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Plasma screening within Rydberg atoms in circular states

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Abstract. A Rydberg atom embedded in a plasma can experience penetration by slowly moving electrons within its volume. The original pure Coulomb potential must now be replaced by a screened Coulomb potential which contains either a screening length R_s or a screening factor $A = R_s^{-1}$. For any given discrete energy level, there is a Critical Screening Factor (CSF) A_c beyond which the energy level disappears (by merging into the continuum). Analytical results are obtained for the classical dependence of the energy on the screening factor, for the CSF, and for the critical radius of the electron orbit for Circular Rydberg States (CRS) in this screened Rydberg atom. The results are derived for any general form of the screened Coulomb potential and are applied to the particular case of the Debye potential. We also show that CRS can temporarily exist above the ionization threshold and are therefore the classical counterparts of quantal discrete states embedded into continuum. The results are significant not only to Rydberg plasmas, but also to fusion plasmas, where Rydberg states of multi-charged hydrogen-like ions result from charge exchange with hydrogen or deuterium atoms, as well as to dusty/complex plasmas.

PACS. 34.60.+z Scattering in highly excited states (e.g., Rydberg states) – 31.70.-f Effects of atomic and molecular interactions on electronic structure – 31.50.Df Potential energy surfaces for excited electronic states

1 Introduction

A Rydberg atom embedded in a relatively cold plasma can experience penetration by slowly moving electrons within its volume, resulting in plasma screening of the Rydberg electron. Plasma screening of a test charge is a well-known phenomenon. For a hydrogen atom or a hydrogen-like ion (an H-atom, for short), it is effected by replacing the pure Coulomb potential by a screened Coulomb potential which contains a physical parameter-the screening length R_s or the screening factor $A = R_s^{-1}$. For example, the Debye-Hückel (or Debye) interaction of an electron with the electronic shielded field of an ion of charge Z is

$$V(R) = -(Ze^2/R)\exp(-R/R_s), \qquad (1)$$

where $R_s = [kT/(4\pi^2 N_e)]^{1/2} \approx 1.304 \times 10^4 (10^{10}/N_e)^{1/2} \times T^{1/2} a_0$ for plasmas of the electron density N_e (cm^{-3}) and of the temperature T(K).

The rms-radius of a Rydberg atom is (see, e.g. [1]) $r_a = \{n^2[5n^2 + 1 - 3l(l+1)]/2\}^{1/2} a_0$, where n and l are the principal and orbital-momentum quantum numbers, a_0 is the Bohr radius. At $n \gg l$ the rms-radius simplifies to $r_a = (5/2)^{1/2} n^2 a_0$. Then for the ratio R_s/r_a we get $R_s/r_a = (8.22 \times 10^3/n^2)(10^{10}T/N_e)^{1/2}$. For plasmas of $N_e \sim 10^{10}$ cm^{-3} and $T \sim 100$ K, the ratio R_s/r_a becomes smaller than one for $n > 286$. This means that for $n > 286$, plasma screening weakens the interaction of the Rydberg electron with the nucleus at least by a factor of 3. We also note that for the same plasma parameters, a noticeable weakening of this interaction by about 20% occurs already for $n = 120$. Thus, the effects of screening (including the elimination of bound states above some critical value of n) may be important for low temperature Rydberg plasmas[1].

As the screening becomes stronger, R_s decreases and the screening factor A increases, so that the number of Discrete Energy Levels (DELs) of a screened H-atom becomes reduced and the degree of degeneracy of the DELs also reduces from n^2 to $2l + 1$ (because the degeneracy of l-states is lifted). For any specific DEL, there is some Critical Screening Factor (CSF) A_c, such that for $A > A_c$ this DEL disappears by merging into the continuum.

The DELs and A_c's were calculated for a (Debye) screened H-atom by various authors (e.g., see a relatively recent reference [15] and references therein). However, most of this work was concerned only with numerical results for relatively low lying n, l states. Because Rydberg plasmas involve high $n > 20$ and high l, it is important

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[1] The study of the plasma screening for ultra-cold plasmas [2–14], where $T \ll 100\,K$, would require a separate investigation, which is beyond the scope of the present paper.

to have A_c and the corresponding DELs for screened Rydberg atoms where quantal numerical calculations become prohibitively difficult and ultimately impractical.

Some analytical results have already been published [16–18]. Smith [16] presented DELs for arbitrary states of a screened H-atom, calculated by the perturbation theory using the basis of the wave functions of the unscreened Coulomb potential. These results [16] are therefore only valid when the difference between the screened and unscreened Coulomb potentials is relatively small. The CSFs for high n-levels correspond, however, to the opposite case and thus cannot be obtained from the results of reference [16]. Bessis et al. [17] presented DELs for a screened H-atom, calculated by the perturbation theory using the basis of the wave functions of the Hulthen potential (see also references therein to previous results of this kind). The method, however, provides rigorous results only for the states of zero angular momentum ($l = 0$). As for the $l > 0$ states most relevant to Rydberg atoms, only some model results were obtained by adding an approximate rotational term.

As for classical analytical results, which are at the focus of the present paper, we point out paper by Rogers et al. [18]. In Section 2 of [18], some classical analytical results for the energy of circular Rydberg states in a screened H-atom were presented. However, it was only some basic starting formula for the classical energy – the dependence of the classical energy on the screening factor was not derived analytically in any usable form. We also note that reference [18] contained no classical calculations of the CSF and/or the critical radius of the electron orbit where DELs disappear.

All the above referenced results were obtained for the Debye potential – the most commonly used form of the screened Coulomb potential. The actual screened Coulomb potential in plasmas may, however, be more complicated than the Debye potential (see, e.g., Ref. [19]).

In the present paper, we provide classical analytical results for the dependence of the energy on the screening factor, for the CSF, and for the critical radius of the electron orbit for Circular Rydberg States (CRS) in a screened H-atom. The results are obtained for a general form of the screened Coulomb potential. As far as we know, there are, as yet, no published results of any kind on the CSF and the critical radius of the electron orbit for the general form of the screened Coulomb potential.

After deriving the results for general screened interactions, we consider a particular case of the Debye potential. Here, we obtain even more explicit analytical results for the dependence of the energy on the screening factor, for the CSF, and for the critical radius of the electron orbit. We also obtain the analytical dependence of the energy on the screening parameter. Finally, we demonstrate the existence of the CRS above the ionization threshold. They are the classical counterparts of quantal discrete states embedded into continuum [1]. We show that some of these states correspond to unstable motion, while the remainder of the CRS above the ionization threshold corresponds to stable motion.

Before proceeding with our theory, we note that CRS have been extensively studied both theoretically and experimentally for several reasons (see, e.g., [20–23] and references therein). Firstly, CRS have long radiative lifetimes and highly anisotropic collision cross-sections, thereby enabling experimental observation of inhibited spontaneous emission and other cold Rydberg gases phenomena [12–14]. Secondly, classical CRS correspond to quantal coherent states that are objects of fundamental importance. Thirdly, the classical description of CRS provided here serves as the leading and primary term in the quantal theory based on the $1/n$-expansion (see, e.g. [24] and references therein).

2 Classical analytical results for the general form of the screened Coulomb potential

Consider the H-atom, with nucleus of charge Z stationary at the origin, embedded in a plasma. Rydberg plasmas correspond to the $Z = 1$ case. We confine ourselves to circular electronic orbits of constant radius R. The classical Hamilton function in atomic units $e = m_e = 1$ is

$$H(R, A) = M^2/(2R^2) - f(AR)Z/R = E, \qquad (2)$$

where E and M are the energy and the absolute value of the angular momentum which are constant. The screened Coulomb potential in its general form (i.e., not necessarily the Debye potential) is $V(R) = -f(AR)/R$ where $A \equiv 1/R_s$ is the screening factor, the inverse value of the screening radius R_s. The function $f(x)$ which represents the departure from the pure Coulomb attraction has the following properties

$$f(x) > 0 \text{ at } 0 < x < \infty, \qquad f(0) = 1, \quad f(\infty) = 0, \quad (3)$$

so that the pure Coulomb potential is recovered for $A = 0$, while the potential vanishes as $A \to \infty$.
On introducing the following scaled quantities,

$$r \equiv RZ/M^2, \; a \equiv AM^2/Z, \; v \equiv VM^2/Z^2, \; \varepsilon \equiv EM^2/Z^2, \qquad (4)$$

the scaled Hamilton function is

$$h(r, a) \equiv HM^2/Z^2 = 1/(2r^2) - f(ar)/r. \qquad (5)$$

Dynamic equilibrium occurs when

$$dh/dr = -1/r^3 + f/r^2 - af'/r = 0, \qquad f' \equiv df/dx, \quad (6)$$

one of the conditions required to determine the equilibrium value $r_0(a)$ of the scaled radius of the orbit for a given scaled screening factor a. It can be re-written in the form:

$$a = [\,f(s) - s\,f'(s)]s, \qquad (7)$$

where $s \equiv ar_0$. The scaled energy $\varepsilon_0$at $r = r_0$ is

$$\varepsilon_0 = 1/2r_0^2 - f(s)/r_0. \qquad (8)$$

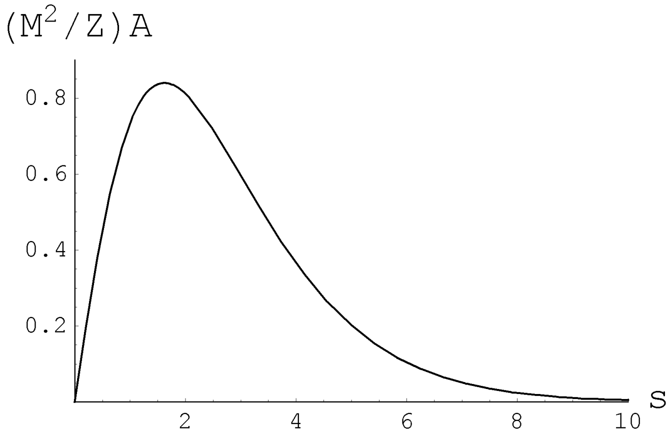

Fig. 1. Scaled screening factor $a = AM^2/Z$ versus the effective range s of the scaled Debye potential $v = -[\exp(-s)]/r$.

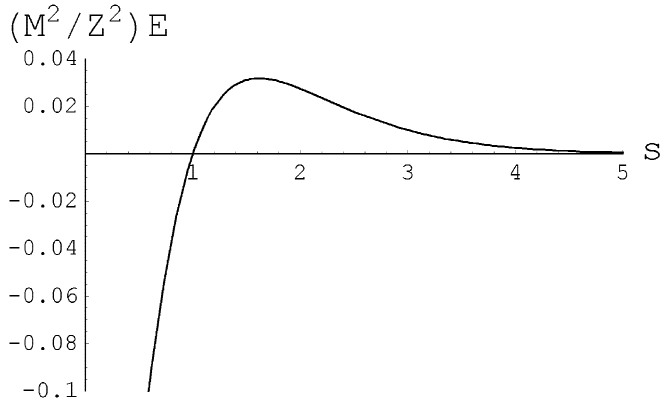

Fig. 2. Scaled energy $\varepsilon_0 = EM^2/Z^2$ versus the effective range s of the scaled Debye potential $v = -[\exp(-s)]/r$.

As the scaled screening factor a increases and exceeds some critical value a_c, the scaled energy becomes positive, which corresponds to the disappearance of the bound state of the Rydberg atom (i.e., to the merging of the bound state into the continuum). This critical value a_c is determined by substituting $a = a_c$ into the right side of equation (8) with $\varepsilon_0 = 0$ to give

$$2r_0 f(s_c) = 1, \tag{9}$$

where $s_c \equiv a_c\ r_0$. Equation (9) can be rewritten in the form:

$$a_c = 2s_c\ f(s_c), \tag{10}$$

which, with equation (7) for $a = a_c$, yields

$$2s_c\ f(s_c) = [f(s_c) - s_c\ f'(s_c)]s_c, \tag{11}$$

or the equivalent equation

$$f(s_c) = -s_c\ f'(s_c) \tag{12}$$

with respect to only one unknown quantity s_c. The solution s_{c0} of equation (12) is then substituted into the right side of equation (10) to finally give the critical value of the scaled screening factor as

$$a_c = 2s_{c0}\ f(s_{c0}). \tag{13}$$

Because the corresponding critical value of the scaled radius of the orbit is $r_{0c} = s_{c0}/a_c$, from equation (9), we also obtain

$$r_{0c} = 1/[2f(s_{c0})]. \tag{14}$$

By substituting $r_0 = s/a$ in equation (8) and then using the expression for $a(s)$ from equation (7), we obtain the analytical dependence of the energy $\varepsilon(s)$,

$$\varepsilon(s) = \{[s\, f'(s)]^2 - [f(s)]^2\}/2, \tag{15}$$

on the screening factor $a(s)$, from equation (7), via the one parameter s ($s = ar_0$).

3 Classical analytical results for the Debye potential

Application of the preceding general theory is now made to the important particular case of the Debye potential

$$v(r, a) = -[\exp(-ar)]/r. \tag{16}$$

The scaled energy at the equilibrium radius $r = r_0$ is

$$\varepsilon_0(s, r_0) = 1/2r_0^2 - \exp(-s)/r_0. \tag{17}$$

Equation (7) for the screening parameter yields

$$a(s) = s(1 + s)\exp(-s). \tag{18}$$

On expressing $\exp(-s)$ from equation (18) and substituting the result in equation (17), we obtain

$$\varepsilon_0(s, r_0) = (s - 1)/[2r_0^2\ (s + 1)] \tag{19}$$

in agreement with an equivalent expression previously presented by Rogers et al. [18]. Because the equilibrium scaled radius is

$$r_0 = s/a(s) = \exp(s)/(1 + s). \tag{20}$$

Equation (17) can be expressed as the pure function

$$\varepsilon_0(s, r_0) = -[(1 - s^2)/2]\exp(-2s) \tag{21}$$

of s alone.

Equation (21) predicts that the critical value s_c at which $\varepsilon_0 = 0$ is $s_{c0} = 1$. Then equation (18) predicts that the critical screening factor $a_c = a(s_{c0})$ at which the corresponding DEL is just about to merge into the continuum is

$$a_c = 2/e \cong 0.735759. \tag{22}$$

The classical scaled radius of this CRS orbit is

$$r_{0c} = s_{c0}/a_c = e/2 \cong 1.359141. \tag{23}$$

Equations (18) and (21) provide the analytical dependence of the energy ε_0 on the screening factor a via one parameter s. The variation of $a(s)$ and $\varepsilon_0(s)$ with s is illustrated

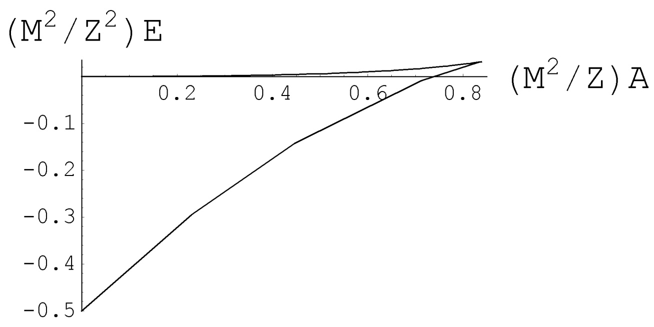

Fig. 3. Scaled energy $\varepsilon_0 = EM^2/Z^2$ of the circular state versus the scaled screening factor $a = AM^2/Z$ for the scaled Debye potential $v = -[\exp(-ar)]/r$.

in Figures 1 and 2, respectively. Both functions display their maximal values

$$a_m \cong 0.839962, \qquad \varepsilon_m \cong 0.0318091 \tag{24}$$

at $s = s_m = (1 + 5^{1/2})/2 \cong 1.61803$. Figure 3 exhibits directly the dependence of the energy ε_0 on the screening parameter a. The maxima of the functions $a(s)$ and $\varepsilon_0(s)$ in Figures 1 and 2 correspond to the "$>$"-shape crossing of the two energy branches in Figure 3. A simple analysis shows that the lower energy branch in Figure 3 corresponds to stable equilibrium, while the upper energy branch in Figure 1 corresponds to unstable equilibrium. For the case of two crossing classical energy branches, identification of the lower branch with stable equilibrium and the upper branch with unstable equilibrium was also previously shown in several different classical problems [25–27].

From Figure 1, it is seen that there are two equilibrium values of r: r_1 and $r_2 > r_1$ for any $a < a_m \cong 0.839962$. The radius r_1 corresponds to stable equilibrium and thus to a bound (or quasi-bound) state. The value r_2 associated with unstable equilibrium corresponds to the electron escaping to become free.

From the combination of Figures 1 and 2, it is seen that there are only quasi-bound states for $a_c < a < a_m$ (i.e., for $0.735759 < a < 0.839962$). Indeed, the range $0.735759 < a < 0.839962$ corresponds to the range $1 < s < 1.61803$ (see Fig. 1 and Eqs. (22), (24)). Then Figure 2 shows that for this range of s, the scaled energy takes non-negative values from 0 to 0.0318091 (see also Eq. (24)); since these energies are non-negative, the Rydberg electron is only quasi-bounded. These are the classical counterparts of quantal discrete states embedded into continuum [1].

Our classical analytical results for the critical screening factor (CSF) for Rydberg atoms can now be compared with the quantal numerical calculations for relatively low lying states available in the literature. Harris [28] and Rogers et al. [18] have both presented quantal numerical results up to the level with $n = 9$ and $l = 8$, i.e., up to the quasi-circular state 9k. For this state, Harris obtained $a_c^{Har} \cong 0.77$ (Tab. 6 of Ref. [28]) – to be compared with our present asymptotic analytical result $a_c = 2/e \cong 0.735759$. For the same 9k-state, Rogers et al. [18] obtained the scaled critical screening length $1/a_c^{Rog} \cong 1.31$ (Tab. 3 of Ref. [17]) – to be compared with our asymptotic analytical result $1/a_c = e/2 \cong 1.359141$. For the rest of our results (i.e., for the overwhelming majority of them), there is, to the best of our knowledge, nothing in the literature available for comparison.

4 Conclusion

For a *general form of the screened Coulomb potential* in a plasma, we have obtained classical analytical results for the dependence of the energy on the screening factor, for the critical screening factor, and for the critical radius of the electron orbit for circular Rydberg states (CRS). We have applied the general theory to a particular example of the Debye potential and derived even more explicit classical analytical results for the above three physical quantities.

We have also demonstrated the existence of the CRS above the ionization threshold. They are the *classical counterparts of quantal discrete states embedded into continuum*. Some of these states correspond to unstable motion, but the remaining CRS above the ionization threshold correspond to stable motion. This result has a fundamental significance. It disproves the paradigm that bound/discrete states embedded into the set of unbound/continuum states is an inherently quantum phenomenon. This result follows in spirit the results of papers [25,26] where another paradigm was disproved: in [25,26] it was shown that crossings of energy levels and charge exchange actually are not inherently quantum phenomena.

Although this entire study is motivated by the new research area of the physics of cold Rydberg plasmas, the results are also relevant to other types of plasmas. One example is fusion plasmas, where Rydberg states of multicharged hydrogenlike ions result from charge exchange with hydrogen or deuterium atoms. Another example is dusty/complex plasmas – see, e.g. [29–31][2].

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