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## Charge transfer between hydrogen atoms and the nuclei of multicharged ions with allowance for the degeneracy of the final states

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The cross sections,  $\sigma$ , for charge transfer between hydrogen and the nuclei of multicharged ions are computed with allowance for the degeneracy of the final hydrogen-like ion states. Allowance for the transitions, induced by the rotation of the internuclear axis, between these states leads to a qualitative change in the  $v$  dependence of  $\sigma$  at low  $v$  (a power-law decrease of the cross sections instead of the exponential decrease found in the Landau-Zener model), as well as to a significant increase in the cross section at the peak. The solution is based on the use of the symmetry properties of the hydrogen atom; this approach makes it possible to take account of the rotation effects in a wide range of velocities. Concrete computations are carried out for the ions  $C^{+6}$  and  $O^{+8}$ .

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### §1. INTRODUCTION

Calculations of the cross sections for charge transfer between neutral hydrogen and multicharged ions are of considerable interest from both the practical and methodological points of view. The practical importance of this problem is due to its connection with the problems of high-temperature-plasma heating and diagnostics. At the same time, charge transfer between hydrogen and nuclei is the simplest type of process in which a large number of degenerate states participate, a process which is of general physical interest (see below).

Of the number of papers devoted to this problem let us note Gershtein's paper,<sup>[1]</sup> in which charge transfer between mesic hydrogen atoms and ions is computed in the Landau-Zener model. Charge transfer between a hydrogen-like ion and its nucleus has been considered by Smirnov.<sup>[2]</sup> The distinctive feature of hydrogen-like systems stems from the presence of the additional symmetry connected with the separability in the field of the two-Coulomb centers of the variables in elliptic coordi-

nates.<sup>[3]</sup> This fact was also used recently by Olson and Salop,<sup>[4,5]</sup> who undertook charge-transfer cross-section calculations within the framework of the Landau-Zener model with allowance for numerical data<sup>[6]</sup> for the electronic terms of the molecular ion  $(HZ)^{+Z}$ , composed of hydrogen, H, and the nucleus of a multicharged ion,  $X^{+Z}$ , with charge  $Z$ .

In Ref. 7, to compute the charge-transfer cross sections, Presnyakov and Ulantsev use the Landau-Zener formula for low speeds together with the Vainshtein-Presnyakov-Sobel'man formula,<sup>[8]</sup> which allows us to follow the transition to the region of high speeds of the charge-exchanging particles. An important distinctive feature of Presnyakov and Ulantsev's paper<sup>[7]</sup> is the description of the transition from the Landau-Zener model to the Brinkman-Kramers model,<sup>[9]</sup> which is valid for fast collisions.

In Ref. 10, Chibisov uses the concept of the decay of the initial "neutral atom+nucleus" term into the continuum of the final "proton+level system of multicharged ion" states. An advantage of the method is its simplicity

and clearness, which allows us to obtain the final results in analytic form. Notice that in its idea content the decay model is equivalent to the "absorbing-sphere" model used in Ref. 5.

It should be pointed out that the enumerated papers contain different opinions concerning the dependence of the total charge-transfer cross section  $\sigma$  on the ion charge  $Z$  even in the low-velocity region. Thus, in Ref. 7 it is found on the basis of numerical computations that  $\sigma \propto Z^2$ ; in Ref. 4, it is assumed, also on the basis of numerical computations, that  $\sigma \propto Z^{3/2}$ ; in the decay model<sup>[10]</sup> the analytic dependence of the cross section has the form  $\sigma \propto Z \ln Z$ ; and, finally, in the similar "absorbing-sphere" model,<sup>[5]</sup>  $\sigma \propto Z \ln^2 Z$ .

The indicated discrepancies are connected, in our opinion, with two circumstances: first, different analytic approximations are used in the various papers for the exchange-interaction potential  $V_{12}(R)$  and, secondly, the region of applicability of the various models strongly depends on the quantity  $Z$ . As to the exchange potential, here the most correct is, apparently, the approximation used in Refs. 4 and 5, which agrees well with the results of the numerical computations<sup>[6]</sup>:

$$V_{12}(R) = \frac{9.13}{Z^2} \exp \left[ -1.324 \frac{R}{Z} \right]. \quad (1.1)$$

It can be seen from this that the effective distances,  $R_{eff}$ , that contribute to the charge transfer are proportional to  $Z^{1/2}$ . Quite close to this form is the exchange potential used in the decay model.<sup>[10]</sup>

As regards the applicability of the decay<sup>[10]</sup> and absorbing-sphere<sup>[5]</sup> models, let us note that these models require fairly high  $Z$  values ( $Z \geq 10$ ). The point is that one of the consequences of the above-noted symmetry of the one-electron system in the field of two Coulomb centers is the fact that only one out of all the  $n^2$  ion states belonging to the level with the principal quantum number  $n$  gets occupied in charge transfer made from the initial term.<sup>[6]</sup> This state corresponds to the maximum component of the dipole moment of the hydrogen-like level of the ion along the direction of the electric field,  $F$ , produced by the proton, and is consequently characterized by the parabolic quantum numbers  $n_2 = n - 1$ ,  $n_1 = 0$ ,  $m = 0$ . For ions of low multiplicity ( $Z \leq 10$ ), the number of levels that contribute to the charge transfer is quite limited (two-three); therefore, the replacement of these levels by an equivalent continuum becomes problematic.

The foregoing discussion indicates first and foremost two distinctive features of charge transfer between a hydrogen atom and a bare nucleus: 1) the high degree ( $n^2$ -fold) of degeneracy of the final states of the hydrogen-like ion and 2) the existence of selection rules according to which there can be charge transfer to only one of these degenerate states, namely, the state with the quantum numbers  $n_2 = n - 1$ ,  $n_1 = 0$ ,  $m = 0$ , which we shall hereafter denote by the symbol  $|0\rangle$ . These two circumstances lead to the appearance of a new type of effects not considered in previous papers. Basically, they amount to the following. The total transition probability is made up of contributions from transitions at two

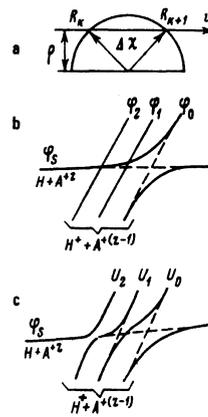


FIG. 1. Collision geometry (a) and scheme of the terms of the system undergoing charge exchange: adiabatic terms (b) and dynamic terms (c).

points: during the approach ( $R_k$ ) and during the separation ( $R_{k+1}$ ); see Fig. 1(a). Then during the motion of the system from the point  $R_k$  to the point  $R_{k+1}$  there can occur transitions between the populated state  $|0\rangle$  and the remaining  $n^2 - 1$  degenerate states, which can lead, in particular, to the depopulation of the state  $|0\rangle$  as the system approaches the point  $R_{k+1}$ . Thus, the total transition probability is determined not only by the population of the states  $|0\rangle$  at the points  $R_k$  and  $R_{k+1}$ , but also by the nature of the interaction of the  $n^2$  degenerate states between these points.

The existence of effects of this type was first discussed by Bates.<sup>[11]</sup> An estimate of their role for the case of charge transfer between non-hydrogen-like ions in states with nonzero orbital angular momenta is given by Zhdanov and Chibisov in Ref. 12. An important experimental confirmation of the significant role played by the effects of the rotation of the internuclear axis is presented for the reaction  $\text{He}^{2+} + \text{He}$  by Afrosimov *et al.* in Ref. 13.

The specific properties of hydrogen-like states are connected with the fact that the effects of mixing of the states in the process of charge transfer can be taken into account exactly in spite of the high degree ( $n^2$ -fold) of level degeneracy. It is to these problems that the present paper is devoted.

## §2. THE PHYSICAL PICTURE OF THE CHARGE-TRANSFER PROCESS. BEHAVIOR OF THE CROSS SECTION IN THE REGIONS OF HIGH AND LOW RATES OF ROTATION

The principal distinctive features of the charge-transfer process consist, as has already been noted by Gershtein,<sup>[1]</sup> Olson and Salop,<sup>[4,5]</sup> Presnyakov and Ulantsev,<sup>[7]</sup> and Chibisov,<sup>[10]</sup> in the following. The initial term,  $E_0(R)$ , of the quasi-molecule  $H(1S) + X^{+Z}$  for an internuclear distance  $R \rightarrow \infty$  coincides with the ground level of hydrogen and varies slowly as the particles approach each other on account of the weak polarization interaction ( $\propto 1/R^4$ ). The final  $H^+ + X^{+(Z-1)}$  term,  $E_n(R)$ , for  $R \rightarrow \infty$  coincides with the level of the multicharged ion with energy  $E_n = -Z^2/2n^2$ , and, for finite  $R$ , contains a strong Coulomb interaction between the proton  $H^+$  and the multicharged ion  $X^{+(Z-1)}$ , so that<sup>1)</sup>

$$E_n(R) = -Z^2/2n^2 + (Z-1)/R. \quad (2.1)$$

It is easy to see that the initial term  $E_0(R)$  has a set of points of intersection,  $R_n$ , with the hydrogen-like system of levels of the final term. These points are given by the relation

$$R_n = 2(Z-1)n^2/(Z^2-n^2), \quad n < Z. \quad (2.2)$$

At relative velocities of the nuclei lower than the atomic velocities (i.e., for  $v \ll 1$ ), the points of intersection make the dominant contribution to the charge-transfer probability. As usual, the system passes through the points of intersection twice—once when the nuclei are approaching each other and once when they are separating.

Let us discuss the possibility of using one-center wave functions to describe the evolution of the electron states on the nucleus.<sup>2)</sup> The point is that the electronic level on the proton disappears at a distance  $R \approx 2(2Z)^{1/2}$  (the estimate follows from the condition for the disappearance of the potential barrier in the elliptic coordinate  $n$ ). This, however, does not yet imply that the electron states on the nucleus of the multicharged ion will be strongly distorted at the distance,  $R$ , in question. Indeed, since the dimensions of the potential well of the multicharged ion are much greater than the dimensions of the well on the proton and the self-field ( $Z/R$ ) of the ion in this region is much stronger than the proton field ( $1/R$ ), the final levels of the electron on the nucleus  $Z$  are weakly distorted. Since we are interested in the mixing of precisely the states on the nucleus of the ion, we can use the unperturbed hydrogen-like states on this nucleus. The indicated circumstance is confirmed by the exact numerical computations carried out in Ref. 6 and analyzed in Refs. 4 and 5, and finds its expression in the smallness of the effective exchange-interaction potential (1.1) at these distances.

Let us estimate the characteristic parameters of the problem. The relation (2.2) allows us, if  $R_{\text{eff}}$  is known, to estimate the effective values of the principal quantum number of the levels,  $n_{\text{eff}}$ , at which the charge transfer occurs:

$$n_{\text{eff}} \approx \frac{Z}{[1+2(Z-1)/R_{\text{eff}}]^{1/2}}. \quad (2.3)$$

Assuming, on the basis of the discussion in §1, that  $R_{\text{eff}} \sim Z^{1/2}$ , we obtain  $n_{\text{eff}} \sim Z^{3/4}$ .

The distance,  $\Delta E_{nn'}$ , between neighboring levels is equal to:

$$\Delta E_{nn'} \approx Z^2/n^3 \sim Z^{-1/4}.$$

The adiabatic approximation is fulfilled provided

$$\Delta E_{nn'} R/v \gg 1 \quad \text{or} \quad v \ll Z^{1/4}. \quad (2.4)$$

Let us compare the Stark splitting,  $\Delta E_S$ , of the hydrogen-like level in the electric field,  $F$ , of the proton with the quantity  $\Delta E_{nn'}$ :

$$\Delta E_S \sim \frac{n^2}{Z} F \sim \frac{1}{Z^{1/2}}, \quad \frac{\Delta E_S}{\Delta E_{nn'}} \sim Z^{-1/4} \ll 1. \quad (2.5)$$

In practice, the inequality (2.5) is weak, since  $Z^{1/4} \sim 1$  right up to  $Z \sim 100$ . This pertains also to the applicability of the asymptotic formulas for the interaction potentials. Therefore, instead of the general order-of-magnitude relations, we should compare the corresponding parameters for the specific cases. Such a comparison, carried out on the basis of the numerical data given in Ref. 4, shows that the use of the asymptotic formulas for the potentials falls within the limits of that accuracy (~30%) which can, in general, be counted on in the analytic solution of the problem. In particular, the values of the intersection radii  $R_n$  computed from the asymptotic formula (2.2) coincide with the results of the numerical term computations<sup>[6]</sup> to within roughly 10%. Therefore, following the authors of Refs. 1, 4, 5, 7, and 10, we shall use the asymptotic potentials.

Let us discuss the applicability of the Landau-Zener model<sup>[3]</sup> to the computation of the transition probability at the points of intersection. The applicability of the model requires the smallness of the transition region  $\Delta R \propto (v/F)^{1/2}$  ( $F = -\partial u/\partial R = (Z-1)/R^2$ ) is the force at the point of intersection) in comparison with the characteristic region,  $\Delta R_V$ , of variation of the interaction potential  $V$ . For the potential (1.1) we have  $\Delta R_V \sim Z^{1/2}$ , so that (with allowance for the fact that  $R_{\text{eff}} \propto Z^{1/2}$ )

$$\Delta R \ll \Delta R_V, \quad \text{if} \quad v \ll Z. \quad (2.6)$$

In fact, the applicability of the model is limited, apparently, to the region  $v \leq 1$ , outside which the results should be described by the Brinkman-Kramers model.<sup>[9]</sup>

The condition (2.6) also expresses the smallness of the size of the transition region,  $\Delta R$ , around each of the two points of intersection in comparison with the distance,  $R_{\text{eff}}$ , between them.

Let us consider the mechanism of charge-transfer to one level,  $n$ , within the framework of the two approximate models, which, as will be seen below, are valid in the region of high and low velocities  $v$ . The first of these models is based on the independence of the contributions of the charge-transfer and degenerate-state-mixing regions. The smallness of the charge-transfer regions,  $\Delta R$ , around the points of intersection in comparison with the mixing regions,  $R_{\text{eff}}$ , between these points [see (2.6)] serves as the physical basis of this assumption.

Let the transition probabilities,  $p$ , at the points of intersection  $R_k$  and  $R_{k+1}$  (see Fig. 1 (a)) be known. Let the operator,  $\hat{U}(\Delta\chi)$ , of evolution of the system of  $n^2$  degenerate sublevels between the points  $R_k$  and  $R_{k+1}$  separated by an angle  $\Delta\chi$  of rotation of the internuclear axis be also known. Since the exchange interaction  $V(R)$  (and along with it the transition probability  $p$ ) has a simple form in the coordinate system oriented along the internuclear axis, it is convenient to carry out all the computations in this rotating system. Within the framework of the model under consideration, it is not difficult to derive an expression for the total transition probability,  $W$ , with allowance for the operator  $\hat{U}$ :

$$W = 2p(1-p) + (1-p)^2[1 - |U_{00}(\Delta\chi)|^2], \quad (2.7)$$

where  $U_{00}$  is the matrix element of the operator  $\hat{U}$ , taken with respect to the states  $|0\rangle$ , to which the charge is transferred. Below we shall call the effects connected with the rotation of the internuclear axis rotation effects.

For the transition probability  $p$ , we have the Landau-Zener formula<sup>[3]</sup>

$$p = \exp[-2\pi V^2(R_n)/v_n F], \quad (2.8)$$

where the magnitudes of the exchange interaction  $V$ , the force,  $F$ , acting on the electron, and the radial velocity  $v_R = v(1 - \rho^2/R^2)^{1/2}$  are evaluated at the point of intersection of the terms  $R_n$ , (2.1). We shall assume the motion of the nuclei is rectilinear:  $R^2 = \rho^2 + v^2 t^2$  ( $\rho$  is the impact parameter and  $v$  is the relative velocity at infinity).

The evolution operator  $\hat{U}(\Delta\chi)$  of the degenerate hydrogen-like states with a given  $n$  in the field of the charge flying by is known from calculations of the Stark broadening of spectral lines.<sup>[14]</sup> Its explicit form is given in Ref. 15.<sup>3)</sup> In the Appendix we show that it is possible to simplify significantly the analytic form of this operator, as a result of which the matrix element  $U_{00}^J(\Delta\chi)$  assumes the form

$$U_{00}^J(\Delta\chi) = (1 - \sin^2 \beta \sin^2(v/2))^{1/2}, \quad J = (n-1)/2, \quad (2.9)$$

$$\tan \beta = \rho v / \alpha, \quad \alpha = 3n/2Z, \quad v = \Delta\chi(1 + (\alpha/\rho v)^2)^{1/2}.$$

Substituting (2.9) into (2.7), and defining in the usual manner the cross section

$$\sigma = 2\pi \int_0^{R_n} \rho d\rho W(\rho),$$

we find

$$\sigma_n = 2\pi R_n^2 [f_{L-Z}(\Delta) + f_{\text{rot}}(\delta, \Delta)], \quad (2.10)$$

$$f_{L-Z} = \int_0^1 dx \exp(-\Delta/\sqrt{x}) [1 - \exp(-\Delta/\sqrt{x})], \quad (2.11)$$

$$f_{\text{rot}}(\delta, \Delta) = \int_0^1 dx [1 - \exp(-\Delta/\sqrt{1-x^2})]^2 [1 - |U_{00}|^2]. \quad (2.12)$$

Here  $\Delta = 2\pi V^2/Fv$  and  $\delta = \alpha/R_n v$ ; the function  $f_{L-Z}(\Delta)$  describes the usual velocity dependence of the cross section in the Landau-Zener model<sup>[3]</sup> and the function  $f_{\text{rot}}(\delta, \Delta)$  takes account of the contribution of the rotation effects.

The influence of the rotation effects can easily be elucidated directly from the general formulas (2.7)–(2.9). Let us assume that  $p \rightarrow 0$ , so that the system moves along adiabatic terms. Then the charge-transfer probability is wholly determined, according to (2.7), by the probability,  $1 - |U_{00}|^2$ , for the depopulation of the state  $|0\rangle$ . The depopulation of the state  $|0\rangle$  is caused, as has been noted, by transitions into other degenerate states not interacting with the initial term (Fig. 1(b)).

If the velocity is sufficiently high, so that  $\delta = \alpha/R_n v \ll 1$ , then, as can be seen from (2.9), the probability for the depopulation of the state  $|0\rangle$  is constant (since  $\sin \beta \approx 1$ ,  $v \approx \Delta\chi \sim 1$ ). In this case the charge-transfer cross section is of the order of  $\pi R_n^2$ , i. e., it is also constant (instead of the exponential decrease in the Landau-Zener model as  $p \rightarrow 0$ ). The physical meaning of this result consists in the following. In the case of a quick flight of the proton from the first charge-transfer point to the second (Fig. 1(a)) the wave function of the level  $n$  in the fixed coordinate system does not, in general, have time to change. As a result, in the rotating system (in which the charge-transfer is being considered) the wave function turns out to be turned through an angle of  $\Delta\chi$ , so that  $1 - |U_{00}|^2 \neq 0$ . This effect is purely geometric, and does not depend on the specific form of the interaction. Essentially, there occurs here an instantaneous change of basis—a “shaking up:” the system at one point is recharged into a state oriented along  $R_n$ , while at the other point it is recharged into a state oriented along  $R_{n+1}$  and rotated through an angle of  $\Delta\chi$  (Fig. 1(a)); the charge transfer is made consistently to states with the maximum component of the dipole moment ( $n_1 = 0$ ,  $n_2 = n - 1$ ,  $m = 0$ ), but along different directions. Therefore, the transitions occurring at the two points are essentially into different states, which leads to an increase in the total transition probability.

At low velocities,  $\delta = \alpha/R_n v \gg 1$ , the mixing of the states is slight (the function  $|0\rangle$  is the “true” function), and, consequently,

$$\lim_{v \rightarrow 0} (1 - |U_{00}(\Delta\chi)|^2) = 0,$$

i. e.,  $W \rightarrow 0$  as  $v \rightarrow 0$ . The foregoing is also valid for a quadrupole interaction; therefore, the estimate,  $\lim_{v \rightarrow 0} W|_{v \rightarrow 0} = \text{const}$ , obtained in Ref. 12 overestimates the contribution of the rotation effects. In the case under consideration, however, the assumption that the effects of the charge transfer and of the mixing of the states are independent does not hold, and the contribution to the charge transfer of the regions,  $\Delta R$ , around the charge-transfer points not considered in the present model becomes appreciable.<sup>4)</sup>

Summarizing the main results of the model based on the independence of the contributions of the charge-transfer and rotation regions, let us note that it correctly describes the region  $\delta \lesssim 1$ , which corresponds to fairly fast collisions. In this case, as is clear from analysis of the asymptotic behavior of the functions  $f_{L-Z}(\Delta)$  and  $f_{\text{rot}}(\delta, \Delta)$ , (2.10)–(2.12), the rotation effects are appreciable in the region  $\Delta \geq 1$ , where  $f_{L-Z} \propto e^{-\Delta}$ , whereas  $f_{\text{rot}}(\delta, \Delta) \rightarrow \text{const}$  [in the region  $\Delta \ll 1$ , however, the function  $f_{L-Z}(\Delta) \propto \Delta$ , while  $f_{\text{rot}}(\delta, \Delta) \propto \Delta^2 \ll f_{L-Z}(\Delta)$ ]. It is clear that these results are in accord with the qualitative estimates.

It is clear from the foregoing that it is convenient to characterize the contribution of the rotation effects by the parameter

$$\epsilon = \frac{\delta}{\Delta} = \frac{3n(Z-1)}{4\pi Z R^2 V^2} \approx \frac{n}{4R^2 V^2}. \quad (2.13)$$

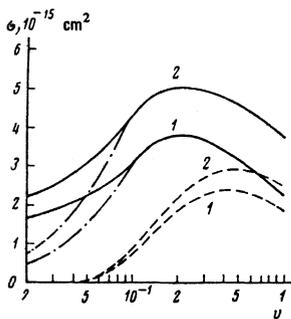


FIG. 2. Cross sections for charge transfer between the hydrogen atom and the ions  $C^{+6}$  (curve 1) and  $O^{+8}$  (curve 2) as functions of the speed. Dashed curves—the Landau-Zener model without allowance for the rotation effects; continuous curves—with allowance for the rotation effects; dash-dot curves—model of independent contributions of the charge-transfer and rotation effects.

If  $\epsilon \ll 1$ , then the rotation appreciably changes the cross section even at its maximum. Using (1.1), (2.1), and (2.13), we can easily determine the value of  $\epsilon$  for different levels of specific ions:  $C^{+6}(n=4) \sim 0.6$ ;  $N^{+7}(n=5) \sim 4.6$ ,  $(n=4) \sim 0.134$ ;  $O^{+8}(n=5) \sim 0.6$ ,  $(n=4) \sim 0.147$ ;  $Ne^{+10}(n=7) \sim 40$ ,  $(n=6) \sim 0.61$ ,  $(n=5) \sim 0.167$ . It can be seen that allowance for rotation is necessary in the majority of practical cases.

The conclusions drawn are confirmed by the results of the more general computations carried out in Sec. III. In Fig. 2 a comparison of the present model with a more rigorous computation is presented which allows us to make a judgment on the region of applicability of the model.

Let us proceed to the consideration of the behavior of the charge-transfer cross section at low velocities ( $v \rightarrow 0$ ).<sup>5)</sup> For this purpose, let us use the adiabatic theory of perturbations.<sup>[3]</sup> The scheme of the adiabatic terms is shown in Fig. 1(b), from which it can be seen that the set of terms  $\varphi_1, \varphi_2, \dots$  that do not interact with the initial term  $\varphi_s$  has a series of points of intersection that make the dominant contribution to the cross section when  $v \rightarrow 0$ . In this case there arises (in first-order perturbation theory) on account of the rotation effects a coupling between only the states  $\varphi_0$  and  $\varphi_1$ .

The probability of transition between an adiabatic term (denoted by  $\Psi_I$ ) and the term  $\varphi_1$ , which intersects it, is given by the expression

$$w = \left| \int_{-\infty}^{+\infty} \langle \Psi_I | L_x | \varphi_1 \rangle \exp \left\{ -i \int_{-\infty}^t [E_I(R) - E_1(R)] d\tau \right\} \right|^2, \quad (2.14)$$

where  $L_x$  is the component of the orbital angular momentum perpendicular to the collision plane.

The wave function  $\Psi_I$  is a linear combination of the functions  $\varphi_s$  and  $\varphi_0$  with well-known coefficients,  $b_+(R)$  and  $b_-(R)$  (see Ref. 3, problem No. 1 to 39), which, in our case, depend on the strengths of the exchange and dipole interactions. This pertains also to the energy,  $E_I(R)$ , of the term. Substituting the expression for  $\Psi_I$  into (2.14), we obtain

$$w = | \langle L_x \rangle_{10} |^2 \left| \int_{-\infty}^{+\infty} dt b_+ [R(t)] \dot{\varphi} [R(t)] \right|^2 \quad (2.15)$$

$$\times \exp \left[ -i \int_{-\infty}^t (E_I - E_1) d\tau \right]^2.$$

The dominant contribution to the integral (2.15) for  $v \rightarrow 0$  is, as has been noted, made by the point,  $R_0$ , of intersection of the terms:  $E_I(R_0) = E_1(R_0)$ . Going through the usual procedure for evaluating an integral by the stationary-phase method near the point of intersection, we find

$$w = | \langle L_x \rangle_{10} |^2 2\pi | \dot{\varphi} |^2 | b_+ |^2 (\partial(E_I - E_1)/\partial t)^{-1} |_{R=R_0}. \quad (2.16)$$

The value of the derivation  $\partial(E_I - E_1)/\partial t$  at the point  $R = R_0$  can be expressed in terms of the coefficient  $|b_-(R)|^2$  if we allow for the fact that the dominant terms here are connected with the derivatives of the Coulomb repulsion energy of the nuclei:

$$\frac{\partial}{\partial t} \left[ \frac{Z-1}{R} \right] = v_n \frac{Z-1}{R^2} = v_n F.$$

As a result, for  $w$  we obtain the final expression (with allowance for the equality  $\dot{\varphi} = \rho v R^{-2}$  and the doubling of the result when the system passes through the points of intersection twice):

$$w = 4\pi | \langle L_x \rangle_{10} |^2 \left| \frac{\rho v}{R^2} \right|^2 \frac{1}{v_n F(R)} \left| \frac{b_+(R)}{b_-(R)} \right|^2_{R=R_0}. \quad (2.17)$$

The matrix element  $\langle L_x \rangle_{10}$ , evaluated with the parabolic wave functions, is equal to  $(n-1)^{1/2}/2$  in the case, being considered, of a transition from the state  $|0\rangle = |n_1 = 0, n_2 = n-1, m = 0\rangle$ . In this case it is necessary to take into consideration the fact that the state  $|0\rangle$  is coupled by rotation to the twofold degenerate state  $|n_1 = 0, n_2 = n-2, m = \pm 1\rangle$ .

The transition cross section

$$\sigma = 2\pi \int_0^{2\pi} \rho d\rho w(\rho),$$

computed on the basis of (2.17), has the form

$$\sigma = \frac{16\pi^2}{3} \frac{n-1}{2(Z-1)} R_0^2 \left| \frac{b_+(R)}{b_-(R)} \right|^2 v. \quad (2.18)$$

The law  $\sigma \propto v$  is characteristic of transitions induced by rotation (see Ref. 3, problem No. 2 to 90). The values of the coefficients  $b_{\pm}$  depend strongly on the location of the point of intersection  $R_0$ , which, in its turn, is determined by the ratio of the strengths of the exchange ( $V$ ) and dipole ( $V_d \propto \alpha/R^2$ , where  $\alpha = 3n/2Z$ ) interactions. In the case of a small value of  $V \ll V_d$  the coefficient  $b_+ \sim 1$ , while  $b_- \ll 1$  (the function  $\Psi_I$  is close to  $\varphi_s$ ), and therefore the ratio  $|b_+/b_-|^2$  is also small. On the other hand, in the case when  $V \gg V_d$ , the ratio  $|b_+/b_-|^2$  is large ( $b_+ \sim 1$ , while  $b_- \ll 1$ : the function  $\Psi_I$  is close to  $\varphi_0$ ; see Fig. 1(b)). In this case the cross section (2.18) assumes the form

$$\sigma = \frac{16\pi^2}{3} \frac{n-1}{2(Z-1)} R_0^2 \left( \frac{VR_0^2}{\alpha} \right)^2 v. \quad (2.19)$$

The result (2.19) can also be obtained easily from the more general approach followed in §3 and, as analysis shows, is valid under the conditions

$$V_0^2/vF \gg 1, \quad \delta = \frac{\alpha}{R_0 v} \gg 1, \quad \frac{nV_0^2}{Fv\delta^2} \ll 1. \quad (2.20)$$

In practice, the cross section approaches its asymptotic value (2.19) at very low velocities, which are of little interest for charge transfer in a plasma. For example, for the  $C^{+6}$  ion (Fig. 2) this value is roughly equal to  $v \approx 5 \times 10^{-3}$  a.u. Here, however, an appreciable role can be played by the effects connected with the quantum motion of the nuclei.<sup>[1]</sup>

### §3. THE DYNAMIC-TERM MODEL. CALCULATION OF THE CROSS SECTIONS IN THE REGION OF INTERMEDIATE RATES OF ROTATION

Let us combine the results of §2, obtained for high and low rates of rotation, within the framework of a unified model that will also allow us to calculate the cross section for charge transfer in the intermediate region. For this purpose, let us use at the very first stage of the problem the wave functions  $u_{n'n''}$ , which diagonalize in the dipole approximation the Hamiltonian for the system of degenerate hydrogen-like sublevels with allowance for the rotation effects.<sup>[14,15]</sup> The evolution of these functions in time is analogous to the evolution of the adiabatic states:

$$u_{n'n''}(t) = u_{n'n''}(0) \exp \left[ -i \int_0^t E_{n'n''}(\tau) d\tau \right], \quad (3.1)$$

$$E_{n'n''} = -\frac{Z-1}{R} - \frac{n'+n''}{R^2} (\alpha^2 + \rho^2 v^2)^{-1/2}.$$

The quantum numbers  $n'$  and  $n''$  for  $v \rightarrow 0$  coincide with the quantum numbers  $i_1$  and  $i_2$ , which are expressible in terms of the parabolic quantum numbers  $n_1$  and  $n_2$ :

$$i_1 = (n_1 - n_2 + m)/2, \quad i_2 = (n_2 - n_1 + m)/2.$$

The evolution operator  $\hat{U}$  (see the Appendix) is diagonal in the representation  $u_{n'n''}$ .

The connection between the wave functions  $u_{n'n''}$  and the parabolic wave functions  $u_{i_1 i_2}$  is determined by the Wigner rotation matrices,<sup>[16]</sup> which parametrically depend on the speed (more precisely on the parameter  $\delta = \alpha/\rho v$ ):

$$u_{n'n''} = \sum_{i_1 i_2} D_{n' i_1}^j(\beta) D_{n'' i_2}^j(\pi - \beta) u_{i_1 i_2}, \quad (3.2)$$

(g)  $\beta = \rho v/\alpha, \quad J = (n-1)/2.$

It can be seen from (3.1) and (3.2) that, when allowance is made for the rotation effects, the system of degenerate states moves along distinctive "terms" that depend parametrically on the speed. It is appropriate to call these "terms" dynamic terms, following Demkov, Ostrovskii, and Solov'ev, who introduced this concept in their calculation<sup>[15]</sup> of the cross section for the reaction  $He^+(2s) + A^+ Z \rightarrow He^+(2p) + A^+ Z$ . The possibility of introducing dynamic terms is due entirely to the specific

character of hydrogen-like states that allows the coupling of the dynamic and static amplitudes to be accomplished, according to (3.2), with the aid of constant (time independent) matrices. The main purpose of the introduction of the dynamic terms is to have the rotation effects automatically taken into account, treating the charge transfer as occurring directly between the initial term and the system of (mutually independent) dynamic terms. With allowance for (3.2), we obtain the value of the effective exchange matrix element,  $V_{n'n''}$ , coupling the state  $u_{n'n''}$  to the initial state  $\varphi_s$  (we have taken account of the fact that the only nonzero matrix element couples  $\varphi_s$  to  $|0\rangle = |i_1 + J, i_2 = -J\rangle$ ):

$$V_{n'n''} = D_{n' i_1}^j(\beta) D_{n'' i_2}^j(\pi - \beta) V. \quad (3.3)$$

It can be seen that this interaction also depends parametrically on the speed. In Fig. 1(c) we show the scheme of the intersections of the dynamic terms  $u_{n'n''}$  with the initial term  $\varphi_s$ . Let us emphasize that the states  $u_{n'n''}$  no longer interact with each other. Thus, the problem of two-level charge exchange with subsequent mixing of the states has been reduced to the problem of transitions upon the intersection of the initial term with a system of levels. To solve this latter problem, we can use the results of Demkov and Osherov,<sup>[17]</sup> who have considered the transitions from a given term when it intersects a system of parallel terms.

Let us point out that, according to (3.1), the positions of the points of intersection also depend parametrically on the speed. However, in the framework of the dipole approximation such a dependence changes little the positions of these points, and we shall neglect it. Let us also note that the states  $u_{n'n''}$  are degenerate in the values of  $n'$ ,  $n''$  that satisfy the condition  $n' + n'' = \text{const}$ . For such terms, the square of the matrix element of the interaction should be replaced by the sum of the squares of the matrix elements belonging to the degenerate term. We can convince ourselves of the existence of a simple relation allowing the computation of the matrix elements for the various sublevels:

$$\sum_{n'+n''=2J-k} D_{n' i_1}^j(\beta) D_{n'' i_2}^j(\beta) = C_{4J}^k \left( \sin^2 \frac{\beta}{2} \right)^k \left( \cos^2 \frac{\beta}{2} \right)^{J-k}, \quad (3.4)$$

where the  $C_{4J}^k$  are binomial coefficients.

Let us discuss the correspondence between the dynamic-term model and the approximate models discussed in §2, which are valid at low and high rates of rotation. Let  $v \rightarrow 0$ , so that the probability,  $p$ , of transition to the term  $U_0$  is exponentially small ( $\Delta = 2\pi V^2/Fv \gg 1$ ). It can be seen from (3.3), however, that the effective exchange matrix element for the neighboring term  $U_1$  (Fig. 1(c)) is proportional to  $v$  (so that  $\beta \propto \delta^{-1} \sim v$ ); for the term  $U_2$ , proportional to  $v^3$ , etc. Therefore, the probability of transition to these sublevels is not exponentially small. Indeed, using the general Landau-Zener formula (2.8), and substituting into it the effective exchange element (3.3), we can verify that the transition probability has the form

$$p = \exp \left[ -4J \frac{2\pi V^2 \delta^{-2}}{Fv} \right]. \quad (3.5)$$

It can easily be verified that, when the conditions (2.20) are fulfilled, the computation of the cross section from the Landau-Zener formula with the probability (3.5) leads to (2.19).

At high speeds ( $\delta \approx \alpha/\rho v \ll 1$ ) the quantity  $\beta \approx \pi/2$  [see (3.2)], and all the effective exchange matrix elements,  $V_{n'n''}$ , given by (3.3) do not depend on the speed. As functions of  $n'n''$ , however, these elements form some distribution (of the type of the statistical Poisson distribution). Therefore, if, as before,  $\Delta = 2\pi V^2/Fv \gg 1$ , then it is clear that from this matrix-element distribution will always be found an element for which  $\Delta_{n'n''} = 2\pi V_{n'n''}^2/Fv \sim 1$ . Thus, the existence of a distribution over the quantities  $V_{n'n''}$  guarantees (in a definite speed range) a transition-probability value  $p$  of the order of unity and, thus, a cross-section value  $\sigma \propto \pi R_0^2$ . This effect is exactly analogous to the effect obtained in §2 in the approximation in which the charge-transfer and the mixing regions are assumed to be independent. The agreement with this approximation for the ions  $C^{+6}$  and  $O^{+8}$  is shown in Fig. 2.

The charge-transfer cross-section calculations in the dynamic-term model requires, as has been noted, knowledge of the multilevel transition probability. Let us therefore briefly discuss the computation of this probability. For this purpose, let us introduce the following notation: Let  $p_k$  be the probability for a single transition for the  $k$ th term;  $w_k$  the total transition probability for the  $k$ th term without allowance for the rest of the levels;  $W_k$  the probability of transition to the  $k$ th term with allowance for the remaining levels;

$$S_k = \sum_{i=1}^k W_i.$$

The terms are numbered, starting from the inner term, the outer term having the number  $N$ . When the interference effects are neglected, it is not difficult to derive the relation

$$W_k = p_N \dots p_{k+1} w_k - (1-p_k) S_{k-1}, \quad S_0 = 0. \quad (3.6)$$

This equality is a recursion relation that allows us to determine successively the population of the terms and the total probability  $S_N$ :

$$S_N = w_N + p_N^2 [w_{N-1} + p_{N-1}^2 (w_{N-2} + \dots)]. \quad (3.7)$$

The formula (3.7) coincides with the corresponding expression of Ref. 1. From this formula follow the simple conclusions:

- 1) if some  $p_k \rightarrow 0$ , then all the subsequent terms with numbers  $i < k$  do not contribute to the total probability ( $p_i < p_k$  for  $i < k$ );
- 2) if for the outer terms  $p_k \rightarrow 1$  and, consequently,  $w_k \rightarrow 0$ , then all of them also do not influence the total probability.

For the particular cases when  $N=2; 3$ , it follows from (3.7) that

$$S_2 = w_2 + p_2^2 w_1, \quad S_3 = w_3 + p_3^2 w_2 + p_3^2 p_2^2 w_1. \quad (3.8)$$

If the values of  $p_k$  differ greatly from each other, then it is clear that the dominant contribution to the charge transfer is made by a small number of levels. As  $Z$  increases, however, the exchange interaction  $V(R)$ , (1.1), decreases more and more slowly with increasing  $R$ , and contributions to the charge transfer are made by a larger and larger number of levels.

Let us note a useful formula connecting the total transition probability  $S_N$  with the characteristics of the  $N$ th level:

$$S_N = (w_N - p_N W_N) / (1 - p_N). \quad (3.9)$$

Despite the simple form, it should be borne in mind that this formula contains a contribution of the levels  $k < N$  through the quantity  $W_N$ .

Let us point out that in the calculation of the total cross section the limits of the integration over  $\rho$  for each term of the sum (3.7) are determined by the term with the smallest value of the number  $k$ . Indeed, as  $\rho \rightarrow R_k$ , the probability  $p_k \rightarrow 0$  and, consequently,  $w_k \rightarrow 0$ , so that the contribution of this term vanishes when  $\rho > R_k$ .

Thus, in the considered formulation the problem is essentially a many-level problem, to wit: both the contribution of the levels with different  $n$  and the contribution of the various sublevels within a level with a given  $n$  are important.

#### §4. THE RESULTS OF THE NUMERICAL COMPUTATIONS. DISCUSSION

The charge-transfer cross-section calculations were carried out both on the basis of the approximate formulas (2.10)–(2.12) and in the general formulation given in §3 for the ions  $C^{+6}$  and  $O^{+8}$ , which are of the greatest interest for the plasma of the tokamak installations. The number of levels contributing to the charge exchange is determined by the strength of the exchange interaction: for  $C^{+6}$  one level ( $n=4$ ); for  $O^{+8}$  two levels ( $n=4, 5$ ); cf. Ref. 4.

In Fig. 2 we show the total charge-transfer cross sections for the  $C^{+6}$  and  $O^{+8}$  nuclei, computed with allowance (the solid curves) and without allowance (dashed curves) for the rotation effects. It can be seen that allowance for rotation leads to an appreciable increase in the magnitude of the cross sections even in the region of their maximum. At speeds  $v \lesssim 5 \times 10^{-3}$  (not shown in Fig. 2), there occurs a transition to the asymptotic result (2.19).

The nature of the variation of the cross sections is determined largely by two factors: 1) the rotation effects and 2) the influence of several levels  $n$ . The first group of effects leads to a smoother variation of the cross section in the region of low speeds; the second in the region of high speeds. As a result, instead of the clearly marked maximum in the Landau-Zener model, there appears a tendency towards the formation of a plateau in the speed dependence of the cross sections.

A comparison with the other models shows that the Landau-Zener model with rotation occupies some med-

ian position between the same model without rotation<sup>[4]</sup> and the decay models.<sup>[5,10]</sup> Let us note that the decay-model calculations<sup>[5]</sup> are in good accord with the curve obtained from the Landau-Zener model with rotation under the assumption that the various transition points are independent of each other.

The obtained results can also be applied to incompletely stripped ions in the case when the influence of the core is not great. Apparently, this is valid at low speeds, but this question, like the problem of the transition to speeds  $v \gg 1$ , needs to be further investigated.

The published experiments<sup>[18]</sup> were performed largely on accelerators. Therefore, the appearance of an ion with a given multiplicity was attended by a simultaneous increase in its energy, so that the investigated speed range corresponded to  $v \approx 1$ . Nevertheless, let us point out that computations carried out in the above-exposed scheme for the model case of  $Z=4$  lead to a result that agrees satisfactorily with experiment<sup>[18]</sup> for the  $C^{4+}$  ion with  $v \sim 1$ . Let us also note that the results of Ref. 18 for the  $Fe^{10+}$  ion reveal a dependence on  $Z$  more critical than the linear. This is due, apparently, to the presence of a substantial electron core.

The analysis carried out indicates an appreciable increase in the charge-transfer cross sections on account of the rotation effects. This leads, accordingly, to a more optimistic assessment of the possibility, discussed by Afrosimov *et al.*,<sup>[19]</sup> of using a beam of neutral atoms for active diagnostics of the impurities in a hot plasma. The latest experimental publication,<sup>[20]</sup> although it does not contain direct data on the cross section for the reaction  $H+O^{+8} \rightarrow H^+ + O^{+7}$ , confirms this possibility.

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## APPENDIX: THE EVOLUTION OPERATOR FOR DEGENERATE HYDROGEN-LIKE STATES IN THE FIELD OF A PASSING CHARGE

The evolution operator  $\hat{U}$ , expressed in terms of the parabolic quantum numbers  $i_1, i_2$ , has the form (see Ref. 15)<sup>6)</sup>

$$\langle i_1' i_2' | \hat{U} | i_1 i_2 \rangle = \sum_{n, n', n''} D_{i_1' n'}^j(\beta) D_{i_2' n''}^j(\pi - \beta) \times D_{i_1 n}^j(\beta) D_{i_2 n''}^j(\pi - \beta) \exp[-iv(n' + n'')], \quad (A.1)$$

where the  $D_{in}^j$  are Wigner functions<sup>[23]</sup> and the quantities  $\beta, \alpha$ , and  $\nu$  are defined in (2.9).

The state  $|0\rangle$ , to which the charge transfer is made, has the form  $|0\rangle = |i_1 i_2\rangle = |J, -J\rangle$ . The formula (A.1) contains a sum of  $n^2$  terms, and is therefore too complex for specific calculations when  $n \gg 1$ . It turns out, however, that it can be significantly simplified by means of the following transformations. Let us write the double sum over  $n' n''$  in (A.1) in the form of a product of two sums:

$$\sum_{n, n'} = \left( \sum_{n'} \dots \right) \left( \sum_n \dots \right). \quad (A.2)$$

It is easy to see that each of the sums is a product of three rotations, which can be replaced by one resultant rotation described by one  $D$ -function (see, for example, Ref. 16). As a result, we obtain

$$\langle i_1' i_2' | \hat{U} | i_1 i_2 \rangle = D_{i_1' i_1}^j(\alpha_1, \beta_0, \gamma_1) D_{i_2' i_2}^j(\alpha_2, \beta_0, \gamma_2). \quad (A.3)$$

The angles  $\beta_0, \alpha_{1,2}$ , which define the resultant rotation, are connected with the original angles  $\beta$  and  $\Delta\chi$  by the relations

$$\begin{aligned} \text{ctg } \alpha_{1,2} &= \cos \beta (\text{ctg } \nu + 1/\sin \nu), & \text{ctg } \gamma_{1,2} &= -\text{ctg } \alpha_{1,2}, \\ \cos \beta_0 &= 1 - 2 \sin^2 \beta \sin^2 (\nu/2). \end{aligned} \quad (A.4)$$

Since into the expression (2.6) for the transition probability enters the modulus,  $|U|$ , of the  $\hat{U}$  operator, with allowance for the relation  $D_{pq}^j(\alpha, \beta, \gamma) = e^{i\beta\alpha} D_{pq}^j(\beta) e^{i\alpha\gamma}$ , we have

$$|\langle i_1' i_2' | \hat{U} | i_1 i_2 \rangle|^2 = D_{i_1' i_1}^j(\beta_0) D_{i_2' i_2}^j(\beta_0). \quad (A.5)$$

Let us consider the form of the evolution operator in the limiting cases of low and high speeds. For  $\alpha/\rho v \gg 1$ , it follows from (A.4) that  $\beta \rightarrow 0, \beta_0 \rightarrow 0$ , and the evolution operator is diagonal in the rotating coordinate system (since  $D_{i_1 i_1}(0) = \delta_{i_1 i_1}$ ). This means that the excited state of the ion has time to "follow" the electric field of the proton flying by. (More trivial is the diagonality of  $\hat{U}$  for  $\Delta\chi \rightarrow 0$ .)

In the other limiting case,  $\alpha/\rho v \ll 1 (\beta \rightarrow \pi/2)$ , from (A.4) we have  $\cos \beta_0 \approx \cos \nu \approx \cos \Delta\chi$ . In this case the effect of the evolution operator amounts to the rotation of the wave function through the angle  $\Delta\chi$ , which is equal to the angle of rotation of the internuclear axis. The above-presented properties of the  $\hat{U}$  operator are in accord with the qualitative arguments set forth in §2.

The diagonal matrix element  $U_{00}$  has the simple analytic form (see Ref. 16 and Ref. 3, §58):

$$U_{00} = \cos^{i'}(\beta_0/2) = (1 - \sin^2 \beta \sin^2 (\nu/2))^{i'}. \quad (A.6)$$

<sup>1)</sup>We use the atomic system of units:  $e = \hbar = m = 1$ .

<sup>2)</sup>We are grateful to M. I. Chibisov for participating in a discussion of this question.

<sup>3)</sup>Notice that the analytic computation of the  $\hat{U}$  operator is possible only in the dipole approximation. However, the general conclusions about the nature of the variation of the cross section are not connected with the specific form of  $\hat{U}$  (for example, they are also valid for the quadrupole interaction<sup>[12]</sup>).

<sup>4)</sup>We are grateful to V. P. Zhdanov for pointing out to us the substantial contribution of these regions when  $v \rightarrow 0$ .

<sup>5)</sup>In this case the particle motion is assumed to be still classical. An assessment of the role of the quantum effects is given in Ref. 1.

<sup>6)</sup>The notation used here differs from the notation used in Ref. 15 in the choice of the quantization axis (directed along the electric field of the outer particle).

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## Absorption line shape of homogeneously broadened degenerate transition

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The effect of degeneracy in the magnetic quantum number  $M$  on the saturation of the absorption of a homogeneously broadened line is investigated. It is shown that the shape of the saturated contour depends on the polarization of the incident wave. The question of the limits of applicability of the approximation of spherical symmetry of the relaxation processes is discussed.

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### 1. INTRODUCTION

The angular-momentum selection rule causes at least one of the two levels between which a radiative transition is allowed to be degenerate. Moreover, in the case of light absorption by a molecule, both levels are as a rule strongly degenerate in the magnetic quantum number  $M$ . Therefore elastic-collision processes accompanied by reorientation of the angular momentum of an atom or a molecule make a discernible contribution to the broadening of the spectral line. The role of these processes in the formation of the linear-absorption line contour was taken into account in a large number of studies (see, e.g.,<sup>[1-3]</sup>), although not fully enough in most cases. Usually, owing to difficulties connected with the calculation of the collision  $S$  matrix, the shape of the contour was determined without taking into account the role of the interference between the transitions that connect various  $M$ -components of the lower and upper levels.<sup>[1,2]</sup>

In problems of nonlinear absorption (the so-called saturation effect) the role of interference of  $M-M'$  transitions, to our knowledge, has not been discussed at all. In this case it is customary to use for the absorbed power the formula derived for an isolated transition by Karplus and Schwinger back in 1948.<sup>[6]</sup>

In this paper we wish to discuss some qualitative effects that result from the interference of transitions that connect various  $M$ -components of the upper and lower levels. We assume here that the density of the perturbing particles is high enough so that the line contour can be regarded as homogeneously broadened and that the broadening due to the Doppler effect can be neglected.

### 2. EQUATIONS FOR THE DENSITY MATRIX

To describe the absorption line shape we start from a system of equations for the density matrix with a