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High-order harmonic generation in a two-color strong laser field with Bohmian trajectory theory*

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We theoretically study the high-order harmonic generation (HHG) in a two-color laser field using the Bohmian mechanics. Our results show that, for the case of a weak second-color laser field, the simulation of the HHG with only one central Bohmian trajectory is in a good agreement with the *ab initio* time-dependent Schrödinger equation (TDSE) results. In contrast, with the increase of the amplitude of the second-color laser field, the HHG spectra from the single central Bohmian trajectory deviate from the TDSE results more and more significantly. By analyzing the Bohmian trajectories, we find that the significant deviation is due to the fact that the central Bohmian trajectory leaves the core quickly in the two-color laser field with the breaking of inversion symmetry. Interestingly, we find that another Bohmian trajectory with different initial position, which keeps oscillating around the core, could qualitatively well reproduce the TDSE results. Furthermore, we study the HHG spectrum in a two-color laser field with inversion symmetry and find that the HHG spectrum in TDSE can be still well simulated with the central Bohmian trajectory. These results indicate that, similar to the case of one color laser field, the HHG spectra in a two-color laser field can be also reproduced with a single Bohmian trajectory, although the initial position of the trajectory is dependent on the symmetry of the laser field. Our work thus demonstrates that Bohmian trajectory theory can be used as a promising tool in investigating the HHG process in a two-color laser field.

Keywords: high-order harmonic generation, two-color laser field, Bohmian trajectory

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1. Introduction

High-order harmonic generation (HHG) first observed in experiment in 1988[1] has attracted much attention due to its potentially broad applications, such as table-top extreme ultraviolet (XUV) and soft x-ray sources,[2] the generation of the attosecond laser pulses,[3–5] and the coherent imaging of molecular structures.[6–8] The process of HHG can be well described with a semiclassical three-step model:[9,10] (i) the bound electron is liberated by the strong laser field, (ii) the ionized electron is accelerated in the laser field, and (iii) the ionized electron may recombine with the parent ion accompanied by the emission of a high-energy photon. The corresponding HHG spectrum exhibits a plateau with a cutoff energy of $3.17U_p + I_p$, where U_p is the ponderomotive potential of the laser field and I_p is the ionization potential of the atomic target under investigated.

Recently, the study of the HHG in a two-color strong laser field has become a hot topic in the strong-field community. The atomic ionization amplitude and the ultrafast dynamics of the ionized electron in a two-color laser field can be accurately controlled and thus the HHG can be well designed. For example, Jin *et al.*[11] showed that the harmonics can be enhanced by one to two orders of magnitude by synthesizing a two- or three-color field. Brugnera *et al.*[12] showed that the short and long quantum trajectories in high harmonic emission can be controlled through the use of an orthogonally polarized two-color field. Very recently, the bright phase-matched circularly polarized high harmonics are generated by using a circularly polarized, counterrotating two-color driving pulse.[13,14]

To well understand the HHG process and its underlying ultrafast electronic dynamics in a two-color laser field, an appropriate theoretical modeling is in demand. Usually, the HHG process is investigated by numerically solving the *ab initio* time-dependent Schrödinger equation (TDSE). However, the TDSE can not provide a clear physical picture to reveal the underlying physics. To overcome this problem, many theoretical models are developed,[15–18] e.g., the Bohmian mechanics[19–21] (also called the quantum trajectory theory[22,23]). Bohmian mechanics, which is exactly derived from TDSE, describes the dynamics of the electron with the concept of trajectories. Thus Bohmian mechanics can not only well simulate the HHG, but, more importantly, it can provide an intuitive picture on the electron dynamics in a laser field. Recently, Bohmian mechanics has been successfully used to study HHG and the photoionization from simple atom to molecule and from the single ionization to the double ionization.[24–39] Generally speaking, the strong-field phenomena can be well simulated with a large number of

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Bohmian trajectories. Recently, however, it is found that, interestingly, just a few Bohmian trajectories are enough to qualitatively reproduce the HHG spectra and hence it provides a very convenient way to understand the HHG process by analyzing these Bohmian trajectories. For example, Song *et al.*[32] showed that the harmonic emission calculated by randomly selected 20 Bohmian trajectories is qualitatively identical to the TDSE calculations. Wu *et al.*[33,34] further showed that the HHG spectrum can be qualitatively well reproduced with only one central trajectory in a monochromatic laser field. However, for a two-color laser field, whether the HHG spectra can be well simulated with the single central Bohmian trajectory is still not clear. An answer to this question would be important for a comprehensive understanding of the HHG processes in a two-color laser field from the Bohmian trajectory perspective.

In this paper, we theoretically study the HHG in a parallel-polarized two-color laser field using the Bohmian mechanics. Our results show that the simulations of the HHG with only one central Bohmian trajectory can well reproduce the TDSE results for the case of a weak second-color laser field. However, with the increase of the amplitude of the second-color laser field, a significant deviation is observed. By analyzing the Bohmian trajectories, we find that the significant deviation is ascribed to the breaking of inversion symmetry in the two-color laser field. Interestingly, another Bohmian trajectory with different initial position qualitatively well reproduces the TDSE result. To further show the influence of the symmetry of a laser field on the HHG with Bohmian trajectory, we study the HHG in a two-color laser field with inversion symmetry and find that the HHG spectrum can be still well simulated with the central Bohmian trajectory. Therefore, our work indicates that the HHG spectra in a two-color laser field can be also reproduced with a single Bohmian trajectory, although the initial position of the trajectory is dependent on the symmetry of the laser field.

2. Theoretical methods

2.1. TDSE method

As a benchmark, we take the *ab initio* TDSE simulation of the interaction of atom with strong laser field. For the sake of simplicity, we solve the one-dimension TDSE

$$\mathrm{i}\frac{\partial}{\partial t}\Psi(\boldsymbol{x},t)=\left[-\frac{1}{2}\boldsymbol{\nabla}^2+V(\boldsymbol{x})-\boldsymbol{x}E(t)\right]\Psi(\boldsymbol{x},t), \tag{1}$$

where $\Psi(\boldsymbol{x},t)$ denotes the electronic wave function. In order to avoid the singularity, we have used the so-called "soft-Coulomb" potential

$$V_c(\boldsymbol{x})=-\frac{1}{\sqrt{\boldsymbol{x}^2+c}}. \tag{2}$$

With $c=1.41$, the ground state energy is $\varepsilon_0=-0.5799$ a.u., which is the same as that for Ar atoms. Atomic units (a.u.) are used throughout unless otherwise indicated.

The two-color laser field is given by

$$E(t)=\begin{cases}\dfrac{E_0}{\sqrt{1+\beta^2}}\sin^2\left(\dfrac{\pi t}{2T}\right)[\cos(r\omega t)+\beta\cos(s\omega t+\phi)], & 0\le t<T,\\ \dfrac{E_0}{\sqrt{1+\beta^2}}[\cos(r\omega t)+\beta\cos(s\omega t+\phi)], & T\le t\le 7T,\\ \dfrac{E_0}{\sqrt{1+\beta^2}}\sin^2\left(\dfrac{\pi t-7\pi T}{2T}\right)[\cos(r\omega t)+\beta\cos(s\omega t+\phi)], & 7T<t\le 8T,\\ 0, & \text{otherwise,}\end{cases} \tag{3}$$

where β is the intensity ratio of the two-color laser field, ϕ is the relative phase of the two-color laser field, s and r are the integers, $E_0/\sqrt{1+\beta^2}$ is the peak electric field, ω is the frequency, and $T=2\pi/\omega$. In this work, the time-dependent wave function of the electron is obtained by solving Eq. (1) with the imaginary-time evolutionary algorithm and split-operate method[40] using the fast Fourier transform technique.[41]

To ensure that all relevant dynamics are incorporated for the parameter range of interest, we have set the box boundaries located far enough away from the core region, e.g., $x_{\max}=512$ a.u. Furthermore, we have employed a mask function to avoid reflections and spurious effects near the box edges, which is

$$\mathrm{Mask}(x)=\begin{cases}\cos^{\frac{1}{8}}\left[\dfrac{\pi|\boldsymbol{x}+x_l|}{2\left(-\dfrac{x_{\max}}{2}+x_l\right)}\right], & \boldsymbol{x}<-x_l,\\ 1, & -x_l\le\boldsymbol{x}<x_l,\\ \cos^{\frac{1}{8}}\left[\dfrac{\pi|\boldsymbol{x}-x_l|}{2\left(\dfrac{x_{\max}}{2}-x_l\right)}\right], & \boldsymbol{x}\ge x_l,\end{cases} \tag{4}$$

where the absorbing boundary x_l is equal to 362. The time-dependent wavefunction is multiplied by the mask function to avoid nonphysical reflections of the electron wavepacket near the boundaries. The expectation value of the dipole accelera-

tion is calculated as

$$\bar{a}(t) = -\left\langle \psi(\boldsymbol{x},t)\left|\frac{\partial V(\boldsymbol{x},t)}{\partial \boldsymbol{x}}\right|\psi(\boldsymbol{x},t)\right\rangle. \tag{5}$$

where $V(\boldsymbol{x},t) = V_{\rm c}(\boldsymbol{x}) - \boldsymbol{x}E(t)$. The HHG spectra are obtained with the standard Fourier transform of the dipole acceleration

$$I(\Omega) = \left|\int \bar{a}(t)\mathrm{e}^{-\mathrm{i}\Omega t}\mathrm{d}t\right|^2. \tag{6}$$

2.2. Bohmian trajectory method

In order to construct the Bohmian trajectories, $\Psi(\boldsymbol{x},t)$ is recast in the polar form[19,20]

$$\begin{aligned}\Psi(\boldsymbol{x},t) &= R\cos(S) + \mathrm{i}R\sin(S)\\ &= R\mathrm{e}^{\mathrm{i}S},\end{aligned} \tag{7}$$

where $R = R(\boldsymbol{x},t)$ is the real-valued amplitude and $S = S(\boldsymbol{x},t)$ is the real-valued phase. Substitution of Eq. (7) in the TDSE leads to two coupled differential equations in R and S. The real part of the resulting equation is

$$\frac{\partial S}{\partial t} + \frac{(\boldsymbol{\nabla} S)^2}{2} + V + Q = 0, \tag{8}$$

and the imaginary part has the form

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho \boldsymbol{v}) = 0, \tag{9}$$

where $Q(\boldsymbol{x},t) = -\frac{1}{2}\frac{\boldsymbol{\nabla}^2 R}{R}$, $\rho(\boldsymbol{x},t) = R^2(\boldsymbol{x},t)$, and $\boldsymbol{v} = \boldsymbol{\nabla} S(\boldsymbol{x},t)$. These two equations are analogous to the classical Hamilton–Jacobi equation and the continuity equation, respectively, except that the equation (8) has an extra term Q which is usually called quantum potential in Bohmian mechanics. Thus the equation (8) is called the quantum Hamilton–Jacobi equation governed by an external potential V and the quantum potential Q. The motion of the electron is guided by Bohm–Newton equation of motion, $\mathrm{d}^2\boldsymbol{x}/\mathrm{d}t^2 = -\boldsymbol{\nabla}(V+Q)$, or, equivalently, by[25,31,33,34]

$$\mathrm{d}\boldsymbol{x}/\mathrm{d}t = \boldsymbol{\nabla} S(\boldsymbol{x},t). \tag{10}$$

The distribution of the initial position x_0 is given by

$$P = |\Psi(x_0,0)|^2, \tag{11}$$

where $\Psi(x_0,0)$ is the initial electron wavefunction.

In Bohmian mechanics, the dipole acceleration of each Bohmian trajectory with the initial position x_0 is given by[25,31,33,34]

$$\bar{a}_{\rm B}(t) = -\frac{\partial V(\boldsymbol{x}(t),t)}{\partial \boldsymbol{x}}\Big|_{\boldsymbol{x}(0)=x_0}. \tag{12}$$

The corresponding HHG spectrum is obtained with the standard Fourier transform of the dipole acceleration

$$I(\Omega) = \left|\int \bar{a}_{\rm B}(t)\mathrm{e}^{-\mathrm{i}\Omega t}\mathrm{d}t\right|^2. \tag{13}$$

3. Results and discussion

In Fig. 1, we show the HHG spectra simulated with TDSE and Bohmian mechanics in a monochromatic laser field ($\beta = 0$ and $r = 1$ in Eq. (3)). In the simulation of the HHG spectrum with Bohmian mechanics, we only consider the central Bohmian trajectory with the initial position $x_0 = 0$. We find that the single central Bohmian trajectory can qualitatively well reproduce the HHG spectrum, e.g., the plateau structure and the cut-off position of HHG spectrum, which is consistent with the result got by Wu *et al.*[33,34] In the following, we study whether a single Bohmian trajectory in a two-color laser field can also simulate the HHG spectrum well.

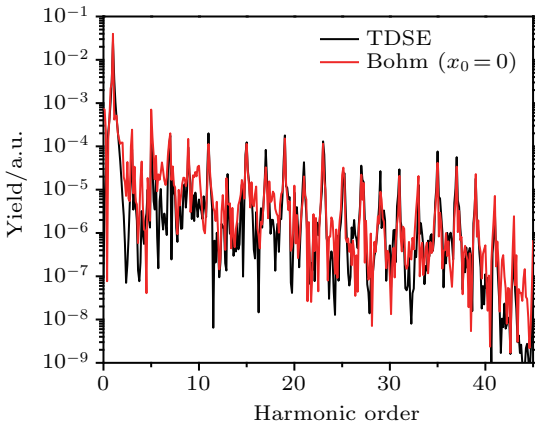


Fig. 1. (color online) HHG spectra simulated with TDSE (black lines) and Bohmian mechanics (red lines) in the monochromatic laser field of intensity $I = 2.0\times10^{14}$ W/cm^2 and wavelength 800 nm with $\beta = 0$ and $r = 1$ in Eq. (3). During the simulation of the HHG spectrum with Bohmian mechanics, we only consider the central Bohmian trajectory with the initial position $x_0 = 0$.

In Fig. 2, we present the HHG spectra simulated with TDSE (black lines) in a two-color laser field with $r = 1$ and $s = 2$ for different intensity ratio β and relative phases ϕ. With the increase of the value of β, the plateau and cut-off of HHG spectra are changed significantly and moreover, similar changes of the HHG spectra with β can be also observed at the different relative phases ϕ. Interestingly, it is found that there are even-order harmonics in the spectra. To show it more clearly, the harmonics from 21th to 24th order are enlarged in the inset of Fig. 2(a). The appearance of the even-order harmonics has been observed in experiment[42,43] and can be understood from the energy conservation and the dipole selection rules[44] that $\Omega = n\times\omega + m\times 2\omega$ and $n+m$ is an odd integer, where n and m denote the numbers of the photons absorbed from the two-color laser field. For example, for the 24th-order harmonic, it can be obtained with $m = 9$ and $n = 6$.

Next, we calculate the HHG spectra with the single central Bohmian trajectory with $x_0 = 0$ (red lines in Fig. 2). For the small intensity ratio β, the main features of the HHG spectra solved from Bohmian trajectory is qualitatively consistent

with the TDSE results, e.g., the pronounced plateau, its cutoff, and even the even-order harmonics. The appearance of the even-order harmonics will be also explained in the view of the Bohmian mechanics in the following. In contrast, with the increase of the value of β, the HHG spectra from the single central Bohmian trajectory deviate from the TDSE results more and more significantly. For example, in Fig. 2(i), the harmonics around the 28th order from the Bohmian trajectory is much lower than that from TDSE calculations. Therefore, in general, in a two-color laser field, the central Bohmian trajectories can not reproduce the TDSE results well.

To understand the influence of the two-color laser field on the HHG simulated with the single central Bohmian trajectory, we analyze the trajectory in the monochrome and two-color laser field, respectively. In Figs. 3(a) and 3(d), we show the electric fields of the laser pulses as a function of time. For the monochrome laser field, the electric field is inversion symmetric with $E(t) = -E(t + \frac{T}{2})$. The central Bohmian trajectory keeps oscillating near the core (see Fig. 3(b)) and the corresponding HHG spectrum is in a good agreement with the TDSE calculation (see Fig. 3(c)). In contrast, for the two-color laser field with $\beta = 1$, the electric field is asymmetric and hence the electron experiences an asymmetric force. Figure 3(e) shows that the central Bohmian trajectory quickly moves to the detector after the time $t > 4.5T$. According to the three-step model,[10] the HHG process is from the recombination of the ionized electron with the core. The central Bohmian trajectory, which leaves the core quickly in the asymmetric electric field, can not well reproduce the HHG spectra, especially for the laser field with the stronger second-color laser field.

Interestingly, we find that even though the central Bohmian trajectory leaves the core quickly in the two-color laser field, there is another Bohmian trajectory which is bounded near the parent ion in the laser field and the ionic Coulomb potential. For example, figure 3(e) shows that for the laser field with $\beta = 1$, the Bohmian trajectory with the initial position $x_0 = 0.3$ keeps oscillating around the core. The corresponding HHG spectrum from Bohmian trajectory with $x_0 = 0.3$ qualitatively agrees well with the TDSE simulations, including the even-order harmonics in the spectrum (see the red line in Fig. 3(f)). The appearance of the even-order harmonics can be also understood from the symmetry of the Bohmian trajectories. The inset in Fig. 3(e) shows that due to the breaking of inversion symmetry of the electric field of the two-color laser field, the Bohmian trajectory is also not inversion symmetric and thus the Fourier transform of the dipole results in the HHG spectrum with energy interval of one photon energy of ω. Therefore, our results show that the HHG spectra in the two-color laser field can be also reproduced with a single Bohmian trajectory, but the initial position of the trajectory is dependent on the symmetry of the laser field.

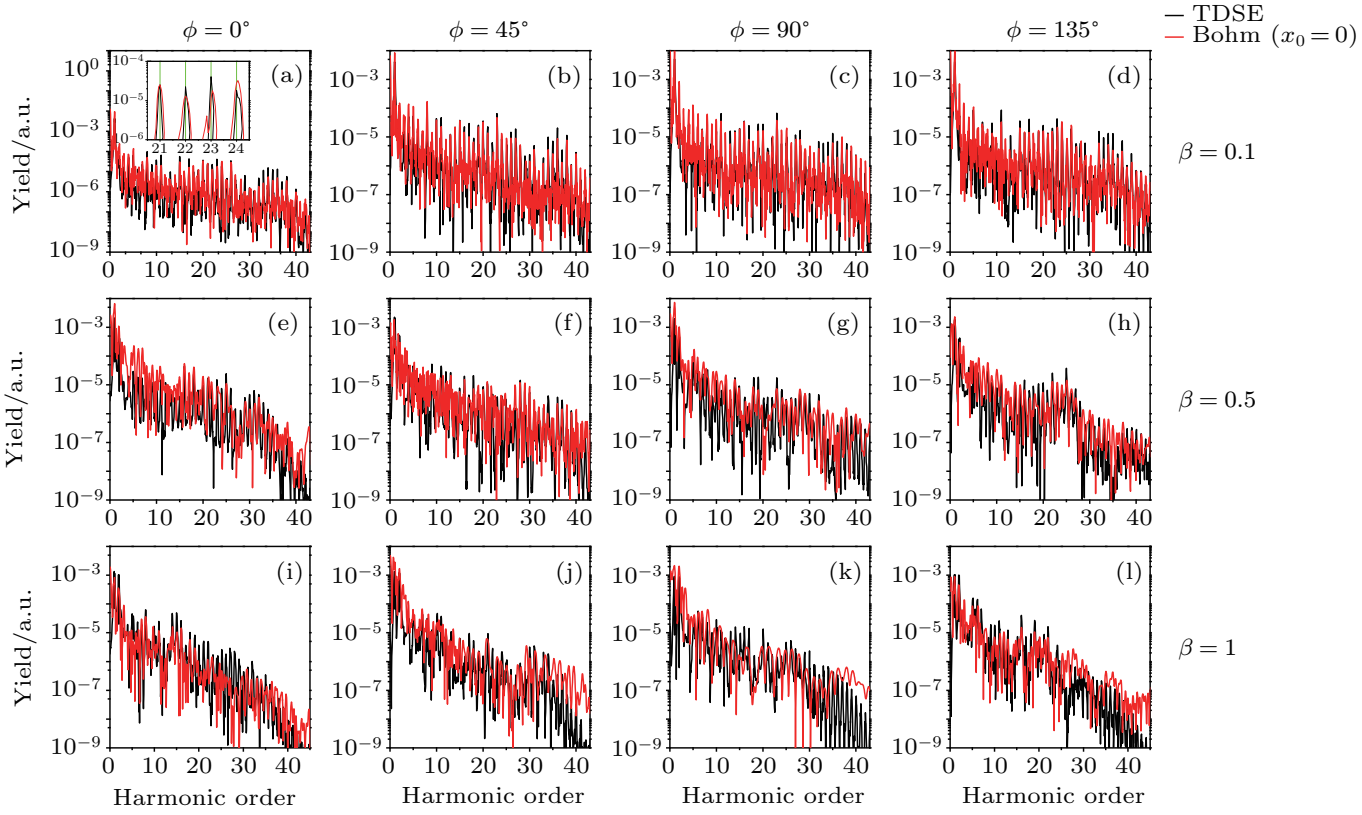


Fig. 2. (color online) HHG spectra simulated with TDSE (black lines) and Bohmian mechanics (red lines) in a two-color laser field with $r = 1$ and $s = 2$ at different intensity ratio β and relative phases ϕ. During the simulation of the HHG spectrum with Bohmian mechanics, we only consider the central Bohmian trajectory with the initial position $x_0 = 0$. Inset: the enlargement of the harmonics from 21th to 24th order in panel (a).

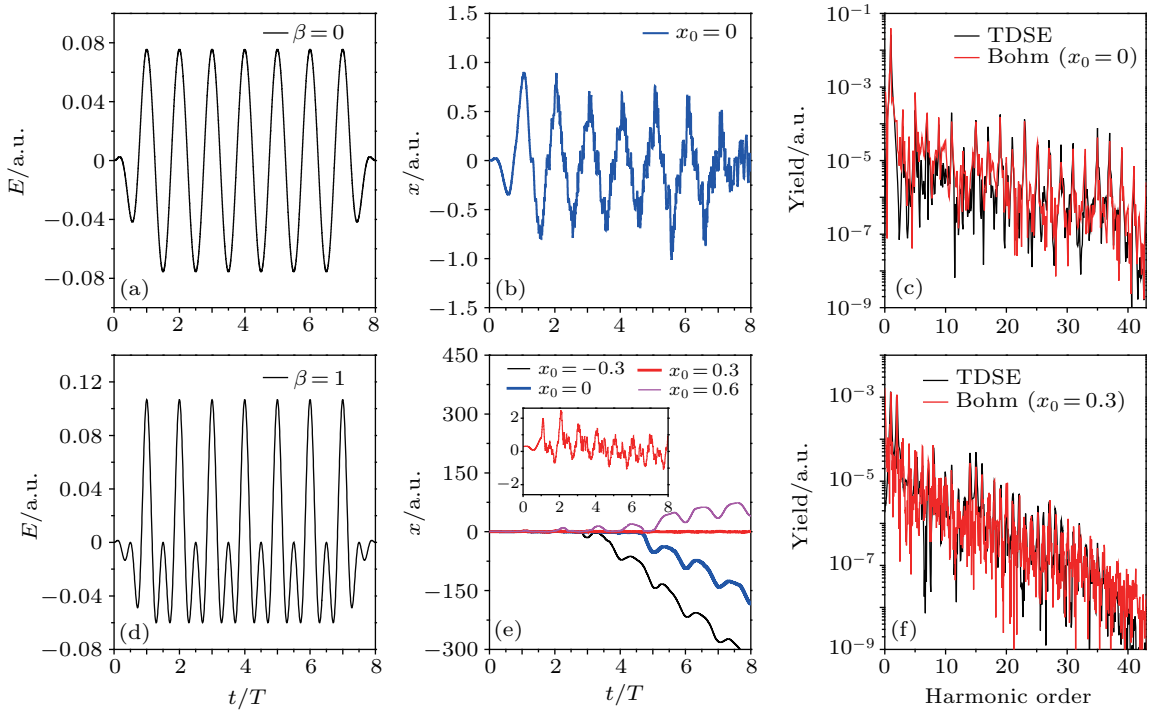


Fig. 3. (color online) From left to right: electric field of the laser field, the Bohmian trajectories with different initial positions, and the HHG spectra simulated with TDSE (black lines) and the Bohmian trajectory (red lines), respectively, (a)–(c) for the monochromatic laser field and (d)–(f) for the two-color laser field with $\beta = 1$, $r = 1$, $s = 2$, and $\phi = 0$. Inset in panel (e) shows the enlargement of the Bohmian trajectory with the initial position $x_0 = 0.3$.

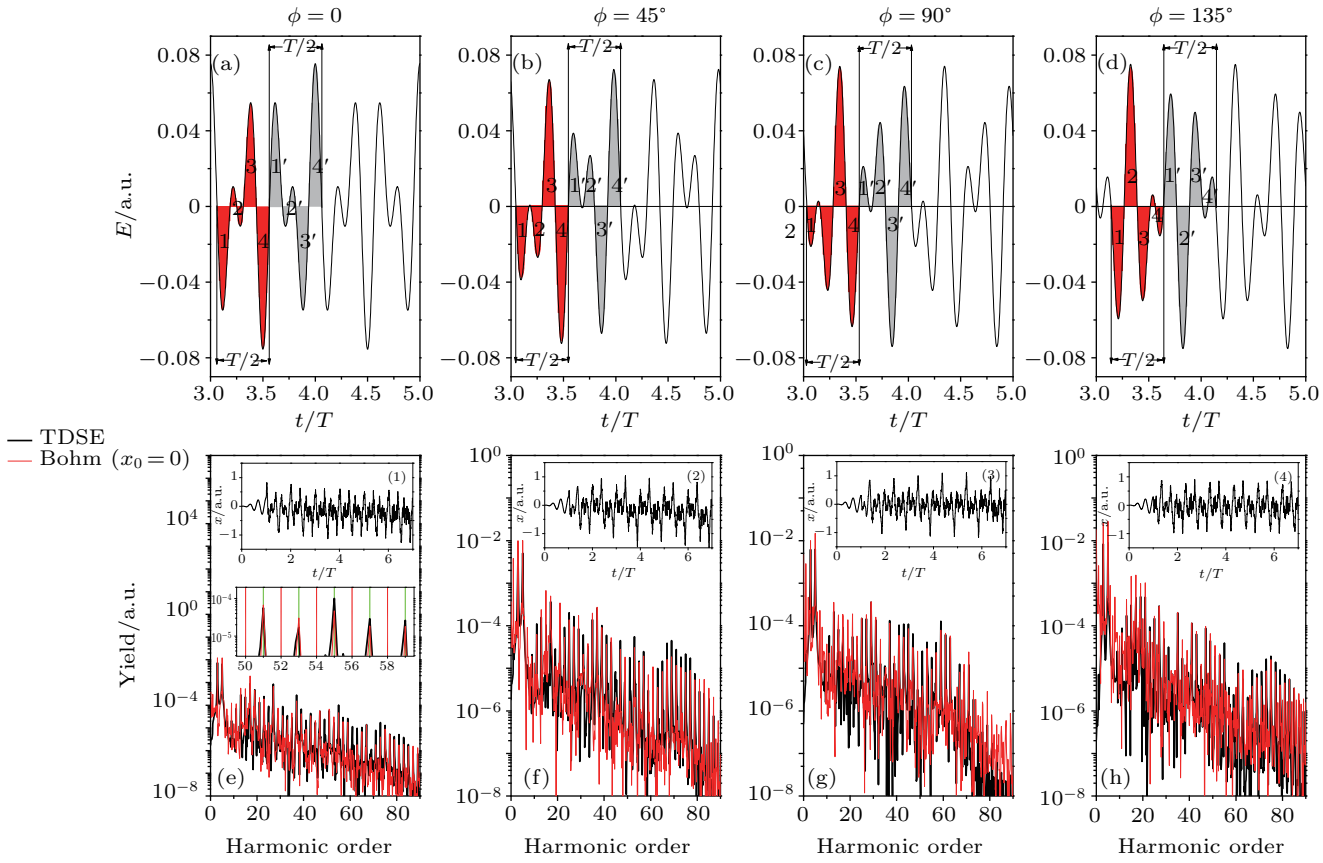


Fig. 4. (color online) (a)–(d) Two-color laser fields with inversion symmetry at four different relative phases in the time regions of $3T < t < 5T$. (e)–(h) HHG spectra simulated with TDSE (black lines) and the central Bohmian trajectory (red lines). Insets (1)–(4) show the corresponding central Bohmian trajectories. Another inset in panel (e) shows the enlargement of the harmonics from 51th to 59th order in panel (e). The laser intensity is $I = 1.0 \times 10^{14}$ W/cm^2 with $\beta = 1$, $r = 3$, $s = 5$, and $\omega = 0.019$ a.u. in Eq. (3).

Furthermore, to more clearly understand the influence of the symmetry of a laser field on the simulation of the HHG spectrum with Bohmian trajectory, we choose a two-color laser field with inversion symmetry with $r = 3$, $s = 5$, $\beta = 1$, and $\omega = 0.019$ a.u. in Eq. (3). In Figs. 4(a)–4(c), we exhibit the two-color laser field at different relative phases ϕ. For a better visualization, we just show a part of the laser fields, e.g., $3T < t < 5T$. As one can see, the electric field of the laser pulse is inversion symmetric with $E(t) = -E(t + \frac{T}{2})$. To show it more clearly, the peaks of the electric fields in one optical cycle are marked with 1–4 and 1′–4′, respectively. One sees that, for example, for the peaks 1 and 1′, $E(t_1) = -E(t_{1'})$. The insets in Figs. 4(e)–4(h) show the central Bohmian trajectory as a function of time, which keeps oscillating around the core as expected. Figures 4(e)–4(h) present the HHG spectra from the TDSE and the single central Bohmian trajectory, respectively. It is interesting to find that the simulations with the central Bohmian trajectory can qualitatively reproduce the TDSE results well. Moreover, since the Bohmian trajectory is also inversion symmetric in the two-color laser field, the energy interval of the harmonics is 2ω, which is consistent with the TDSE simulation shown in the inset of Fig. 4(e).

4. Conclusion

We theoretically studied the HHG in a two-color laser field using the Bohmian mechanics, in comparison with the TDSE calculations. Our results show that the simulation of the HHG with only one central Bohmian trajectory is in a good agreement with the TDSE results for the case of a weak second-color laser field. However, with the increase of the amplitude of the second laser pulse, a significant deviation of the HHG spectra is observed. By analyzing the Bohmian trajectories, we find that the significant deviation is ascribed to that the central Bohmian trajectory leaves the core quickly in the two-color laser field with the breaking of inversion symmetry. Interestingly, we find that another Bohmian trajectory with different initial position, which keeps oscillating around the core, could qualitatively reproduce the HHG spectrum well. Furthermore, we study the HHG spectrum in a two-color laser field with inversion symmetry and find that the HHG spectrum can be still well simulated with the central Bohmian trajectory. Therefore, our work indicates that the HHG spectrum in a two-color laser field can be also reproduced with a single Bohmian trajectory, although the initial position of the trajectory is dependent on the symmetry of the laser field. This result suggests that Bohmian trajectory theory provides a promising tool to explore the HHG of atoms and molecules[45,46] in a two-color laser field and to reveal the underlying electronic dynamics.

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