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# Atomic magneto-dipole photoionization

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The special features of magneto-dipole photoionization of $s$-atomic states are analyzed and the possibilities of experimental observation of this effect are discussed. It has been shown that despite the smallness of total cross sections of magnetic processes as compared with electric-dipole ones, the experimental observation of magnetic effects is possible, in principle, if photoelectrons are registered in the directions perpendicular to both the polarization vector of photon and its momentum; i.e. in the directions where the differential cross section of electric-dipole ionization of s-atomic states is close to zero. The possibilities of the derived general formulas for the magneto-dipole cross sections are illustrated by numerical calculations for s-subshells of He and Be atoms.

The investigation of atomic photoeffect has started more than eighty years ago (see, e.g. [1] and references therein). All this period only its electric component was considered, since it was clear that the magnetic contribution is small and almost non-observable. We will show here that the situation nowadays is different and the magnetic photoeffect, being determined to large extent by electron correlations, is at some angles observable and dominative.

The magnetic transitions are due to interacting of the magnetic field of the electromagnetic wave with the electron spin. Within the non-relativistic approach, the electron behaves as a particle having along with the electric charge a magnetic moment $\boldsymbol{\mu} = \boldsymbol{\sigma}/2c$ as well. Here $c$ is the speed of light, $\boldsymbol{\sigma}$ is the spin operator[1)]. In the one-electron approximation the Pauli equation for the atomic electron in the presence of the vector-potential $\mathbf{A}$ and scalar potential $\Phi$ has the form [2]

$$I\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \left[\frac{1}{2}\left(\mathbf{p}-\frac{1}{c}\mathbf{A}\right)^2 + V(r) + \Phi - \frac{1}{2c}(\boldsymbol{\sigma}\cdot\mathrm{rot}\,\mathbf{A})\right]\psi(\mathbf{r},t). \quad (1)$$

Here $\mathbf{r}$ and $\mathbf{p}$ are the electron coordinate and momentum, $V(r)$ is the spherically symmetric self-consistent potential of the nuclei and other atomic electrons. Choosing the calibration of the 4-vector-potential as $\mathrm{div}\mathbf{A} = 0$ and $\Phi = 0$, and neglecting the term $\sim \mathbf{A}^2$ in Eq. (1), we write the Hamiltonian of electron interaction with the electromagnetic field as follows

$$\hat{H}_{\mathrm{int}} = -\frac{1}{2}\left[(\mathbf{A}\cdot\mathbf{p}) + \frac{1}{2}(\boldsymbol{\sigma}\cdot\mathrm{rot}\,\mathbf{A})\right]. \quad (2)$$

[1)] Throughout the paper we use the atomic system of units $e = m = \hbar = 1$.

The vector-potential of radiation propagating as a plane wave with the wave vector $\boldsymbol{\kappa}$ and frequency $\omega$ can be written in the form

$$\mathbf{A} = A_0\mathbf{e}\cos(\boldsymbol{\kappa}\cdot\mathbf{r} - \omega t). \quad (3)$$

Let us choose a coordinate system where the photon polarization vector $\mathbf{e}$ is directed along the $Z$-axis and the photon wave vector $\boldsymbol{\kappa}$ along the $X$-axis. In this coordinate system the Hamiltonian of interaction Eq. (2) is presented in the following form

$$\hat{H}_{\mathrm{int}} = -\frac{A_0}{2c}\left\{\left[(\mathbf{e}\cdot\mathbf{p}) - \frac{i}{2}\kappa(\boldsymbol{\sigma}\cdot\mathbf{j})\right]e^{-i(\boldsymbol{\kappa}\cdot\mathbf{r}-\omega t)} + \left[(\mathbf{e}\cdot\mathbf{p}) + i\frac{1}{2}\kappa(\boldsymbol{\sigma}\cdot\mathbf{j})\right]e^{-i(\boldsymbol{\kappa}\cdot\mathbf{r}-\omega t)}\right\}. \quad (4)$$

Here the unit vector $\mathbf{j}$ is directed along the $Y$-axis. The firs term in this formula is responsible for the process of photon adsorption and the second for spontaneous photon emission. The imaginary unit in Eq. (4) corresponds to a phase shift between the electric and magnetic fields of electromagnetic wave and it is evidence of the absence of interference between the terms due to interacting with the electron charge and magnetic moment [3].

Within accuracy up to the second order in photon momentum $\boldsymbol{\kappa}$ a part of the operator (4) responsible for electric transitions accompanying photon absorption is presented in the form

$$H'_{\mathrm{el}} \approx i\frac{A_0}{2c}\left[1 + i(\boldsymbol{\kappa}\cdot\mathbf{r}) - \frac{1}{2}(\boldsymbol{\kappa}\cdot\mathbf{r})^2\right](\mathbf{e}\cdot\nabla)e^{-i\omega t}. \quad (5)$$

A part of this operator corresponding to the magnetic photoionization is

$$\hat{H}'_{\mathrm{mag}} \approx i\frac{A_0\omega}{4c^2}(\boldsymbol{\sigma}\cdot\mathbf{j})e^{-i\omega t}. \quad (6)$$

The terms in Eq. (5) result in the electric-dipole (E1) and electric-quadrupole (E2) electron transitions. The

operator Eq. (6) is responsible for the magneto-dipole transitions (M1) accompanied with spin flip of the optical electron. This operator acts only on the spin parts of the wave functions so the matrix element of the transition due to this operator is simply an overlap integral between the wave functions of the initial and final states of the optical electron. According to these formulas, the amplitude of the magneto-dipole transitions is the same order as the amplitude of the quadrupole transitions. However, because of interference of the dipole (E1) and quadrupole (E2) electric amplitudes, the probability of the magnetic transitions proves to be $1/\alpha$ less than that of the E1–E2 electric transition ($\alpha$ is the fine structure constant).

Because of absence of interference between the photoelectron partial waves generated by the electric and magnetic operators, the differential cross section of an atom is a sum of the cross sections of the photoelectric and photo-magnetic processes

$$\frac{d\sigma_{\rm tot}(\omega)}{d\Omega_k} = \frac{d\sigma_{\rm el}(\omega)}{d\Omega_k} + \frac{d\sigma_{\rm mag}(\omega)}{d\Omega_k}. \qquad (7)$$

Here $d\Omega_k$ is the solid angle in which the electron wave vector $\mathbf{k} = \mathbf{p}$ is as a result of atomic photoionization.

Magneto-dipole photoionization in the s-state results in the isotropic angular distribution of photoelectrons. The differential cross section of this process is defined by the formula

$$\frac{d\sigma_{\rm mag}(\omega)}{d\Omega_k} = \frac{\sigma_{\rm mag}(\omega)}{4\pi}, \qquad (8)$$

where the total magnetic cross section is

$$\sigma_{\rm mag}(\omega) = 2\pi n_s \alpha^3 \omega p M_0^2. \qquad (9)$$

Here $n_s$ is the number of electrons in the $s$-atomic state. The matrix element of the magneto- dipole $s$–$s$-transition with spin flip of the optical electron has the form

$$M_0 = \int R^{\uparrow}_{n0}(r) R^{\downarrow}_{k0}(r) r^2 dr. \qquad (10)$$

The arrows at the radial parts of the photoelectron wave functions designate the directions of electron spin in the bound ns-state and continuum $ks$-one. This integral is non-zero, if exchange between atomic electrons is taken into account.

The asymptotic behavior of the continuum wave function is defined as follows

$$R^{\downarrow}_{k0}(r)_{r\to\infty} \approx (kr)^{-1} \sin(kr + \delta^{\downarrow}_l). \qquad (11)$$

Here $\delta^{\downarrow}_l(k)$ are the phase shifts of the wave functions.

The numerical calculation of the magnetic cross section (9) for He atom was performed in the Hartree–Fock approximation with the codes [4]. First, the wave function of the ortho-He ground state, in which the electrons with opposite spines are in the $1s^{\downarrow}1s^{\uparrow}$-state was calculated. An optical electron in the initial state was described by the function $R^{\uparrow}_{10}(r)$. The continuum wave function is an excited state of para-He. Therefore, the next stage of calculation is that of the ground state $1s^{\downarrow}2s^{\downarrow}$ of para-He, in which both electrons have the same spin. This ground state of para-He is used in calculating the frozen core approximation continuum wave function $R^{\downarrow}_{k0}(r)$. This approximation assumes that the electron wave functions of the atomic core remain unchanged during optical electron transition to the continuum. The wave functions $R^{\uparrow}_{10}(r)$ and $R^{\downarrow}_{k0}(r)$ are used for calculation of the overlapping integral (10) and the cross section (9). The calculations of the para-He wave function $R^{\downarrow}_{k0}(r)$ were performed also for the $1s^{\downarrow}ns^{\downarrow}$ ground states of para-He where the principal quantum number is $n = 3$–$5$. It was found that the results of magnetic cross-section calculations are practically independent of n, which evidences the correctness of the frozen core approach.

The calculation results for $\sigma_{\rm mag}(\omega)$ are presented in Fig. 1. The magnetic cross section of $1s$-photoionization

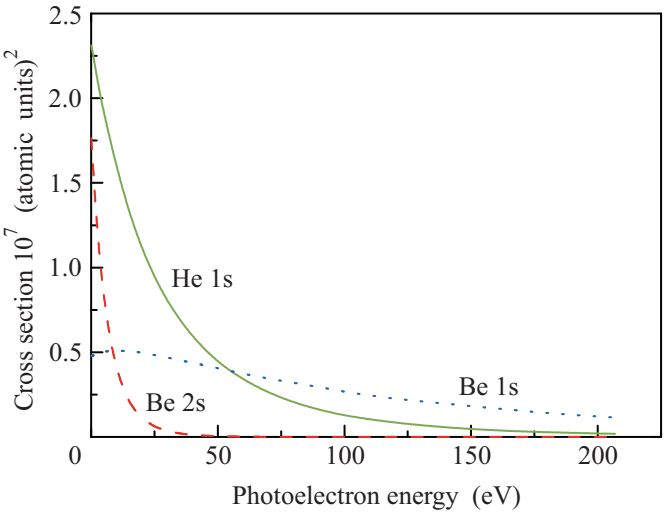


Fig.1

monotonic decreases with the growth of photon energy. At the process threshold the cross-section has the value $\sigma_{\rm mag}(I_{1s}) = 6.64 \cdot 10^{-24}\,{\rm cm}^2$ that is significantly less than the electric cross-sections of atomic photoionization. However the cross-sections of such an order are quite accessible for experimental observation and study (see, for example, [3, 5]). The calculation results of the cross sections for $1s$- and $2s$-subshells of Be atom are derived similar to that for $1s$-shell of He and are also presented in this figure.

In spite of smallness of the magnetic cross section as compared to the electric one, under some conditions the magnetic-dipole transitions become a main channel

of atomic photoionization. Unlike the isotropic angular distribution for magneto-dipole $s$–$s$-photoionization (8), the differential cross section $d\sigma_{\rm el}/d\Omega_k$ has anisotropy form. It is easy to show that within accuracy up to the $\sim\kappa^2$ terms the cross section $d\sigma_{\rm el}/d\Omega_k$ is defined by a linear combination of the following spherical functions: $Y_{10}(\mathbf{k})$, $Y_{2\pm1}(\mathbf{k})$, $Y_{30}(\mathbf{k})$ and $Y_{3\pm2}(\mathbf{k})$ [6]. Here $Y_{lm}(\mathbf{k}) \equiv Y_{lm}(\vartheta_k, \varphi_k)$, where $\vartheta_k$ and $\varphi_k$ are the polar and azimuthal angles of the vector $\mathbf{k}$ in the above described coordinate system. All these spherical functions go to zero for $\vartheta_k = \varphi_k = \pi/2$ [7]. Hence in experiment registering photoelectron emission in the direction of the $Y$-axis the electric cross section is $d\sigma_{\rm el}/d\Omega_k = 0$[2)], the differential photoionization cross section (7) is equal to the magneto-dipole $s$–$s$ one

$$\frac{d\sigma_{\rm tot}}{d\Omega_k}\left(\vartheta_k = \varphi_k = \frac{\pi}{2}\right) = \frac{\sigma_{\rm mag}(\omega)}{4\pi}. \qquad (12)$$

Thus, the study of photoelectron emission at $\vartheta_k = \varphi_k = \pi/2$ opens the possibility of the direct experimental observation of magnetic photoeffect.

A possible scheme of such experiment is given in Fig. 2, where the detector d fixes the photoelectrons

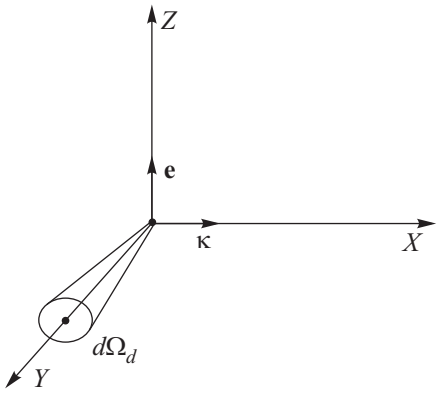


Fig.2

ejecting along the $Y$-axis to a small solid angle

$$d\Omega_d = \int\limits_{\pi/2-\varepsilon/2}^{\pi/2+\varepsilon/2} \sin\vartheta_k \vartheta_k \int\limits_{\pi/2-\varepsilon/2}^{\pi/2+\varepsilon/2} d\varphi_k = \varepsilon^2. \qquad (13)$$

It is evident that the angular size of the detector should be such that the photoelectron current due to electric photoeffect to this detector be small as compared to the magneto-dipole one. For this the following inequality should be met

$$\int\limits_{\pi/2-\varepsilon/2}^{\pi/2+\varepsilon/2} \frac{d\sigma_{\rm el}}{d\Omega_k}\sin\vartheta_k d\vartheta_k \int\limits_{\pi/2-\varepsilon/2}^{\pi/2+\varepsilon/2} d\varphi_k < \frac{d\sigma_{\rm mag}}{d\Omega_k} d\Omega_k. \qquad (14)$$

[2)] The electric cross section along the axis $Y$ is equal to zero for all the orders in photon momentum. It is easy to see it using the plane wave as continuum wave function.

Within accuracy up to the first order in photon momentum $\boldsymbol{\kappa}$ the photoelectric cross section of the atomic s-state photoionization has the form [6]

$$\frac{d\sigma_{\rm el}(\omega)}{d\Omega_k} = \frac{\sigma_{\rm el}(\omega)}{4\pi}[3\cos^2\vartheta_k + \gamma_s(\omega)\cos^2\vartheta_k \sin\vartheta_k \cos\varphi_k]. \qquad (15)$$

Here $\gamma_s(\omega) \sim \kappa$ is one of the nondipole parameters of the photoelectron angular distribution. The terms of the next order $\sim\kappa^2$ in the cross section (15) make a negligibly small contribution to the integral (14). Substituting (15) into (14), we obtain the following limitation for the detector solid angle

$$d\Omega_d < 4\frac{\sigma_{\rm mag}(\omega)}{\sigma_{\rm el}(\omega)}. \qquad (16)$$

Taking into account that the photoionization cross-section of He atom at the threshold has the value $\sigma_{\rm el}(I_{1s}) \approx 8\cdot10^{-18}\,{\rm cm}^2$ [8], we obtain from (16) the following rather rigid limitation for the detector angular size: $d\Omega_d < 3\cdot10^{-6}$ steradian.

It follows from (16) that the less is $d\sigma_{\rm el}(\omega)$, the more favorable is the possibility of experimental observation of magnetic photo-transitions. It is this situation that is realized in the processes of photodetachment of s-states of negative ions (as for any atomic-like system formed by the short-range forces, e.g. deuterons [9], for which the electric dipole photodetachment cross section goes to zero at the processes threshold. Magnetic photodetachment of negative ions we will consider elsewhere.

The experimental discovery and study of here-described magnetic effects is *per se* a new avenue in investigations of electromagnetic radiation interaction with atomic systems, which sheds light on earlier unknown delicate effects of quantum electrodynamics.

1. M. Ya. Amusia, *Atomic photoeffect*, Plenum Press, New York and London, 1990.
2. V. B. Berestetskii, E. M. Lifshitz, and L. P. Pitaevskii, *Relativistic Quantum Theory*, Pergamon Press, Oxford, 1974.
3. S. De Benedetti, *Nuclear Interactions*, John Willey & Sons, Inc., New York–London–Sydney, 1964.
4. M. Ya. Amusia and L. V. Chernysheva, *Computation of Atomic Processes*, Bristol, Philadelphia: "Adam Hilger" Institute of Physics Publishing, 1997.
5. N. Hulthen and M. Sugawara, Handbook of Physics **39**, 112 (1957).
6. J. W. Cooper, Phys. Rev. A **42**, 6942 (1990); **47**, 1841(1993).
7. D. A. Varshalovich, A. N. Moskalev, and V. K. Khersonskii, *Quantum Theory of Angular Momentum*, World Scientific, Singapore-New Jersey-Hong Kong, 1988.
8. J. B. West and G. V. Marr, Proc. Roy. Soc. (London) A **349**, 397 (1976).
9. E. Fermi, Phys. Rev. **48**, 570 (1935).