ASYMPTOTIC APPROACH TO THE PROCESSES OF TWO-ELECTRON CAPTURE AT SLOW ION-ATOM COLLISIONS

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Two-electron capture at slow ion-atomic collision is under consideration within the framework of asymptotic approach. Cross section of one- and two-electron capture at separate final state is calculated using the method of strong-coupling channels. Different ways of two-electron transfer (straight and step-by-step) and their relative contribution to the total cross-section of process is investigated.

Introduction

Processes of two-electron exchange at slow multicharged ion and atom collisions similar to

$$A^{(Z_a-2)+} + B^{Z_b+} \to A^{Z_a+} + B^{(Z_b-2)+}(n_1l_1, n_2l_2), \quad (1)$$

attract increasing attention of both theoretical [1-5] and experimental groups [6-9]. Firstly, importance of these processes for application is explained by possibilities of using them for controlled thermonuclear synthesis [10], obtaining particles with great excitation energy what is interesting for inverse density of population creation. Secondly, theory of atomic collisions needs furthermore investigation of the correlation of electrons at the dynamics of two-electron exchange [2–4]. And finally, detailed studying of two-electron processes leads to better understanding of the mechanism of three- and four-electron exchange detected experimentally [11] (resonance exchange of three electrons was theoretically investigated [12] in the framework of asymptotic approach). At present time one of the most successful theoretical descriptions of the process similar to (1) is achieved in the framework of asymptotic theory of atomic collisions [2-4]. In work [3], using a quasi-classical approach, most general analytic expression for matrix element of two-electron exchange interaction of atom and multicharged ion with different nuclei charge is obtained. Built in [3] theory corresponds with the cases when probabilities of the one-electron transfer are smaller then those for two-electron transfer, and one-electron channels of reaction are negligible comparatively with those for the two-electron case. However, while distance between particles decreases, the possibility of one-electron transfer at the excited state of the ion $B^{(Z_b-1)+*}$ increases and exceeds two-electron capture. This fact on the first view closes two-electron channels the more strongly the greater is the probability of one-electron transfer. Nevertheless, two-electron capture is probable as a sequence of two-electron process which consists of simultaneous transition of a preliminary captured electron from the excited state $|nl\rangle$ of $B^{(Z_b-1)+*}$ to the ground state $|n_1l_1\rangle$ of $B^{(Z_b-1)+}$ and an electron capture from the ground state of the $A^{(Z_a-1)+}$ ion to an excited state $|n_2l_2\rangle$ of $B^{(Z_b-2)+}$ ion:

$$A^{(Z_a-2)+} + B^{Z_b+} \to A^{(Z_a-1)+} + B^{(Z_b-1)+*}(nl) \to \to A^{Z_a+} + B^{(Z_b-2)+}(n_1l_1, n_2l_2)\,. \quad (2)$$

The chain of reaction (2) occurs during a single act of collision, thus great probability of one-electron exchange makes possible another so-called step-by-step mode of two-electron transfer which is under consideration in this work. A similar possibility of two-electron capture was considered earlier [13] in the case of collision of an atomic

particle with the same particle but without two electrons. Reaction

$$He\,(1s^2) + Ar^{6+}\,(3s^2) \rightarrow$$
$$\rightarrow He^{++} + Ar^{4+}(3s^2\, n_1 l_1\, n_2 l_2), \quad (3)$$

is considered as an example of the asymptotic approach application.

Matrix element calculation

Here we designate as $1/2n_{1a,2a}^2$ and $1/2n_{1b,2b}^2$ the first and the second ionization potentials of $A^{(Z_a-2)+}, B^{(Z_b-2)+}$ particles, respectively. Further we shall be restricted to considering a quite general case when ionization potentials satisfy $n_{1a,1b} > n_{2a,2b}$ condition. Then the leading term of two-electron exchange matrix element of interaction between highly charged ion and atom is determined by configuration when tunneling electrons make transition at the different nuclei and independent electrons approximation is correct [2–4].

The approximation of "frozen" cores of particles A and B reduces problems to the consideration of two active electrons motion in the field of A^{Z_a+} and B^{Z_b+} ions. Here we designate by $\Psi_a(\vec{r}_1,\vec{r}_2)$ wave function of $A^{(Z_a-2)+}$ ion and by $\Psi_b(\vec{r}_{1b},\vec{r}_{2a})$ wave function of $B^{(Z_b-2)+}$ ion. In detail the analytic representation and the scheme of obtaining these functions is described at [3]. Our task is to evaluate the matrix element [2-4]:

$$H_{ab} = <\Psi_a|\hat{H}|\Psi_b> - <\Psi_a|\Psi_b><\Psi_a|\hat{H}|\Psi_a> \quad (4)$$

where $\hat{H}$ – is full Hamiltonian of the system at the two-electron approximation:

$$\hat{H} = -\frac{\Delta_1}{2} - \frac{\Delta_2}{2} + V_a(r_{1a}) + V_a(r_{2a}) + V_b(r_{1b}) + V_b(r_{2b}) + \frac{Z_a Z_b}{R} + \frac{1}{r_{12}} \quad (5)$$

Here Z_a, Z_b are effective charges of A and B particles' atomic core, $r_{ia}, r_{ib}, (i = 1,2)$ are distances from the i-th electron to the core of A and B; $V_a(r_{1a})$ and $V_b(r_{1b})$- interaction potentials of the $i = 1$ electron with A^{Z_a+} and B^{Z_b+} respectively; $V_a(r_{2a})$ and $V_b(r_{2b})$ - the same values for the $i = 2$ electron; R - the distance between A and B nuclei. In [2-4] it was shown that only the operator of interaction between electrons makes non-zero contribution to the matrix element (3). It is convenient to represent interaction between electrons as an expansion of a small parameter R^{-1} (multipole expansion):

$$r_{12}^{-1} = \frac{4\pi}{R}\sum_{l_1 m_1}\sum_{l_2 m_2}\frac{(-1)^{l_2}}{R^{l_1+l_2}}\delta_{-m_1,m_2}(l_1+l_2)!\,\Lambda_1(\vec{r}_1)\Lambda_2(\vec{r}_2)\times$$
$$[(2l_1+1)(2l_2+1)(l_1+m_1)!(l_1-m_1)!(l_2+m_2)!(l_2-m_2)!]^{-1/2}, \quad (6)$$

where $\Lambda_q = r_q^l Y_{lm}(\Omega_q)$. In order to keep the leading term of the matrix element we should limit summation at (5) up to minimal multipole term, which corresponds to the allowed transition (dipolar transition in most cases).

Further for the asymptotic of two-electron wave functions $\Psi_a(\vec{r}_{1b},\vec{r}_{2a})$ and $\Psi_b(\vec{r}_{1b},\vec{r}_{2a})$ [3]: we use an analytic representation:

$$\Psi_a(\vec{r}_{1b},\vec{r}_{2a}) = \varphi_{1ab}(\vec{r}_{1b})\cdot\varphi_{2a}(\vec{r}_{2a}); \quad \Psi_b(\vec{r}_{1b},\vec{r}_{2a}) = \varphi_{1b}(\vec{r}_{1b})\cdot\varphi_{2ba}(\vec{r}_{2a}), \quad (7)$$

$$\varphi_{1ab}(\vec{r}_b) = D_{ab}\sum_{l=0}^{\infty}\frac{f_{ll}(r_b)}{r_b}Y_{l0}(\theta_b,\phi_b)(-1)^l B_{l0};\quad B_{l0}=\sqrt{\frac{2l+1}{2}}$$

$$D_{ab} = \frac{A_{1a}n_{1a}}{\sqrt{2}}(2l_1+1)^{l/2}\left(\frac{2}{n_{1a}^2 Z_b}\right)^{n1a(Za-1)}\left(\frac{n_{1a}^2 Z_b}{2e}\right)^{n_{1a}Z_b} Q(R) \quad , \qquad (8)$$

$$Q(R) = R^{2n_{1a}(Z_a-1)-1}\exp\left(-\frac{R}{n_{1a}}\right)\left(\sqrt{\frac{R}{2Z_b n_{1a}^2}}-\sqrt{\frac{R}{2Z_b n_{1a}^2}+1}\right)^{\frac{2(Z_b-Z_a+1)}{\sqrt{\frac{1}{n_{1a}^2}+\frac{2Z_b}{R}}}}$$

$f_{1l}(r_b)$ being regular at origin partial solution of equation for radial Green's function [3] at the model potential $V_{mod} = -\frac{Z}{r}+\frac{A_l}{r^2}$ of particle B;

$$f_{ll}(r_b) = \left(\frac{2}{n_{1a}}\right)^{n_{1a}Z_b}\frac{\Gamma(1+S_l-n_{1a}Z_b)}{\Gamma(2S_l+2)}M_{n_{1a}Z_b;S_l+\frac{1}{2}}\left(\frac{2r_b}{n_{1a}}\right), \qquad (9)$$

here S_l - is an effective orbital quantum number at the model potential $V_{mod} = -\frac{Z}{r}+\frac{A_l}{r^2}$, A_l - an empirical value depending on the electron energy, calculation procedure of these parameters is described in detail in [3,14]; $\varphi_{1ab}, \varphi_{2ba}$- one-electron wave functions in the vicinity of the distant particle; $Y_{lm}(\theta,\phi)$- spherical harmonic; $M_{\lambda;\mu}(x)$- Whittaker's function; A_{1a}- an asymptotic coefficient of the first transferring electron, (wave function φ_{2ba} is gained by formal replacement $a \Leftrightarrow b$). We obtain the next expression for matrix element, which corresponds to the straight mode of the two-electron capture (1):

$$H_{ab} = -\begin{pmatrix} l_2 & l_1 & L \\ 0 & 0 & 0 \end{pmatrix}\cdot\frac{2}{R^3} < \varphi_a\left|Q_{2,0}^{(a)}\right|\varphi_{ba} >_A \cdot < \varphi_{ab}\left|Q_{1,0}^{(b)}\right|\varphi_b >_B, \qquad (10)$$

$$<|\,|>_A = \sqrt{2}\cdot Z_a^{3/2}D_{ab}\cdot\left(\frac{2}{n_{1b}}\right)^{n_{1b}Z_a-3}\frac{4\Gamma(2-n_{1b}Z_a)}{\left(\frac{1}{2}+\frac{Z_a n_{1b}}{2}\right)^5}\cdot{}_2F_1\left(5,2-n_{1b}Z_a;4;\frac{2}{Z_a n_{1b}+1}\right)\delta_{0,q}, \qquad (11)$$

$$<|\,|>_B = \delta_{0,-q}\cdot\frac{(-1)(2\beta_2)^{3/2+S_1}}{\sqrt{6\cdot\Gamma(3+2S_1)}}D_{ab}\left(\frac{2}{n_{1a}}\right)^{n_{1a}Z_b-S_1-3}\times$$

$$\left\{\sqrt{1-q^2}\,\frac{\Gamma(1+S_0-n_{1a})}{\Gamma(2S_0+2)}\,\frac{\Gamma(S_1+S_0+4)}{\left(\frac{1}{2}+\frac{n_{1a}}{2n_{2b}}\right)^{S_0+S_1+4}}\cdot{}_2F_1\left(S_0+S_1+4,-n_{1a}Z_b+S_0+1;2S_0+2;\frac{2}{\frac{n_{1a}}{n_{2b}}+1}\right)+\right. \qquad (12)$$

$$\left.\sqrt{4-q^2}\,\frac{\Gamma(1+S_2-n_{1a}Z_b)}{\Gamma(2S_2+2)}\,\frac{\Gamma(S_1+S_2+4)}{\left(\frac{1}{2}+\frac{n_{1a}}{2n_{2b}}\right)^{S_1+S_2+4}}\cdot{}_2F_1\left(S_1+S_2+4,-n_{1a}Z_b+S_2+1;2S_2+2;\frac{2}{\frac{n_{1a}}{n_{2b}}+1}\right)\right\}.$$

Within the framework of our approach the straight mode of the two-electron capture can be described as a sequence of their correlation interaction: the first captured electron passes from the excited to the ground state of $B^{(Z_b-1)+}$, another electron transfers from the ground level of $A^{(Z_a-1)+}$ to the wave function "tail" of the excited state $|n_1l_1,n_2l_2\rangle$ of $B^{(Z_b-2)+}$ ion. Under the selected condition $n_{1a,1b} > n_{2a,2b}$ on ionization potentials, $\varphi_{2a},\varphi_{1b}$ functions are non-perturbed atomic wave functions, which we consider to be known.

The matrix element, which describes the step-by-step mode of the two-electron capture, can be represented in the same form (10). However, the transfer at the particle B, which is contained in (10) as matrix element $<\varphi_{ab}|Q_{1,0}^{(b)}|\varphi_b>_B$, corresponds to the electron transition from the excited state $|nl\rangle$ of $B^{(Z_b-1)+*}$ to the ground state $|n_1l_1\rangle$ of $B^{(Z_b-1)+}$, and taking into account the relation

$$\int_0^{2\pi}\int_0^{\pi} d\Omega \cdot Y_{l_1}^{m_1}(\theta,\phi)Y_{l_2}^{m_2}(\theta,\phi)Y_{l_3}^{m_3}(\theta,\phi) = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l_3+1)}}\begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix}, \quad (13)$$

expressed in the form

$$<|\ |>_B = \pm\delta_{0,-q}\frac{2^{3+S_l^{(i)}+S_l^{(f)}}\beta_i^{3/2+S_l^{(i)}}\beta_f^{3/2+S_l^{(f)}}}{\sqrt{\Gamma\left(3+2S_l^{(i)}\right)\Gamma\left(3+2S_l^{(f)}\right)}}\frac{\Gamma\left(4+S_l^{(i)}+S_l^{(f)}\right)}{\left(\beta_i+\beta_f\right)^{4+S_l^{(i)}+S_l^{(f)}}}\sqrt{\frac{2l_i+1}{2l_f+1}}\cdot\begin{pmatrix} l_i & 1 & l_f \\ 0 & 0 & 0 \end{pmatrix}^2. \quad (14)$$

$\begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$ - the Clebsch-Gordan coefficient; $\frac{\beta_i^2}{2}, \frac{\beta_f^2}{2}, l_i, l_f$ - the ionization energy, and orbital quantum number of electron at $B^{(Z_b-1)+*}$ and $B^{(Z_b-1)+}$ states, respectively. Deriving (14) we have simulated the bound states of $B^{(Z_b-1)+*}$ by the wave function of the ground state at the above mentioned model potential V_{mod} with appropriate orbital quantum number [3,14]. Such assumption is justified because of closed shell of Ar^{6+} $(3s^2)$. However when the dipole transition is forbidden (for example, *4p-3p*), we should considesr *4p* level as the first excited after "ground" *3p* state, and keep a quadrupole term in (6). The sign in (11) is selected from the condition of coincidence model and Hartree-Fock wave function [15] at large distance from the electron to the nuclei.

Results and discussion

In Fig. 1 diabatic terms of initial ($He + Ar^{6+}$) and final ($He^{2+} + Ar^{4+}$) configuration corresponding with the channels of creation Ar^{4+} ions at *3p3d*, *3p4s*, *3p4p* and *3p4d* excited levels, as well as diabatic terms of ($He^{+} + Ar^{5+}$) configuration of Ar^{5+} ground *3p* and excited *3d*, *4s*, *4p* levels are presented. For more excited states of Ar^{4+} and Ar^{5+} appropriate channels make negligible contribution into the total and partial cross section and these states were not taken into account. As shown in Fig. 1, quasicrossing of one-electron terms, associated with one-electron captures, occurs at larger distances R than in the case of the two-electron capture.

Expression for the one-electron capture matrix element was taken from [14], where the procedure of deriving them is described in detail. The cross-section value obtained by numerical integration of the strong-coupled channels system is presented in Fig.2. Our theoretical predictions are seen to be in good agreement with the experimental data [7,8].

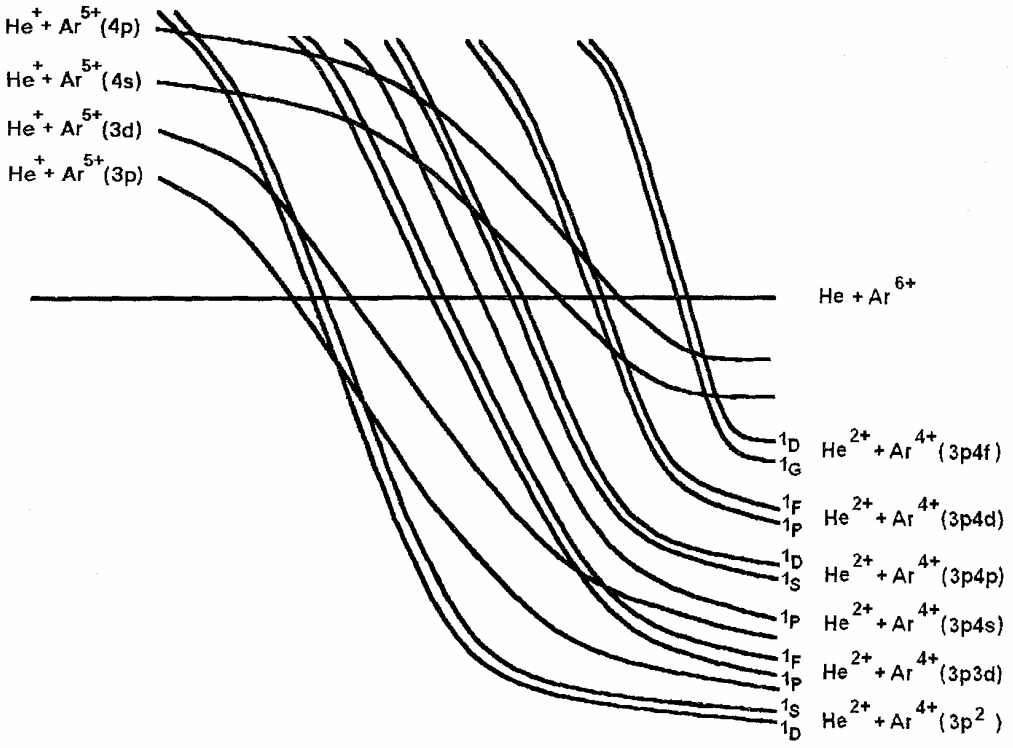

Fig. 1 Principal scheme of adiabatic energy levels for reaction (3)

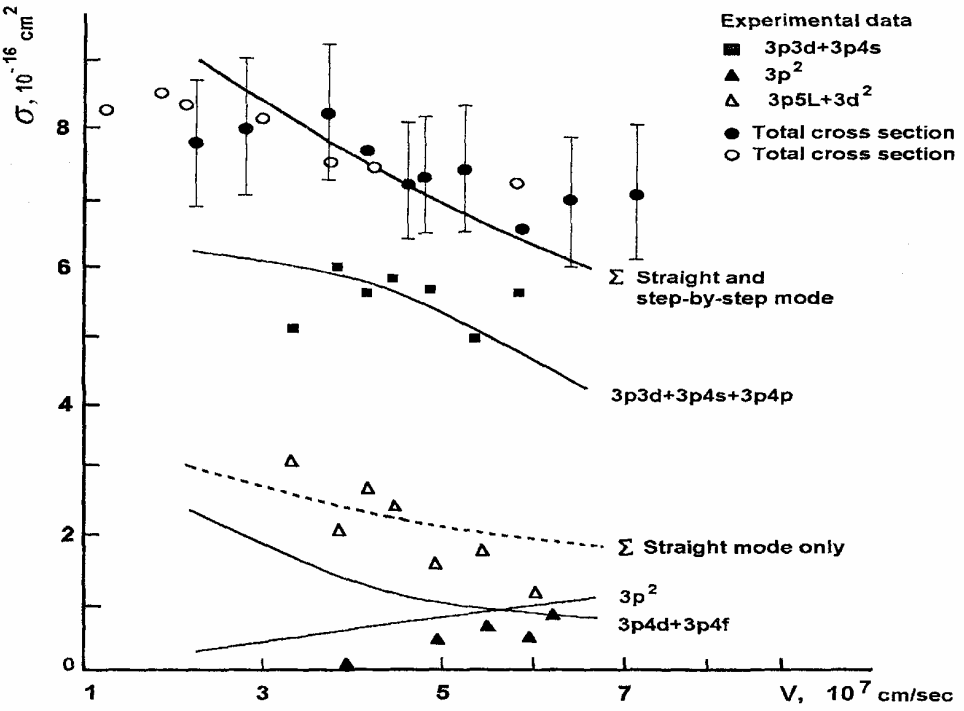

Fig.2. Total and partial cross section for two-electron capture (3). Experimental data from [7]; ■ - *3p3d + 3p4s*; ▲- $3p^2$; Δ - *3p5L + 3d²*; ● - total cross-section; ○ - total cross-section [8]. Solid lines – theoretical prediction, this work. Dashed line – total cross-section for two-electron capture when the straight mode of transfer taken into account only.

There is a nonconformity with our interpretation of the partial final state and that presented as experimental data. For example, data marked as solid squares corresponds to *3p3d* and *3p4s* final state of Ar^{4+} but we interpreted these data group as *3p3d*, *3p4s* and *3p4p* – levels. Besides, a mechanism of final state of Ar^{4+} formation was established. The straight mode of the two-electron capture makes contribution to the total cross-section about 30% only, but step-by-step mode makes about 70% contribution. The charge exchange to the ground state of Ar^{5+} $(3s^23p)$ and Ar^{4+} $(3s^23p^2)$ appears to be less then the transition to the excited states what is in good agreement with the experimental data.

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АСИМПТОТИЧНИЙ ПІДХІД ДО ПРОЦЕСІВ ДВОЕЛЕКТРОННОГО ЗАХОПЛЕННЯ ПРИ ПОВІЛЬНИХ ІОН-АТОМНИХ ЗІТКНЕННЯХ

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Розглянуто процеси двоелектронного захоплення в рамках асимптотичного підходу. Перерізи одно- та двоелектронних процесів захоплення у парціальні стани обчислено методом сильного зв'язку каналів. Розглянуто різні механізми двоелектронного захоплення (прямий та постадійний), та проаналізовано їх відносний внесок у повний переріз процесу.