lem, which is of interest to the physics of the Stark effect, can serve as the object of independent study.

<sup>1)</sup>Formulas of this type, but different from (4, 6), were proposed without sufficient corroboration in Refs. 7 and 9.

- <sup>4</sup>R. Ya. Damburg and V. V. Kolosov, Asimptoticheskii podkhod k zadache Shtarka dlya atoma vodoroda (Asymptotic Approach to the Stark Problem for the Hydrogen Atom), Zinatne, Riga, 1977; J. Phys. B 9, 3149 (1976); 11, 1921 (1978); 12, 2637 (1979); Opt. Commun. 24, 21 (1978).
- <sup>5</sup>G. F. Drukarev, Zh. Eksp. Teor. Fiz. **75**, 473 (1978) [Sov. Phys. JETP 48, 237 (1978)].

- <sup>6</sup>S. Feneuille, S. Liberman, J. Pinard, and P. Jacquinot, Compt. Rend. B238, 291 (1977); S. Liberman and J. Pinard, Phys. Rev. A 20, 507 (1979).
- <sup>7</sup>R. R. Freeman, N. P. Economou, G. C. Bjorklund, and K. T. Lu, Phys. Rev. Lett. **41**, 1463 (1978).
- <sup>8</sup>S. Feneuille and P. Jcquinot, Proc. 6th Conf. on Ateomic Physics, 1978, p. 636.
- <sup>9</sup>A. R. P. Rau, J. Phys. B 12, L193 (1979).
- <sup>10</sup>L. D. Landau and E. M. Lifshitz, Mekhanika (Mechanics), Nauka, 1973 [Pergamon].
- <sup>11</sup>E. Clementi and C. Roetti, Atomic Data and Nuclear Data Tables 14, Nos. 3-4, 1974.
- <sup>12</sup>V. V. Beletskii, Kosmicheskie issledovaniya 2, 408 (1964).
   <sup>13</sup>V. V. Beletskii, Proc. Conf. on Gen. and Appl. Problems of Celestial Mechanics, Nauka, 1972, p. 213.
- <sup>14</sup>V. V. Beletskii, Ocherki o dvizhenii kosmicheskikh tel (Studies of the Motion of Cosmic Bodies), Nauka, 1977.

Translated by J. G. Adashko

## Alignment of hydrogenlike atoms produced by electron capture in collisions of heavy charged particles with target atoms

E. G. Berezhko and N. M. Kabachnik

Nuclear Physics Research Institute of the Moscow State University (Submitted 31 January 1980) Zh. Eksp. Teor. Fiz. **79**, 409–421 (August 1980)

We investigate the alignment of excited states of hydrogenlike atoms produced by electron capture in collisions of heavy charged particles with target atoms. The degree of alignment, as well as the degree of polarization of the photons emitted upon decay of the excited states, is calculated in the Oppenheimer-Brinkman-Kramers approximation for a number of concrete cases. The dependence of these quantities on the velocity of the incident particle is investigated for various charge ratios of the particle and of the target-atom nucleus. The effect of cascade population of the excited state on the polarization of the radiation is investigated. The calculation results are compared with the available experimental data.

PACS numbers: 34.70. + e

1. This paper is devoted to a theoretical study of the alignment of the excited states of a single-electron  $B^{+(Z-1)}$ , which are produced as a result of capture of an electron when nuclei  $B^{+Z}$  collide with target atoms:

 $B^{+z} + A \rightarrow B^{+(z-1)} + A^+. \tag{1}$ 

The ion  $B^{+(z-1)*}$  turns out to be in an aligned state because of the differences between the probabilities of populating the sublevels with different values of the projection |m| of the electron angular momentum on the direction of the incident beam. The degree of alignment of the excited state determines the polarization and the anisotropy of the angular distribution of the radiation produced in the successive transitions of the electrons to lower-lying states.<sup>1</sup>

The electron-capture cross sections in reactions (1) has recently been the subject of a tremendous number of theoretical as well as experimental studies (see, e.g., Ref. 2 and the literature therein), since these reactions play an important role in astrophysics, atmosphere physics, and plasma physics. Of particular interest, in connection with the problem of impurities in thermonuclear plasma, are investigations of the capture into excited states.<sup>3</sup> Since the cross sections for capture into the excited states are determined in practice from the intensity of the radiation emitted at a definite angle as a result of the decay of these states, it is essential to know the angular distribution of this radiation. In addition, investigations of the excitation<sup>1</sup> and ionization<sup>4</sup> of atoms in collisions have shown that the study of the angular distribution and of the polarization of the radiation can yield additional information on the charge-exchange process itself, and is therefore of independent theoretical interest.

There are at present no published systematic data on the alignment of the excited states produced in the electron-capture process. Measurements of the degree of polarization of the  $L_{\alpha}$  emission of the hydrogen atom following capture of an electron by a proton in certain inert gases are reported in Refs. 5 and 6. These data, however, are not in agreement and are even contradictory. Measurement of the angular distribution of the characteristic x radiation produced when an elec-

<sup>&</sup>lt;sup>1</sup>L. D. Landau and E. M. Lifshitz, Kvantovaya Mekhanika (Quantum Mechanics), Nauka (1974) [Pergamon].

<sup>&</sup>lt;sup>2</sup>H. A. Bethe and E. E. Salpeter, Quantum Mechanics of Oneand Two-electron systems, Springer, 1958.

<sup>&</sup>lt;sup>3</sup>M. H. Rice and R. H. Good, J. Opt. Soc. Am. 52, 239 (1962).

tron is captured by multiply charged fluorine ions in argon and helium have been recently reported.<sup>7</sup>

The polarization of the radiation was considered theoretically only for electron capture by protons. In Ref. 8 they calculated the radiation polarization of several hydrogen-atom lines in the process

 $\mathrm{H}^{+}+\mathrm{H}^{+}\mathrm{H}^{+}(nl)+\mathrm{H}^{+}.$ 

Using the first Born approximation and the impact-parameter method, the authors of Ref. 8 have shown that the radiation is quite strongly polarized, and that the degree of polarization depends little on the energy of the incident proton. Close results were obtained in Ref. 9 for the same process by the method of strong coupling of the channels. Mapleton *et al.*<sup>10</sup> investigated the polarization of the radiation of several hydrogenatom Balmer-series lines excited upon electron capture in the reaction

 $H^++He \rightarrow H^{\bullet}(3l)+He^+$ .

It turned out that in this case, too, the polarization changes little with energy.

The main purpose of the present study was an investigation of the alignment of the excited states produced in the process (1), as well as of the anisotropy and polarization of the radiation as functions of the energy of the incident particles, of their charge, and of the properties of the target atoms at sufficiently high velocities of the colliding particles. In addition, we investigated the influence of the cascade transitions on the polarization of the radiation. This influence can be substantial when an electron is captured by a multiply charged ion in a collision with a complex atom. We describe the electron-capture process by the simplest Oppenheimer-Brinkman-Kramers (OBK) approximation.<sup>11, 12</sup> Although the absolute values of the cross sections obtained in this approximation are several times larger than those obtained in experiment, the OBK approximation yields the correct dependence of the cross sections on the energy and the correct ratio for capture on various subshells.<sup>2</sup> Moreover, introduction of simple corrections within the framework of this approximation leads to satisfactory agreement with experimentalso with respect to the magnitudes of the cross sections in a wide range of energies.<sup>13, 14</sup> The OBK approximation is therefore still extensively used to interpret the experimental data. Our first calculations of the radiation polarization in the OBK approximation<sup>15</sup> were in satisfactory agreement with experiment. Taking all the foregoing into account, we hope to obtain, using the OBK approximation, the correct principal regularities of the alignment of the state and of the polarization of the radiation.

2. To describe the polarization properties of the excited states of an atom  $B^{+(Z-1)}$ , which are produced in the reaction (1), we use the polarization-tensor formalism (see, e.g., Ref. 16), which is widely used in nuclear physics. The polarization tensors  $\rho_{kx}(j,j')$  are constructed on the basis of the density matrix  $\langle jm | \rho | \times j'm' \rangle$  in the representation of the total angular momentum j of the system:

$$p_{kx}(j,j') = \sum_{mm'} (-1)^{j-m'} \langle jmj'-m'|kx\rangle \langle jm|\rho|j'm'\rangle,$$
(2)

where  $\langle j_1 m_1 j_2 m_2 | j_3 m_3 \rangle$  are Clebsch-Gordan coefficients; the summation in (2) is over all the values of the projection of the angular momentum *m* on the quantization axis *z*.

The symmetry properties of the system determine the number of independent nonzero components of the tensors  $\rho_{kx}(j,j')$ . If unpolarized particles take part in the process (1) and the atoms in the final state are not registered, the excited state of the hydrogenlike atom  $B^{+(Z-1)}$  turns out to be aligned relative to the direction of the incident beam. (We choose this direction to be the quantization axis). In an aligned system, only the components of the polarization tensors of even rank with  $\varkappa = 0$  differ from zero.<sup>16</sup>

The polarization tensors determine completely all the polarization and correlation characteristics of the system decay products. Thus, the angular distribution of the dipole photons emitted in the decay of an aligned system is defined by the expression<sup>4</sup>

$$W(\theta) = \frac{W_0}{4\pi} (1 + \alpha_2 \mathscr{A}_{20} P_1(\cos \theta)), \qquad (3)$$

where  $W_0$  is the total probability of decay per unit time,  $\mathscr{A}_{20} = \rho_{20}(j,j)/\rho_{00}(j,j)$  is the degree of alignment of the initial state with angular momentum j, and  $P_2(\cos\theta)$  is a Legendre polynomial. The coefficient  $\alpha_2$ depends only on the values of angular momenta j and  $j_1$ of the initial and final states, respectively<sup>4</sup>:

$$\alpha_2 = (-1)^{j+j_1+1} \left(\frac{3}{2}\right)^{j_2} \hat{j} \left\{ \frac{j \ j \ 2}{1 \ 1 \ j_1} \right\}.$$
(4)

Here  $\{\dots\}$  is the Wigner 6*j*-symbol and  $\hat{j} \equiv (2j+1)^{1/2}$ . The same sole parameter  $\mathscr{A}_{20}$  determines also the degree of linear polarization of the photons:

$$P=3\alpha_2\mathcal{A}_{20}/(\alpha_2\mathcal{A}_{20}-2). \tag{5}$$

In the OBK approximation chosen by us, the electron capture is due to the spin-independent Coulomb interaction. We neglect therefore the spins of the particles in the first stage of the calculation. The question of the influence of the fine and hyperfine splitting will be considered specially later on. In the absence of spins, the polarization state of a single-electron atom will be described by a set of polarization tensors  $\rho_{kx}(l,l)$  that are connected with the density matrix  $\langle lm | \rho | lm' \rangle$  in the representation of the orbital momentum l of the electron by an equation similar to (2). We normalize the density matrix to the cross section for the capture of the electron in an excited state, and then we have for the density-matrix elements<sup>1</sup>

$$\langle lm|\rho|lm'\rangle = \sum_{n_0l_0m_0} \int d\Omega_{\mathbf{k}_f} \frac{k_f}{k_i} F_{nlm}(n_0l_0m_0\mathbf{k}_i\mathbf{k}_f) \dot{F}_{nlm'}(n_0l_0m_0\mathbf{k}_i\mathbf{k}_f), \quad (6)$$

where  $F_{nl_m}(n_0l_0m_0\mathbf{k}_i\mathbf{k}_f)$  is the amplitude of the process of electron capture from the state  $n_0l_0m_0$  to the state nlm on scattering of an incident particle with momentum  $\mathbf{k}_i$  into a state with momentum  $\mathbf{k}_f$  by the target atoms. The summation in (6) means that we take into account the contributions of all the target-atom shells.

In the OBK approximation, in which account is taken

of only the Coulomb interaction of the incident nucleus with the captured electron, and in the single-particle model of the atom, the amplitude of the process can be expressed in the form

$$F_{nlm}(n_0 l_0 m_0 \mathbf{k}_i \mathbf{k}_j) = -2\pi^2 \mu_j (B^2 + 2\mathscr{F}_{nl}) \Psi_{n_0 l_0 m_0}(\mathbf{A}) \Psi^{\bullet}_{nlm}(\mathbf{B}).$$
(7)

Here  $\mu_f$  is the reduced mass of the system in the final state,  $\mathscr{G}_{nl}$  is the binding energy of the electron in the hydrogenlike atom  $B^{+(Z-1)}$ ,  $\Psi_{nlm}(Q)$  is the wave function of the electron in the momentum representation, and the vectors **A** and **B** are connected with the vectors of the incident-particle momenta in the initial and final states by the relations

$$A = M_{A}k_{i}/(M_{A}+1) - k_{i},$$

$$B = k_{i} - M_{B}k_{i}/(M_{B}+1),$$
(8)
(9)

where  $M_B$  and  $M_A$  are the mass of the incident particle and the mass of the ion  $A^+$  (the electron mass is unity). Substituting (7) in (6) and in (2) and summing over the projections of the angular momenta, we obtain

$$\rho_{kx}(l,l) = \delta_{x0} \frac{2\pi}{v_i^2} \hat{l}^2 \langle l0l0|k0\rangle (-1)^l$$

$$\times \sum_{n_0 l_0} \hat{l}_0^2 \int_{A_{nln}} A \, dA \, (B^2 + 2\mathscr{E}_{nl})^2 \, P_k(\cos\theta_B) \, |R_{nl}(B)|^2 |R_{n_0 l_0}(A)|^2. \tag{10}$$

Here  $v_i$  is the velocity of the incident particle,  $P_k(\cos\theta)$  is a Legendre polynomial,  $\theta_B$  is the angle between the direction of the vector B and the z axis, and  $R_{nl}(Q)$  is the Fourier transform of the radial wave function:

$$R_{nl}(Q) = \int_{0}^{\infty} R_{nl}(r) j_{l}(Qr) r^{2} dr, \qquad (11)$$

where  $j_i(x)$  is a spherical Bessel function and  $R_{ni}(r)$  is the radial part of the single-particle wave function of the electron.

Using (8) and (9) and the energy conservation law, we easily obtain an expression for the cosine of the angle  $\theta_B$ :

$$\cos \theta_{B} = \frac{k_{i}^{2} + B^{2} - M_{B}^{2} k_{i}^{2} / (M_{B} + 1)^{2}}{2k_{i} B},$$
 (12)

and readily establish the connection between |A| and |B|:

$$B^{2} \frac{M_{B}+1}{M_{B}} = A^{2} \frac{M_{A}+1}{M_{A}} - 2(\mathscr{E}_{nl} - \mathscr{E}_{n_{sl}e}).$$
(13)

The integration limits in (10) are determined from the relation (8):

$$A_{max}^{min} = \frac{M_A}{M_A + 1} k_i \mp k_j. \tag{14}$$

Using (10)-(14) we can calculate the polarization tensors for capture of an electron by any shell nl of the incident ion.

3. To clarify the qualitative features of the behavior of the alignment of the ion as a function of the parameters of the problem (the velocity of the incident particle and the ratio of the particle charges), we consider the following simple problem. Let a particle with charge Z capture in the 2p state an electron from a filled shell of the target atom with principal quantum number  $n_0$ , which we describe by hydrogenlike functions with effective charge  $Z_{eff}$ . Then, using the relation<sup>17</sup>

$$\sum_{l_0=0}^{n_0-1} \sum_{m_0=-l_0}^{l_0} |\Psi_{n_0l_0m_0}(\mathbf{A})|^2 = \frac{8}{\pi^2} \frac{a^3}{(A^2+a^2)^3} n_0^2,$$
(15)

where  $a = Z_{eff}/n_0$ , we can integrate (10) analytically and obtain the following expression for the degree of alignment:

$$\mathscr{A}_{20} = -2^{-\frac{N_2}{2}} \frac{11s^2 - 4}{7s^2 + 4} \left[ 1 + \frac{30\beta s \left(s^2 + 4\right) + 6\beta^2 \left(s^2 + 4\right)^2}{5\left(11s^2 - 4\right)} \right];$$
(16)

$$\beta = \frac{1}{4\mu_i u_i}, \quad u_i = \frac{2\nu_i}{Z}, \quad s = \frac{(Z_{eij}/Z)^2 n^2/n_0^2 - 1}{u_i} + u_i.$$
(17)

In the range of velocities  $v_i$  where the capture cross section is large enough  $(u_i \sim 1)$ , we have  $\beta \ll 1$  and therefore, neglecting the terms  $\sim \beta$  and  $\beta^2$ , we obtain a simple expression for  $\mathscr{A}_{20}$ :

$$\mathscr{A}_{20} = -2^{-\frac{1}{2}} \frac{11s^2 - 4}{7s^2 + 4}.$$
 (18)

We note that the numerical comparison has shown that Eq. (18) approximates expression (16) with goodaccuracy in the region of applicability of the OBK approximation.

If  $Z \leq Z_{eff}/n_0$ , then  $s^2$  is always larger than unity and, according to (18), the degree of alignment, and hence also the polarization of the radiation, is a slowly varying single-sign function of the velocity. At high velocities,  $u_i \gg 1$ ,

$$\mathscr{A}_{20} \to -\frac{1}{\sqrt{2}} \frac{11}{7}.$$
 (19)

At  $Z > Z_{eff}$  the alignment can change considerably with velocity, and can even reverse sign. An estimate with the aid of (18) shows that the reversal of the sign of the alignment and of the polarization can occur under the condition

$$Z > \left(\frac{11}{3}\right)^{\nu_2} \frac{Z_{eff}}{n_0}.$$
 (20)



FIG. 1. Degrees of alignment of the 2p (a), 3p (b, solid lines), and 3d (b, dashed) states vs. the reduced velocity of the incident particle for different values of the ratio  $Z/(Z_{eff}/n_0)$ : a) 1-1.0; 2-1.667; 3-2.0; 4-2.5; 5-4.0; b) 1-1.0; 2-2.0; 3-4.0.

Figure 1a shows the dependence of the degree of alignment of the state 2p on the velocity of the incident particle for different ratios of Z and  $Z_{eff}/n_0$ . The case  $Z/(Z_{eff}/n_0) = 1$  corresponds to that considered in Ref. 8. It is seen that in all cases the alignment reaches large values and can reverse sign at large Z.

We can similarly obtain simple expressions for the alignment of the states 3p and 3d:

$$\mathscr{A}_{20}^{(3p)} = -2^{-\frac{1}{2}} \frac{33s^{6} - 216s^{4} + 384s^{2} - 64}{21s^{6} - 108s^{4} + 144s^{2} + 64},$$

$$(21)$$

$$\mathscr{A}_{20}^{(3d)} = -\frac{1}{2} \left(\frac{10}{2}\right)^{\frac{1}{2}} \frac{117s^{4} + 12s^{2} - 32}{21s^{6} - 108s^{4} + 12s^{2} - 32},$$

$$(22)$$

 $\mathscr{A}_{20}^{(3d)} = -\frac{1}{16} \left(\frac{10}{7}\right)^{\frac{1}{2}} \frac{117s^4 + 12s^2 - 32}{9s^4 + 9s^2 + 4},$  (22) The corresponding curves for three different values of

 $Z/(Z_{\rm eff}/n_0)$  are shown in Fig. 1b.

4. We consider now the influence of the fine and hyperfine level splittings of a hydrogenlike ion on the alignment of the ion and on the polarization of the radiation. This question was first considered in Ref. 18 for a case when the radiation registration time is much longer than the lifetime of the state. A generalization of this theory to the case of an arbitrary ratio of these times was carried out in Ref. 19, and is directly applicable to the charge-exchange processes considered here. A survey of the entire problem as a whole can be found in Ref. 1.

The excited state of the ion becomes oriented on account of the alignment of the orbital angular momentum of the electron during the course of its Coulomb interaction with the incident nucleus. The spin orbit (SO) and hyperfine (HF) interactions lead to a certain depolarization of the state. The physical cause is the precession of the orbital angular momentum under the influence of the interaction. We note that the principal results of the theory of depolarization are common with those of the theory of perturbed angular correlations in nuclear spectroscopy,<sup>20</sup> since the physical gist of these phenomena is the same.

It can be shown that allowance for the SO interaction makes it necessary to multiply the polarization tensors  $\rho_{k0}(l,l)$  contained in the quantity  $\mathcal{A}_{20}$  in Eqs. (3) and (5) by the additional factors  $D_{b}(l)$ :

$$D_{k}(l) = \sum_{jj'} \frac{(jj')^{2}}{2} \left\{ j' \quad j \quad k \\ l \quad l^{-1/2} \\ \times \left( \cos \omega_{jj'} \Delta t - \varepsilon_{jj'} \sin \omega_{jj'} \Delta t \right) \right\}, \qquad (23)$$

where  $\omega_{jj} = (E_j - E_{j'})$  is the distance between the finestructure levels,  $\gamma_l$  is the decay width of the excited state,  $\varepsilon_{jj'} = \omega_{jj'}/\gamma_l$ , and  $\Delta t$  is the time during which the photons are registered, starting with the instant of formation of the excited state, i.e., the time during which the excited atom moves in the field of view of the recording apparatus.

Equation (23) is derived in Ref. 26 in a rather simple manner, using the polarization-tensor formalism. Equations analogous in meaning and close in form are obtained also in Refs. 19 and 20, but by other more cumbersome procedures.

It is easily seen that the factor  $D_k(l)$  lies in the range  $0 \le D_k \le 1$  (we recall that

$$\sum_{jj'} \frac{(jj')^2}{2} \left\{ j \ j' \ k \\ l \ l \ 1/2 \right\} = 1 \right).$$

This means precisely that the splitting of the energy levels on account of the SO interaction leads in fact to depolarization of the excited state. We shall therefore name  $D_{\mathbf{k}}$  the depolarization coefficients.

In the limiting case when the interaction is weak and the level splitting is much less than their width,  $\omega_{jj}$ ,  $\ll \gamma_1, \varepsilon_{jj}, -0, D_k - 1 - \exp(-\gamma_1 \Delta t)$ , the depolarization coefficient is independent of k and consequently neither the angular distribution nor the polarization changes when account is taken of the SO interaction.

In the other limiting case, when the level widths are much less than the distances between them:

$$\omega_{jj'} \gg \gamma_i, \quad \frac{1}{1+\varepsilon_{jj'}} = \begin{cases} \sim 0 & j \neq j' \\ 1 & j = j' \end{cases},$$

only terms with j = j' are left in the sum over j and j', i.e., the fine-structure levels are incoherently excited, and their emission is simply the sum of the emissions from each of the sublevels. In this case, if the experimental resolution permits separation of individual finestructure lines, it is convenient to use the polarization tensors for each sublevel of the fine structure  $\rho_{kx}(j,j)$ , which are connected with the orbital-momentum polarization tensors by the relation (see, e.g., Ref. 16)

$$\rho_{\mathbf{A}\mathbf{x}}(j,j) = \frac{1}{2} (-1)^{\nu_{l+k+l+j}} \hat{j}^{2} \begin{cases} l & j & \nu_{2} \\ j & l & k \end{cases} \rho_{\mathbf{A}\mathbf{x}}(l,l).$$
(24)

The depolarization coefficients depend on the photon registration time t, i.e., on the construction of the concrete experimental setup. In concrete calculations we shall hereafter always assume that this time is long enough,  $\Delta t \gg 1/\gamma_1$ , and then obtain  $D_k$  the simpler expression

$$\overline{D}_{k}(l) = \sum_{jj'} \frac{(jj')^{2}}{2} \left\{ j j' k \atop l l^{-1/2} \right\}^{2} \frac{1}{1 + \varepsilon_{jj'}^{2}} \frac{1}{\gamma_{l}}.$$
(25)

We point out finally that if the HF interaction must be taken into account, this can be done by replacing the depolarization coefficient by

$$\overline{D}_{k}(l) = \sum_{j,j' \in F'} \frac{(j\tilde{j}' \tilde{F} F')^{2}}{2l^{2}} \left\{ \begin{array}{c} j \ j' \ k \\ l \ l \ 1/_{2} \end{array} \right\}_{l}^{2} \left\{ \begin{array}{c} F' \ F \ k \\ j \ j' \ I \end{array} \right\}^{2} \frac{1}{1 + a_{FF'}^{2}} \frac{1}{\gamma_{l}}, \qquad (26)$$

where F is the total angular momentum of the ion, including the spin I of the nucleus: F = I + j.

5. Before we proceed to discuss the results of the calculation for concrete cases and to compare them with experiment, we examine the role of two-stage cascade processes. The investigated state can be populated not only by direct capture of an electron, but also by capture from a higher state followed by decay with transition to the investigated state. Naturally, the alignment of the latter will differ considerably from the case of direct population. In the particular case, a two-step process via an intermediate state with l=0 produces no anisotropy whatever, and the contribution of this process leads to a decrease of the total alignment. The degree of the influence of a two-stage process is determined by the ratio of the lifetime  $\tau_i$  of the intermediate state and the observation time  $\Delta t$ , i.e., it depends on

the parameters of the concrete experimental setup.

Since we do not know the parameters of the experimental setups used in the experiments of interest to us, the calculations presented below were performed for the following two limiting cases: In the first case the cascade population of the considered state was disregarded. In practice this corresponds to an experiment in which  $\Delta t/\tau_i \gg 1$  for all states  $n_i l_i$  located above the considered state. In the second calculation variant it was assumed that the time  $\Delta t$  is long enough, so that  $\Delta t/\tau_i \gg 1$  at least for a number of closely lying levels. In this case the polarization tensors of the investigated state can be approximately calculated from the formula

$$\rho_{k_{\varkappa}}^{\Sigma}(l, l) = \rho_{k_{\varkappa}}(l, l) + \sum_{l_{i}} (-1)^{l_{i}+l_{i}+1+k} \hat{l}_{i}^{2} \begin{cases} ll_{i} \ 1 \\ l_{i}l \ k \end{cases} \frac{1}{\gamma_{l_{i}l}} \\ \times \sum_{j_{i}} \frac{1}{2} (2j_{i}+1)^{2} \left\{ \frac{j_{i} \ j_{i} \ k}{l_{i} \ l_{i} \ l_{2}} \right\}^{2} \rho_{k_{\varkappa}}^{i}(l_{i}, l_{i}),$$
(27)

where  $\gamma_{i_{j}i}$  and  $\gamma_{i_{j}i}$  are the partial and total widths of the *i*-th level. (In the derivation of this formula we have assumed that the distance between the fine-structure levels is much larger than their widths,  $\omega_{jj'} \gg \gamma$ , an assumption valid in the cases considered below.) Understandably, these two variants are two limiting cases. Their comparison permits an estimate of the influence of the cascade population on the alignment of an excited state of a hydrogenlike atom, as well as on the angular distribution and polarization of the emitted photons.

6. We have calculated the alignment and polarization of the radiation for the 2p + 1s transition in the hydrogen atom and in the hydrogenlike ion  $F^{+8}$ , which are produced as a result of charge exchange in the collisions  $p + \text{Ne}, p + \text{Ar}, F^{+9} + \text{He}, \text{ and } F^+ + \text{Ar}$ . The tensors  $\rho_{k0}(l, l)$  and  $\rho_{k0}{}^{C}(l, l)$  were calculated from formulas (10) and (27). Wave functions in the Hartree-Slater approximation<sup>21</sup> for the Ne and Ar atoms were used and Hartree-Fock wave functions were used for the He atom.

The distances between the levels of the fine and hyperfine structures for the hydrogen atom, and the transition rates, which are needed for the calculation of the depolarization coefficients  $D_k$  and the tensors  $\rho_k \sum_{x}^{c}$ , were taken from Sobel'man's book.<sup>22</sup> We present the values of the coefficients  $\overline{D}_k$  for the investigated case of the 2p state of hydrogen. Allowance for the fine splitting [see (25)] yields  $\overline{D}_k^{SO} = 0.3333$ . Allowance for the hyperfine splitting for this case produces only a small change in  $\overline{D}_k$ , viz.,  $\overline{D}_k^{HF} = 0.3364$ . Since both the magnitude of the fine splitting and the decay rate are proportional to  $Z^4$ , the coefficient  $\overline{D}_k^{SO}$  will have the same value for any Z [i.e., also for  $F^{+8}(2p)$ ]. On the other hand, since the hyperfine structure is  $\sim Z^3$ , its influence will decrease with increasing Z. In the case of  $F^{+8}(2p)$ , it is negligibly small (<10<sup>-4</sup>).

Figure 2a shows the results of the calculation of the tensors  $\mathscr{A}_{20}$  and  $\mathscr{A}_{20}^{\mathbb{D}}$  for the 2p state of the hydrogen atom produced in the reaction  $p + \operatorname{Ne}$ , as a function of the energy  $E_i$  of the incident proton. Our calculation, based on the OBK approximation, can claim to describe the phenomenon correctly only if the proton velocity exceeds that of the captured electron, i.e., at  $E_i > 20$ 



FIG. 2. Degree of alignment of the 2p state of the hydrogen atom (a) and degree of polarization of the  $L_{\alpha}$  line (b) in p +Ne collisions, as functions of the incident-proton energy. The letter  $\Sigma$  marks curves calculated with allowance for cascade population of the 2p state via 3s, 3d, and 4s states (0-data of Ref. 5,  $\Delta$ -data of Ref. 6).

keV. To illustrate the method, however, we present the calculation result also for lower energies. The tensor  $\mathscr{A}_{20}$  was calculated without allowance for cascade population, while  $\mathscr{A}_{20}^{\mathbb{E}}$  was calculated with account taken of cascade population from the 3s, 3d, and 4s states. The contributions of the other states were neglected. It is seen that the tensor  $\mathscr{A}_{20}$  has the same sign in a wide energy range, in agreement with the conclusion of Sec. 3, and its value varies little and deviates nowhere greatly from the maximum (absolute) value. (Using expressions (2) and (6), it is easy to establish the following relation between the degree of alignment  $\mathscr{A}_{20}$  for the 2p state and the cross section  $\sigma(2pm)$  for capture into a state with a definite projection m of the orbital angular momentum on the z axis:

$$\mathscr{A}_{20} = 2^{-1} \frac{\sigma(2p1) - \sigma(2p0)}{2\sigma(2p1) + \sigma(2p0)}.$$
 (28)

It is seen from this equation, in particular, that  $\mathscr{A}_{_{20}}$  can vary in the range from  $-\sqrt{2}$  to  $1/\sqrt{2}$ .)

It is seen from Fig. 2a that allowance for the cascade population changes quite strongly the course of the degree of alignment. The tensor  $\mathscr{A}_{20}^{\mathbb{C}}$  is smaller in absolute value than  $\mathscr{A}_{20}^{\mathbb{C}}$  in the entire energy range, and when the energy is increased to  $E_i \ge 100 \text{ keV}$  the value of  $\mathscr{A}_{20}^{\mathbb{D}}$  tends rapidly to zero. The reason is that in this energy region the 2p state is populated mainly via the 3s and 4s states. This is easily understood by starting from Eqs. (8)-(14): when the energy is high and increases,  $A_{\min}$  and the associated quantity  $B_{\min}$  increase. And since, with increasing B, the Fourier transform in expression (10) which is the slowest to decrease with increasing B is  $R_{nl}(B)$  at l=0, the result is that at very high energies  $E_i$  the capture into the ns states predominates. In this case  $\mathscr{A}_{20}^{\mathtt{E}}$  tends to zero, since the population of the 2p states via the s states makes no contribution to the alignment tensor  $\rho_{20}^{\Sigma}$ .

Figure 2b shows the values of the degree of polarization of the  $L_{\alpha}$  line. The two theoretical curves were obtained from Eq. (5) using the tensors  $\mathscr{A}_{::0}$  and  $\mathscr{A}_{::0}^{\mathbb{D}}$   $(\alpha_2 = 1/\sqrt{2})$ . The experimental values were taken from Refs. 5 and 6.



FIG. 3. The same as in Fig. 2, but for p + Ar collisions.

Similar results are shown in Fig. 3 for the case p + Ar. The character of the energy dependence of the tensors  $\mathscr{A}_{20}$  and  $\mathscr{A}_{20}^{\mathcal{L}}$  is here the same as in the preceding case.

As seen from the figures, in both considered cases the degree of polarization of the emission of the hydrogen  $L_{\alpha}$  line is quite appreciable (about 30%) and varies little with energy. Allowance for the cascade population decreases the polarization somewhat, and with increasing energy the influence of the cascade transitions increases and the polarization decreases. Unfortunately, the available experimental data<sup>5,6</sup> were obtained mainly at energies for which the approximation used by us is not valid. We note that the data of these two papers<sup>5,6</sup> differ greatly from one another, and in the region of the highest measured energies  $E_i > 10 \text{ keV}$ the experimental data differ even in sign. Our calculation confirms more readily the results of Ref. 5.

At low energies  $(E_i < 10 \text{ keV})$  an additional maximum is observed in the cross section of electron capture from Ne and Ar into the 2p state.<sup>23</sup> In Ref. 24 was considered a stepwise electron-capture mechanism, consisting of capture in the 1s state followed by excitation of the 2p state. This mechanism explained the presence of the additional maximum. It is useful to estimate the alignment of the 2p state for this mechanism. It is clear that alignment can occur only during the second stage, in the 1s-2p excitation. On the other hand, as shown in Ref. 25, at low velocities only transitions at  $\Delta m = 0$  are possible in the excitation process. In our case this means that at low energies of the incident proton only the sublevel with projection m = 0 will be populated in the 2p state. This, as follows from (28), yields an alignment limit  $\mathscr{A}_{20} = -\sqrt{2}$ . The same value, as seen from Eq. (10), is obtained in the OBK approximation. This coincidence is apparently accidental, but it does give grounds for hoping that the curves calculated by us show correctly the dependences of the alignment and of the polarization on the energy.

Figure 4a shows the calculated degree of alignment of the 2p state of the  $F^{*8}$  ion produced in collision of  $F^{*9}$  nuclei with He atoms. The curves labeled by the letter  $\Sigma$  corresponds in this figure to the value of the alignment tensor calculated with allowance for population via the 3s, 3d, and 4s states. The same, but for the case of  $F^{*9}$ +Ar, is shown in Fig. 4b.



FIG. 4. Degree of alignment of 2p state of  $F^{+8}$  ion produced in  $F^{+9}$  +He (a) and  $F^{+9}$  +Ar (b) collisions. The letter  $\Sigma$  marks the curve calculated with allowance for population via 3s, 3d, and 4s states. The experimental point ( $\Delta$ ) was obtained from the data of Ref. 7.

In contrast to the case of capture by a proton, for electron capture by  $F^{+9}$  nucleus one could expect a reversal of the signs of the alignment and of the polarization of the radiation with change of energy. Indeed, in the case of  $F^{+9}$  + He the inequality (20) is satisfied with some margin. In the case  $F^{+9} + Ar$  it does not hold only for the K shell. Therefore in the energy region where the main contribution to the  $F^{+8}(2p)$  production is made by the higher shells of the Ar atom one should expect a reversal of the sign of  $\mathscr{A}_{20}$ . Calculation by formula (10) (see Fig. 4) has confirmed our expectations. In the case  $F^{+9}$  + He the alignment is positive at energies close to 10 MeV and negative at lower and higher energies. In the  $F^{+9}$  + Ar case, positive value of the alignment are obtained at energies 300 keV-5 MeV.

The  $\mathscr{A}_{20}$  and  $\mathscr{L}_{20}^{c}$  curves of Fig. 4b differ little in the entire represented energy region. The picture is different in the case of He atoms (Fig. 4a). The  $\mathscr{A}_{20}$  and  $\mathscr{A}_{20}^{\Sigma}$  curves differ greatly in the entire represented energy region, owing to the substantial contribution of the cascade population at all energies.

In both figures, the points at energy  $E_i = 33$  MeV mark the values of  $\mathcal{A}_{20}$  obtained by recalculation, with the aid of Eq. (5), from the experimental values of the degree of polarization of the  $2p \rightarrow 1s$  line of  $F^{+8}$ , taken from Ref. 7. In both cases, the theory and experiment agree very well.

7. Investigations of the alignment of excited states yield additional information on the capture of electrons by fast ions. Simple calculations reveal qualitatively different dependences of the degree of alignment on the velocity for different pairs of colliding atoms. In some cases, a substantial influence of cascade transitions is predicted. An experimental investigation of the alignment of the excited state by measuring the polarization or the angular distribution of the subsequent radiation can be a useful means of studying the electron capture process.

- <sup>1</sup>U. Fano and J. Macek, Rev. Mod. Phys. 45, 553 (1973).
- <sup>2</sup>D. Basu, S. C. Mukherjee, and D. P. Sural, Phys. Repts. 42, 145 (1978).
- <sup>3</sup>F. Garett, 9th Internat. Conf. on Physics of Electronic and Atomic Collisions, Seattle, 1975, p. 846.
- <sup>4</sup>E. G. Berezhko and N. M. Kabachnik, J. Phys. B10, 2467 (1977).
- <sup>5</sup>T. D. Gaily, D. H. Jaecks, and R. Geballe, Phys. Rev. 167, 81 (1968).
- <sup>6</sup>P. B. Needham, P. J. O. Teubner, and B. D. Sartwell, Phys. Rev. A2, 1686 (1970).
- <sup>7</sup>E. H. Pedersen, S. J. Czuchlewski, M. D. Brown, L. D. Ellsworth, and J. R. Macdonald, Phys. Rev. A11, 1267 (1975).
- <sup>8</sup>J. van den Bos and F. J. de Heer, Physica (Utrecht) **34**, 333 (1967); **40**, 161 (1968).
- <sup>9</sup>L. Wilets and D. F. Gallaher, Phys. Rev. 147, 147, 13 (1966).
- <sup>10</sup>R. A. Mapleton, R. W. Doherty, and P. E. Meehan, Phys. Rev. A9, 1013 (1974).
- <sup>11</sup>J. R. Oppenheimer, Phys. Rev. 31, 349 (1928).
- <sup>12</sup>H. C. Brinkman and H. A. Kramers, Proc. Acad. Sci. Amst. 33, 973 (1930).
- <sup>13</sup>V. S. Nikolaev, Zh. Eksp. Teor. Fiz. 51, 1263 (1966) [Sov. Phys. JETP 24, 847 (1967)].

- <sup>14</sup>G. Lapicki and W. Losonsky, Phys. Rev. A 15, 896 (1977).
- <sup>15</sup>E. G. Berezhko and N. M. Kabachnik, 11th Internat. Conf. on Physics of Electronic and Atomic Collisions, Kyoto, 1979, p. 560.
- <sup>16</sup>A. Ferguson, Angular Correlation Methods in Gamma Ray Spectroscopy, Am. Elsevier, 1965.
- <sup>17</sup>R. M. May, Phys. Rev. A 136, 669 (1964).
- <sup>18</sup>I. C. Percival and M. J. Seaton, Phil. Trans. Roy. Soc. London A251, 113 (1958).
- <sup>19</sup>J. Macek and D. H. Jaecks, Phys. Rev. A4, 2288 (1971).
- <sup>20</sup>H. Frauenfelder and R. Steffen, in: Alpha, Beta and Gamma Spectroscopy, K. Siegbahn, ed., Collier-Macmillan, 1965.
- <sup>21</sup>F. Herman and S. Skillman, Atomic Structure Calculation, Prentice-Hall, 1963.
- <sup>22</sup>I. I. Sobel'man, Vvedenie v teoriyu atomnykh spektrov (Introduction to the Theory of Atomic Spectra), Nauka, 1977.
- <sup>23</sup>D. Jaecks, B. Van Zyl, R. Geballe, Phys. Rev. 137, A340, (1965).
- <sup>24</sup>I. A. Poluektov and L. P. Presnyakov, Zh. Eksp. Teor. Fiz.
   54, 120 (1968) [Sov. Phys. JETP 27, 67 (1968)].
- <sup>25</sup>L. A. Vainshtein, I. I. Sobel'man, and E. A. Yukov, Vozbuzhdenie atomov i ushirenie spektral'nykh linii (Excitation of Atoms and Broadening of Spectral Lines), Nauka, 1979.
- <sup>26</sup>E. G. Berezhko, Candidate's dissertation, Moscow State Univ., 1979.

Translated by J. G. Adashko

## Luminescence of excitons bound to phosphorus atoms in silicon subjected to a magnetic field

A. S. Kaminskiĭ, V. A. Karasyuk, and Ya. E. Pokrovskiĭ

Institute of Radio Engineering and Electronics, Academy of Sciences of the USSR, Moscow (Submitted 11 February 1980) Zh. Eksp. Teor. Fiz. **79**, 422–430 (August 1980)

An investigation was made of the luminescence spectra of excitons bound to phosphorus atoms in silicon. A magnetic field of 18-55 kOe intensity directed along the [001] and [111] crystallographic axes was applied to the samples in the Faraday and Voigt configurations. The values of the electron  $(g_e = 2.0)$  and hole  $(g_1 = 0.83, g_2 = 0.22)$  g factors and the diamagnetic shifts were determined; these were found to depend on the initial state of holes in bound excitons. The amplitudes of the Zeeman components in these spectra were in satisfactory agreement with the calculations carried out using the shell model approximation for bound excitons.

PACS numbers: 71.35. + z, 78.55.Hx, 78.20.Ls, 71.70.Ej

## **1. INTRODUCTION**

Recent progress in the understanding of the structure of many-particle exciton—impurity (EI) complexes<sup>1</sup> has largely been due to the application of the shell model proposed in Refs. 2 and 3. In particular, this model has made it possible to interpret satisfactorily the main features of the luminescence spectra of EI complexes in silicon subjected to magnetic fields.<sup>4,5</sup> However, we must bear in mind that the luminescence bands of EI complexes formed as a result of binding *m* excitons to neutral group III or V atoms in silicon have a fine structure if m > 1 even if there are no external perturbations.<sup>6</sup> Separations between the individual components of a luminescence band can reach 200  $\mu$ eV, i.e., they are comparable with the separations between the Zeeman components in magnetic fields  $H \leq 50$  kOe. The Zeeman spectra of EI complexes can be interpreted simply if we know exactly the constants (in particular, the electron and hole g factors) representing the initial and final states of bound carriers in magnetic fields.

We must bear in mind that, in the case of EI complexes bound to donors in silicon, the  $\alpha$ -series luminescence lines<sup>2,3</sup> appear on recombination of electrons from the state  $\Gamma_1$  in which there cannot be more than two electrons and which is filled even for a bound exciton if m=1. We shall assume that the necessary constants can be determined sufficiently accurately by analyzing the Zeeman spectra of excitons bound to neutral donors in silicon (i.e., by analysing the spectra of EI complexes with m=1), which can then be used to