Publ. Astron. Obs. Belgrade No. 84 (2008), 165 - 168 *Contributed Paper*

RESONANT *vs.* NON-RESONANT NEUTRALIZATION OF MULTIPLY CHARGED IONS IN THE INTERACTION WITH SOLID SURFACES

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Abstract. The two-state vector model is used to investigate the intermediate stages of the electron capture into the Rydberg states of multiply charged ArVIII ion, escaping solid surface. Two cases of the ionic velocities are considered: the low velocities ($v \approx 0$ a.u.) and the intermediate velocities ($v \approx 1$ a.u.). Within the framework of the two-state vector description of the neutralization dynamics the two wave functions are used to determine the state of a single active electron. The intermediate stages of the process are characterized by the two-amplitude, the neutralization probability and rate. These quantities are obtained in two different analytical forms in the two considered cases of the projectile velocities. The key difference of the intermediate velocity case in respect to the low-velocity case, is the non-resonant character of the electron transitions. The obtained rates in the low velocity case are well localized. The neutralization rates in the intermediate velocity case are oscillatory in character. At larger ion-surface distances R the neutralization is stabilized; the behavior of the rates becomes similar to that obtained for the low ionic velocities.

1. INTRODUCTION

One of the recently developed model for description of the non-resonant neutralizations process during the interaction of multiply charged ions with the solid surface is the quantum teleological model, known as the two-state vector model (TVM), see e.g. Nedeljković et al. (1994, 2003) and Nedeljković and Nedeljković (1998). This model is appropriate for description of the intermediate stages of the ion-surface interaction, when we consider the problem at which distance from the surface the process is the most probable. Within the framework of TVM, we define the intermediate probabilities and rates, from which the problem of localization of the process can be resolved.

The TVM represents a form of the time-symmetric quantum model in which the two state functions are used for description of a single electron exchange dynamics. The first wave function $\Psi_1(t)$ evolves from the preselected state of the electron, initially localized in the solid, which is described by the parabolic set of quantum numbers $\mu_M = (\gamma_M, n_{1M}, m_M)$. The second wave function $\Psi_2(t)$ describes the state which will evolve into the given postselected final state of the electron bound to the ion, labeled by the spherical quantum number set $\nu_A = (n_A, l_A, m_A)$. In the TVM formalism, the

electron capture process from the solid surface into the moving ion is described via mixed flux through the Firsov plane S_F, separating the solid and the ionic subsystems.

In this paper we consider the neutralization of ArVIII ions in a normal emergence geometry. The main output of this analysis are the normalized neutralization rates for the ions finally detected in a given Rydberg state ν_A. We apply the TVM, considering both the neutralization at small ionic velocities as well as the neutralization process at intermediate projectile velocities.

2. THE TVM OF NEUTRALIZATION

Neutralization process represents the capture of the active electron from the solid surface into the field of moving ion. Within the framework of TVM it can be considered as a transition $\Psi_1(t) \to \Psi_2(t)$ at some intermediate time t, due to the "measurement" of the electron localization in the ionic region V_A.

Hamiltonians $\hat{H}_1$ and $\hat{H}_2$, which determine the evolutions of the states Ψ_1 and Ψ_2 are adapted to the fact that in the first scenario, inside the solid, electron can moves infinitely. Also, in the second scenario and outside the solid, the polarization effect of the ionic core has to be included. Therefore, inside the solid we have $\hat{H}^{(1)} = -(1/2)\nabla^2 - U_0$ and $\hat{H}^{(2)} = -(1/2)\nabla^2 - Z/r_A$, where U_0 is the the mean electronic potential inside the solid, and r_A is the distance of the electron from the ionic core. Outside the solid we have $\hat{H}^{(i)}(R) = -(1/2)\nabla^2 + U_A^{(i)} + U_S^{(i)}$, where $U_A^{(i)}$ is the effective potential energy of the active electron in the field of polarized ionic core; the surface potential $U_S^{(i)}$ is the electron potential energy in the field of polarized solid. In the second scenario the Simons-Bloch potential $U_A^{(2)} = -Z/r_A + \sum_{l'=0}^{\infty}(c_{l'}/r_A^2)\hat{P}_{l'}$ can be used, where $\hat{P}_{l'} = |l'\rangle\langle l'|$ is the projection operator onto the subspace of a given angular momentum l'. The quantity $U_S^{(i)}$ can be expressed in the electrostatic approximation; furthermore, in the low-l case the radial electron coordinate can be neglected in comparison to the ion-surface distance R.

Following the general TVM-formalism, the neutralization is described by the two-state probability amplitude $A_{\mu_M,\nu_A}(t) = \langle\Psi_2(t)|\hat{P}_A(t)|\Psi_1(t)\rangle$, where $\hat{P}_A(t) = \int_{V_A}|\vec{r}_A\rangle\langle\vec{r}_A|$ is the projecting operator onto the ionic region V_A. Using the two-amplitude we can define the intermediate neutralization probability, as well as the normalized probability $\tilde{P}_{\nu_A}(t)$ and the corresponding rate $\tilde{\Gamma}_{\nu_A}(t)$. The advantage of the TVM is that the probabilities and rates can be expressed via mixed flux through the boundary surface S_A of the region V_A, which partially consists of the Firsov plane S_F. In this way, we obtain the relatively simple expressions for the normalized probability and rate; these expressions have different forms in the low and intermediate velocity regions.

The normalized neutralization rate is given by $\tilde{\Gamma}_{\nu_A}(t) = d\tilde{P}_{\nu_A}/dt$. In the low-velocity case for the normalized probability $\tilde{P}_{\nu_A}$ we have, see e.g. Nedeljković and Majkić (2007)

$$\tilde{P}_{\nu_A}(t) = \left[1 - \left(\frac{R}{R_{in}^*}\right)^{\tilde{\alpha}} \mathrm{e}^{-\tilde{\beta}(R-R_{in}^*)}\right]^2, \tag{1}$$

where R_{in}^* is the minimal ion-surface distance at which the resonant neutralization is possible. In the case of intermediate velocities, the expression for the normalized

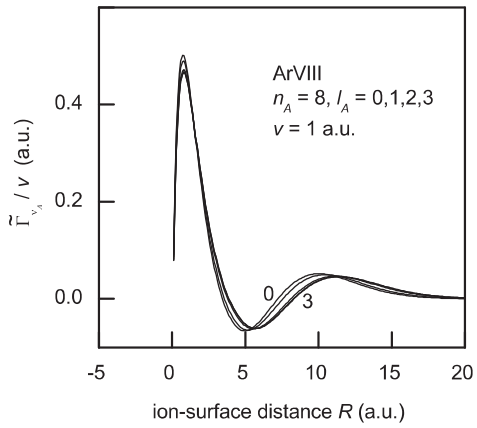

Figure 1: Normalized intermediate rates $\tilde{\Gamma}_{\nu_A}(t)$ (scaled by v) via ion surface distances R for the ArVIII ion escaping the solid surface with velocity $v = 1$ a.u.

probability is more complicated:

$$\tilde{P}_{\nu_A}(t) = 1 + f^2(R) - 2f(R)\cos\left(\frac{w}{v}R + \arg\mathcal{B}\right), \tag{2}$$

where

$$f(R) \approx \left(1 + \frac{|\beta|^{\tilde{\alpha}}}{\Gamma(\tilde{\alpha}+1)}R^{\tilde{\alpha}}\right)e^{-\tilde{\beta}R}, \tag{3}$$

whereas $|\beta| = [\tilde{\beta}^2 + (\omega/v)^2]^{1/2}$, and

$$\arg\mathcal{B} = \arctan\frac{|\beta|^{\tilde{\alpha}}R^{\tilde{\alpha}}\sin[(\tilde{\alpha})\arctan(\omega/v)]}{1 + |\beta|^{\tilde{\alpha}}R^{\tilde{\alpha}}\cos[(\tilde{\alpha})\arctan(\omega/v)]}. \tag{4}$$

The quantities $\tilde{\alpha}$ and $\tilde{\beta}$ are the given functions of the energy parameter $\tilde{\gamma}_A$ for the electron in the field of polarized ionic core and energy parameter γ_M: $\tilde{\alpha} = Z/\tilde{\gamma}_A - 1/2 + 1/4\gamma_M$ and $\tilde{\beta} = \gamma_M + (\tilde{\gamma}_A - \gamma_M)g$. Parameter g defines the kinematics of the Firsov plane, and the quantity w is defined by $w = (1/2)\left(\gamma_M^2 - \tilde{\gamma}_A^2\right) - (v^2/2)(1-2g)$.

3. RESULTS

In Fig. 1. we present the normalized intermediate rates $\tilde{\Gamma}_{\nu_A}(t)$ (scaled by v) via ion-surface distances R, for the ArVIII ion interacting with Al solid surface. We considered the case of the electron capture into the Rydberg state $n_A = 8, l_A = 0-3, m_A = 0$, for the ionic velocity $v = 1$ a.u., which belongs to the domain of intermediate velocities. The case of the point-like core (dashed curve) nearly coincide with the curve obtained for $l_A = 3$. From Fig. 1 we recognize that in the initial stages of the ionic motion, at smaller distances from the surface, we have a kind of instability. That is, the electron is firstly captured (neutralization); after that, the sign of the rate is changed, which means that the electron become partially recaptured by the solid. At larger R, the neutralization process is stabilized.

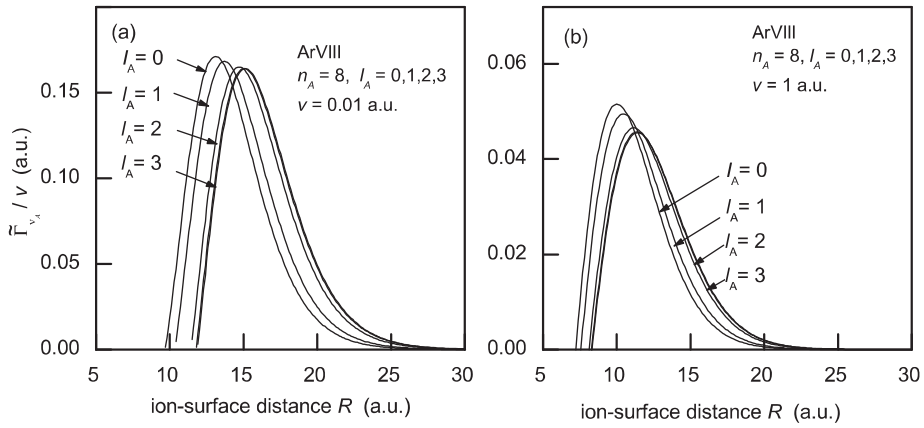

Figure 2: Normalized intermediate rates $\tilde{\Gamma}_{\nu_A}(t)$ (scaled by v) via ion-surface distances R for the ion ArVIII escaping the solid surface with velocity (a) $v = 0.01$ a.u. and (b) $v = 1$ a.u.

In Fig. 2. we present the normalized intermediate rates $\tilde{\Gamma}_{\nu_A}(t)$ (scaled by v) analyzing the cases of small and intermediate ionic velocities, Figs. 2(a) and 2(b), respectively. Again, we consider the electron capture into the Rydberg state $n_A = 8, l_A = 0 - 3, m_A = 0$, for the ionic velocities $v = 0.01$ a.u., see e.g. Nedeljković and Majkić (2007), and Nedeljković et al. (2008) and $v = 1$ a.u. In Fig. 2(b), we present only the stabilized part of the rate, i.e., the last oscillation. We recall that the neutralization of the ionic projectile escaping the surface with small velocity, Fig 2(a), is resonant in type; it begins at the ion-surface distance R^*_{in}, which can be determined on the base of the energy condition. On the other hand, in the case of intermediate velocities, Fig. 2(b), the beginning of the stable regime coincide with the last zero of the rate.

Two effects can be recognize from Fig. 2. First, the rates are shifted toward the smaller R with increasing ionic velocity v. Indeed, the non-resonant transitions ($v = 1$ a.u.) are localized at smaller ion-surface distances R comparing to the resonant transitions ($v = 0.01$ a.u.). Second, the rates are additionally shifted toward the smaller ion-surface distances R due to the ionic core polarization.

We point out that the velocity dependence obtained within the TVM is nontrivial, and different comparing to the velocity dependence obtained within the framework of rate equation.

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