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THE EFFECT OF CORE POLARIZATION ON THE POPULATION OF THE RYDBERG STATES OF ArVIII IONS ESCAPING SOLID SURFACES

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Abstract. The appearance of maxima at $n_A = n_{\max}$ in the population distributions for the Rydberg states of multiply charged ions ArVIII escaping solid surfaces at intermediate velocities ($v \approx 1$ a.u.) is discussed. Within the framework of the time-symmetrized two-state vector model, in which the state of a single active electron is described by two wave functions Ψ_1 and Ψ_2, the regular maxima appear as a consequence of the electron tunneling through the potential barrier created between the ionic core and the polarized solid. The pronounced peaks (resonances) in the population distributions are addressed to the electron tunneling in the vicinity of the potential barrier top. The appropriate etalon equation method is used in the calculation of the function Ψ_1; the effect of core polarization is expressed via the function Ψ_2.

1. INTRODUCTION

Considering the final population of the Rydberg states ($n_A >> 1$) of multiply charged ions interacting with solid surfaces, one can recognize the Rydberg states with principal quantum number $n_A = n_{\max}$ that are dominantly populated in the process. Classically, these Rydberg states are populated over-the-barrier (COB model), from the Fermi level of the solid; Burgdörfer (1993). The quantum mechanical analysis yields somewhat different picture of the population process. Within the framework of two-state vector model (TVM), Nedeljković et al. (1994), Nedeljković et al. (1998), in the intermediate velocity case, the Rydberg states are populated through the non-resonant electron pickup from the foil conducting band. In the population distribution for the ArVIII ion, the regular population maxima at $n_A = n_{\max} \approx 8$ are accompanied by the pronounced maxima at $n_A = n_{\max} \approx 11$ (resonances).

We recall that, according to the TVM, the state of a single electron of the ion-surface system is described by two state vectors $|\Psi_1(t)\rangle$ and $|\Psi_2(t)\rangle$. The first state evolves toward the future (first scenario) from the initial parabolic state $|\mu_M\rangle$, corresponding to the electron localized in the solid at the time $t = t_{in}$; the second state evolves "teleologically" (second scenario) towards the fixed final state $|\nu_A\rangle$ at the time $t = t_{fin}$. The population mechanism is simultaneously governed by the functions $|\Psi_1(t)\rangle$ and $|\Psi_2(t)\rangle$: from the standpoint of the fist scenario, the regular population is via the deep subbarrier electron tunneling, while the resonant Rydberg states are mainly populated in the vicinity of the potential barrier top. The both population mechanisms can be treated by the TVM if the appropriate etalon equation method (EEM), with two different scaling parameters α, is used for the calculation of the function Ψ_1; Nedeljković et al. (1998).

Recently, it was demonstrated that the polarization of the ionic core could play an important role in the regular population mechanism; Nedeljković et al. (2009). The aim of the present work is to analyze the effect of core polarization (expressed via the function Ψ_2) on the resonances in the final population distributions of the ions ArVIII escaping solid surface at intermediate velocity.

2. POPULATION DYNAMICS -TVM

The final TVM-population probability $P_{\nu_A}^{fin}$, where $\nu_A = (n_A, l_A, m_A)$ is the set of the final spherical quantum numbers, can be expressed by the appropriate multichannel expression, in which the transition probabilities $T_{\nu'_A}^{fin}$ into different Rydberg states ν'_A are combined, Nedeljković et al. 1998

Using the model, together with the mixed flux concept, first we obtain the analytical expressions for the intermediate transition probabilities per unit γ_M, $T_{\mu_M \nu_A}(t)$, and the transition probability $T_{\nu_A}(t) = \int \sum T_{\mu_M, \nu_A}(t) d\gamma_M$, which represents a "sum" over the initial parabolic quantum numbers $\mu_M = (\gamma_M, n_{1M}, m_M)$. The final expressions for the quantities $T_{\nu_A}^{fin}$ we obtain in the limit $t \to t_{fin}$. We point out that in the non-resonant TVM, the overall conduction band of the solid participate in the population process, i.e., the energy parameter $\gamma_M \in [\gamma_\phi, \gamma_{U_0}]$, where $\phi = \gamma_\phi^{\;2}/2$ and $U_0 = \gamma_{U_0}^{\;2}/2$ are the solid work function and the depth of the solid potential well (in the Sommerfeld model).

The following physical picture of the population of the Rydberg state $|\nu_A\rangle$ emerges from the analysis of the present paper. The states with lower n_A are mainly populated from the bottom of the solid conduction band via the deep subbarrier tunneling (scaling parameter $\alpha \to \infty$; one-large-parameter asymptotic for the function Ψ_1); the states with larger n_A are mainly populated from the Fermi level via the electron transitions in the vicinity of the potential barrier top (scaling parameter $\alpha \approx 1$; two-large-parameter asymptotic); the population is selective with maxima at $n_A = n_{\max}$. In our quantum model, the values $n_{\max}$ for both the regular and the resonant population mechanisms depend on Z and ϕ (as in the COB model), but also on the quantities U_0, v, and l_A, as well as on the state of polarization of the ionic core.

3. RESULTS

In Fig. 1(a,b) we present (full curves) the final transition probabilities $T_{\nu_A}^{fin}$ and the population probabilities $P_{\nu_A}^{fin}$ for the ion ArVIII with core charge $Z = 8$ escaping the conducting solid surface. Dashed curves are the final probabilities obtained in the absence of core polarization, i.e., in the point-like core approximation. Solid circles in Fig. 1(a) are the properly normalized beam-foil experimental results, Bashkin et al. (1982).

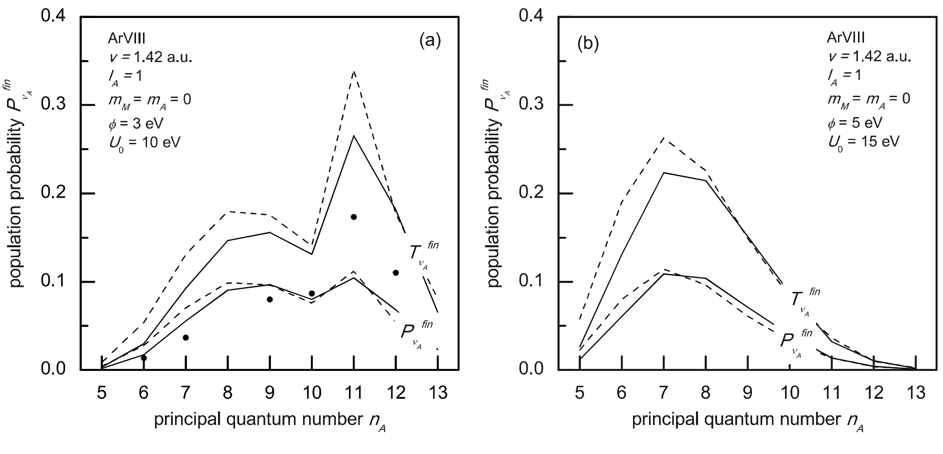

Figure 1: Final probabilities $T_{\nu_A}^{fin}$ and $P_{\nu_A}^{fin}$ for the ArVIII ion escaping solid surface at velocity $v = 1.42$ a.u. via principal quantum numbers n_A, for (a) the surface (type I) with $\phi = 3$ eV and $U_0 = 10$ eV and (b) the surface (type II) with $\phi = 5$ eV and $U_0 = 15$ eV. Dashed curves correspond to the point-like cores. Solid circles in (a) are the beam-foil experimental results, Bashkin et al. (1982).

In Figs. 1(a) and 1(b) we analyze the final population distributions for two type of solid surfaces, with different values of the parameters ϕ and U_0; surfaces of the type I and the type II, respectively. Considering the surface of the type I, for $n_A \in [5,10]$, we obtain the same final population probabilities as those obtained recently by Nedeljković et al. (2009), with the population maxima at $n_{\max} = 9$ for the polarized core (solid line), and at $n_{\max} = 8$ if the polarization is neglected (dashed curve). In the considered case the resonance appears at $n_{\max} = 11$. The final population probabilities with the polarization included are smaller in comparison to the probabilities in the point-like core approximation (compare the solid and the dashed curves in Fig. 1(a)). The obtained final probabilities are in qualitative agreement with the experimental results, Bashkin et al. (1982). We expect that the more accurate multichannel expression for the final population probability $P_{\nu_A}^{fin}$ will be in a better agreement with the experimental findings.

The final population distribution for the surface with larger ϕ (type II) presented in Fig. 1(b) are different in comparison to the distributions obtained in the case of the surface of the type I. The population maxima are located at $n_{\max} = 7$, for both the polarized and the nonpolarized cores, without resonances in the large-n_A region.

From Figs. 1(a,b) we recognize that the electron transitions in the vicinity of the potential barrier top induce the pronounced maxima in the final population distribution for ArVIII ion, for the surfaces with lower values of the work function ϕ (contaminated surfaces, effectively included image states effect, etc.). We point out that the core polarization distinguishes the ions ArVIII, KrVIII, and XeVIII (all with core charges $Z = 8$). Our preliminary analysis show that the population probabilities for KrVIII and XeVIII ions are significantly lower in comparison to the probabilities for ArVIII ion presented in Fig. 1. The population of KrVIII ion also exhibits the resonance at $n_{\max} = 11$, but less pronounced than for the ArVIII ion. The population distribution for XeVIII ion is characterized by only one maximum at $n_{\max} = 10$.

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