INFLUENCE OF SPIN–ORBIT COUPLING ON THE INELASTIC SCATTERING OF HIGH ENERGY ELECTRONS

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This paper presents a technique for calculating cross sections of excitation of atoms by fast electrons. To do this a technique of expansion over partial wave functions taking into account the antisymmetric properties of the wave function, is used. The scattering operator takes into account spin–dependent interactions. Using Born approximation we have calculated a cross section of the intercombination transition $1^1S - 3^3S$ of helium atoms. Calculational results show that at energies of electrons about 10 keV *and above the corrections of the scattering operator for relativistic effects should be done.*

Effect of spin symmetry in the scattering theory results in a number of phenomena of the fundamental importance.[1,2] In connection with the development of the polarization spectroscopy the scattering processes leading to the polarization of atomic states are of particular interest. In the case of electron–atom collisions an account of spin characteristics explains an effect of spin polarization of electrons and occurrence of intercombination transitions in atoms.

In the context of the quantum theory of scattering a spin–dependent scattering amplitude is a consequence of exchange effects between the states of a bombarding electron and of an electron in the atom. However, the exchange fraction of the scattering amplitude falls off with increasing energy[4] as ε^{-3} and at energies of several hundreds of electron volts becomes negligible. The other way of taking the spin characteristics of particles into account is to involve relativistic corrections into the scattering operator. In Breit approximation[5] these corrections are described by "spin–own orbit" (H_1), "spin–foreign orbit" (H_2), and "spin–spin" (H_3) interaction operators

$$H_1 = \frac{e^2}{2m^2c^2} \sum_{i=1}^{N} \frac{1}{r_i^3} (\mathbf{l}_i s_i) , \quad (1)$$

$$H_2 = -\frac{e^2}{2m^2c^2} \sum_{i \neq j}^{N} \frac{1}{r_{ij}^3} [\mathbf{r}_{ij}\mathbf{p}_i] (\mathbf{s}_i + 2\mathbf{s}_j) , \quad (2)$$

$$H_3 = -\frac{e^2}{m^2c^2} \sum_{i>j}^{N} \left\{ -\frac{8\pi}{3} \mathbf{s}_i\, \mathbf{s}_j)\, \delta(r_{ij}) + \frac{1}{r_{ij}^3} \times \right.$$

$$\left. \times \left[(\mathbf{s}_i\, \mathbf{s}_j) - \frac{3}{r_{ij}^2} (\mathbf{s}_i\, \mathbf{r}_{ij})\, (\mathbf{s}_j\, \mathbf{r}_{ij}) \right] ,\right\} \quad (3)$$

where $\mathbf{s}_i$ and $\mathbf{l}_i$ are the spin and orbital moments of an electron with the momentum $\mathbf{p}_i$ and radius–vector $\mathbf{r}_i$.

Small parameter (ζ) implicitly entering into the operators describing the spin–dependent interactions well explains their weakness. It can be separated out in an explicit form by considering the dimensional factors of corresponding operators. As a result we obtain that for spin–orbit coupling

$$\zeta = \alpha \frac{\beta}{\sqrt{1 - \beta^2}} \, \mathrm{Ry} \quad (4)$$

and for spin–spin coupling

$$\zeta = 2\, \alpha^2\, \mathrm{Ry} , \quad (5)$$

where α is the fine–structure constant and $\beta = (v/c)$. Consequently, the most essential contribution to the cross section of inelastic scattering comes from the spin–foreign orbit interaction because it explicitly depends on the momentum of a bombarding electron. The cross section of an electron scattering process described by the H_3 operator is proportional to the value $\alpha^4 \ln \varepsilon$, while the cross section of excitation of the intercombination transition of an atom rapidly falls off with increasing energy. The estimates show that for forbidden optical transitions at energies of several keV the contribution from the process described by H_2 operator to the scattering amplitude becomes comparable to that coming from electrostatic interaction.

Mittleman[6] has derived a formula for the cross section of intercombination transition in the Born approximation involving the H_2 operator into the scattering operator. Calculations done for the transition $1^1S - 2^3S$ in the helium atom show that the interaction process described by operator H_2 noticeably contributes to the scattering cross section in the energy range near 8 keV.

In this paper we develop a more general method of calculating the cross section of the atomic excitation that involves the H_2 operator and uses expansion over partial waves.

Let an atomic state, in the case of the LS–type coupling, be described by quantum numbers γ, L_1, S_1, M_{L_1} and M_{S_1} and the state of an incident electron by a wave vector $\mathbf{k}$ and by a spin projection μ on the Z axis. Amplitude of the transition

$$\Gamma = (\gamma_0 L_1 S_1 M_{L_1} M_{S_1};\, \mathbf{k}_0\, \mu_0) - \Gamma' = (\gamma' L_1' S_1' M_{L_1}' M_{S_1}';\, \mathbf{k}\mu)$$

has the form

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$$f_{\Gamma\Gamma'} = -\frac{2\pi m}{h^2} \cdot \langle\Gamma' \,|V|\, \Gamma\rangle , \tag{6}$$

where V is the interaction operator involving the electrostatic interaction and spin–orbit coupling operators

$$V = \sum_{i=1}^{N-1} \frac{e^2}{r_{Ni}} - \frac{e^2 h}{2m^2c^2} \sum_{i=1}^{N-1} \frac{1}{r_{Ni}^3} [\mathbf{r}_{Ni}\, \mathbf{p}_N]\, (\mathbf{s}_N + 2\mathbf{s}_i) . \tag{7}$$

In the general case based on the antisymmetry properties of the wave functions the scattering amplitude is

$$f_{\Gamma'\Gamma} = -\frac{m}{2\pi h^2} \int A\Phi^*_{\gamma'}(\xi)\, \chi^*_{\mu'}(\eta_N) \exp(-\,i\mathbf{k}\mathbf{r}_N)\; V\, \Psi(\zeta)\; \mathrm{d}(\zeta), \tag{8}$$

where A is the antisymmetrizing operator and $\Psi(\zeta)$ is the wave function of the "electron + atom" system.

Now we expand the Ψ function over eigenfunctions of the Hamiltonian of an atom

$$\Psi = \sum_{\gamma\mu} AF_{\gamma\mu}(\mathbf{r})\; \Phi_\gamma(\xi)\; \chi_\mu(\eta_N) . \tag{9}$$

To separate the angular and radial variables let us expand the wave functions of the incident electron before and after the collision over spherical harmonics

$$F_{\gamma\mu} = \sum_{\lambda m} i^{\,\lambda} \sqrt{4\pi\, (2\lambda + 1)}\; g_{\gamma\lambda\mu}(\kappa_0\, r)\; Y_{\lambda_0}(\hat{\mathbf{r}}) , \tag{10}$$

$$e^{i\mathbf{kr}} = 4\pi \sum_{\lambda m} i^{\,\lambda} \sqrt{(2\lambda + 1)}\; j_\lambda(\kappa r)\; Y^*_{\lambda m}(\hat{\mathbf{k}})\; Y_{\lambda m}(\hat{\mathbf{r}}) . \tag{11}$$

Then, by substituting these expansions in Eq. (8) we obtain

$$f_{\Gamma'\Gamma} = -\frac{2m}{h^2} \sum_{\lambda\lambda' m'} i^{\,\lambda-\lambda'} \sqrt{4\pi\, (2\lambda' + 1)\, (2\lambda + 1)}\; Y_{\lambda' m'}(\hat{\mathbf{k}}) \times$$

$$\times \sum_{\gamma\mu} \langle\gamma';\, \lambda'\, m'\, \mu' \,|V|\, \gamma'\, ;\, \lambda 0 \mu\rangle . \tag{12}$$

Let us now pass to the representation of coupled momenta $\boldsymbol{L} = \boldsymbol{L}_1 + \lambda$, $\boldsymbol{S} = \boldsymbol{S}_1 + \boldsymbol{s}$, and $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$, where $\boldsymbol{L}$, $\boldsymbol{S}$, $\boldsymbol{J}$ are the total momenta of the "electron + atom" system. Let us denote the new set of quantum numbers as $\Lambda : \Lambda = L_1\, S_1\, \lambda s\, LS\, JM$. Then the scattering amplitude can be written as

$$f_{\Gamma'\Gamma} = -\frac{2m}{h^2} \sum_{\lambda\lambda' m'} i^{\,\lambda-\lambda'} \sqrt{4\pi\, (2\lambda' + 1)\, (2\lambda + 1)}\; Y_{\lambda' m'}(\hat{\mathbf{k}}) \times$$

$$\times \sum_{\gamma\mu} \sum_{\Gamma|\Lambda\Gamma'|\Lambda'} (\Gamma|\Lambda)(\Gamma'|\Lambda')\, \langle\Lambda'|\mathrm{V}|\Lambda\rangle , \tag{13}$$

where $(\Gamma|\Lambda)$ denotes the coefficient of Γ to Λ transform and is equal to

$$(\Gamma|\Lambda) = \langle L_1 M_{L_1},\, \lambda m | LM_L\rangle\, \langle S_1 M_S,\, s\mu | SM_S\rangle$$

$$\langle LM_L,\, SM_S | JM\rangle . \tag{14}$$

Summation in Eq. (13) is performed over those quantum numbers from the set Λ which do not enter into Γ, i.e., $\Gamma/\Lambda = LM_L SM_S\, JM$.

Matrix elements being involved from Eq. (13) are calculated using the technique of the angular moment theory.[5] In the below formulas we use the following designations for matrix elements of different interactions: $V^{(\mathrm{el})}_{\Lambda'\Lambda}$ for the electrostatic interaction, $V^{(\mathrm{ex})}_{\Lambda'\Lambda}$ for the exchange one, and $V^{(\mathrm{so})}_{\Lambda'\Lambda}$ for the spin–orbit coupling.

$$V^{(\mathrm{el})}_{\Lambda'\Lambda} = (-\,1)^{L+L'_1+L_1+L_0}\, [L'_1,\, L_1,\, \lambda',\, \lambda,\, l',\, l] \times$$

$$\times \sum_\kappa \begin{Bmatrix} L_1 & \lambda' & L \\ \lambda & L_1 & \kappa \end{Bmatrix} \begin{Bmatrix} L'_1 & l' & L_0 \\ l & L_1 & \kappa \end{Bmatrix} F^{\,\kappa}(\gamma\gamma',\, \lambda\lambda') , \tag{15}$$

$$V^{(\mathrm{ex})}_{\Lambda'\Lambda} = (-\,1)^{S'_1+S_1+l'+l+1} \sum_\kappa [L'_1,\, L_1,\, S'_1,\, S_1,\, \lambda',\, \lambda,\, l',\, l] \times$$

$$\times \begin{Bmatrix} \lambda' & l & \kappa \\ L & L_1 & \lambda \\ L'_1 & L_0 & l' \end{Bmatrix} \begin{Bmatrix} 1/2 & S_0 & S_1 \\ 1/2 & S & 1 \end{Bmatrix} G^\kappa(\gamma\gamma',\, \lambda'\, \lambda) , \tag{16}$$

$$V^{(\mathrm{so})}_{\Lambda'\Lambda} = \alpha^4\, [L',\, L,\, S',\, S,\, L'_1,\, L_1,\, S'_1,\, S_1,\, l',\, l,\, \lambda',\, \lambda]\, (3/2)^{1/2} \times$$

$$\times \begin{Bmatrix} L' & S' & J \\ S & L' & 1 \end{Bmatrix} \begin{Bmatrix} S_1 & S & 1/2 \\ S' & S_1 & 1 \end{Bmatrix} \begin{Bmatrix} S_1 & 1/2 & S_0 \\ 1/2 & S'_1 & 1 \end{Bmatrix} \Bigg[\sum_k (-\,1)^\kappa \times$$

$$\times \Bigg\{ \Bigg[(\kappa + 2)\, (2\kappa + 3)\, T_{\kappa+1\ \kappa+1} \begin{Bmatrix} \kappa+1 & 1 & \kappa+1 \\ \lambda & \lambda' & \lambda \end{Bmatrix} +$$

$$+ (2\kappa + 1)\, (2\kappa + 3)\, T_{\kappa+1\ \kappa} \begin{Bmatrix} \kappa+1 & 1 & \kappa \\ \lambda & \lambda' & \lambda \end{Bmatrix} \Bigg] \sqrt{\lambda(\lambda + 1)\, (2\lambda + 1)} \times$$

$$\times R^b_\kappa(\gamma\gamma',\, \lambda\lambda') - \sqrt{(\kappa + 1)\, (\kappa + 2)\, (2\kappa + 3)}\; T_{\kappa+1\ \kappa+1} \times$$

$$\times \xi^b_{\kappa+1}(\gamma\gamma',\, \lambda\lambda') \Bigg\} + \sum_\kappa (-\,1)^\kappa \Bigg\{ \Bigg[\kappa\, (\kappa + 1)\, T_{\kappa\kappa} \begin{Bmatrix} \kappa & 1 & \kappa \\ \lambda & \lambda' & \lambda \end{Bmatrix} +$$

$$+ (2\kappa + 1)\, (2\kappa + 3)\, T_{\kappa\ \kappa+1} \begin{Bmatrix} \kappa & 1 & \kappa+1 \\ \lambda & \lambda' & \lambda \end{Bmatrix} \Bigg] \sqrt{\lambda(\lambda + 1)\, (2\lambda + 1)} \times$$

$$\times R^a_\kappa(\gamma\gamma',\, \lambda\lambda') - \sqrt{\lambda(\lambda + 1)\, (2\lambda + 1)}\; T_{\kappa\,\kappa}(\gamma\gamma',\, \lambda\lambda') \Bigg\} \Bigg], \tag{17}$$

where the following designations are introduced:

$$[j_1,\, j_2,\, \ldots] \equiv \sqrt{(2\, j_1 + 1)\, (2\, j_2 + 1)\, \ldots} , \tag{18}$$

$$F^{\,\kappa}(\gamma\gamma',\, \lambda\lambda') = \begin{pmatrix} l' & \kappa & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda' & \kappa & \lambda \\ 0 & 0 & 0 \end{pmatrix} \times$$

$$\times \int \frac{r^\kappa_<}{r^{\kappa+1}_>} R_{\gamma'}(r_1)\, j_{\gamma'}(\kappa r_2)\, R_\gamma(r_1)\, g_{\gamma\lambda\mu}(\kappa_\gamma\, r_2)\, r_1^2\, r_2^2\, \mathrm{d}r_1\, \mathrm{d}r_2 , \tag{19}$$

$$G^\kappa(\gamma\gamma',\, \lambda\lambda') = \begin{pmatrix} l' & \kappa & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda' & \kappa & l \\ 0 & 0 & 0 \end{pmatrix} \times$$

$$\times \int \frac{r^\kappa_<}{r^{\kappa+1}_>} R_{\gamma'}(r_2)\, j_{\lambda'}(\kappa r_1)\, R_\gamma(r_1)\, g_{\gamma\lambda\mu}(\kappa_\gamma\, r_2)\, r_1^2\, r_2^2\, \mathrm{d}r_1\, \mathrm{d}r_2 , \tag{20}$$

$$R^a_\kappa(\gamma\gamma',\lambda\lambda') = \begin{pmatrix} l' & \kappa & l \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \lambda' & \kappa & \lambda \\ 0 & 0 & 0 \end{pmatrix} \times$$

$$\times \int_0^\infty \mathrm{d}r_2\, j_{\lambda'}(\kappa r_2)\, g_{\gamma\lambda\mu}(\kappa_\gamma r_2)\frac{1}{r_2^{\kappa+1}}\int_0^{r_2} r_1^{\kappa+2} R_{\gamma'}(r_1)\,\mathrm{d}r_1 , \qquad (21)$$

$$R^b_\kappa(\gamma\gamma',\lambda\lambda') = \begin{pmatrix} l' & \kappa & l \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \lambda' & \kappa & \lambda \\ 0 & 0 & 0 \end{pmatrix} \times$$

$$\times \int_0^\infty \mathrm{d}r_2\, j_{\lambda'}(\kappa r_2)\, g_{\gamma\lambda\mu}(\kappa_\gamma r_2) r_2^{\kappa+2}\int_{r_2}^{\infty} \frac{1}{r_1^{\kappa+1}} R_{\gamma'}(r_1)\, R_\gamma(r_1)\,\mathrm{d}r_1 , \qquad (22)$$

$$\xi^a_\kappa(\gamma\gamma',\lambda\lambda') = \begin{pmatrix} l' & \kappa & l \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \lambda' & \kappa & \lambda \\ 0 & 0 & 0 \end{pmatrix} \times$$

$$\times \int_0^\infty \mathrm{d}r_2 j_{\lambda'}(\kappa r_2)\frac{\mathrm{d}}{\mathrm{d}r_2} g_{\gamma\lambda\mu}(\kappa_\gamma r_2)\frac{1}{r_2^{\kappa+1}}\int_0^{r_2} r_1^{\kappa+2} R_{\gamma'}(r_1) R_\gamma(r_1)\mathrm{d}r_1 , \qquad (23)$$

$$\xi^b(\gamma\gamma',\lambda\lambda') = \begin{pmatrix} l' & \kappa & l \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \lambda' & \kappa & \lambda \\ 0 & 0 & 0 \end{pmatrix} \times$$

$$\times \int_0^\infty \mathrm{d}r_2 j_{\lambda'}(\kappa r_2)\frac{\mathrm{d}}{\mathrm{d}r_2} g_{\gamma\lambda\mu}(\kappa_\gamma r_2) r_2^{\kappa+2}\int_0^{\infty} \frac{1}{r^{\kappa+1}} R_{\gamma'}(r_1) R_\gamma(r_1)\mathrm{d}r_1 , \qquad (24)$$

$$T_{\kappa r} = \begin{Bmatrix} L_1' & \lambda' & L' \\ L_1 & \lambda & L \\ \kappa & \mathrm{k} & 1 \end{Bmatrix}\begin{Bmatrix} L_1 & l & L_0 \\ l' & L_1' & \kappa \end{Bmatrix} . \qquad (25)$$

In calculations it is assumed that only an optical electron of an atom takes part in the transitions and that the parentage scheme is valid for the outer electron shell.

Taking into account Eqs. (15)–(17) we can write the scattering amplitude as follows:

$$f_{\Gamma'\Gamma} = -\,2a_0 \sum_{\lambda\lambda' m'} i^{\,\lambda-\lambda'}\sqrt{4\pi\,(2\lambda'+1)\,(2\lambda+1)}\; Y_{\lambda' m'}(\hat{\mathbf{k}}) \times$$

$$\times \sum_{\gamma\mu}\ \sum_{\Gamma|\Lambda\Gamma'|\Lambda'} (\Gamma\,|\,\Lambda)(\Gamma'\,|\,\Lambda')\,[V^{(\mathrm{el})}_{\Lambda'\Lambda} + V^{(\mathrm{ex})}_{\Lambda'\Lambda} + V^{(\mathrm{so})}_{\Lambda'\Lambda}] . \qquad (26)$$

Calculation of matrix elements (15)–(17) is reduced to calculation of radial integrals (19)–(25). To determine an unknown radial function of an incident electron $g_{\gamma\lambda\mu}(r)$ it is necessary to solve the equation

$$D^{(l)}_\beta(r)\, g^{JM}_\beta(r) =$$

$$= \frac{2m}{(h/2\pi)^2}\sum_{\mathrm{b}'}\sqrt{\frac{(2j'+1)}{(2j+1)}}\; i^{\,J'-J} \langle\Lambda\,|\,V\,|\,\Lambda'\rangle\, g^{JM}_{\beta'}(r) , \qquad (27)$$

where β is the set of quantum numbers $\{\gamma, J, j\}$, $D^{(l)}_\beta(r)$ is the differential operator, and $D^{(l)}_\beta(r) = \dfrac{\mathrm{d}^2}{\mathrm{d}r^2} - \dfrac{l(l+1)}{r^2} + \kappa^2\beta$.

In the simplest case of the Born approximation $g_{\gamma\lambda\mu}(r) = j_\lambda(r)\delta_{\gamma\gamma_0}$, where γ_0 denotes the initial atomic state.

The angular dependence of the scattering amplitude is separated out explicitly and is determined by spherical functions $Y_{\lambda' m'}$.

In the region of high energies of electrons a great number of partial waves should be taken into account. The estimates demonstrate that at ε equal approximately 10 keV about 100 partial waves will be needed.

The developed method is applied to calculation of the excitation cross section of the helium atom transition 1^1S – 3^3S. The results of calculations are given in Table I.

As can be seen from the table, the cross section of scattering caused by exchange process between an electron and the electrostatic potential descreases while the cross section corresponding to the spin–orbit coupling increases with increasing ε. Thus at 10 keV their ratio is about 0.14, i.e., the spin–orbit coupling begins to contribute appreciably to the scattering cross section. At higher energies the cross section is determined by the spin–orbit coupling alone, since the cross section of scattering due to exchange processes continues to decrease.

The energy range under study, where the relativistic corrections contribute significantly to the scattering cross section, is now available in experiments. As an example, the gas discharges initiated by a beam of runaway electrons[7] can be mentioned. The energy transfer from the electron component of plasma mainly occurs through allowed optical transitions. Intercombination transitions can be used in this case as a diagnostic mean of the high–energy portion of the electron energy distribution function and its anisotropic characteristics.

TABLE I. Excitation cross sections for the transition $1^1S - 3^3S$ in the helium atom for different energies of an incident electron.

Electron energy,	Excitation cross section, πa_0^2	
keV	exchange	spin–orbit
1	$8.89\cdot10^{-6}$	$6.67\cdot10^{-11}$
2	$1.25\cdot10^{-6}$	$1.26\cdot10^{-10}$
3	$3.93\cdot10^{-7}$	$2.20\cdot10^{-10}$
5	$9.00\cdot10^{-8}$	$1.01\cdot10^{-9}$
7	$3.39\cdot10^{-8}$	$1.44\cdot10^{-9}$
8	$2.30\cdot10^{-8}$	$1.56\cdot10^{-9}$
9	$1.63\cdot10^{-8}$	$1.65\cdot10^{-9}$
10	$1.20\cdot10^{-8}$	$1.72\cdot10^{-9}$

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