# Transitions between <sup>2</sup>P and <sup>3</sup>P multiplet sublevels in collisions between atoms and ions

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The cross sections for transitions between  ${}^{2}P$  and  ${}^{3}P$  sublevels in collisions between various types of atoms and ions are considered. The calculation is based on the assumption of the energy splitting between the respective sublevels being small and on the multiplet being more or less isolated from the other terms. The results of the investigation may be of interest for a theoretical investigation of gas lasers based on elements considered in the paper.

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## **1. QUALITATIVE DISCUSSION**

1. Gas lasers operating with a great variety of elements and compounds have now been or are being developed. Of great interest for theoretical investigation is the consideration of the transitions from their working levels to other levels as a result of collisions of the atoms or molecules. The cross sections of such transitions are particularly large when both the working level and the level to which the transition takes place belong to one and the same multiplet. In a gas laser there is always a large number of ions, and the cross sections of the transitions of interest to us in collisions between atoms and ions are particularly large, as will be shown later on. The most important of all the possible interactions of an atom with an ion is the charge-quadrupole interaction, since it varies like R<sup>-3</sup>, while the polarization interaction (i.e., the interaction of the charge with the dipole moment induced by its field) varies like  $R^{-4}$ (R is the distance between the nuclei of the atom and the ion). Apart from the charge-quadrupole interaction, such transitions can be produced only by resonant dipoledipole interaction (the order of magnitude of its decrease with increasing R is the same).

Transitions induced by resonant dipole-dipole interaction were considered in a number of papers<sup>[1-9]</sup>, and precisely for the transition  ${}^{2}P_{1/2} \rightarrow {}^{2}P_{3/2}$  in<sup>[3, 4, 8, 9]</sup>. In<sup>[7]</sup> they considered also the depolarization of atoms under the influence of charge-quadrupole interaction. The purpose of the present study is to find the cross sections of the transitions between the sublevels of the multiplets  ${}^{2}P$  and  ${}^{3}P$  in collisions between different atoms and ions.

2. The following three approximations are used in the paper:

1) The motion of the nucleus of the ions relative to the nucleus of the atoms is assumed to be classical and along a straight-line trajectory. The satisfaction of the first of these conditions requires that in the c.m.s. the wavelength corresponding to the motion be small in comparison with the impact parameter  $\rho_0$ :

$$\lambda = 1/Mv \ll \rho_0; \tag{1.1}$$

Here M is the reduced mass of the atom and the ion, and v is their relative velocity (we use an atomic system of units:  $\hbar = m_e = e = 1$ ). Satisfaction of the second of these conditions requires that the momentum transfer  $\Delta P$  be small in comparison with the momentum P of the motion in the c.m.s.:

$$\Delta P \sim F \Delta t \sim \frac{|ZQ|}{\rho_0^4} \frac{\rho_0}{v} = \frac{|ZQ|}{\rho_0^3 v} \ll P = Mv,$$

where F is the largest force of interaction between the particles,  $\Delta t$  is the characteristic interaction time, Z is the ion charge, and Q is the quadrupole moment of the atom. From this we obtain the condition

$$_{0}^{3} \gg |ZQ|/Mv^{2}.$$
 (1.2)

2) We neglect the difference between the energies of the considered states of the atom. To this end it is necessary that the frequency  $\omega$  of the transition between the sublevels be small in comparison with the reciprocal characteristic time of the collision:

$$\omega = \delta E \ll v/\rho_0, \quad \rho_0 \ll v/\Delta E, \quad (1.3)$$

where  $\delta E$  is the difference of the energies of the considered sublevels.

3) We neglect the polarization interaction. To ascertain the region where this neglect is valid, we compare the charge-quadrupole and polarization interactions of the atom with the ion. The energy of the first of these is  $\overline{r^2}/5R^3$ , where r is the distance of the valence p-electron from the nucleus of the atom (as is well known, for such an electron we have  $Q = (2/5)\overline{r^2}$ ). The energy of the second interaction is  $\overline{r^2}/3R^4\Delta E$ , where  $\Delta E$  is the energy difference between the given level and the nearest level to which the electric dipole transition is allowed. Comparing these two expressions, we obtain

$$\rho_0 \sim R \gg 1/\Delta E. \tag{1.4}$$

(This derivation is rigorously valid only for alkalimetal atoms, for they are the only ones having a single valence electron. However, in the case of any atom, the energy of the charge-quadrupole interaction is equal to  $Q/2R^3$ , and the energy of the polarization interaction is  $\alpha/R^4$ , where  $\alpha$  is the polarizability of the atom, with  $\alpha \Delta E \sim Q.$ )

3. The impact distance  $\rho_0$  can be estimated by two means :

a) The largest contribution to the transition probability is made by those  $\rho$  for which the parameter B in (3.4) is of the order of unity. This yields  $\rho_0 \sim (|ZQ|/v)^{1/2}$ .

b) The obtained cross sections are of the order of  $\pi |\mathbf{ZQ}| / \mathbf{v}$ . Since the cross section is  $\sigma \sim \pi \rho_0^2$ , it follows that  $\rho_0 \sim (|\mathbf{ZQ}| / \mathbf{v})^{1/2}$ .

Taking this condition into account, requirements (1) and (1.2) yield

$$1/|ZQ|M^2 \ll v \ll |ZQ|.$$
 (1.5)

On the other hand, from (1.3) it follows that

$$v \gg [|ZQ| (\delta E)^2]^{\frac{1}{3}}.$$
 (1.6)

Finally, the requirement (1.4) yields

$$v \ll |ZQ| (\Delta E)^2. \tag{1.7}$$

It must be assumed that  $|\mathbf{Q}| \sim 1$  and  $|\mathbf{Z}| = 1$ . Therefore condition (1.5) is practically always satisfied at thermal velocities (thus, for helium  $M^{-2} \sim 5 \times 10^{-7}$  and  $v \sim 5 \times 10^{-4}$  (at a temperature 300°K). On the other hand, the conditions (1.6) and (1.7) depend on the quantities  $\delta E$  and  $\Delta E$ . The values of  $\delta E$  and  $\Delta E$  should be such as to satisfy the inequality

$$[|QZ| (\delta E)^{2}]^{\mathbb{Z}} \ll |QZ| (\Delta E)^{2}, \qquad (1.8)$$

which follows from the conditions (1.6) and (1.7); otherwise our approximations are incorrect. On the other hand, the inequality (1.8) is satisfied for the ground, metastable, or resonant <sup>2</sup>P or <sup>3</sup>P terms of the following elements: helium, all the elements of period 2 of the periodic system with the exception of neon, and also chlorine. The values of  $\delta E$  and  $\Delta E$  and the resultant minimal and maximal values of the relative velocities  $v_{min}$  and  $v_{max}$  of the atoms and ions and of the temperatures  $T_{min}$  and  $T_{max}$  for the indicated elements are listed in Table I. It is assumed that the atoms collide with their own ions. The values of  $\delta E$  and  $\Delta E$  are taken from<sup>[10]</sup>.

In addition to the charge-quadrupole polarization interactions, transitions between the sublevels of the multiplets  ${}^{2}P$  and  ${}^{3}P$  can also result from exchange interaction. However, since the characteristic impact distances are large in comparison with the atomic distances, the exchange integrals will be very small (the electron shells of the atom and ions do not overlap, and the probability of transferring of an electron from the atom to the ion or vice versa is practically excluded). Therefore the exchange interaction plays practically no role at all in this situation. Indeed, the cross sections of the transitions due to the exchange interaction should be of the same order of or smaller than the charge-exchange cross section (charge exchange can, of course, also occur in collisions between atoms and ions, especially of the same element). Let us compare, for example, the cross sections obtained by us for the  $1s2p^{3}P^{0}$  transitions in helium (see (4.2) and Table II below) with the cross sections of the charge exchange occurring when a helium atom collides with an  $He^+$  ion (see<sup>[11]</sup>), at an incidention energy 0.1 eV. Our cross sections are of the order of  $10^3 \pi a_0^2$  ( $a_0$  is the atomic unit of length), and the chargeexchange cross sections are of the order of  $30\pi a_0^2$ .

4. It is of interest to investigate the opposite, adiabatic case, when  $\rho_0 \gg v/\delta E$ . In this case the adiabatic perturbation theory is applicable. As is well known, it yields an exponentially small result if the terms of the states for the transition between which the cross section is sought do not intersect and do not converge asymptotically (the terms are taken as functions of the distance between the nuclei of the atom and the ion).

An investigation, which we do not report here, shows that the terms coming from the sublevels  ${}^{2}P_{1/2}$  and  ${}^{2}P_{3/2}$ indeed do not intersect and do not converge asymptotically (in the case of collision of excited and unexcited atoms of an alkali metal, the terms intersect and therefore the adiabatic cross sections are large, see<sup>[3, 8, 9]</sup>). For a collision of an atom with an ion in the adiabatic limiting case, the cross sections of the transitions between the sublevels of the doublet  ${}^{2}P$  are exponentially small, and are of no interest to us.

TABLE I

|                            | 1               | 1               | 1                   |                 | 1                            | 1                |                 |                  |                   |
|----------------------------|-----------------|-----------------|---------------------|-----------------|------------------------------|------------------|-----------------|------------------|-------------------|
| Element                    | He              | Li              | Be                  | В               | с                            | N                | 0               | F                | CI                |
| Term •                     | 2p 3P0<br>(res) | 2p *Po<br>(res) | 2p 3Po<br>(res)     | 2p *P•<br>(gnd) | 2p <sup>2 3</sup> P<br>(gnd) | 2p3 #P0<br>(met) | 2p4 3P<br>(gnd) | 2pš *P0<br>(gnd) | 3p\$ 2P0<br>(gnd) |
| δE. cm−1                   | 1.064           | 0.39            | 4.5                 | 16              | 43.5                         | 0                | 226             | 405              | 878               |
| r <sub>min</sub> , at. un. | 3.10-4          | 2.10-4          | 7.10-4              | 2.10-3          | 4-10-3                       | 0                | 1.10            | 2.10-1           | 3-10-1            |
| T <sub>min</sub> , K       | 70              | 30              | 1 · 10 <sup>3</sup> | 6.5.103         | 3.104                        | 0                | 3.10*           | 9·103            | 4.10              |
| $\Delta E$ , eV            | 1.14            | 1.85            | 2,195               | 4,94            | 4.18                         | 9.34             | 9.12            | 12.68            | 8.87              |
| rmax, at. un.              | · 2·10-*        | 4-10-3          | 6.5.10-3            | 3-10-*          | 2.10-1                       | 1-10-1           | 1-10-1          | 2.10~1           | 2.10-1            |
| T <sub>max</sub> , K       | 2.109           | 3.104           | 7.104               | 2.10*           | 1.10•                        | 4.107            | 4-107           | 2.10             | 2.10*             |

\*The abbreviations in the parentheses under the designations of the terms are the following: res-resonant, gnd-ground, met-metastable.

| TABLE II    |                |  |  |  |  |  |  |  |
|-------------|----------------|--|--|--|--|--|--|--|
|             | J              |  |  |  |  |  |  |  |
| J,          | . 0            | 1  | 2  |  |  |  |  |  |
| 0<br>1<br>2 | 0.692<br>2.169 | $\frac{1}{3a} \xrightarrow{(0 \to 1)} 3.715$ | $^{1/_{5}a} (0 \rightarrow 2)$<br>$^{3/_{5}a} (1 \rightarrow 2)$ |  |  |  |  |  |

The foregoing pertains to the case  $R \gg 1$ . Therefore in the adiabatic limiting case the cross sections of the transitions between the sublevels of the doublets <sup>2</sup>P are actually not small, but are of the order of  $\pi$ , which is small in comparison with the ballistic cross sections obtained below. An analogous investigation shows that the terms from the sublevels <sup>3</sup>P<sub>0</sub>, <sup>3</sup>P<sub>1</sub>, and <sup>3</sup>P<sub>2</sub> likewise do not intersect, but that some of them converge asymptotically. Adiabatic transitions therefore occur between them (these will be discussed elsewhere).

#### 2. FUNDAMENTAL EQUATIONS

1. It is convenient to choose the coordinate axes in the following manner: the y axis is directed along the velocity vector of the incident ion, the x axis also lies in the scattering plane, and the z axis is perpendicular to the latter; the origin is aligned with the nucleus of the atom. Solving the problem by perturbation theory, we can show that the transitions between the different electron configurations of the atoms, and also between the different L and S terms, are negligibly small. Therefore the electron wave function of the atom can be written in the form (we consider <sup>2</sup>P or <sup>3</sup>P terms)

$$\Psi(t) = \sum_{J,J_z} a(J,J_z;t) | J,J_z\rangle \exp\{-iE_J t\},\$$

where  $|J, J_Z\rangle$  are the wave functions of the stationary states of the atoms with total electron angular momentum J and its projections  $J_Z$  on the z axis (the principal and orbital numbers of the individual electrons, and the total orbital and spin angular momenta of the electron shell of the atom remain unchanged, and we therefore omit the symbols for these quantum numbers as well as the radial parts of the wave functions).  $E_J$  is the energy of this state;

$$|J, J_z\rangle = \sum_{M, S_z} \langle 1, M; S, S_z | J, J_z \rangle Y_{1M} \chi_{SS_z},$$

where  $Y_{1,M}$  is the angular wave function of the state with orbital quantum number L = 1 and with magnetic quantum number M = -1, 0, +1,  $\chi_{S,SZ}$  is a spin state with spin S and projection  $S_Z$  on the z axis, and  $\langle 1, M; S, S_Z | J, J_Z \rangle$  are Clebsch-Gordan coefficients.

The Schrödinger equation for this function takes the form

$$i\partial \Psi/\partial t = [\ddot{H}_0 + \ddot{V}(t)] \Psi(t),$$
 (2.1)

where  $\widehat{H}_0$  is the Hamiltonian of the free atom and  $\widehat{V}(t)$  is the operator of the interaction of the atom with the ion. Multiplication of both sides of (2.1) by  $\langle J, J_Z|$  and integration over the configuration space yield

$$\frac{da(J, J_{z})}{dt} = \sum_{J, J_{z}} \langle J, J_{z} | \hat{V}(t) | J', J_{z}' \rangle a(J', J_{z}'; t) \exp\{i\delta(J, J')t\},\\\delta(J, J') = E_{J} - E_{J'}.$$
(2.2)

By virtue of the condition  $v/\rho_0 \gg \delta(J, J')$ , it can be assumed that  $\exp \{i\delta(J, J')t\} = 1$  over the entire time interval in which the transitions take place. Equations (2.2) become simpler:

$$\frac{da(J, J_{z})}{dt} = \sum_{J, J_{z}} \langle J, J_{z} | \hat{V}(t) | J', J_{z}' \rangle a(J', J_{z}'; t).$$
(2.3)

2. An atom in the P-state can have no nonzero *l*-pole angular momenta with  $l \neq 2$ . Therefore the interaction of the atom with the ion is charge quadrupole. Its operator is given by

$$\hat{V} = Z \hat{Q}_{ik} n_i n_k / 2R^3,$$

where n = R/R; R is the radius vector of the nucleus of the ion relative to the nucleus of the atom;  $\hat{Q}_{ik}$  is the operator of the quadrupole moment of the atom. The latter is equal to

$$\hat{Q}_{ik} = \frac{3}{2}Q(\hat{L}_{i}\hat{L}_{k} + \hat{L}_{k}\hat{L}_{i} - \frac{4}{3}\delta_{ik}),$$

where  $\hat{\mathbf{L}}$  is the operator of the total orbital angular momentum of the electron shell of the atom with  $\mathbf{L} = 1$ . Thus,

$$\hat{V} = \frac{3}{2} ZQ((\hat{L}n)^2 - \frac{2}{3})/R^3.$$
 (2.4)

### 3. TRANSITION CROSS SECTIONS IN THE DOUBLET 과

1. The total spin of the atom is S = 1/2, and its projection on the z axis is  $S_z = \pm 1/2$ . Therefore the function  $|J, J_z\rangle$  takes the form

$$|J, J_z\rangle = \sum_{M, S_z} \langle 1, M; {}^{i}/{}_{z}, S_z | J, J_z\rangle Y_{1M}\chi_{h,S_z}.$$
(3.1)

Substituting (3.1) and (2.4) in (2.3), we obtain two similar systems of equations (the system (2.3) is separable):

$$i \frac{da({}^{3}/_{2}, \pm^{3}/_{2})}{dt} = \frac{ZQ}{4R^{3}} \{-a({}^{3}/_{2}, \pm^{3}/_{2}) + \sqrt{3} e^{\pm 2i\varphi} [a({}^{3}/_{2}, \pm^{1}/_{2}) \pm \sqrt{2} a({}^{1}/_{2}, \pm^{1}/_{2})]\},$$
(3.2)

$$i \frac{da(\frac{3}{2}, \pm \frac{1}{2})}{dt} = \frac{ZQ}{4R^3} \left[ \sqrt{3} e^{\pm 2i\varphi} a(\frac{3}{2}, \pm \frac{3}{2}) + a(\frac{3}{2}, \pm \frac{1}{2}) \mp \sqrt{2} a(\frac{1}{2}, \pm \frac{1}{2}) \right],$$
  
$$i \frac{da(\frac{1}{2}, \pm \frac{1}{2})}{dt} = \pm \frac{ZQ}{2\sqrt{2}R^3} \left[ \sqrt{3} e^{\pm 2i\varphi} a(\frac{3}{2}, \pm \frac{3}{2}) - a(\frac{3}{2}, \pm \frac{1}{2}) \right].$$

Here  $\varphi$  denotes the angle between the x axis and the radius vector **R**.

The reasons for the separation of the system (2.3) into two systems consists in the following. The operator  $\hat{V}(t)$ , as seen from (2.4), is quadratic in the orbital angular momentum operator  $\hat{L}$ . Since the z axis is always perpendicular to the radius vector  $\mathbf{R}$ , it follows that, by acting on the angular wave functions  $Y_{1M}$ , the operator  $\hat{V}(t)$  changes the magnetic quantum number of the atom M by 0 or  $\pm 2$ . Since the operator  $\hat{V}(t)$  does not act at all on the spin variables, it follows that by acting on the state on the atom  $|\mathbf{J}, \mathbf{J}_{\mathbf{Z}}\rangle$ , it also changes the projection  $J_{\mathbf{Z}}$  of its total electron angular momentum on the z axis by 0 or  $\pm 2$ . Therefore all the matrix elements  $\langle \mathbf{J}, \mathbf{J}_{\mathbf{Z}} | \hat{V}(t) | \mathbf{J}', \mathbf{J}'_{\mathbf{Z}} \rangle$ , where  $\mathbf{J}_{\mathbf{Z}} - \mathbf{J}'_{\mathbf{Z}} \neq 0, \pm 2$ , vanish.

2. We change over from the vector  $\mathbf{\Phi}$ , the components of which are the coefficients  $a(J, J_Z; t)$ , to the vector X, whose components are the coefficients  $b_{\mathbf{M}}^{\mathbf{L}}(t) = b(\mathbf{M}, \pm 1/2; t)$  of the expansion of the wave function of the atom

$$\Psi(t) = \sum_{\boldsymbol{M}, \boldsymbol{S}_{z}} b(\boldsymbol{M}, \boldsymbol{S}_{z}; t) Y_{\boldsymbol{1}\boldsymbol{M}} \chi_{\boldsymbol{1}\boldsymbol{h}, \boldsymbol{S}_{z}}$$

over the states with definite projections of the total orbital and spin angular momenta of the atom on the z axis. Equations (3.2) are simplified even further:

$$i\frac{db_{+1}^{\pm}}{dt} = \frac{ZQ}{4R^{3}}(-b_{+1}^{\pm}+3e^{-2i\varphi}b_{-1}^{\pm}),$$

$$i\frac{db_{-1}^{\pm}}{dt} = \frac{ZQ}{4R^{3}}(3e^{2i\varphi}b_{+1}^{\pm}-b_{-1}^{\pm}),$$

$$i\frac{db_{\Phi}^{\pm}}{dt} = \frac{ZQ}{4R^{3}}b_{0}^{\pm}.$$
(3.3)

The reason for the separation of the equation for  $b_0$  is the vanishing of the matrix elements of the operator  $\hat{V}(t)$  for transitions with  $\Delta M = \pm 1$  and with  $\Delta S_z \neq 0$ .

We change from the vector X to the vector  $\Psi$ , whose components are the coefficients  $c_i^{\pm}(t) = c(i, S_Z; t)$  of the expansion of the wave function of the atom

$$\Psi(t) = \sum_{i,S_t} c(i,S_z;t) Y_{i}\chi_{\lambda_z,S_z};$$

here  $\mathtt{Y}_{1i}$  are the angular wave functions, chosen in the form

$$\mathbf{Y}_{i} = \left(\frac{3}{4\pi}\right)^{1/2} \frac{\mathbf{r}}{r}$$

(**r** is the radius vector of the "effective electron" that would have interacted with the electric field of the ion in the same manner as all the electrons of the unfilled p shell of the atom taken together (in the particular case this can be a real p electron or p hole)).

In addition, we make the change of variable

$$\xi = vt/R$$
.

As t changes from  $-\infty$  to  $+\infty$ , the quantity  $\xi$  covers the interval from -1 to +1. We obtain the system of equations

$$ic_{x}' = B[-(2-3\xi^{2})c_{x}+3\xi(1-\xi^{2})^{t_{y}}c_{y}],$$
  

$$ic_{y}' = B[3\xi(1-\xi^{2})^{t_{y}}c_{x}+(1-3\xi^{2})c_{y}],$$
  

$$ic_{x}' = Bc_{x},$$
  
(3.4)

where the prime denotes differentiation with respect to  $\xi$ , and

 $B = ZQ/2\rho^2 v$ 

(we have left out the  $\pm$  symbols of the coefficients  $c_i^{\pm}$ ).

The solution for  $c_z$  is obtained directly:

$$c_i = Ce^{-iB_i}$$
.

From  $c_x$  and  $c_y$  we change over to u and v:

$$c_x = u e^{iB\xi/2}, \quad c_y = v e^{iB\xi/2}$$

From (3.4) we easily obtain a system of equations for u and v. It was first obtained and investigated by Vain-shtein and Galitskii<sup>[1]</sup>. On going from  $\xi = -1$  to  $\xi = +1$ , the solution changes in the following manner:

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \rightarrow \begin{pmatrix} fe^{i\phi} \\ g \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \rightarrow \begin{pmatrix} -g \\ fe^{-i\phi} \end{pmatrix}$$

Here

 $\binom{u(\xi)}{v(\xi)}$ 

is the solution of the system of equations for u and v,

while f, g, and  $\varphi$  are real functions of the parameter B. The exact values of f, g, and  $\varphi$  were obtained by numerical computer integration of the aforementioned system of equations for u and v.

3. Let us express the results of the collision in terms of f, g, and  $\varphi$ . The state  $\Psi_{\text{out}}$  after the collision can be expressed in terms of the state  $\Psi_{\text{in}}$  prior to the collision with the aid of the unitary matrix S:

$$\Psi_{out} = S \Psi_{in}, \quad SS^+ = 1.$$

The matrix S takes the form

$$S = \begin{pmatrix} R & 0 \\ 0 & R \end{pmatrix}$$

where R is the unitary matrix

$$R = \begin{pmatrix} fe^{i(B+q)} & -ge^{iB} & 0\\ ge^{iB} & fe^{i(B-q)} & 0\\ 0 & 0 & e^{-2iB} \end{pmatrix}.$$

The vector  $\Phi_{in}$  is transformed into  $\Phi_{out}$  by the matrix S':

$$\Phi_{out} = S' \Phi_{in}, \quad S' = K^+ S K.$$

Here K denotes the unitary matrix that effects the transition from the vector  $\Phi$  to the vector  $\Psi$ :

$$\Psi = K \Phi, \quad K K^{-} = 1.$$

4. Let us consider the transition of a completely unpolarized atom whose state is  ${}^{2}P_{1/2}$  into the state  ${}^{2}P_{3/2}$ , and the analogous transition from the state  ${}^{2}P_{3/2}$  to the state  ${}^{2}P_{1/2}$ . Averaging over the initial states and summing over the final states, we obtain

$$w(J + J') = \frac{1}{2J + 1} \sum_{J_z, J_z'} |S'(J, J_z; J', J_z')|^2$$

where  $w(J \rightarrow J')$  are the probabilities of the corresponding transitions;  $S'(J, J_Z, J', J'_Z)$  is the S' matrix element corresponding to a transition from the state  $|J, J_Z\rangle$  to the state  $|J', J'_Z\rangle$ .

The probabilities  $w(1/2 \rightarrow 3/2)$  and  $w(3/2 \rightarrow 1/2)$  are given by

$$w({}^{1}/_{2} \rightarrow {}^{3}/_{2}) = {}^{4}/_{9}(1 - f\cos 3B\cos\varphi + f^{2}\sin^{2}\varphi);$$
  
$$w({}^{3}/_{2} \rightarrow {}^{4}/_{2}) = {}^{2}/_{9}(1 - f\cos 3B\cos'\varphi + f^{2}\sin^{2}\varphi).$$

The cross section of the transition  $J \rightarrow J'$  is equal to

$$\sigma(J \to J') = 2\pi \int_{0}^{\infty} w(J \to J', \rho) \rho \, d\rho = \frac{\pi}{2} \frac{|QZ|}{v} \int_{0}^{\infty} \frac{dB}{B^2} w(J \to J', B).$$

The integral

$$I_{i} = \int_{0}^{\infty} \frac{dB}{R^{2}} (1 - f \cos 3B \cos \varphi + f^{2} \sin^{2} \varphi)$$
 (3.5)

was calculated with a computer. As a result, the following values were obtained for the cross sections of interest to us:

$$\sigma({}^{1}/_{2} \rightarrow {}^{3}/_{2}) = 4,800\pi e |ZQ|/\hbar v,$$
  
$$\sigma({}^{3}/_{2} \rightarrow {}^{1}/_{2}) = {}^{1}/_{2}\sigma({}^{1}/_{2} \rightarrow {}^{3}/_{2})$$

(in ordinary units). Although all the foregoing pertains to the case QZ > 0, it is easy to show that the final results are the same also at  $QZ \le 0$ .

## 4. CROSS SECTIONS OF TRANSITIONS IN THE TRIPLET <sup>3</sup>P

1. The total spin of the atom is S = 1, and its projection in the z axis is  $S_z = -1$ , 0, +1. Therefore the function  $|J, J_z\rangle$  takes the form

$$|J,J_z\rangle = \sum_{M,S_z} \langle 1,M;1,S_z|J,J_z\rangle Y_{1M}\chi_{1S_z}.$$
(4.1)

Substituting (4.1) and (2.4) in (2.3), we obtain two systems of equations (the system (2.3) is separable). Each of them describes the time variation of the coefficients  $a(J, J_Z; t)$ , one of them with even  $J_Z$  and the other with odd  $J_Z$ . The reason for the separation of the system of equations (2.3) into two equations is the same as in Sec. 3.

2. We now proceed as in Sec. 3. We arrive at the system (3.4). The only difference is that the matrix K is more complicated and cumbersome, and hence so is S' (these matrices like S, are not 6 by 6 as in Sec. 3, but  $9 \times 9$ ). In addition to the integral I<sub>1</sub> (see (3.5)), we need in this case also the values of two other integrals:

$$I_2 = \int_0^\infty \frac{dB}{R^2} g^2,$$

$$I_3 = \int_0^\infty \frac{dB}{R^2} f[f(1+\sin^2\varphi) - \cos 3B\cos\varphi],$$

which were also calculated with a computer. Each cross section is equal to

$$\sigma(J \to J') = a(J \to J') \pi e |ZQ|/\hbar v \qquad (4.2)$$

(we have used here ordinary units), and the values of  $a(J \rightarrow J')$  obtained with the computer are listed in Table II. Just as in Sec. 3, the final results do not depend on the sign of ZQ.

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