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THE INFLUENCE OF INITIAL VELOCITY DISTRIBUTION ON IONIZATION DYNAMICS OF RYDBERG ATOMS APPROACHING SOLID SURFACES IN THE ELECTRIC FIELD

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Abstract. We analyze the ionization dynamics of slow hydrogenlike Rydberg atoms (principal quantum number $n >> 1$) approaching solid surface in a weak electric field. The recently obtained etalon-equation method results for the simulation of experimental signal are used to investigate the influence of the initial velocity distribution. It is demonstrated that an agreement with the experimental signal can be obtained with the broadened velocity distributions.

1. INTRODUCTION

Rydberg atoms in which one electron is excited to a state of large principal quantum number n form a sensitive probe of atom-surface interactions. Because of their large physical size ($\sim n^2$ a.u.) and weak binding, even relatively far from a surface the motion of the excited electron can be strongly affected by image charge interactions, leading to the formation of the hybridized Stark-like states; Nordlander (1996). Providing that the appropriate energy conditions have been met, the ionization of Rydberg atoms preferentially occurs via tunneling of the excited electron in the vicinity of the potential barrier top into a vacant level in the surface. Recent theoretical studies based on the wave package propagation method by So et al. (2009) and the etalon equation method by Nedeljković and Nedeljković (2005) suggested that such ionization process is well localized in the atom-surface distance range of approximately 50 a.u. On the other hand, landmark experimental investigations of Dunning and co-workers; see, for example, the most recent publication by Pu et al. (2010), performed by collecting the surface-ionized xenon Rydberg atoms using a weak electric field, showed that ionization occurs over a much broader separation range.

Several possible explanations have been proposed in order to elucidate the origin of this discrepancy. First suggestion, proposed by Sjakste et al. (2006), stated that the applied electric field strongly influences the ionization process and so the ionization distance. However their analysis was performed for the system parame-

ters (applied electric field, projectile velocity) well above those used in the experiment. Wethekam et al. (2006), attributed the delocalization of the ionization process to the presence of local stray electric "patch" fields near the surface resulting from potential variations across the surface associated with surface inhomogeneities. Model calculations were undertaken assuming a simple periodic variation in potential and an over-the-barrier model showed that such patch fields might indeed account for the experimental observations. More recently, Nedeljković and Božanić (2010) presented a detailed analysis of the ionization process in the experiment based on the quantum decay model and etalon equation method (EEM). The ionization distances R_c^I (e.g. distances at which the ionization per unit time is the most probable) were obtained from the model. The projectile motion and the decay of the electron cloud have been treated simultaneously. The functional dependence between the critical velocity v_c and the applied field F was obtained. As a consequence, the estimation of the ionization distances from the experimental values of $F_{\min}$ could not performed using an arbitrary values of projectile velocity as done previously by Hill et al. (2000), but rather using the critical value v_c, characteristic for the given Rydberg state and minimal electric field. This suggests that the velocity distribution of the atoms within the impinging beam can also contribute to the observed delocalization of the experimental signal.

In this article, we use the EEM results for the simulation of experimental signal (the normalized number of the detected ions) to investigate the influence of the initial velocity distribution on the signal shape.

2. FORMULATION OF THE PROBLEM

We consider the ionization of a beam of slow hydrogenlike Rydberg atoms impinging a solid surface in a presence of a weak external electric field F (directed from the solid to the vacuum). The described model of beam ionization, corresponding to the experimental situation, is presented schematically in Fig. 1. Each trajectory stands for the representative member of the subensemble of Rydberg atoms/ions with a given initial perpendicular velocity $v_{\perp 0}$. Only the projectiles with $v_{\perp 0} < v_c(\mu, F)$, after the ionization (mainly localized at ionization distance $R_c^I(\mu, v_{\perp 0}, F)$), will be collected by the external electric field F and detected experimentally. The trajectories of these projectiles are characterized by the minimal ion-surface distance $R_{\min}$.

According to the model, the decaying Rydberg state Ψ_μ of the active electron is considered as an eigenfunction of the Hamiltonian: $\hat{H}(R)\Psi_\mu(R) = E_\mu(R)\Psi_\mu(R)$, corresponding to the complex eigenenergies $E_\mu(R) = \mathrm{Re}\, E_\mu(R) - i\Gamma_\mu(R)/2$, where $\Gamma_\mu(R)$ are the ionization rates and μ designates the set of parabolic quantum numbers (n_1, n_2, m). Eigenenergies

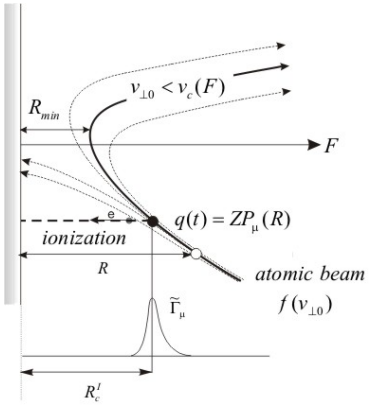

Figure 1: Decay model of ionization dynamics of the beam of atomic particles, with initial perpendicular velocity distribution $f(v_{\perp 0})$.

$E_\mu(R)$ can be obtained using the EEM without explicit calculation of the wave-functions. Details of solving the complex energy eigenvalue problem are given explicitly by Nedeljković and Nedeljković (2005). The probability $P_\mu(R; v_{\perp 0}, F)$ that the representative member of the subensemble of particles from the atomic beam with a given initial velocity is ionized at ion-surface distance R is given by

$$P_\mu(R; v_{\perp 0}, F) = 1 - \exp\left[-\int_R^\infty \frac{\Gamma_\mu(R')}{v_{\perp 0}(R')} dR' \right]. \quad (1)$$

The intermediate stages of ionization are characterized by the total ionization rates $\tilde{\Gamma}_\mu(R; v_{\perp 0}, F) = dP_\mu / dt$. The positions of maxima of the total ionization rates are the ionization distances $R_c^I(\mu, v_{\perp 0}, F)$. Note that the velocities $v_{\perp 0}$ in Eq. (1) also depend on the ionization probability, so that the iterative procedure has to be used for resolving the problem.

The experimental procedure (Wethekam et al. (2006), Pu et al. (2010)) produces a normalized number of ionized atoms as a function of the applied field F. These results can be compared with the averaged probability $\Pi_\mu(F)$ of the probability $P_\mu(R_{\min}; v_{\perp 0}, F)$ over the initial velocity distribution $f(v_{\perp 0})$. In the case of Gaussian distribution of initial velocities, we get

$$\Pi_\mu(F) = \frac{1}{2}\left[1 + erf\left(\frac{v_c(\mu, F) - \bar{v}}{\Delta} \right) \right], \quad (2)$$

where $\bar{v}$ is the mean velocity and Δ is the distribution width. The field dependence of critical velocity $v_c(\mu, F)$ is characteristic of each state μ and is explicitly given by Nedeljković and Božanić (2010).

3. RESULTS

In Fig. 2(a,b) we present the averaged probabilities $\Pi_\mu(F)$ for $n=17$ and $n=20$, respectively, for some characteristic values of the quantities $\bar{v}$ and Δ, and the corresponding experimental data.

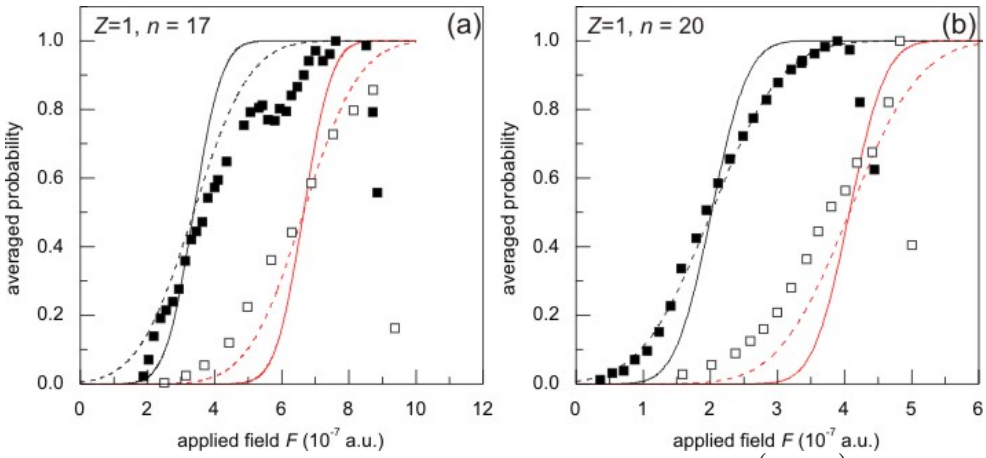

Figure 2: Averaged ionization probabilities $\Pi_\mu(F)$ for (a) H-like $(n=17)$ and (b) H-like $(n=20)$ atomic projectiles for $\bar{v}=1.4\times10^{-5}$ a.u., $\Delta=0.7\times10^{-5}$ a.u. (solid curves), $\bar{v}=1.4\times10^{-5}$, $\Delta=1.4\times10^{-5}$ a.u. (dashed curve), $\bar{v}=3.8\times10^{-5}$ a.u., $\Delta=0.7\times10^{-5}$ a.u. (shifted solid curve), and $\bar{v}=3.8\times10^{-5}$ a.u., $\Delta=1.4\times10^{-5}$ (shifted dashed curve). Available experimental data for Xe atom, for $\bar{v}=1.4\times10^{-5}$ a.u. (black squares) and $\bar{v}=3.8\times10^{-5}$ a.u. (open squares) is taken from Pu et al. (2010).

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