

SELF-CONSISTENT PROCEDURE FOR TREATMENT OF THE IONIZATION DYNAMICS OF RYDBERG ATOMS APPROACHING SOLID SURFACES IN THE ELECTRIC FIELD

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Abstract The self-consistent procedure for the analysis of the ionization dynamics of slow hydrogenlike Rydberg atoms approaching solid surface in a weak electric field has been developed. The complex energy eigenvalue problem is solved in the critical region of the ion-surface distances R using an etalon equation method. The problem of motion of a representative member of the atomic beam is resolved by including the R -dependent expression for the perpendicular velocity into the expression for the ionization probability iteratively. The results of the procedure were employed to calculate the averaged ionization probabilities which were compared to the available experimental results.

1. INTRODUCTION

The investigations of interactions between Rydberg atoms and solid metallic surfaces represent a significant challenge from both the experimental and theoretical point of view. The charge transfer processes from the atom to the surface and vice versa can be influenced by variety of parameters including electron state in the atom, direction and velocity of the core motion, or the presence of external electric and magnetic fields. Furthermore, due to weak binding between the excited electron and the atomic core, the polarization of the Rydberg electron states by the surface can occur at distances far away from the surface. This provides an opportunity to investigate the intermediate stages of the ionization process using the appropriate asymptotic methods (Nedeljković and Božanić 2010).

Recent experiments by Hill et al. (2000) give a direct insight in the intermediate stages of the ionization processes between Rydberg atoms and metallic surfaces. That is, an effort was made to determine the distances at which the ionization mostly occurs (e.g. ionization distances R_c^I) by directing a beam of slow Xe atoms to a flat metallic surface. Upon ionization, the positively charged particles were collected by an electric field and driven into a detector. The applied electric fields were sufficiently low so that it can not induce the ionization. The depen-

dence of the number of collected particles on the intensity of the electric field was determined (ion signal) and the ionization distances were estimated from the onset of the signal using a classic formula derived under assumption that ionization occurs at a specific distance. The experimental results coincided with the theoretical R_c^I values obtained directly from the etalon equation method (EEM) results, Nedeljković and Nedeljković (2005). However, latest quantum mechanical analysis by Nedeljković and Božanić (2010) of the ionization process in the experiments implied that the influences of image acceleration and the electric field on core motion must be included in a self-consistent manner. The precise treatment of the core motion, with perpendicular velocity $v_{\perp}(R)$, of the decaying projectile (which decays with the ionization probability $P_{\mu}(R; v_{\perp 0}, F)$) is of particular importance for the theoretical treatment of the signal.

In this article, we present the iteration procedure for the determination of core motion and ionization probabilities of Rydberg atoms approaching solid surfaces in the presence of a weak electric field. The results of the analysis are employed to elucidate the novel experimental finding by Pu *et al.* (2010).

2. SIMULTANEOUS TREATMENT OF THE IONIZATION AND THE PROJECTILE MOTION

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 complex eigenenergies $E_{\mu}(R) = \text{Re} E_{\mu}(R) - i\Gamma_{\mu}(R)/2$ of the system Hamilton (that includes the possibility of a decay of atomic projectile) can be obtained using the appropriate EEM. The quantities $E_{\mu}(R)$ can be obtained without the explicit calculation of the intermediate eigenfunctions Ψ_{μ} of the active electron (μ designates the set of parabolic quantum numbers (n_1, n_2, m)). From the ionization rates $\Gamma_{\mu}(R)$, the ionization probabilities can be calculated using the relation

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

where $v_{\perp 0}$ stands for initial perpendicular velocity and F is the applied electric field. It can be seen that the probability $P_{\mu}(R; v_{\perp 0}, F)$ depends on the ionic motion via perpendicular velocity $v_{\perp}(R)$. However, at the same time the motion of the atomic projectile depends on the ionization probability via the charge $q = q(t) = ZP_{\mu}(R)$. The charge q decay moving toward the surface in the external electric field F , under the classical image acceleration opposite to the effect of the external electric field.

Therefore, in order to determine the core motion $v_{\perp}(R)$, a kind of self-consistent procedure is necessary. The problem can be resolved by including the R -dependent expression for the perpendicular velocity into the expression for the ionization probability iteratively. That is, in the i^{th} iterative step ($i = 0, 1, 2, \dots$) we assume that

$$P_{\mu}^{(i)}(R; v_{\perp 0}, F) = 1 - \exp \left[- \int_R^{\infty} \frac{\Gamma_{\mu}(R')}{v_{\perp}^{(i)}(R')} dR' \right], \quad (2)$$

where, for $i = 1, 2, \dots$,

$$v_{\perp}^{(i)2}(R) = v_{\perp 0}^2 - \frac{2FZ}{M} \int_R^{\infty} P_{\mu}^{(i-1)}(R') dR' + \frac{Z^2}{2M} \int_R^{\infty} \frac{P_{\mu}^{(i-1)2}(R')}{R^2} dR', \quad (3)$$

and, for $i = 0$, $v_{\perp}^{(0)} = v_{\perp 0}$. An important fact concerning the motion of the core is that there exists a critical field value F_c for which $v_{\perp}(R) = 0$. An example of the obtained $v_{\perp}(R)$ dependence (for $i = 2$) that describes the behavior of the curves for three different values of the electric field is given in the Fig. 1.

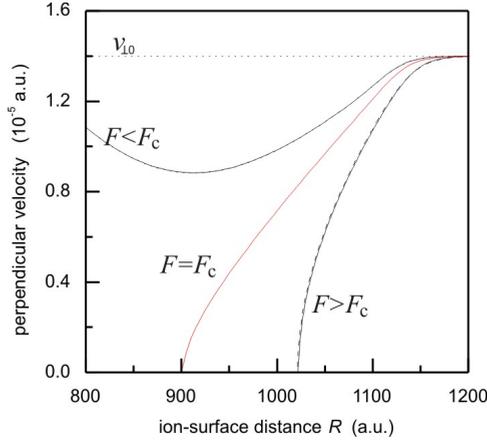


Figure 1: An example of $v_{\perp}^{(i=2)}(R)$ dependance for $Z = 1$, $n = 17$, $v_{\perp 0} = 1.4 \times 10^{-5}$ a.u., and for three typical values of the electric field F .

The F_c values change with the change in the initial velocity of the projectiles. The corresponding $v_c(\mu, F)$ dependencies are presented in Fig. 2(a). These values are crucial for the comparison of our results to the ion signal obtained experimentally. In our approach, the experimental signal can be simulated by the field dependent averaged probability $\Pi_{\mu}(F)$ given by

$$\Pi_{\mu}(F) = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{v_c(\mu, F) - \bar{v}}{\Delta} \right) \right], \quad (4)$$

where \bar{v} and Δ are the experimental values of mean and width of the Gaussian velocity distribution, Wethekam *et al.* (2006).

3. RESULTS

In Fig. 2(b) we present the averaged probabilities $\Pi_\mu(F)$ for $n = 26$, $n = 31$, and $n = 36$, for the values of the quantities \bar{v} and Δ characteristic for the available experimental data.

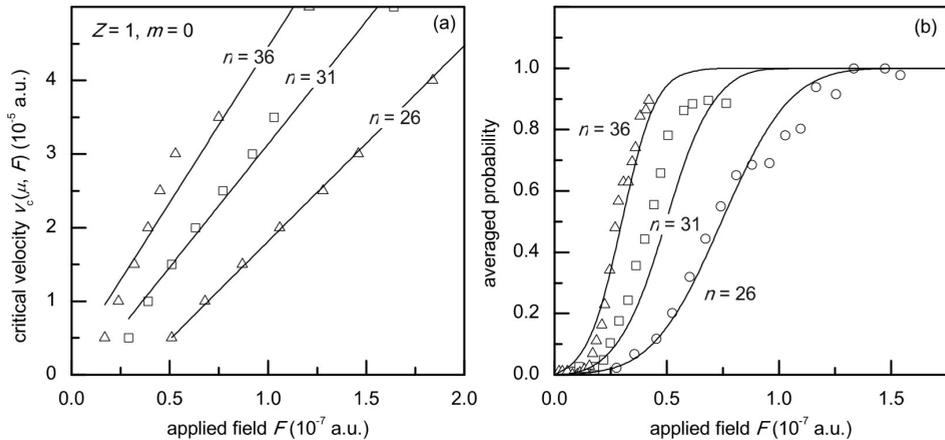


Figure 2: (a) Critical velocity $v_c(\mu, F)$ via applied electric field F . (b) Averaged ionization probabilities $\Pi_\mu(F)$ for $H(n = 26)$, $H(n = 31)$, and $H(n = 36)$ atomic projectiles for $\bar{v} = 1.4 \times 10^{-5}$ a.u., $\Delta = 0.7 \times 10^{-5}$ a.u. (solid line). Available experimental data (symbols) obtained for Xe atoms are taken from Pu *et al.* (2010).

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