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NEUTRALIZATION OF MULTIPLY CHARGED RYDBERG IONS INTERACTING WITH SOLID SURFACES UNDER THE GRAZING INCIDENCE GEOMETRY

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Abstract. We elaborated the time-symmetric, two-state vector model to investigate the intermediate stages of the electron capture into the Rydberg states of multiply charged ions interacting with solid surface under the grazing incidence geometry. The neutralization distances for the ions Xe^{Z+} interacting with Al-surface are calculated, for core charges $Z \in [5,30]$. The corresponding mean neutralization distances are in agreement with the data deduced from the measured kinetic energy gain due to the image acceleration of the ions.

1. INTRODUCTION

The electron exchange during the interaction of ions with solid surfaces has been intensively studied both theoretically and experimentally; see, for example, Burgdörfer (1993) and Winter (2002). However, the quantum description of the events in the time interval between the initial and final "measurements" is still uncompleted. This kind of problem has been recently considered within the framework of two-state vector model (TVM) by Nedeljković et al. (2007) and Nedeljković et al. (2008), concerning the quasi-resonant electron capture into the Rydberg states of multiply charged ions escaping solid surfaces at low velocity. The scattering geometry that provides interesting new phenomena and insight into atom-surface interactions has not been considered by the TVM.

In the present paper, we analyze the electron capture (neutralization) into the Rydberg states of multiply charged ions ($Z >> 1$) in the scattering geometry (under the grazing incidence condition) at low perpendicular velocity ($v_{\perp} << 1$ a.u.). We formulate the TVM for the collision geometry, by taking into account the appropriate initial and final conditions. We assume that at the initial time t_{in}, when the projectile is at the distance $R = R_{in} \to \infty$ from the surface, the active electron is in the metallic parabolic state $|\mu_M\rangle$ mainly localized in the solid, and that at the final time $t = t_{fin}$, when the ionic projectile is at the finite ion-surface distance $R = R_{fin}$, the electron is bound to the ion, in the "atomic" spherical Rydberg state $|\nu_A\rangle$. Both the initial and the final states determine the electron behavior at the intermediate stages of the neutralization process.

The neutralization process of the Xe^{Z+} ion is mainly localized at ion-surface distances R_c^N (neutralization distances). These distances can be obtained from the electron capture probability P_{ν_A} into the considered final state $|\nu_A\rangle$. The mean neutralization distances $\langle R_c^N \rangle$ for the cascade neutralization: $Z \to Z-1 \to Z-2...$ can be compared with the values deduced from the measured projectile kinetic energy gain; Winter (1992), Winter et al. (1993).

2. NEUTRALIZATION - TVM

The quantum TVM ensemble under consideration consists of the active electrons in the field of moving polarized ionic cores (core charge Z) and polarized solid (Fig. 1).

At the intermediate time $t \in [t_{in}, t_{fin}]$ the state of the considered active electron is described by two state vectors:

$$|\Psi_1\rangle = \exp\left(-\frac{i}{\hbar}\int_{t_{in}}^{t} \hat{H}_1 dt\right)|\mu_M\rangle, \quad |\Psi_2\rangle = \exp\left(-\frac{i}{\hbar}\int_{t_{fin}}^{t} \hat{H}_2 dt\right)|\nu_A\rangle. \qquad (1)$$

By $\hat{H}_1$ and $\hat{H}_2$ we denoted the "in- and out-channel" Hamiltonians, respectively. The final perpendicular ion-surface distance R_{fin} is determined by the intersection of the electron energy term $E_A(R)$ with the Fermi level: $E_A(R) = -\phi$, where ϕ is the solid work function. We point out that the scattering geometrical conditions considered in the present paper induce the modifications in the in- and out Hamiltonians in comparison to the normal emergency geometry case considered in our previous TVM treatment of the neutralization process. At the ion-surface distance $R \approx R_c^N$, the electron capture is mainly through the narrow cylindrical region around the instant perpendicular ion-surface direction; see Fig. 1.

The interaction of the active electron with polarized ionic core in the first scenario is simply the Coulomb interaction. In the second scenario the active electron moves closer to the charge cloud of the electrons already bound to the nucleus. In that case, the Simons-Bloch potential can be used.

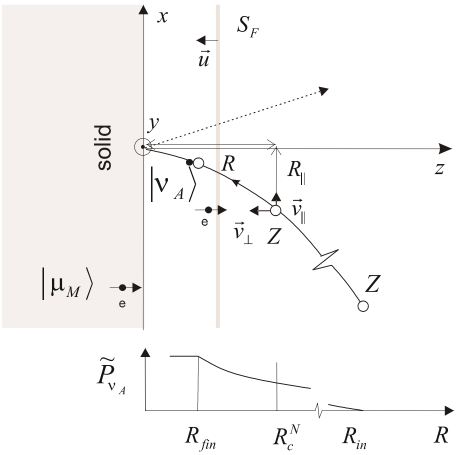

Figure 1: The TVM description of neutralization under the scattering condition. The electron capture is mainly localized at ion-surface distance R_c^N (neutralization distance) at which the normalized neutralization probability $\tilde{P}_{\nu_A} = 1/2$.

The intermediate stages of the neutralization can be characterized by the normalized probability $\tilde{P}_{\nu_A} = P_{\nu_A} / P_{\nu_A}^{fin}$, where $P_{\nu_A}^{fin} = \lim_{t \to t_{fin}} P_{\nu_A}$. Within the framework of the TVM, the normalized probability is expressed via the mixed flux through the moving Firsov plane S_F, see Fig. 1. We get

$$\tilde{P}_{\nu_A} = \left(\frac{R}{R_{fin}} \right)^{2\tilde{\alpha}} e^{-2\tilde{\beta}(R - R_{fin})}, \tag{2}$$

where the parameters $\tilde{\alpha}$ and $\tilde{\beta}$ are expressed in terms of the initial and final electron energies and the kinematics of the S_F plane.

3. NEUTRALIZATION DISTANCES

In Fig. 2(a) we present (full curves) the neutralization distances R_c^N for the ion Xe^{Z+} slowly escaping the Al surface, for the electron capture into the Rydberg states $\nu_A = (n_{A,} l_A = 0, m_A = 0)$. Dashed curves are the neutralization distances obtained in the case of pointlike cores. From Fig. 2(a) we recognize that the polarization of the ionic cores plays an important role in the considered low-l_A case; the neutralization distances are significantly overestimated if the polarization is neglected.

At present, the experimental evidence concerning the intermediate stages of neutralization of the considered multiply charged ions for the projectiles impinging the surface under grazing geometry is very restricted. From the measured projectile kinetic energy gains $\Delta E = Z^2 / 4\langle R_c^N \rangle$, Winter (1992), Winter et al. (1993), one can only deduce the mean neutralization distances $\langle R_c^N \rangle$. The quantity $\langle R_c^N \rangle$ can be considered as a neutralization distance R_c^N for the Rydberg level $\langle n_A(Z) \rangle$, where $\left| E_A\left(R_c^N\right) \right| \big/_{n_A = \langle n_A \rangle} = \phi + \Delta\phi$; the shift $\Delta\phi = \phi/3$ is estimated according to the classical over-barrier model. In Fig. 2(b) we present the TVM mean neutralization distances (the R_c^N values for $n_A = \langle n_A(Z) \rangle$) together with the experimental data.

We found that the polarization of the ionic core has no influence on the mean neutralization distances; see Fig. 2(b).

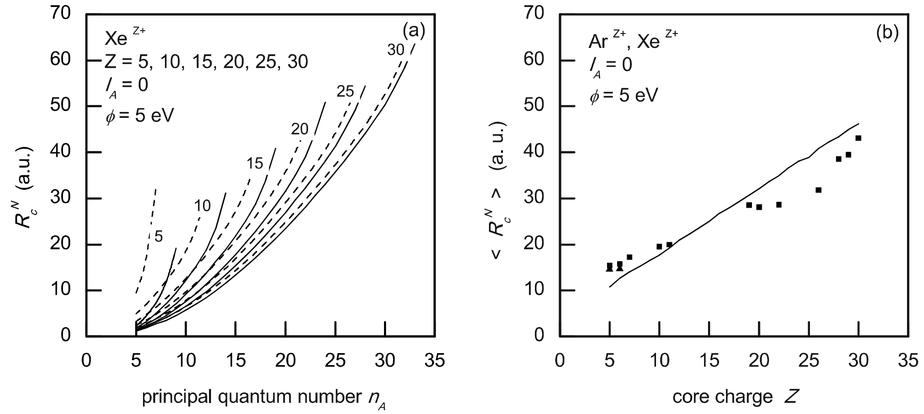

Figure 2: (a) Neutralization distances R_c^N of the ion Xe^{Z+} interacting with Al surface. Dashed curves correspond to the point-like cores. (b) The mean distances $\langle R_c^N \rangle$. Symbols are the experimental results, Winter (1992), Winter et al. (1993).

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