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Resonances in the final Rydberg state population of multiply charged ions ArVIII, KrVIII, and XeVIII escaping solid surfaces

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The appearance of resonances (pronounced maxima at $n_A = n_{res}$) in the probability distributions for the population of the Rydberg state (n_A, l_A, m_A) of multiply charged ions ($Z \gg 1$) 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 resonances are explained by means of an electron tunneling in the very vicinity of the ion–surface potential barrier top. To include this specific feature of electron transitions into the model, the appropriate etalon equation method is used in the calculation of the function Ψ_1. We consider the ions ArVIII, KrVIII, and XeVIII with the same core charges $Z = 8$ a.u., but with different core polarizations. The effect of the ionic core polarization is associated with the function Ψ_2. The population probabilities for $n_A \approx n_{res}$ are complemental to those obtained recently for $n_A < n_{res}$, and in sufficiently good agreement with available beam-foil experimental data. The pronounced resonances in the final population distributions are recognized only in the case of ArVIII ion and for the lower values of the solid work function (argon anomaly).

1. Introduction

Considering the population of the Rydberg states ($n_A \gg 1$) of multiply charged ions ($Z \gg 1$) interacting with solid surfaces, two aspects of the process can be considered. The first aspect is devoted to the intermediate stages of the population dynamics. These stages are characterized by the neutralization rates and the neutralization distances R_c^N. The final population probabilities represent an another important aspect of the process; namely, from the population distributions one can recognize the Rydberg states $|\nu_A\rangle = |n_A, l_A, m_A\rangle$, with principal quantum number n_A and angular momentum quantum number l_A, that are dominantly populated. The both aspects of the population process have been considered in the last twenty years [1–3], and still represent an open theoretical problem [4–6].

The population of the Rydberg states of multiply charged ions has been recognized under different geometrical conditions: in the beam-foil experiments [7–10], for the ions traversing through the microcapillary foils [11], and in the scattering (grazing incidence) geometry [2]. The basic population mechanism can be rather different for these different geometries and for different projectile velocities. The present paper is mainly devoted to the beam-foil (normal emergence) geometry and the intermediate projectile velocities ($v \approx 1$ a.u.). In the corresponding experiments the final (relative) population probabilities of the Rydberg ions CIV, NV, OVI [7], ArVIII, KrVIII [8], XeVIII [9], SVI, and ClVII [10] interacting with carbon foil have been measured by the methods of optical spectroscopy. We point out that the recent experimental data are for the Rydberg ions ArVII and ArVIII interacting with the microcapillary foil [11], for the large-l_A Rydberg states.

The beam-foil experimental data have been analyzed theoretically within the framework of the time-symmetrized two-state vector model (TVM), both for lower values of l_A [12,13], and in the large-l_A case [14]. It was assumed that the Rydberg states $|\nu_A\rangle$ are populated through the non-resonant electron pickup from the foil conducting band, in the outgoing part of the ionic trajectory. This assumption was originally based on the idea [7–9] that Rydberg states $|\nu_A\rangle$ with geometrically large size cannot exist inside the foil. That is, the mean radius $\langle r_{n_A l_A}\rangle$ of the considered Rydberg states is large in comparison with mean distances between foil atoms. Using a dynamical threshold estimation for existence of excited electronic states in sold [15], we also conclude that in the intermediate velocity case the considered Rydberg states cannot be formed in the solid. The overall qualitative agreement of the TVM results [12–14] with the available beam-foil experiments (for different ions and for both the low-l_A and the large-l_A Rydberg states with $n_A \approx Z$) support the assumption that the electron capture from the foil along the outgoing part of the ionic trajectory is the basic population mechanism. Moreover, the considered Rydberg states are formed preferably at sufficiently large ion–surface distances R where stable “orbits” of captured electrons are possible. We note that the bulk effect become relevant for the multiply charged ions traversing thin foils at high velocities ($v \gg 1$ a.u.) [16].

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In all cited TVM studies, the ionic cores have been considered as a point-like one. A more general TVM analysis in the intermediate velocity region, with the ion core polarization effectively taken into account, is given in Ref. [6]. Differences in the population distributions for the ions with the same core charges Z, but with different core polarizations, have been recognized; see, for example, the probability curves for the sodium-like ArVIII, copper-like KrVIII, and silver-like XeVIII [6]. The positions of maxima of the population distributions ($n_A \approx n_0$) obtained in Ref. [6] are shifted toward larger n_A due to the core polarization; also, the core polarization systematically suppressed the final population probabilities comparing to the pointlike core approximation. The results obtained in the cited reference [6] correspond to the Rydberg states with $n_A \in \mathcal{N}$, for which the subbarrier tunneling population mechanism was assumed.

The aim of the present work is to analyze the population curves in the vicinity of the resonant quantum numbers $n_{res} > n_0$, i.e., for $n_A \in \mathcal{N}_r$, where the set $\mathcal{N}_r$ is complemental to the set $\mathcal{N}$ considered in Ref. [6]. We are looking for the existence of an extra pronounced maximum (resonance) in the final population distribution at $n_A = n_{res}$. Such a situation has been experimentally recognized for the ArVIII ions, for $n_A = n_{res} = 11$ and $l_A = 1$ and 2 [8]. The corresponding experimental situation has been previously addressed as argon anomaly [13], and explained within the TVM-study [13]. The model predicted well the positions and the shapes of resonances in the population distribution, but the results were the same for ArVIII, KrVIII, and XeVIII ions, because of the pointlike core approximation. In the present article we consider the resonances using the Simons–Bloch potential [18] for a more realistic description of the electron capture into the field of closed-shall ions [6]. It is an intriguing question whether the resonances are characteristic only for the ArVIII ion, or they also appear in the case of KrVIII and XeVIII ions.

According to the TVM, the state of a single active 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 from the initial parabolic state $|\mu_M\rangle = |\gamma_{M0}, n_{1M}, m_M\rangle$ toward the future, while the second state evolves "teleologically" toward the fixed final state $|\nu_A\rangle = |n_A, l_A, m_A\rangle$, within the first and the second scenario, respectively. The initial state (at the time $t = t_{in}$) describes the electron mainly localized in the solid, with energy $-\gamma_{M0}^2/2$, while the final state (at the time $t = t_{fin}$) describes the electron bounded to the ion. During the time interval $t \in [t_{in}, t_{fin}]$, the electron can be captured from the solid surface into the Rydberg state of the moving ion with the intermediate transition probability per unit γ_M, $T_{\mu_M,\nu_A}(t)$ (probability density). For the nonresonant electron transitions the overall conduction band of the solid participate in the process, so that the transition probability $T_{\nu_A}(t)$ represents an integral over the energy parameter γ_{M0} and a sum over the n_{1M} and m_M.

In the case $n_A \in \mathcal{N}_r$, i.e., for $n_A \approx n_{res}$, it is necessary to adapt the wave function Ψ_1 for the electron transitions in the very vicinity of the potential barrier top. The function Ψ_1 will be calculated within the framework of the etalon equation method (EEM) of solving the effective one-dimensional energy eigenvalue problem corresponding to the close turning point configuration [13]. The appropriate EEM contains the scaling parameter α, as a measure of the distance between the turning points. With the adapted function Ψ_1 and the core polarization included in the TVM via the function Ψ_2, we obtain the final transition probabilities T_{μ_M,ν_A}^{fin} and $T_{\nu_A}^{fin}$ (at the final time $t = t_{fin}$) for $n_A \in \mathcal{N}_r$. The final population probability $P_{\nu_A}^{fin}$ can be expressed via the appropriate multichannel expression [13], in which all the background states $n'_A \in \mathcal{N}$ and $n'_A \in \mathcal{N}_r$, $n'_A \neq n_A$, are taken into account. In the limit $\alpha \to \infty$, the TVM predictions of the present article overcome to the predictions valid for $n_A \in \mathcal{N}$, considered previously in Ref. [6].

The following physical picture of the population dynamics of the ions ArVIII, KrVIII, and XeVIII follows from the TVM analysis of the present paper. The regular population of the states $n_A \in \mathcal{N}$ is mainly via the non-resonant electron tunneling mechanism, with population maxima at $n_A = n_0$, where the values n_0 are different for the ions ArVIII, KrVIII and XeVIII and for different solid work functions. For some combination of the ion–surface parameters an additional population of the resonant states $n_A \in \mathcal{N}_r$ occurs. These states are populated in the vicinity of the potential barrier top (within the first scenario of the TVM) and mainly from the Fermi level. The values n_{res} for the ions ArVIII, KrVIII, and XeVIII, for the given solid work function ϕ, are arranged around the classical overbarrier (COB) model values n_c^{class} [17] because the population mechanism of the level n_{res} is close to be of the over-barrier resonant type. The extra pronounced maxima for $n_A = n_{res} \in \mathcal{N}_r$ in the final population distributions are obtained only in the case of ArVIII for $l_A = 1$ and 2, and for lower values of ϕ, e.g., for $\phi = 3$ eV ($n_{res} = 11$), in agreement with the argon anomaly recognized experimentally [8]. With increasing ϕ, the extra maximum in the population of the ArVIII ion decreases, so that, for $\phi = 5$ eV, the Rydberg levels $n_A = n_0$ and $n_A = n_{res}$ are populated with equal probabilities. For $\phi = 3$ eV, the population curve for KrVIII has two maxima of the same magnitude at $n_A = n_0 = 9$ and $n_A = n_{res} = 12$, and the population distribution for XeVIII has only one maximum at $n_A = n_0 = 10$. Due to presence of the other open background channels, the distributions are also changed, and the resonances become less pronounced and disappear in some cases.

This article is organized as follows. In Section 2 some aspects of the TVM characteristic for the appearance of the resonances in the final population probability distributions are presented. In Section 3 we derive the expressions for the mixed flux, and the quantities T_{μ_M,ν_A}^{fin}, $T_{\nu_A}^{fin}$ and $P_{\nu_A}^{fin}$. In Section 4 we present the results, considering the population of the Rydberg levels of the ArVIII, KrVIII, and XeVIII ions (with $Z = 8$) escaping the solid surface at velocity $v = 1.42$ a.u., for the two types of the surfaces ($\phi = 3$, $U_0 = 10$ and $\phi = 5$, $U_0 = 15$; in eV). The final population probabilities for $n_A \in \mathcal{N}$ and $n_A \in \mathcal{N}_r$, for the ArVIII, KrVIII, and XeVIII ions, are calculated and compared with the available beam-foil experimental data [8,10]. The concluding remarks are given in Section 5.

Atomic units ($e^2 = \hbar = m_e = 1$) will be used throughout the paper unless indicated otherwise.

2. Formulation of the problem

2.1. The TVM of the resonances

We consider the TVM of the non-resonant electron capture into the low-l_A Rydberg state $|\nu_A\rangle$ with $n_A \in \mathcal{N}_r$ of multiply charged ions (core charge Z) escaping a surface of the semi-infinite polarized conducting solid along the z axis perpendicular to the surface, Fig. 1. In this range of principal quantum numbers a pronounced maximum (observable resonance) in the final population distribution is expected, for the resonant quantum number $n_A = n_{res}$. Restricting ourselves to the case of the intermediate projectile velocities $v = dR/dt \approx 1$ a.u., where $R = vt$ is the instant ion–surface distance, we assume that the ionic core is polarized due to the internal electronic

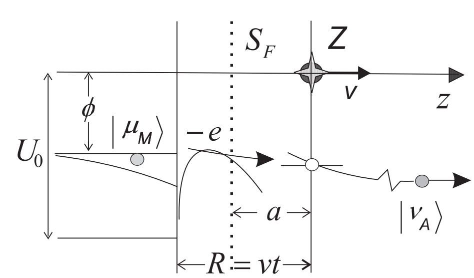

Fig. 1. The TVM-scheme of the population of the Rydberg state $|\nu_A\rangle$ for $n_A \in \mathcal{N}_r$. The initial state $|\mu_M\rangle$ describes the electron mainly localized in the solid.