

A Classical Description of Electric-Field Induced Crossings of Energy Levels Enhancing Charge Exchange and Ionization

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ABSTRACT: Charge exchange and crossings of corresponding energy levels that enhance charge exchange are strongly connected with problems of energy losses and of diagnostics in high temperature plasmas. Besides, charge exchange was proposed as one of the most effective mechanisms for population inversion in the soft x-ray and VUV ranges. One of the most fundamental theoretical playgrounds for studying charge exchange is the problem of electron terms in the field of two stationary Coulomb centers (TCC) of charges Z and Z' separated by a distance R . It presents fascinating atomic physics: the terms can have crossings and quasicrossings. These rich features of the TCC problem also manifest in a different area of physics such as plasma spectroscopy: a quasicrossing of the TCC terms, by enhancing charge exchange, can result in an unusual structure (a dip) in the spectral line profile emitted by a Z -ion from a plasma consisting of both Z - and Z' -ions, as was shown theoretically and experimentally. Before year 2000, the paradigm was that the above sophisticated features of the TCC problem and its flourishing applications were inherently quantum phenomena. In year 2000 there was presented a purely classical description of the crossings of energy terms. In the present paper we study the effect of an electric field (along the internuclear axis) on circular Rydberg states of the TCC system. We provide analytical results for strong fields, as well as numerical results for moderate fields. We show that the electric field has several effects. First, it leads to the appearance of an extra energy term: the fourth classical energy term – in addition to the three classical energy terms at zero field. Second, but more importantly, the electric field creates additional crossings of these energy terms. We show that some of these crossings significantly enhance charge exchange while other crossings enhance the ionization of the Rydberg quasi-molecule.

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1. INTRODUCTION

Charge exchange and crossings of corresponding energy levels that enhance charge exchange are strongly connected with problems of energy losses and of diagnostics in high temperature plasmas – see, e.g., [1, 2] and references therein. Besides, charge exchange was proposed as one of the most effective mechanisms for population inversion in the soft x-ray and VUV ranges [3-6]. One of the most fundamental theoretical playgrounds for studying charge exchange is the problem of electron terms in the field of two stationary Coulomb centers (TCC) of charges Z and Z' separated by a distance R . It presents fascinating atomic physics: the terms can have crossings and quasicrossings.

The crossings are due to the fact that the well-known Neumann-Wigner general theorem on the impossibility of crossing of terms of the same symmetry [7] is not valid for the TCC problem of $Z' \neq Z$ – as shown in paper [8]. Physically it is here a consequence of the fact that the TCC problem allows a separation of variables in the elliptic coordinates [8]. As for the quasicrossings, they occur when two wells, corresponding to separated Z - and Z' -centers, have states Ψ and Ψ' , characterized by the same energies $E = E'$, by the same magnetic quantum numbers $m = m'$, and by the same radial elliptical quantum numbers $k = k'$ [9 – 11]. In this situation, the electron has a much larger probability of tunneling from one well to the other (i.e., of charge exchange) as compared to the absence of such degeneracy.

These rich features of the TCC problem also manifest in a different area of physics such as plasma spectroscopy as follows. A quasicrossing of the TCC terms, by enhancing charge exchange, can result in unusual structures (dips)

in the spectral line profile emitted by a Z -ion from a plasma consisting of both Z - and Z' -ions, as was shown theoretically and experimentally [12–17].

Before year 2000, the paradigm was that the above sophisticated features of the TCC problem and its flourishing applications were inherently quantum phenomena. But then in year 2000 one of us published papers [18, 19] presenting a purely classical description of both the crossings of energy levels in the TCC problem and the dips in the corresponding spectral line profiles caused by the crossing (via enhanced charge exchange). These classical results were obtained analytically based on first principles without using any model assumptions. Later applications of these results included a magnetic stabilization of Rydberg quasi-molecules [20] and a problem of continuum lowering in plasmas [21].

In papers [18, 20, 21] the study was focused at Circular Rydberg States (CRS) of the TCC system (the analysis in paper [19] 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 [22 – 25] 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 [26, 27], (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. [28] and references therein).

While the authors of paper [20] studied analytically the effect of a magnetic field (along the internuclear axis) on CRS of the TCC system, in the present paper we study the effect of an electric field (along the internuclear axis) on CRS of the TCC system. We provide analytical results for strong fields, as well as numerical results for moderate fields. We show that the electric field leads to the following consequences.

First, it leads to the appearance of an extra energy term: the fourth classical energy term – in addition to the three classical energy terms at zero field. Second, but more importantly, the electric field creates additional crossings of these energy terms. We show that some of these crossings enhance charge exchange while other crossings enhance the ionization of the Rydberg quasi-molecule.

2. CALCULATIONS OF THE CLASSICAL STARK EFFECT FOR A RYDBERG QUASI-MOLECULE IN A CIRCULAR STATE

We consider a TCC system, where the charge Z is at the origin and the Oz axis is directed to the charge Z' , which is at $z = R$ (here and below the atomic units $\hbar = e = m_e = 1$ are used). A uniform electric field F is applied along the internuclear axis – in the negative direction of Oz axis. We study CRS where the electron moves around a circle in the plane perpendicular to the internuclear axis, the circle being centered at this axis.

Two quantities, the energy E and the projection L of the angular momentum on the internuclear axis are conserved in this configuration. We use cylindrical coordinates to write the equations for both.

$$E = ((d\rho/dt)^2 + \rho^2 (d\phi/dt)^2 + (dz/dt)^2)/2 - Z/r - Z'/r' - Fz \quad (1)$$

$$L = \rho^2 d\phi/dt \quad (2)$$

In the equations above, ρ is the distance of the electron from the internuclear axis, ϕ is its azimuthal angle, z is the projection of the radius-vector of the electron on the internuclear axis, r and r' are the distances of the electron from the particle to Z and Z' .

The circular motion implies that $d\rho/dt = 0$; as the motion occurs in the plane perpendicular to the z -axis, $dz/dt = 0$. Further, expressing r and r' through ρ and z , and taking $d\phi/dt$ from (2), we have:

$$E = L^2/(2\rho^2) - Z/(\rho^2 + z^2)^{1/2} - Z'/(\rho^2 + (R - z)^2)^{1/2} - Fz \quad (3)$$

With the scaled quantities

$$w = z/R, v = \rho / R, b = Z'/Z, \varepsilon = -ER/Z, m = L/(ZR)^{1/2}, f = FR^2/Z, r = ZR/L^2, \quad (4)$$

our energy equation takes the form below:

$$\varepsilon = 1/(w^2 + v^2)^{1/2} + b/((1 - w)^2 + v^2)^{1/2} + fw - m^2/(2v^2) \quad (5)$$

We can seek the equilibrium points by finding partial derivatives of ε by the scaled coordinates w , v and setting them equal to zero. This will give the following two equations.

$$f + b(1 - w)/((1 - w)^2 + v^2)^{3/2} = w/(w^2 + v^2)^{3/2} \quad (6)$$

$$m^2/v^4 = 1/(w^2 + v^2)^{3/2} + b/((1 - w)^2 + v^2)^{3/2} \quad (7)$$

From the definitions of the scaled quantities (4), $m^2 = 1/r$ and $E = -(Z/R)\varepsilon$. Since $r = ZR/L^2$, $E = -(Z/L)^2\varepsilon/r$, where $r = 1/m^2$ can be obtained by solving (7) for m . Substituting m into the energy equation, we get the three master equations for this configuration.

$$\varepsilon_1 = p^2 (1/(w^2 + p)^{3/2} + b/((1 - w)^2 + p)^{3/2}) ((w^2 + p/2)/(w^2 + p)^{3/2} + b((1 - w)^2 + p/2)/((1 - w)^2 + p)^{3/2} + fw) \quad (8)$$

$$r = 1/(p^2 (1/(w^2 + p)^{3/2} + b/((1 - w)^2 + p)^{3/2})) \quad (9)$$

$$f + b(1 - w)/((1 - w)^2 + p)^{3/2} = w/(w^2 + p)^{3/2} \quad (10)$$

In these equations $E = -(Z/L)^2\varepsilon_1$ and $p = v^2$. Thus, ε_1 is the “true” scaled energy, whose equation for E does not include R . The scaled energy ε_1 and internuclear distance r in (8) and (9) now explicitly depend only on the coordinates w and p (besides the constants b and f). Therefore, if we solve (10) for p and substitute it into (8) and (9), we will have the parametric solution $\varepsilon_1(r)$ with the parameter w .

Our focus is at crossings of energy terms of the *same symmetry*. In the quantum TCC problem, “terms of the same symmetry” means terms of the same magnetic quantum number m [8 – 11]. Therefore, in our classical TCC problem, we fixed the angular momentum projection L and study the behavior of the classical energy at $L = \text{const} \geq 0$ (the results for L and $-L$ are physically the same).

Equation (10) does not allow an exact analytical solution for p . Therefore, we will use an approximate analytical method.

Figure 1 shows a contour plot of Eq. (10) for a relatively weak field $f = 0.3$ at $b = 3$, with w on the horizontal axis and p on the vertical. The plot has two branches. The left branch spans from $w = 0$ to $w = w_1$. The right one actually has a small two-valued region between some $w = w_3$ and 1 ($w_3 < 1$). Indeed, at $w = 1$, there are two values of p : $p = 0$ and $p = f^{-2/3} - 1$. Thus, the two-valued region exists only for $f < 1$.

The right branch touches the abscissa at $w = 1$ and at some $w = w_2$. Analytical expressions for w_1 and w_2 are given in Appendix A. The quantity w_3 is a solution of the equation

$$f^{2/5} (2w_3 - 1)^{3/5} = w_3^{2/5} - b^{2/5} (1 - w_3)^{2/5} \quad (11)$$

The method, by which w_3 was found from Eq. (11), is presented in Appendix B.

Figure 2 shows a contour plot of Eq. (10) for a relatively strong field $f = 20$ at $b = 3$. It is seen that there is no two-valued region.

From now on we consider the situation where the radius of the electronic orbit is relatively small, meaning that $p \ll 1$. Physically this corresponds to strong fields $f > f_{\min} \sim 10$.

Solving Eq. (10) in the small- p approximation, we obtain

$$p = (w/(f + b/(1 - w)^2))^{2/3} - w^2 \quad (12)$$

for the left branch ($0 < w < w_1$) and

$$p = (b(1 - w)/(1/w^2 - f))^{2/3} - (1 - w)^2 \quad (13)$$

for the right branch ($1 < w < w_2$). Substituting these results into Eqs. (8) and (9), we get approximate solutions for energy terms $-\varepsilon_1(r)$ in both regions in a parametric form, w being the parameter. Now we plot classical energy terms $-\varepsilon_1(r)$ by varying the parameter w over both regions, using the appropriate formula for each one.

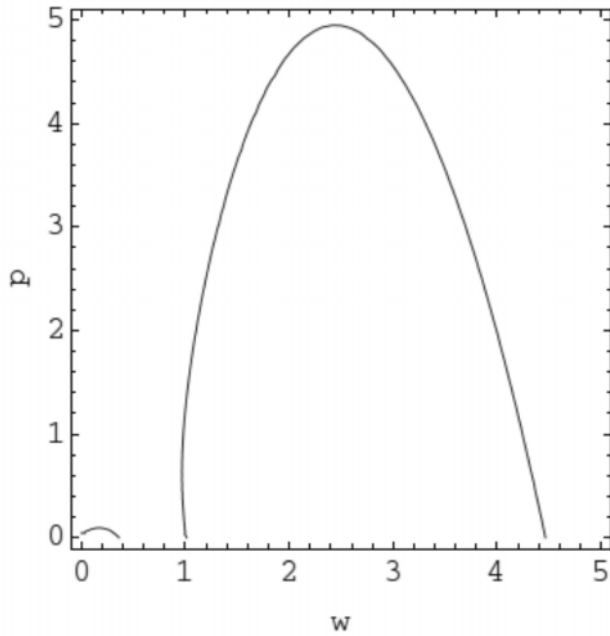


Figure 1: Contour Plot of Eq. (10) for a Relatively Weak Field $f = FR^2/Z = 0.3$ at $b = Z'/Z = 3$

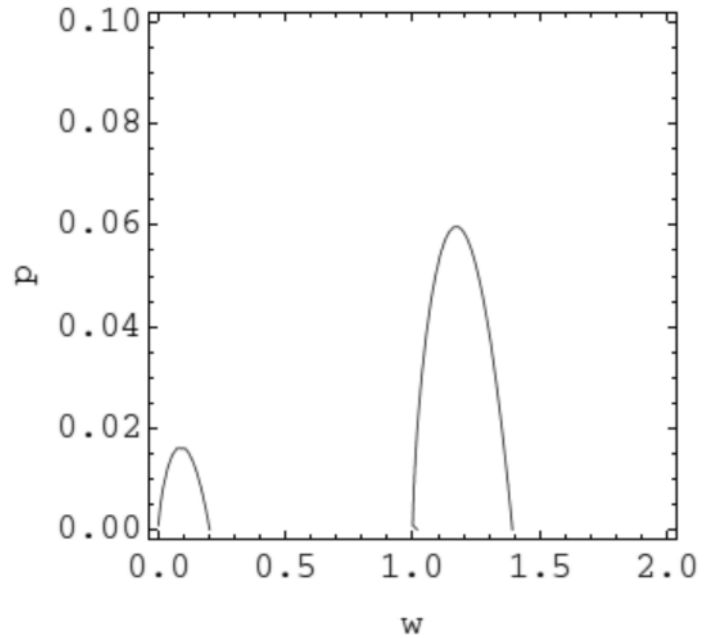


Figure 2: The Same as in Fig. 1, but for a Relatively Strong Field $f = FR^2/Z = 20$

Figure 3 shows classical energy terms at $b = 3$ for $f = 20$. Figure 4 presents classical energy terms at $b = 3$ for $f = 5$.

We also solved the same problem numerically. By comparison we found that the approximate analytical solution is accurate for fields $f = 5$ and above.

Figures 5 and 6 show the numerically obtained classical energy terms at $b = 3$ for $f = 2$ and $f = 0.1$, respectively. For comparison, Fig. 7 shows the classical energy terms at $b = 3$ at the absence of the electric field (it had been previously presented by one of us in papers [18, 19]).

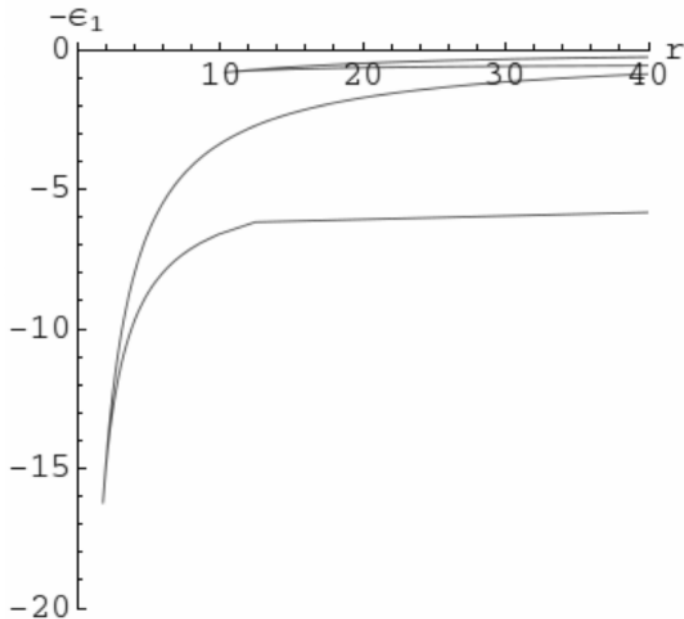


Figure 3: Classical Energy Terms at $b = 3$ for $f = 20$

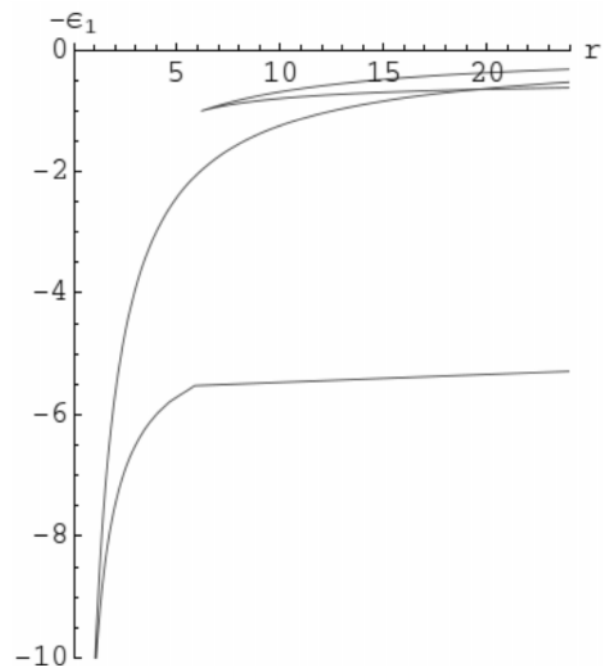


Figure 4: Classical Energy Terms at $b = 3$ for $f = 5$

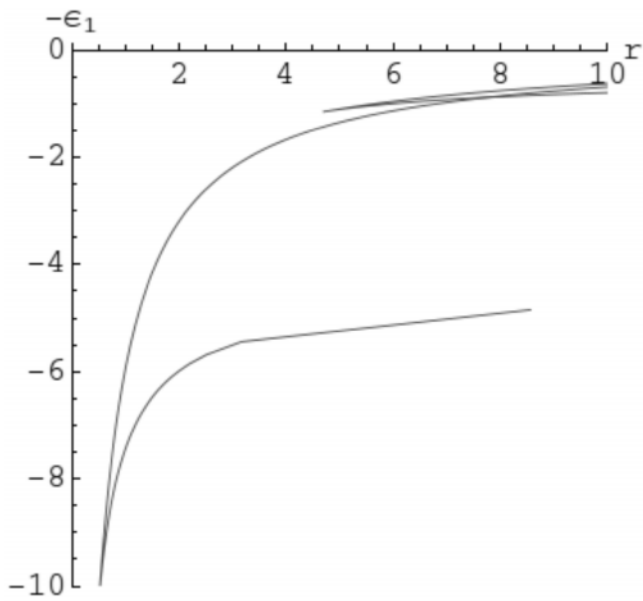


Figure 5: Classical Energy Terms at $b = 3$ for $f = 2$

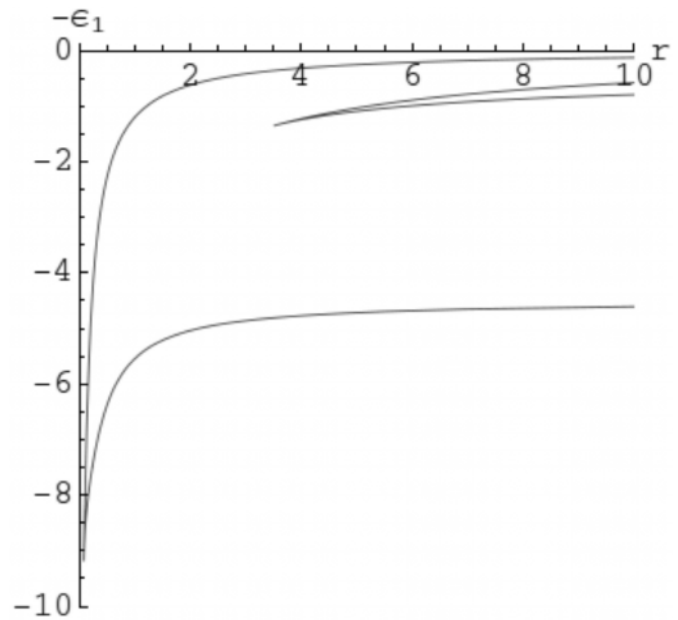


Figure 6: Classical Energy Terms at $b = 3$ for $f = 0.1$

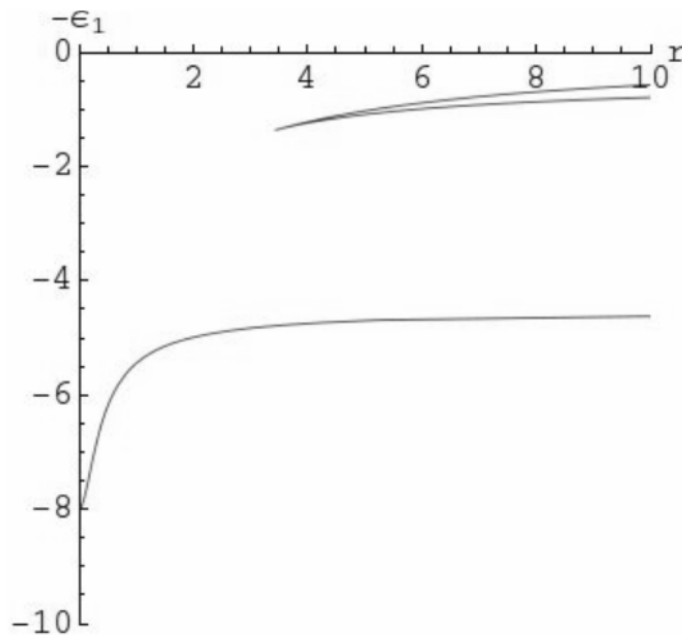


Figure 7: Classical Energy Terms at $b = 3$ at the Absence of the Electric Field

The electric field causes several important new features compared to the zero-field case. While at $f=0$ there are three classical energy terms, the electric field brings up the fourth classical energy term. Indeed, let us take as an example the case of $f=5$ at $b=3$ presented in Fig. 4. There are four energy terms that we label as follows:

- #1 – the lowest term;
- #2 – the next term up (which has a V-type crossing with term 1);
- #3 – the next term up;
- #4 – the highest term (which has a V-type crossing with term 3).

We will use this labeling also while discussing all other plots (except the plot in Fig. 7 for $f=0$): terms 1 and 2 will be those having the V-type crossing at the lower energy, terms 3 and 4 will be those having the V-type crossing at the higher energy,

At $f=0$ term 2 is absent, but it appears at any non-zero value of f – no matter how small. Actually, as f approaches zero, this term behaves like $-f/r$, which is why it disappears at $f=0$.

The existence of this additional term can be explained physically as follows. When $f=0$, equilibrium of the orbital plane to the right of Z' (i. e., for $w > 1$) does not exist, so that the values of w_1 and w_3 reduce to the ones presented in papers [18, 19] and the right branch of $p(w)$ asymptotically goes to infinity when w goes down to w_3 . When an infinitesimal field f appears, the right branch flips over positive infinity and ends up on the abscissa at $w_2 \rightarrow \infty$, thus enabling the whole region $w > 1$ for equilibrium. As the field grows, w_2 decreases. Physically, the force from the electric field at $w > 1$ balances out the Coulomb attraction of the Z, Z' system on the left – the situation not possible for $f=0$. This term is obtained by varying the parameter w from 1 to w_2 .

We emphasize that the above examples presented for $Z'/Z=3$ represent a typical situation. In fact, for any pair of Z and $Z' \neq Z$, at the presence of the electric field, there are four classical energy terms of the same symmetry for CRS.

Another important new feature caused by the electric field is X-type crossings of the classical energy terms. This kind of crossings and their physical consequences are discussed in the next section.

3. X-TYPE CROSSINGS OF CLASSICAL ENERGY TERMS AND THEIR PHYSICAL CONSEQUENCES

Figure 8 shows a magnified version of the energy terms 2, 3, and 4 at $b=3$ for $f=2$. Figure 9 shows a further magnified version of the energy terms 2 and 4 at $b=3$ for $f=2$. Compared to Fig. 5 for the same b and f , in Figs. 8 and 9 we decreased the exhibited energy range, but increased the exhibited range of the internuclear distances r .

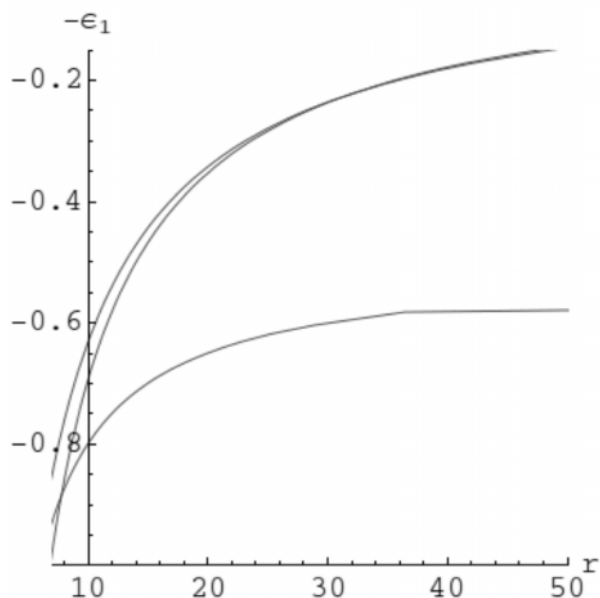


Figure 8: Magnified Plot of the Classical Energy Terms 2, 3, and 4 at $b=3$ for $f=2$

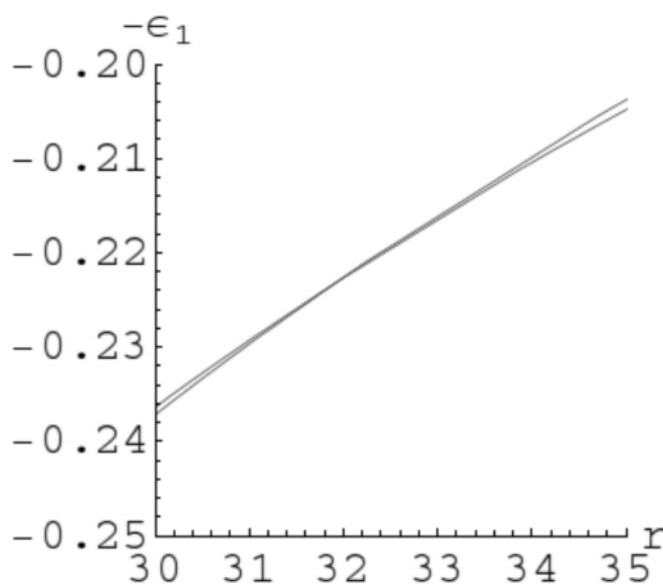


Figure 9: Further Magnified Plot of the Classical Energy Terms 2 and 4 at $b=3$ for $f=2$

It is seen that term 2 has the X-type crossing with term 3 at $r=7.8$ and the X-type crossing with term 4 at $r=32$. The situation where there are two X-type crossings exists in a limited range of the electric fields. For example, for $b=3$:

- two X-type crossings exist at $1.31 < f < 2.4$;

- there are no X-type crossings at $f < 1.31$;
- there is one X-type crossing at $f > 2.4$ (the crossing of terms 2 and 3).

To reveal physical consequences of the X-type crossings, let us first discuss the origin of all four classical energy terms for arbitrary $Z'/Z \neq 1$. At $r \rightarrow \infty$, term 3 corresponds to the energy of a hydrogenlike ion of the nuclear charge $Z_{\min} = \min(Z', Z)$, slightly perturbed by the charge $Z_{\max} = \max(Z', Z)$, as shown in [18, 19].

At $r \rightarrow \infty$, term 4 corresponds to a near-zero-energy state (where the electron is almost free), as shown in [18, 19]. If the ratio Z'/Z is of the order of (but not equal to) unity, this term at $r \rightarrow \infty$ can be described only in the terminology of elliptical coordinates (rather than parabolic or spherical coordinates), meaning that even at $r \rightarrow \infty$ the electron is shared between the Z - and Z' -centers. However, in the case of $Z' \gg Z$, this term can be asymptotically considered as the Z' -term, as shown in [18, 19]. It has the V-type crossing with term 3, which asymptotically is the Z -term (since $Z_{\min} = Z$ for $Z' > Z$). Likewise, in the case of $Z' \ll Z$, term 4 can be asymptotically considered as the Z -term, as shown in [18, 19]. It has the V-type crossing with term 3, which asymptotically is the Z' -term (since $Z_{\min} = Z'$ for $Z' < Z$).

At $r \rightarrow \infty$, term 1 corresponds to the energy of a hydrogenlike ion of the nuclear charge Z_{\max} slightly perturbed by the charge Z_{\min} , as shown in [18, 19]. As for the term 2, at $r \rightarrow \infty$ it has properties similar to term 4, but with the interchange of Z_{\max} and Z_{\min} . In particular, in the case of $Z' \gg Z$, this term can be asymptotically considered as the Z -term, having the V-type crossing with term 1, which asymptotically is the Z' -term (since $Z_{\max} = Z'$ for $Z' > Z$). In the case of $Z' \ll Z$, term 2 can be asymptotically considered as the Z' -term, having the V-type crossing with term 1, which asymptotically is the Z -term (since $Z_{\max} = Z$ for $Z' < Z$).

Thus, when Z and Z' 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. This situation *classically depicts charge exchange*, as explained in papers [18, 19]. Indeed, say, initially at $r \rightarrow \infty$, the electron was a part of the hydrogenlike ion of the nuclear charge Z_{\min} . As the charges Z and Z' come relatively close to each other, the two terms undergo a V-type crossing and the electron is shared between the Z - and Z' -centers. Finally, as the charges Z and Z' go away from each other, the electron ends up as a part of the hydrogenlike ion of the nuclear charge Z_{\max} .

So, the first distinction caused by the electric field is an additional, second V-type crossing leading to charge exchange – compared to the zero-field case where there was only one such crossing. However, the second V-type crossing (the crossing of terms 1 and 2) occurs at the internuclear distance $r_{v2} \ll r_{v1}$, where r_{v1} is the internuclear distance of the first V-type crossing (the crossing of terms 3 and 4). Therefore the cross-section of the charge exchange corresponding to the second V-type crossing is much smaller than the corresponding cross-section for the first V-type crossing.

Now let us discuss the X-type crossing from the same point of view. When Z and Z' differ significantly from each other, the X-type crossing of terms 2 and 4 is the crossing of terms that can be asymptotically labeled as Z - and Z' -terms. Thus, this situation again *classically depicts charge exchange*. The most important is that this crossing occurs at the internuclear distance $r_{x1} \gg r_{v1} \gg r_{v2}$. Therefore, the cross-section of charge exchange due to this X-type crossing is much greater than the corresponding cross-sections for the V-type crossings. This is the most fundamental physical consequence caused by the electric field: a *significant enhancement of charge exchange*.

When Z and Z' differ significantly from each other, the X-type crossing of terms 2 and 3 is the crossing of terms having the same asymptotic labeling: either both of them are Z -terms or both of them are Z' -terms. Therefore this second X-type crossing (at $r = r_{x2}$) does not correspond to charge exchange – rather it represents an *additional ionization channel*. Indeed, say, initially at $r \rightarrow \infty$, the electron resided on term 3 of the hydrogenlike ion of the nuclear charge Z . As the distance between the charges Z and Z' decreases to $r = r_{x2}$, the electron can switch to term 2, which asymptotically corresponds to a near-zero-energy state (of the same hydrogenlike ion of the nuclear charge Z) where the electron would be almost free. So, as the charges Z and Z' go away from each other, the system undergoes the ionization. Thus, another physical consequence caused by the electric field is the appearance of the additional ionization channel. This should have been expected since the electric field promotes the ionization of atomic and molecular systems.

4. CONCLUSIONS

We studied the effect of an electric field (along the internuclear axis) on circular Rydberg states of the two Coulomb centers system. We provided analytical results for strong fields, as well as numerical results for moderate fields. We showed that the electric field had the following effects.

The first effect is the appearance of an extra energy term: the *fourth classical energy term* – in addition to the three classical energy terms at zero field. This term exhibits a V-type crossing with the lowest energy term. The two highest energy terms continue having a V-type crossing like at the zero field. In the situation where the charges Z and Z' differ significantly from each other, both V-type crossings correspond to charge exchange.

The second effect is the appearance of a new type of crossings – X-type crossings. One of the X-type crossings (existing in a limited range of the electric field strength) corresponds to charge exchange at a much larger internuclear distance compared to the V-type crossings. Therefore the cross-section of charge exchange due to this X-type crossing is much greater than the cross-section of charge exchange due to V-type crossings. Thus, the electric field can *significantly enhance charge exchange*. We believe that this is the most important result of the present paper.

The other X-type crossing does not correspond to charge exchange. Instead, it represents an *additional ionization channel*.

Appendix A. The limits w_1 and w_2 on the graph of $p(w)$ in Eq. (10)

The analytical results for the quantities w_1 and w_2 , obtained using the software Mathematica, have the following form.

For w_1 :

$$\frac{1}{6} \left(-\sqrt{3} \sqrt{\frac{\sqrt[3]{6\sqrt{3}} \sqrt{bf(b^2+3b^2(f-1)+3b(f(f+7)+1)+(f-1)^2)} + (b+f-1)^2 + 54f(b+f-1) - 54f^2 + 54f}{f}} + \frac{(b+f-1)^2}{f \sqrt[3]{6\sqrt{3}} \sqrt{bf(b^2+3b^2(f-1)+3b(f(f+7)+1)+(f-1)^2)} + (b+f-1)^2 + 54f(b+f-1) - 54f^2 + 54f}} - \frac{2(b+f-1)}{f} + 3 \right) + \sqrt{3} \sqrt{\frac{\sqrt[3]{6\sqrt{3}} \sqrt{bf(b^2+3b^2(f-1)+3b(f(f+7)+1)+(f-1)^2)} + (b+f-1)^2 + 54f(b+f-1) - 54f^2 + 54f}{f}} - \frac{(b+f-1)^2}{f \sqrt[3]{6\sqrt{3}} \sqrt{bf(b^2+3b^2(f-1)+3b(f(f+7)+1)+(f-1)^2)} + (b+f-1)^2 + 54f(b+f-1) - 54f^2 + 54f}} + \frac{(6\sqrt{3}(b+1))}{f \sqrt{\frac{\sqrt[3]{6\sqrt{3}} \sqrt{bf(b^2+3b^2(f-1)+3b(f(f+7)+1)+(f-1)^2)} + (b+f-1)^2 + 54f(b+f-1) - 54f^2 + 54f}{f}} + \frac{(b+f-1)^2}{f \sqrt[3]{6\sqrt{3}} \sqrt{bf(b^2+3b^2(f-1)+3b(f(f+7)+1)+(f-1)^2)} + (b+f-1)^2 + 54f(b+f-1) - 54f^2 + 54f}} - \frac{2(b+f-1)}{f} + 3 \right) - \frac{4(b+f-1)}{f} + 6 \Bigg) + 3$$

For w_2 :

$$\frac{1}{6} \left(\sqrt{3} \sqrt{\left(\frac{\sqrt[3]{-b^3 + 3b^2(f-1) + 6\sqrt{3}\sqrt{bf(3(b+1)f^2 - 3((b-7)b+1)f + (b+1)^3 - f^3)} - 3b(f(f+16)+1) + (f-1)^3}}{f} \right.} \right. +$$

$$\frac{(b-f+1)^2}{f^2 \sqrt[3]{-b^3 + 3b^2(f-1) + 6\sqrt{3}\sqrt{bf(3(b+1)f^2 - 3((b-7)b+1)f + (b+1)^3 - f^3)} - 3b(f(f+16)+1) + (f-1)^3}} +$$

$$\left. \left. \frac{2(b+1)}{f} + 1 \right) + \right.$$

$$\sqrt{3} \sqrt{\left(-\frac{\sqrt[3]{-b^3 + 3b^2(f-1) + 6\sqrt{3}\sqrt{bf(3(b+1)f^2 - 3((b-7)b+1)f + (b+1)^3 - f^3)} - 3b(f(f+16)+1) + (f-1)^3}}{f} \right.} +$$

$$\frac{(b-f+1)^2}{f^2 \sqrt[3]{-b^3 + 3b^2(f-1) + 6\sqrt{3}\sqrt{bf(3(b+1)f^2 - 3((b-7)b+1)f + (b+1)^3 - f^3)} - 3b(f(f+16)+1) + (f-1)^3}} +$$

$$\left. \left. \frac{6\sqrt{3}(b-1)}{f} \right) / \right.$$

$$\left(f \sqrt{\left(\frac{\sqrt[3]{-b^3 + 3b^2(f-1) + 6\sqrt{3}\sqrt{bf(3(b+1)f^2 - 3((b-7)b+1)f + (b+1)^3 - f^3)} - 3b(f(f+16)+1) + (f-1)^3}}{f} \right.} + \right.$$

$$\frac{(b-f+1)^2}{f^2 \sqrt[3]{-b^3 + 3b^2(f-1) + 6\sqrt{3}\sqrt{bf(3(b+1)f^2 - 3((b-7)b+1)f + (b+1)^3 - f^3)} - 3b(f(f+16)+1) + (f-1)^3}} +$$

$$\left. \left. \left. \left. \frac{2(b+1)}{f} + 1 \right) + \frac{4(b+1)}{f} + 2 \right) + 3 \right) \right)$$

Appendix B. Finding the Lower Limit w_3 of the Two-valued Region on the Graph of $p(w)$ in Eq. (10)

Defining a function

$$F(p, w) = f + b(1-w)/((1-w)^2 + p)^{3/2} - w/(w^2 + p)^{3/2}, \quad (B.1)$$

we can rewrite Eq. (10) as $F(p, w) = 0$. From the graph it is seen that at w_3 , $dw/dp = 0$. Since $F(p, w) = 0$, $dF/dp = 0$ as well. On the other hand, $F(w, p) = F(w(p), p) = 0$ and

$$dF/dp = \partial F/\partial w \, dw/dp + \partial F/\partial p = 0, \quad (B.2)$$

from where we get

$$dw/dp = -(\partial F/\partial p) / (\partial F/\partial w). \quad (B.3)$$

Setting the right side of Eqs. (B.1) and (B.3) to zero, we obtain the system of two equations, solving which for w will give us the point on the contour plot of $F(p, w) = 0$ where the derivative dw/dp vanishes, i. e., the desired point. Excluding p from the system, we reduce the equation to

$$f^{2/5} (2w_3 - 1)^{3/5} = w_3^{2/5} - b^{2/5} (1 - w_3)^{2/5} \quad (B.4)$$

where w was renamed to w_3 for clarity. This is Eq. (11) of the main text.

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