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THE TIME-SYMMETRIC DESCRIPTION OF ELECTRON EXCHANGE IN ION-ION COLLISION

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Abstract. In this work we consider the process of one electron exchange between the Rydberg states of ions using two-wave-function (TWF) model. Investigation of atomic collision processes is very important for a detailed understanding of the elementary processes in plasma, especially in order to develop appropriate diagnostic methods of plasma fusion. The specific approach within the model imposes the use of two wave functions necessary for determining the transition probability and corresponding rates and finally estimating of the neutralization distances. We study the intermediate stages of the population of the Rydberg states of highly charged SiIV, PV and SVI ions escaping the targets ArVIII and KrVIII.

1. INTRODUCTION

We analyze one electron transfer into the Rydberg state of multiply charged projectile ion with core charge Z_A after collision with stationary multiply charged target ion with core charge Z_B (see Janev, R. K. 1986). A specific feature of the time-symmetric model under consideration is the description of representative electron transfer from ion B to ion A in two scenarios with two wave functions: $\Psi_B(\vec{r},t)$ and $\Psi_A(\vec{r},t)$.

For fixed initial $\Psi_{\nu_B=(n_B,l_B,m_B)}$ $(t = t_{in})$ and final states $\Psi_{\nu_A=(n_A,l_A,m_A)}$ $(t = t_{fin})$, by using the evolution operators $\hat{U}_B(t_1,t_2)$ and $\hat{U}_A(t_1,t_2)$, we are able to find evolution of the system, i.e. $\Psi_B(\vec{r},t) = \hat{U}_B(t_{in},t)\Psi_{\nu_B}$ and $\Psi_A(\vec{r},t) = \hat{U}_A(t_{fin},t)\Psi_{\nu_A}$, taking into account that the mentioned evolution operators are determined by Hamiltonians $\hat{H}_B$ and $\hat{H}_A$, respectively, which can be presented in the following form:

$$\hat{H}_B = -\frac{1}{2}\nabla^2 - \frac{Z_B}{r_B} + \sum_{l=0}^{\infty}\frac{c_{l_B}}{r_B^2}\hat{P}_l + \hat{U}_{B,A}, \tag{1}$$

$$\hat{H}_A = -\frac{1}{2}\nabla^2 - \frac{Z_A}{r_A} + \sum_{l=0}^{\infty}\frac{c_{l_A}}{r_A^2}\hat{P}_l + \hat{U}_{A,B}. \tag{2}$$

In both equations, the second and third terms are the potential energy of the electron in the field of polarized ionic core expressed over Simons-Bloch potential form in which the projection operator $\hat{P}_l$ onto the subspace of an orbital quantum number l are appears. On the other hand, by $\hat{U}_{B,A}$ and $\hat{U}_{A,B}$ we introduce the potential energy of the electron due to the presence of ion A and B, respectively. At large distances between ions $R \gg 1$, it is justified to use approximations $\hat{U}_{B,A} = -Z_A/r_A$ and $\hat{U}_{A,B} = -Z_B/r_B$. Even more, in cases where the narrow cylindrical area around the ion trajectory is considered (the case of small values of angular momentum) which are the subject of this paper, a quite satisfactory approximation is given in the form $\hat{U}_{B(A)} \approx -Z_{A(B)}/R$.

Normalized transition probability $\tilde{T}_{\nu_B,\nu_A}(t) = T_{\nu_B,\nu_A}(t)/T^{t\to t_{fin}}_{\nu_B,\nu_A}$ and corresponding normalized rate $\tilde{\Gamma}_{\nu_B,\nu_A}(t) = d\tilde{T}_{\nu_B,\nu_A}(t)/dt$ can be obtained from mixed flux $I_{\nu_B,\nu_A}(t)$ (see Nedeljković et al. 2012.) by following expression:

$$T_{\nu_B,\nu_A}(t) = \left| \int_{t_{in}}^{t} I_{\nu_B,\nu_A}(t)dt \right|^2, \tag{3}$$

whose analytical expression is given in the reference Galijaš et al. 2021, 2019. Finally, taking the position of the maximum of the normalized rate, it is possible to give an estimate of the partial neutralization distance under different conditions in which the appropriate system can be found.

2. RESULTS

In Fig. 1 we present normalized transition probability and corresponding rate for population of the high charged ion SVI ($n_A = 6, l_A = 0, m_A = 0$) escaping KrVIII ($n_B = 8, l_B = 0, m_B = 0$) for two different velocities a) $v = 3$ a.u. and b) $v = 7$ a.u. We point out that $\tilde{\gamma}_B$ and $\tilde{\gamma}_A$ are the most important parameters appearing in the mixed flux function $I_{\nu_B,\nu_A}(t)$ and are related to the values of the considered energy levels of ions and can be determined by spectroscopic measurements, see Ralchenko Yu. et al. 2007. Here we discussed only values corresponding to the ground state of the ionic cores. Comparing atomic collision processes under the same conditions but at different projectile ion velocities, it can be concluded that the significance of the value of the orbital angular momentum l_A decreases with increasing of the velocity in case of estimation of the most likely neutralization distances.

On the other hand, at a fixed value of the angular momentum $l_A = 0$, different ions with same paired electronic core configurations are considered: SiIV($n_A = 4$, solid curves), PV($n_A = 5$, dotted curves) and SVI($n_A = 6$, dashed curves) in a wider range of intermediate velocities v. It is obvious from Fig. 2a, that neutralization distances move towards higher values with increasing of core charge (with the same ratio Z/n) so that the difference is greater with increasing of relative ion-ion velocity. In order to compare, data for KrVIII($n_A = 8$, circles) and XeVIII($n_A = 8$, squares) taken from Ref. Galijaš et al. 2021., were entered on the graph.

Finally, Fig. 2b presents the normalized neutralization rates $\tilde{\Gamma}_{\nu_A}(t)$ (scaled by v) for PIII, PIV, PV ($n_A = 5, l_A = 0$) and for SIV, SV, SVI ($n_A = 6, l_A = 0$). As can be stated in both cases, ion-ion neutralization distance R_{ec} is significantly reduced in the case when in addition to the closed projectile ionic core $2p^6 3s^2$ we have electron capture in the far $^2S_{1/2}$ (Rydberg) empty shell. Moreover, at higher projectile velocities, this effect becomes even more pronounced.

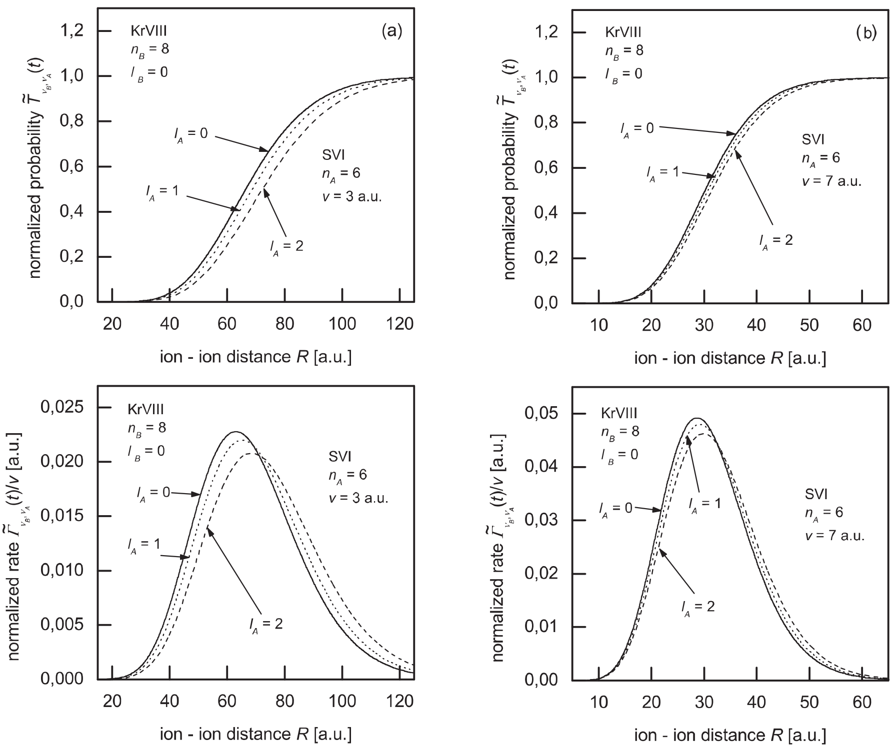

Figure 1: Population of the Rydberg levels of SVI ion for $n_A = 6$ and $l_A = 0, 1$ and 2. Normalized transition probabilities $\tilde{T}_{\nu_B,\nu_A}$ and corresponding normalized neutralization rates $\tilde{\Gamma}_{\nu_B,\nu_A}$ (scaled by v) are presented for two different ion-projectile (ion A) velocities a) $v = 3$ a.u. and b) $v = 7$ a.u.

3. DISCUSSION

All the results presented in this paper clearly indicate the conclusion that the application of the two-wave-function model is extremely useful in understanding the process of the electron capture in ion-ion collisions. We analyzed only atomic particles with ground state of the ionic cores, i.e.: PV($2p^6$), PIV($3s$), PIII($3s^2$), SVI($2p^6$), SV($3s$), SIV($3s^2$). The neutralization distances R_{ec} were estimated for electron capture in the state $n_A = 5$ in the case of P ions and in the state $n_A = 6$ in the case of S ions, with the lowest possible energies: PV($^2S_{1/2}$), PIV($^3S_1$), PIII($^2S_{1/2}$) and SVI($^2S_{1/2}$), SV($^3S_1$), SIV($^2S_{1/2}$). For PIII($3s^25s, {}^2S_{1/2}$) i SIV($3s^26s, {}^2S_{1/2}$) a significant reduction in the neutralization distance was observed.

Additionally, despite the fact that a pronounced velocity dependence of electron capture distance has been found, the model has not yet been tested outside the limits of intermediate velocities.

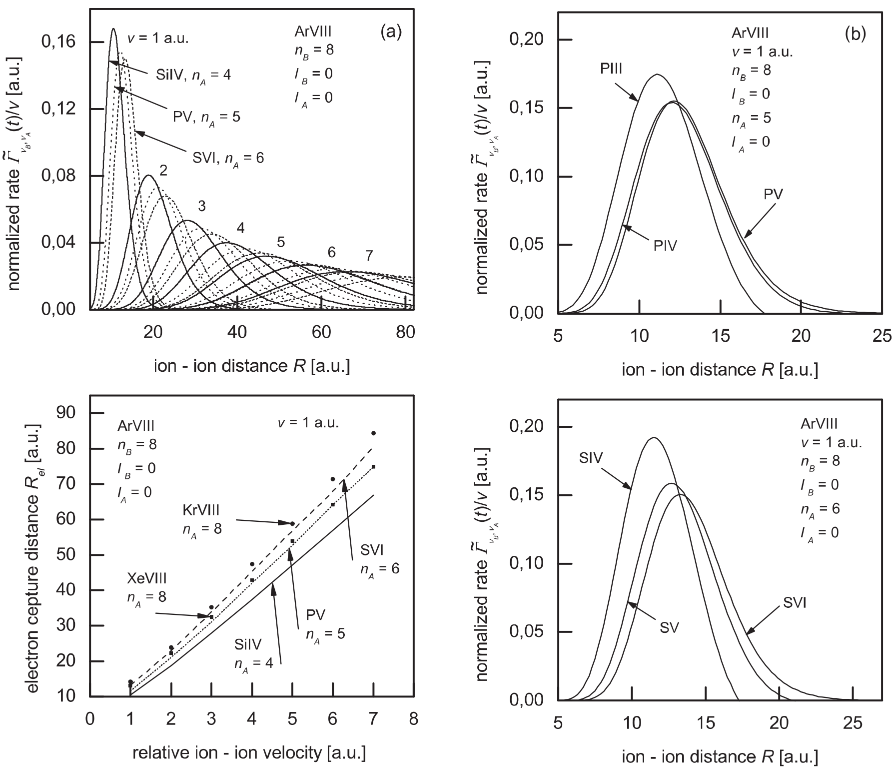

Figure 2: a) Normalized neutralization rates $\tilde{\Gamma}_{\nu_A}(t)$ scaled by v and appropriate velocity dependence of the electron capture distance R_{ec} in the velocity region $1 \leq v \leq 7$ a.u. Electron capture in the Rydberg state $(n_A, l_A) = (4, 0)$, $(5, 0)$ and $(6, 0)$ of the SiIV (solid curves), PV (dotted curves) and SVI (dashed curves) ions, respectively, escaping the ArVIII ($n_B = 8, l_B = 0$) was considered. b) Normalized neutralization rates $\tilde{\Gamma}_{\nu_B,\nu_A}$ (scaled by v) are presented for P and S ions with a different core charge.

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