Efficient time-sampling method in Coulomb-corrected strong-field approximation

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(Received 21 August 2016; published 23 November 2016)

One of the main goals of strong-field physics is to understand the complex structures formed in the momentum plane of the photoelectron. For this purpose, different semiclassical methods have been developed to seek an intuitive picture of the underlying mechanism. The most popular ones are the quantum trajectory Monte Carlo (QTMC) method and the Coulomb-corrected strong-field approximation (CCSFA), both of which take the classical action into consideration and can describe the interference effect. The CCSFA is more widely applicable in a large range of laser parameters due to its nonadiabatic nature in treating the initial tunneling dynamics. However, the CCSFA is much more time consuming than the QTMC method because of the numerical solution to the saddle-point equations. In the present work, we present a time-sampling method to overcome this disadvantage. Our method is as efficient as the fast QTMC method and as accurate as the original treatment in CCSFA. The performance of our method is verified by comparing the results of these methods with that of the exact solution to the time-dependent Schrödinger equation.

DOI: 10.1103/PhysRevE.94.053310

I. INTRODUCTION

Many novel phenomena arise when atoms and molecules are exposed to intense laser fields, such as above-threshold ionization (ATI) [1], high-order harmonic generation (HHG) [2], multiple ionization [3], and dissociative ionization and Coulomb explosion [4], etc. By exploiting the HHG, it is possible generate laser pulses with durations in the attosecond regime, which have made a revolution in the ultrafast sciences [5–7].

To understand the electronic dynamics of few-body atomic and molecular systems in strong laser fields, the most exact way is to numerically solve the time-dependent Schrödinger equation (TDSE) [8–11]. From the final wave function after the completion of the interaction, one can extract the momentum spectrum of the photoelectron by projecting it onto the scattering states. However, the numerical solution to TDSE is very time consuming and sometimes it is not easy to get a transparent physical picture about the underlying process.

Therefore, several semiclassical methods have been proposed to understand the observed structures of the ionization spectrum in an intuitive way. The simple man model [12–14] gives a basic perspective to understand the dynamics in a semiclassical way. When the laser pulse is shined on the atom, the Coulomb potential barrier is suppressed through which the bound electron can tunnel out [15,16]. Then the electron is dragged by the laser electric field and may rescatter with the core to induce many different processes. After the end of the laser pulse, one of the fates of the electron is to get emitted with a very wide energy spectrum. To calculate such a spectrum semiclassically, one needs to know the tunneling probability of the electron at a certain moment and its corresponding initial position and velocity. The theories proposed by Perelomov, Popov, and Terent’ev (PPT) and by Ammosov, Delone, and Krainov (ADK) [17–19] can provide an applicable ionization rate. After the tunneling of the electron, the subsequent dynamics of the electron is governed by the Newtonian equation in the combined Coulomb and laser field. By a large ensemble of the initial electrons, one can statistically calculate the final electron momentum distribution. This is the well-known classical trajectory Monte Carlo (CTMC) method [20,21] and it has successfully explained the basic processes in the above-threshold ionization [1].

In order to account the interference structures in the spectrum, the quantum trajectory Monte Carlo (QTMC) [22,23] was recently proposed. As the same treatment used in the Feynman’s path-integral [24,25], the phase information of each trajectory of the electron is considered by employing the classical action as the phase. In this way, the contribution of the electrons with the same final velocity can be added up coherently. This method can efficiently reproduce the ionization spectrum qualitatively in the adiabatic regime.

The Coulomb-corrected strong-field approximation (CCSFA) [26–29] is another popular semiclassical method with a nonadiabatic nature, which is based on the strong-field approximation (SFA) [16,30,31]. Unlike the QTMC, the CCSFA can provide a proper ionization rate [32] and initial velocity in the nonadiabatic regime. Thus, the CCSFA works well in a much wider range of laser parameters [33,34]. Recently, some details in realization of the CCSFA method have been studied [35–37], which is helpful to improve the performance of CCSFA. The key step to get a correspondence between the quantum and the classical description from the SFA is the saddle-point method [38–40]. Each solution to the saddle-point equation, called the saddle point, corresponds to a complex ionization time. However, it is very time consuming to solve these saddle-point equations for a large number of the initial ensemble.

Since semiclassical methods provide a direct way to understand the motion of the electron, they have found many applications in different circumstances [22,41–49]. Therefore, it is desirable to have a numerical method with a high efficiency and a wide range of applicability. In the present contribution, we present an alternative numerical scheme, the time-sampling method, to overcome the time-consuming disadvantage of the CCSFA. It turns out to be as efficient as the fast QTMC method.
and as accurate as the original treatment in the CCSFA. The key step of our scheme is that we choose the solution of the saddle-point equation \( t_s \) as a parameter. All other variables can be expressed by \( t_s \) analytically so one does not need to solve the saddle-point equations. Compared with the original numerical scheme of CCSFA, our method can save the computational consumption by tens of times.

The rest of the paper is organized as follows. In Sec. II, we start by introducing the SFA and saddle-point method and then present how we avoid solving the saddle-point equations by approximation and the saddle-point method. Then we will draw a short conclusion in Sec. IV. Atomic units are employed throughout unless otherwise stated.

II. NUMERICAL METHODS

In this section, we will first briefly introduce the strong-field approximation and the saddle-point method. Then we will present how we avoid solving the saddle-point equations by an improved Monte Carlo sampling method.

A. Strong-field approximation

For an atomic system starting from an initial state \( |\Psi_0(t_0)\rangle \) at \( t_0 \) and then driven by a laser field from then on, the full Hamiltonian can be written as

\[
H(t) = -\nabla^2 + \mathbf{r} \cdot \mathbf{E}(t) + V(\mathbf{r}),
\]

(1)

where the interaction term has been expressed in the form of length gauge. By solving the corresponding time-dependent Schrödinger equation, one can get the state at any subsequent time \( |\Psi(t)\rangle = U(t,t_0)|\Psi_0(t_0)\rangle \), where \( U(t,t_0) \) is the time-evolution operator of \( H(t) \).

To get the transition amplitude of an photoelectron with a final momentum \( \mathbf{p} \), one can project the final wave function onto the scattering state \( |\Psi_p(t)\rangle \)

\[
M_p = \langle \Psi_p(t)|U(t,t_0)|\Psi_0(t_0)\rangle.
\]

(2)

With the help of the Dyson equation [38]

\[
U(t,t_0) = U_a(t,t_0) + i \int_{t_0}^{t} dt' U(t,t')\mathbf{r} \cdot \mathbf{E}(t)U_a(t',t_0),
\]

(3)

we can rewrite Eq. (2) in the form

\[
M_p = i \int_{t_0}^{t} dt' \frac{e^{i S_p(t',t)}}{S_p(t_0)}|\Psi_p(t)|U(t,t')\mathbf{r} \cdot \mathbf{E}|\Psi_0(t_0)\rangle.
\]

(4)

Note that, in Eq. (3), \( U_a(t',t_0) \) is the time-evolution operator of the field free Hamiltonian \( H_a(t) = -\nabla^2 + V(\mathbf{r}) \), whose initial state is the eigenstate with an eigenenergy of \(-I_p\).

If one supposes the laser field is intense and that only the first-order effect is considered (which means that the electron never interacts with the atomic core later on), then it comes to the most crucial step of the strong-field approximation that one makes the substitutions \( |\Psi_p(t') \rangle \rightarrow |\Psi^S_p(t')\rangle \) and \( U(t,t') \rightarrow U_0(t,t') \). Here, \( U_0 \) denotes the time-evolution operator of Hamiltonian without the Coulomb binding potential, i.e., \( H_0(t) = -\nabla^2 - \mathbf{r} \cdot \mathbf{E}(t) \). The Volkov state \( |\Psi^S_p(t')\rangle \) is the eigenstate of \( H_f \) and has the following form [50,51]:

\[
|\Psi^S_p(t')\rangle = |\mathbf{p} + \mathbf{A}(t')\rangle e^{-i S(p,t')},
\]

(5)

where \( |\mathbf{p} + \mathbf{A}(t')\rangle \) is a plane-wave state and the phase is given by

\[
S_p(t') = \int_{t_0}^{t'} d\tau \frac{[\mathbf{p} + \mathbf{A}(\tau)]^2}{2},
\]

(6)

with \( \mathbf{A}(t) \) being the vector potential of the laser pulse. Note that one has the relation of \( \mathbf{E}(t) = -\frac{\partial \mathbf{A}(t)}{\partial t} \).

In the above SFA framework, by omitting a global phase at time \( t_0 \), one can achieve a final simple expression for the transition amplitude

\[
M_p = i \int_{t_0}^{t} dt' e^{i S_p(t')}(\mathbf{p} + \mathbf{A}(t'))\mathbf{r} \cdot \mathbf{E}|\Psi_0\rangle,
\]

(7)

with the phase given by

\[
S_p(t') = \int_{t_0}^{t'} d\tau \left\{ \frac{[\mathbf{p} + \mathbf{A}(\tau)]^2}{2} + I_p \right\}.
\]

B. Saddle-point method

In principle, the ionization probability \( |M_p|^2 \) at each final momentum \( \mathbf{p} \) can be calculated by carrying out the multiple integration in Eq. (7). However, one can simplify the computation by using some mathematical tricks and it turns out that a transparent physical picture can be achieved. Usually, for most of the common laser parameters used, the phase \( S_p(t') \) in the integral of Eq. (7) varies more rapidly than the prefactor \( \langle \mathbf{p} + \mathbf{A}(t')\rangle\mathbf{r} \cdot \mathbf{E}|\Psi_0\rangle \). Therefore, one can adopt the saddle-point method (method of steepest descents [52]) to deal with the integration.

After using the saddle-point method, the integration can be approximated by the sum of the integrand value at every saddle point,

\[
M_p \sim \sum_s \sqrt{\frac{2\pi i}{S_p'(t_s)}} (\mathbf{p} + \mathbf{A}(t_s))|\mathbf{r} \cdot \mathbf{E}|\Psi_0\rangle e^{i S_p(t_s)},
\]

(9)

where the saddle point \( t_s \) is the stationary phase point that satisfies the saddle-point equation

\[
\frac{\partial S_p(t)}{\partial t} \bigg|_{t=t_s} = \frac{[\mathbf{p} + \mathbf{A}(t_s)]^2}{2} + I_p = 0.
\]

(10)

Unfortunately, for the Coulomb potential, the element \( \langle \mathbf{p} + \mathbf{A}(t')\rangle\mathbf{r} \cdot \mathbf{E}|\Psi_0\rangle \) is a singularity at the saddle point \( t_s \), which makes the direct usage of Eq. (9) inapplicable. But, as shown by Milošević and coworkers [40], one can bypass this problem by starting from Eq. (7). In doing so, one can finally get the ionization amplitude in the following concise form:

\[
M_p \sim \sum_s \sqrt{\frac{2I_p}{2!E(t_s)}} \frac{1}{3!} (\mathbf{p} + \mathbf{A}(t_s))^2 e^{i S_p(t_s)}.
\]

(11)

It is obvious that the solutions \( t_s \) of Eq. (10) are complex numbers. Denoting \( t_s = t_s + i\tau_s \), we can consider that the process from the complex time \( t_s \) to the real time \( t_r \) is under the Coulomb barrier. The electron moves classically after tunneling out at real time \( t_r \). The initial velocity while tunneling
out at \( t_f \) can be defined as

\[
v_0 = p + A(t_f).
\]

The initial position can be defined as the real displacement under the barrier \[53\]

\[
r_0 = \text{Re} \int_{t_0}^{r_f} [p + A(\tau)]d\tau = \text{Re} \int_{t_0}^{r_f} A(\tau)d\tau.
\]

The ionization rate can be extracted from \( M_p \). We rewrite the phase into two parts

\[
\hat{S}_p(t) = -\int_{t_0}^{r_f} d\tau \left\{ \frac{|p + A(\tau)|^2}{2} + I_p \right\} - \int_{t_0}^{\infty} d\tau \left\{ \frac{|p + A(\tau)|^2}{2} + I_p \right\}.
\]

The second part is the phase accumulation after the ionization and makes no contribution to the ionization rate. The first part of the phase accumulation under barrier is a complex number, whose real part gives the initial tunneling phase and the imaginary part gives the ionization rate. Let us define

\[
\hat{S}_p = -\int_{t_0}^{r_f} d\tau \left\{ \frac{|p + A(\tau)|^2}{2} + I_p \right\},
\]

and then we have the transition amplitude corresponding to the saddle point \( t_s \)

\[
M_s = \frac{(2I_p)^{5/4}}{2^{1/2}E(t_f)[|p + A(t_f)|]} e^{\hat{S}_p}.
\]

C. Time-sampling Monte Carlo method

In order to present our time-sampling Monte Carlo method, we now consider a specific case where a linear polarized laser field with a \( \cos^2 \) envelope is employed. The polarization direction is along \( z \) axis and the laser field has the form

\[
A(t) = A_c e^{i\beta t} = A_c \cos^2(\beta t) \sin(\omega t + \phi) e^z,
\]

where \( \beta = \frac{2\pi}{T} = \frac{2\pi}{2N} \), \( T \) is the laser pulse duration, and \( N \) is the total number of laser cycles. Since the laser field is along \( z \) axis, the ionization spectrum should show cylindrical symmetry along \( z \) axis. Thus, one only needs to consider the electrons in the \( x-z \) plane so the position and velocity along the \( y \) axis can be set to zero, \( y = 0, v_y = 0 \). For each final momentum \( p = p_x e_x + p_z e_z \), the saddle-point equation \(10\) can be written as

\[
\frac{1}{2}[p_z^2 + A_z(t_f)]^2 + \frac{1}{2}p_x^2 + I_p = 0.
\]

The solution \( t_s = t_f + i t_i \) is a complex number and \( A_z \) should be a complex function

\[
A_z(t_r, t_i) = A_z(t_r, t_i) + i A_i(t_r, t_i).
\]

Then the saddle-point equation \(18\) can be derived into the following algebraic equations:

\[
p_z + A_z(t_r, t_i) = 0,
\]

\[
p_z^2 + 2I_p - A_i^2(t_r, t_i) = 0.
\]

After the tunneling, one can describe the electron in a classical point of view. Let us focus on the electron with a final momentum \( p \). The electron tunnels out at time \( t_f \), which is the solution to Eqs. \(20\) and \(21\) with an initial position

\[
x_0 = 0,
\]

\[
y_0 = 0,
\]

\[
z_0 = \text{Re} \int_{t_0}^{t_f} A_z(\tau)d\tau,
\]

and the initial velocity

\[
v_x = \left[ A_i^2(t_r, t_i) - 2I_p \right]^{1/2},
\]

\[
v_y = 0,
\]

\[
v_z = -A_z(t_r, t_i) + A_z(t_r, 0).
\]

The ionization amplitude with an initial phase is given by Eq. \(16\), where

\[
\hat{S}_p = -\int_{t_0}^{r_f} d\tau \left\{ \frac{1}{2} p_z^2 + \frac{1}{2} p_x^2 + I_p + p_z A_z(\tau) + \frac{1}{2} A_z^2(\tau) \right\},
\]

\[
= i \left\{ \frac{1}{2} p_z^2 + \frac{1}{2} p_x^2 + I_p \right\}t_i - p_z \int_{t_i}^{r_f} A_z(\tau)d\tau - \frac{1}{2} \int_{t_i}^{r_f} A_z^2(\tau)d\tau.
\]

Note that the integrals in Eqs. \(24\) and \(28\) can be derived analytically for the specific laser pulse considered. One can write them into the following forms:

\[
\int_{t_i}^{r_f} A_z(\tau)d\tau = I_z(t_r) - I_z(t_s),
\]

\[
\int_{t_i}^{r_f} A_z^2(\tau)d\tau = I_z(t_r) - I_z(t_s),
\]

where the functions \( I_z(\cdot) \) and \( I_z^2(\cdot) \) are defined as

\[
I_z(t) = \frac{A_z^2}{64} \left[ 6t + 8 \sin(2\beta t) + \frac{2 \sin(4\beta t)}{4\beta} - \frac{6 \sin(2\omega t + 2\phi)}{2\omega} \right],
\]

\[
I_z^2(t) = \frac{A_z^2}{64} \left[ 6t + 8 \sin(2\beta t) + \frac{2 \sin(4\beta t)}{4\beta} - \frac{6 \sin(2\omega t + 2\phi)}{2\omega} \right],
\]

\[
- \frac{4 \sin(2\omega t + 2\beta + 2\phi)}{2\omega + 2\beta} - \frac{4 \sin(2\omega t - 2\beta + 2\phi)}{2\omega - 2\beta} \right],
\]

\[
- \frac{4 \sin(2\omega t + 4\beta + 2\phi)}{2\omega + 4\beta} - \frac{4 \sin(2\omega t - 4\beta + 2\phi)}{2\omega - 4\beta} \right].
\]

In the ordinary SFA method, one first solves the saddle-point equations \(20\) and \(21\) for every momentum grid point \( (p_x, p_z) \) and calculate the time when electron tunnels out. The electrons emitted at different times are then driven solely by the laser field. The electrons which reach a same final momentum
when the laser is over will interfere with each other. The final ionization amplitude at each momentum grid point can be calculated by Eq. (11). One note that the Coulomb effect is absent in the whole process of the SFA calculation.

The quantum trajectory Monte Carlo method [22,23] is an easily understood method that takes into account both the Coulomb effect after the tunneling and the interference effect. In the QTMC, the electron tunnels out the suppressed barrier when the laser electric field is applied. The ionization rate and the initial momentum distribution are given from the ADK theory while the initial position can be found by the Landau’s static tunneling theory [15]. One first chooses the ionization time and initial momentum randomly, after which the initial position and tunneling rate can be calculated. The subsequent classical motion is governed by the Newtonian equations in the combined laser field and the Coulomb potential. Therefore, one can calculate the trajectory of the electron according to

\[
\frac{dr}{dt} = v, \quad (33)
\]

\[
\frac{dv}{dt} = -\mathbf{E} - \frac{r}{r^3}. \quad (34)
\]

The interference effect can be included by considering the classical action of each trajectory as the phase [22,23]

\[
S_c = -\int_0^\infty dt \left[ \frac{v^2}{2} - \frac{1}{r} + I_p \right]. \quad (35)
\]

which can be regarded as the second part of Eq. (14) with a Coulomb correction.

Recently, a more proper Coulomb-corrected phase was presented in Ref. [54]

\[
S_c = -\int_0^\infty dt \left[ \frac{v^2}{2} - \frac{2}{r} + I_p \right]. \quad (36)
\]

One can notice a difference of a factor of 2 in the Coulomb-corrected part, which plays an important role in realizing a better agreement in the low-energy angular spectrum [55–57]. In the present work, we will use Eq. (36) instead of Eq. (35) as the classical action in the following calculations.

Electrons with different trajectories and phases may get interferences with each other if they reach the same final momentum. In practice, we collect the electrons whose final momenta fall into the same grid box \((p_x, p_z)\), whose solution are analytically given by

\[
P_x = N / \int_0^\infty \frac{dx}{J(x)}. \quad (38)
\]

Since \((p_x, p_z)\) can be analytically expressed, it is straightforward to calculate the above derivatives analytically. Alternatively, it is more convenient to employ the 5-point finite-difference method to get the derivatives numerically, which can work for an arbitrary pulse shape.

We can finally calculate the effective transition amplitude at time \(t_s\),

\[
M_x^\text{eff} = M_x J(t_s), \quad (38)
\]

which is a modified version of Eq. (16). Our method can be understood as a nonadiabatic quantum trajectory model.
The electrons begin to tunnel out randomly at complex time $t_s$, and then they become free at real time $t_r$ with a nonzero longitudinal velocity. The tunneling probability is given by $|M_{ss}|^2$. The subsequent dynamics is governed by the Newtonian equation and can be equally treated as the QTMC method. The final momentum distribution is a coherent sum of all the electrons which reach the same grid in the final momentum plane. Due to the nature of our method, we will call it the time-sampling method.

Our method is always valid if the original sample method has two degrees of freedom. It works well if the laser field is in a two-dimensional (2D) configuration, e.g., an elliptically polarized pulse or orthogonally polarized two-color laser field. Quite remarkably, if the original sample method has to sample three variables ($p_x, p_y, p_z$), in the case of a three-dimensional laser field, our method is difficult to use, as the mapping from the three-momentum variables to the two time variables is not defined. However, even for the original momentum sampling case, to the best of our knowledge, we have not seen any semiclassical methods which sample three degrees of freedom that have been successfully implemented. Therefore, the 3D semiclassical method is worth further studying.

III. RESULTS AND DISCUSSIONS

In this section, we will first discuss the importance of the Jacobian matrix in our time-sampling method, in which case we temporarily neglect the Coulomb potential. Then, we will make a comparison study on a realistic case where the Coulomb potential is taken into account. We will show the results of several semiclassical methods and of the exact TDSE result and discuss their differences together with a trajectory analysis. Finally, we systematically carry out a series of calculations at various laser parameters. By tabulating the different time costs of these numerical methods, one can see clearly that our time-sampling method overwhelms the previous semiclassical methods.

A. Importance of the Jacobian matrix

The Jacobian matrix (37) is very important in our time-sampling method. To see how it works, we first calculate the photoelectron momentum distributions without the Coulomb potential. We take the hydrogen atom as an example. The atom is driven by a 4-cycle linearly polarized laser pulse at wavelength of 800 nm and peak intensity of $1 \times 10^{14}$ W/cm², with a cos² envelope.

In Fig. 1(a), we present the exact photoelectron momentum distributions, calculated by a direct numerical integration of Eq. (7). Of course, by the saddle-point method, one can get almost the same momentum distributions if we sum up the transition amplitude $M_{ss}$, as shown in Eq. (16), for every solution $t_s$.

In our time-sampling method, we take advantage of Monte Carlo to replace the numerical solution process of the saddle-point equations. We prepare the sample electrons by setting $t_r$.

FIG. 1. The top panels show the 2D photoelectron momentum distributions of hydrogen atom, ionized by a 4-cycle linearly polarized laser pulse at wavelength of 800 nm and peak intensity of $1 \times 10^{14}$ W/cm², with a cos² envelope: (a) direct numerical integration from Eq. (7) and [(b) and (c)] our time-sampling method without and with the Jacobian matrix respectively. The low panels show the normalized momentum spectra for $p_z$ at $p_x = 0, 0.02, 0.1$ respectively in (d), (e), and (f). The red solid line is extracted from the exact result in panel (a), and the green long-dashed line is extracted from our method in panel (c). Note that the Coulomb potential is temporally neglected in these calculations.
and \( t_c \) randomly in a uniform distribution. At a random time \( t_c \), there is a sample electron tunneling out. It is driven by the laser field and flies to the detector with a final momentum \( \{ p_x(t_f), p_y(t_f), p_z(t_f) \} \). The electrons are regarded to have the same final momentum if they drop into the same small momentum grid box. If the number of the sample electrons is sufficiently large, the grid box will collect sample electrons from all relevant saddle points. These steps are almost the same as what one does in the QTMC method.

If we sum up the probability amplitude (16) of all the sample electrons in each grid box, one will get the momentum distributions, as shown in Fig. 1(b), which is not correct, as expected. The reason is that our sample is prepared in a uniform distribution in the time space. It will surely lead to the nonuniform distribution in the momentum space. We can see in Fig. 1(b) that there are far fewer sample electrons along \( p_z = 0 \) than along \( p_z = 0.2 \). For these reasons, the Jacobian matrix should be taken to compensate the nonuniform distribution in the momentum space. Figure 1(c) shows the photoelectron momentum distribution calculated by including the Jacobian matrix, which gives the correct result, as can be seen by comparing with Fig. 1(a).

There are two points that we should pay attention to. The first one is that the small number of sample electrons in the vicinity of \( p_z = 0 \) means a large noise. We can see that the spectrum along \( p_z = 0 \) [cf. Fig. 1(d)] is quite far from being satisfactory. It can be overcome by launching more sample electrons. However, as we will discuss below, these electrons will become less important if one takes the Coulomb potential into account. The second point is the asymmetry of the distribution, which can be noticed from the green line in Figs. 1(e) and 1(f). The electrons in the same grid box are not exactly the same final momentum as the grid point, so there is error in summing up the transition amplitude, depending on the grid resolution. The error is accumulating during the electron’s propagation in the combined Coulomb and laser field. The electrons with the nonsymmetric final momentum in the \( z \)-axis direction tunnel out at earlier time, so the error of the transition amplitude is larger. It leads to the difference between the left and the right plane in the momentum distribution. However, one can apparently reduce the asymmetry by decreasing the size of the momentum grid box.

**B. Comparison studies and trajectory analysis**

Now let us consider a realistic case where the Coulomb potential is taken into account. For the purpose of comparison, we present in Fig. 2(a) the exact momentum distributions calculated by a numerical solution to the TDSE [58,59], using the same laser parameters as those in Fig. 1. The result simulated by the QTMC method and by the original CCSFA method is shown in Fig. 2(b) and Fig. 2(c), respectively. Finally, in Fig. 2(d), we show the result of our time-sampling method for the CCSFA method, which looks essentially the same as Fig. 2(c) by the original time-consuming CCSFA method.

Both of the semiclassical methods can reveal the scattering ring [60] and the maximum momentum boundary qualitatively because of rescattering of the electron with the core. However, the structures in the result of TDSE cannot be well reproduced quantitatively. The reason is that the tunneling probability of the electrons with a final momentum \( p_z \) is derived without the Coulomb potential. If the Coulomb potential effect is added in the electron’s propagation, the electron can be scattered to get a very large final momentum, which differs considerably from the momentum before rescattering. Therefore, the quantitative difference between the quantum mechanical and semiclassical methods implies that improper rates are used for scattering electrons. A more proper rate of the rescattering electrons should be derived by considering the higher-order terms in the expansion of the transition amplitude [61].

In the present work, we only concentrate on the low-energy part of the spectrum below \( 2U_p \) [55–57,62–65], whose main structures can be reproduced qualitatively by both the QTMC and CCSFA methods. However, by a careful examination, one notices that a much better agreement has been achieved by the CCSFA method because the nonadiabatic effect is taken into account in the initial tunneling dynamics. The electrons within the marked and zoomed black boxes in Figs. 2(a)–2(c) may reach a larger final momentum in the CCSFA method than in the QTMC method, because there exists a nonzero initial longitudinal momentum in the nonadiabatic SFA treatment [44]. In addition, in the adiabatic QTMC method, the finer interference structures roughly perpendicular to the \( p_z \) axis, as zoomed in the left-top corner in these panels, cannot be reproduced at all.

In both of the semiclassical methods, one can trace the motion of the electron [66] to see what kind of trajectories contribute to the interference structures. In Fig. 3, we show the trajectories and the tunneling time of the electrons with a final
sample electrons are selected with the final momentum around the propagation. For better comparisons, all results have been scaled into dealing with 1 million electrons per core.

In the CCSFA, the time is divided into two parts, namely, time cost in solving saddle-point equations and time cost in complex ionization time (right panels) of the sample electrons that nonadiabatic regime than the QTMC method. However, the

Table I. All three methods are trivially parallelized and we use 120 cores to deal with about 500 million electrons in total for each case. In this table, we show the time spent in dealing with 1 million electrons on each core. In the original CCSFA method, the time is separated into two parts, respectively for solving saddle-point equations and for carrying out the subsequent propagation of the electrons. We can see that, for all three methods, it naturally costs more time in the propagation step for a longer duration of laser pulse. We have optimized our programs so they cost less time in both the QTMC and the CCSFA method in the propagation. In the ordinary CCSFA method, solving saddle-point equations costs the most time. Our time-sampling method should be as efficient as the QTMC, because now the most time-consuming step is the electron’s propagation.

To show the performance of our numerical method, we carry out a series of calculations at different laser parameters, using different semiclassical methods. The times are listed in Table I. All three methods are trivially parallelized and we use 120 cores to deal with about 500 million electrons in total for each case. In this table, we show the time spent in dealing with 1 million electrons on each core. In the original CCSFA method, the time is separated into two parts, respectively for solving saddle-point equations and for carrying out the subsequent propagation of the electrons. We can see that, for all three methods, it naturally costs more time in the propagation step for a longer duration of laser pulse. We have optimized our programs so they cost less time in both the QTMC and the CCSFA method in the propagation. In the ordinary CCSFA method, solving saddle-point equations costs the most time. Our time-sampling method cleverly avoids this step and achieves a high efficiency as that in the QTMC method.

IV. CONCLUSIONS

In this paper, we have developed a highly efficient time-sampling method to treat the nonadiabatic tunneling ionization of atoms semiclassically. In this numerical scheme, one prepares sample electrons in the time space, so all the classical initial conditions derived from the SFA can be calculated directly without solving the saddle-point equations. Through careful comparison studies, we show that our method achieves the same high efficiency as the fast QTMC method but can
work well in the nonadiabatic regime. The time consumption of our method is tens of times faster than the original CCSFA scheme, which needs to solve the transcendental equations involving trigonometric functions.

We emphasize that, although the efficiency of our method has been demonstrated by a specific pulse shape, our method equally works for any other pulse shapes. For those cases where the integrations \( I_1(t) \) and \( I_2(t) \) do not have analytical forms, one can easily do it numerically, where the time cost is still much cheaper than that needed to solve the nonlinear saddle-point equations. Finally, the present method can be straightforwardly generalized to deal with the elliptically polarized laser fields or orthogonally polarized two-color fields.

**ACKNOWLEDGMENTS**

This work is supported by National Natural Science Foundation of China (NSFC) under Grants No. 11322437 and No. 11574010 and by the National Program on Key Basic Research Project of China (973 Program) under Grant No. 2013CB922402.