

Lithium Atoms or Lithium-like Ions in a High-Frequency Laser Field: Circular Rydberg States

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ABSTRACT: We analyze a lithium atom or a lithium-like ion, one of the three electrons being in a Rydberg state, subjected to a laser field of high frequency. We used the generalized method of the effective potentials. We describe analytically the following two outcomes for circular Rydberg states. One of the outcomes is the precession of the plane of the orbit of the highly excited electron – the precession whose frequency we calculate analytically. It leads to the following modification of the radiation spectrum: the appearance of satellites at the distances from the unperturbed frequency of the spectral line equal to multiples of the precession frequency. The other outcome is an energy shift of the Rydberg electron. Its dependence on the nuclear charge was found to be a non-monotonic function. This is a counterintuitive result.

KEYWORDS: circular Rydberg states; lithium atoms and lithium-like ions; high-frequency laser field; precession of the orbital plane; energy shift

1. INTRODUCTION

We consider a Li atom or a Li-like ion in a high-frequency laser field. (This is the follow-up to paper [1] where we studied a He atom or a He-like ion in a high-frequency laser field.) The atom/ion has two inner electrons in the state 1s, while the third, outer, electron is in a highly excited (Rydberg) state. The potential Φ of a system consisting of a nucleus of charge Z and two inner electrons in state 1s is (see, e.g., [2, 3])

$$\Phi = \frac{Z-2}{r} + 2\left(\left(Z - \frac{5}{16}\right)\mu + \frac{1}{r}\right)e^{-2\left(Z - \frac{5}{16}\right)\mu r} \quad (1)$$

where $\mu = M_n m_e / (M_n + m_e)$ is the reduced mass of the pair “nucleus Z – electron” (M_n is the mass of the nucleus and m_e is the mass of the electron) and r is the distance from the center of the atom to the electron. Here we use atomic units: $\hbar = e = m_e = 1$. The atom is placed into a laser field of high frequency ω and amplitude F . The case of Rydberg electrons can be treated classically or semi-classically.

2. NEW RESULTS

2.1. Linearly-polarized laser field

First, we study the case of the linearly-polarized laser field. The Hamiltonian for the outer electron in this system can be written in the following way:

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

where $\mu_1 = m_e(M_n + 2m_e)/(M_n + 3m_e)$ is the reduced mass of the pair “nucleus Z with the two inner electrons – outer electron”, the z -axis is parallel to the laser field \mathbf{F} , (r, θ, φ) are the spherical coordinates of the electron. μ and μ_1 are approximately equal to 1: their physical values are between 0.999922 (for lithium, $Z = 3$) and 0.999998 (for Li-like oganesson, $Z = 118$). For the analysis of systems subjected to a high-frequency field, with the field frequency much greater than the highest frequency of the unperturbed system, the formalism of effective potentials [4-8] is appropriate. After the application of this formalism, a time-independent term gets added to the Hamiltonian H_0 . The zeroth-order effective potential,

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

where $V = zF$ and $[P, Q]$ are the Poisson brackets, is an energy shift that does not depend on the coordinates and thus does not affect the system dynamics. The first non-zero effect on the system dynamics comes from the first-order effective potential:

$$U_1 = \frac{1}{4\omega^4} [[V, H_0], [[V, H_0], H_0]] = \\ = -\frac{F^2((Z - \frac{5}{16})\mu)^3(Z - 2)}{4\mu_1^2\omega^4x^3} \left(\frac{8x^3}{3(Z - 2)} e^{-2x} + (3\cos^2\theta - 1) \left(1 + \frac{2g(x)}{3(Z - 2)} e^{-2x} \right) \right) \quad (4)$$

where x is the corresponding analogue of the notation introduced in paper [1],

$$x = \mu \left(Z - \frac{5}{16} \right) r \quad (5)$$

and

$$g(x) = 3 + 6x + 6x^2 + 4x^3 \quad (6)$$

In the limit of $x \ll 1$, the first-order effective potential simplifies to:

$$U_1 \approx \frac{F^2 Z}{4\mu_1^2\omega^4} \frac{1 - 3\cos^2\theta}{r^3} \quad (7)$$

It differs only by the factor Z from the corresponding first-order effective potential, derived in paper [4] for a hydrogen Rydberg atom in a linearly-polarized high-frequency laser field. As noted in paper [4], this kind of effective potential is also a mathematical analogue of the potential energy of a satellite orbiting around the oblate Earth [9].

As it was shown in paper [1] and references therein, the perturbing potential of the type given by Eq. (4), modifies the unperturbed Coulomb potential and exhibits the following physical behavior: in the general case of an elliptic orbit, the orbit engages in two kinds of precession. One kind is the precession of the elliptic orbit in its own plane. Another kind is the precession of the plane of the orbit about the vector \mathbf{F} . The frequencies of both precessions are of the same order of magnitude; the electron’s Kepler frequency is much greater than any of the two precession frequencies. As in paper [1], we study the case of a circular unperturbed orbit of the outer electron. In this case the first precession – of the elliptic orbit in its plane – becomes irrelevant and we take into account only the second precession – the one of the orbital plane.

The potential from Eq. (4) is similar to the potential for the He-like case (Eq. (9) in paper [1]), which we reproduce here for comparison:

$$U_1 = -\frac{F^2(Z\mu)^3(Z - 1)}{4\mu_1^2\omega^4x^3} \left(\frac{4x^3}{3(Z - 1)} e^{-2x} + (3\cos^2\theta - 1) \left(1 + \frac{g(x)}{3(Z - 1)} e^{-2x} \right) \right) \quad (8)$$

Thus, the quantity

$$\frac{\Delta\Omega}{\Omega} = \frac{2g(x)}{3(Z-2)} e^{-2x} \quad (9)$$

is a relative correction to the precession frequency of the plane of the orbit, and the quantity

$$\delta E = -\frac{F^2((Z-\frac{5}{16})\mu)^3(Z-2)}{4\mu_1^2\omega^4x^3} \frac{8x^3}{3(Z-2)} e^{-2x} = -\frac{2F^2((Z-\frac{5}{16})\mu)^3}{3\mu_1^2\omega^4} e^{-2x} \quad (10)$$

corresponds to an energy shift. In a circular orbit, the outer electron has energy $E = -(Z-2)/(2r)$ and, using Eq. (5), we get the dependence of x on the unperturbed energy as

$$x(E) = \mu(Z - \frac{5}{16})r = -\frac{\mu(Z - \frac{5}{16})(Z-2)}{2E} \quad (11)$$

and we rewrite the energy shift in the form:

$$\delta E = -\frac{2F^2((Z - \frac{5}{16})\mu)^3}{3\mu_1^2\omega^4} e^{\frac{\mu(Z-\frac{5}{16})(Z-2)}{E}} \quad (12)$$

Fig. 1 shows the energy shift as a function of the unperturbed electron energy for $Z = 4, 6$ and 9 in the laser field with $F = 1$ and $\omega = 80$.

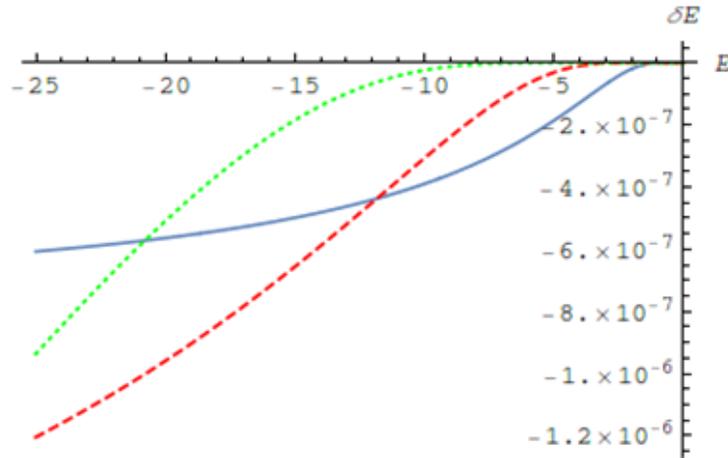


Fig. 1. The energy shift versus the unperturbed electron energy for $Z = 4$ (blue, solid curve), $Z = 6$ (red, dashed curve) and $Z = 9$ (green, dotted curve) for $F = 1$, $\omega = 80$.

We see that the energy shift is zero at the zero unperturbed energy and approaches the limit $-2F^2((Z - 5/16)\mu)^3/(3\mu_1^2\omega^4)$ as the absolute value of the unperturbed energy increases. Taking the ratio of the energy shift in our case to the energy shift in the He-like case (Eq. (14) in paper [1]), which is

$$\frac{\delta E}{\delta E_{He}} = 2(1 - \frac{5}{16Z})^3 e^{-\frac{(21Z-10)\mu}{16E}} \quad (13)$$

we see that for negative E and $Z \geq 2$, the ratio is always greater than 1, so for the given energy of the outer electron, the energy shift is always greater by the absolute value in the Li-like case than in the He-like case.

Figure 2 shows the energy shift as a function of the nuclear charge Z . Comparing it with Fig. 3 in paper [1], we see that it is similar, and the shift is greater in the Li-like case.

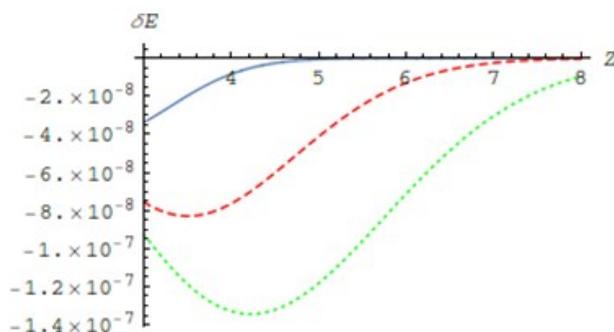


Fig. 2. The energy shift versus the nuclear charge Z for $E = -2$ (blue, solid curve), $E = -5$ (red, dashed curve) and $E = -8$ (green, dotted curve) for $F = 1$, $\omega = 100$.

It is seen that with the growth of Z , the energy shift has the non-monotonic dependence on the nuclear charge, which is a *counterintuitive* result.

Figure 3 shows the ratio of the energy shift in the Li-like case to the one in the He-like case given by Eq. (13) depending on the energy of the electron, for the nuclear charge $Z = 4$.

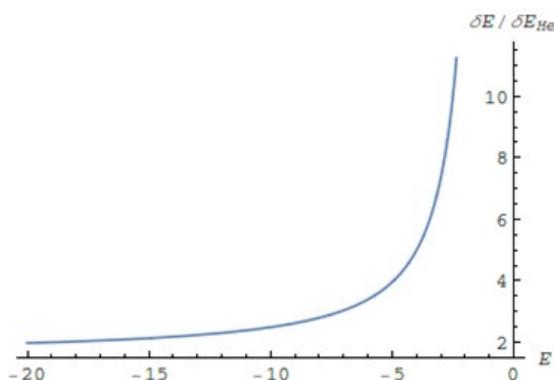


Fig. 3. The ratio of the energy shift in the Li-like case to the one in the He-like case, depending on the energy of the electron, for $Z = 4$.

Figure 4 shows the ratio of the energy shift in the Li-like case to the one in the He-like case given by Eq. (13) depending on the nuclear charge, for the value of electron energy $E = -10$.

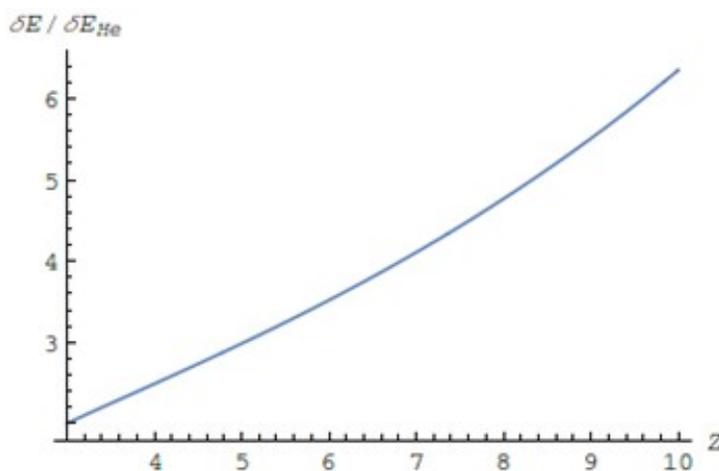


Fig. 4. The ratio of the energy shift in the Li-like case to the one in the He-like case, depending on the nuclear charge, for $E = -10$.

The relative correction to the precession frequency of the plane of motion is given by Eq. (9). Using the energy of the outer electron in the case of circular orbits, $E = -(Z - 2)/(2r)$, and Eq. (5), we express the relative correction to the precession frequency, $\delta\Omega$, as a function of E and Z :

$$\delta\Omega = \frac{\Delta\Omega}{\Omega} = \frac{2g(x(E))}{3(Z-2)} e^{-2x(E)}. \quad (14)$$

where $g(x)$ is given in Eq. (6) and $x(E)$ is given in Eq. (11).

Figure 5 shows the relative correction to the precession frequency of the orbital plane of the Rydberg electron versus the electron energy for several values of the nuclear charge Z .

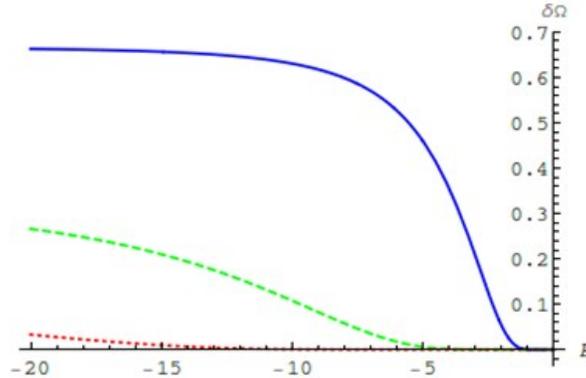


Fig. 5. The dependence of the relative correction to the precession frequency of the orbital plane of the Rydberg electron on the electron energy for several values of the nuclear charge: $Z = 5$ (blue solid curve), $Z = 8$ (green dashed curve), and $Z = 12$ (red dotted curve).

It is seen that for $Z = 5$, the relative correction is about $2/3$ for most of the energy range considered. The correction $\delta\Omega = \Delta\Omega/\Omega$ approaches the limit of $2/(Z-2)$ at large negative values of the energy of the electron.

For comparing the relative correction $\delta\Omega$ in the present Li-like case to the corresponding quantity in the previously studied He-like case, we take the ratio of the correction in the present case, given by Eq. (14), to the one in the He-like case. The correction in the He-like case is given in Eqs. (28) and (25) in paper [1]:

$$\delta\Omega_{He} = \frac{g(x_{He}(E))}{3(Z-1)} e^{-2x_{He}(E)}, \quad x_{He}(E) = -\frac{\mu Z(Z-1)}{2E} \quad (15)$$

The ratio of the relative corrections has the form:

$$\frac{\delta\Omega}{\delta\Omega_{He}} = 2 \frac{Z-1}{Z-2} \frac{g(x(E))}{g(x_{He}(E))} e^{-\frac{(21Z-10)\mu}{16E}} \quad (16)$$

where $g(x)$ is given in Eq. (6), $x(E)$ is given in Eq. (11), and $x_{He}(E)$ is given in Eq. (15). For $Z \geq 2$ and negative E , the ratio from Eq. (16) is strictly greater than unity, so the relative correction $\delta\Omega$ is always greater than in the He-like case for the given values of the outer electron energy and the nuclear charge Z .

It should be emphasized that in the radiation spectrum, this precession would lead to satellites, whose distance from the spectral line at the Kepler frequency is equal to multiples of the precession frequency. Therefore, our result on the more precise value of the precession frequency seems to be important for the comparison with experiments.

2.2. Circularly-polarized laser field

Now we study the case of the circularly-polarized laser field of the amplitude F and frequency ω , with the polarization field perpendicular to the z -axis, which can be represented in the following way:

$$\mathbf{F} = F(\mathbf{e}_x \cos\omega t + \mathbf{e}_y \sin\omega t) \quad (17)$$

where \mathbf{e}_x and \mathbf{e}_y are the unit vectors on the x - and y -axes (perpendicular to the z -axis). The Hamiltonian for the outer electron in this system can be written in the following way:

$$H = H_0 + xF\cos\omega t + yF\sin\omega t \quad (18)$$

where H_0 is given in Eq. (2). Denoting

$$V = xF = Fr\sin\theta\cos\varphi, W = yF = Fr\sin\theta\sin\varphi \quad (19)$$

where (r, θ, φ) are the spherical coordinates, and applying the formalism of effective potentials [4-8], we obtain the following zeroth-order effective potential

$$U_0 = \frac{1}{4\omega^2} ([V, [V, H_0]] + [W, [W, H_0]]) = \frac{F^2}{2\mu_1\omega^2} \quad (20)$$

and the first-order effective potential

$$\begin{aligned} U_1 &= \frac{1}{4\omega^4} ([[V, H_0], [[V, H_0], H_0]] + [[W, H_0], [[W, H_0], H_0]]) + \frac{-1}{2\omega^3} [[V, H_0], [W, H_0]] = \\ &= \frac{F^2((Z - \frac{5}{16})\mu)^3(Z - 2)}{4\mu_1^2\omega^4x^3} (-\frac{16x^3}{3(Z - 2)}e^{-2x} + (3\cos^2\theta - 1)(1 + \frac{2g(x)}{3(Z - 2)}e^{-2x})) \end{aligned} \quad (21)$$

From the form of Eq. (21), by comparing it to Eq. (8) related to the case of linear polarization, we see that the energy shift is twice as that of the linear-polarization case, and the correction to the precession frequency is the same as in the linear-polarization case.

3. CONCLUSIONS

We studied a Li atom or a Li-like ion in a high-frequency laser field. We derived the effective potential and showed that, if the outer electron would be at a relatively small distance r from the nucleus, the effective potential would differ just by a factor Z from the corresponding effective potential, derived in paper [4] for a hydrogen Rydberg atom in a linearly-polarized laser field of high frequency. We noted that in this situation, the effective potential is analogous to the potential of a satellite moving around the oblate Earth.

For circular Rydberg states we calculated analytically a more precise value of the frequency of the precession of the plane of the orbit of the Rydberg electron. This precession would lead to satellites, whose distance from the spectral line at the Kepler frequency is equal to multiples of the precession frequency. Therefore, our result on the more precise value of the precession frequency seems to be important for the comparison with experiments.

We also calculated analytically the red shift of the energy of the highly-excited electron caused by the high-frequency laser field. It turned out that, as the unperturbed binding energy of the Rydberg electron increases, the absolute value of the shift increases monotonically. However, the dependence of the shift on the nuclear charge Z was found to be non-monotonic. This is a *counterintuitive* result.

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