Polarization effects in inelastic electron–atom collisions accompanied by a change in the atomic spin

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A theoretical description is given of the polarization effects which occur in three-electron systems in collisions which give rise to singlet–triplet transitions in an atom. The operators of a transition are derived and these make it possible to calculate the polarization of all the electrons of the system as a result of excitation of the atom and a change in its spin by unity. The results of this calculation are in agreement with recent experimental data on the depolarization of electron beams caused by the excitation of triplet atomic states.

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1. INTRODUCTION

Theory of the polarization effects in inelastic collisions of electrons with atoms is developed less than for elastic collisions. In particular, until recently there has been no general theory of polarization effects in collisions of electrons with atoms accompanied by a change in the atomic spin.

The problem has become urgent after the appearance of the experimental paper of Hanne and Kessler,[1] who measured the change in the initial polarization of an electron beam as a result of excitation of one of the triplet levels of the mercury atom. The same authors were subsequently able to determine the depolarization of electrons by exciting separate components of the fine structure of the ^3P level of the mercury atom.[2]

A consistent theory of such processes should include spin variables of all the electrons, incident and atomic, participating in a transition. Clearly, in the simplest case of singlet–triplet transitions, we are dealing with a three-electron system. We shall consider the problem of the polarization of electrons in inelastic collisions in a three-electron system accompanied by a change in the spin. We shall derive the operators of a transition which can be used to calculate in a unified manner the polarization of all the electrons as a result of the exchange excitation of an atom accompanied by a change in its spin by unity. This approach is more general and consistent than that employed by Hanne,[3] who described a three-particle system by an amplitude matrix of a transition in the spin space of one incident electron. Clearly, in this approach it is *a priori* impossible to calculate the polarization characteristics of an atom which appear on transition to a triplet state resulting from a collision with polarized electrons.

Our results are in agreement with the experimental data given in[2]. It follows from our theory that, in particular, the spin–orbit interaction inside an atom does not polarize an electron beam if there is no initial polarization in the beam. In this respect our results differ from those obtained by Hanne,[3] who concluded that in this situation a polarization should appear in the electron beam.

2. TRANSITION AMPLITUDE

We shall consider inelastic transitions in a two-electron atom ignoring completely at first the spin–orbit interaction between the atomic electrons. Then, the spin S of the atom and its total angular momentum L are conserved separately. We shall denote the quantum numbers representing the state of the atom and incident electron by LSM_LM_S and sm_s. We shall select the normal to the scattering plane as the quantization axis:

$$\mathbf{n}=[\mathbf{k}\times\mathbf{k}']/|[\mathbf{k}\times\mathbf{k}']|$$

($\mathbf{k}$ and $\mathbf{k}'$ are the wave vectors of an electron before and after scattering). The scattering amplitude is a matrix of the spin variables. Elements of this matrix can be represented in the form

$$g_{LM_L}(E,\vartheta)\langle S'M_S'^{1}/_{2}m_s'|\hat{A}|SM_S{}^{1}/_{2}m_s\rangle, \tag{1}$$

where the function g_{LM_L} depends on the scattering angle ϑ and the initial electron energy E.

The operator $\hat{A}$ governs all the polarization characteristics of electrons and atoms and the changes in these characteristics as a result of an inelastic collision. The explicit form of the operator $\hat{A}$ can be found by introducing the state vectors $|SM_S\frac{1}{2}m_s\rangle$, expressed in terms of one-electron spinors α and β. The spinor α describes a state with a positive projection of the spin on the quantization axis and the spinor β describes a corresponding state with the negative projection. If we use the index 1 for the incident electron and the indices 2 and 3 for the atomic electrons, the vector of the three-electron system with the atom initially in the singlet state can be described by

$$|00^{1}/_{2}{}^{1}/_{2}\rangle=2^{-1/2}\alpha_1(\alpha_2\beta_3-\alpha_3\beta_2). \tag{2}$$

The eigenvectors of the system, corresponding to the triplet state of the atom with the spin projections $M_S=0$ and $M_S=\pm1$, are, respectively,

$$\left.\begin{aligned}&|10^{1}/_{2}{}^{1}/_{2}\rangle=2^{-1/2}\alpha_1(\alpha_2\beta_3+\alpha_3\beta_2),\\ &|11^{1}/_{2}-{}^{1}/_{2}\rangle=\beta_1\alpha_2\alpha_3,\quad |1-1^{1}/_{2}{}^{1}/_{2}\rangle=\alpha_1\beta_2\beta_3.\end{aligned}\right\} \tag{3}$$

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We shall introduce an operator $\hat{A}(M_S)$ which transforms the initial state into one of the final states in accordance with the definition

$$\hat{A}(M_S)\,|SM_S{}^1/_2m_s\rangle=|S'M_S'{}^1/_2m_s'\rangle. \tag{4}$$

The operator $\hat{A}$ should contain combinations of the spin matrices σ_1, σ_2, and σ_3 and of the vector $\mathbf{n}$, which are invariant under rotation, reflection, and coordinate-shift transformations. These combinations are

$$\sigma_1\sigma_2,\ \sigma_1\sigma_3,\ \sigma_2\sigma_3,\ \sigma_1\mathbf{n},\ \sigma_2\mathbf{n},\ \sigma_3\mathbf{n}.$$

We can easily check that in the case of a transition accompanied by the spin change $S=0\to S'=1$, we have

$$\left.\begin{aligned}\hat{A}(M_S=0)&=-{}^1/_2(\sigma_1\mathbf{n})\,[\,(\sigma_2\mathbf{n})-(\sigma_3\mathbf{n})\,],\\ \hat{A}(M_S=\pm1)&=2^{-1/2}\{\sigma_1(\sigma_2-\sigma_3)-(\sigma_1\mathbf{n})\,[\,(\sigma_2\mathbf{n})-(\sigma_3\mathbf{n})\,]\}.\end{aligned}\right\} \tag{5}$$

If the components of the term with different values of M_S can be regarded as degenerate, we can introduce a more general operator $\hat{A}$ which transforms the initial singlet state into a triplet state representing a superposition of states with different values of M_S. In accordance with the law of conservation of the total spin of the system ($j=1/2$), a superposition of such states can be represented by the vector

$$\chi=6^{-1/2}[2\beta_1\alpha_2\alpha_3-\alpha_1(\alpha_2\beta_3+\alpha_3\beta_2)\,], \tag{6}$$

and we can easily show that the operator satisfying

$$\hat{A}\,|00{}^1/_2{}^1/_2\rangle=\chi, \tag{7}$$

is

$$\hat{A}=\frac{1}{2\cdot3^{1/2}}\sigma_1(\sigma_2-\sigma_3). \tag{8}$$

We can demonstrate that this operator transforms purely triplet states with a fixed value of M_S into the state $|00\,\frac{1}{2}m_s\rangle$.

We shall now calculate the polarization characteristics of electrons after scattering and we shall do this in the general case of mixed states.

3. TRANSITIONS IN THE *LS*-COUPLING APPROXIMATION

We shall assume that the atom under consideration is initially in a singlet state. Then, the initial density matrix of the whole system is

$$\rho={}^1/_8(I+\mathbf{p}\sigma_1)\otimes(I\otimes I-\sigma_2\otimes\sigma_3). \tag{9}$$

Here, I is a two-dimensional unit matrix and the symbol $\otimes$ denotes a direct product of the matrices. After scattering accompanied by the excitation of the atom, the density matrix becomes

$$\rho'=\sum_{M_SM_L}\hat{A}\rho\hat{A}^+|g_{LM_L}|^2=3\hat{A}\rho\hat{A}^+\sum_{M_L}|g_{LM_L}|^2, \tag{10}$$

where $\hat{A}$ is given by Eq. (8) and the vector $\mathbf{p}$ represents the initial polarization of the electron beam.

The excitation cross section is

$$\sigma=(k'/k)\mathrm{Tr}\,\rho', \tag{11}$$

whereas the average values of the quantities represented by the operator $\hat{L}$ are

$$\langle L\rangle=\mathrm{Tr}\,L\rho'/\mathrm{Tr}\,\rho'. \tag{12}$$

It follows from these calculations that

$$\sigma=3\frac{k'}{k}\sum_{M_L}|g_{LM_L}|^2. \tag{13}$$

Before we give the polarization characteristics of the electrons after the scattering, we can demonstrate directly that they refer to a state in which the atomic spin is $S=1$. In fact, the correlation of electrons in the atom is represented by the average value of the quantity $q_{23}=\langle\sigma_2\otimes\sigma_3\rangle$. Before a collision, we have $q_{23}=-3$, which corresponds to an atom in a singlet state. After the collision, the quantity

$$q_{23}'=\mathrm{Tr}\,(\sigma_2\otimes\sigma_3\rho')/\mathrm{Tr}\,\rho'$$

assumes the value

$$q_{23}'=1, \tag{14}$$

as expected for an atom in a triplet state. The correlation of the other two pairs is $q_{12'}=q_{13'}=-2$ and, consequently,

$$\sum_{k>i}q_{ik}'=-3.$$

We can show that this condition corresponds to the total spin $j=1/2$ of the system, which is conserved in inelastic collisions.

The excitation of an atom by a polarized electron beam causes depolarization of this beam and the atom transferred to the triplet state acquires partial polarization. The degree of depolarization of the beam is characterized by the ratio of the final polarization $p_{1\alpha'}$ of the scattered electrons to the initial polarization $p_{1\alpha}$. In the LS-coupling approximation, this quantity is

$$p_{1\alpha}'/p_{1\alpha}=-{}^1/_3. \tag{15}$$

The polarization of the atom is

$$P_{1\alpha}={}^2/_3p_{1\alpha}. \tag{16}$$

Clearly, the factor which gives rise to the polarization of the atom is the exchange interaction, which redistributes the initial polarization of the electron beam. If initially the beam is not polarized ($p_{1\alpha}=0$), the pure exchange interaction does not give rise to a polarization after the scattering.

We shall now consider triplet–singlet transitions. In this case the initial density matrix is

$$\rho=\frac{1}{8}\Big[I+\sum_\alpha p_{1\alpha}\sigma_{1\alpha}\Big]\otimes\Big[I\otimes I+\sum_{\alpha'}P_{\alpha'}(\sigma_{2\alpha'}\otimes I+I\otimes\sigma_{3\alpha'})+\frac{1}{3}\sigma_2\otimes\sigma_3\Big], \tag{17}$$

where $p_{1\alpha}$ and $P_{\alpha'}$ are the components of the polarization vectors of a continuum electron and of an atom before a collision.

The necessary calculations of the transition cross section give

$$\sigma = \frac{k'}{k}(1-\mathbf{p}\cdot\mathbf{P})\sum_{M_L}|g_{LM_L}|^2. \tag{18}$$

The cross section depends on the scalar $\mathbf{p}\cdot\mathbf{P}$ and it vanishes for $\mathbf{p}\cdot\mathbf{P}=1$. This circumstance agrees with the Wigner rule of conservation of the total spin. In fact, if $\mathbf{p}\cdot\mathbf{P}=1$, the total spin of the system is 3/2, but in the final channel it is 1/2.

A calculation based on pair spin correlations shows that after the scattering the atom now goes over to a singlet state. It follows from the calculations that

$$q_{23}'=-3;$$

this corresponds to the spin $S=0$. We can also show that the condition

$$\sum_{k>i} q_{ik}'=-3,$$

corresponding to the conservation of the initial spin of a three-electron system, is satisfied by the transition in question.

An independent check of this formulation of the problem is provided by a calculation of the polarization of an atom formed with the spin $S=0$, which is exactly zero. A calculation gives the expected result $P_{\alpha'}=0$.

The electron polarization after an inelastic transition is

$$p_{1\alpha}'(1-\mathbf{p}\cdot\mathbf{P})=(P_\alpha-{}^1/_3 p_{1\alpha}). \tag{19}$$

Hence, it follows that if an atom is initially unoriented ($P_\alpha=0$), the depolarization of the electron beam is

$$p_{1\alpha}'/p_{1\alpha}=-{}^1/_3.$$

A more interesting case is provided by a situation in which an unpolarized electron beam is scattered by an oriented atom. It follows from Eq. (19) that the scattered beam acquires a polarization equal to the initial polarization of the atom:

$$p_{1\alpha}'=P_\alpha. \tag{20}$$

Thus, the exchange interaction in a triplet–singlet transition results in a complete transfer of the initial atomic polarization to the scattered electrons. It is important to draw attention to the circumstance that the polarization of these electrons is independent of the scattering angle or initial energy. This allows us to consider the triplet–singlet transition as a possible mechanism for generating polarized electrons.

A situation of this kind may be realized, for example, in the process

$$\mathrm{He}(2\,{}^3S)\uparrow + e \to \mathrm{He}(1\,{}^1S) + e(\uparrow), \tag{21}$$

where helium atoms are first oriented in some way by, for example, optical pumping.

The results obtained are a function of the type of binding. In the next section we shall allow for the multiplet structure of a level resulting from the spin–orbit interaction inside an atom.

4. ALLOWANCE FOR THE MULTIPLET STRUCTURE IN THE *LS*-COUPLING APPROXIMATION

If the spin–orbit interaction inside an atom is slight, then—in the first approximation—a state $|^{2S+1}L;\, JM_J\rangle$ can be produced from a state $|SLM_SM_L\rangle$ in accordance with the rule:

$$|^{2S+1}L;\, JM_J\rangle = \sum_{M_SM_L} C^{JM_J}_{LSM_LM_S}|LSM_LM_S\rangle, \tag{22}$$

where $C^{JM_J}_{LSM_LM_S}$ are the coefficients of the Clebsch–Gordan vector coupling. The transition matrix becomes

$$\hat{A}(JM_J)=\sum_{M_LM_S} C^{JM_J}_{LSM_LM_S}\hat{A}(LSM_LM_S), \tag{23}$$

where

$$\hat{A}(LSM_LM_S)=g_{LM_L}\hat{A}(M_S).$$

We shall now give the explicit form of the operators $\hat{A}(M_S)$ directing the z axis along the vector n:

$$\left.\begin{aligned}\hat{A}(0)&\equiv A_0=-{}^1/_2\sigma_{1z}\otimes(\sigma_{2z}\otimes I - I\otimes\sigma_{3z}),\\ A(\pm1)&\equiv A_1=2^{-1/2}[\sigma_1\otimes(\sigma_2\otimes I - I\otimes\sigma_3)-\sigma_{1z}\otimes(\sigma_{2z}\otimes I - I\otimes\sigma_{3z})].\end{aligned}\right\} \tag{24}$$

Bearing in mind applications in the special case of excitation of the ^3P_J states, because the experimental results are available for this case,[2] we shall now give the operators $\hat{A}(JM_J)$ for $J=0$, 1, and 2.

1) For $J=0$ and $M_J=0$, we have

$$\hat{A}(00)=3^{-1/2}g_0A_0; \tag{25a}$$

2) for $J=1$ and $M_J=-1$, 0, 1, we obtain

$$\left.\begin{aligned}\hat{A}(11)&=2^{-1/2}(g_0A_1+g_1A_0),\ \hat{A}(10)=-2^{1/2}g_1A_1,\\ \hat{A}(1-1)&=-2^{-1/2}(g_0A_1-g_1A_0);\end{aligned}\right\} \tag{25b}$$

3) for $J=2$ and $M_J=-2$, -1, 0, 1, 2, we find that

$$\left.\begin{aligned}\hat{A}(22)&=g_1A_1,\quad \hat{A}(21)=2^{-1/2}(g_0A_1-g_1A_0),\\ \hat{A}(20)&=-(2/3)^{1/2}g_0A_0,\ \hat{A}(2-1)=2^{-1/2}(g_0A_1+g_1A_0),\ \hat{A}(2-2)=-g_1A_1.\end{aligned}\right\} \tag{25c}$$

The density matrix is

$$\rho'(J)=\sum_{M_J}\hat{A}(JM_J)\rho\hat{A}^+(JM_J). \tag{26}$$

For example, for the excitation of a $^3P_0$ level, this matrix can be written in its explicit form as follows:

$$\rho'(0)={}^1/_{24}|g_0|^2A_0(I+\mathbf{p}\sigma_1)\otimes(I\otimes I-\sigma_2\otimes\sigma_3)A_0^+. \tag{27}$$

The expressions for the matrices $\rho'(1)$ and $\rho'(2)$ are similar although they look much more complex.

5. RESULTS OF CALCULATIONS OF THE POLARIZATIONS AND CROSS SECTIONS IN THE EXCITATION OF ^3P_J STATES

We shall first give the expressions for the excitation cross sections of the individual components of the fine structure of a ^3P level $[\sigma(J)=(k'/k)\mathrm{Tr}\rho'(J)]$:

$$\left.\begin{aligned}\sigma(0)&=(k'/k)\,|g_0|^2/3\equiv(k'/k)\sigma^{(0)},\\ \sigma(1)&=(k'/k)\,(|g_0|^2+3|g_1|^2)\equiv(k'/k)\sigma^{(1)},\\ \sigma(2)&=(k'/k)\,(^5/_3|g_0|^2+3|g_1|^2)\equiv(k'/k)\sigma^{(2)}.\end{aligned}\right\}\qquad(28)$$

In the nonrelativistic limit, when the components of the fine structure are regarded as degenerate, we obtain the total cross section

$$\sigma=(k'/k)\,(3|g_0|^2+6|g_1|^2)=3(k'/k)\sum_{M_L}|g_{LM_L}|^2$$

which is in agreement with Eq. (13).

We shall now consider the polarization of an electron after the excitation of the relevant sublevels. For the $^3P_0$ state, we obtain

$$p'_{x,y}=-p_{x,y},\quad p_z'=p_z,\qquad(29)$$

i.e., the scattering transforms the initial polarization vector $\mathbf{p}(p, \vartheta, \varphi)$ into a vector $\mathbf{p}(p, -\vartheta, \varphi)$; in other words, it rotates the vector through the angle 2ϑ in the $\varphi=\text{const}$ plane. We can show that $q_{23'}=1$, as expected for the transition in question. For a $^3P_1$ level,

$$\left.\begin{aligned}\sigma^{(1)}p'_{x,y}&=-|g_1|^2p_{x,y},\\ \sigma^{(1)}p_z'&=-(|g_0|^2+|g_1|^2)p_z.\end{aligned}\right\}\qquad(30)$$

In the excitation of the $^3P_2$ state,

$$\left.\begin{aligned}\sigma^{(2)}p'_{x,y}&=-(^2/_3|g_0|^2+|g_1|^2)p_{x,y},\\ \sigma^{(2)}p_z'&=-(^1/_3|g_0|^2+|g_1|^2)p_z.\end{aligned}\right\}\qquad(31)$$

In the forward scattering, when the amplitude g_1 vanishes, the values of the components $p_{x,y}$ of the polarization vector orthogonal to the normal n become constant and, in accordance with Eqs. (29)–(31), their values are given by

$$p'/p=-1\ (^3P_0);\quad p'/p=0\ (^3P_1);\quad p'/p=-0{,}4\ (^3P_2).\qquad(32)$$

It follows from the experimental data of Ref. 2 for the $^3P_1$ and $^3P_2$ levels that, within the limits of their error, they are in agreement with the calculated depolarization (32). The experimental conditions under which the depolarization was measured (low near-threshold collision energies and zero scattering angle) were the most favorable for a comparison with the calculations because one could ignore the contribution of the spin–orbit interaction in the continuum, which was not allowed for in our calculations.

Summarizing the results, we can state once again that an exchange transition redistributes the initial polarization. If initially an electron beam and an atom are unpolarized, the pure exchange interaction does not produce any polarization as a result of an inelastic transition. In this respect results differ from the conclusions reached by Hanne,[3] where it is predicted that the polarization should appear as a result of pure exchange excitation. It follows from general considerations that the polarization can appear in an initially unoriented system if allowance is made for the spin–orbit interaction in the continuous spectrum. However, this effect requires separate treatment.

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