# SURVIVAL OF LARGE-*l* RYDBERG STATES OF HIGHLY CHARGED IONS IN THE VICINITY OF METAL SURFACES

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**Abstract.** The probabilities for ionization of large-*l* multiply charged Rydberg ions approaching metallic surfaces at thermal velocities in the normal incidence geometry were calculated. The ionization process was treated within the framework of decay model using the appropriate etalon equation method for solving the complex energy eigenvalue problem. It is shown that, in contrast to corresponding low-*l* states, the large-*l* Rydberg states exhibit non-zero survival probabilities.

## 1. INTRODUCTION

The charge transfer events between the Rydberg atoms/ions and a metallic surfaces represent complex quantum processes that require detailed clarification of their intermediate stages. It is well known that the motion of the excited electron, in a given Rydberg state described by set of spherical quantum numbers, can be strongly affected by the presence of the metallic surface leading to formation of hybridized Stark-like states, best described by parabolic symmetry $\mu = (n_1, n_2, m)$ (Nordlander 1996). The decay of these intermediate states was treated theoretically by different quantum mechanical models such as coupled angular-mode (CAM) method by Borisov et al. (1996) or etalon equation method (EEM) by Nedeljković & Nedeljković (2005) and Nedeljković et al. (2006). However, the problem of ionization of multiply charged Rydberg ions and atoms, as well as the reionization of the previously populated Rydberg states, was treated in the low-*l* case only.

Major difference in theoretical analysis of low- and large-*l* Rydberg states is in the fact the electron cloud of the low-*l* atoms/ions is highly eccentric and therefore the radial coordinate $\rho$ of the active electron can be practically neglected. On the other hand, for the large-*l* states the radial coordinate is comparable to ion-surface distance $R$. Thus, the quantity $\rho$ represents a key parameter for the investigation of the intermediate stages of the ionization processes. Recently, we have developed a variational condition for $\rho$ in order to solve the complex energy eigenva-

lue problem (of the active electron in the process of decay of multiply charged Ryderg ion slowly approaching metallic surface) by the EEM (Nedeljković et al. 2008). The ionization rates and corresponding energy terms were calculated and it was shown that large-$l$ states ionize at similar ion-surface distance as vacuum oriented low-$l$ states, but much closer to the surface than surface oriented low-$l$ states. Also, from the Clebsh-Gordon (CG) series expansion it was demonstrated that the initial large-$l$ states correspond to states with $n_1 \approx n_2$ at the intermediate stages of the process.

In this study, we present the probabilities for ionization of multiply charged ($Z \gg 1$) ions approaching solid surfaces at velocity $v$, being initially populated in the large-$l$ Rydberg states ($n \gg 1$; $l \approx n-1$; $m = 0$). It is shown that in contrast to the low-$l$ states of the same $n$, the large-$l$ states exhibit non-zero survival probability in the near surface region.

## 2. THE IONIZATION PROBABILITIES

The ionization process $A^{(Z-1)+} + M = A^{Z+} + M(e)$ of the ionic projectile $A$ initially in the large-$l$ Rydberg state approaching a solid surface $M$ at velocity $v = -dR/dt$, along the $z$ axis orthogonal to the surface is considered. At the initial time $t_{in}$ the active electron is in the initial state $\Psi_{\nu,in}$, where $\nu = (n,l,m)$ represents a set of spherical quantum numbers. Prior to ionization, the state $\Psi_{\nu,in}$, in the presence of the metallic surface, evolves into an intermediate state $\Psi_\mu$, characterized by the parabolic quantum numbers $\mu = (n_1,n_2,m)$. By expansion of the inital spherical state over the parabolic ionic states, using the CG coefficients, it can be shown that the large-$l$ wave function at the intermediate stages of the ion-surface interaction behaves as parabolic wave function corresponding to parabolic quantum numbers for which $n_1 \approx (n-1)/2$. The ionization of the Rydberg ion is treated as a decay of the intermediate state, e.g., $\Psi_\mu \to \overline{\Psi}_\mu$, where $\overline{\Psi}_\mu$ are the decaying eigenstates of the system Hamiltonian (with radial coordinate $\rho$ of the active electron considered as parameter) that correspond to the complex eigenenergies $E_\mu(\rho,R) = \operatorname{Re} E_\mu(\rho,R) - i\Gamma_\mu(\rho,R)/2$, where $\Gamma_\mu(\rho,R)$ are the ionization rates and $R$ is the ion-surface distance.

The energy eigenvalue problem can be solved using an appropriate EEM. However, the appearance of the non-vanishing intrinsic parameter $\rho$ requires an analytic criterion for determination of the physically relevant values $\rho = \rho_0(\mu;R)$. To do this, we have developed a variation procedure for resolving $\rho_0$, which can be reduced to the following condition

$$\left.\frac{\partial \Gamma_\mu(\rho,R)}{\partial \rho}\right|_{\rho=\rho_0(\mu;R)} = 0 \ . \tag{1}$$

At a given ion-surface distance $R$, and for the given set of parabolic quantum number $\mu$, the parameter $\rho_0$ represents the radial coordinate of the region through which the decay process is the most probable. Thus, it can be expected that at large $R$, i.e., far from the decay region, the quantity $\rho_0$ is equal to the mean electron radius pertaining to the eigenstate $\Psi_{v,in}$. Therefore $\rho = \min\{\rho_0, [3n^2 - l(l+1)]/2Z\}$. The probability that incident ion will bi ionized at a given ion-surface distance (e.g. ionization probability) $P_\mu^I(R)$ is given by

$$P_\mu^I(R) = 1 - \exp\left[-\frac{1}{v}\int_R^\infty \Gamma_\mu(\rho_0(\mu;R'),R')\,dR'\right]. \tag{2}$$

## 3. RESULTS
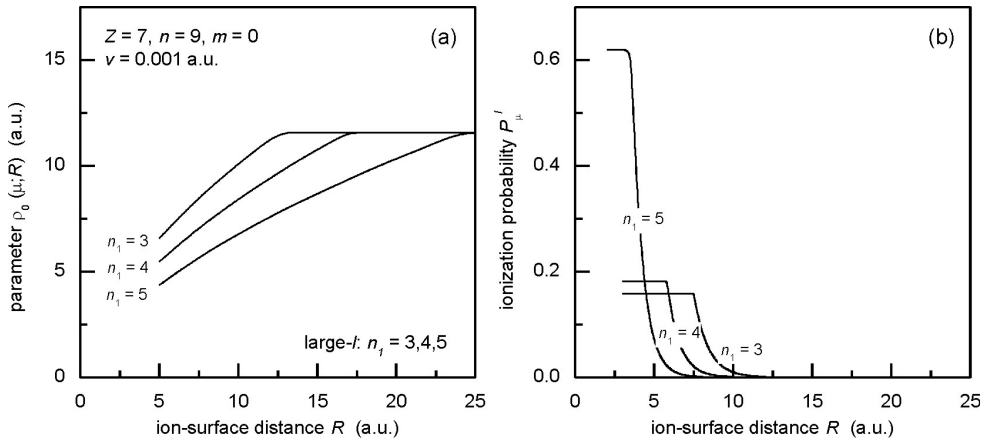


**Figure 1:** (a) Parameter $\rho_0(\mu;R)$ expressed via ion-surface distance $R$ for $Z = 7$, $n = 9$, $m = 0$, $v = 0.001$ a.u. and $n_1 = 3,4$, and 5 and (b) the corresponding ionization probabilities given by Eq. (2).

The result of the analyzed ionization dynamics of multiply charged Rydberg ions approaching metallic surface are presented in Fig. 1. Fig. 1(a) shows the values $\rho_0(\mu;R)$ as a function of ion-surface distance $R$. It can be seen that that in the decay region the variational parameter $\rho_0$ decreases with decreasing R. The analysis also shows the change in averaged radial coordinate occurs at distances of about 10 – 20 a.u. Using the $\rho_0(\mu;R)$ dependence and Eq. (2), the ionization probabilities $P_\mu^I(R)$ were calculated and presented in the Fig. 1(b). The probability curves depict typical behavior for the case of ionization of ions in the presence of the metallic surface and exhibit the decrease in the onset position with the increase of $n_1$. However, at the lower end of the investigated ion-surface separations the probabilities reach non-unity values.

This specific feature of the large-$l$ Rydberg ions indicates that there is a non-zero survival probability $P_\mu^{surv}(R) = 1 - P_\mu^I(R)$ that the intermediate states can survive in the near surface region. This effect was verified for $Z = 6,7$, and 8 and $n = 10-12$ and are presented in Fig. 2. It can be seen that the survival probability decreases with the increase in principal quantum number $n$, but increases as the charge $Z$ of the core increases. These results suggest the possibility of further investigation of charge exchange properties of the ion surface in the near surface region by use the decaying intermediate Rydberg states $\overline{\Psi}_\mu$.
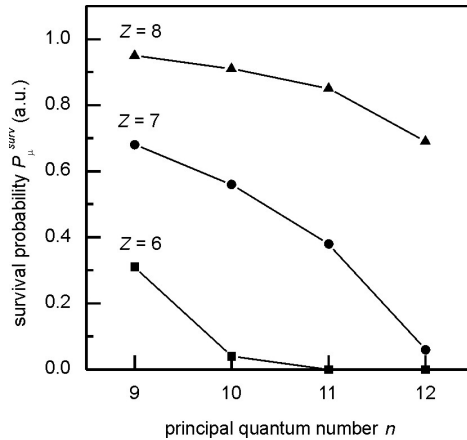


**Figure 2:** Survival probability dependence on $Z$ and $n$ for $n_1 = 5$, $m = 0$ and $v = 0.001$ a.u.

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