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Classical Analytical Description of Helium Atoms or Helium-like Ions in Highly-Excited States under a High-Frequency Laser Field

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ABSTRACT: Rydberg states of hydrogenic atoms/ions in a high-frequency laser field were studied for many years. In particular, it was shown that the motion of the Rydberg electron is analogous to the motion of a satellite around an oblate planet (for a linearly-polarized laser field) or around a (fictitious) prolate planet (for a circularly-polarized laser field): it exhibits two kinds of the precession – one of them is the precession within the orbital plane and another one is the precession of the orbital plane. In the present paper we study a helium atom or a helium-like ion with one of the two electrons in a Rydberg state, the system being under a high-frequency laser field. For obtaining analytical results, we use the generalized method of the effective potentials. We find two primary effects of the high-frequency laser field on circular Rydberg states. The first effect is the precession of the orbital plane of the Rydberg electron. We calculate analytically the precession frequency and show that it differs from the case of a hydrogenic atom/ion. In the radiation spectrum this precession would manifest as satellites separated from the spectral line at the Kepler frequency by multiples of the precession frequency. The second effect is a shift of the energy of the Rydberg electron, also calculated analytically. We find that the absolute value of the shift increases monotonically as the unperturbed binding energy of the Rydberg electron increases. We also find that the shift has a non-monotonic dependence on the nuclear charge Z: as Z increases, the absolute value of the shift first increases, then reaches a maximum, and then decreases. The non-monotonic dependence of the laser-field-caused energy shift on the nuclear charge is a counterintuitive result.

Keywords: *circular Rydberg states; helium atoms; helium-like ions; high-frequency laser field; precession of the orbital plane; energy shift.*

1. INTRODUCTION

Rydberg states of hydrogenic atoms/ions in a high-frequency laser field were studied for many years. In particular, in papers [1-3] there were studies of a hydrogenic atoms/ions in a high-frequency laser field. In papers [2, 3] the focus was at Rydberg states in the classical description. By "high-frequency" it meant that the laser frequency ω is much greater than the Kepler frequency $\omega_K = m_e e^4/(n^3 \hbar^3)$ of the highly-excited hydrogen atom: $\omega >> \omega_K$. Here m_e and e are the electron mass and charge, respectively; $n >> 1$ is the principal quantum number. In this situation, the laser field and the Rydberg atom can be considered as the fast and slow subsystems, respectively, thus allowing the analytical treatment of the problem. In particular, the authors of paper [2] generalized Kapitza's method of effective potentials [4, 5].

In papers [1-3] it was revealed that this fundamental problem exhibits rich physics. When the laser field is linearly-polarized or circularly-polarized, the system has the axial symmetry, so that the square of the angular momentum M^2 should not be conserved (only its projection M_z on the axis of the symmetry is conserved). However, in papers [1-3] it was shown that M^2 is approximately conserved in this situation, so that there is an approximate algebraic symmetry higher than the geometrical symmetry.

In addition, when the laser field is linearly-polarized or circularly-polarized, the system has celestial analogies. Namely, in the linearly-polarized laser field, the motion of the Rydberg electron is analogous to the motion of a satellite around an oblate planet: it exhibits two kinds of the precession – one of them is the precession within the orbital plane and another one is the precession of the orbital plane. In the circularly-polarized laser field, the motion of the Rydberg electron is analogous to the motion of a satellite around a (fictitious) prolate planet: it exhibits the same two kinds of the precession.

In the present paper we study a helium atom or a helium-like ion with one of the two electrons in a Rydberg state, the system being under a high-frequency laser field. For obtaining analytical results, we use the generalized method of the effective potentials from works [2, 6], presented also in book [7] in Appendix A.

Then we focused at circular Rydberg states. We show that the high-frequency laser field causes the precession of the orbital plane of the Rydberg electron. We calculate analytically the precession frequency and demonstrate that it differs from the case of a hydrogenic atom/ion. In the radiation spectrum this precession would manifest as satellites separated from the spectral line at the Kepler frequency by multiples of the precession frequency.

We also show that the high-frequency laser field also causes a red shift of the energy of the Rydberg electron. We calculate analytically this energy shift and study its dependence on parameters of the system.

2. NEW RESULTS

We study a He-like atom or ion in a high-frequency laser field. The atom/ion has the inner electron in state 1s and the highly excited (Rydberg) outer electron. The potential Φ of a quasinucleus consisting of the nucleus Z and a spherically-symmetric charge distribution corresponding to the inner electron in state 1s is (see, e.g, paper [8])

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

where $\mu = M_n m_e/(M_n + m_e)$ is the reduced mass of the pair "nucleus Z – electron" (M_n is the nuclear mass and m_e is the electron mass) and r is the distance from the center of symmetry to the electron. In this study we use atomic units $\hbar = e = m_e = 1$. The atom is subjected to a high-frequency laser field of amplitude F and frequency ω. For Rydberg electrons, a classical or semi-classical treatment is appropriate.

2.1. Linear polarization of the laser field

First, we consider the case of the linear polarization of the laser field. The semi-classical Hamiltonian for the outer (Rydberg) electron in this configuration can be represented in the form

$$H = H_0 + zF\cos\omega t, H_0 = \frac{1}{2\mu_1}(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\varphi^2}{r^2\sin^2\theta}) - \Phi(r) \tag{2}$$

where $\mu_1 = m_e(M_n + m_e)/(M_n + 2m_e)$ is the reduced mass of the pair "nucleus Z with the inner electron – outer electron", the z-axis is in the direction of the laser field $\mathbf{F}$, (r, θ, φ) are the spherical coordinates of the electron, F is the magnitude and ω is the frequency of the laser field. Both μ and μ_1 are very close to unity: their physical values lie in the range between 0.999864 (for helium, $Z = 2$) and 0.999998 (for He-like oganesson, $Z = 118$). For the systems in a high-frequency field, when the frequency of the field is much greater than the highest frequency of the unperturbed system, it is appropriate to use the formalism of effective potentials [2, 4-7]. As a result, the Hamiltonian H_0 acquires a time-independent term. The zeroth-order effective potential,

$$U_0 = \frac{1}{4\omega^2}[V,[V,H_0]] = \frac{F^2}{4\mu_1\omega^2} \tag{3}$$

where $V = zF$, [P, Q] are the Poisson brackets, is a coordinate-independent energy shift that does not affect the dynamics of the system. The first non-vanishing effect on the dynamics of the system originates from the first-order effective potential:

$$U_1 = \frac{1}{4\omega^4}[[V, H_0], [[V, H_0], H_0]] =$$
$$= -\frac{F^2(Z\mu)^3}{8\mu_1^2\omega^4x^3}((Z-1)(1+3\cos 2\theta) + ((1+2x)(1+2x^2) + (3+6x+6x^2+4x^3)\cos 2\theta)e^{-2x}) \quad (4)$$

where we use the notation

$$x = \mu Z r \quad (5)$$

so that the effective potential energy of the electron is

$$U_{eff} = U + U_0 + U_1 \quad (6)$$

where U is the unperturbed potential energy.

In paper [2], where the authors studied a hydrogen Rydberg atom in a linearly-polarized high-frequency laser field, it was shown that the effective potential energy has the form

$$U_{eff}(r,\theta) = -\frac{e^2}{r} - \frac{\gamma}{r^3}(3\cos^2\theta - 1), \gamma = \frac{e^4F^2}{4m_e^2\omega^4} \quad (7)$$

where θ is the polar angle, that is, the angle between the radius-vector **r** of the electron and the *z*-axis chosen along the vector-amplitude **F** of the laser field. This effective potential energy, which is mathematically equivalent to the potential energy of a satellite around the oblate Earth (see, e.g., book [9]), has the following property: in the general case, where the unperturbed electron orbit is elliptical, the orbit undergoes simultaneously two precessions. One is the precession of the ellipse in its plane, another – the precession of the orbital plane about the vector **F**. Both of the precession frequencies are of the same order of magnitude and are much smaller than the Kepler frequency of the electron.

In our case the effective potential energy is generally more complicated. Therefore, we limit ourselves by the situation where the unperturbed orbit of the outer electron is circular. In this situation the precession in the orbital plane loses its meaning and we deal only with the precession of the orbital plane.

So, we fix r = const and only the angle θ remains as the dynamic variable. Then our effective potential energy can be brought to the form (7) with an additional θ-independent form, as shown below.

Introducing the functions

$$f(x) = (1+2x)(1+2x^2), g(x) = 3+6x+6x^2+4x^3 \quad (8)$$

we can rewrite (4) in the following form

$$U_1 = -\frac{F^2(Z\mu)^3(Z-1)}{4\mu_1^2\omega^4x^3}((3\cos^2\theta - 1)(1 + g(x)\frac{e^{-2x}}{3(Z-1)}) + \frac{3f(x)-g(x)}{2}\frac{e^{-2x}}{3(Z-1)}) \quad (9)$$

Therefore, the total energy can be represented in the form

$$U_{eff} \approx -\frac{Z-1}{r} + \Delta U_1(r) + \Delta U(r, \cos\theta) \quad (10)$$

where the second term is the energy shift with respect to the unperturbed energy, and the third term is responsible for the precession.

From (9) and (7) we see that the term

$$g(x)\frac{e^{-2x}}{3(Z-1)} \tag{11}$$

is a relative correction to the precession frequency of the orbital plane, and the term

$$\frac{3f(x)-g(x)}{2}\frac{e^{-2x}}{3(Z-1)} = 4x^3\frac{e^{-2x}}{3(Z-1)} \tag{12}$$

corresponds to an energy shift. Taking into account the factor in the beginning of (9), the energy shift is

$$\delta E = -\frac{F^2(Z\mu)^3}{3\mu_1^2\omega^4}e^{-2x} \tag{13}$$

For circular orbits, the energy of the outer electron is $E = -(Z-1)/(2r)$, and, using (5), we write the energy shift as

$$\delta E = -\frac{F^2(Z\mu)^3}{3\mu_1^2\omega^4}e^{\frac{\mu Z(Z-1)}{E}} \tag{14}$$

Figure 1 shows the dependence of the energy shift on the unperturbed electron energy for $Z = 4$, $F = 1$, $\omega = 100$. The electron Kepler frequency at these energies,

$$\omega_K = \frac{1}{Z-1}\sqrt{\frac{8|E|^3}{\mu_1}} \tag{15}$$

is indeed much smaller than the laser frequency.

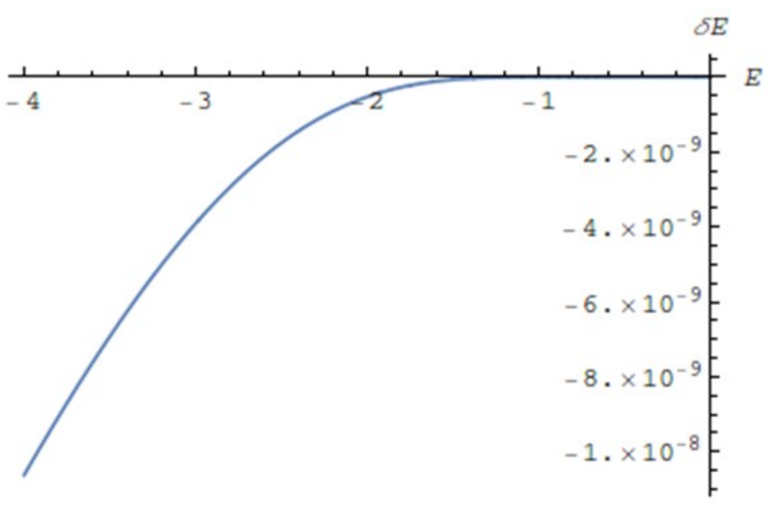

Fig. 1. The energy shift versus the unperturbed electron energy for $Z = 4$, $F = 1$, $\omega = 100$.

The shift is zero at the zero unperturbed energy, and approaches the limit $-F^2(Z\mu)^3/(3\mu_1^2\omega^4)$ as the unperturbed energy increases by the absolute value.

Figure 2 presents the dependence of the energy shift on the nuclear charge Z at $F = 1$ and $\omega = 100$ for two values of the unperturbed energy: $E = -2$ (blue, solid line) and $E = -5$ (red, dashed line). It has a minimum at the point $Z_m \approx (1 + (1 + 24|E|)^{1/2})/4$ (in the approximation $\mu = \mu_1 = 1$). The non-monotonic dependence of the energy shift on the nuclear charge is a *counter-intuitive result*.

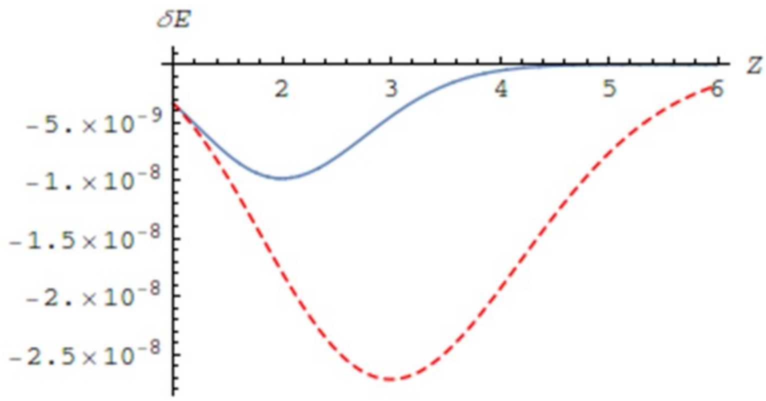

Fig. 2. The energy shift versus the nuclear charge *Z* for *E* = –2 (blue, solid line) and *E* = –5 (red, dashed line) for *F* = 1, ω = 100.

Figure 3 shows a 3D-plot of the dependence of the energy shift on both the nuclear charge and the unperturbed energy for *F* = 1 and ω = 100. It is seen that the location of the minimum of the energy shift with respect to the nuclear charge indeed moves to higher values of *Z* as the unperturbed energy increases in the absolute value.

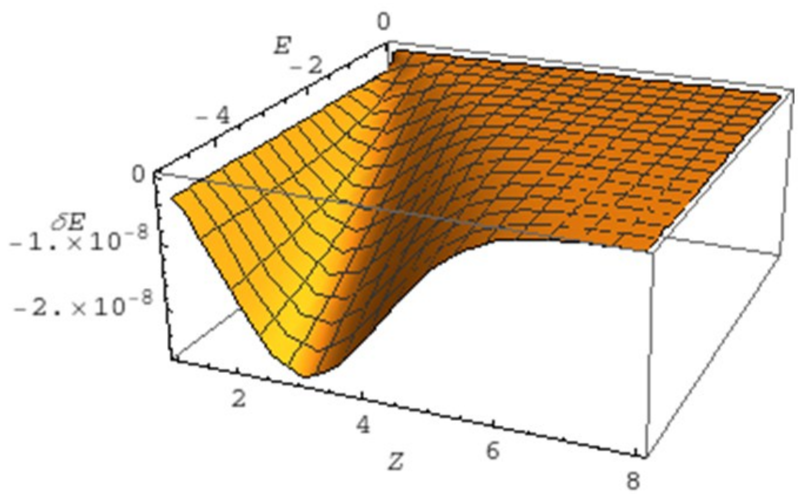

Fig. 3. The dependence of the energy shift on *Z* and *E* for *F* = 1, ω = 100.

The motion characterized by the effective potential energy

$$U_{eff} = -\frac{(Z-1)e^2}{r} - \frac{(Z-1)\gamma}{r^3}(3\cos^2\theta - 1) \tag{16}$$

is mathematically equivalent to the motion of a satellite around the oblate Earth, in the latter case the effective potential being (according, e.g., to book [9]):

$$V_E = -\frac{GM_E m}{r} - \frac{GM_E m|I_2|R^2}{2r^3}(3\cos^2\theta - 1) \tag{17}$$

Here M_E and m are the Earth and the satellite masses, respectively; R is the equatorial radius of the Earth, and I_2 is a constant characterizing the relative difference between the equatorial and polar diameters of the Earth. The ratio of the precession frequency of the satellite plane Ω to the Kepler frequency ω_K is [9]:

$$\frac{\Omega}{\omega_{E,K}} = \frac{3|I_2|}{2}\left(\frac{R}{p}\right)^2 \cos i \tag{18}$$

where

$$\omega_{E,K} = \sqrt{\frac{G(M_E + m)}{A_s^3}} \tag{19}$$

is the Kepler frequency of the satellite, m and A_s being the satellite mass and the major semi-axis of its unperturbed elliptical orbit, respectively. In Eq. (18), i is the *inclination*, that is, the angle between the plane of the satellite orbit and the equatorial plane of the Earth. The quantity p is the semi-latus rectum of the unperturbed elliptical orbit.

If in Eq. (17) we would redefine (i.e., bring into the correspondence)

$$GM_E m = (Z-1)e^2, |I_2|R^2 = \frac{2\gamma}{e^2} \tag{20}$$

then the effective potential energy from Eq. (17) would become identical to Eq. (16). By substituting $|I_2|R^2 = 2\gamma/e^2$ in Eq. (18), we obtain the corresponding ratio for our case

$$\frac{\Omega}{\omega_K}|_0 = \frac{3\gamma}{e^2 p^2}\cos i \tag{21}$$

where the Kepler frequency ω_K is given by Eq. (15) and the index "0" denotes the unperturbed case.

For circular orbits one has

$$p = r = \frac{Z-1}{2|E|} \tag{22}$$

so that the ratio from Eq. (21), corresponding to the unperturbed case, takes the form

$$\frac{\Omega}{\omega_K}|_0 = \frac{12\gamma|E|^2}{(Z-1)^2}\cos i \tag{23}$$

where in our case the quantity γ is (see Eq. (9)):

$$\gamma = \frac{F^2}{4\mu_1^2\omega^4} \tag{24}$$

For circular orbits, the dependence of the quantity x from Eq. (23) on the unperturbed energy is

$$x(E) = \mu Z r = \frac{\mu Z(Z-1)}{2|E|} \tag{25}$$

In (10), $\Delta U_1(r)$ is a relatively small shift of the energy of the electron. The dynamics of the motion beyond the plane of the unperturbed circular orbit is controlled by the following truncated $U_{eff,\,tr}$ (see (9), (10)):

$$U_{eff,tr} = -\frac{Z-1}{r} - \frac{(Z-1)\gamma}{r^3}\left(1 + g(x)\frac{e^{-2x}}{3(Z-1)}\right)(3\cos^2\theta - 1) \tag{26}$$

where $g(x)$ is given by (8), r is given by (22) and x by (25). Thus, the ratio of the precession frequency to the Kepler frequency of the electron is

$$\frac{\Omega}{\omega_K} = \frac{3\gamma}{r^2}\left(1 + g(x)\frac{e^{-2x}}{3(Z-1)}\right)\cos i = \frac{12\gamma|E|^2}{(Z-1)^2}\left(1 + g(x)\frac{e^{-2x}}{3(Z-1)}\right)\cos i \tag{27}$$

and the relative correction to the precession frequency is

$$\frac{\Delta\Omega}{\Omega} = g(x(E))\frac{e^{-2x(E)}}{3(Z-1)} \tag{28}$$

with $g(x)$ given in (8) and $x(E)$ given in (25).

Figure 4 presents the dependence of the relative correction to the precession frequency of the orbital plane of the Rydberg electron on the electron energy for selected values of Z.

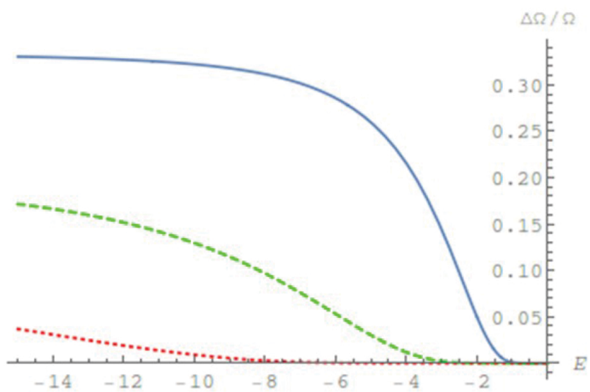

Fig. 4. Dependence of the relative correction to the precession frequency of the orbital plane of the Rydberg electron on the electron energy for Z = 4 (blue solid curve), Z = 6 (green dashed curve), and Z = 9 (red dotted curve).

The correction $\Delta\Omega/\Omega$ approaches the limit of $1/(Z-1)$ at large negative values of the electron energy.

2.2. Circular polarization of the laser field

Now we consider the case of the circular polarization of the laser field of the amplitude F and frequency ω, the polarization field being perpendicular to the z-axis. The laser field varies as

$$\mathbf{F} = F(\mathbf{e}_x \cos\omega t + \mathbf{e}_y \sin\omega t) \tag{29}$$

where $\mathbf{e}_x$ and $\mathbf{e}_y$ are the unit vectors along the x- and y-axes (which are perpendicular to the z-axis). The semi-classical Hamiltonian for the outer (Rydberg) electron in this case can be represented in the form

$$H = H_0 + xF\cos\omega t + yF\sin\omega t \tag{30}$$

where H_0 is given in (2). Denoting

$$V = xF = Fr\sin\theta\cos\varphi, W = yF = Fr\sin\theta\sin\varphi \tag{31}$$

where (r, θ, φ) are the spherical coordinates, and using the formalism of effective potentials [2, 6, 7], we obtain the zeroth-order effective potential

$$U_0 = \frac{1}{4\omega^2}([V,[V,H_0]] + [W,[W,H_0]]) = \frac{F^2}{2\mu_1\omega^2} \tag{32}$$

and the first-order effective potential

$$U_1 = \frac{1}{4\omega^4}([[V,H_0],[[V,H_0],H_0]] + [[W,H_0],[[W,H_0],H_0]]) + \frac{-1}{2\omega^3}[[V,H_0],[W,H_0]] =$$
$$= \frac{F^2(Z\mu)^3}{8\mu_1^2\omega^4 x^3}((Z-1)(1+3\cos 2\theta) + ((1+2x+2x^2-4x^3) + (3+6x+6x^2+4x^3)\cos 2\theta)e^{-2x}) \tag{33}$$

where x is given in (5). Using the same procedure as in the case of the linear polarization, we can rewrite U_1 in the form as in (9):

$$U_1 = \frac{F^2(Z\mu)^3(Z-1)}{4\mu_1^2\omega^4x^3}((3\cos^2\theta - 1)(1 + g(x)\frac{e^{-2x}}{3(Z-1)}) + \frac{3f_1(x) - g(x)}{2}\frac{e^{-2x}}{3(Z-1)}) \quad (34)$$

It differs from (9) by the sign in the beginning and a different function $f_1(x)$, which is given by

$$f_1(x) = 1 + 2x + 2x^2 - 4x^3 \quad (35)$$

From (34) we find that the energy shift in the case of circular polarization is

$$\delta E = -\frac{2F^2(Z\mu)^3}{3\mu_1^2\omega^4}e^{-2x} \quad (36)$$

which is twice as much as in the linear case. The relative correction to the precession frequency of the orbital plane is the same as in the linear-polarization case (given in (11) and (28)).

3. CONCLUSIONS

We studied a helium atom or a helium-like ion with one of the two electrons in a Rydberg state while the system is subjected to a high-frequency laser field. For obtaining analytical results, we use the generalized method of the effective potentials from works [2, 6, 7].

Then we concentrated on circular Rydberg states. We found two primary effects of the high-frequency laser field. The first effect is the precession of the orbital plane of the Rydberg electron. We calculated analytically the precession frequency and showed that it differs from the case of a hydrogenic atom/ion. In the radiation spectrum this precession would manifest as satellites separated from the spectral line at the Kepler frequency by multiples of the precession frequency.

We also demonstrated that the high-frequency laser field causes a red shift of the energy of the Rydberg electron – the shift that we calculated analytically. We studied its dependence on parameters of the system. We found that the absolute value of the shift increases monotonically as the unperturbed binding energy of the Rydberg electron increases. We also found that the shift has a non-monotonic dependence on the nuclear charge Z: as Z increases, the absolute value of the shift first increases, then reaches a maximum, and then decreases. The non-monotonic dependence of the laser-field-caused energy shift on the nuclear charge is a *counterintuitive* result.

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