Coulomb-corrected strong-field approximation based on a genetic algorithm

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1. Introduction

Atomic and molecular photoionization under intense laser irradiation is a fundamental process in strong-field light–matter interaction. The solution to the time-dependent Schrödinger equation (TDSE) is assumed to be the numerical experiments of strong-field physics. However, the calculation by solving TDSE is very time consuming, and it is difficult to get a distinct underlying physical mechanism from the final calculated results, which is the reason that the numerical solution to the TDSE is referred to as a ‘black box’. As the complementarity to the TDSE, semiclassical methods adopting the...
classical concept of trajectory provide a transparent physical picture of the underlying process.

Generally, in the semiclassical description, the electron being considered as a classical particle is accelerated by the laser field after a quantum transition from its ground state to a continuum [1, 2]. The standard strong-field approximation (SFA) [3–5] is a widely used nonperturbative approach, which considers the following assumptions: (i) only the ground state contributes to the evolution of the system; (ii) the depletion of the ground state is neglected; (iii) in the continuum, the electron is treated as a free particle moving in the laser field without the effect of the potential [2]. Assumption (iii) means that the short-range potential is adopted in the standard SFA, which is valid when the electron moves under the influence of a very strong laser field in the continuum.

In recent years, a low-energy structure (LES) [6–9] has been observed in many experiments due to the effect of the long-range Coulomb potential. It can be reproduced by solving the TDSE rather than SFA [6]. However, the LES can be well depicted and explored by the classical trajectory Monte Carlo (CTMC) method [7, 10] in which assumption (iii) is modified and the electron in the continuum is driven by the combined Coulomb and laser field [11–13]. In the CTMC method, the ionization process is described by the adiabatic tunneling ionization theory of Ammosov, Delone and Krainov [14, 15]. The evolution of the electron after ionization is simulated by launching a number of electron trajectories with random initial conditions. For each electron trajectory, the motion of the electron is governed by the Newton equation. Based on the CTMC and the Feynman’s path-integral [16, 17], the quantum trajectory Monte Carlo (QTMC) method [18], employing the classical action as the phase, was proposed to simulate the interference structures in the spectrum. However, the CTMC and QTMC methods, which treat ionization with quasistatic approximation, are only rigorously valid in the adiabatic tunneling regime [3]. Very recently, a generalized quantum trajectory Monte Carlo method, integrating the nonadiabatic ionization theory [19, 20], classical dynamics with combined laser and Coulomb fields [11–13], and the Feynman’s path integral approach [16–18], has been proposed to reproduce the experimental results and TDSE simulations [21–26].

On the other hand, Coulomb-corrected strong-field approximation (CCSFA) came into being after applying the Coulomb-correction to the standard SFA in which the nonadiabatic ionization effect is included in the calculation of the transition amplitude [27–32]. The transition amplitude in the SFA/CCSFA is calculated by saddle-point approximation [33], i.e. the method of steepest descents [34], which is a mathematical treatment for solution of the Fourier-type integrals. However, in order to achieve convergence of the interference oscillations in the photoelectron spectrum, a huge number of trajectories (~ 109) and the saddle-point equation of each trajectory should be calculated in the CCSFA simulation, which is very time consuming. Very recently, a time-sampling method has been proposed to avoid solving the saddle-point equation and overcome the time-consuming disadvantage of the CCSFA [35, 36]. With the development of attosecond pump-probe technology, sophisticatedly tailored laser fields have been applied to extract the spatio-temporal dynamics information in more and more newly emerging experiments [39–41]. For the complicated laser fields, such as elliptically polarized laser fields and orthogonally polarized two-color fields, it is difficult to find the accurate solution of saddle-point equation in the original treatment of SFA and CCSFA.

The genetic algorithm (GA) is a metaheuristic inspired by the process of natural selection. Usually, it is used to efficiently generate high-quality solutions to optimize and search problems [37]. For whatever the mathematic formula that is in a specific physical problem, the optimized solution can be found by the self-propelled evolution of the initial population of the GA. In the present work, we propose an improved CCSFA based on the GA (CCSFA-GA) in which the GA is applied to autonomously find the optimized solution of the saddle-point equation with a complicated laser pulse shape. By comparing our result with the results of the original saddle-point treatment in CCSFA and TDSE, the accuracy of the CCSFA-GA is verified.

This paper is organized as follows. In section 2, we present the theoretical background on which the CCSFA-GA is built and our numerical scheme. In section 3, we take the hydrogen atom for an example to compare CCSFA-GA with the original treatment in CCSFA with a linearly polarized pulse and the numerical solution of the TDSE with an elliptically polarized pulse. The conclusions are presented in section 4.

2. Theoretical model

2.1. Saddle-point method in strong-field approximation

First, the Keldysh–Faisal–Reiss (KFR) [3–5, 32] amplitude is given by

\[
M_p = -i \int_{-\infty}^{\infty} dt \langle \chi_p(t) | \mathbf{r} \cdot \mathbf{E}(t) | \psi_0(t) \rangle \tag{1}
\]

where \( |\psi_0(t)\rangle \) is the atomic ground state with energy \(-I_p\), and

\[
|\chi_p(t)\rangle = |p + A(t)\rangle \exp[-iS_p(t)] \tag{2}
\]

is the Volkov state with drift momentum \(p\). According to the Feynman’s path integral approach, the phase is given by the classical action

\[
S_p(t) = J^t_0 dt' e^{iS_p(t)} \left\{ \frac{|p + A(t)|^2}{2} + I_p \right\}. \tag{3}
\]

Hence, the KFR amplitude can be expressed as

\[
M_p(t) = -i \int_0^t dt' e^{iS_p(t)} \langle p + A(t) | \mathbf{r} \cdot \mathbf{E}(t) | \psi_0 \rangle. \tag{4}
\]

This KFR amplitude can be obtained through the saddle-point method, which is a mathematical means to solve the Fourier-type integrals with the asymptotic expansion [34]. The objective of this method is to derive the leading term of the contribution to the asymptotic expansion from the saddle-point.
Saddle-point is the stationary phase point at which the first-order derivative of the phase is equal to zero,
\[ \frac{\partial S_p(t)}{\partial t} \bigg|_{t=t_s} = \frac{|\mathbf{p} + \mathbf{A}(t)|^2}{2} + \mathbf{I_p} = 0 \] (5)
where \( t = t_s \) is saddle-point, \( 0 < \text{Re}(t_s) < T_p, \text{Im}(t_s) > 0, T_p \)
the time when the laser pulse is switched off and the vector potential remains unchanged before and after the pulse, and \( \mathbf{A}(0) = \mathbf{A}(T_p) \). Generally, there exists a small neighborhood \( N_c \) of the saddle-point, within as \( \partial S_p(t)/\partial t \) does not equal zero. In this neighborhood, the integrand is approximately equal to zero as the integrand \( \langle \mathbf{p} + \mathbf{A}(t) \rangle \cdot \mathbf{E} |\psi_0\rangle \) oscillates around zero [33, 34]. Then, the integration can be approximated by the summation of the integrand value over all saddle-points. Thus, the KFR amplitude can be expressed as
\[ M_{\text{SP}} = -i \sum_n \sqrt{\frac{2\pi i}{S''(t_s)}} \langle \mathbf{p} + \mathbf{A}(t_s) | \mathbf{r} \cdot \mathbf{E} |\psi_0\rangle e^{i S_p(t_s)}, \] (6)
where \( S'' = d^2 S_p(t)/d\tau^2 \) is the second derivative of the phase. The standard saddle-point method cannot be used to solve equation (6) since the integrand is singular for \( S'(t) = 0 \). However, one can find the steepest descent directions of the saddle-point method for \( |S''(t_s)| = |S''(t_s)| \exp(i\alpha) \) [33, 34]. Thus, the ionization amplitude can be expressed as
\[ M_{\text{SP}} = - \sum_n \frac{2^{3/4} (t_p^{5/4})}{\mathbf{E}(t_s) \cdot (\mathbf{p} + \mathbf{A}(t_s)) e^{i S_p(t_s)}, \] (7)

### 2.2. Coulomb-corrected strong-field approximation

In order to understand the Coulomb potential effect in strong-field phenomena, the Coulomb-correction is applied to the trajectories in the SFA. The classical action of the CCSFA can be separated into two parts,
\[ S_C(t_s) = S_C^I [\text{Im}(t_s)] + S_C^T [\text{Re}(t_s)] = \int_{t_s}^{\text{Re}(t_s)} \frac{\sqrt{v^2 + I_p}}{2} + \int_{\text{Re}(t_s)}^{\infty} dr \left( \frac{v^2}{2} - \frac{1}{r} + I_p \right) \] (8)
where \( S_C^I [\text{Im}(t_s)] \) and \( S_C^T [\text{Re}(t_s)] \) are the sub-barrier and the real-time contribution to the phase, respectively [38]. The classical motion of electrons in the combined laser and Coulomb fields is governed by the Newtonian equation:
\[ \frac{d^2 \mathbf{r}}{dt^2} = -\mathbf{E}(t) - \nabla[V(\mathbf{r})]. \] (9)
After the electric field is switched off, the motion of the electron is only governed by the Coulomb force and follows Kepler’s law. According to the energy conservation, one could transfer the potential energy into the kinetic energy in infinity and get the asymptotic momentum of the free electron.

### 2.3. Coulomb-corrected strong-field approximation based on a genetic algorithm

In fact, the saddle-point equation is a transcendental equation, it will take a lot of time if we solve billions of saddle-point equations by finding roots in the whole complex time plane. Moreover, for a special laser pulse shape, it is hardly the case to find the solution of the saddle-point equation with the original treatment of SFA and CCSFA. To overcome this disadvantage, we propose a new method to solve this root-finding process by applying GA to the original treatment of CCSFA.

We now consider a simple case where a linearly polarized laser field is employed. Suppose the hydrogen atom \( (t_p = 0.5) \) is ionized by a 1-cycle linearly polarized laser field of frequency \( \omega = 0.0228 \), the peak intensity of the laser fields is \( E_0 = 0.0543 \), the vector potential is \( \mathbf{A}(t) = -A_0 \sin(\omega t) \), where \( A_0 = E_0/\omega \). Thus, the saddle-point equation can be written as:
\[ f = \frac{\partial S_p(t)}{\partial t} = \frac{1}{2} p_0^2 + \frac{1}{2} [p_0 + A(t)]^2 + \mathbf{I_p} = 0. \] (10)

The transcendental equation can be solved by the GA in five steps, as shown in the following.

Step 1: generate the initial population. The process begins with a set of randomly generated individuals in which each individual is a solution to the problem. An individual is characterized by a set of parameters known as genes. Genes are usually represented in binaries as strings of 0 and 1. As the solution of our saddle-point equation is a complex number \( t_s = t_r + i \cdot t_i \), we apply two genes for each individual, representing the real and imaginary part of \( t_s \), respectively. The population size should be as large as possible because more initial individuals gives a higher possibility to evolve the best result.

Step 2: reconstruct a fitness function \( H = 1/(t + 0.01) \) as \( f \) approaching 0, \( H_{\max} = 100 \). The fitness function evaluates the fitness of each individual in the population. The probability that an individual will be selected for reproduction is based on its fitness score.

Step 3: extract a subset of genes as parents from the current population according to their fitness scores.

Step 4: generate a new population. With a crossover probability crossing over the parents to form a new offspring (child), with a mutation probability mutating new offspring at each position in individuals. Place new offspring in the new population.

Step 5: return the current population as the best solution if the end condition is satisfied. Otherwise, go to Step 2.

Parameters such as the mutation probability, crossover probability, and population size play important roles in the GA’s performance. A very small mutation rate may lead to genetic drift (which is non-ergodic in nature). A recombination rate that is too high may lead to the premature convergence of the genetic algorithm. A mutation rate that is too high may lead to loss of good solutions, unless the elitist selection is employed [37].
3. CCSFA-GA numerical implementation

In this section, we apply two different electric fields into our two-dimensional calculations, one is the linearly polarized pulse and the other is the elliptically polarized pulse. Atomic units are used unless otherwise noted.

3.1. CCSFA-GA with a linearly polarized pulse

In our calculation, the fitness value has a great effect on the precision of the result. The greater the fitness value, the more precise the result, the longer time it takes. The individual switch fitness values that are greater than 90 (H > 90) are recorded as the best individuals by taking the two above factors into consideration.

Figure 1 describes the distributions of different generations in the complex time plane. The individuals concentrate gradually from random distributed spots to a few dense areas marked as A, B, C, and D.

The saddle-points obtained by traversing method and genetic algorithm under the linearly polarized pulse are shown in figure 2. The results from these two methods match well. As can be seen from figures 2(a)–(b), there are two saddle-points for a given asymptotic momentum per cycle under the linearly polarized pulse. Thus, there are in total four saddle-points, causing a pair of asymptotic momenta with negative and positive values to exist. The results are in agreement with that in [29].

Figure 3 compares the results of the standard CCSFA and CCSFA-GA methods. It is shown in figure 3(a)–(b) that the photoelectron momentum distributions (PMDs) simulated with the two methods agree with each other very well. Figures 3(c)–(d) present the corresponding normalized photoelectron yields along $p_x = 0.0$ and $p_x = 0.45$, respectively.

From figures 3(c)–(d), it can be found that the normalized photoelectron spectra simulated by the CCSFA and CCSFA-GA methods are almost the same.

3.2. CCSFA-GA with an elliptically polarized pulse

We consider the following elliptically polarized pulse in the ($x$, $z$) plane with a $\sin^2$ type envelope. Lately, the elliptically polarized pulse has played an important role in attoclock research [35]. The CCSFA-GA here provides a new idea for studying the electron dynamics under the elliptically polarized pulse and other complex pulse. The vector potential can be written as
Figure 4. The two-dimensional PMDs of the hydrogen atom at a laser intensity of $1 \times 10^{14}$ W/cm$^2$ calculated by the standard-CCSFA (a), TDSE (b), and CCSFA-GA (c). (d) The corresponding energy spectra calculated from (a), (b), and (c).

$$A(t) = -\frac{E_0}{\omega} \sin^2 \left( \frac{\omega t}{\pi} \right) \left[ \cos \frac{\theta}{2} \cos(\omega t + \varphi) \mathbf{e}_x - \sin \frac{\theta}{2} \sin(\omega t + \varphi) \mathbf{e}_z \right]$$

where $E_0$ is the peak intensity of the electric field, $n/2$ is the optical period, and $\omega$ is the laser angular frequency. The ellipticity of this field is defined as $\varepsilon = \cos(\frac{\theta}{2}) / \sin(\frac{\theta}{2})$. The saddle-point equation of the elliptically polarized pulse can be obtained by substituting the vector potential into equation (9).

We compare the results of the standard CCSFA, CCSFA-GA calculation, and TDSE in figure 4, in which their parameters are same. The PMD obtained by the standard CCSFA is shown in figure 4(a), with two lobes distributed in the upper region. The yield of the left lobe is relatively higher than that of the right one. Similarly, the PMD obtained by the TDSE and CCSFA-GA are shown in figures 4(b)–(c), respectively. The PMD in figure 4(c) is almost the same as that in figure 4(a). The distribution obtained by the TDSE in figure 4(b) is in general agreement with those in figures 4(a) and (c). We also illustrate the energy spectra in figure 4(d), which are consistent with each other.

4. Conclusions

In summary, we have developed a new method based on the genetic algorithm for solving the saddle-point equation and applied it into CCSFA calculation. For the linearly polarized pulse, it keeps the precision of its roots compared with the saddle-point method, i.e., searching the whole complex time space. For the cases of more complicated laser fields such as the elliptically polarized pulse, it keeps precision effectively. No matter how complex the electric field is, the precise solutions can be obtained by the GA method after evolving enough generations.

Acknowledgments

The work was supported by the National Key Research and Development Program of China (Grant No. 2019YFA0307700 and No. 2016YFA0401000), the NNSF of China (Grant No. 11674209, No. 11774215, No. 11334009, No. 11425414, No.91950101, and No.11947243), the Sino-German Mobility Programme (Grant No. M-0031), the Department of Education of Guangdong Province (Grant No. 2018KCXTD01), the High Level University Projects of the Guangdong Province (Mathematics, Shantou University), and the Open Fund of the State Key Laboratory of High Field Laser Physics (SIOM).

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