Electron dynamics under the influence of the strong laser field: a classical approach

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We present the classical ionization trajectory of hydrogen atoms in a strong laser field by numerically solving Newton's equation using the Monte-Carlo method. The electron ionization trajectories are scrutinized for different optical periods (T_D = 1T, 3T, and 5T), and it is found that the pulse duration of the laser field has significantly influenced the ionization trajectory of the ionized electron. For the short optical period, the electron gains enough energy and be ionized, while for a long optical period, when the pulse duration has not attained an optical period, the absorbed energy is not enough to ionize the atom. Moreover, the trajectory of the ionized electrons alters correspondingly with the change in the carrier-envelope phase of the laser field.

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1. Introduction

In the past two decades, the process of laser-atom interactions in intense laser fields has attracted much attention due to the highly nonlinear optical phenomena [1-4]. Among these phenomena, above-threshold ionization (ATI), high-order harmonic generation (HHG), and non-sequential double ionization (NSDI) are the most well-known examples [5-8]. Particularly, HHG offers a favourable technique to originate the coherent extreme ultraviolet (XUV) light source in the attosecond time scale [9-11], which leads to unique applications such as the observation and control of the real-time electronic dynamical behaviour [12-14]. Different theoretical approaches are employed to comprehend these diverse phenomena, for example, the numerical solution of the time-dependent Schrödinger equation (TDSE), the strong-field approximation (SFA) [15-17], and semiclassical models [18, 19]. In the classical models, the detached electron is described as a classical corpuscle that obeys the Newtonian laws of motion [20]. The two-step model for ionization [21, 22] and the three-step models for HHG and rescattering are widely used based on the semiclassical approaches [23]. In the two-step model, the electron tunnels out of an atom, and then it propagates in the applied laser field. In the third step, the electron is driven back toward the residual ion to recombine to the ground state and emits the harmonic photons. The three-step model describes a qualitative picture of the rescattering-induced process, i.e., high-order ATI, HHG, and NSDI [24].

Over the last two decades, although significant advancement has been made in the development of the theoretical approaches based on SFA and TDSE [25, 26], still, the semiclassical approaches are extensively used in strong laser field physics. The semiclassical simulations have a number of advantages as it helps to provide an illustrative picture in terms of classical trajectories. The essential features such as cutoffs and plateaux in HHG and high-order ATI spectra [27-29], the maximum angles in the photoelectron angular distributions [30], and the characteristic momenta of recoil ions of the NSDI [31] are explained by means of classical and semiclassical models. In both the two-step and three-step models, the effect of the Coulomb potential of the parent ion on the electron motion after ionization is neglected [24]. The presence of the Coulomb potential in the two-step model reveals the Coulomb focusing effect [32]. The Coulomb cusp in the angular distribution of strong-field ionized electrons can be identified by employing classical trajectory Monte Carlo (CTMC) simulations [33].

In this work, we focus on the classical treatment of the one-electron atom embedded in a strong laser field using the CTMC technique. The classical ionization trajectories are investigated for different optical periods. It is found that the duration of the laser field pulse significantly affects the ionization trajectory of the ionized electron. The electron can easily be ionized in the short optical period by gaining sufficient energy, while in the case of the long optical period, the absorbed energy is not enough to ionize the atom. Furthermore, the carrier-envelope phase (CEP) has a significant impact on the electron trajectory and represents the difference between the optical phase of the carrier wave and the envelope position. The CEP of the laser field alters the direction of the laser pulse, which can help in further understanding the characteristics of the change in the CEP.

2. Classical description of electron motion

We employ the classical treatment of a one-electron system using Coulomb's potential and external laser field.

The trajectory of the electron is obtained using Newton's equation:

$$\begin{cases} m_e\ddot{x}(t) = F(t) - \nabla V(x) \\ \dot{x}(t) = v(t) \end{cases}, \tag{1}$$

where m_e = 1 (in atomic units) and $V(a,Q;x) = -\frac{Q^2}{(a^2+x^2)^{1/2}}$ is quasi-Coulombic potential [34]. The parameters a and Q are introduced to remove the singularity at the origin and to adjust the depth of the potential well. The total energy obtained by the electron is [35]:

$$E = \frac{p^2}{2} + V(r). \tag{2}$$

The electric field component at a fixed value for z is given as [36];

$$F(t) = \frac{\varepsilon_0}{\sqrt{1+\chi^2}} f(t)((\sin \omega t\hat{x} + \varphi) + \chi \cos(\omega t\hat{y} + \varphi)), \tag{3}$$

where -1 ≤ χ ≤ 1 is the ellipticity parameter, which determines the degree of linear and circular polarization. Here ε_0 is the peak amplitude of the laser pulse electric field, ω is the centre frequency of the laser pulse, φ is the carrier-envelope phase, and $f(t) = \sin^2(\frac{\pi t}{T_D})$ is the laser field pulse envelope, where T_D is the total optical period of the laser pulse. When $\chi = 0$, the laser pulse is linearly polarized light field; therefore, the Eq. 2 becomes as;

$$F(t) = \frac{\varepsilon_0}{\sqrt{1+\chi^2}} f(t)(\sin \omega t + \varphi). \tag{4}$$

The CTMC method is used to investigate the classical trajectories of the electron ionization in a strong laser field, and a large number of initial values are selected to describe the real dynamics. For fixed initial energy (-0.5 a.u.), a series of initial distributions (-0.8 a.u. ~ 0.8 a.u.) of electrons with a set of initial position and momentum are obtained. The peak amplitude of the electric field and the centre frequency of laser pulse are considered as ε_0 = 0.063 a.u. and ω = 0.056 a.u., respectively. We investigated the electron's energy distributions and trajectories at the optical periods 1T, 3T, and 5T for the phase angles 0 and π.

3. Results and discussion

Assuming the positive vibration direction of the laser field, selecting the initial state, the electron energy distribution of the electrons in different carrier-envelope phases, and the classical ionization trajectories of the electrons in different optical periods are obtained using Eq. (4).

The electron energy distributions under different CEPs at T_D = 1T are shown in Fig. 1. It can be seen from Fig. 1 that at φ = 0, the energy obtained by the electrons changes homogenously with the optical period of the laser pulse. At φ = π, initially, the energy distribution is uniform, but later there are two intense and energy peaks that are relatively dispersed. Using Eq. (2) and Eq. (1) for obtaining the ionization trajectory of the electrons at φ = 0 and π, as shown in Fig. 2.

From Fig. 2, it is found that the electrons are ionized in the negative direction, and the obtained energy is small at T_D = 1T, φ = 0. When T_D = 1T, φ = π, the electric field direction of the laser field is reversed; as a result, the electric field strength of the electron in the opposite direction is increased, and later, the electron trajectory is concentrated in the positive direction. By comparing it with Fig. 1, it is clear that in less than one optical period, electrons have reached the peak energy, and hence ionization occurs.

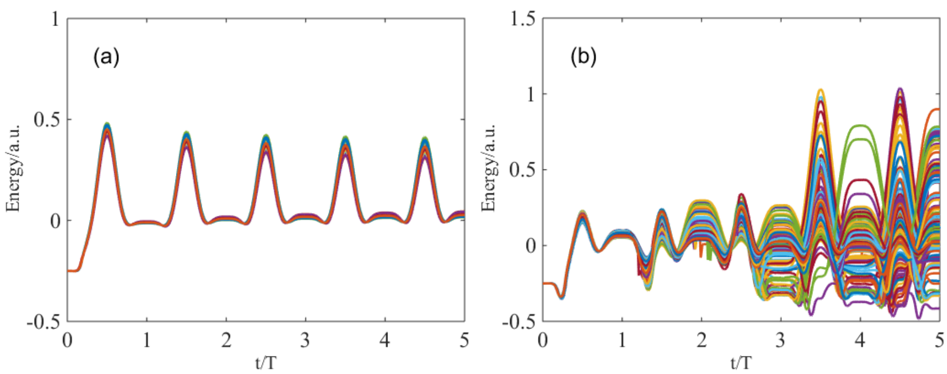

Fig. 1. Energy distribution of electrons at (a) φ = 0 and (b) φ = π (color online)

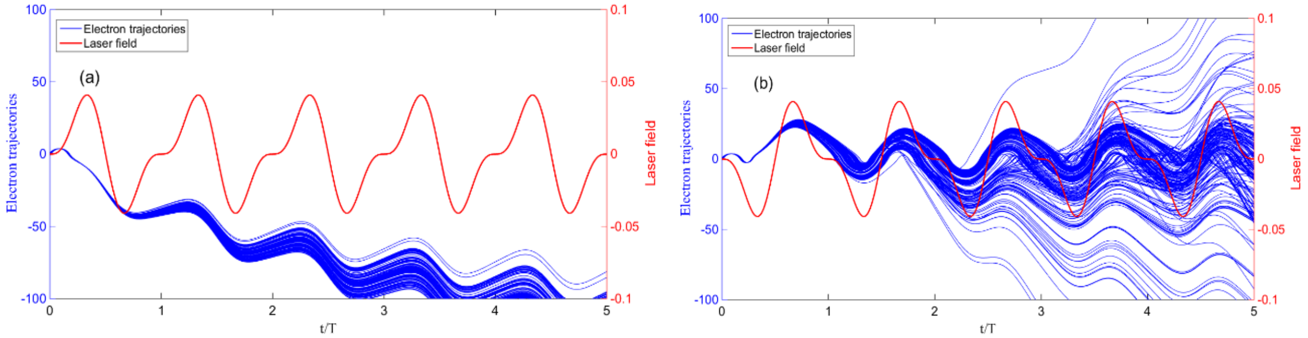

Fig. 2. Electron ionization trajectories at (a) $\varphi = 0$ and (b) $\varphi = \pi$ (color online)

Fig. 3 shows the energy distribution of the electrons at $T_D = 3T$. The initial peak appears in the first optical cycle. The energy increases, and the trajectories of the electron are dispersed with the increase in time. The corresponding electron trajectories are shown in Fig. 4. It can be seen from Fig. 4 (a) that at $\varphi = 0$, the electrons first oscillate along the laser field and then gradually diverge to both positive and negative directions with the increase in the pulse time. In contrast, at $\varphi = 0$, the electron trajectories are more dispersed at a later time.

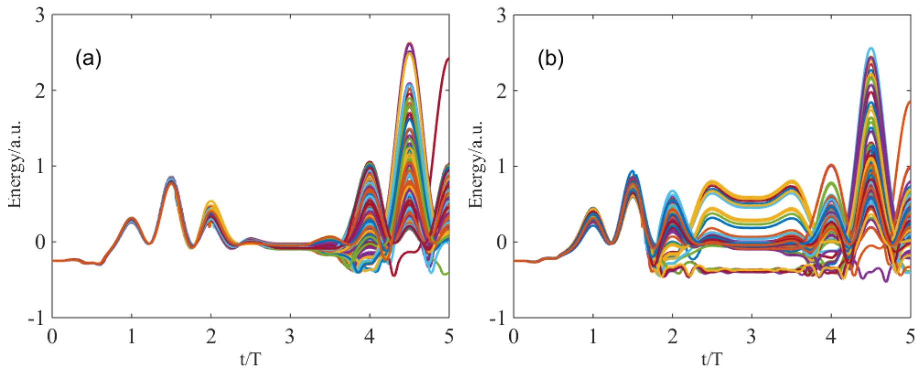

Fig. 3. Energy distribution of electrons at (a) $\varphi = 0$ and (b) $\varphi = \pi$ (color online)

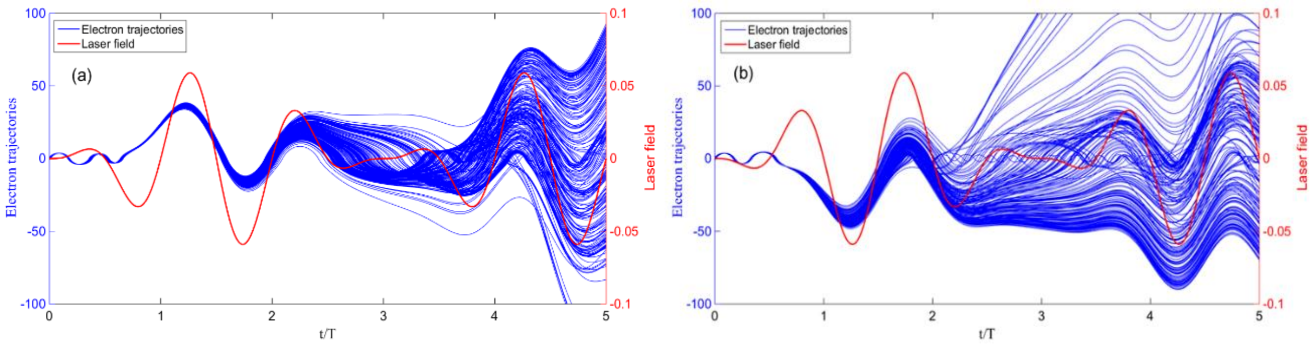

Fig. 4. Electron ionization trajectories at (a) $\varphi = 0$ and (b) $\varphi = \pi$ (color online)

The electron energy distribution under different CEPs at $T_D = 5T$ of the optical period of the linearly polarized laser field is shown in Fig. 5.

Relative to energy distribution at $T_D = 3T$, the energy increases with the pulse time at $T_D = 5T$. The electrons still have some energy at the first cycle of the laser field and are almost distributed in an equal amount but not concentrated. The relative electron trajectories are shown in Fig. 6.

At $T_D = 5T$ of the laser pulse time, the ionization trajectory no longer tends to one side; as a result, the electrons diverge to both positive and negative sides in the case of $\varphi = 0$. The effect of the changing CEPs on the ionization trajectory is significantly reduced. The positive part decreases and concentrates in the case of $\varphi = \pi$, which is due to the change in the pulse waveform.

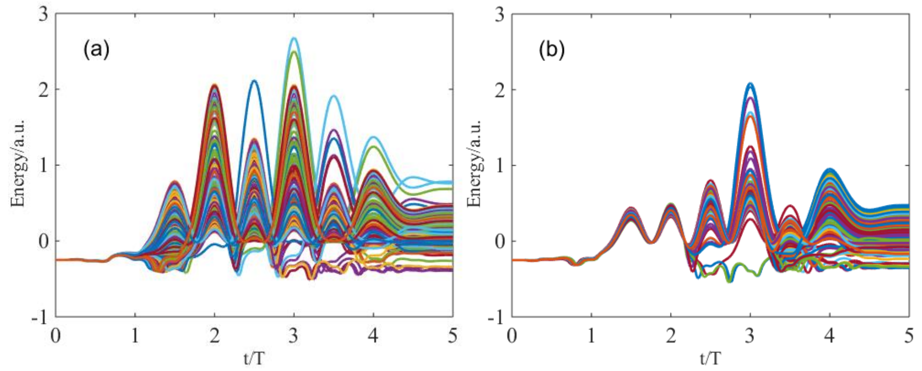

Fig. 5. Energy distribution of electrons at (a) $\varphi = 0$ and (b) $\varphi = \pi$ (color online)

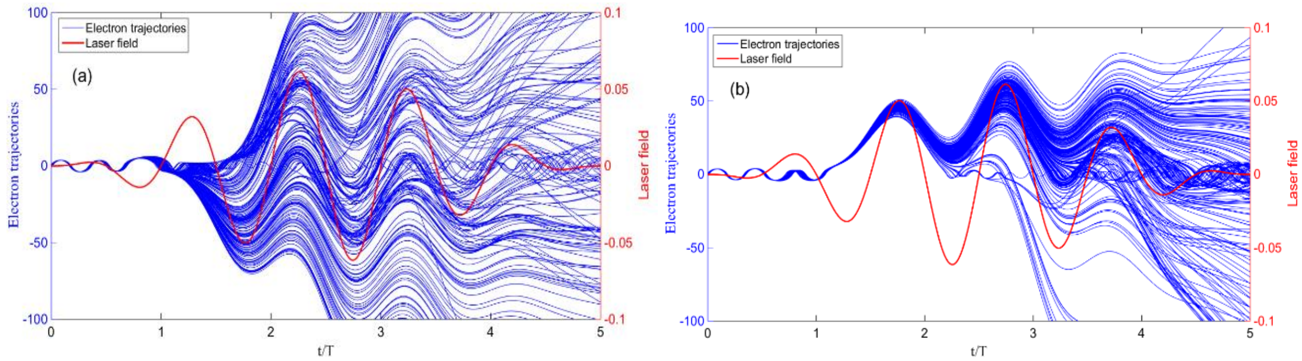

Fig. 6. Electron ionization trajectories at (a) $\varphi = 0$ and (b) $\varphi = \pi$ (color online)

The electrons in atoms and molecules are precisely described by quantum mechanics and their wave representation. The state of the electrons before ionization can be treated quantum mechanically. After ionization, the motion of the electron is treated purely classically in terms of trajectories. At the maximum external electric field, the total potential of the atom and the laser field forms a barrier through which the electron may ionize by the tunnelling process. After ionization, the electron is accelerated by the oscillating electric field, gaining kinetic energy. When the field changes its sign, the electron is accelerated back to the vicinity of the ion core, where it can scatter off. This scattering can happen either elastically, inelastically, or it recombines, and its energy is released in the form of a photon. Whether the electron is actually driven back to the ion core or not depends on the time of tunnelling with respect to the phase of the laser field. The phase of the laser field at which the electron is born in the continuum controls whether the electron can return to the ionic core at a later time or not, as well as the momentum and energy transfer from the field to the electron. In a short pulse regime, for many cycles of the laser pulse, the laser field turns off before the electron has a chance to leave the laser focus. The direct electrons returned electrons, and backscattered electrons can attain maximum kinetic energies.

4. Conclusion

A classical treatment of a one-electron atom embedded in a strong laser field using the CTMC technique is demonstrated. The electron energy distributions and ionization trajectories are investigated for different optical periods and CEPs. It is concluded that the laser pulse duration significantly affects the ionization trajectory of the ionized electron. The electron can easily be ionized in the short optical period by gaining sufficient energy, while in the case of the long optical period, the absorbed energy is not enough to ionize the atom. Moreover, the CEP has a significant impact on the electron trajectories, which alters the direction of the laser pulse and can help in a better understanding of the characteristics of the change in the CEPs.

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References

[1] M. Protopapas, C. H. Keitel, P. L. Knight, Rep. Prog. Phys. **60**(4), 389 (1997).
[2] F. Krausz, M. Ivanov, Rev. Mod. Phys. **81**(1), 163 (2009).

[3] M. Chini, K. Zhao, Z. Chang, Nat. Photon. **8**(3), 178 (2014).
[4] P.-C. Li, Y.-L. Sheu, H. Z. Jooya, X.-X. Zhou, S.-I. Chu, Sci. Rep. **6**(1), 1 (2016).
[5] W. Becker, F. Grasbon, R. Kopold, D. B. Milošević, G. G. Paulus, H. Walther, Adv. At. Mol. Opt. Phys. **48**, 35 (2002).
[6] D. B. Milošević and F. Ehlotzky, Adv. At. Mol. Opt. Phys. **49**, 373 (2003).
[7] A. Becker, F. H. M. Faisal, J. Phys. B: At. Mol. Opt. Phys. **38**(3), R1 (2005).
[8] C. F. de Morisson Faria, X. Liu, J. Mod. Opt. **58**(13), 1076 (2011).
[9] P. B. Corkum, F. Krausz, Nat. Phys. **3**(6), 381 (2007).
[10] A. Paul, R. Bartels, R. Tobey, H. Green, S. Weiman, I. Christov, M. Murnane, H. Kapteyn, S. Backus, Nature **421**(6918), 51 (2003).
[11] J. Seres, V. Yakovlev, E. Seres, C. Streli, P. Wobrauschek, C. Spielmann, F. Krausz, Nat. Phys. **3**(12), 878 (2007).
[12] E. Gagnon, P. Ranitovic, X.-M. Tong, C. L. Cocke, M. M. Murnane, H. C. Kapteyn, A. S. Sandhu, Science **317**(5843), 1374 (2007).
[13] S. Baker, J. S. Robinson, C. Haworth, H. Teng, R. Smith, C. Chirilă, M. Lein, J. Tisch, J. P. Marangos, Science **312**(5772), 424 (2006).
[14] S. Haessler, J. Caillat, W. Boutu, C. Giovanetti-Teixeira, T. Ruchon, T. Auguste, Z. Diveki, P. Breger, A. Maquet, B. Carré, Nat. Phys. **6**(3), 200 (2010).
[15] L. Keldysh, Sov. Phys. JETP **20**(5), 1307 (1965).
[16] F. H. M. Faisal, J. Phys. B: At. Mol. Opt. Phys. **6**(4), L89 (1973).
[17] H. R. Reiss, Phys. Rev. A **22**(5), 1786 (1980).
[18] A. Perelomov, V. Popov, M. Terentev, Sov. Phys. JETP **23**(5), 924 (1966).
[19] M. V. Ammosov, Sov. Phys. JETP **64**, 1191 (1987).
[20] P. Botheron, B. Pons, Phys. Rev. A **80**(2), 023402 (2009).
[21] T. F. Gallagher, Phys. Rev. Lett. **61**(20), 2304 (1988).
[22] P. B. Corkum, N. H. Burnett, F. Brunel, Phys. Rev. Lett. **62**(11), 1259 (1989).
[23] P. B. Corkum, Phys. Rev. Lett. **71**(13), 1994 (1993).
[24] N. Shvetsov-Shilovski, M. Lein, L. Madsen, E. Räsänen, C. Lemell, J. Burgdörfer, D. Arbó, K. Tőkési, Phys. Rev. A **94**(1), 013415 (2016).
[25] H. Muller, Laser Phys. **9**(1), 138 (1999).
[26] D. Bauer, P. Koval, Comput. Phys. Commun. **174**(5), 396 (2006).
[27] J. L. Krause, K. J. Schafer, K. C. Kulander, Phys. Rev. Lett. **68**(24), 3535 (1992).
[28] M. Lewenstein, P. Balcou, M. Y. Ivanov, A. L'Huillier, P. B. Corkum, Phys. Rev. A **49**(3), 2117 (1994).
[29] G. G. Paulus, W. Nicklich, H. Xu, P. Lambropoulos, H. Walther, Phys. Rev. Lett. **72**(18), 2851 (1994).
[30] G. G. Paulus, W. Becker, W. Nicklich, H. Walther, J. Phys. B: At. Mol. Opt. Phys. **27**(21), L703 (1994).
[31] D. B. Milošević, W. Becker, Phys. Rev. A **68**(6), 065401 (2003).
[32] T. Brabec, M. Y. Ivanov, P. B. Corkum, Phys. Rev. A **54**(4), R2551 (1996).
[33] K. I. Dimitriou, D. G. Arbó, S. Yoshida, E. Persson, J. Burgdörfer, Phys. Rev. A **70**(6), 061401 (2004).
[34] Q. Su, J. H. Eberly, Phys. Rev. A **44**(9), 5997 (1991).
[35] D. Banks, J. Leopold, J. Phys. B: At. Mol. Opt. Phys. **11**(1), 37 (1978).
[36] N. L. Manakov, V. D. Ovsiannikov, L. P. Rapoport, Phys. Rep. **141**(6), 320 (1986).

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