

# Neutralization in Quantum Teleology of the Ion-Surface Interaction

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**Abstract.** The total neutralization rates of the multiply charged Rydberg ions escaping solid surfaces are obtained within the framework of teleological (two-state) model (QTM). These rates are characterized by set of parabolic quantum numbers  $\mu_M$  of the electron initially localized in the solid and the spherical quantum numbers  $v_A$  of the electrons finally detected in the ions.

**Keywords:** Ion, neutralization, surface, quantum teleology

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## QUANTUM TELEOLOGICAL MODEL (QTM)

In the last two decades several theoretical methods were developed, which can be principally used for an investigation of the neutralization of one-electron multiply charged Rydberg ions. The proposed methods are very heterogenous in nature; here we mention the classical over-barrier (COB) method [1, 2], and its extended dynamic version [3, 4], perturbation method [5], coupled angular mode (CAM) method [6, 7], complex scaling method (CSM) [8, 9, 10, 11], stabilization method [12, 13], time dependent close-coupling technique [14, 15], and quantum teleological model (QTM) [16, 17] in combination with the etalon equation method (EEM) [18, 19, 20].

In the present paper we apply the QTM to obtain the total neutralization rates of multiply charged Rydberg ions. Within the framework of the teleological model the state of a single electron is described by two state vectors  $|\Psi_1(t)\rangle$  and  $|\Psi_2(t)\rangle$ . The first state evolves (in the first scenario) from the initial state  $|\Psi_1(t_{in})\rangle = |\mu_M\rangle$  towards the future:

$$|\Psi_1(t)\rangle = \hat{U}_1(t_{in}, t) |\Psi_1(t_{in})\rangle. \quad (1)$$

The second state  $|\Psi_2(t)\rangle$  evolves "teleologically" (in the second scenario) towards the fixed final state  $|\Psi_2(t_{fin})\rangle = |v_A\rangle$  postselected in the final time  $t = t_{fin}$ , according to the law

$$|\Psi_2(t)\rangle = \hat{U}_2(t_{fin}, t) |\Psi_2(t_{fin})\rangle. \quad (2)$$

QTM represents a time symmetrized description of the intermediate stages of the process. Namely, the results of any measurements performed in the time  $t \in (t_{in}, t_{fin})$  depend on both the initial and final quantum conditions <sup>1</sup>.

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<sup>1</sup> The time symmetrized quantum mechanic which is the base of QTM was introduced by Aharonov et al [21].

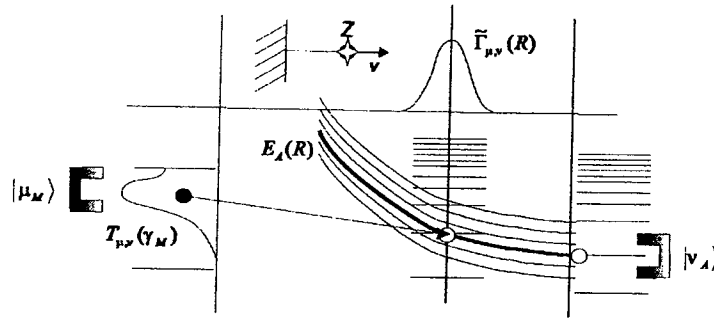


FIGURE 1. Quantum teleology of neutralization, schematically

## NEUTRALIZATION IN THE QTM

We consider the neutralization of multiply charged Rydberg ions escaping the solid surface with velocity  $v = dR/dt$ , where  $R$  is the instant ion-surface distance. We assume that the teleological conditions are satisfied, i.e., the system is preselected in the parabolic state  $|\mu_M\rangle$ , where  $\mu_M = (\gamma_M, n_{1M}, m_M)$  and postselected in the spherical state  $|\nu_A\rangle$ , where  $\nu_A = (n_A, l_A, m_A)$ , and calculate the intermediate probabilities and rates, for the neutralization process, see Fig. 1.

In order to control intermediate stages of the neutralization, we define the teleological transition amplitude

$$A_{\mu,\nu}(t) = \langle \Psi_2(t) | \hat{P}_2(t) | \Psi_1(t) \rangle, \quad (3)$$

where  $\hat{P}_2(t) = \int_{V_2} |\vec{r}_A\rangle \langle \vec{r}_A| dV$  is the projecting operator onto the ionic region  $V_2$ . Intermediate neutralization probability is defined as an integral over the solid conduction band energy parameter  $\gamma_M$  of the quantity  $T_{\mu,\nu}(t) = |A_{\mu,\nu}(t)|^2$ :

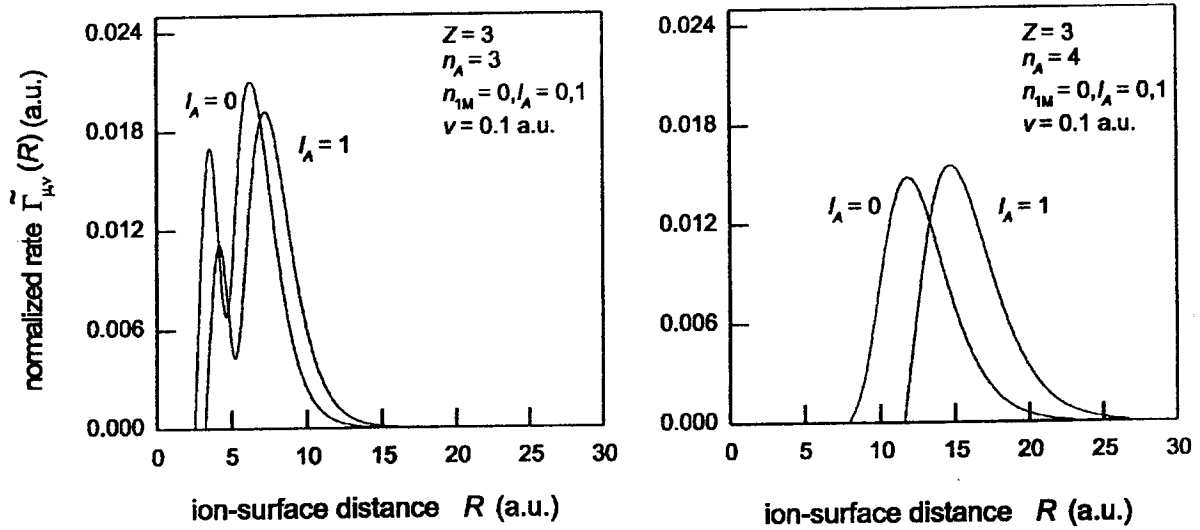
$$P_{\mu,\nu}(R) = \int T_{\mu,\nu}(t) d\gamma_M. \quad (4)$$

Probability  $T_{\mu,\nu}$  can be expressed via mixed flux  $I_{\mu,\nu}(t)$  through the surface  $S_2(t)$  containing the ion, which in parts consists of the Firsov plane  $S_F$  positioned between the ion and the surface, i.e., we get  $T_{\mu,\nu}(t) = \left| \int_{t_{in}}^t I_{\mu,\nu}(t) dt \right|^2$ , where

$$I_{\mu,\nu}(t) = - \oint_{S_2(t)} \left( \vec{j}_{12} - \rho_{12} \vec{u} \right) \cdot d\vec{S}, \quad (5)$$

whereas  $\vec{u}$  is the velocity of the surface element  $d\vec{S}$ . We see that the mixed flux is determined by the two-amplitude  $\rho_{12}(\vec{r}, t) = \Psi_1(\vec{r}, t) \Psi_2^*(\vec{r}, t)$  and the two-current density  $\vec{j}_{12} = (\Psi_2^* \nabla \Psi_1 - \Psi_1 \nabla \Psi_2^*) / (2i)$ . Moreover, the neutralization dynamics is completely determined by the behaviors of these quantities exclusively on the Firsov plane  $S_F$ , i.e., in the region of the negligible ion-surface interaction.

The neutralization of multiply charged Rydberg ions occurs at large ion-surface distances  $R$ . Therefore it is possible to apply appropriate asymptotic methods. In the present paper we use the JWKB method to obtain the wave function  $\Psi_1(\vec{r}, t)$  analytically continued from the solid region to the vicinity of the Firsov plane. The function  $\Psi_2(\vec{r}, t)$  on



**FIGURE 2.** Normalized neutralization rates  $\tilde{\Gamma}_{\mu,\nu}(R)/P_{\mu,\nu}$  of the  $C^{3+}$  ion ( $Z=3$ ) in the Rydberg states  $n_A=3,4$  escaping the Al-surface with velocity  $v=0.1$  a.u. We consider the case  $m_M=m_A=0$ ,  $n_{1M}=0$  and  $l_A=0,1$ .

the  $S_F$  plane represents the second component of the twostate, for the active electron in the field of screened Coulomb potential and polarized solid.

## TOTAL NEUTRALIZATION RATES

Within the framework of QTM, we get

$$P_{\mu,\nu}(R) \approx \left| 1 - \left( \frac{R}{R_{in}} \right)^{\frac{Z}{\tilde{\gamma}_A} - \frac{1}{2} + \frac{1}{4\gamma_M}} e^{-(\gamma_M + (\tilde{\gamma}_A - \gamma_M)g - i\frac{w}{v})(R - R_{in})} \right|^2 P_{\mu,\nu}, \quad (6)$$

where  $P_{\mu,\nu}$  is the final neutralization probability, and  $\gamma_M$  and  $\tilde{\gamma}_A$  are the energy parameters of the first and second scenarios, respectively. The quantity  $w$  in Eq. (6) is defined by  $w = (\gamma_M^2 - \tilde{\gamma}_A^2)/2 - v^2(1 - 2g)/2$ , where  $g = a/R$ , whereas  $a$  represents the position of the Firsov plane  $S_F$  with respect to the ion. The parameter  $g$  follows from the variational requirement  $\delta \tilde{P}_{\mu,\nu}(R)/\delta g = 0$ , where  $\tilde{P}_{\mu,\nu}(R) = P_{\mu,\nu}(R)/P_{\mu,\nu}$  is the normalized (teleological) probability. We get  $g \approx (1 + (\tilde{\gamma}_A^2 - \gamma_M^2)/v^2)/2$ . For  $v < 1$ , the last expression can be applied only in combination with the condition  $\tilde{\gamma}_A \approx \gamma_M$ . For the energy parameter  $\tilde{\gamma}_A$  we take the experimentally obtained values  $\gamma_{A0}$  (from the energy spectra of the considered ion) shifted due to the image forces:  $\tilde{\gamma}_A \approx \sqrt{\gamma_{A0}^2 - (2Z - 1)/(2R)}$ . By  $\gamma_{max}$  we denoted the energy parameter  $\gamma_M$  for which the probability  $T_{\mu,\nu}$  is maximal. In the quasi-resonant approximation we have  $\gamma_{max} \approx \tilde{\gamma}_A$ .

The total neutralization rate is defined as a first derivative with respect to time of the intermediate probability  $P_{\mu,\nu}(R)$ , i.e., we have

$$\tilde{\Gamma}_{\mu,\nu}(R) = 2vf \left\{ \left( \frac{\alpha}{R} - \beta \right) \left[ f - \cos \left( \frac{w}{v}(R - R_{in}) \right) \right] + \frac{w}{v} \sin \left( \frac{w}{v}(R - R_{in}) \right) \right\} P_{\mu,\nu}, \quad (7)$$

where  $f(R) = (R/R_{in})^\alpha \exp(-\beta(R - R_{in}))$ , whereas  $\alpha = Z/\tilde{\gamma}_A - 1/2 + 1/(4\gamma_M)$  and  $\beta = \gamma_M + (\tilde{\gamma}_A - \gamma_M)g$ . By  $R_{in} = (2Z - 1)/(2(\gamma_{A0}^2 - 2\phi))$ , where  $\phi$  is the solid work function, we denoted the minimal distance from the surface at which the neutralization is energetically possible.

In Fig. 2 we present the normalized total neutralization rates  $\tilde{\Gamma}_{\mu,\nu}(R)/P_{\mu,\nu}$  considering the combination of the first parabolic quantum number  $n_{1M} = 0$  and the spherical quantum numbers  $l_A = 0, 1$ , for the partial neutralization of  $C^{3+}$ -ion at Al-surface. We assume that the quasi-resonant conditions are satisfied for the ionic velocity  $v = 0.1$  a.u., discussed in Fig. 2.

The maxima of the presented rates determine the neutralization distances  $R_c^N$  (ion-surface distances at which the neutralization is mainly localized). With increasing of  $n_A$  we obtain the expected increasing of  $R_c^N$  values (scaled as  $n_A^2/Z$ ). The  $R_c^N$  values for  $l_A = 0$  are less than the values of  $R_c^N$  for  $l_A = 1$ . This behavior is a consequence of the inequality  $\gamma_{A0}(l_A = 0) > \gamma_{A0}(l_A = 1)$ . We point out that the influence of the first parabolic quantum number  $n_{1M}$  is pronounced only in the case of intermediate velocities ( $v \approx 1$  a.u.), when the quasi-resonant approximation is not valid. In that case, instead of  $\gamma_{max} = \tilde{\gamma}_A$ , we obtain the  $n_{1M}$ -dependent value.

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