Shake-off mechanism of two-electron transitions in slow ion-atom collisions

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The shake-off mechanism, known in photon impact, has been applied to the analysis of two-electron transitions in slow ion-atom collisions. The mechanism consists of relaxation of the electronic state of an outer target electron upon relocalization of the inner-electron wave function from the target to projectile nucleus. Based on this mechanism, a method is proposed to estimate cross sections of two-electron processes. The method is demonstrated by calculating cross sections of double capture, transfer excitation, and transfer ionization for collisions of the excited He $(1s2l)$ atom with the B^{5+} ion. The dependence of the cross sections of double capture and transfer excitation on the principal quantum number n of the final state is presented. [S1050-2947(98)02206-9]

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I. INTRODUCTION

While the physics of one-electron transfer processes in slow ion-atom collisions is considered to be well understood both theoretically and experimentally, two-electron transitions such as double capture, transfer excitation, and transfer ionization present a much less studied field. Such transitions occur most efficiently in collisions of atoms with slow, highly charged ions. A particular aspect of these processes is the simultaneous activity of two electrons during the collision. The interaction between the two electrons is known to play an important role because probabilities of one-step and two-step two-electrons transitions for a number of cases studied have comparable values [1,2].

The situation in theoretical studies of two-electron transitions in slow ion-atom collisions is described in a recent review by Barat and Roncin [3] and briefly can be formulated as follows: there is no efficient theoretical approach to this problem yet. The reasons lie both in specific features of two-electron transitions and in the difficulties of numerical implementation of theoretical models for such collision systems. There are two basic theoretical approaches used for the description of the ion-atom collisions at low velocities ($v<1$ a.u.): the classical description of the collision process in terms of independent electrons moving in the potential wells of ionic cores and the quasimolecular description based on the close-coupling method.

The representative of the first approach is the classical over-barrier model that was introduced by Bohr and Lindhart in 1954 [4] and applied to multicharged ions by Ryufuku *et al.* [5] to describe single-electron-capture process. Extension to multiple-electron capture was considered by Barany *et al.* [6]. The most refined development of this model is the molecular classical over-barrier model (MCBM) introduced by Niehaus [7]. The MCBM is an independent electron model in which electrons are captured successively at different nuclear distances. The main defects of the model are the lack of dynamic aspects and complete neglect of the possibility of capturing *simultaneously* two electrons at the same distance. Due to these defects the MCBM cannot describe correctly the physical pattern of the collision process and therefore cannot provide accurate numerical results. The second approach is considered to be most suitable for collisions at low velocities and theoretical models based on the close-coupling method [1,2,8–10] are widely applied to describe two-electron transitions in slow ion-atom collisions. However, taking into account the fact that during such collisions a large number of the electronic states are populated and in most cases the double capture populates high-n doubly excited states, the close-coupling method faces considerable problems because calculations of individual populations of highly excited states require a large number of basis functions [for example, the calculations of individual populations of $(n,n')=(3,3)$ and $(3,4)$ manifolds in O^{8+}-He collisions require more than 100 basis functions]. Therefore, difficulties in actual implementation of the close-coupling method for the slow collisions restrict its practical applicability, while active experimental studies require a wide spectrum of theoretical data, including cross sections of double capture and transfer excitation to highly excited states, as well as transfer ionization.

In the present paper we suggest a theoretical model of two-electron transitions in slow ion-atom collisions that takes into account the interaction between two active electrons based on the so-called *shake-off* mechanism. To our knowledge, this simple mechanism has not been discussed so far in applications to two-electron transitions [3]. We consider here three types of two-electron processes, namely, double capture (DC), transfer excitation (TE), and transfer ionization (TI), described by the equations

$$A+B^{q+}\rightarrow A^{2+}+B^{(q-2)+} \quad \text{(DC)}, \tag{1}$$

$$A+B^{q+}\rightarrow A^{1+}*+B^{(q-1)+} \quad \text{(TE)}, \tag{2}$$

$$A+B^{q+}\rightarrow A^{2+}+B^{(q-1)+}+e \quad \text{(TI)}, \tag{3}$$

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where an asterisk indicates an excited state. We study the collision processes of He in the excited state $1s2l$ and the B^{5+} ion. The choice of the particular state of He is due to requirement of the present theoretical model and will be explained in the next section.

II. THEORETICAL MODEL

For a qualitative understanding of the interelectron interaction effects we consider the following simple model. Our collision system is assumed to consist of two electrons and two bare nuclei of the charge Z_T (target) and Z_P (projectile). Both electrons, initially bound on the target, are not equivalent, i.e., one can be treated as an *inner* electron and the other as an *outer* electron. For a given internuclear distance R, we approximate the wave functions of the inner and the outer electrons by solutions of the two-center Coulomb problems for the charges (Z_T,Z_P) and (Z_T-1,Z_P), respectively. We consider a situation where in the course of the collision the inner electron undergoes the charge-transfer transition, i.e., the region of localization of its wave function jumps from Z_T to Z_P. This happens while passing some narrow range of R around a point of avoided crossing of the one-electron adiabatic potential curves in the field of the nuclear charges (Z_T,Z_P). This transition is seen by the outer electron as an abrupt change of the nuclear charges defining its own wave function from (Z_T-1,Z_P) to (Z_T,Z_P-1), which may result in the change of its state. This shake-off mechanism is of first order both in nonadiabatic coupling at the point of avoided crossing and in the interelectron interaction. It reproduces the effect of the interelectron interaction on the final state of the outer electron.

The theoretical ground for this qualitative description of the model suggested is as follows. The starting point for studying our collision system is the time-dependent Schrödinger equation for two active electrons, which can be written as (atomic units are used throughout this paper)

$$i\frac{\partial}{\partial t}\psi(\mathbf{r}_1,\mathbf{r}_2,t)=H(\mathbf{r}_1,\mathbf{r}_2)\psi(\mathbf{r}_1,\mathbf{r}_2,t), \tag{4}$$

with the Hamiltonian

$$H(\mathbf{r}_1,\mathbf{r}_2)=-\frac{1}{2}\Delta_1-\frac{1}{2}\Delta_2-\frac{Z_T}{r_1}-\frac{Z_P}{|\mathbf{r}_1-\mathbf{R}(t)|}-\frac{Z_T}{r_2}-\frac{Z_P}{|\mathbf{r}_2-\mathbf{R}(t)|}+\frac{1}{\mathbf{r}_{12}}, \tag{5}$$

where the indices 1 and 2 correspond to the inner and outer electrons, respectively, and $\mathbf{R}(t)$ is the internuclear distance. The fact that in the present case the motion of the nuclei is much slower than the motion of the electrons allows us to apply the adiabatic theory to solve this equation. First we shall solve the stationary problem

$$H(\mathbf{r}_1,\mathbf{r}_2)\tilde{\psi}(\mathbf{r}_1,\mathbf{r}_2)=E\tilde{\psi}(\mathbf{r}_1,\mathbf{r}_2) \tag{6}$$

and find the two-electron wave functions $\tilde{\psi}(\mathbf{r}_1,\mathbf{r}_2)$ for each moment t, i.e., for the corresponding internuclear distance $\mathbf{R}$. Using these functions, the solution of the time-dependent equation (4) can be found in the form

$$\psi(\mathbf{r}_1,\mathbf{r}_2,t)=\sum_i c_i(t)\tilde{\psi}_i(\mathbf{r}_1,\mathbf{r}_2). \tag{7}$$

Since we assume that the electrons are not equivalent [one of them is the inner (fast) and the other is the outer (slow) electron], the Bohr-Oppenheimer adiabatic separation of variables can be applied to solve Eq. (6). We seek the solution in the form

$$\tilde{\psi}(\mathbf{r}_1,\mathbf{r}_2)=\phi(\mathbf{r}_1;\mathbf{r}_2)\varphi(\mathbf{r}_2). \tag{8}$$

To find the solution for the inner electron we shall separate the $\mathbf{r}_1$-dependent terms of the Hamiltonian (5) and solve the equation

$$\left[-\frac{1}{2}\Delta_1-\frac{Z_T}{r_1}-\frac{Z_P}{|\mathbf{r}_1-\mathbf{R}(t)|}+\frac{1}{\mathbf{r}_{12}}\right]\phi(\mathbf{r}_1;\mathbf{r}_2)=V(\mathbf{r}_2,t)\phi(\mathbf{r}_1;\mathbf{r}_2), \tag{9}$$

where the eigenvalue $V(\mathbf{r}_2,t)$ parametrically depends on $\mathbf{r}_2$ and t. Let us suppose that we have found $V(\mathbf{r}_2,t)$. In order to find the solution for the outer electron $\mathbf{r}_2$ we average Eq. (6) over the motion of the inner electron. Combining Eq. (8) with Eq. (6) we obtain

$$\left(\int \phi(\mathbf{r}_1;\mathbf{r}_2)H(\mathbf{r}_1,\mathbf{r}_2)\phi(\mathbf{r}_1;\mathbf{r}_2)d\mathbf{r}_1\right)\varphi(\mathbf{r}_2)=E\varphi(\mathbf{r}_2). \tag{10}$$

This gives us the equation for the outer electron

$$\left[-\frac{1}{2}\Delta_2-\frac{Z_T}{r_2}-\frac{Z_P}{|\mathbf{r}_2-\mathbf{R}(t)|}+V(\mathbf{r}_2,t)\right]\varphi(\mathbf{r}_2)=E\varphi(\mathbf{r}_2), \tag{11}$$

where the potential $V(\mathbf{r}_2,t)$ is defined by the motion of the inner electron.

Equations (9) and (11) should be solved simultaneously, which constitutes our model for describing two-electron transitions. Similar equations were recently considered by Kazansky [11]. In the present paper, in order to investigate the basic features of this model we adopt the following approximation for the solution of Eq. (9). The only term in Eq. (9) that depends on $\mathbf{r}_2$ is the interelectron interaction $1/\mathbf{r}_{12}$. Let us suppose that a transition where the inner electron is transferred to the projectile ion occurs at the moment $t=t_c$ corresponding to the internuclear distance R_c. At this moment the region of localization of the wave function of the inner electron jumps from Z_T to Z_P. Using a simple screening approximation for the interelectron interaction and assuming that $r_1 \ll r_2$ before the transition and $|\mathbf{r}_1-\mathbf{R}(t)| \ll r_2$ after the transition, the potential $V(\mathbf{r}_2,t)$ can be approximated by

$$V(\mathbf{r}_2,t)=\begin{cases}\dfrac{1}{r_2}+a_1, & t<t_c\\[2ex] \dfrac{1}{|\mathbf{r}_2-\mathbf{R}(t)|}+a_2, & t>t_c,\end{cases} \tag{12}$$

where a_1 and a_2 are some constants that do not depend on $\mathbf{r}_2$. In this approximation the model allows simple quantitative analyses as follows.

Substituting the explicit form of the potential $V(\mathbf{r}_2,t)$ into Eq. (11), we obtain the stationary Schrödinger equation for the outer electron moving in the field of two Coulomb centers, whose charges change abruptly at the moment $t=t_c$, as is described by the Hamiltonian

$$H(\mathbf{r}_2,t)=\begin{cases} -\frac{1}{2}\Delta_2-\frac{Z_T-1}{r_2}-\frac{Z_P}{|\mathbf{r}_2-\mathbf{R}(t)|}, & t<t_c \\ -\frac{1}{2}\Delta_2-\frac{Z_T}{r_2}-\frac{Z_P-1}{|\mathbf{r}_2-\mathbf{R}(t)|}, & t>t_c . \end{cases} \tag{13}$$

In order to adjust its state to new conditions at the moment $t=t_c$, the outer electron undergoes the shake-off transition with the probability

$$P_{\mathrm{sh}}(q_2\rightarrow h_2)=\left|\int \varphi_{q_2}(\mathbf{r}_2)\varphi_{h_2}(\mathbf{r}_2)d\mathbf{r}_2\right|^2, \tag{14}$$

where q_2 and h_2 are the set of the quantum numbers describing the state of the outer electron in the field of two Coulomb charges (Z_T-1,Z_P) and (Z_T,Z_P-1) before and after the transition of the inner electron, respectively. An equation similar to Eq. (14) but for the shake-off transition in the one-center Coulomb problem was used by Migdal and Feinberg in 1941 [12], who considered the β decay of the nuclei. In 1966 Krause and Carlson applied the same method to study the photoionization from the inner shells [13]. As mentioned already, our system consists of two bare nuclei with charges Z_T and Z_P and two electrons in states i_1 (inner electron) and i_2 (outer electron) bound on the target before the collision. The probability for these two electrons to be found in the discrete states f_1 and f_2 after the collision can be expressed as

$$P(i_1,i_2\rightarrow f_1,f_2)=P_{\mathrm{LZ}}(i_1\rightarrow f_1)\sum_{\nu}\sum_{\mu}[P^{in}_{\mathrm{LZ}}(i_2\rightarrow q_2^{(\nu)}) \times P_{\mathrm{sh}}(q_2^{(\nu)}\rightarrow h_2^{(\mu)})P^{\mathrm{out}}_{\mathrm{LZ}}(h_2^{(\mu)}\rightarrow f_2)]. \tag{15}$$

Here $P_{\mathrm{LZ}}(i_1\rightarrow f_1)$ is the Landau-Zener probability for the inner electron to pass the avoided crossing between the one-electron potential curves corresponding to the states i_1 and f_1 in the field of the nuclear charges (Z_T,Z_P) diabatically on the way in and adiabatically on the way out. $P^{\mathrm{in}}_{\mathrm{LZ}}(i_2\rightarrow q_2^{(\nu)})$ is the Landau-Zener probability of the transition of the outer electron from its initial state i_2 to the νth state of the same symmetry $q_2^{(\nu)}$ $(\nu=1,\ldots,N)$, N being the number of the avoided crossings between the one-electron adiabatic potential curves in the field of the nuclear charges (Z_T-1,Z_P) before the transition of the inner electron, i.e., the probability for the outer electron to be in state $q_2^{(\nu)}$ at the moment of the inner-electron transition. $P_{\mathrm{sh}}(q_2^{(\nu)}\rightarrow h_2^{(\mu)})$ is the shake-off probability defined by Eq. (14), $\mu=1,\ldots,M$, where M is the number of possible discrete states to which the electron can change its state due to the shake-off effect. Finally, $P^{\mathrm{out}}_{\mathrm{LZ}}(h_2^{(\mu)}\rightarrow f_2)$ is the Landau-Zener probability of the transition of the outer electron to the final state f_2 in the field of the charges (Z_T,Z_P-1) on the way out. The probability of the transfer ionization at the moment of the shake-off can be expressed as

$$P(i_1,i_2\rightarrow f_1,k_2) = P_{\mathrm{LZ}}(i_1\rightarrow f_1) \times\sum_{\nu}\left[P^{\mathrm{in}}_{\mathrm{LZ}}(i_2\rightarrow q_2^{(\nu)})1-\sum_{\mu}P_{\mathrm{sh}}(q_2^{(\nu)}\rightarrow h_2^{(\mu)})\right], \tag{16}$$

where k_2 is the final state of the outer electron in a continuum. The cross section σ of the two-electron transition is given as

$$\sigma=2\pi\int_0^{\infty}P(b)b\,db, \tag{17}$$

where b is the impact parameter, $P(b)$ is defined by Eq. (15) for double capture and transfer excitation and by Eq. (16) for transfer ionization, and the upper limit of integration is actually defined by the internuclear distance at the moment of the transition of the inner electron R_c.

III. CALCULATIONS AND RESULTS: COLLISIONS OF THE B^{5+} ION WITH He ($1s2l$)

The probability of a transition between two adiabatic potential curves at a pseudocrossing has been calculated within the framework of the Landau-Zener model:

$$p=\exp\left[-\frac{\pi\Delta^2(R)}{2v_{\mathrm{rad}}\Delta F(R)}\right]_{R=R_c}, \tag{18}$$

where $\Delta(R)=U_1(R)-U_2(R)$ and $\Delta F(R)=dU_1/dR-dU_2/dR$ are the energy splitting (difference) between two curves and the difference of their derivatives at the avoided crossing R_c. The radial velocity v_{rad} is defined as

$$v_{\mathrm{rad}}=v\left(1-\frac{b^2}{R^2}\right)^{1/2}. \tag{19}$$

Here v is the relative velocity of nuclear motion. To calculate the adiabatic potential curves the Shrödinger equation for the two-center Coulomb problem [14]

$$[\Delta+2(U-V)]\psi=0 \tag{20}$$

has been solved in prolate spheroidal coordinates ξ,η,φ. In these coordinates the Laplace operator can be expressed as

$$\Delta=\frac{4}{R^2(\xi^2-\eta^2)}\left\{\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi}+\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta} +\frac{\xi^2-\eta^2}{(\xi^2-1)(1-\eta^2)}\frac{\partial^2}{\partial\varphi^2}\right\} \tag{21}$$

and the potential is

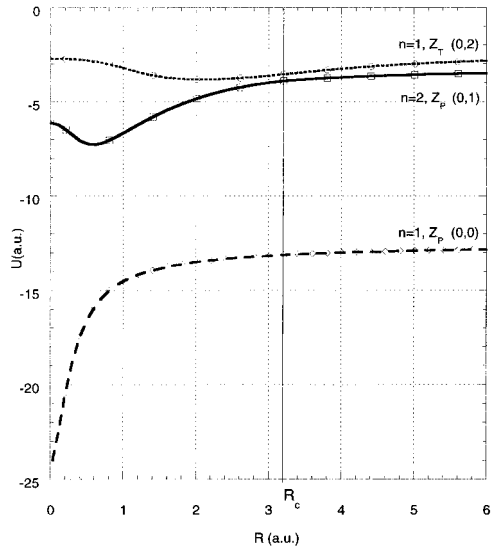

FIG. 1. Potential curves of the inner electron in the field of the charges $Z_T=2$ and $Z_P=5$.

$$V=-\frac{2Z_1}{R(\xi+\eta)}-\frac{2Z_2}{R(\xi-\eta)}. \tag{22}$$

We find the solution of Eq. (20) in the form

$$\psi=f(\xi)g(\eta)e^{\pm im\varphi} \tag{23}$$

and after separation of the variables one obtains for ξ and η

$$\left[\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi}-\frac{m^2}{\xi^2-1}+(Z_2+Z_1)R\xi+\frac{1}{2}UR^2(\xi^2-1)-A(R)\right]f(\xi)=0,$$

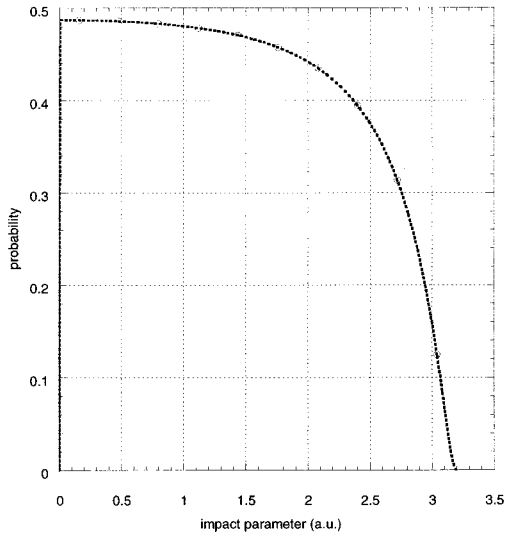

FIG. 2. Probabilities of the inner-electron transition from the state $1s$ on He to the state with $n=2$ on B^{5+}.

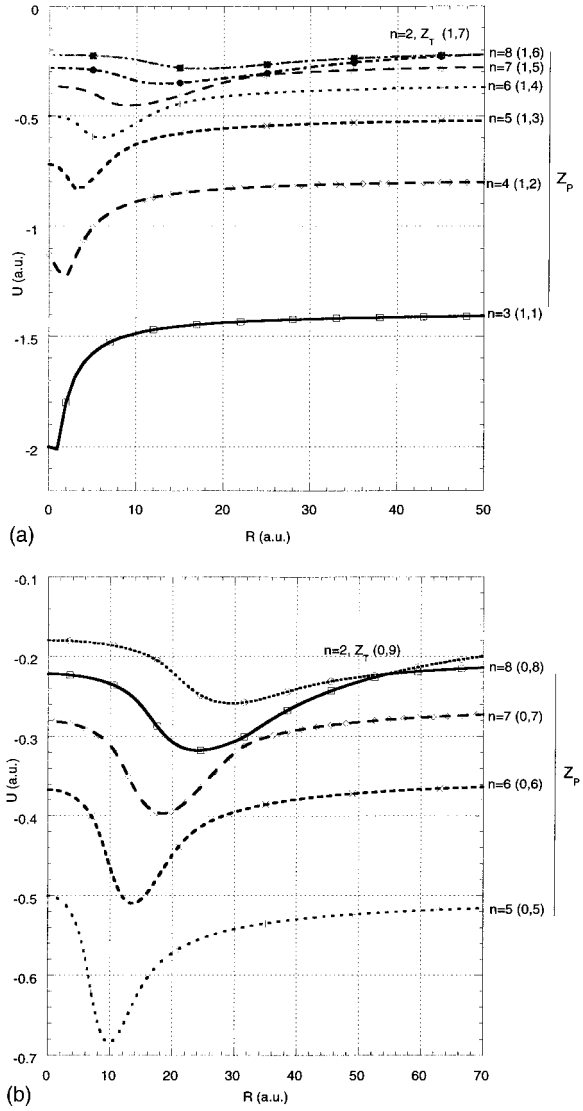

FIG. 3. Potential curves of the outer electron in the field of the charges $Z_T=1$ and $Z_P=5$ for the initial states (a) $(n_\xi,n_\eta)=(1,7)$ and (b) $(n_\xi,n_\eta)=(0,9)$.

$$\left[\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta}-\frac{m^2}{1-\eta^2}+(Z_2-Z_1)R\eta+\frac{1}{2}UR^2(1-\eta^2)+A(R)\right]g(\eta)=0, \tag{24}$$

where $A(R)$ is a separation constant. These equations have been numerically solved using the discrete variable representation method, which allows us to calculate the energy $U(R)$ for the electron state characterized by the elliptic quantum numbers n_ξ, n_η, and m.

We shall illustrate how our method works by calculating probabilities and cross sections of the double capture, transfer excitation, and transfer ionization for collisions of the B^{5+} ion with the He $(1s2l)$ atom. Figure 1 shows the potential curves of the inner electron in the field of the charges $Z_T=2$ and $Z_P=5$. In the limit of $R\to\infty$ the upper curve corresponds to the $1s$ electron state on He and the two lower curves correspond to the $n=2$ and $n=1$ states on the B^{5+}

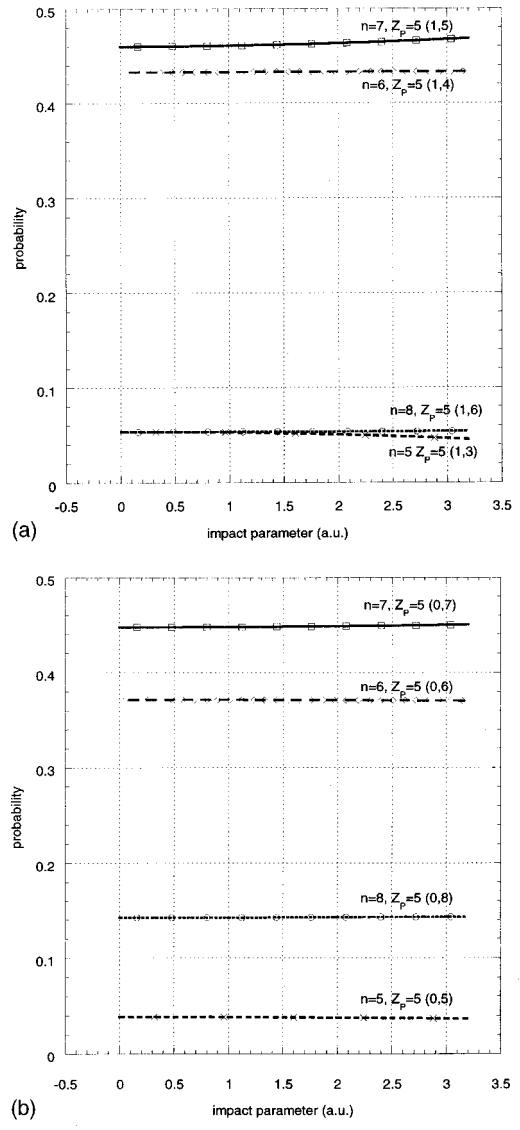

FIG. 4. Probabilities of the outer-electron states on the way in for the initial states (a) $(n_\xi, n_\eta)=(1,7)$ and (b) $(n_\xi, n_\eta)=(0,9)$.

ion (the corresponding elliptic quantum numbers n_ξ and n_η are given in parentheses and $m=0$ throughout the calculation). It can be seen from the figure that the transition of the inner electron from its initial $1s$ state on He to the $n=2$ state on B^{5+} occurs at the avoided crossing at the internuclear distance $R_c=3.21$ a.u. and the transition to the $n=1$ state on B^{5+} at $R_c=1.01$ a.u. Since the first transition has much higher probability than the second one we consider the $n=2$ state on the B^{5+} ion as a final state of the inner electron. Evaluating the radius of the electron as $r_e=n^2/Z$, we find that the radius of the inner electron, while bound on He, is 0.5 a.u. and the one after the transition to the state with $n=2$ on B^{5+} ion is 0.8 a.u., which is in agreement with our statement that the region of localization of the inner electron wave function jumps from Z_T to Z_P. The probability for the inner electron to pass this avoided crossing diabatically on the way in and adiabatically on the way out, i.e., the first factor in Eq. (15), is

$$P_{\mathrm{LZ}}(i_1 \to f_1) = p_1(1-p_1)(1-p_2)^2, \tag{25}$$

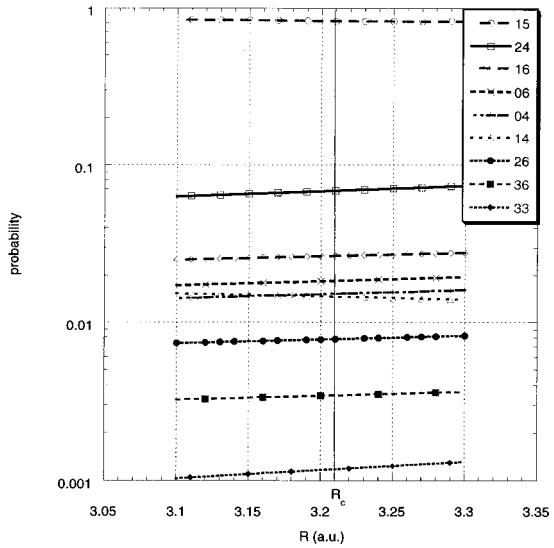

FIG. 5. Shake-off probability of the outer-electron transition from the state (1,5) of nuclear charges $Z_T-1=1$ and $Z_P=5$ to the states in the field of nuclear charges $Z_T=2$ and $Z_P-1=4$.

where i_1 is the $1s$ state on He, f_1 is the $n=2$ state on the B^{5+} ion, and p_1 and p_2 are the Landau-Zener probabilities of the diabatic transitions defined by Eq. (18) in the avoided crossings at 3.21 a.u. and 1.01 a.u., respectively. The probability of the inner-electron transition from the $1s$ state on He to the $n=2$ state on B^{5+} is shown in Fig. 2 as a function of the impact parameter at the relative velocity of the nuclear motion of 0.5 a.u. Since the transition of the inner electron occurs at the internuclear distance of 3.21 a.u., from here on we can restrict ourselves to considering the case when the impact parameter is less than or equal to 3.21 a.u. According to our model, the outer electron before the collision occupies the $2s$ or $2p$ state on He, which corresponds to the state characterized by a pair of elliptic quantum numbers $(n_\xi, n_\eta)=(1,7)$ and (0,9) in the field of nuclear charges $Z_T=1$ and $Z_P=5$, while the distance between two nuclei is infinite. The potential curves of the states (1,7) and (0,9) and

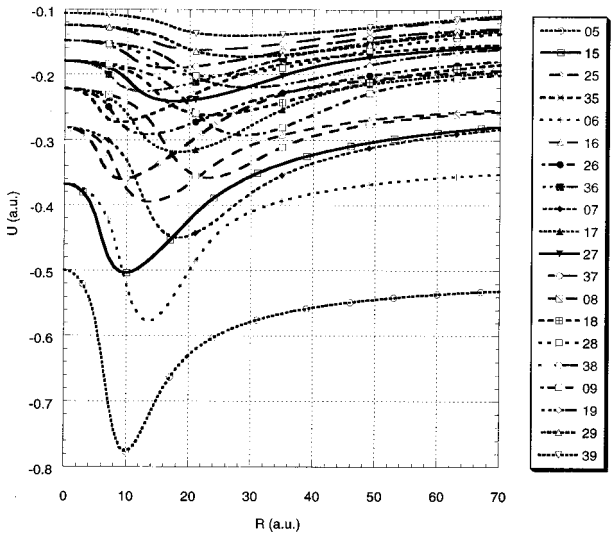

FIG. 6. Potential curves of the outer electron in the field of charges $Z_T=2$, $Z_P-1=4$.

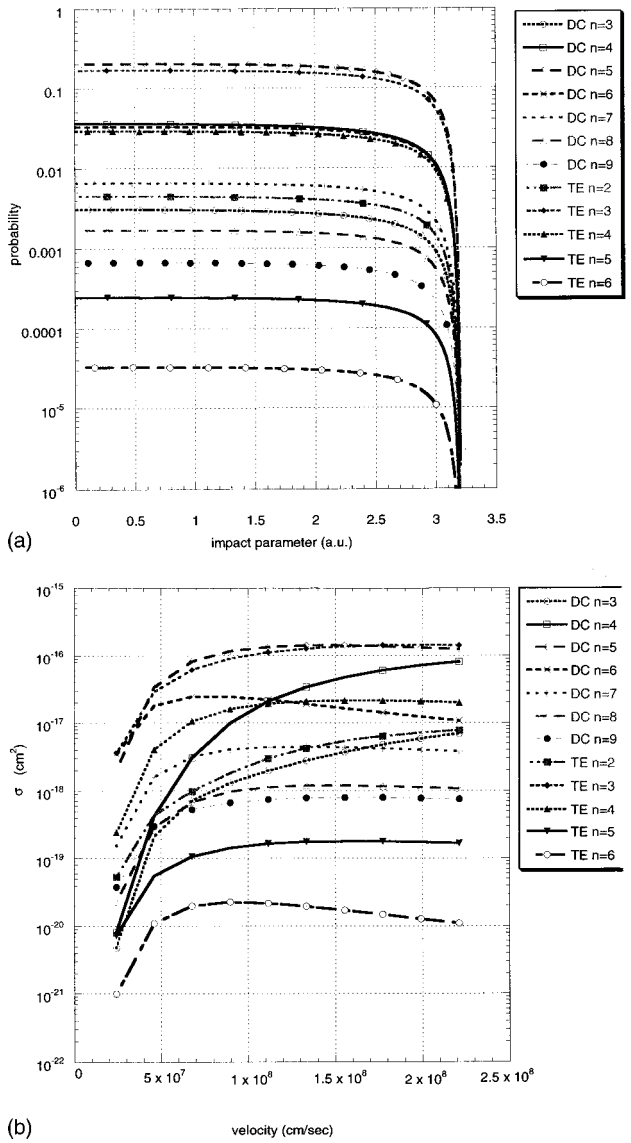

FIG. 7. (a) Probability and (b) cross section of the DC and TE to the n state of the outer electron at the collision velocity of 0.5 a.u.

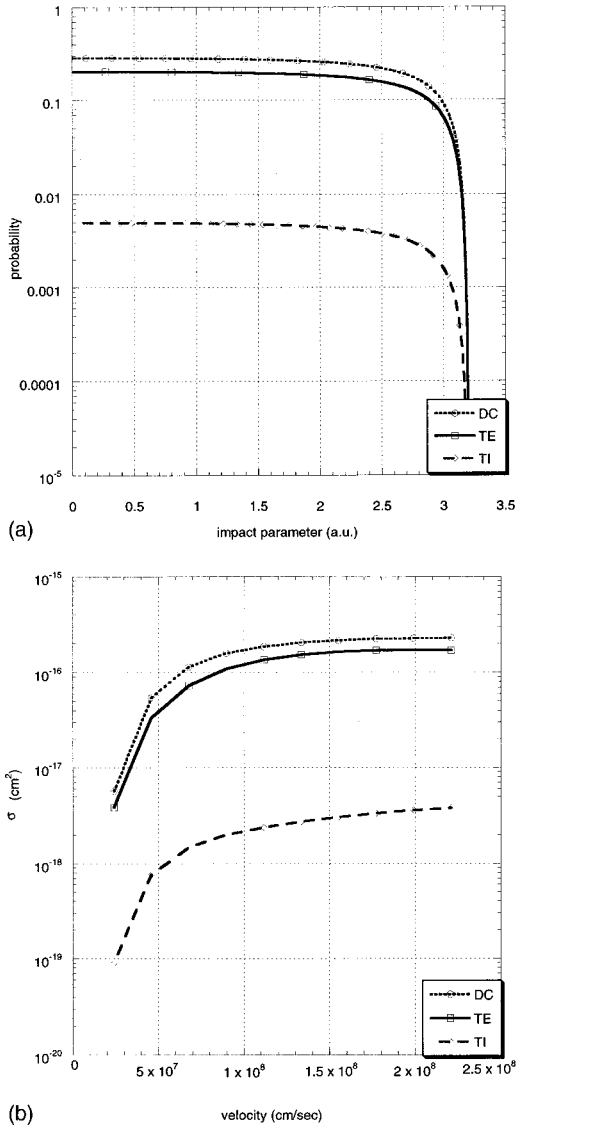

FIG. 8. (a) Total probability and (b) total cross section of the DC, TE, and TI at the collision velocity of 0.5 a.u.

of the states with the same elliptic quantum numbers n_ξ and m are shown in Figs. 3(a) and 3(b), respectively. To calculate the probability of the outer-electron states on the way in or the second factor in Eq. (15), the following formula has been used:

$$P_{\mathrm{LZ}}^{\mathrm{in}}(i_2 \to q_2^{(\nu)}) = p_1 p_2 \cdots p_\nu (1 - p_{\nu+1}), \tag{26}$$

where $\nu = 1, \ldots, N$, N being the number of the avoided crossings between the potential curves shown in Figs. 3(a) and 3(b), and p_ν is the Landau-Zener probability of the diabatic transition in the νth avoided crossing defined by Eq. (18). The nonzero probabilities of the states of the outer electron with the initial states $(n_\xi, n_\eta) = (1,7)$ and (0,9) are shown in Figs. 4(a) and 4(b). The most probable state of the outer electron with the initial state (1,7) at the moment of the transition of the inner electron is the state (1,5), with $Z_T = 1$ and $Z_P = 5$ [Fig. 4(a)]. Figure 5 shows the probabilities of the outer-electron transitions from this state to several states in the field of charges $(Z_T, Z_P) = (2,4)$ due to the shake-off effect calculated at the internuclear distance $R_c = 3.21$ a.u. This probability, defined by Eq. (14), gives us the third factor in Eq. (15). Some of the potential curves of the outer-electron states that are the result of the shake-off effect are shown in Fig. 6. The probabilities of the transitions of the outer electron on the way out [the fourth factor in Eq. (15)] have been calculated in the same way as the ones on the way in [see Eq. (26)] considering the outer-electron state after shake-off as the initial state for the transitions. The probabilities and cross sections of the two-electron transitions during collisions of the B^{5+} ion with the He $(1s2l)$ atom have been calculated separately for the two possible initial states of the outer electron $(n_\xi, n_\eta) = (1,7)$ and (0,9). The final probability P and cross section σ are then given by

$$P = \frac{1}{2}(P_{(1,7)} + P_{(0,9)}), \quad \sigma = \frac{1}{2}(\sigma_{(1,7)} + \sigma_{(0,9)}). \tag{27}$$

The final probabilities and cross sections of the DC

$$B^{5+} + \mathrm{He}(1s2l) \to B^{3+}(n_1 = 2, n_2 = 3-9) + \mathrm{He}^{2+} \tag{28}$$

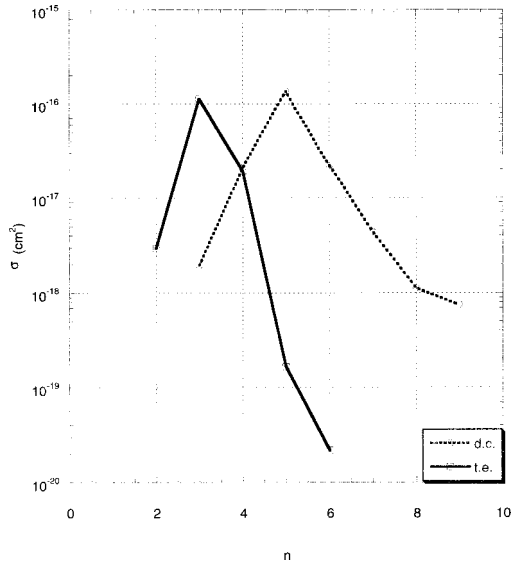

FIG. 9. n dependence of the DC and TE cross sections at the collision velocity of 0.5 a.u.

and TE

$$B^{5+}+He(1s2l)\rightarrow B^{4+}(n_1=2)+He^{1+}(n_2=3-6) \tag{29}$$

are shown in Figs. 7(a) and 7(b), respectively. Figure 8 shows the total probabilities and cross sections of DC, TE, and TI. The n dependence of the cross section of DC and TE are presented in Fig. 9. Unfortunately, no experimental data are available for collisions of ions with the excited-state He atom target. From these results, the following conclusions can be drawn about the collisions of the B^{5+} ion with the He $1s2l$ atom: (i) The cross section and the probability of DC and TE have comparable values at the collision velocity up to 1 a.u. and (ii) the most probable products in collisions of the B^{5+} ion with the He $1s2l$ atom are (a) the B^{3+} ($n_1=2$ and $n_2=5$) ion and He^{2+} ion in DC and (b) the B^{4+} ($n=2$) ion and He^{1+} ($n=3$) ion in TE.

IV. CONCLUSIONS

A theoretical model based on the shake-off mechanism is proposed for two-electron transitions in slow ion-atom collisions. This mechanism is similar to the shake-off mechanism well known in the theory of atomic photoionization, though it has not been applied to atomic collisions so far. This model allows us to estimate probabilities of different two-electron processes (DC, TE, and TI). This model has several advantages over MCBM and the close-coupling method.

(i) The model takes into account the interelectron interaction and dynamics of the collision process.

(ii) The present method is simple in implementation and permits one with the same ease to consider a wide range of processes, i.e., initial or final states of the collision system, including those that are hardly accessible by other methods (e.g., close coupling calculation).

(iii) The present method also allows us to calculate the transfer ionization probability, a process that no other theoretical approach can treat today. Moreover, it makes the computation of the spectrum of ionized electrons tractable.

We hope the shake-off mechanism will help to clarify the dynamics of two-electron transitions and the present method will be very useful for analyses of the experiments on collision of ions with the excited-state target. The extension of the present model to collisions of ions with the target with the equivalent electrons such as those in the ground state and the calculations of the spectrum of ionized electrons are under way.

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