) with $N_{1s}<1$.

Approximation 3 is the second approximation with allowance for the formation of intermediate states of the virtual one-photon double excitation/ionization, (10) and (12). The wave functions of the $n_1 l_1$- and $n_2 l_2$-electrons were obtained by solving the Hartree–Fock equations for the $1s^1 4p^5 n_1 l_1 n_2 l_2$ configuration after averaging over the ^{2S+1}P and LS states. The wave functions of the atomic core electrons were obtained by solving the Hartree–Fock equations for the $1s^1 4p^5$ configuration after averaging over the $^{1,3}P$ states, i.e., we allowed for the relaxation of the atomic core in the field of the $1s$- and $4p$-vacancies.

The effect of monopole transformation of the electron shells and the correlations of the random-phase approximation with exchange play an important role only when photon absorption energies are close to the ionization thresholds of the nl-shells of the atom. Since the ionization threshold of the $1s$-shell of the Kr atom is far from the ionization thresholds of the other atomic core shells (e.g., $\omega_{1s} - \omega_{2s} = 12.646$ keV), the matrix elements of the transition operator, $D_{nl}^{m(l\pm1)}$, and the corresponding anomalous-
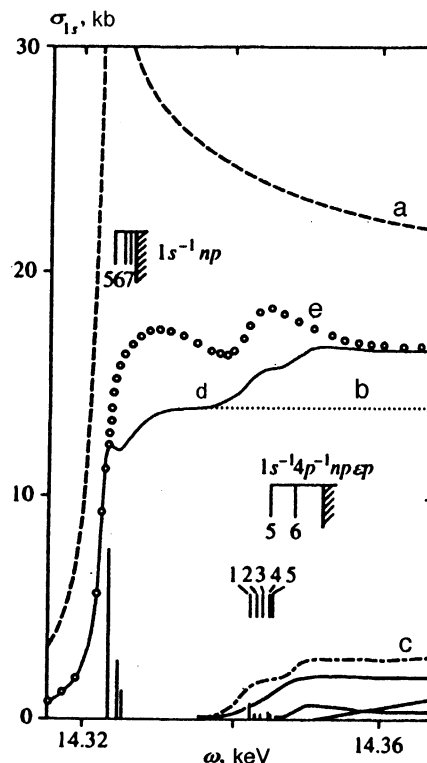

FIG. 2. The cross section for absorption of an x-ray photon by the $1s$-shell of the Kr atom (the theory developed in this paper): curve a, approximation 1; curve b, approximation 2; curve c, the total cross section of one-photon double excitation/ionization; the curves below c are the partial cross sections of one-photon double excitation/ionization for $n=5$, 6, and ε, respectively; curve d, approximation 3; and curve e, the experimental data of Ref. 11. The identification of the double photoionization states denoted by numbers is given in the text. The decay width of the $1s$-vacancy is $\Gamma_{1s}=2.69eV$ (see Ref. 24), and ω is the energy of the absorbed photon.

dispersion terms in the elastic scattering amplitude for these shells were obtained in approximation 1.

To identify the main virtual photoionization processes in the anomalous-dispersion scattering range, we calculated the cross section for absorption of an x-ray photon by a Kr atom near the ionization threshold of the $1s$-shell:

$$\sigma_{1s}(\omega) = \frac{4\pi^2}{3c} S_{m>F} \, \rho_{1s}(\omega,\omega_m)\omega_m |D_{1s}^{mp}|^2, \qquad (13)$$

where we have defined the Cauchy–Lorentz spectral function ρ as follows:

$$\rho_{1s}(\omega,\omega_m) = \frac{\Gamma_{1s}}{2\pi}\left[(\omega-\omega_m)^2 + \frac{\Gamma_{1s}^2}{4}\right]^{-1}.$$

When calculating the discrete structure of the cross section (13) for photon energies below the ionization threshold of the $1s$-shell, we allow in all approximations only for the transitions to the virtual $5p$-, $6p$-, and $7p$-states of the photoelectron that have the highest intensities (Fig. 2). These transitions result in a broad resonance in the theoretical elastic scattering spectrum in the region $\omega \approx 14\,325 \pm 3$ eV (Fig. 3).

The calculated value of the ionization threshold of the $1s$-shell of the Kr atom is $\omega_{1s} = 14\,325.911$eV (here we have allowed for the total relativistic correction $\Delta\omega_{1s}=224.0eV$;

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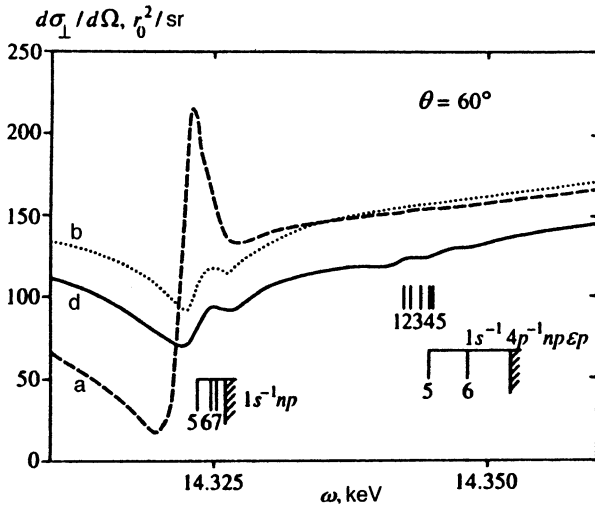$d\sigma_\perp/d\Omega,\ r_0^2/\mathrm{sr}$

FIG. 3. Differential cross section of elastic scattering of a linearly polarized x-ray photon by the Kr atom near scattering resonances (the notation is the same as in Fig. 2); ω is the energy of the scattered photon.

TABLE I. Dependence of $\eta_\perp(\omega;\theta)$ for the Kr atom on the scattering angle θ at $\omega_{1s}=14325.911$ eV.

θ	0°	30°	60°	90°	120°
$\eta_\perp(\omega;\theta)$	0.90	0.81	0.64	0.39	0.23

see Ref. 23). For the total decay width of the $1s$-vacancy we have taken the theoretical value $\Gamma_{1s}=2.69\mathrm{eV}$ (see Ref. 24).

The discrete part of the near fine structure of the absorption spectrum of an x-ray photon by the $1s$-shell of the Kr atom (Fig. 2) is caused by transitions to the following states:

$$|1\rangle=-0.8\gamma_3 5p^2(^3P)+0.5\gamma_1 4d^2(^1D),$$

$$|2\rangle=0.7\gamma_1 5p^2(^1D)-0.5\gamma_3 4d^2(^3P),$$

$$|3\rangle=0.5\gamma_3 5p6p(^3D),\qquad(14)$$

$$|4\rangle=0.7\gamma_1 5p6p(^1D),$$

$$|5\rangle=0.5\gamma_1 4d5d(^1D),$$

where $\gamma_{1,3}=1s^1 4p^5(^{1,3}P)$, and in the complete structure of states (10) we have retained the terms with configuration mixing coefficients whose absolute values are at least 0.50. The virtual components $1s^1 4p^5 n_1 dn_2 d$ and $1s^1 4p^5 n_1 sn_2(s,d)$ of the states (14) manifest themselves in the elastic scattering spectrum only through their mixing with the $1s^1 4p^5 n_1 pn_2 p$ components of the transition in the final photoabsorption state, since in the dipole approximation they contribute nothing to the matrix element of the transition operator. Indeed, transitions to the $1s^1 4p^5 n_1 dn_2 d$ states are forbidden in view of the selection rules in the orbital quantum number l, and transitions to the $1s^1 4p^5 n_1 sn_2(s,d)$ states are practically forbidden if we insist that the wave functions of these states must be orthogonal to wave functions of states of the same symmetry but with lower energies. The orthogonality condition specified here and in the building of transition amplitudes of type (9) was realized by employing the Gram–Schmidt orthogonalization procedure.[25]

The channels of one-photon excitation/ionization and double ionization (12) of the Kr atom (Fig. 2) open up at the corresponding energies of the scattered x-ray photon: 14 344.70, 14 348.21, and 14 351.97 eV.

The virtual processes of one-photon double excitation/ionization of the ground state of the Kr atom lead to the

emergence of a faint extended resonance structure in the theoretical elastic scattering spectrum in the range with $\omega\geq 14\ 341\mathrm{eV}$ (Fig. 3).

The results of calculating the characteristics of large-angle elastic scattering of a linearly polarized x-ray photon by a Kr atom in the anomalous-dispersion scattering range are depicted in Figs. 3–5 and listed in Table I.

The main conclusions of the present work in accordance with these results are given below.

1. The effect of monopole transformation of electron shells in the field of the virtual $1s$-vacancy leads to (Fig. 3)

(a) a strong suppression of the amplitudes and a shift toward the short-wave energies of resonances calculated in approximation 1;

(b) a redistribution in the intensity of scattering calculated in approximation 1 from the short-wave region of the scattering spectrum to the long-wave region.

2. Allowing for the virtual processes of one-photon double $1s^{-1}4p^{-1}-n_1 l_1 n_2 l_2$ excitation/ionization of the ground state of the Kr atom leads to

(a) a noticeable reduction in the scattering intensity calculated in approximation 2 (Fig. 3). For instance, at a scattering angle θ of 60° and x-ray photon energies close to the ionization threshold of the $1s$-shell, the scattering intensity is reduced by approximately 20–25 percent. In turn, this result allows for a radical refinement of the theoretical description of the "degree of opacity" of the atomic system, i.e., its ability to elastically scatter the incident x-ray radiation. For instance, when the x-ray photon energies are near the ionization threshold of the $1s$-shell of the Kr atom, the behavior of the "degree of opacity" of the atom changes not only quantitatively but also qualitatively as we go from approximation 1 to approximation 3;

(b) a redistribution in the intensity of scattering calculated in approximation 2 from the long-wave region of the scattering spectrum to the short-wave region (Fig. 3). Here the result of the effect of the monopole transformation of the electron shells for x-ray photon energies far from the ionization threshold of the $1s$-shell is practicably balanced;

(c) a situation in which the theoretical results of the present work practically coincide with those of the S-matrix formalism of quantum electrodynamics and the experimental data of Ref. 14 for x-ray photon energies considerable higher than the ionization threshold of the $1s$-shell (Fig. 4). The explanation is that in this energy range the cross sections of absorption of an x-ray photon by the $1s$-shell of the Kr atom calculated in approximations 1 and 3 practically coincide.

3. As the scattering angle grows, the relative effect of the monopole transformation of the electron shells in the field of the virtual $1s$-vacancy and the virtual processes of one-photon multiple excitation/ionization of the ground state of
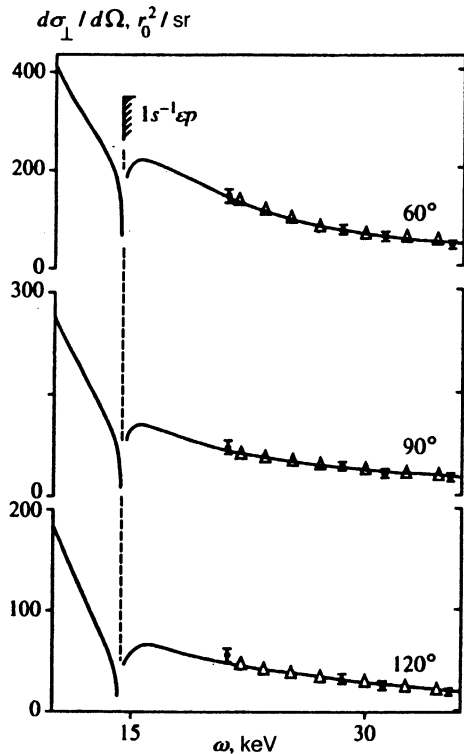
FIG. 4. Differential cross section of elastic scattering of a linearly polarized x-ray photon by the Kr atom far from scattering resonances. The dots and triangles stand for the experimental and theoretical data of Ref. 14, and the solid curves follow from the theory developed in the present paper (approximation 3).
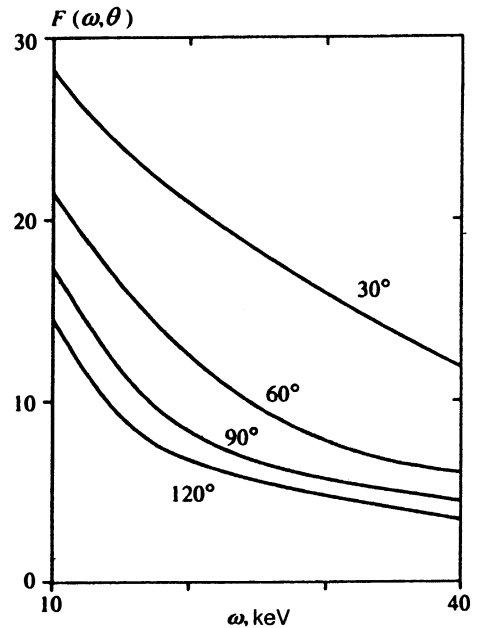

FIG. 5. The form factor of the Kr atom vs the scattering angle θ in the anomalous-dispersion range of energies Ω of the scattered x-ray photon (the theory developed in the present paper).

the Kr atom on the differential elastic scattering cross section increases. To illustrate this, we define the quantity

$$\eta_\perp(\omega;\theta) = \frac{(d\sigma_\perp/d\Omega)_3}{(d\sigma_\perp/d\Omega)_1}, \qquad (15)$$

which characterizes the degree of suppression or enhancement of the theoretical intensity of elastic scattering of a linearly polarized x-ray photon by the Kr atom as we go from approximation 1 (the subscript 1) to approximation 3 (the subscript 3). Table I illustrates the dependence of (15) on the scattering angle for the x-ray photon energy equal to the ionization threshold of the $1s$-shell of the Kr atom. Two factors determine the behavior of (15): the dependence of the form factor (5) of the Kr atom on the scattering angle and energy of the x-ray photon (Fig. 5), and the fact that the anomalous-dispersion terms in the elastic scattering amplitude in the dipole approximation for the matrix element (7) of the transition operator are independent of the scattering angle. Such a decrease in the form factor when the scattering angle grows with the energy of the scattered x-ray photon fixed is equivalent to a decrease in its relative effect on the differential elastic scattering cross section in the anomalous-dispersion scattering region. The fact that in the process the relative role of the anomalous-dispersion terms in the elastic scattering amplitude grows leads to a situation in which the quantity specified by (15) noticeably differs from unity.

4. As the electric charge of the atomic nucleus is increased, the region in which many-electron effects strongly

affect the differential elastic scattering cross section in the anomalous-dispersion energy range of the x-ray photon corresponds to large scattering angles. This is a corollary of the previous conclusion and the fact that, according to Eq. (5), at a zero scattering angle the atomic form factor coincides with the charge of the nucleus. Thus, for heavy atoms the predictions of the theoretical models based on the independent-particle approximation in describing the wave functions of the atomic states should differ considerably from the experimental data primarily for large scattering angles. This fact was mentioned in the Introduction.

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