01

Double Compton scattering of a photon by an atomic ion

© A.N. Hopersky, A.M. Nadolinsky¶

Rostov State University for Railway Transportation,
344038 Rostov-on--, Russia

¶e-mail: amnrnd@mail.ru

Received January 17, 2023
Revised February 15, 2023
Accepted February 16, 2023.

The analytical structure, absolute values, and angular anisotropy of the four-fold differential cross sections of the nonlocal and local double Compton scattering are theoretically predicted when an X-ray photon is scattered by a multicharged helium-like atomic ion.

Keywords: Helium-like ion, X-ray photon, inelastic scattering, four-fold differential cross sections, angular anisotropy.

DOI: 10.61011/EOS.2023.04.56365.4538-22

Introduction

Scattering of a photon by an electron with the emission of two photons (double Compton scattering) is one of the fundamental processes in the microcosm. A large number of experimental [1–5] and theoretical [6–10] papers are devoted to his research. In the present work, we carry out the first theoretical study of this process in the scattering of a photon by an atomic ion. In this case, the photon absorbed by the atomic ion gives rise to a virtual electron of a continuous energy spectrum, and the probability amplitudes of the double nonlocal (radiation at different space-time points (Fig. 1, *a*)) and local (radiation at one spatiotemporal point (Fig. 1, *b*)) Compton scattering arise as substructures of the full amplitude of the scattering probability. 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 [11,12]. A helium-like ion of a neon atom (Ne^{8+}, nuclear charge $Z = 10$, configuration and term of the ground state $[0] = 1s^2[^1S_0]$) was taken as the object of study. The choice is due to the spherical symmetry of the ground state of the Ne^{8+} ion, its accessibility in the gas phase during high-precision experiments, for example, with an X-ray free electron laser [13], and the pronounced presence of its (r, i, f) - triplet of $K\alpha$- lines in observed X-ray emission spectra from hot astrophysical objects [14,15].

Method theory

Let us overview the processes of nonresonant inelastic scattering of a photon by a helium-like atomic ion:

$$\omega + [0] \to X \to \begin{Bmatrix} K_s \\ K_d \end{Bmatrix} \to W, \tag{1}$$

$$X = 1sxp(^1P_1), \tag{2}$$

$$\begin{Bmatrix} K_s \\ K_d \end{Bmatrix} = \begin{Bmatrix} 1sys(^1S_0) \\ 1syd(^1D_2) \end{Bmatrix} + \omega_n, \quad n = 1, 2, \tag{3}$$

$$W = 1s\varepsilon p(^1P_1) + \omega_1 + \omega_2, \tag{4}$$

$$\omega + [0] \to X \to W. \tag{5}$$

In (1), (3), (4), (5) and further, the atomic system of units ($e = \hbar = m_e = 1$), $\omega\,(\omega_n)$ — energy of the incident (scattered) photon, $x(\varepsilon)$ — electron energy of the continuous spectrum of the intermediate (final) scattering state, $x \in [0; \infty)$, $\varepsilon = \omega - I_{1s} - \omega_1 - \omega_2$, I_{1s} — shell ionization threshold energy $1s^2$. Scattering along the channel (1) corresponds to nonlocal double Compton scattering (Fig. 1, *a*) along the radiative transition operator:

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

where $\hat{p}_n$ — the momentum operator$n$- of the electron, $\hat{A}_n$ — the electromagnetic field operator in the second quantization representation, c — the speed of light in vacuum, N — the number of electrons in the ion. Scattering along channel (5) corresponds to local Compton scattering (Fig. 1, *b*) according to the contact interaction operator:

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

When constructing the scattering probability amplitudes, the third order (in terms of the fine structure constant) of the quantum-mechanical perturbation theory is taken. Meanwhile, the probability amplitudes of spontaneous production „of particles“ (photons, electrons, vacancies) before the moment of photon absorption (Fig. 1, *c, d*) are discarded (Tamm–Dankov approximation [16]).

Analytical structures of four times differential scattering cross sections for channels (1) and (5) were obtained by methods of the algebra of photon creation (destruction)

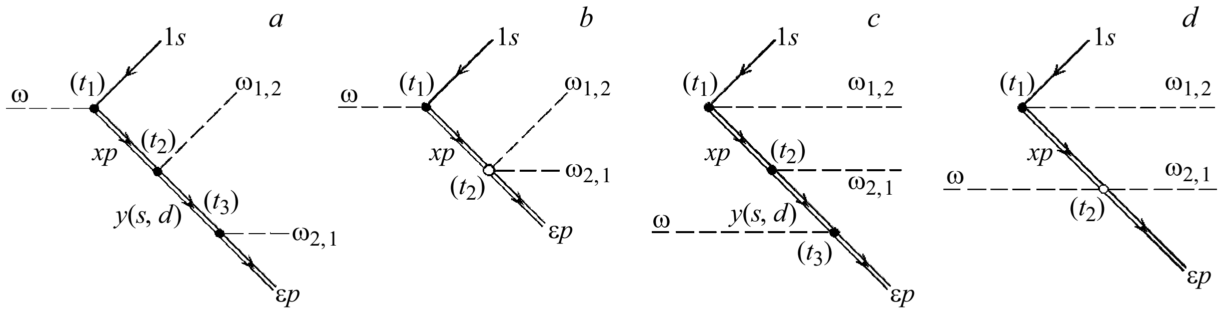

Figure 1. Probability amplitudes of inelastic photon scattering by a helium-like atomic ion (Ne^{8+}) in the representation of Feynman diagrams: (a) nonlocal double Compton scattering, (b) local double Compton scattering, (c, d) scattering „over – time – ago". Right arrow — electron, left arrow — vacancy. Double line — the state was obtained in the Hartree-Fock field of the $1s$--vacancy. Black (light) circle — top of radiative (contact) transition, $\omega(\omega_n)$ — incident (scattered) photon. Time direction — left to right ($t_1 < t_2 < t_3$).

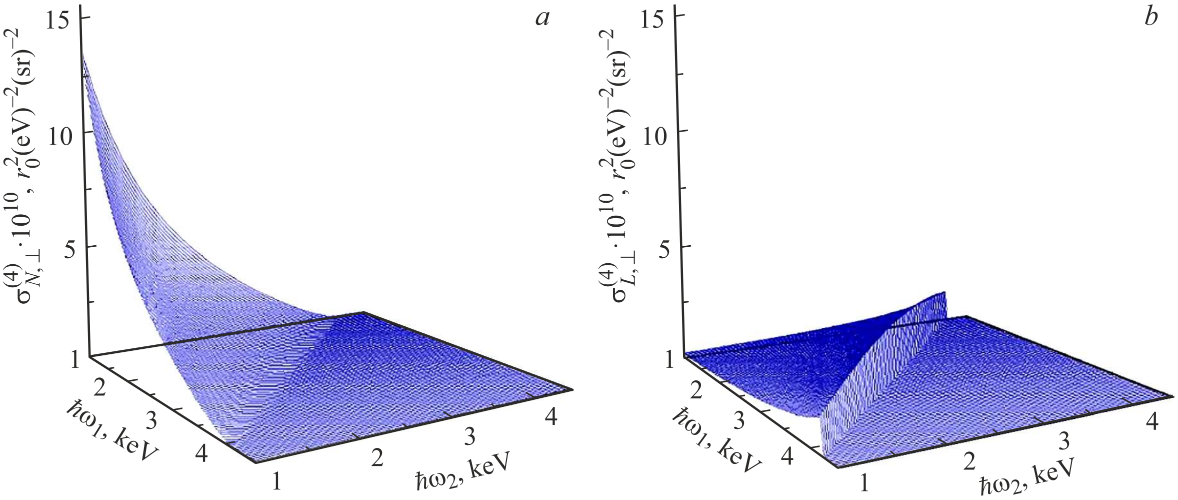

Figure 2. Partial quadruple differential cross sections for inelastic photon scattering by a Ne^{8+} ion for the $\perp$ - experimental scheme: cross section of (a) nonlocal ($\rho^{\perp} = 1$) and (b) local ($\mu^{\perp} = 1$) double Compton scattering. Angle of scattering $\theta = 90°$. Incident photon energy $\hbar\omega = 6.40$ keV, $\hbar\omega_n$ — scattered photon energy ($n = 1, 2$).

operators, the theory of irreducible tensor operators, and the theory of non-orthogonal orbitals [17] in the approximation of zero natural disintegration width 1s-vacancies. For the cross section of nonlocal double Compton scattering (NDCS, Fig. 1,a, 2,a) in the dipole approximation for the $\hat{R}$- operator, taking into account the quantum interference of virtual scattering states K_s and K_d we have

$$\frac{d^4\sigma_N}{d\omega_1 d\omega_2 d\Omega_1 d\Omega_2} \equiv \sigma_N^{(4)} = r_0^2\,\frac{\omega_1\omega_2}{\omega}\,\beta\rho N^2, \tag{8}$$

$$N = \frac{\sqrt{6}}{5}\,\frac{\varepsilon(\varepsilon + I_{1s})}{\omega_1\omega_2}\,\langle 1s_+/1s_0\rangle\langle 1s_0|\hat{r}|\varepsilon p_+\rangle, \tag{9}$$

where Ω_n — spatial angle of departure of the scattered ω_n-photon, r_0 — classical electron radius, $\beta = \alpha r_0 \in_0 /(a_0\pi^2)$, α — fine structure constant, $\in_0 = 27.21$ and a_0 — Bohr radius. In (9), the indices „0" and „+" correspond to the radial parts of the electron wave functions obtained by solving the equations of the self-consistent Hartree–Fock field for the configurations initial ([0]) and final ([$1s_+$]) states of the ion. In (8) the polarization factor ρ determines the effect of the angular anisotropy of the NDCS cross section of the - process. It is specified according to the three schemes of the supposed coplanar [$\mathbf{k}, \mathbf{k}_n \in P$; $\mathbf{k}\,(\mathbf{k}_n)$ — wave vector of the incident (scattered) photon, P — scattering plane] and axisymmetric (with respect to the vector $\mathbf{k}$) experiment. The first scheme — photon polarization vectors are perpendicular to the scattering plane ($\mathbf{e}, \mathbf{e}_n \perp P$). The second scheme — photon polarization vectors are parallel to the scattering plane ($\mathbf{e}, \mathbf{e}_n \parallel P$). The third scheme — scheme with unpolarized (UP) photons. This results in

$$\rho^{\perp} = 1, \tag{10}$$

$$\rho^{\parallel} = \cos^2\theta + \frac{1}{12\pi}\,\sin^4\theta + f\,\sin^2(2\theta), \tag{11}$$

$$\rho_{NP} = \frac{1}{2}\,(\rho^{\perp} + \rho^{\parallel}), \tag{12}$$

$$f = \frac{1}{4\pi}\left(1 + \frac{1}{16\pi}\right) - \frac{1}{9}\,\frac{(\omega_1 + 2\omega_2)(\omega_2 + 2\omega_1)}{(\omega_1 + \omega_2)^2}, \tag{13}$$

where θ — scattering angle (angle between the vectors $\mathbf{k}$ and $\mathbf{k}_n$). Singular one-electron amplitudes of the emission probability during the transition from continuum to continuum (Fig. 1, a) are obtained in the form of velocity in the plane wave approximation for the radial parts of the wave functions of the continuous spectrum, $|x\rangle \cong \left(\frac{2}{\pi^2 x}\right)^{1/4} \sin(r\sqrt{2x})$:

$$(x-y)\langle xp_+|\hat{r}|y(s,d)\rangle \cong i\sqrt{2x}\delta(x-y), \tag{14}$$

$$(y-\varepsilon)\langle y(s,d)_+|\hat{r}|\varepsilon p_+\rangle \cong i\sqrt{2y}\delta(y-\varepsilon), \tag{15}$$

where δ — delta- Dirac function. The analytical structure of the section (8) qualitatively reproduces the results for single Compton scattering [18]. Namely, the occurrence „of the infrared divergence" of the cross section at $\omega_{1,2} \to 0$ is reproduced:

$$\lim_{\omega_{1,2}\to 0} \sigma_N^{(4)} = \infty, \tag{16}$$

becoming zero of the section at $\varepsilon \to 0$ (Fig. 2, a: line $\omega_1 + \omega_2 = \omega - I_{1s}$ on the plane $(\omega_1,\ \omega_2)$):

$$\lim_{\varepsilon\to 0} \sigma_N^{(4)} = 0, \tag{17}$$

and implementation of the asymptotic condition at $\omega \to \infty$:

$$\lim_{\omega\to\infty} \sigma_N^{(4)} = 0. \tag{18}$$

For the cross section of local double Compton scattering (LDCS; Fig. 1, b, 2, b) outside the framework of the dipole approximation for the operator $\hat{Q}$ we have [19,20]

$$\sigma_L^{(4)} = r_0^2 \frac{\omega_1\omega_2}{\omega} \beta\mu L^2, \tag{19}$$

$$L = \frac{1}{\sqrt{6}} \left(1 - \frac{\omega}{\omega_1 + \omega_2}\right) \langle 1s_+|1s_0\rangle\langle 1s_0|\hat{r}\hat{j}_0(qr)|\varepsilon p_+\rangle, \tag{20}$$

where $\hat{j}_0(qr) = (1/qr)\cdot\sin(qr)$, $q = |\mathbf{k} + \mathbf{k}_2|$ and polarization factor

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

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

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

determines the effect of angular anisotropy of the LDCS process cross section. Let us note that (20) takes into account the factor $1\sqrt{6}$, which was lost in [19,20]. This adjustment does not change the physical results of the papers [19,20]. For the section (19) „there is no infrared divergence", at $\varepsilon \to 0$ a break occurs and the asymptotic condition is satisfied.

Restricting to the mathematically simplest $\perp$ - scheme of the proposed experiment, for the total cross section of double Compton scattering, taking into account the quantum interference of the probability amplitudes of the NDCS (1) process and the LDCS (5) process, we have

$$\sigma_\perp^{(4)} = \chi^2 \sigma_{L,T}^{(4)}, \tag{24}$$

$$\chi = \frac{6}{5}\varepsilon\left(\frac{1}{\omega_1} + \frac{1}{\omega_2}\right) - 1, \tag{25}$$

where $\sigma_{L,T}^{(4)}$ is determined by expression (19) at $\mu^\perp = 1$. As expected, at $\varepsilon \to 0$ $\sigma_{N,\perp}^{(4)} \to 0$ and $\sigma_\perp^{(4)} \to \sigma_{L,\perp}^{(4)}$.

Results and discussion

The calculation results are presented in Fig. 2–4. For the parameters of the sections (8) and (19) the values $I_{1s} = 1.195\,\text{keV}$ [19] and $\omega = 6.400\,\text{keV}$ (energy $K\alpha$- of the emission line of the iron atom [21]) are taken. In this case, the criterion of applicability of the dipole approximation $[\exp(i\mathbf{k}\cdot\mathbf{r}_n) \cong 1]$ for the $\hat{R}$- operator is complied with: $\lambda_\omega/\langle r_{1s}\rangle \gg 1$,where the average shell radius $1s^2$ of the Ne^{8+} $\langle r_{1s}\rangle = 0.08\,\text{Å}$ ion and the wavelength of the radiation incident on the $\lambda_\omega = 1.94\,\text{Å}$ion.

The result in Fig. 2, a demonstrates the leading role of the NDCS -process at $\varepsilon \to \omega - I_{1s}$ (tendency to „infrared divergence" (16)). Meanwhile, taking into account the quantum interference of the scattering channels K_s and K_d from (3) almost doubles the theoretical values of the cross section NDCS- of the process, obtained taking into account only the channel K_s. At I $\varepsilon \to 0$, the LDCS-process becomes leading (Fig. 2, b). The result in Fig. 3 demonstrates the effect of the angular anisotropy of the cross sections of the NDCS- process (Fig. 3, a; predominant scattering in the direction of the angles $\theta = 0°,\ 180°$) and the LDCS- process (Fig. 3, b; predominant scattering in the direction of the angles $\theta = 0°,\ \pm 90°,\ 180°$) for $\parallel$ - experimental scheme and the experiment with unpolarized photons. The results in Fig. 3, a qualitatively reproduce those for single Compton scattering [18,22]. However, these results acquire the following feature — the polarization factors $\rho^\parallel$ and ρ_{NP} formally become mathematically dependent (through the f- function from (13)) on the energies ω_n- of photons. Comparison of the results in Fig. 4, a and Fig. 4, b demonstrates the effect of destructive (quenching) quantum interference of the probability amplitudes NDCS- and LDCS- of processes entering with different signs into the full amplitude of the scattering probability. Meanwhile, the scattering probability is redistributed into the area of dominance of the NDCS- process.

Conclusions

A nonrelativistic version of the quantum theory of the process of double Compton scattering of an X-ray photon by a multiply charged helium-like atomic ion is formulated. (a) energy domains of dominance, (b) effects of angular anisotropy (in the corresponding schemes of the proposed experiment), and (c) effect of destructive quantum interference of nonlocal and local double Compton scattering processes are specified. The results obtained are predictive. The theory can be modified, in particular, by replacing the

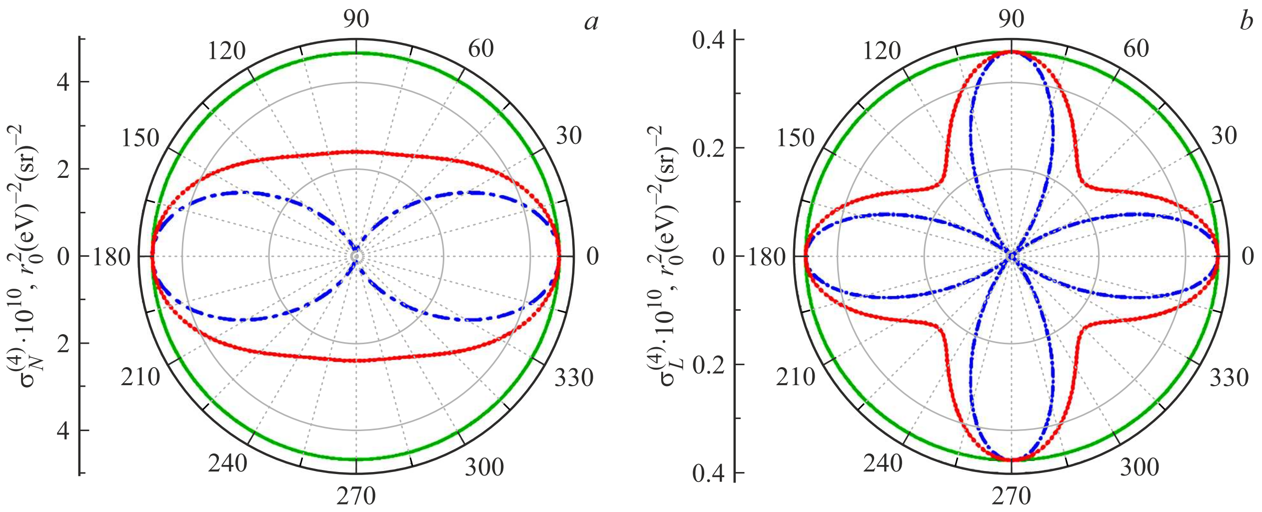

Figure 3. The indicatrices of (*a*) nonlocal (Fig. 2, *a*) and (*b*) local (Fig. 2, *b*) of double Compton scattering of a photon by Ne^{8+} ion with a polar radius $\sigma^{(4)}$ and a polar angle θ at fixed energies of the incident ($\hbar\omega = 6.40\,\mathrm{keV}$) and scattered ($\hbar\omega_1 = \hbar\omega_2 = 1.50\,\mathrm{keV}$) photons. Experiment setup: $\perp$ (solid green curve), $\|$ (dashed-dotted blue curve), unpolarized photons (dashed red curve).

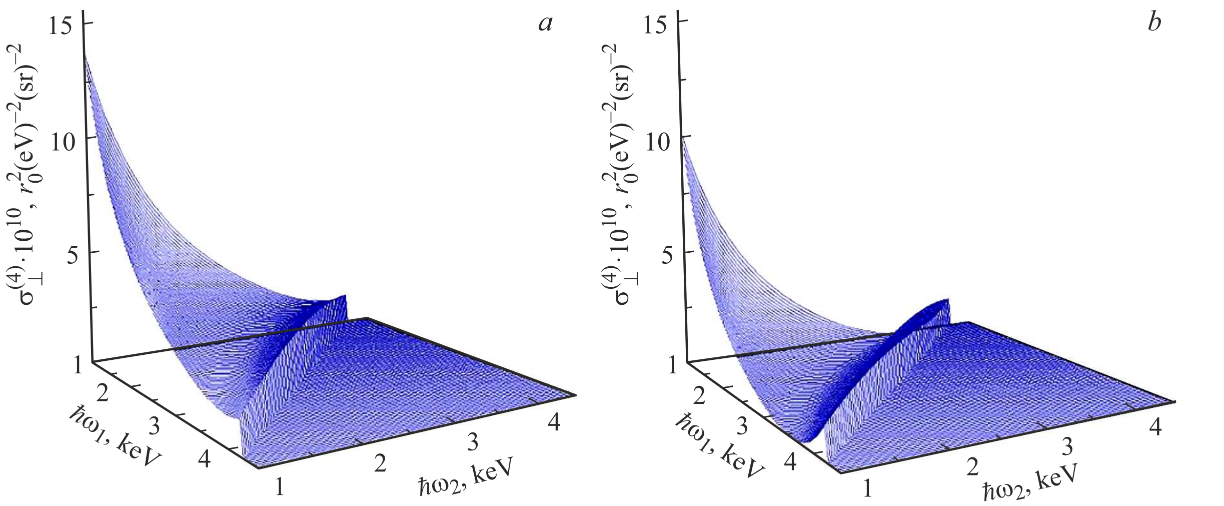

Figure 4. The total quadruple differential cross sections for inelastic photon scattering by a Ne^{8+} ion for the $\perp$ - experimental scheme: (*a*) excluding (sum (8) and (19) at $\rho^\perp = \mu = 1$) and (*b*) taking (24) quantum interference of probability amplitudes of processes of nonlocal and local double Compton scattering. Angle of scattering $\theta = 90°$. Incident photon energy $\hbar\omega = 6.40\,\mathrm{keV}$, $\hbar\omega_n$ — scattered photon energy ($n = 1,\ 2$).

δ- Dirac function in the „golden rule" Fermi [23] with the spectral Gaussian– Laplace function:

$$\delta(\varepsilon - \varepsilon_0) \to G = \frac{1}{\gamma_b\sqrt{\pi}}\exp\left\{-\left(\frac{\varepsilon - \varepsilon_0}{\gamma_b}\right)^2\right\},$$

$$\gamma_b = \frac{1}{2\sqrt{\ln 2}}\Gamma_{beam},$$

to take into account the non-zero width of the spectral resolution of modern experiments (for example, $\Gamma_{beam} = 0.50\,\mathrm{eV}$ in experiments with X-ray free-electron lasers [24] and $\Gamma_{beam} = 5\,\mathrm{eV}$ in astrophysics [25]). Finally, let us add the following. It can be assumed that the experimental detection of the process of double Compton scattering of a photon by an atomic ion is possible, in particular, by the methods of papers [1–5]. In this case, the estimate of the value of the expected double differential cross section for double Compton scattering of a photon by Ne^{8+} $[\sigma^{(2)} \sim 10^{-8}(r_0^2 eV^{-1} sr^{-1})]$ into two– three orders of magnitude smaller than the value of the doubly differential cross section of single Compton scattering of a photon by a helium-like (and „close" to the Ne^{8+} ion) Si^{12+} ion [26].

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] A. Bracci, C. Coceva, C. Colli, E. Lonati. Nuovo Cimento, **3**, 203 (1956). DOI: 10.1007/BF02746210

[2] M.R. Mc Gie, F.P. Brady, W.J. Knox. Phys. Rev., **152** (4), 1190 (1966). DOI: 10.1103/PhysRev.152.1190

[3] B.S. Sandhu, R. Dewan, B. Singh, B.S. Ghumman. Phys. Rev. A, **60**, 4600 (1999). DOI: 10.1103/PhysRevA.60.4600

[4] A. Sharma, M.B. Saddi, B. Singh, B.S. Sandhu. Nucl. Sci. Eng., **148**, 445 (2004). DOI: 10.13182/NSE04-A2470

[5] M.B. Saddi, B. Singh, B.S. Sandhu. Nucl. Technology, **175** (1), 168 (2011). DOI: 10.13182/NT11-A12286

[6] L.M. Brown, R.P. Feynman. Phys. Rev., **85** (2), 231 (1952). DOI: 10.1103/PhysRev.85.231

[7] F. Mandl, T.H.R. Skyrme. Proc. R. Soc. (London) A, **215** (1123), 497 (1952). DOI: 10.1098/rspa.1952.0227

[8] M. Ram. Phys. Rev. D, **12** (7), 2043 (1975). DOI: 10.1103/PhysRevD.12.2043

[9] W. Heitler. *The Quantum Theory of Radiation* (Dover, N.Y., 1984).

[10] F. Bell, arXiv: 0809.1505 [quant-ph]. DOI: 10.48550/arXiv.0809.1505

[11] P. Beiersdorfer. J. Phys. B, **48** (14), 4017 (2015). DOI: 10.1088/0953-4075/48/14/144017

[12] P. Indelicato. J. Phys. B, **52** (23), 2001 (2019). DOI: 10.1088/1361-6455/ab42c9

[13] G. Doumy, C. Roedig, S.-K. Son, C.I. Blaga, A.D. Di Chiara, R. Santra, N. Berrah, C. Bostedt, J.D. Bozek, P.H. Bucksbaum, J.P. Cryan, L. Fang, S. Ghimire, J.M. Glownia, M. Hoenner, E.P. Kanter, B. Krässig, M. Kuebel, M. Messerschmidt, G.G. Paulus, D.A. Reis, N. Rohringer, L. Young, P. Agostini, L.F. Di Mauro. Phys. Rev. Lett., **106** (08), 3002 (2011). DOI: 10.1103/PhysRevLett.106.083002

[14] Y. Tanaka, H. Uchida, T. Tanaka, Y. Amano, Y. Koshiba, T. Go Tsuru, H. Sano, Y. Fukui. Astrophys. J., **933**, 101 (2022). DOI: 2205.10038

[15] G. Rauw, Y. Naze, C. Motch, M.A. Smith, J.G. Flŏ, R. Lopes de Oliveira. Astron. Astrophys., **664**, A 184 (2022). DOI: 10.1051/0004-6361/202243679

[16] A.L. Fetter, J.D. Waleska. *Quantum Theory of Many-Particle System* (Mc Graw-Hill, N.Y., 1971). DOI: 10.1063/1.3071096

[17] A.N. Hopersky, A.M. Nadolinsky, S.A. Novikov. Phys. Rev. A, **98** (6), 3424 (2018). DOI: 10.1103/PhysRevA.98.063424

[18] P.M. Bergstrom, T. Surič, K. Pisk, R.H. Pratt. Phys. Rev. A, **48** (2), 1134 (1993). DOI: 10.1103/PhysRevA.48.1134

[19] A.N. Hopersky, A.M. Nadolinsky, S.A. Novikov, R.V. Koneev. J. Phys. B, **54** (15), 5601 (2021). DOI: 10.1088/1361-6455/ac04c5

[20] A.N. Hopersky, A.M. Nadolinsky, R.V. Koneev. ZhETF, **162** (1), 27 (2022). (in Russian) DOI: 10.31857/S0044451022070000

[21] A. Shimaguchi, K.K. Nobukawa, S. Yamauchi, M. Nobukawa, Y. Fujita. Publ. Astron. Soc. Japan, **74**, 656 (2022). DOI: 10.48550/arXiv.2203.03136

[22] A.N. Hopersky, A.M. Nadolinsky, I.D. Petrov, R.V. Koneev. ZhETF, **158** (6), 1032 (2020). (in Russian) DOI: 10.31857/S0044451020110000

[23] R. Loudon. *The Quantum Theory of Light* (Oxford Science Publications, 2001).

[24] V.M. Kaganer, I. Petrov, L. Samoylova. Acta Crystallogr. A, **77**, 1 (2021). DOI: 10.1107/S2053273321003697

[25] P. Gandhi, T. Kawamuro, M. Diaz Trigo, J.A. Paice, P.G. Boorman, M. Cappi, C. Done, A.C. Fabian, K. Fukumura, J.A. Garčia, C.L. Greenwell, M. Guainazzi, K. Makishima, M.S. Tashiro, R. Tomaru, F. Tombesi, Y. Ueda. Nature Astron., **6**, 1364 (2022). DOI: 10.1038/s41550-022-01857-y

[26] A.N. Hopersky, A.M. Nadolinsky. Pis'ma v ZhETF, **115** (8), 469 (2022) (in Russian). DOI: 10.31857/S1234567822080110

Translated by E.Potapova