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Trajectory-based analysis of low-energy electrons and photocurrents generated in strong-field ionization

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The three-dimensional classical-trajectory Monte Carlo method is employed to investigate low-energy photoelectron spectra in above-threshold ionization by strong laser fields. By connecting the tunneling coordinates with the final momentum-energy spectra, we identify the effects of the Coulomb potential on electron trajectories and the final energy spectra. In addition, we verify that the photoelectron spectra, depending on the energy region, can be controlled with a two-color laser pulse by varying the phase delay. The modulations of the electron spectra and yields as well as the generated photocurrents reveal the connections among them, which support our previous work [Phys. Rev. Lett. 109, 243002 (2012)] on terahertz wave generation from two-color laser pulses.

I. INTRODUCTION

Since the observation of above-threshold ionization (ATI) in 1979 [1], studies on the photoionization of atoms by strong laser fields have been continuously advanced, attracting much interest in the last three decades [2,3]. The dynamics involved are well understood with a three-step model [4,5], where the strong-field approximation (SFA) [6–8] serves as an analytical tool to describe the rescattering process. In this model, the electron released at a certain laser phase is subsequently driven back towards the parent ion and its elastic backscattering off the nucleus leads to the generation of high-energy ATI electrons. This semiclassical picture of ionization dynamics pioneered by Keldysh [6] can well describe the detachment of electrons from negative ions, in the tunneling regime where the Keldysh parameter \( \gamma \ll 1 \). Here, \( \gamma = \sqrt{I_p/2U_p} \), \( I_p \) is the ionization potential, and \( U_p \) is the ponderomotive energy.

For the ionization of neutral atoms, however, the Coulomb field of the atomic core was found non-negligible in recent experimental findings such as double-hump structures in electron momentum spectra [9–11] and frustrated tunneling ionization [12–15]. In particular, two experiments by Blaga et al. [16] and Quan et al. [17] reported an “ionization surprise.” They found an unexpected characteristic spikelike structure at the low-energy area in the photoelectron spectra, when probing electrons along the laser polarization direction in strong mid-infrared laser fields. These features of low-energy structure (LES) are in contrast to the prediction of the SFA [6–8] or the SFA with Coulomb corrections [18]. Various numerical methods [19–24] have been proposed and a similar conclusion was drawn that LES is attributable mainly to soft collisions [21] or forward rescattering [19], as pointed out by Blaga et al. [16]. More recently, Xie et al. [25] further demonstrated that two-color sculpted laser fields could control and modify the relative importance of the Coulomb field effect on the electron wave packet by subcycle tuning of the instantaneous electric field, which will benefit further studies on low-energy electrons.

A transient plasma current (PC) model was proposed to study terahertz (THz) generation in two-color fields by considering the subsequent electron dynamics following ionization [26]. After considering the Coulomb potential, the optimal phase delay for maximization of the THz pulse energy is 0.8\( \pi \) in the PC model, as proposed in our previous work [27,28]. However, the contribution of low-energy electrons to the photocurrent in strong-field ionization remains obscure.

In this work, we employ the three-dimensional classical-trajectory Monte Carlo (CTMC) method to clarify the dependence of the electron spectra on the tunneling coordinates. We define the tunneling coordinates as the laser vector potential and the electron’s transverse momentum at the instant when the electron tunnels out. Our definition is slightly different from that in the work of Yuan et al. [29], in that the laser vector potential has units of momentum. We show that the Coulomb potential has profound effects on the low-energy photoelectron by analyzing the trajectories of photoelectrons with different tunneling coordinates. In addition, we study how the photoelectron spectra vary when a second harmonic pulse is applied to accompany the fundamental pulse at different phase delays. The dependence of the modulation on the electrons’ final energy demonstrates again the importance of the Coulomb potential. After weighting the final electron velocity with the corresponding probability, we obtain the photocurrents by summing over all the possible trajectories. In a three-dimensional (3D) classical-trajectory Monte Carlo simulation, we find that the current attains its maximum around a phase delay of 0.8\( \pi \) in accordance with the previous findings [27,28].

The paper is organized as follows. In Sec. II, we briefly summarize our method. In Sec. III we present the simulation results and discuss the effects of the Coulomb potential in detail. Finally we draw a conclusion in Sec. IV. Atomic units are used throughout unless indicated otherwise.

II. THEORETICAL METHODS

In our 3D CTMC simulations, the hydrogen atom is taken as an example for discussion. The laser field is assumed to be polarized in the \( z \) direction with the form \( F(t) = F_0 f_1(t) \sin(\omega t) \) for a monochromatic field and \( F(t) = F_0 f_2(t) [\cos(\omega t) + \epsilon \cos(2\omega t + \varphi)] \) for two-color fields, where

\[ F_0 = \frac{\hbar c}{m_e} \]
$F_0$ is the peak electric field, $f_1(t)$ and $f_2(t)$ are the pulse envelopes, $\varphi$ is the relative phase, and $\epsilon$ denotes the intensity ratio of the two color fields.

In the case of a monochromatic field interacting with the hydrogen atom, we use a half-trapezoidal laser envelope which is constant for the first ten cycles and ramped off within the last three cycles. For simplicity, we focus on the electrons launched in the first half cycle and follow their dynamics classically in the monochromatic field after tunneling ionization. When the field is off, the final energy of the electron is obtained by summing up the kinetic energy and the potential energy. Electrons are considered as ejected if the final energy is greater than zero.

At each instant within the first half cycle, we assume the electron tunnels out with initial momentum distribution and ionization rate predicted by Ammosov-Delone-Krainov (ADK) theory [30]. The initial position is derived from Landau’s effective potential theory [31,32]. The initial longitudinal momentum (along the $x$ axis) is fixed at zero and the initial transverse momenta are set as $p_x^i = p_z^i \cos \alpha$, $p_y^i = p_z^i \sin \alpha$. Here $\alpha$ is the angle between $p_z^i$ and the $x$ axis, distributed equally within the interval of $(0,2\pi)$. About $10^9$ trajectories are launched to account for the initial lateral momentum distribution from ADK theory. Therefore, each electron trajectory [30,33] is weighted by

$$W(t_0, p_x^i) = W_0(t_0)W_1(p_x^i),$$

$$W_0(t_0) = 4[2L_p^2/|F(t_0)|^2]^{\sqrt{2/\pi}}1 - \exp[-(2L_p^2)/|3F(t_0)|],$$

$$W_1(p_x^i) = p_x^i/\pi[\sqrt{2L_p^2}/|F(t_0)|]\exp[-(\sqrt{2L_p^2}/|F(t_0)|)^2/|3F(t_0)|]. \tag{1}$$

where $W_0(t_0)$ is the tunneling rate and $W_1(p_x^i)$ corresponds to the initial transverse momentum distribution. After tunneling, the electrons’ motion is governed by the classical Newtonian equation under both the Coulomb potential and the laser field, which is solved using the Runge-Kutta method. All calculated electron three-dimensional asymptotic momenta at the virtual detector are transformed using the energy conservation law [34].

### III. Results and Discussion

Typical photoelectron energy spectra in the tunneling regime, calculated in a 3D CTMC simulation, are shown in Fig. 1(a). The entire energy spectrum considering the Coulomb potential exhibits behaviors consistent with the three-step model, e.g., escaping electrons forming a slope, rescattering electrons forming a plateau ($E > 2U_p$), and a cutoff ($E = (8-10)U_p$), where $U_p = 56.25$ eV for 150 TW/cm$^2$, 2.0 $\mu$m pulses. As for the energy spectrum without the Coulomb potential, the maximum energy is about $2U_p$ because no rescattering exists. In Fig. 1(b), our results are compared with experimental data [16] for Ar under the same laser parameters, showing qualitative agreement in the LES. Figure 1(c) shows the calculated angular distributions of photoelectrons integrated in the energy interval [2.25 eV, 2.75 eV] for laser fields with central wavelengths of 800 nm and 2.0 $\mu$m at the same peak intensity $I = 10^{14}$ W/cm$^2$, respectively. For comparison, experimental data [35] under the same laser parameters are shown as well. It can be seen that both the theoretically and experimentally obtained angular distributions exhibit Gaussian profiles. The full width at half maximum (FWHM) is found to be three times narrower at the longer wavelength [35]; this will be discussed based on electron trajectories later.

Now we turn to the classical illustration of photoelectron spectra. By tracing back to the initial tunneling coordinates [tunneling vector potential $A = -\frac{e\omega}{\hbar} \cos(\omega t)$ and initial transverse momentum] of the electrons, the correspondence between the electron final energies and the initial tunneling coordinates can be easily figured out as shown in Fig. 2. In order to identify the effects of the Coulomb potential, the distributions calculated with and without Coulomb potential are shown in Figs. 2(a) and 2(b), respectively. Without the Coulomb potential, the distribution [Fig. 2(b)] forms a circular annulus centered at $A = 0$ that corresponds to the maximum electric field. When the Coulomb potential is taken into consideration in Fig. 2(a), the electron final energy distribution changes from a circle to a heart shape, due to the distortion effect of the Coulomb potential [36]. The center of the heart is shifted left to a negative $A$. This suggests that the electrons gain additional longitudinal momenta from the Coulomb potential, in accordance with the findings in terahertz wave generation [27,28]. Additionally, in the central region in Fig. 2(a), an irregular pattern is formed by electrons with random final energy up to $(8-10)U_p$, which indicates that chaotic processes are occurring [29,32].

To further identify the effects of the Coulomb potential, we analyze the electron trajectories in various initial tunneling
coordinates. First we consider the electron trajectories at a given lateral initial momentum $p_x = 0.04$ a.u., $p_y = 0$ with the vector potential $A$ varying from $-2.0$ a.u. to $2.0$ a.u. corresponding to different tunneling instants. Figures 3(a) and 3(b) illustrate the trajectories with and without Coulomb potential, respectively. It can be seen clearly from Fig. 3(b), that the final momentum of the ejected electron is given by $\vec{p} = (p_x, p_y, -A)$ when the Coulomb potential is neglected. However, when the Coulomb potential is taken into account in Fig. 3(a), the trajectories are strongly distorted at certain tunneling coordinates. Figures 3(c), 3(d), and 3(e) show detailed plots of various trajectories around the origin.

It can be seen from Fig. 3(c) that electrons with $A < -0.4$ a.u. escape directly from the nucleus after tunneling. The transverse momenta are being decreased due to the Coulomb potential as they move away from the nucleus, when compared with Fig. 3(b). In this case the Coulomb potential plays the role of focusing. Electrons with $A > 0$, shown in Fig. 3(e), make turns after tunneling, travel toward the nucleus, and eventually exit in the positive $z$ direction. When passing by the nucleus, they make rescollisions due to Coulomb potential. Interestingly, they experience a transverse momenta transfer and escape eventually in the direction opponent to the initial transverse momentum, revealing the forward scattering or softly collision (with scattering angle $\theta < 90^\circ$).

For electrons with $-0.4 \text{ a.u.} \leq A \leq 0$, in Fig. 3(d), a different scenario occurs: the electron trajectories are strongly modified by the Coulomb potential. Electrons with $A = -0.4$ a.u. have multiple collisions with the nucleus before they are backscattered away, while electrons with $A = 0$ return to the nucleus in the first cycle. In both cases electrons make hard collisions, leading to large-angle scattering or even backscattering. In the backward scattering, the electron gains very large kinetic energy giving rise to high-energy ATI photoelectrons. This explains why high-energy ATI spectra can be observed only when the Coulomb potential is taken into account in Fig. 1(a). For $A = 0$, one would expect that the electron could be recombined into excited states including the Rydberg states, which might be one of the reasons for frustrated tunneling ionization [12,15].

Trajectories of electrons with larger initial transverse momenta ($p_x = 0.2$ a.u., $p_y = 0$) are shown in Fig. 4. Coulomb focusing decreases the final transverse momenta and makes the trajectories deviate toward the positive $z$ axis, which is the reason why the shape changes from circle to heart when Coulomb potential is considered in Fig. 2. In this case, there is no clear boundary between the escaping and rescattering events, since the electrons in both cases leave rapidly from the nucleus. For the escape process, the electrons make a half collision with the atomic core during the first half cycle, while the rescattering electrons make a turn and pass through the atomic core at a large impact parameter in a full collision during the first half cycle.

Based on the analysis above, the electrons with energy less than $2U_p$ make soft collisions with the atomic core. Regardless of whether the electrons escape or rescat
the Coulomb potential, respectively. We determine the optimal phases when the yield attains maximum at each energy; they are indicated by the solid black circles. Contour data are rescaled within each energy interval to make the electron yield modulation clearer. Without the Coulomb potential in Fig. 5(e), the optimal phase jumps from 0 to $-0.5\pi$ as energy increase. However, when Coulomb potential is considered in Fig. 5(f), the low-energy electrons attain their maximum yield at a phase delay of $0.1\pi$, resulting from the negative center in Fig. 2(a).

As the energy increases, the phase of the maximum yields changes gradually to $-0.4\pi$.

In order to understand the difference, we separate the total electrons into escaping electrons and rescattering electrons by their tunneling coordinates, i.e., $A < 0$ for escaping electrons and $A > 0$ for rescattering electrons as shown in Fig. 6. It can be seen from Fig. 6(b) that without Coulomb potential, the rescattering electrons attain maximum yields at phases similar to those of the total electrons shown in Fig. 5(f), while the escaping electrons exhibit mirroring behavior. However, when the Coulomb potential is taken into consideration, the energy spectra contributed by escaping electrons show an unclear modulation behavior in a comparatively high-energy range ($E > 1.2U_p$) as shown in Fig. 6(c). This dispersion results from the mixture of electrons with different kinds of trajectories when the initial $A$ is around 0. As for the energy spectra contributed by rescattering electrons shown in Fig. 6(d), the dispersion phenomenon is not as obvious as that of escaping electrons and only a slight shift of 0.1$t$ exists between the maximum phase delays in Figs. 6(b) and 6(d).

Based on the analysis of Figs. 5 and 6, we conclude that the phase-delay dependence of the total electron yields is dominated by the rescattering electrons shown in Fig. 5(f) when the Coulomb potential is taken into account, while in

![Figure 5](image)

**FIG. 5.** (Color online) Modulated momentum spectra and energy spectra with the phase delay of the two-color field. (a),(b) Parallel momentum distribution; (c),(d) vertical momentum distribution; and (e),(f) energy distribution as a function of the relative phase. In the left column, electrons propagate in only the laser field, while the Coulomb potential is taken into account in the right column. The optical phases at which the yields attain maximum values are indicated by black filled circles in (e) and (f). The laser parameters are the same as in Fig. 1 while the second harmonic pulse has an intensity of 0.005 times the fundamental.

this soft collision, the longitudinal momenta are dominated by the laser acceleration which is proportional to the laser wavelength. The electron’s final kinetic energy is $E_{\text{kin}} = (p_x^2 + p_y^2)/2$ and $\cos(\theta) = p_x/p = (1/\omega)/p = \lambda/p$, where $\theta$ is the angle between the final momentum $p$ and the laser polarized axis. Obviously, if $p$ is fixed, $\cos(\theta)$ is proportional to the wavelength $\lambda$, so $\theta$ is inversely correlated with $\lambda$, which can explain why the longer wavelength has a narrower FWHM in Fig. 1(c).

Now we consider the case of the hydrogen atom interacting with a two-color laser pulse. In Fig. 5, we show the parallel and vertical momentum distributions as well as the energy distribution of the ejected electrons, against the phase delay between the two-color laser fields. The centers of the parallel momentum distribution, shown in Figs. 5(a) and 5(b), are found to vary with the phase delay. While the maximum shift of the center occurs at a delay of $-0.5\pi$ for the Coulomb-field-free case in Fig. 5(a), it occurs at a delay of $-0.2\pi$ in Fig. 5(b) when the Coulomb potential is considered. This is closely connected to the experimental finding that terahertz wave yields attain a maximum at $0.8\pi$ ($-0.2\pi$) [27,28]. When the center of the parallel momentum distribution has its maximum shift to one side, the asymmetry distribution of parallel momenta and the currents will be the largest; this is most efficient for terahertz wave generation.

In contrast, the vertical momentum distribution hardly changes with the phase delay as shown in Figs. 5(c) and 5(d). When the Coulomb potential is considered in Fig. 5(d), the distribution gets much narrower than that in the case without Coulomb potential [Fig. 5(e)], which demonstrates clearly the focusing effect of the Coulomb potential. In Figs. 5(e) and 5(f) we draw the contour plots of the distribution of the final energy versus the phase delay for the cases of neglect and inclusion of

![Figure 6](image)

**FIG. 6.** (Color online) Energy spectra contributed by escaping and rescattering electrons, respectively, against the phase delay of the two-color field. (a),(b) Electrons propagate with the Coulomb potential. (c),(d) Electrons propagate without the Coulomb potential. In the left column, only escaping electrons are considered, while only rescattering electrons are taken into account in the right column. Optimal phases when the yields attain maximum at each energy are indicated by the solid black circles and contour data are rescaled within each energy interval. The laser parameters are the same as in Fig. 5.
maximum at delay $\varphi = 0$. However, the yields of electrons collected in the $6^\circ$ range parallel and antiparallel to the laser polarization vary strongly with the relative phase and attain maxima at $\varphi = -0.25\pi$ and $\varphi = 0.7\pi$, respectively. The corresponding currents are found to attain maximum magnitude at phase delay $0.7\pi$, in accordance with the previous investigation [27,28], where it was attributed to the soft collisions of electrons in the combination of the laser field and the Coulomb potential.

IV. CONCLUSION

By reproducing the experimental results of LES and angular distributions, we show that 3D CTMC calculations are in good agreement with the experimental findings. Based on the simulation, we analyze in detail how the trajectories of electrons depend on the initial tunneling coordinates. In particular, we clarify the role of the Coulomb potential in recollisions and laser-assisted soft collisions, which give rise to the generation of high- and low-energy photoelectrons. It is found that the focusing effects from the Coulomb potential modify both the final energy and the lateral momentum distribution. Calculations employing two-color fields further suggest that the modulations of both the momentum and the energy spectra can be greatly changed by the Coulomb potential. The forward and backward electron yields within a narrow cone along the laser polarization are found to be closely related to generation of the terahertz wave.

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