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Entangled trajectories during ionization of an H atom driven by n-cycle laser pulse

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ABSTRACT

We study the ionization of an H atom in a linearly polarized laser field with different optical cycle numbers by calculating the entangled trajectories in phase space. The results indicate that, for a two-cycle laser pulse, the entangled trajectory is simple owing to the simple laser electric distribution. As the number of optical cycles increases, the complexity of the laser electric field distribution, and subsequently, that of the entangled trajectories increase. From these entangled trajectories, re-scattering ionization can be observed. Further, we investigate the effect of quantum force on trajectories by comparing them with classical trajectories. We find that for few-cycle laser pulses ($n_p = 2$ and 4), the effect of the quantum force is more distinct than classical behavior, whereas for longer laser pulses ($n_p = 6$ and 8), it is quite similar to the classical behavior. Because of the quantum force, the final kinetic energy is slightly higher than that obtained by classical calculation. The different initial positions have some influence on the individual trajectories, but the individual trajectories still keep similar configuration to the mean trajectories.

1. Introduction

Interaction between atoms or molecules and few-cycle laser pulses can result in many fundamental strong-field physics phenomena such as above-threshold ionization (ATI), high harmonic generation (HHG), and non-sequential double ionization (NSDI) [1–8]. Ionized electrons from atoms and molecules in a few-cycle pulsed laser field are emitted in direct ionization or are pulled back by the laser field when the laser electric field changes direction. The ionized electrons can carry information about the laser field and the electronic structure of the atoms or molecules. For example, Milošević et al. observed and measured the carrier-envelope (CE) phase of a laser pulse through the strong left-right asymmetry of the emitted electrons[9,10]. Paulus et al. investigated the ionization of an H atom exposed to an intense few-cycle laser pulse by calculating the left-right asymmetry of the photoelectron momentum distributions, and they found an asymmetry parameter as a function of laser intensity for a particular CE phase range [11]. The results reported by Morishita et al. implied that existing few-cycle infrared lasers can be implemented for the ultrafast imaging of transient molecules with a temporal resolution of a few femtoseconds [12]. Huismans et al. formulated a new method to record the underlying electron dynamics on a sub-laser-cycle timescale, enabling photoelectron spectroscopy with a temporal resolution using the holographic structures of the ionization of a Xe atom [13]. Few-cycle laser pulses are characterized by parameters such as the frequency and intensity of the laser electric field, CE phase, and number of optical cycles. The effect of frequency and intensity on ionization has been reported. The actual shape of a few-cycle pulse crucially depends on the number of optical cycles, and so does the physical processes. In our earlier studies [14,15], we investigated the ionization behaviors of an H atom in a few-cycle pulse with different optical cycle numbers and found that photoelectron angular distributions exhibit energy-dependent phenomena for different ATI peaks, and ionization behaviors of the atom extend to those of an atom in an infinitely monochromatic plane wave when the optical cycle numbers are very large.

Theoretical calculations for interactions between atoms or molecules and intense few-cycle laser pulses are typically carried out using different methods. The main theoretical approaches can be divided into two groups: the first kind is the direct integration of the time-dependent Schrödinger equation (TDSE), or the Bohmian formulation basing on the TDSE [16], and the second kind

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is analytical theory, such as the Keldysh–Faisal–Reiss (KFR) model [17–19], the analytical R-matrix method [20,21]. In addition to the above methods, many people have used the Wigner function to investigate the ionization of atoms or molecules in strong laser field [22–24]. The Wigner function [25–28] is a quasiprobability function in phase space that allows one to study position-momentum correlations. These correlations give a physical interpretation of the emergence of the above-threshold-ionization (ATI) energy spectrum. The Wigner function enables us to show the dependence of ionization probability on time and explicitly demonstrates the transition of the ionization process. In this study, we follow the approach of our recent work [22], however, we do not seek further detailed improvements on this approach. We perform comprehensive calculations of the entangled trajectories of the electrons which have been ionized irrespective of the ionization mechanism (tunneling ionization or over barrier ionization). From these trajectories, we can investigate the effect of the optical cycle number on entangled trajectories. Further, we demonstrate the effect of quantum force on the trajectories by comparing them with classical trajectories.

This paper is arranged as follows: we introduce the Wigner function used in this paper in Sec. 2 The results and discussions are in Sec. 3. In Sec. 4 we conclude.

2. Theoretical methods

Under the dipole approximation, using the minimal-coupling Hamiltonian the Schrödinger equation describing the interaction between an atom and a laser field is

$$\left\{\frac{[-i\hbar\nabla + e\mathbf{A}(t)]^2}{2m_e} + U_c(x)\right\}\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}, \tag{1}$$

where $\mathbf{A}(t)$ is the vector potential of the laser field. And $U_c(\mathbf{r})$ is the atomic Coulomb potential, which has many different models for H atom. In the early study, Loudon [29] had used the model potential, $-1/|x|$, to investigate the energy-level degeneracy because of the potential singularity, which affects the low-energy photoelectron nearby the nucleus. In this paper we will mainly study the common ionization phenomenon. So we will use a soft Coulomb potential, $U_c(x) = -Q/\sqrt{x^2+a}$ which are commonly used[30–32]. The parameters a and Q are introduced to remove the singularity at the origin and to adjust the depth of the potential well. For H atom [33], the parameters a and Q are 0.367 and 0.561, respectively, to set the ionization potential of H atom −0.5 a.u. and make the system less polarization. This model potential has three bound states: one ground state and two excited states, and has an acceptable trade off. In this paper we will investigate the ionization from the ground state, and neglect the contribution of the excited states to the ionization because of the small contribution [34]. $E(t) = -\frac{\partial\mathbf{A}(t)}{\partial t}$ is the electric field of the laser used in this paper. The time-dependent wavefunction $\Psi(x,t)$ can describe the ionization dynamics of H atom in position space. An equivalent phase space description more closely analogous to classical mechanics is given in terms of the Wigner function $W(x,p,t)$. The Wigner function was introduced at the dawn of quantum mechanics to get a natural connection with classical mechanics [25] and became an indispensable tool for studying the classical world as an emergent and effective description based on the more fundamental quantum mechanics [36]. In this paper, the time-dependent Wigner function can be gotten by a Fourier transform of the shifted position time-dependent wave functions, and has the following form

$$W(x,p,t) = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} d\xi\,\Psi(x-\frac{\xi}{2},t)\Psi^*(x+\frac{\xi}{2},t)e^{i\xi p/\hbar}. \tag{2}$$

According to Refs. [36–40], the equations of the trajectory at point (x,p), are

$$\frac{\partial x}{\partial t} = \frac{p}{m_e}, \tag{3}$$

$$\frac{\partial p}{\partial t} = -\left[U_c'(x) + eE(t)\right] + \frac{\hbar^2}{24}\left[U_c'''(x)\right]\frac{1}{W}\frac{\partial^2 W}{\partial p^2} \tag{4}$$

$$+\frac{1}{5!}U_c^{(5)}(x)\left(\frac{\hbar}{2}\right)^4\frac{\partial^4 W}{\partial p^4} + \cdots \tag{5}$$

where $\frac{\hbar^2}{24}\left[U_c'''(x)\right]\frac{1}{W}\frac{\partial^2 W}{\partial p^2} + \frac{1}{5!}U_c^{(5)}(x)\left(\frac{\hbar}{2}\right)^4\frac{\partial^4 W}{\partial p^4} + \cdots$ are the quantum terms and show the quantum force, which are not found in the equations of the classical trajectory. For time integration in the above equation, a fourth-order Runge–Kutta method was used to obtain the values of (x,p).

Before presenting the main results, we must numerically check the convergence of the summation given by Eq. (4) and Eq. (5) which includes more terms comparing with Eq. (4). What we must know is up to which term in Eqs. (4) or (5) for the numerical convergence. In Fig. 1, we have ensured the numerical convergence of the summation. The blue dashed line is for the summation in Eq. (4), and the red solid line is for the summation in Eq. (5) including one higher order term $\frac{1}{5!}U_c^{(5)}(x)\left(\frac{\hbar}{2}\right)^4\frac{\partial^4 W}{\partial p^4}$. From this figure we can know the entangled trajectories calculated by using the Eq. (4) and Eq. (5), respectively, have indescribable difference, and the Eq. (5) are the numerical convergence. It is acceptable for neglecting the error due to neglecting the higher order terms in Eq. (5). In this paper, we will use the Eq. (5) to calculate the entangled trajectories.

3. Numerical results and discussion

As for the laser field we assume that it is linearly polarized along the x axis throughout this paper, and the electric field amplitude E = 0.08 a.u. (a.u. means the atomic units), and corresponds to the laser peak intensity of I = 1.126 $\times 10^{14}$ W/cm^2, with the carrier-envelope phase, ϕ, is zero. The laser pulse shape is

$$E(t) = E_0\,\mathrm{sech}\left(\frac{t-t_f/2}{\pi\omega}\right)\sin(\omega t+\phi), \tag{6}$$

where E_0 is the amplitude of the electric field of the laser pulse, and $t_f = n_p T$. n_p is the number of laser pulse cycle. ϕ is the carrier-envelope phase. The laser electric field force is on the ionized electrons is shown in Fig. 2. From these plots, we can find that the oscillation of the force f on the ionized electrons becomes stronger with an increase in the optical cycle number of the laser pulse. This indicates that the entangled trajectories are affected by the optical cycle number.

In this paper, we will choose 500 ionization trajectories and plot the mean trajectories in the following figure. The initial positions are distributed according to $|\Psi(x,0)|^2$, and the initial velocities are set $v_i(t=0)=0$ for the stationary state [35].

Fig. 3 shows the mean trajectories produced using Eqs. (3) and (5), which correspond to the entangled trajectories (blue dashed line), and the trajectories by setting $\hbar = 0$, which correspond to the classical trajectories (red solid line). From Fig. 3 we can find the influence of the optical cycle numbers and the quantum force on the trajectories.

First, we talk about the influence of the optical cycle numbers. Fig. 3 (a) depicts a simple entangled trajectory, which shows