Dynamic stabilization of ionization for an atom irradiated by high-frequency laser pulses studied with the Bohmian-trajectory scheme

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We study the atomic ionization process in high-frequency laser pulses by the Bohmian-trajectory scheme. Combined with the analysis of the trajectories of Bohmian particles and the time-dependent potential well based on the Kramers-Henneberger transformation, we find that there are two kinds of forces that act on each Bohmian particle (BP): the classical force from the combined potential of the atomic Coulomb potential and the laser field and the quantum force. By investigating the forces acting on different BPs, we find that the quantum force plays an important role in the atomic ionization process in the laser pulse.

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I. INTRODUCTION

Recently, with the development of the laser technique, especially, the application of the high-order harmonic sources and the realization of the free-electron laser pulses [1–6], it is possible to experimentally investigate the ionization process of an atom in a high-frequency intense laser pulse. On the other hand, the ionization of an atom in a superintense high-frequency laser field has been studied theoretically for more than 20 years. Based on the theoretical research, a counterintuitive phenomenon has been found: The ionization probability of an atom in a superintense high-frequency laser field may decrease with the laser intensity when the laser intensity exceeds a critical value [7–9]. This ionization stabilization phenomenon has attracted a lot of interest since it was found [9–15]. Using the numerical solution of the time-dependent Schrödinger equation (TDSE), it was found that the dynamical stabilization of the atomic ionization exists in both one- and three-dimensional calculations. Furthermore, the influence of the laser conditions on the stabilization of atomic ionization has been considered [9–12]. Then, similar phenomena have been found in the ionization process of Rydberg atoms in intense laser fields and have been confirmed by relevant experiments [13–15]. More recently, the ionization stabilization process has also been studied in the two-electron atomic system, and the influence of the correlation between electrons on it has been investigated [16,17].

In general, the stabilization phenomenon of an atom in a high-frequency laser field can be explained by the Floquet theory under the Kramers-Henneberger (K-H) transformation [9,18]. Under the K-H transformation, the interaction between laser and atom can be expressed by a unified time-dependent potential function. If the laser's electric field can be treated as a monochrome plane wave, the time-dependent problem of the atom-laser system can be transformed into a time-independent problem. As the duration of the high-frequency laser pulse is very long, the behavior of the electron in an atom can be well described by a Floquet ground state. However, as the pulse duration dwindles, several Floquet excited states (shake up) and even Floquet ionized states (shake off) need to be considered to express the behavior of the electron. In such cases, the Floquet method does not have an obvious advantage for explaining the ionization of the atom explicitly and succinctly.

Although the TDSE calculation may provide an accurate simulation result, it cannot present a clear physics picture about the origin of the atomic ionization stabilization. To overcome this difficulty, we employ the Bohmian-trajectory (BT) scheme to investigate the atomic ionization under the action of high-frequency laser pulses. In the BT scheme, the electron is described by an ensemble of Bohmian particles (BPs) whose motions are ushered by the wave function of the atom [19,20]. This method has been applied successfully in the study of quantum chaos [21] and double-slit experiments [21,22]. Recently, the BT scheme has been used to investigate the interaction between strong laser pulses and atoms or molecules [23–26]. For example, Lai *et al.* [23] investigated the quantum-classical correspondence in the atomic ionization process in an intense laser field. Takemoto and Becker [24] studied the ultrafast electron dynamics of a hydrogen molecular ion in a strong laser pulse. Sanz *et al.* [25] investigated the mechanism of high harmonic generation of an atom irradiated by a laser pulse.

In this paper, we study the ionization stabilization of an atom in a high-frequency laser pulse using the BT scheme. We first solve the TDSE and obtain the time-dependent atomic wave function, then calculate the dynamical behaviors of Bohmian particles by using the wave function and, at last, obtain the ionization information of the atom. The BT method is presented in Sec. II. Using the selected Bohmian trajectories, we study the dynamic process of the atomic ionization. The dynamic profile of the Bohmian trajectory in different laser intensities is analyzed in Sec. III. Finally, the main conclusion is summarized in Sec. IV.

II. THEORETICAL METHODS

In order to analyze the atomic ionization process in a laser pulse by the BT scheme, we need to solve the TDSE

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that describes the interaction between an atom and a laser pulse. Since the stabilization phenomenon of the atomic ionization exists in one- or three-dimensional cases, we can reasonably investigate the dynamic ionization process of an atom by using the one-dimensional model for simplicity. The one-dimensional TDSE for an atom in an intense laser pulse is given by (atomic units are used throughout, unless otherwise stated)

$$i\frac{\partial\psi(x,t)}{\partial t}=\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2}+V(x)-E(t)x\right]\psi(x,t), \quad (1)$$

where $V(x)$ is the soft Coulomb potential describing the interaction between the electron and the nucleus,

$$V(x)=-q/\sqrt{x^2+\alpha}. \quad (2)$$

In this paper, we set $q=1$ and $\alpha=2$, hence, the lowest bound energy is -0.5, which corresponds to the ground-state energy of the hydrogen atom. The laser's electric field $E(t)$ in Eq. (1) is as follows: $E(t)=-\frac{\partial A(t)}{\partial t}$, where $A(t)$ is the laser's vector potential,

$$A(t)=E_0 f(t)\sin(\omega t+\phi). \quad (3)$$

Here, E_0, ω, and ϕ are the peak amplitude, the frequency, and the carrier-envelope phase, respectively, of the laser pulse, and $f(t)=\sin^2(\omega t/2\tau_R)$ is the envelope of the laser's electric field with τ_R being the pulse duration. To solve Eq. (1), in this paper, a symmetric splitting Fourier-transformation scheme is adopted [27,28].

To obtain the Bohmian trajectories, we need to generate an ensemble of Bohmian particles $x_{i,i=\{1,\ldots,N_{\rm tr}\}}$ by using the probability density distribution of the atomic ground state where the initial position of each BP is determined by this density distribution. Here, we assume that the weight of each trajectory is the same, i.e., $1/N_{\rm tr}$ with $N_{\rm tr}$ being the total number of BTs. According to Bohmian mechanics [19,29], the velocity of the kth BP is

$$v_k(t)=\mathrm{Im}\left[\frac{1}{\psi(x,t)}\frac{\partial}{\partial x}\psi(x,t)\Big|_{x=x_k(t)}\right], \quad (4)$$

where the wave function $\psi(x,t)$ is obtained by solving Eq. (1).

Integrating the above equation, the position of the Bohmian particle at moment t can be obtained by $x_k(t)=x_k\ (t=0)+\int_0^t v_k(t')dt'$. According to position x_k and velocity v_k of each BP, its potential energy in the combined potential of the atomic Coulomb and the laser field is $V_k=V(x_k)-E(t)x_k$, and its kinetic energy is $E_k=-\mathrm{Re}\{\psi^*(x,t)\psi''(x,t)/[\psi^*(x,t)\psi(x,t)]\}/2|_{x=x_k}=v_k(t)^2/2+Q(x_k)$, where $v_k(t)^2/2$ is the classical kinetic energy and $Q(x_k)$ is the quantum potential. Summing up the potential energy V_k and the kinetic energy E_k, the total energy of each BP is obtained. Therefore, if the BP's total energy is larger than zero, it is ionized; otherwise, it is still bound. By counting the number of the ionized Bohmian particles at the end of the laser pulse, we may obtain the ionization probability by the Bohmian-trajectory method.

For the purpose of comparison, we also calculate the ionization of an atom in a laser pulse using the TDSE method. By projecting each bound state onto a wave function at the end of the laser pulse, one can obtain the population amplitude of the bound state $c_n=\langle\phi_n|\psi\rangle$, and hence, the ionization probability of the atom is as follows:

$$P_{ion}=1-\sum_i |c_i|^2. \quad (5)$$

III. RESULTS AND DISCUSSIONS

In this paper, without loss of generality, we set the laser parameters as that the pulse duration is $\tau_R=10$ optical cycles, the laser carrier frequency is $\omega=1$, and the peak intensity of the laser pulse changes from 10^{15} W/cm^2 to about 10^{17} W/cm^2. We should mention that, for the laser conditions considered here, the dipole approximation is still suitable. This is because the laser intensity we used here is much smaller than 10^{18} W/cm^2 where Sorngard *et al.* [16] pointed out that the nondipole effects begin to play an important role as the laser's electric-field strength is larger than 20 (i.e., the intensity is larger than 10^{18} W/cm^2). Moreover, since we find that our results are insensitive to the carrier-envelope phase ϕ of the laser pulse, we set $\phi=0$ for simplicity throughout this paper.

Figure 1 presents the atomic ionization probability as a function of the peak strength of the laser's electric field. The solid square in Fig. 1 is the result by solving the TDSE, whereas, the solid circle and the solid triangle are the results by the Bohmian-trajectory method with $N_{\rm tr}=5000$ and 50 000, respectively. One can find that the ionization suppression occurs in Fig. 1 where the atomic ionization probability increases with laser intensity until it gets its maximum value at about $E_0=1.8$, then the probability decreases with the laser intensity. In Fig. 1, it shows that the results by the Bohmian-trajectory method agree well with that by the quantum numerical calculation, which indicates that we may study the ionization mechanism by analyzing the characteristics of the Bohmian trajectories in the ionization process.

In order to understand the mechanism of the atomic ionization stabilization in a high-frequency laser pulse, we now consider the time evolution of the density distribution of the electron in the combined potential of the Coulomb and the laser's electric field by solving the TDSE. Figure 2 presents the time evolution of the density distribution as the peak amplitude of the laser's electric fields as follows: (a) $E_0=1$, (b) 1.8, and

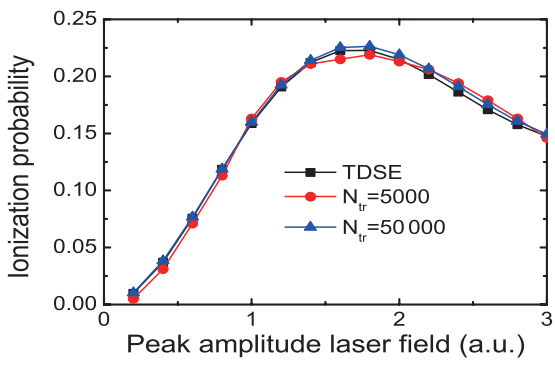

FIG. 1. (Color online) Change in the ionization probability with the peak amplitude of the laser electric field.

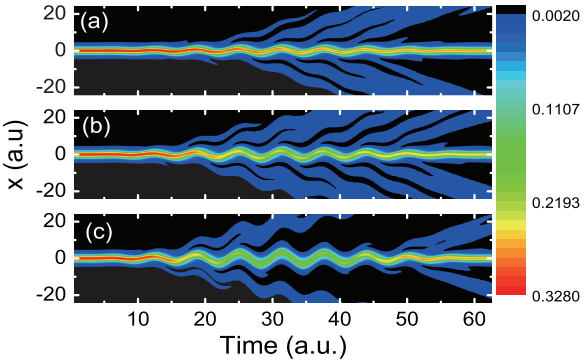

FIG. 2. (Color online) Evolution of the time-dependent probability density in different electric fields: (a) $E_0 = 1$ a.u.; (b) $E_0 = 1.8$ a.u.; (c) $E_0 = 2.8$ a.u.

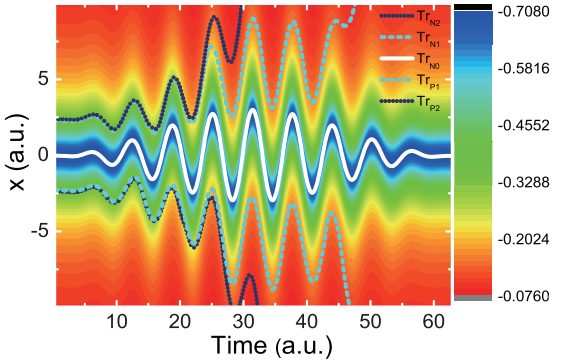

FIG. 4. (Color online) Change in the K-H potential $V_{\text{K-H}}(x,t)$ and BTs as a function of time.

(c) 2.8. As shown in Fig. 2(a), when the laser intensity is low [Fig. 2(a)], no ionization occurs at the rising and falling edges of the laser pulse, and the ionization mainly occurs at the peak of each half-optical cycle around the peak region of the laser pulse. As the peak amplitude of the laser's electric field increases to $E_0 = 1.8$ in Fig. 2(b), the evolution of electron density is similar to the case of $E_0 = 1$, and the difference is that more laser cycles are involved in the ionization process and the ionization probability increases due to the higher peak amplitude of the laser's electric field. However, as the peak amplitude increases to $E_0 = 2.8$ as shown in Fig. 2(c), there exhibits a very different ionization situation: The ionization of the electron mainly occurs at the rising and falling edges of the laser pulse, whereas, there is no electron being ionized around the peak of the laser field. Consequently, the phenomenon of the atomic ionization suppression in such a high-frequency laser pulse can be attributed to the existence of a time region around the peak of the laser pulse that no ionization has happened.

In the following, we will explain the above quantum numerical results by analyzing the characteristics of the corresponding Bohmian trajectories. Figure 3 presents 200 BTs in the laser field with its peak amplitude: (a) $E_0 = 1$, (b) 1.8, and (c) 2.8. From Fig. 3, it can be seen that the behaviors of the BTs agree with the time-evolution features of the electron-density

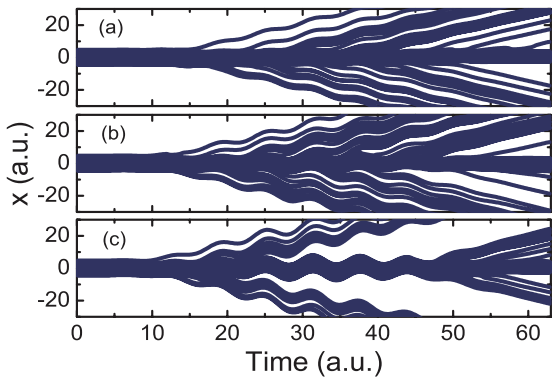

FIG. 3. (Color online) Time evolution of BTs in different electric fields: (a) $E_0 = 1$ a.u.; (b) $E_0 = 1.8$ a.u.; (c) $E_0 = 2.8$ a.u.

distribution shown in Fig. 2 where a few Bohmian particles are ionized around the peak of the laser pulse when $E_0 = 1$, and then the number of the ionized BPs increases as the amplitude E_0 increases to $E_0 = 1.8$. Especially when the amplitude increases further to $E_0 = 2.8$, there is no Bohmian particle running out of the nuclear zone during the time from about 25–45 a.u., indicating that no ionization occurs in this period.

To investigate the origin why the atom is not ionized around the peak of the laser pulse when $E_0 = 2.8$, we calculate the time-dependent potential function of the system under the K-H transformation and compare it with the evolution of BPs. Applying the K-H transformation, we can obtain the TDSE in the acceleration form

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} + V_{\text{K-H}}(x,t)\right]\Phi_{\text{K-H}} = i\frac{\partial \Phi_{\text{K-H}}}{\partial t}, \tag{6}$$

where $V_{\text{K-H}}(x,t) = V_a[x + \alpha(t)]$ and $\alpha(t) = -\frac{1}{c}\int^t A(t')dt'$ can be regarded as the motion trajectory of a free electron in the intense laser pulse. Under this framework, the laser-electron interaction potential and the nuclear Coulomb potential are replaced by the unified potential $V_{\text{K-H}}(x,t)$. The evolution of the unified potential is shown in Fig. 4 where the peak amplitude of the laser field is $E_0 = 2.8$. From the figure, it can be seen that the central position of the potential changes as the amplitude of laser field varies. In order to facilitate the analysis, we present five Bohmian trajectories Tr_{N2}, Tr_{P2} (dotted navy lines), Tr_{N1}, Tr_{P1} (dashed cyan lines) and Tr_{N0} (solid white line) in Fig. 4. We can see that trajectory Tr_{N0} is initially located at the center of the unified potential well, and during the subsequent motion, it remains located at the central position of the time-dependent potential $V_{\text{K-H}}(x,t)$. For particles Tr_{P1} and Tr_{N1}, they initially locate at the edge of the potential well, then, during the time from the rising edge to the peak of the electric field, they follow the profile of the time-dependent potential $V_{\text{K-H}}(x,t)$, whereas, during the falling edge of the laser pulse, they get rid of the time-dependent potential, and thus, these two BPs are ionized at the end of the laser pulse. For the BPs Tr_{P2} and Tr_{N2}, which are initially far away from the center of the atomic potential, they fail to catch up with the change in time-dependent potential $V_{\text{K-H}}(x,t)$ and, hence, are ionized rapidly during the rising edge of the laser pulse.

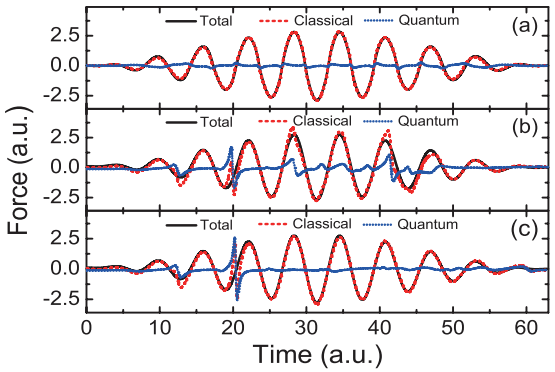

FIG. 5. (Color online) Force analysis of the BPs: (a) Tr_{N0}, (b) Tr_{N1}, and (c) Tr_{N2}. Where the solid black curve denotes the total force, the dotted blue one denotes the quantum force, and the dashed red one denotes the classical force.

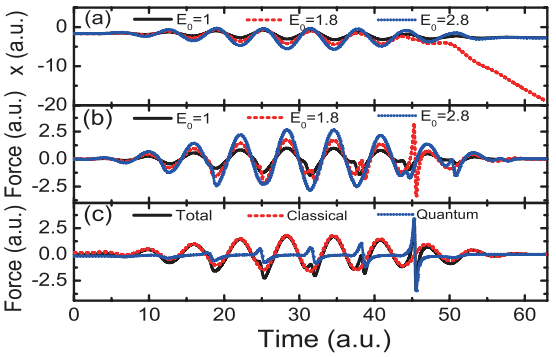

FIG. 6. (Color online) (a) Change in Bohmian trajectory and (b) total force as a function of time in different laser fields. In (c), we present the force analysis of the Bohmian particle in the laser field whose peak amplitude is 1.8 a.u. [dotted red line in (b)].

We now consider the time-dependent forces that act on the BPs Tr_{N0}, Tr_{N1}, and Tr_{N2}, which are shown in Figs. 5(a)–5(c), respectively. Based on the Bohmian-trajectory theory, the force that can influence the trajectory of a BP in our atom-laser system can be classified as two kinds: the classical force $F_{\mathrm{classical}}(t)$, which comes from the combined potential of the atomic Coulomb and the laser's electric field, i.e., $F_{\mathrm{classical}}(t) = -\frac{\partial v_k(t)}{\partial x}$, and the quantum force $F_{\mathrm{quantum}}(t)$, which comes from the interaction between this BT and other BTs, i.e., $F_{\mathrm{quantum}}(t) = -\frac{\partial Q}{\partial x}$. From Fig. 5(a), it can be seen that the force felt by the BP on trajectory Tr_{N0} is identical to the classical force (dashed red line), hence, the quantum force (dotted blue line) plays a negative role in its evolution process, and its behavior agrees well with the classical trajectory $\alpha(t)$. On the other hand, from Fig. 5(c), we can find that the BP on Tr_{N2} bears a large quantum force at about time $t = 20$, then this quantum force vanishes rapidly because the BP obtains enough energy from this sudden "push" to get rid of the bondage of the atomic potential, resulting in the fact that this BP is ionized at the end of the laser pulse. Furthermore, as shown in Fig. 5(b), the BP on trajectory Tr_{N1} is also affected by the quantum force at about $t = 20$, but the quantum force is not strong enough to set it free from the bondage of the atomic Coulomb potential. Therefore, the BP continues moving under the influence of the two forces until it is ionized at the end of the laser pulse.

From the above results, we may find that the quantum force plays a crucial role in the ionization process of the BPs in the laser pulse. The above three trajectories can be understood in the following way: For the BP located at the position very close to the nucleus, the classical force from the Coulomb potential and the laser field dominate the behavior of the BP and make it stay in the center of the K-H potential during the time evolution, hence, the interaction between it and other BPs can be ignored; whereas, for the BP initially located at a position far away from the nucleus, the classical force can be weak at some moments when the BP is far away from the nucleus (hence, the Coulomb potential is weak), and the laser's electric field is close to zero. Then, at these moments, the quantum force from other BPs may be larger than the classical force (because the BPs can be very close to each other at these moments during which they oscillate in the laser field) and changes the trajectory of the BP during its oscillation in the K-H potential and makes it free from the bondage of the nucleus at the end of the laser pulse.

From the viewpoint of the BT theory, the ionization suppression of an atom in a laser pulse indicates that some Bohmian trajectories, which are ionized in a weak laser field, become unionized as the laser intensity increases. We present a trajectory which is ionized when $E_0 = 1.8$ and is unionized when E_0 increases to 2.8 in Fig. 6. From Fig. 6(c), we may find that the quantum force makes this BP ionized when $E_0 = 1.8$, and this quantum force decreases as the laser intensity increases, resulting in the unionization of the BP as $E_0 = 2.8$. This result confirms that the quantum force plays a crucial role in the ionization of the BPs in a high-frequency laser pulse.

IV. CONCLUSIONS

In conclusion, we investigate the ionization stabilization of an atom in a high-frequency intense laser pulse by using Bohmian trajectories. We find that there are two kinds of forces that act on each BT: the classical force from the combined potential of the atomic Coulomb potential and the laser field and the quantum force. The competition between these two forces determines the behavior of each BT. Especially for the BT initially located at the center of the K-H potential, the classical force plays a dominate role in it, resulting in the fact that this BT is unionized; whereas, for the BT initially located far away from the center of the K-H potential, the quantum force plays a crucial role in it, resulting in the fact that this BT is ionized after the laser pulse.

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