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The study on ionization of hydrogen atoms in a laser field considering non-dipole approximation and Coulomb corrections

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Abstact. We report a theoretical study of low-energy structures (LES) in the process of the strong-field ionization in the velocity gauge when considering non-dipole approximation and Coulomb corrections respectively. Comparisons have been made between considering non-dipole approximation and Coulomb corrections. A derivation of the photoelectron energy spectra for a hydrogen atom in a strong linearly polarized laser field is presented, which is considering non-dipole approximation and Coulomb corrections in the ground state. Based on the quantum and semiclassical analysis, we calculate ionization rates changed with the energy and variable regular changed with the wavelength and intensity have been also discussed.

1. Introduction

Recently, owing to the rapid advanced laser technology, the photoionization processes of atoms and molecules in strong laser fields have attracted attention in experiment and theory. The strong field ionization processes can be described through Keldysh-Faisal-Reiss (KFR) [1-3] theories or strong field approximation theories (SFA)[4]. S-matrix theories is employed to study ionization. Keldysh proposed the adiabatical parameter γ and got the simpler analytical expressions for ionization rates. When the parameter $\gamma \ll 1$ of Keldysh is tunneling and multiphoton ionization, $\gamma \gg 1$, the parameter $\gamma = \sqrt{I_p/2U_p}$ of Keldysh (I_p is the ionization potential and $U_p = F^2/4\omega^2$ is the ponderomotive potential where the energy of oscillating motion of a free electron can be driven by incident laser field. Herein, F is the amplitude of the electric field). In this work we consistently use atomic units (a.u.) $\hbar = e = m_e = 1$.

Recently, LES was discovered in experiment of the electron spectra. The LES were found to be present in the spectra of different atomic targets, which indicated a general phenomenon. A semi-classical approach based on quantum orbits was presented in these ref.[5,6,7]. In the tunneling regime, LES was found [8, 9]. Semiclassical model [9, 10] was applied to research the LES. In its production, the non-dipole effects and Coulomb potential played the very important roles.

In strong-field ionization, non-non-dipole effects were researched subject to lots of groups and were observed experimentally. Multiply charged ions were studied under the condition of ultrahigh-intensity beams at wavelengths of 800 nm [11–13] and 1053 nm [14,15] and extreme ultraviolet pulses[16].

They also were studied in the course of calculations on photoelectron rescattering processes [17-20], and studied the laser driven ion dynamics [21-25] theoretically. In this work, we present the theoretical study on non-dipole strong-field ionization and then explore the Coulomb potential on the low-energy photoelectron dynamics for the important case of linearly polarized light.

The LES for a hydrogen atom in the strong linearly polarized laser field in the ground state is presented when considering the non-dipole approximation. At the same time, the LES is presened by taking into accounts Coulomb correction. Based on quantum and semi-classical analysis, the roles of the non-dipole approximation and Coulomb correction in the LES are investigated. In addition, we consider the hydrogenlike atom in a linearly polarized laser field, only when the laser field is strong enough to act as a simple theory that can be applied.

2. Theoretical methods

Considering the hydrogen-like atom, we put Z for the hydrogen in our numerical calculation. The approximate probability amplitude of strong-field ionization is

$$(S-1)_{fi} = -i\int_{-\infty}^{\infty} dt(\Psi_f, H_I\Psi_i), \tag{1}$$

The initial state of a hydrogen-like ion can be written as follows:

$$\begin{aligned}\psi_i(r,t) &= \psi_i(r)\exp(iE_Bt)\\ &= \sqrt{\frac{Z^3}{\pi}}\exp(-Zr)\exp(i\frac{Z^2}{2}t)\end{aligned}, \tag{2}$$

and the final state wave function is

$$\psi_f = \frac{1}{(2\pi)^{3/2}}\exp\{\frac{i}{\hbar}p\cdot r - \frac{i}{\hbar}p^2t - \frac{i}{\hbar}\int_{-\infty}^{t}d\tau H(p,\tau)\}, \tag{3}$$

Ψ_f is Volkov state that is eigenstate of H_I.

The laser-atom interaction Hamiltonian H_I is given by

$$H_I = A\cdot P + \frac{1}{2}A^2 = A\cdot(-i\nabla) + \frac{1}{2}A^2, \tag{4}$$

Considering the radiation field is linear polarized, under the non-dipole approximation, the electric field can be written as

$$\vec{A}(\vec{r},t) = a\vec{\varepsilon}\cos(\omega t) + a\vec{\varepsilon}\sin(\omega t)\cdot\vec{k}\cdot\vec{r}, \tag{5}$$

Where A is the amplitude of the vector potential, ω is the frequency of the laser field, k is the wave vector, the ε represents

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the unit vector in the direction of polarization.

A can be expanded near the zero of $u = k \cdot r$ into Taylor series

$$A(r,t) = \varepsilon A_0 \{\cos \omega t + k \cdot r \sin \omega t + \cdots\},\qquad(6)$$

The first expansions $\varepsilon A_0 \cos \omega t$ is the result of long wave approximation and the second expansion $\varepsilon A_0 k \cdot r \sin \omega t$ is the first order correction of non-dipole approximation

$$H_I = H_I^{(0)} + H_I^{(1)},\qquad(7)$$

The Eq. (7) is the Hamiltonian in the non-dipole approximation. Where

$$H_I^{(0)} = \frac{e}{m} \varepsilon \cdot p A_0 \cos \omega t + \frac{e^2 A_0^2}{2m}\cos^2 \omega t,\qquad(8)$$

And

$$H_I^{(1)} = k \cdot r[\frac{e}{m} \varepsilon \cdot p A_0 \sin \omega t + \frac{e^2 A_0^2}{2m}\sin 2\omega t],\qquad(9)$$

the Eq. (9) is the Hamiltonian in the first order correction of dipole approximation.

$$(S-1)_{fi} = (S-1)_{fi}^{(0)} + (S-1)_{fi}^{(1)},\qquad(10)$$

According to Reiss' treatment,

$$(S-1)_{fi}^{(0)} = \frac{i}{\hbar}\phi_i^{(0)}(p)(\frac{p^2}{2m} - E_i)\int_{-\infty}^{\infty} dt \exp\{\frac{i}{\hbar}(p^2 - E_i + U_p)t + i\zeta \sin \omega t + i\frac{z}{2}\sin 2\omega t\}\qquad(11)$$

Where

$$\zeta = \frac{e A_0}{m\hbar\omega}\varepsilon \cdot p,\qquad(12)$$

$$(S-1)_{fi}^{(1)} = -\frac{i}{\hbar\omega}\phi_i^{(1)}\int dx[\zeta \sin x + 2z \sin 2x]\times\exp\{\frac{i}{\hbar\omega}(\frac{p^2}{2m} - E_i + U_p)x$$
$$+ i\zeta \sin x + i\frac{z}{2}\sin 2x\}\qquad,(13)$$

$$U_P = \frac{e^2 A_0^2}{4m},\qquad(14)$$

$$z = \frac{U_p}{\hbar\omega} = \frac{e^2 A_0^2}{4m\hbar\omega},\qquad(15)$$

$\phi_i^{(0)}$ and $\phi_i^{(1)}$ are the Fourier transformation of the bound state.

$$\phi_i^{(0)} = \frac{1}{(2\pi)^{3/2}}\int d^3r \exp[-\frac{i}{\hbar}p \cdot r]\psi_{i(r)},\qquad(16)$$

$$\phi_i^{(1)} = \frac{1}{(2\pi)^{3/2}}\int d^3r k \cdot r \exp[-\frac{i}{\hbar}p \cdot r]\psi_{i(r)},\qquad(17)$$

As a model, we consider a hydrogen atom in the strong laser field. The rate of photoionization for direct transition from the ground state to the continuum state is given as follows:

$$w = |(S-1)_{fi}|^2\qquad(18)$$

$$W = \int_0^\infty wp^2 dp \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi = \int_0^\infty w\sqrt{2E}dE\int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi,\qquad(19)$$

The ionization rate per unit energy is

$$\frac{dW}{dE} = \int_0^\pi w\sqrt{2E}\sin\theta d\theta \int_0^{2\pi} d\phi,\qquad(20)$$

$$\frac{dW}{dE} = \int wpd\Omega$$
$$= \int d\Omega \sum_{n=n_0} \frac{32Z^5\omega^2\sqrt{2E}}{(Z^2 + p^2)^4}\left|J_n(\xi, -\frac{z}{2})\right|^2 (z-n)^2\delta(\frac{p^2}{2m_e} - E_i + z\omega - n\omega)$$
$$- \frac{128\omega^2(p)^2 k}{[(Z/a_0)^2 + (p/\hbar)^2]^5}(\frac{Z}{a_0})^5\{(\zeta_1 + 2z)(n_0 - z)\left|J_{n0}(\zeta_1, -\frac{z}{2})\right|\delta(\frac{p^2}{2m} - E_i - n_0\omega + z\omega)$$
$$+ 2z(n_1 - z)\left|J_{n1}(\zeta_1, -\frac{z}{2})\right|\delta(\frac{p^2}{2m} - E_i - n_1\omega + z\omega)\}$$

$$(21)$$

It is the main result of this paper: a formula for ionization energy spectra of 1s hydrogen atom can be obtained considering non-dipole approximation.

The Coulomb volkov wave function is originates from the

ref.[26]

$$\psi_f^{WKB} = \psi_f \exp[\frac{iZ}{a_0}(\frac{5}{4}t - \frac{1}{8\omega}\sin 2\omega t)],\qquad(22)$$

a_0 is the Bohr radius. In the non-non-dipole approximation, thevector potential

$$A(t) = A\varepsilon \cos \omega t,\qquad(23)$$

And

$$H_I = \frac{e}{m}\varepsilon \cdot p A_0 \cos \omega t + \frac{e^2 A_0^2}{2m}\cos^2 \omega t,\qquad(24)$$

$$(S-1)_{fi} = -i(2\pi)\phi_i^0\omega\sum(2-n)$$
$$\times J_n(\zeta_1 + \frac{ZA}{8\omega\alpha_0}, -\frac{\pi}{2})\qquad,(25)$$
$$\times \delta(E_f + (2-n)\omega - \frac{5ZA}{4\alpha_0} + E_B)$$

3. Results and discussion

We get numerical results by using our analytical formula for the atomic system. The initial state of the atom in this paper is the ground state. The laser is 2000nm at intensity 100TWcm-2. The calculation result is shown in Fig3.1. We present the low-energy part of the measured photoelectron spectra by considering the non-non-dipole approximation, the non-dipole approximation and the Coulomb correctionsin its ground state, respectively, followed by taking account of the tunneling regime ($\gamma \ll 1$)and ($I_P/\omega \gg 1$). For wavelength value of 2000nm, the above threshold ionization(ATI) peaks can be clearly observed. We can't find obviously the changes caused by non-dipole approximation. There is an obvious change in the curve through the Coulomb corrections.

In Fig. 3.2, we show ionization rates changed with the energy for different wavelength at intensity 520TWcm-2 considering Coulomb corrections. The ATI peaks become less pronounced with wavelength increasing. The ATI peaks cannot be distinguished in the spectrum for 2000nm. Nevertheless, in the long-wavelength spectra[27], the LES[15,16] becomes noticeable .
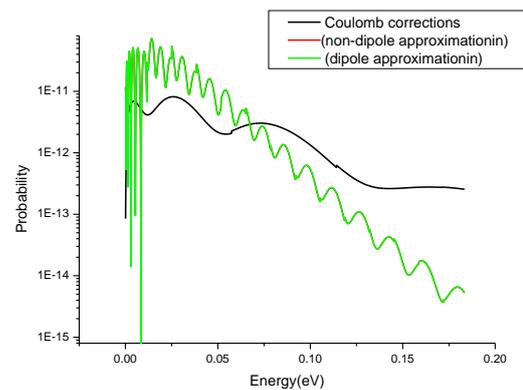

Fig.3.1: The low-energy part of the measured photoelectron spectra considering the non-non-dipole approximation, the non-dipole approximation and the Coulomb corrections respectively in its ground state.

In Fig.3.3, these ionization rates are similar kind of lines as before, but for the wavelength 2000nm, the ionization rates changed with the energy for different intense of the laser field I. With increasing intense of the laser field, the ATI peaks become more pronounced.
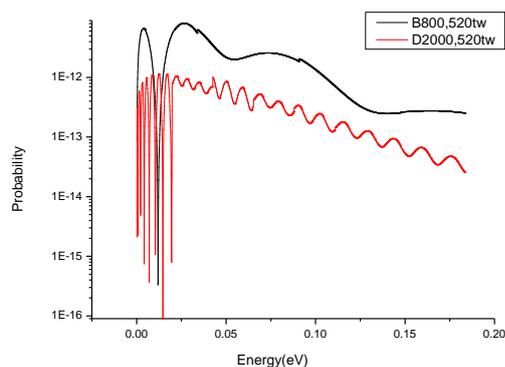
Fig.3.2: The ionization rates changed with the energy for different wavelength at intensity 520TWcm^{-2} considering Coulomb corrections.
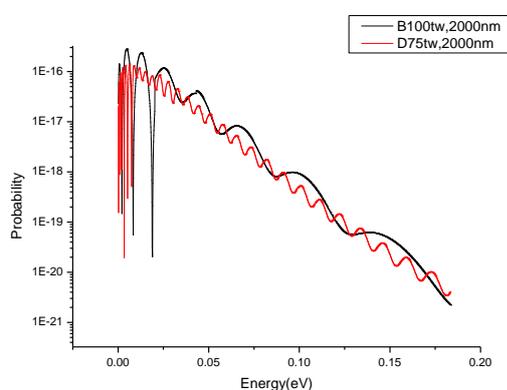
Fig.3.3. Plot of the ionization rates changed with the energy for different intense of the laser field I for the wavelength 2000nm.

4. Conclusion

In summary, for 1s hydrogen atom, we have derived the LES in the process of the strong-field ionization in the velocity gauge taking into accounts non-dipole approximation and Coulomb corrections respectively for the ground state of a hydrogen atom. An analysis of the numerical result for photoelectron spectra calculated via our formulas Eq. (21), as well as the combined result Eq. (25) shows that discrepancy between considering dipole approximation and considering Coulomb corrections. Based on our quantum and semiclassical analysis, the non-dipole approximation and Coulomb corrections in the production of this LES play an important part. It is the Coulomb attraction between the electron and ionic core which seems to be responsible for the origin of the LES.

Acknowledgements

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