Rydberg Quasimolecules Consisting of a He-like Ion and a Fully-Stripped Ion: Classical Description of Crossings of Energy Terms and of Charge Exchange

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ABSTRACT: In year 2000 one of us published papers [1, 2] presenting a purely classical description of energy terms of Rydberg quasimolecules consisting of one electron and two fully-stripped ions of charges Z and Z', where $Z' \neq Z$. The analysis of the crossings of the energy terms led to a classical description of charge exchange either between a hydrogen-like ion of the nuclear charge Z with a fully-stripped ion of the charge Z' or between a hydrogen-like ion of the nuclear charge Z' with a fully-stripped ion of the charge Z. These papers broke the paradigm, in which charge exchange was considered an inherently quantum phenomenon.

Later applications of these results included the magnetic stabilization of such one-electron Rydberg quasimolecules (hereafter, ORQ), the electric-field-caused enhancement of the ionization of the ORQ and of charge exchange, the effect of the screening by plasma electrons on the classical energy terms of ORQ, continuum lowering in plasmas, the attachment of an electron to a muonic hydrogen atom, and the effect of a laser field on ORQ.

In the present paper we extend the classical description of energy terms to *two-electron* Rydberg quasimolecules (TRQ) that consist of two electrons and two fully-stripped ions of charges Z and Z'. We show that classical energy terms of TRQ also exhibit crossings like the energy terms of ORQ. The crossings of terms of TRQ occur at larger internuclear distances compared to the crossings of the corresponding terms of ORQ, so that the cross-section of the charge exchange for TRQ is larger than the corresponding cross-section for ORQ.

PACS numbers: 32.60.+i, 32.80.Ee, 34.70.+e, 33.80.Be, 31.15.-p

1. INTRODUCTION

In year 2000 one of us published papers [1, 2] presenting a purely classical description of energy terms of Rydberg quasimolecules consisting of one electron and two fully-stripped ions of charges Z and Z', where $Z' \neq Z$. The analysis of the crossings of the energy terms led to a classical description of charge exchange either between a hydrogen-like ion of the nuclear charge Z with a fully-stripped ion of the charge Z' or between a hydrogen-like ion of the nuclear charge Z' with a fully-stripped ion of the charge Z [1, 2]. This meant that papers [1, 2] broke the paradigm, in which charge exchange was considered an inherently quantum phenomenon.

Later applications of these results included the following studies: the magnetic stabilization of such one-electron Rydberg quasimolecules (hereafter, ORQ) [3], the electric-field-caused enhancement of the ionization of the ORQ and of charge exchange [4, 5], the effect of the screening by plasma electrons on the classical energy terms of ORQ [6, 7], the application to the problem of continuum lowering in plasmas [6-8], the effect of a laser field on ORQ [9], and the attachment of an electron to a muonic hydrogen atom [10, 11] or to a muonic hydrogenic ion [12]. All these studies were summarized in review [13].

In papers [1, 3 – 7, 10, 11] the studies were focused at Circular Rydberg States (CRS) of the TCC system (the analysis in papers [2, 9, 12] went beyond CRS). CRS of atomic and molecular systems, with only one electron, correspond to $|m| = (n - 1) \gg 1$, where n and m are the principal and magnetic electronic quantum numbers, respectively. They have been extensively studied [14 - 17] both theoretically and experimentally for several reasons: (a) CRS have long radiative lifetimes and highly anisotropic collision cross sections, thereby enabling experiments

on inhibited spontaneous emission and cold Rydberg gases [18, 19], (b) classical CRS correspond to quantal coherent states, objects of fundamental importance, and (c) a classical description of CRS is the primary term in the quantal method based on the $1/n$-expansion (see, e.g. [20] and references therein).

In the present paper we extend the classical description of energy terms to *two-electron* Rydberg quasimolecules (TRQ) that consist of two electrons and two fully-stripped ions of charges Z and Z'. We show that classical energy terms of TRQ also exhibit crossings like the energy terms of ORQ. The crossings of terms of TRQ occur at larger internuclear distances compared to the crossings of the corresponding terms of ORQ. Therefore the cross-section of the charge exchange for TRQ is larger than the corresponding cross-section for ORQ.

2. ANALYTICAL CALCULATIONS OF CLASSICAL ENERGY TERMS

We consider a Rydberg quasimolecule formed by a He-like ion of the nuclear charge Z, having the inner electron in state 1s and the highly excited outer electron, being in the vicinity of a fully stripped ion of the nuclear charge Z'. The outer electron is in the superposition of the Coulomb potential from charge Z' and the potential Φ of a quasinucleus consisting of the nucleus Z and a spherically-symmetric charge distribution corresponding to the inner electron in the 1s state (see, e.g., [21]):

$$\Phi(r) = \frac{Z-1}{r} + \left(Z\mu + \frac{1}{r}\right)e^{-2Z\mu r} \tag{1}$$

where $\mu = Mm/(M+m)$ is the reduced mass of the pair "nucleus Z – electron", M is the nuclear mass. We use atomic units $\hbar = e = m_e = 1$.

A detailed classical analytical solution of the TCC problem, where an electron revolves around nuclei of charges Z and Z', has been presented in papers [1, 2]. In the case shown here, the Hamiltonian of the highly excited electron is

$$H = \frac{1}{2}(p_z^2 + p_\rho^2 + \frac{p_\phi^2}{\rho^2}) - \Phi(r) - \frac{Z'}{\sqrt{\rho^2 + (R-z)^2}} \tag{2}$$

where $r = (\rho^2 + z^2)^{1/2}$ is the distance from the highly excited electron to the nucleus Z and (ρ, φ, z) are the cylindrical coordinates positioned in such a way that the nuclei Z and Z' are on the z-axis at $z = 0$ and $z = R$ accordingly. The electron is in a circular state, therefore, φ is a cyclic coordinate and its corresponding momentum is conserved:

$$p_\phi = \rho^2 \frac{d\phi}{dt} = L \tag{3}$$

With (3) and (1) substituted into (2), we obtain

$$H = \frac{1}{2}(p_z^2 + p_\rho^2) + E \tag{4}$$

where

$$E = \frac{L^2}{2\rho^2} - \frac{Z-1}{\sqrt{\rho^2 + z^2}} - (Z\mu + \frac{1}{\sqrt{\rho^2 + z^2}})e^{-2Z\mu\sqrt{\rho^2 + z^2}} - \frac{Z'}{\sqrt{\rho^2 + (R-z)^2}} \tag{5}$$

In a circular state, we have $p_z = p_\rho = 0$, and E becomes the total energy of the electron.

Using the scaled quantities

$$\ell = \frac{L}{\sqrt{ZR}}, \; w = \frac{z}{R}, \; v = \frac{\rho}{R}, \; p = v^2, \; \varepsilon = -\frac{R}{Z}E, \; k = \mu R, \; b = \frac{Z'}{Z}, \; r = \frac{Z}{L^2}R \tag{6}$$

we obtain the scaled energy ε of the electron

$$\varepsilon = \frac{1 - 1/Z}{\sqrt{w^2 + p}} + \frac{b}{\sqrt{(1-w)^2 + p}} + (k + \frac{1/Z}{\sqrt{w^2 + p}})e^{-2Zk\sqrt{w^2 + p}} - \frac{\ell^2}{2p} \tag{7}$$

For the equilibrium with respect to the scaled coordinates (w, p), it is required that

$$\frac{d\varepsilon}{dw} = 0, \; \frac{d\varepsilon}{dp} = 0 \tag{8}$$

The first differentiation in (8) being set equal to zero gives us the equilibrium relationship between the coordinates (w, p) for the given values of Z, b and k. The explicit form of this relationship is given by (9):

$$\frac{b(1-w)}{((1-w)^2 + p)^{3/2}} = w\frac{Z - 1 + (1 + 2Zk\sqrt{w^2 + p} + 2Z^2k^2(w^2 + p))e^{-2Zk\sqrt{w^2 + p}}}{Z(w^2 + p)^{3/2}} \tag{9}$$

Fig. 1 shows, as an example, the plot $p(w)$ for $Z = 2$, $b = 3$, $k = 2$.
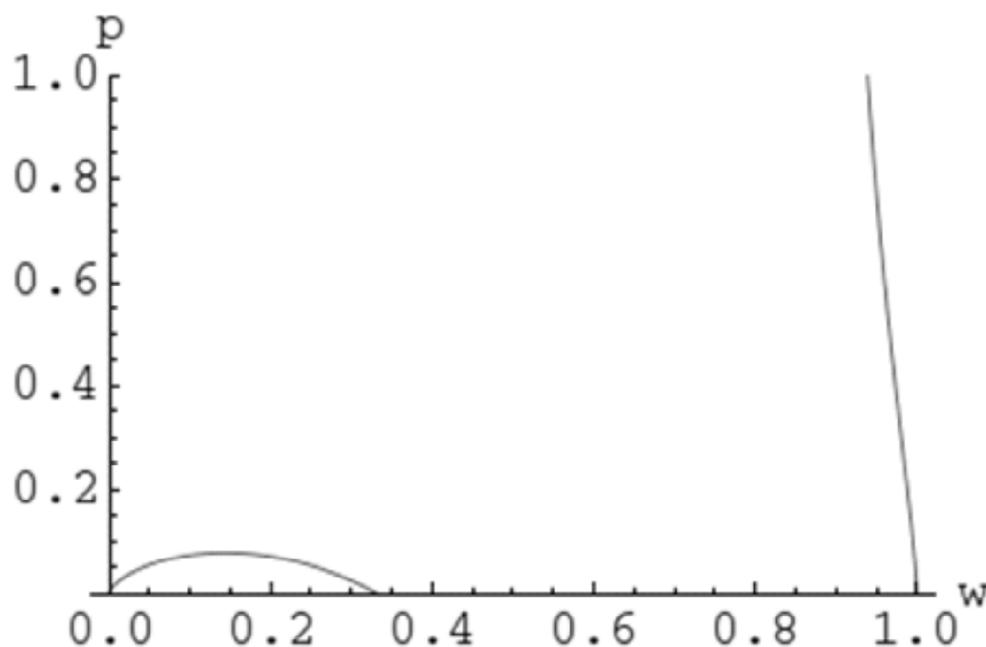
Figure 1: Equilibrium plot of the dependence of the squared scaled radius of the orbit p on the scaled axial coordinate w for $Z = 2$, $b = 3$, $k = 2$.

As in the case of two bare nuclei [1, 2], the equilibrium range is $0 < w < w_1$ and $w_3 < w < 1$. In this case,

$$w_1 = \frac{\alpha}{Zk} \tag{10}$$

where α is the solution of the transcendental equation

$$bZ\alpha^2 = (Zk - \alpha)^2 (Z - 1 + (1 + 2\alpha + 2\alpha^2)e^{-2\alpha}) \tag{11}$$

and the asymptote $w = w_3$ is determined by

$$w_3 = \frac{b}{b + 1 - 1/Z} \tag{12}$$

In the second differentiation the last term in (7) survives and we obtain the equilibrium value of ℓ, which we substitute into (7) and obtain the value of the scaled energy in the circular state:

$$\varepsilon = \frac{(1 - 1/Z)(w^2 + p/2)}{(w^2 + p)^{3/2}} + \frac{b((1 - w)^2 + p/2)}{((1 - w)^2 + p)^{3/2}} +$$
$$+ \frac{w^2 + p/2 + Zk\sqrt{w^2 + p}(w^2 - pZk\sqrt{w^2 + p})}{Z(w^2 + p)^{3/2}} e^{-2Zk\sqrt{w^2 + p}} \tag{13}$$

From the scaling formulas (6) it follows that $r = 1/\ell^2$, that is,

$$r = p^{-2} \left(\frac{1 - 1/Z}{(w^2 + p)^{3/2}} + \frac{b}{((1 - w)^2 + p)^{3/2}} \right.$$
$$\left. + \frac{1 + 2Zk\sqrt{w^2 + p} + 2Z^2k^2(w^2 + p)}{Z(w^2 + p)^{3/2}} e^{-2Zk\sqrt{w^2 + p}} \right)^{-1} \tag{14}$$

Also, from the same formulas we see that $E = - (Z/L)^2 \varepsilon/r$, so if we denote $\varepsilon/r = \varepsilon_1$, then ε_1 and r will have the same scaling.

Thus, we have three master equations: (13), (14) and (9), which depend on w, p, k for the given values of b and Z. Then we solve (9) numerically for p and substitute it into (13) and (14), obtaining ε and r depending on w and k (for the given b and Z). From the 6th and 8th formulas in (6) it follows that $k = (\mu L^2/Z)r$. By denoting $\sigma = \mu L^2/Z$, we obtain

$$\frac{k}{\sigma} = r(w, p(w, k, b, Z), k, b, Z) \tag{15}$$

where the right-hand side is the equation (14) with the p substituted from the numeric solution of (9).

This equation (15) can be solved numerically for $w = w(k, \sigma, b, Z)$. It appears that it may have up to three solutions. Then, the previously defined scaled energy $\varepsilon_1 = \varepsilon/r$, with ε and r from (13) and (14) with p substituted from (9), will depend only on w and k for the given b and Z. Finally, substituting the three solutions for w obtained before into ε_1, we obtain $\varepsilon_1 = \varepsilon_1(k, \sigma, b, Z)$ – the scaled energy dependence on k for the given σ, b and Z.

From (6), $k = \mu R$, where μ is the reduced mass of the pair nucleus – electron. In our units, the mass of the electron is 1, so $\mu = M/(1 + M)$, where M is the nuclear mass $Zm_p + Nm_n$ of the nucleus containing Z protons and N neutrons. In atomic units, $m_p \approx 1849.3596$ and $m_n \approx 1851.9088$. Since

$$\mu = \frac{M}{1 + M} = \frac{1}{\frac{1}{M} + 1} = \frac{1}{\frac{1}{Zm_p + Nm_n} + 1} \approx \frac{1}{\frac{1}{(Z + N)m_p} + 1} \tag{16}$$

the lower limit of μ is realized when $Z = 1$ and $N = 0$ and is approximately 0.99946 and the upper limit is 1. Therefore, the realistic values of μ lie in the range $0.99946 \leq \mu < 1$. The values of R for the case of a Rydberg quasimolecule are of the order of several Bohr radii. Thus, the realistic values of $k = \mu R$ are of the order of $\sim(10 -$

100) and k physically represents the slightly scaled internuclear distance. Therefore, the dependence $\varepsilon_1 = \varepsilon_1(k, \sigma, b, Z)$ obtained earlier is a direct (rather than parametric) dependence of the scaled energy on the (slightly) scaled internuclear distance for the given σ, b and Z. Its plot will represent the energy terms.

As an example, we consider the case of $Z = 6$, $N = 6$, $b = 3$. For this case, according to (16) and the definition of σ, the value of $L = 10$ corresponds to $\sigma = 16.6659$. Figure 2 presents the classical energy terms $\varepsilon_1(k)$ for the two-electron Rydberg quasimolecule (TRQ) for the case $b = 3$, $Z = 6$, $N = 6$, $L = 10$. It is seen that there are three classical energy terms and that the upper two terms undergo a V-type crossing (resembling a letter V rotated clockwise by about 90 degrees).
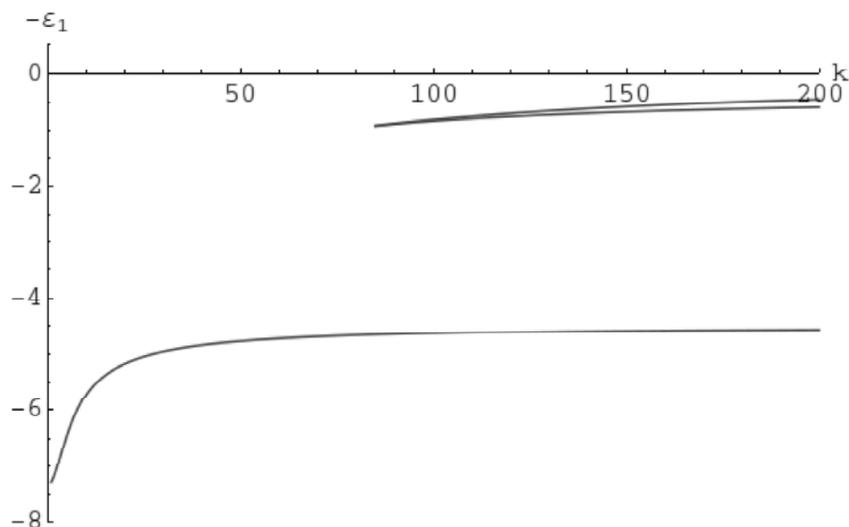
Figure 2: Classical energy terms $\varepsilon_1(k)$ for the two-electron Rydberg quasimolecule for the case of $b = 3$, $Z = 6$, N = 6, L = 10.

Figure 3 shows the comparison of the classical energy terms $\varepsilon_1(k)$ for the case $b = 3$, $Z = 6$, $N = 6$, $L = 10$ for TRQ (thick curves) with the corresponding classical energy terms for the one-electron Rydberg quasimolecule (ORQ) [1, 2] (thinner curves). It is seen that the terms of the TRQ have lower binding energies compared to the corresponding ORQ. This should be expected because of the screening of the charge Z for the TRQ by the nearby electron in the state 1s.
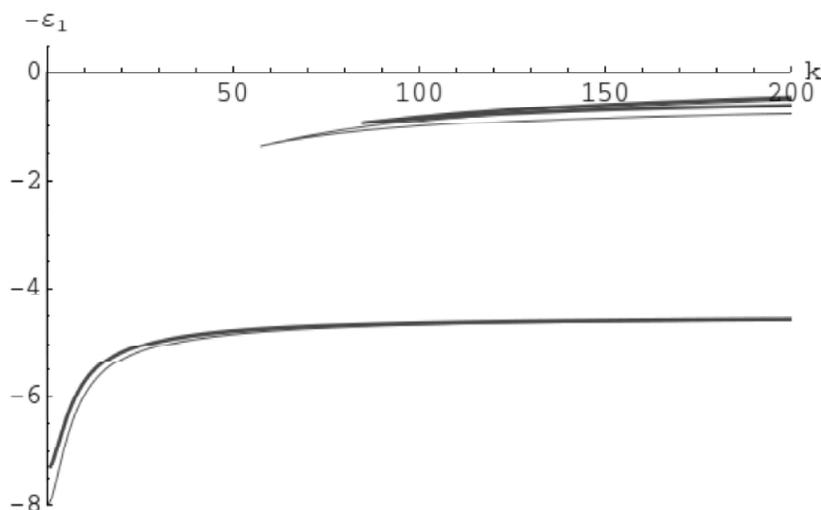
Figure 3: Comparison of the classical energy terms $\varepsilon_1(k)$ for the two-electron Rydberg quasimolecule for the case of $b = 3$, $Z = 6$, $N = 6$, $L = 10$ (thick curves) with the classical energy terms for the corresponding one-electron Rydberg quasimolecule (thinner curves)

3. RELATION TO CHARGE EXCHANGE

When Z and Z' (for ORQ) or $Z_{eff} = Z - 1$ and Z' (for TRQ) differ significantly from each other, the V-type crossings occur between two classical energy terms that can be asymptotically labeled as Z- and Z'-terms (for ORQ) or as Z_{eff}- and Z'-terms (for TRQ). This situation *classically depicts charge exchange*, as explained in papers [1, 2]. Indeed, say, initially at $r \to \infty$, the electron was a part of the hydrogenlike ion of the nuclear charge $Z_{min} = \min(Z', Z)$ for ORQ or $Z_{min} = \min(Z', Z_{eff})$ for TRQ. As the charges Z or Z_{eff} and Z' come relatively close to each other, the two terms undergo a V-type crossing and the electron is shared between the Z- (or Z_{eff}-) and Z'-centers. Finally, as the charges Z (or Z_{eff}) and Z' go away from each other, the electron ends up as a part of the hydrogenlike ion of the nuclear charge $Z_{max} = \max(Z', Z)$ for ORQ or $Z_{max} = \max(Z', Z_{eff})$ for TRQ.

From Fig. 3 it is seen that the V-type crossing of the upper two terms for TRQ occurs at a larger internuclear distance than for ORQ. Therefore the cross-section of the charge exchange for TRQ is larger than the corresponding cross-section for ORQ.

4. CONCLUSIONS

We extended the classical description of energy terms from one-electron Rydberg quasimolecules (ORQ) to *two-electron* Rydberg quasimolecules (TRQ). We obtained the classical energy terms of TRQ and found that they exhibit crossings like the energy terms of ORQ. We explained the relation between the crossings of the energy terms and charge exchange.

The crossings of terms of TRQ occur at larger internuclear distances compared to the crossings of the corresponding terms of ORQ. This means that the cross-section of charge exchange at these crossings is larger for TRQ compared to ORQ.

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