

to the  $X$  axis, we have

$$\operatorname{tg} \varphi = \frac{\Pi_1^2 + \Pi_2^2/4 - \Pi_1 \Pi_2 \cos \Delta\omega\tau_s}{\Pi_1^2 + \Pi_2^2 + 2\Pi_1 \Pi_2 \cos \Delta\omega\tau_s} \operatorname{tg} \psi. \quad (30)$$

As a function of  $\tau_s$ , the plane of polarization of the echo executes quantum beats analogous to the quantum beats of the amplitude (20). By measuring the oscillations of the plane of polarization (30) and of the amplitude (20) we can determine not only the energy difference,  $E_2 - E_1$ , but also the dipole moments of the atomic transitions.

In the case of the broad spectral line in the regions (22) and (24) the polarization plane of the echo at  $t' = \tau_s$  oscillates as a function of  $\tau_s$  and the oscillations are likewise described by formula (30). In the region of (25), the obtained effect can be calculated by numerical methods.

The polarization properties of the light echo in a three-level system with  $J_0 = \frac{3}{2}$  and  $J_1 = J_2 = \frac{1}{2}$  are the same as in a two-level system with atomic transition  $\frac{1}{2} \rightarrow \frac{3}{2}$ . Putting  $\pi_1 = 0$  or  $\pi_2 = 0$  in (29) we obtain the amplitude of the photon echo for two-level systems with atomic transitions  $\frac{3}{2} \rightarrow \frac{1}{2}$  or  $\frac{1}{2} \rightarrow \frac{1}{2}$ , respectively.

If the close levels  $E_1$  and  $E_2$  are formed as a result of hyperfine interaction, then according to (26) the ratio (30) takes the simple form

$$\operatorname{tg} \varphi = 2(1 - \cos \Delta\omega\tau_s) \operatorname{tg} \psi / (5 + 4 \cos \Delta\omega\tau_s),$$

from which it follows that the amplitude of the oscillations of the plane of polarization of the echo is large enough for experimental observation of the obtained effect.

Radiative decay and atomic collisions cause the amplitude of the photon echo to attenuate with time  $t$ ,

mainly in accord with the exponential law  $\propto \exp(-t/2t_r)$ , where  $t_r$  is the time of irreversible relaxation. If  $\tau_s \sim t_r$ , then the echo-amplitude oscillations determined above will be superimposed on this damped component. This amplitude damping, however, does not affect the oscillations (30) of the echo-polarization plane.

- <sup>1</sup>I. D. Abella, N. A. Kurnit, and S. R. Hartmann, *Phys. Rev.* **141**, 391 (1966).
- <sup>2</sup>A. I. Alekseev and I. V. Evseev, *Izv. Akad. SSSR Ser. Fiz.* **37**, 2046 (1973).
- <sup>3</sup>L. Q. Lambert, A. Compaan, and I. D. Abella, *Phys. Lett. A* **30**, 153 (1969).
- <sup>4</sup>V. V. Samartsev and V. R. Nagibarov, *Fiz. Tverd. Tela (Leningrad)* **11**, 3669 (1969) [*Sov. Phys. Solid State* **11**, 3085 (1970)].
- <sup>5</sup>L. Q. Lambert, A. Compaan, and I. D. Abella, *Phys. Rev. A* **4**, 2022 (1971).
- <sup>6</sup>S. M. Zakharov and E. M. Manykin, *Zh. Eksp. Teor. Fiz.* **60**, 1867 (1971) [*Sov. Phys. JETP* **33**, 1009 (1971)].
- <sup>7</sup>P. H. Hu, R. W. Leigh, and S. R. Hartmann, *Phys. Lett. A* **38**, 241 (1972); *A* **40**, 164 (1972).
- <sup>8</sup>P. F. Liao, R. W. Leigh, P. H. Hu, and S. R. Hartmann, *Phys. Lett. A* **41**, 285 (1972).
- <sup>9</sup>L. Q. Lambert, *Phys. Rev. B* **7**, 1834 (1973).
- <sup>10</sup>E. M. Kaveeva, *Izv. Akad. Nauk SSSR Ser. Fiz.* **37**, 2214 (1973).
- <sup>11</sup>R. L. Shoemaker and F. A. Hopf, *Phys. Rev. Lett.* **33**, 1527 (1974).
- <sup>12</sup>A. I. Alekseyev, *Phys. Lett. A* **31**, 495 (1970).
- <sup>13</sup>G. Oliver and R. Lefebvre, *J. Phys. (Paris)* **31**, 761 (1970).
- <sup>14</sup>G. Oliver, *Physica (Utrecht)* **51**, 197 (1971).
- <sup>15</sup>A. Shenzele, S. Grossman, and R. G. Brewer, *Phys. Rev. A* **13**, 1891 (1976).
- <sup>16</sup>A. I. Alekseev and I. V. Evseev, *Zh. Eksp. Teor. Fiz.* **56**, 2118 (1969); **68**, 456 (1975) [*Sov. Phys. JETP* **29**, 1139 (1969); **41**, 920 (1975)].
- <sup>17</sup>A. I. Alekseev, I. V. Evseev, and V. M. Ermachenko, *Zh. Eksp. Teor. Fiz.* **73**, 470 (1977) [*Sov. Phys. JETP* **46**, 246 (1977)].

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## Polarization phenomena in an oriented helium plasma

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The collisions of metastable oriented  $\text{He}(2^3S)$  atoms, accompanied by elastic scattering and by Penning ionization, is analyzed. The amplitude collision matrices are obtained. The cross sections and polarizations of all the particles are calculated, and schemes are proposed for a complete experiment, i.e., for a set of experiments that determine the amplitudes that characterize the scattering process. The obtained formulas are used for numerical estimates of the effects of polarization in the Penning ionization process.

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Spin-polarization phenomena in electron and atom collisions have been experimentally investigated in recent years. The reasons for the noticeable interest in polarization phenomena are in all cases of interference origin, and therefore provide a subtle and most sensitive means of investigating the structure and properties

of matter and of analyzing physico-chemical processes. Even the very first experiments with polarized electrons<sup>1-3</sup> have confirmed that investigations of polarization effects are promising. It has immediately become clear that polarization phenomena constitute a new means of collision spectroscopy of atoms and molecules,

of diagnostics of optically pumped plasma, of investigations of metastable states and of structures of large molecules, of surfaces, etc. As a brief formulation of the significance of the polarization experiments it can be stated that any complete experiment aimed at accounting for all the amplitudes that characterize the scattering process is unthinkable without experiments with polarized electrons.

At first the experiments in a plasma of oriented metastable helium atoms He(2<sup>3</sup>S) were essentially aimed at practical applications, namely obtaining polarized-electron beams suitable for further experiments.<sup>[4,5]</sup> The detachment of the polarized atomic electron in the metastable state occurs most effectively in the Penning ionization process. In particular, by specially selecting the partners it is possible to attain complete transfer of the produced atomic polarization to the continuous spectrum. The influence of the initial orientation of the metastable helium on the electron density and on the emission in the plasma was subsequently established<sup>[6,7]</sup> in experiment.

In this paper we consider polarization phenomena in a system of oriented metastable He(2<sup>3</sup>S) atoms. A unified description of the different types of processes (elastic scattering and Penning ionization) is attained by using the formalism of the amplitude collision matrix and the spin density matrix. A detailed analysis is presented of elastic scattering of metastable helium atoms in a state with vector orientation. The choice of precisely these He(2<sup>3</sup>S) states is dictated by two considerations. First, it is known that such states can be produced in experiment, for example by the scattering of polarized electrons from non-oriented helium atoms.<sup>[8,9]</sup> Second, as shown in the present paper, in this case an experiment is possible in which the moduli of all the amplitudes of the process and their relative phase shifts can be determined. An analysis of this type is of fundamental significance for the theory, since it can yield unambiguous correspondence with experiment. To complete the picture, we consider also some relativistic aspects of this problem. In the Penning ionization, we calculate the spin dependence of the reaction cross section, the polarization of the electrons and their pair correlations corresponding to alignment. It follows from the results that the polarization phenomena are due to interference of amplitudes corresponding to different values of the total spin of the system. The obtained formulas and the known experimental data on Penning ionization in a helium plasma are used for numerical estimates of the polarization effects. These estimates can be used for plasma diagnostics and for the investigation of oriented metastable atomic states.

## 1. ELASTIC SCATTERING IN A SYSTEM OF PARTICLE WITH SPIN $S = 1$

### 1A. Amplitude matrix

The scattering amplitudes describing all the possible processes for any combination of spins in the initial and final states make up a matrix of dimension  $(2S_1 + 1)^2(2S_2 + 1)^2$  ( $S_1$  and  $S_2$  are the spins of the two particles). It

follows from symmetry principles that the amplitude matrix  $M$  is invariant to spatial rotations, to inversion of the coordinate system, and to time reversal. In the considered He(2<sup>3</sup>S) system the total spin  $S = 1$  is made up by two electrons in the triplet state. It can be shown that in the absence of triplet-singlet transitions the spin state of the two-electron system is exactly equivalent to the state of a single particle with spin  $S = 1$ . The elastic scattering of the He(2<sup>3</sup>S) atoms is then described by a wave function that has the following asymptotic behavior:

$$\Psi \rightarrow \Phi_0 \chi_{1\mu}(1, 2) \chi_{1\mu}(3, 4) e^{ikr} + \sum_{\mu_1 \mu_2} \Phi_n M_{\mu_1 \mu_2 \mu_1' \mu_2'}^n \chi_{1\mu'}(1, 2) \chi_{1\mu'}(3, 4) \frac{\exp(ik_n r)}{r} \quad (1)$$

Here  $\Phi$  are the atomic functions and  $\chi_{1\mu}$  are the spin functions of the pair of electrons, and correspond to  $S = 1$  and to its projection  $\mu$ .

The elements  $M_{\mu_1 \mu_2 \mu_1' \mu_2'}$  of the amplitude matrix  $M$  can be expressed in terms of the elements of the scattering  $T$ -matrix, using the standard partial analysis corresponding to the asymptotic form (1). We present the result:

$$M_{\mu_1 \mu_2 \mu_1' \mu_2'} = \frac{1}{2ik} \sum_{J L L' S S'} [4\pi(2L+1)]^{1/2} T_{L L' S S'}^J \times C_{L O S M_S}^{J M_J} C_{L' M_L' S' M_S'}^{J M_J} C_{1\mu_1 \mu_2}^{S M_S} C_{1\mu_1' \mu_2'}^{S' M_S'} Y_{L' M_L'}(\theta, \varphi). \quad (2)$$

Here  $L$  and  $L'$  are the angular momenta of the system,  $S$  and  $S'$  are the values of the total spin, and  $J$  and  $M_J$  are the total angular momentum and its projection. The elements  $M_{\mu_1 \mu_2 \mu_1' \mu_2'}$  form a  $9 \times 9$  matrix that provides a complete description of all the processes in a system of two particles with unity spin. Taking into account the species of the discussed problem (low collision energies), we separate first from the total matrix  $M(2)$  the amplitudes corresponding to the nonrelativistic collision conditions (the conservation of  $L^2, S^2$ , and their projections separately). It is known that these amplitudes are determined by the expansion of (2) at  $M_L^2 = 0$ . Taking this remark, into account, we find that the nonrelativistic  $M$ -matrix can be written in operator form as follows:

$$M = aI_0 + b\hat{S}_1 \hat{S}_2 + c(\hat{S}_1 \hat{S}_2)^2, \quad (3)$$

$$I_0 = I_1 \otimes I_1, \quad \hat{S}_1 = S_1 \otimes I_1, \quad \hat{S}_2 = I_1 \otimes S_2;$$

$a$ ,  $b$ , and  $c$  are known functions of the collision energy and of the scattering angle.

We note that the algebraic structure of expression (3) follows from the requirement that the  $M$ -matrix be invariant. This expression can be rewritten differently, by using the projection spin operators

$$\hat{\Pi}_0 = -1/2 [I_0 - (\hat{S}_1 \hat{S}_2)^2], \quad \hat{\Pi}_1 = 1/2 [2I_0 - (\hat{S}_1 \hat{S}_2) - (\hat{S}_1 \hat{S}_2)^2], \quad (4)$$

$$\hat{\Pi}_2 = 1/6 [2I_0 + 3(\hat{S}_1 \hat{S}_2) + (\hat{S}_1 \hat{S}_2)^2]$$

and by introducing the amplitudes

$$G_0 = \frac{1}{2ik} \sum_L (2L+1) T_{L0} P_L(\cos \theta), \quad (5)$$

which describe the scattering at total spin values  $S = 0, 1,$  and  $2$ . We then obtain from (3) ultimately

$$M = \sum_s G_s \hat{\Pi}_s. \quad (6)$$

Some results for a relativistic  $M$ -matrix are given in Sec. 1D.

### 1B. Scattering cross section and particle polarization

Inasmuch as under conditions of scattering experiments the initial spin state is mixed, it is described by a density matrix  $\rho$ . The spin state after the collision has a density matrix  $\rho' = M\rho M^*$ , which is normalized to the differential cross section  $d\sigma/d\Omega \equiv \sigma = \text{Sp} \rho'$ . We choose as the basis matrices in the expansion of  $\rho$  the matrices  $S_i$  with unity spin and the components of second-rank symmetrical tensor:

$$S_{ij} = 1/2(S_i S_j + S_j S_i) - 2/3 \delta_{ij} I_3, \quad (7)$$

with the condition  $\sum_i S_{ii} = 0$ . The density matrix of each particle then takes the form

$$\rho = \frac{1}{3} \left[ I_3 + \frac{3}{2} \sum_i P_i S_i + 3 \sum_{ij} Q_{ij} S_{ij} \right], \quad (8)$$

where  $P_i = \langle S_i \rangle$  are the polarization-vector components that describe the orientation, and  $Q_{ij} = \langle S_{ij} \rangle$  are the polarization-tensor components that describe the alignment. The state parameters  $P_i$  and  $Q_{ij}$  vary in the ranges  $-1 \leq P_i \leq 1$ ,  $-1 \leq Q_{ij} \leq 1$  ( $i \neq j$ ),  $-2/3 \leq Q_{ii} \leq 1/3$ . In the general case, the state of a target with unity spin is described by eight real parameters, as against three for a particle with spin  $1/2$ .

For further applications, we take notice of the fact that when a polarized electron collides with an initially unoriented target the latter acquires only vector orientation ( $P_i \neq 0, Q_{ij} = 0$ ).<sup>[8,9]</sup> Such states are singled out because they can be obtained experimentally and it is possible to indicate for them a complete-experiment scheme. Therefore, avoiding a formal generalization, we present results for only such states (with vector orientation).

Recognizing that the density matrix of the entire system prior to the collision is  $\rho = \rho_1 \otimes \rho_2$ , we obtain for the cross section

$$\sigma = A + B(\mathbf{P}_a \cdot \mathbf{P}_b), \quad (9)$$

$\mathbf{P}_a$  and  $\mathbf{P}_b$  are the vectors of the initial polarization of the atoms. The polarization  $\mathbf{P}_a$  of the atom  $a$  after scattering is equal to

$$\begin{aligned} \sigma \mathbf{P}_a' = & 1/12 \{ [ |G_1|^2 + 5|G_2|^2 + 4/3(\bar{G}_0 G_1 + G_0 \bar{G}_1) + 2/3(\bar{G}_1 G_2 + G_1 \bar{G}_2) ] \mathbf{P}_a \\ & + [ |G_1|^2 + 5|G_2|^2 - 2/3(\bar{G}_0 G_1 + G_0 \bar{G}_1) - 2/3(\bar{G}_1 G_2 + G_1 \bar{G}_2) ] \mathbf{P}_b \\ & + i [ (G_0 \bar{G}_1 - \bar{G}_0 G_1) + 1/2(G_1 \bar{G}_2 - \bar{G}_1 G_2) ] [\mathbf{P}_a \times \mathbf{P}_b] \}; \quad (10) \end{aligned}$$

the polarization  $\mathbf{P}_b'$  is obtained by interchanging the subscripts,  $a \leftrightarrow b$ . Using (9) and (10), we can propose an experiment for the determination of  $|G_0|$ ,  $|G_1|$ ,  $|G_2|$  and the two relative phases.

### 1C. Complete experiment in elastic scattering

To complete the minimal program—the determination of the moduli of all the scattering amplitudes—three ex-

periments are sufficient. One is traditional and entails the determination of the cross section  $\sigma_0 = A$  of the unpolarized particles. In the two others, the cross section  $\sigma$  is obtained for collision of oriented atoms and depolarization of the particles having initially the same polarization  $P$ . Let us verify this. We have for the depolarization  $D = P'/P$ , according to (10),

$$D = (|G_1|^2 + 5|G_2|^2) / 6\sigma. \quad (11)$$

Combining this expression with expression (9) for  $\sigma$  and for  $\sigma_0 = A$ , introducing the notation  $D\sigma \equiv \sigma_a$ , and noting that  $B = (\sigma - \sigma_0) / P^2$ , we obtain after algebraic transformations the sought results:

$$\begin{aligned} |G_0|^2 = & 1/18(81\sigma_0 - 62\sigma_a - 40B), & |G_1|^2 = & 1/18(45\sigma_0 - 26\sigma_a + 20B), \\ |G_2|^2 = & 1/18(-9\sigma_0 + 28\sigma_a - 4B). \end{aligned} \quad (12)$$

From this we can obtain the moduli of all three amplitudes  $|G_s|$ . We note that the suggested scheme for finding  $|G_s|$  is not the only one, but it is optimal when account is taken of the experimental capabilities. The determination of the relative phases  $\delta_0$  and  $\delta_{12}$  between the amplitude pairs  $G_0, G_1$  and  $G_1, G_2$  calls, as expected, for three additional independent experiments. We present the final results:

$$\begin{aligned} 2|G_0| \sin \delta_{01} + 5|G_2| \sin \delta_{12} = & -12D_N \sigma_0 / |G_1|, \\ 4|G_0| \cos \delta_{01} + 5|G_2| \cos \delta_{12} = & 9d\sigma_0 / |G_1|. \end{aligned} \quad (13)$$

$D_N$  is defined here as the depolarization of the particles in a direction normal to the plane in which the initial vectors  $\mathbf{P}_a \perp \mathbf{P}_b$  are located, subject to the additional condition  $|\mathbf{P}_a| = |\mathbf{P}_b| = P$ . The value of  $d$  is obtained from two experiments on the scattering of the polarized atom ( $a$ ) by the unpolarized one ( $b$ ). The former is depolarized here to  $d_1 = P'_a / P_a$ , while the latter acquires a polarization  $d_2 = P'_b / P_a$ . Then  $d = d_1 + d_2$ . The described program is a development of the idea of a perfect experiment in a system of particles with spin  $1/2$ , where the scattering is characterized by two amplitudes (see, e.g.,<sup>[10]</sup>).

### 1D. Relativistic aspects of the elastic-scattering problem

If spin-orbit interaction  $U_1(r)(\hat{S}_1 + \hat{S}_2)\hat{L}$ , takes place in the system in addition to the central interaction  $U(r)$  then, as can be seen from (2), the matrix  $M$  becomes equal to

$$M_{so} = M + d(\hat{S}_1 + \hat{S}_2)\mathbf{n} + e(\hat{S}_1 \hat{S}_2)(\hat{S}_1 + \hat{S}_2)\mathbf{n}. \quad (14)$$

Here  $M$  takes the form (6) with amplitudes

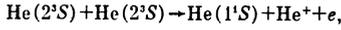
$$\begin{aligned} G_0 = & \frac{1}{2ik} \sum_L (2L+1) T_{2L}^{L+} P_L, & G_1 = & \frac{1}{2ik} \sum_L [(L+1) T_{2L}^{L+1} + L T_{2L}^{L-1}] P_L, \\ G_2 = & \frac{1}{2ik} \sum_L [(L+1) T_{2L}^{L+2} + L T_{2L}^{L-2}] P_L, \\ & d = i(h_2 + 2h_1), & e = & i(h_2 - 2h_1), \\ h_1 = & \frac{1}{8ik} \sum_L [T_{2L}^{L-1} - T_{2L}^{L+1}] P_L^{(1)}, & h_2 = & \frac{1}{8ik} \sum_L [T_{2L}^{L-2} - T_{2L}^{L+2}] P_L^{(1)}. \end{aligned} \quad (15)$$

It follows therefore that the spin-orbit interaction alters the initial state in such a way that one can speak of spin

rotation (the projection of the spin in the atom changes by unity, i.e.,  $M_s = 0 \rightleftharpoons M'_s = \pm 1$ ). Spin-orbit interaction leads to spin flip ( $M_s = \pm 1 \rightarrow M'_s = \mp 1$ ) in higher orders of perturbation theory. It can be shown, by using (2), that an interaction that leads to spin flip even in first order is described by amplitudes of the type  $H = \sum_L h_L P_L^{(2)}$ , while interaction that leads to flipping of the spins of both particles is described by amplitudes of the type  $R = \sum_L r_L P_L^{(4)}$ .

## 2. PENNING IONIZATION IN AN ORIENTED HELIUM PLASMA

In this part we consider the Penning-ionization process



where one of the atoms undergoes a triplet-singlet transition. For this reason, the problem cannot be reduced to a two-particle one, and must be treated as a four-electron problem, i.e., with maximum detail. It follows therefore that a consistent description of the polarization phenomena in this process call for  $16 \times 16$  matrices. Let us find these matrices.

### 2A. Partial analysis and amplitude matrix

We write the solution corresponding to the inelastic reaction channel in the form

$$\Psi = \sum_{nL} [4\pi(2L+1)]^{1/2} i^L \frac{R_{nL}}{r} Y_{L0} \chi_{SM_S}^{(i)} \Phi_n, \quad R \rightarrow \frac{1}{2ik_n} i^L \exp(ik_n r) S_{LS}. \quad (16)$$

It is assumed here that the interaction conserves the total angular momenta and their projections,  $\chi_{SM_S}^{(f)}$  is the eigenfunction of  $S^2$  and  $M_S$  after scattering. We introduce next the amplitude matrix of the transition with change of spin, in accordance with the definition ( $\gamma = S_1 m_1 S_2 m_2$ )

$$\Psi \rightarrow \sum_n M_{\gamma\gamma'}^n \hat{A}_{SM_S}^{(i)} \Phi_n \frac{\exp(ik_n r)}{r}, \quad (17)$$

where  $\chi_{SM_S}^{(i)}$  is the initial eigenfunction of  $S^2$  and  $M_S$ . This function can differ from  $\chi_{SM_S}^{(f)}$  if the spins and the spin projections of the individual particles change in the course of the collision.

We denote by  $\hat{A}_{SM_S}$  the operator that converts the initial spin state into the final state:

$$\hat{A}_{SM_S} \chi_{SM_S}^{(i)} = \chi_{SM_S}^{(f)}. \quad (18)$$

Then, writing (17) in the form

$$\Psi \rightarrow \sum_n M_{\gamma\gamma'}^n \hat{A}_{SM_S}^{-1} \chi_{SM_S}^{(f)} \Phi_n \frac{\exp(ik_n r)}{r} \quad (19)$$

and comparing this expression with (16) as  $r \rightarrow \infty$ , we obtain

$$M_{\gamma\gamma'}^n = \hat{A}_{SM_S} \frac{1}{2ik_n} \sum_L [4\pi(2L+1)]^{1/2} S_{LS} Y_{L0} = \hat{A}_{SM_S} G_S(\theta, \varphi). \quad (20)$$

If the process is allowed for several values of the total

spin, then

$$M_{\gamma\gamma'}^n = \sum_S \hat{A}_{SM_S} G_S(\theta, \varphi), \quad (21)$$

where the amplitudes  $G_S$  correspond to the total spin of the system, at which a process with redistribution of the spins of the individual particles takes place. In the process discussed here we have in the initial state

$$\chi_{SM_S}^{(i)} = \sum_{\mu_1 \mu_2} C_{\mu_1 \mu_2}^{SM_S} \chi_{\mu_1}^{(1,2)} \chi_{\mu_2}^{(3,4)}, \quad (22)$$

whereas in the final state the two electrons (1, 2) produce zero spin, and the two others (3, 4) are described by the spin wave function

$$\chi_{SM_S}^{(f)} = \sum C_{\mu_3 \mu_4}^{SM_S} \chi_{\mu_3}^{(3)} \chi_{\mu_4}^{(4)} \quad (23)$$

at the values  $S=0$  and 1. At  $S=0$  we find that the operator  $\hat{A}_{00}$ , defined by (18), is equal to

$$\hat{A}_{00} = (\sqrt{3}/4) (\hat{\sigma}_2 - \hat{\sigma}_1) (\hat{\sigma}_3 - \hat{\sigma}_4). \quad (24)$$

At  $S=1$  we have

$$\hat{A}_{1M_S} = (\sqrt{3}/4) (\hat{\sigma}_2 - \hat{\sigma}_1) (\hat{\sigma}_3 + \hat{\sigma}_4). \quad (25)$$

From this we obtain, according to (21), the sought transition operator

$$M = G_0 \hat{A}_{00} + G_1 \hat{A}_{1M_S}. \quad (26)$$

It is implied here that  $\hat{\sigma}_i$  are specified in the space of the four electrons, i.e.,  $\sigma_2$ , for example, is  $I_2 \otimes \sigma_2 \otimes I_2 \otimes I_2$ , etc.

### 2B. Cross section and polarization of electrons in Penning ionization

The density matrix  $\rho_a$ , which takes explicit account of the two-electron structure of the helium atom, will be chosen in the form

$$\rho_a(1,2) = 1/4 \left[ I_4 + \sum P_{\alpha i} (\hat{\sigma}_{1i} + \hat{\sigma}_{2i}) + \sum q_{ij} \hat{\sigma}_{1i} \hat{\sigma}_{2j} \right], \quad (27)$$

$$I_4 = I_2 \otimes I_2, \quad \hat{\sigma}_{1i} = \sigma_{1i} \otimes I_2, \quad \hat{\sigma}_{2i} = I_2 \otimes \sigma_{2i}$$

( $i = x, y, z$ ,  $\sigma_i$  are Pauli matrices) with the following normalization of the coefficients

$$P_{\alpha i} = \text{Sp } \rho_a (\hat{\sigma}_{1i} + \hat{\sigma}_{2i}), \quad q_{ij} = \text{Sp } \rho_a \hat{\sigma}_{1i} \hat{\sigma}_{2j}, \quad \sum q_{ii} = 1. \quad (28)$$

The coefficient  $q_{ij}$  and  $Q_{ij}$  are related by  $q_{ij} = Q_{ij} + 1/3 \delta_{ij}$ , from which follow the restrictions

$$-2 \leq q_{ij} \leq 2 \quad (i \neq j), \quad -1 \leq q_{ii} \leq 1. \quad (29)$$

Calculating the complete density matrices of the entire system after the reaction, in accordance with the formula

$$\rho' = M \rho_a(1,2) \otimes \rho_b(3,4) M^+$$

[for a definition of  $M$  see (26)], we obtain the ionization cross section

$$\sigma = \text{Sp } \rho' = 1/4 \left[ |G_0|^2 + 3|G_1|^2 - 2(|G_0|^2 + |G_1|^2) (\mathbf{P}_a \mathbf{P}_b) + (|G_0|^2 - |G_1|^2) \sum_i q_{ii} q_{ii} \right]. \quad (30)$$

For a state with initial vector polarization  $q_{ij} = 1/3\delta_{ij}$  we obtain

$$\sigma = \sigma_0 - B(P_a P_b), \quad \sigma_0 = |G_0|^2 + 2|G_1|^2, \quad B = 2/3(|G_0|^2 + |G_1|^2). \quad (31)$$

For the polarization of the polaron electrons (3, 4) we get

$$P_{\alpha\alpha}' = \sigma^{-1} \text{Sp} \rho' (\hat{\delta}_{\alpha\alpha} + \delta_{\alpha\alpha}) \\ = (3/4\sigma) \{ [2|G_1|^2(1 - q_{\alpha\alpha}^b) + (G_0 \bar{G}_1 + \bar{G}_0 G_1)(1 + q_{\alpha\alpha}^b)] P_{\alpha\alpha} \\ + [2|G_1|^2(1 - q_{\alpha\alpha}^a) - (G_0 \bar{G}_1 + \bar{G}_0 G_1)(1 + q_{\alpha\alpha}^a)] P_{\alpha\alpha} + i(G_0 \bar{G}_1 - G_1 \bar{G}_0) [P_a \times P_b]_{\alpha} \}. \quad (32)$$

For the polarization of the first pair (1, 2), which makes up the He(<sup>1</sup>S) atom, we obtain  $P_i' = 0$ , thus providing an independent confirmation of the correctness of the form of the matrix  $M$  (26) and of the calculation scheme. A change in the spin of one of the atoms changes the initial electron-pair correlation corresponding to alignment. For the correlation of the first pair the calculations yield

$$\sigma \text{Sp} \rho' (\hat{\delta}_{\alpha\alpha} \otimes \hat{\delta}_{\beta\beta}) = \sigma (q_{\alpha\alpha}^a)' = -2/3 \left\{ [2(|G_0|^2 + |G_1|^2)(1 - P_a P_b) \right. \\ \left. + (|G_1|^2 - |G_0|^2)(q_{\alpha\alpha}^a + q_{\alpha\alpha}^b - 2q_{\alpha\alpha}^a q_{\alpha\alpha}^b)] \delta_{\alpha\beta} \right. \\ \left. + (|G_1|^2 - |G_0|^2) \sum_{i,j} q_{ij} q_{\alpha\alpha}^i q_{\beta\beta}^j \right\}. \quad (33)$$

Summing  $(q_{\alpha\alpha}^a)'$  over to  $\alpha$ , we obtain  $\sum_{\alpha} (q_{\alpha\alpha}^a)' = -3$ , which corresponds to the electron correlation at  $S = 0$ . For the other pair we get

$$\sigma (q_{\alpha\alpha}^b)' = 2/3 \left\{ [2(|G_1|^2 - |G_0|^2)(1 - P_a P_b) - 2(|G_1|^2 + |G_0|^2) q_{\alpha\alpha}^a q_{\alpha\alpha}^b \right. \\ \left. - (|G_1|^2 - |G_0|^2)(q_{\alpha\alpha}^a + q_{\alpha\alpha}^b)] \delta_{\alpha\beta} - (|G_1|^2 - |G_0|^2) \sum_{i,j} q_{ij} q_{\alpha\alpha}^i q_{\beta\beta}^j \right. \\ \left. + P_{\alpha\alpha} P_{\beta\beta} (2|G_1|^2 + G_1 \bar{G}_0 + \bar{G}_1 G_0) + P_{\alpha\beta} P_{\beta\alpha} (2|G_1|^2 - G_1 \bar{G}_0 - \bar{G}_1 G_0) \right\}. \quad (34)$$

It follows from (34) that the sum  $\sum (q_{\alpha\alpha}^b)' = -3$ , if the electron and ion are produced in the singlet state, and  $\sum (q_{\alpha\alpha}^b)' = 1$ , if this pair has a spin  $S = 1$ . Both results are obtained if correct account is taken of the pair correlations in the discussed process. In the last section we shall use the obtained formulas for numerical calculations.

## 2C. Complete experiment for the Penning-ionization process, and numerical estimates

Just as in Sec. 1C, we confine ourselves first to a discussion of the experimental setup for the determination of the moduli  $|G_0|$  and  $|G_1|$ —the minimum program in the complete experiment, since such a program is already within the scope of the experimental capabilities. We assume that the states have a vector orientation ( $q_{ij} = 1/3\delta_{ij}$ ), and note, to be more specific, that it follows from the general relations between  $P_i$  and  $q_{ij}$  that the condition  $q_{ij} = 1/3\delta_{ij}$  restricts the maximum value of  $P$  to  $2/3$ , which incidentally exceeds the polarizations presently attainable in experiment. To find  $|G_0|$  and  $|G_1|$  we need two experiments—to determine the ionization cross section  $\sigma_0$  of the unpolarized atoms and the cross section  $\sigma$  for atoms with identical initial polarization  $P$ . We then obtain from (31) ( $B = (\sigma - \sigma_0)/P^2$ )

$$|G_0|^2 = 2/3 B - \sigma_0, \quad |G_1|^2 = -2/3 B + \sigma_0, \quad (35)$$

from which we get the moduli of the amplitudes. To find the relative phases  $\varphi_0 - \varphi_1 = \varphi$  of the amplitudes  $G_0$  and  $G_1$  we must determine the polarization of the produced electron (or ion) under the initial conditions  $P_a = P_b = P$  (the value of  $P_b'/P = D$ ) and the polarizations of the electron in the direction  $N = P_a \times P_b / |P_a \times P_b|$  under the initial conditions  $P_a \perp P_b$ ,  $|P_a| = |P_b| = P$  (the value of  $P_N'/P = D_N$ ). We then obtain from (32)

$$\cos \varphi = D\sigma/4|G_0||G_1|, \quad \sin \varphi = -2D_N\sigma_0/3|G_0||G_1|. \quad (36)$$

We proceed to estimate the amplitudes and the polarizations of the produced electron under typical conditions of experiments on Penning ionization in an aligned helium plasma.<sup>[11]</sup>

We introduce the ratio  $r = \sigma_i/\sigma_s$ , of the triplet and singlet ionization cross sections. According to<sup>[11]</sup>  $r = 0.7-1.0$  at  $\sigma_0 = 10^{-14} \text{ cm}^2$ . Inasmuch as in terms of  $\sigma_i$  and  $\sigma_s$  the total cross section is  $\sigma_0 = 1/4(\sigma_s + 3\sigma_i)$ , we obtain by comparison with (31)

$$\sigma_0 = 4|G_0|^2, \quad \sigma_i = 8|G_1|^2/3, \quad |G_1|^2 = 3r|G_0|^2/2. \quad (37)$$

It follows therefore that in the indicated interval of  $r$  we have  $|G_1| \sim |G_0|$ , and at  $r = 2/3$  this quality is satisfied exactly, with  $|G_1| \approx 0.6 \times 10^{-7} \text{ cm}$ . For the polarization of the produced electron or ion under the initial conditions  $P_a = P_b = P$ ,  $q_{\alpha\alpha}^a = q_{\alpha\alpha}^b = q$  we obtain from (32)

$$\sigma P' = 9r\sigma_0(1-q)P/2(1+3r). \quad (38)$$

From this we can draw the following general conclusions: For an oriented plasma we have

$$\sigma P' = 3r\sigma_0 P/(1+3r). \quad (39)$$

At  $r = 2/3$  we have

$$P' = 2P/3(1-P^2), \quad (40)$$

which corresponds, for an initial value  $P^2 = 1/3$ , to total transfer of the polarization of the atomic electrons to the continuous spectrum. At the other extreme value  $r = 1$  we have

$$P' = 12P/(16-15P^2). \quad (41)$$

Total transfer of the polarization is attained at  $P = 0.517$ , and under typical experimental conditions  $P' = 3P/4$ , i.e., a high degree is likewise reached. Another important feature of this mechanism of production of polarized electrons is the stable value of  $P'$ , i.e., the practical independence of the quantities  $\theta$  and  $E$  at a high value of the cross section. These circumstances allow us to regard Penning ionization of oriented helium atoms as a promising source of polarized electrons.

In conclusion we note that under the conditions  $(P_a \cdot P_b) = 1$  and  $\sum_i q_{ii}^a q_{ii}^b = 1$ , which correspond to an initial pure state with spin  $S = 2$ , the transition cross section  $\sigma$  vanishes identically [see (30)]. This result agrees with the Wigner rule of conservation of the total spin, which was assumed to hold true from the very beginning.

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<sup>1</sup>B. Bederson, *Atomic Physics* 3, 401 (1973).

<sup>2</sup>G. F. Hanne and J. Kessler, *J. Phys. B* 9, 791 (1976).

<sup>3</sup>M. J. Alguard, V. W. Hughes, M. S. Lubell, and P. F. Wainwright, *Abstr. Tenth Intern. Conf. Electr. Atom. Coll., Paris, 1977*, p. 506.

<sup>4</sup>L. D. Shearer, *Phys. Rev.* 166, 30 (1968).

<sup>5</sup>M. V. McCuster, L. L. Hatfield, and G. W. Walters, *Phys. Rev. A* 5, 177 (1972).

<sup>6</sup>B. N. Sevast'yanov and R. A. Zhitnikov, *Zh. Eksp. Teor. Fiz.* 56, 1508 (1969) [*Sov. Phys. JETP* 29, 809 (1969)].

<sup>7</sup>R. A. Zhitnikov, E. V. Blinov, and L. S. Vlasenko, *Zh. Eksp. Teor. Fiz.* 64, 98 (1973) [*Sov. Phys. JETP* 37, 53 (1973)].

<sup>8</sup>G. F. Drukarev and V. D. Ob'edkov, *Abstr. Seventh Intern. Conf. Electr. Atom. Coll., Amsterdam, 1971*, p. 357.

<sup>9</sup>K. Blum and H. Kleinpoppen, *Phys. Rev. A* 9, 1902 (1974).

<sup>10</sup>J. Kessler, *Polarized Electrons*, Springer Verlag, Berlin-Heidelberg, New York, 1976.

<sup>11</sup>A. I. Okunevich, *Zh. Eksp. Teor. Fiz.* 70, 899 (1976) [*Sov. Phys. JETP* 43, 467 (1976)].

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## Application of the Faddeev equations to calculations of dissociative attachment cross sections

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The Faddeev equations have been used to calculate the total and differential cross sections for the dissociative attachment of an electron to  $H_2$ , HD, and  $D_2$  molecules ( $e + AB \rightarrow A^- + B$ ). The adiabatic approximation (at electron energies above the threshold for the dissociation of the molecule to the free atoms  $A + B$ ) and the approximation of separable potentials (at electron energies below this threshold) are used to solve the Faddeev equations. Good agreement is achieved between theoretical calculations and experimental data on dissociative attachment.

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### 1. INTRODUCTION

This paper is concerned with the process of dissociative attachment of an electron to  $H_2$ , HD, and  $D_2$  molecules ( $e + AB \rightarrow A^- + B$ ). The reaction threshold is equal to the difference between the dissociation energy of the molecule into free atoms  $A + B$  (4.48 eV in this case) and the electron affinity of the atom (0.75 eV), and amounts to 3.73 eV.

The basic approximation is that the interaction between the incident electron and the electrons and nuclei in the molecule is replaced by the interaction between the electron and each of the atoms forming the molecule. The complicated many-body problem is thus reduced to the three-body problem. This approximation is reasonable for incident electron energies below the energy corresponding to the electronic excitation of the molecule. Under these conditions, the incident electron energy can be both much greater than the dissociation energy of the molecule in its electronic ground state (4.48 eV) or comparable with it.

We shall use the Faddeev equation<sup>[1]</sup> to solve this problem and will employ different approximations in different energy intervals. When the incident-electron energy is high enough (incident electron energy greater than the energy of dissociation of the molecule in its electronic ground state), we can use the adiabatic ap-

proximation. The set of integral equations is then much simpler and has an exact analytic solution if we use the zero-range potentials for the interaction between the electron and each of the atoms forming the molecule.<sup>[2]</sup>

The adiabatic approximation is not valid in the region near the dissociative attachment threshold, and the use of the zero-range potential outside the framework of the adiabatic approximation is invalid.<sup>[2]</sup> The solution for this region is, therefore, determined in the separable-potential approximation,<sup>[3]</sup> which results in a substantial simplification of the equations (Sec. 2). The advantages and disadvantages of the various approximate potentials can be estimated by comparing such calculations with experimental data.<sup>[4,5]</sup>

In this paper, we report the first attempt at calculations on the dissociative attachment process within the framework of the three-body problem and based on the Faddeev equations.

### 2. COMPUTATIONAL PROCEDURE

Let us first consider the adiabatic approximation in which the two-body potentials for the interaction of the electron and the atoms forming the molecule is taken to be the zero-range potential.

The cross section for the dissociative attachment process then has the following form<sup>[2]</sup>: