The effect of electron initial longitudinal velocity on the non-sequential double ionization process in an elliptically polarized laser field*

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The effect of initial longitudinal velocity of the tunnelled electron on the non-sequential double ionization (NSDI) process in an elliptically polarized laser field is studied by a semiclassical model. We find that the non-zero initial longitudinal velocity has a suppressing effect on single-return collision (SRC) events in the double ionization process, more specifically, it results in an obvious reduction in the center part of the correlation momentum distributions in the direction of the major polarization axis (z axis) and makes the distribution of single-return collision in the minor polarization axis (x axis) become narrower.

Keywords: non-sequential double ionization, initial longitudinal velocity, elliptically polarized laser field, single return collision

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1. Introduction

The nonsequential double-ionization (NSDI) process has attracted considerable interest and has been intensively investigated during the past two decades[1−22] because it is a prototype model to study new aspects of the electron–electron correlation.[20] Rescattering has been widely accepted as the dominant mechanism for NSDI. The rescattering process can be understood from the semiclassical notion: the first electron is released by the laser field via a tunnelling process and is driven back to collide with the core to ionize the second electron. The initial velocity of the tunnelled electron was assumed to be zero corresponding to the situation of tunnelling when the semiclassical was first proposed.[23] However, from the quantum mechanical point of view, the initial wave packet generated in the tunnelling ionization process should possess a finite width of momentum due to the uncertainty principle, which will lead to diffusion in its subsequential propagation process. In addition, the zero initial velocity approximation restricts the model to be essentially a one-dimensional approach which makes it invalid in treatment of some important processes, e.g., double ionization, due to neglect of the quantum diffusion effect. This problem has been partly remedied in Refs. [8] and [15] by introducing a non-zero initial transverse velocity into the semiclassical model to take into account the transverse quantum diffusion effect of the electron after its tunnelling ionization and this extends the previous one-dimensional model[4,23] to a three-dimensional one which is essential in treatment of the double ionization process. However, the longitudinal velocity of the electron is still assumed to be zero therein, and the effect of the diffusion of the wave packet in the longitudinal direction has not been considered. Most recently, the diffusion effect of the wave packet in the longitudinal direction was investigated in a linearly polarized laser field by introducing the non-zero initial longitudinal velocity and it was reported that the results were in better agreement with the experimental observation than that of the zero initial longitudinal velocity.[24]

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Compared with the case of linear polarization, the interaction of the electron with the elliptically polarized field is two-dimensional, and hence the diffusion effect of the wave packet is more complex. Therefore, in this paper we study the effects of the non-zero initial longitudinal velocity of the first tunnelled electron on the NSDI in an elliptically polarized laser field within the rescattering picture. Our results unveil that the non-zero initial longitudinal velocity has a suppressing effect on single-return collision (SRC) events in the DI process in an elliptically polarized laser field.

2. Model and method

Following the same procedure of the previous semiclassical model,[15–19] the ionization of the first outer electron from the bound state to the continuous state is described by the quantum tunnelling ionization theory.[25] The subsequent evolution of this ionized electron and the bound electron is governed by the classical dynamics, in which the motion of the two electrons are described by the classical Newton equation: the motion of two electrons with different initial conditions in the combined Coulomb potential and the time-dependent intense laser field. This classical motion equation can be expressed by (in atomic units $e = m = \hbar = 1$)

$$\frac{\mathrm{d}^2 \boldsymbol{r}_i}{\mathrm{d}t^2} = \boldsymbol{E}(t) - \boldsymbol{\nabla}\left(V_{\mathrm{ne}}^i + V_{\mathrm{ee}}\right), \tag{1}$$

where $\boldsymbol{E}(t) = (E_x(t), 0, E_z(t))$ denotes the elliptically polarized laser field with $E_z(t) = f(t) E_{0z} \cos \omega t$ and $E_x(t) = f(t) E_{0x} \sin \omega t$. The ellipticity is defined as $\varepsilon \equiv E_{0x}/E_{0z} < 1$ ($\varepsilon = 0$ for linearly polarized light while $\varepsilon = 1$ for circularly polarized light). The tunnelling ionized and bounded electrons, with ionization potentials I_{p1} and I_{p2}, are denoted by $i = 1, 2$ respectively. The Coulomb potentials are

$$V_{\mathrm{ne}}^i = -\frac{Z_{\mathrm{eff}}}{|\boldsymbol{r}_i|}, \qquad \text{and} \qquad V_{\mathrm{ee}} = \frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}, \tag{2}$$

where $Z_{\mathrm{eff}} = \sqrt{2I_{\mathrm{p2}}}$ is the effective charge of Ne^{2+} and $\boldsymbol{r}_i$ is the distance between the i-th electron and the nucleus.

To solve the Eq. (1), we need to determine the initial conditions for the two electrons. Assuming the quasi-static approximation is valid for the tunnelled electron under the condition that the ellipticity $\varepsilon \ll 1$, we can obtain its initial conditions along with the method in Ref. [15]. After rotating the z axis to the direction of the instantaneous external field, the tunnelling process can be described by the following Schrödinger equation[25,26]

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}\eta^2} + \left(\frac{I_{\mathrm{p1}}}{2} + \frac{1}{2\eta} + \frac{1}{4\eta^2} + \frac{E\eta}{4}\right)\phi = 0 \tag{3}$$

in parabolic coordinates. Equation (3) describes the tunnelling process for a single electron with energy $K = I_{\mathrm{p1}}/4$ within a one-dimensional effective potential $U(\eta) = -1/4\eta - 1/8\eta^2 - E\eta/8$, where E is the uniform external field. At the moment t_0, the first electron tunnels the effective potential $U(\eta)$ through the turning point (η_0), determined by $U(\eta) = K$.[25]

The initial position of the first electron is expressed as $x_{10} = -\frac{1}{2}\eta_0 \sin\{\arctan[\varepsilon \tan(\omega t_0)]\}$, $y_{10} = 0$, and $z_{10} = -(1/2)\eta_0 \cos\{\arctan[\varepsilon \tan(\omega t_0)]\}$.[23] To include the non-zero initial longitudinal velocity, the initial velocities are set as

$$\begin{aligned} v_{x0} &= v_{\mathrm{per}} \cos\theta \cos\{\arctan[\varepsilon \tan(\omega t_0)]\} \\ &\quad - v_{\mathrm{lon}} \sin\{\arctan[\varepsilon \tan(\omega t_0)]\}, \end{aligned} \tag{4}$$

$$v_{y0} = v_{\mathrm{per}} \sin\theta, \tag{5}$$

$$\begin{aligned} v_{z0} &= -v_{\mathrm{per}} \cos\theta \sin\{\arctan[\varepsilon \tan(\omega t_0)]\} \\ &\quad - v_{\mathrm{lon}} \cos\{\arctan[\varepsilon \tan(\omega t_0)]\}, \end{aligned} \tag{6}$$

where v_{per} and v_{lon} are the transverse and longitudinal velocities, respectively, θ is the angle between v_{per} and x axis after rotation. The weight of each trajectory is evaluated by $w(t_0, v_0) = w(0)\,\overline{w(1)}$,[25] where

$$w(0) = \frac{4(2I_{\mathrm{p1}})^2}{E} \exp\left[-\frac{2}{3E}(2I_{\mathrm{p1}})^{3/2}\right], \tag{7}$$

$$\overline{w(1)} = \frac{(2I_{\mathrm{p1}})^{1/2}}{E\pi} \exp\left(-\frac{v_0^2 (2I_{\mathrm{p1}})^{1/2}}{E}\right), \tag{8}$$

where $v_0 = \sqrt{v_{\mathrm{per}}^2 + v_{\mathrm{lon}}^2}$ is the initial total velocity.[24] The initial condition of the second electron (bound electron) is determined by assuming that the electron is in the ground state of Ne^+ and its initial distribution is a microcanonical distribution.[26]

The parameters in our calculation are chosen as follows: for Ne atom, $I_{\mathrm{p1}} = 0.7928$ a.u. (atomic unit) (21.5646 eV), $I_{\mathrm{p2}} = 1.506$ a.u. (40.964 eV), and the parameters for the corresponding laser field are $I = 1.0 \times 10^{15}$ W/cm^2, $\omega = 0.05695$ a.u. ($\lambda = 800$ nm) and the ellipticity is $\varepsilon = 0.1$. Because the number of the double ionization cases is very low, we have to use the method in Ref. [15] to obtain convergent correlated electron momentum distribution. In the

first step, 3×10^5 points are randomly distributed in the parameter volume $-\pi/2 < \phi_0 < \pi/2$, $v_{\rm per} > 0$, $v_{\rm lon} > 0$, and $0 < \theta < 2\pi$, where $\phi_0 = \omega t_0$. Each trajectory is traced until the electron is actually ionized (e.g., $r_{\rm i} > 300$ a.u.). The double ionization happened only when the energy of both electrons is greater than zero. In the second step, the parameter volume is carefully chosen according to the calculation of the first step. Finally, the cases obtained in the second step are traced until $t_{\rm f} = 13T$ to obtain the momentum distributions. The profile of the intensive laser pulse is taken as

$$f(t) = \begin{cases} 1, & t \le 10T, \\ \cos^2 \dfrac{(t-10T)\,\pi}{6T}, & 10 < t \le 13T, \\ 0, & t > 13T, \end{cases} \quad (9)$$

where T is the optical period.

3. Result and discussion

3.1. Correlated momentum distribution in the direction of the major polarization axis (z axis)

Firstly, we show the correlated electron momentum distribution of double ionization in an elliptically polarized laser field in the direction of the major polarization axis (z axis) in Fig. 1 (for clarity, the cases of zero and non-zero initial longitudinal velocity have been normalized throughout this paper). As we know, the collision can be categorized into two kinds of trajectories: one is single-return collision (SRC) which means that the outer electron collides with the core at its first return, which happens within the first optical cycle after the tunnelling process; the other is multiple-return collision (MRC) which means that the collision happens when the outer electron returns back to the core after passing the core more than once, which may occur after several optical cycles of oscillation in the laser field. These two different collisional trajectories were discussed and the corresponding contributions to the DI are reported in Ref. [15]. We separate the contributions of these two typical collisional trajectories (SRC and MRC). In Fig. 1(a), the two emitted electrons mainly distribute in the first and third quadrants and the center part around zero momentum is also distributed densely. While in Fig. 1(d), the yield in the first and third quadrants remains almost unchanged but yield in the center part is suppressed. This can be seen more clearly in distributions of SRC events (Fig. 1(b) and Fig. 1(e)), in which the dense distribution region around the origin in Fig. 1(b) is significantly reduced after taking into account non-zero initial longitudinal velocity (Fig. 1(e)). This change actually gives rise to the main difference between Figs. 1(a) and 1(d).

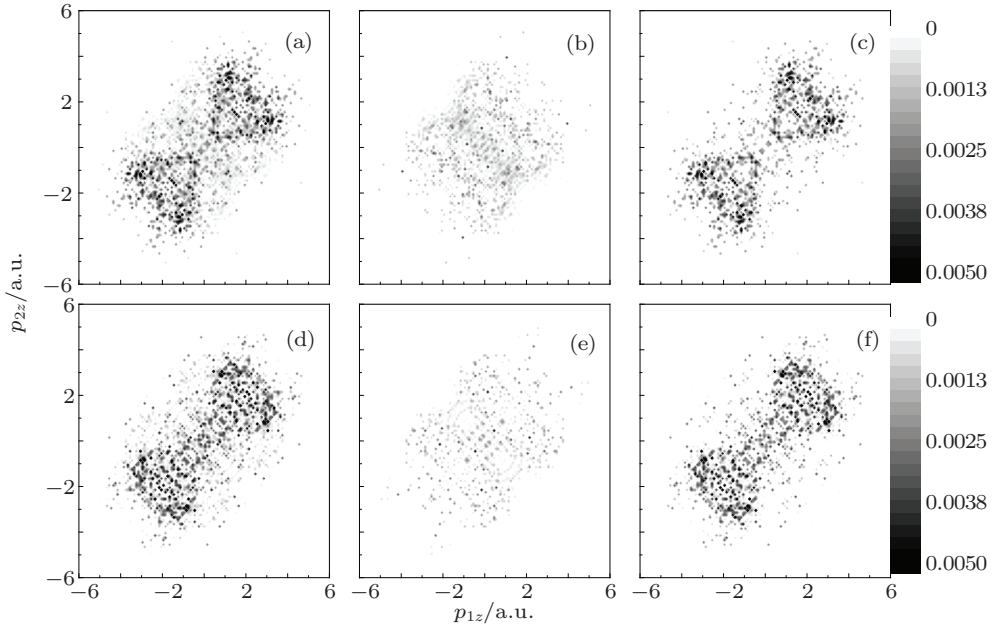


Fig. 1. The correlated electron momentum distributions in z-axis direction in an elliptical polarization field, panels (a), (b), and (c) with zero initial longitudinal velocity; panels (d), (e), and (f) with non-zero initial longitudinal velocity, panels (a) and (d) for all DI events, panels (b) and (e) for only SRC events, panels (c) and (f) for only MRC events.

As we know, the final momenta of the electrons strongly depends on the recollision and DI time, so we show the distributions of the collision time and the double ionization (DI) time in Figs. 2(a) and 2(b) respectively to understand the pattern of the correlated momentum distributions. For the DI time distribution in Fig. 2(b), there are two peaks in the second half of the optical cycle which correspond to 64% of the double ionization cases in the first peak (SRC) of the collision time distribution in Fig. 2(a). In the rescattering picture, the collision can either ionize the second electron directly which is called collision ionization (CI) or only induces excitation of the second electron with subsequent field ionization which is called collision excitation ionization (CEI). Following Ref. [29], we define a parameter $\triangle t$ which is equal to the interval between the collision time and the DI time and it is considered a CI event if $\triangle t < 0.05$ cycle. We found that, in the case of zero initial longitudinal velocity, the proportion of CI is 81% for the first peak and 32% for the second peak in Fig. 2(b), indicating that the first and the second peaks mainly correspond to CI and CEI, respectively. This conclusion is similar to the case of a linearly polarized laser field.[26] We can see clearly that the first peak in Fig. 2(b) almost disappears while the second peak increases after taking into account the non-zero initial longitudinal velocity. In Ref. [24], it is reported that the CI peak is responsible for the distribution in the region near the origin. Therefore, the significant reduction of the center part in the correlated momentum distribution in Fig. 1(e) results from the disappearance of the CI peak in Fig. 2(b).

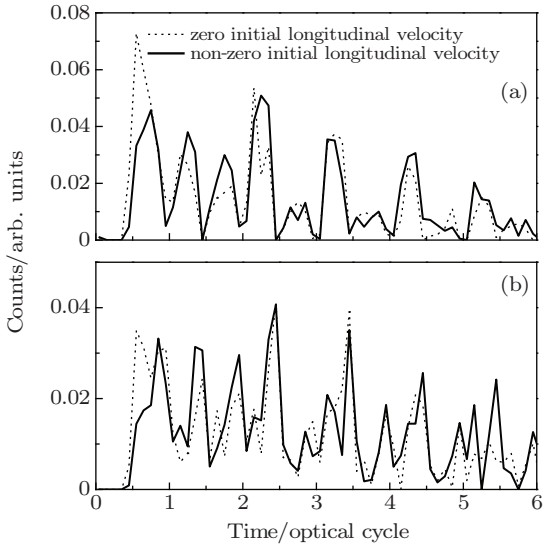


Fig. 2. Distributions of (a) the collision time t_c and (b) the DI time t_i of DI events in an elliptical polarization field.

The disappearance of the CI peak results directly from the delay of the collision time as we can see in Fig. 2(a) in which the first peak shifts to the right and we attribute this delay effect to the delay of the tunnelling time and the change of the first electron's travel time (the interval between tunnelling time and collision time). We present the distribution of the initial phase $\phi_0 = \omega t_0$ leading to double ionization in Fig. 3. We can see clearly that the effect of non-zero initial longitudinal velocity is to make the tunnelling time shift to the right both for SRC and MRC events and this shift of the tunnelling time can be explained by the fact that due to its initial velocity the outer electron has to reduce the time of acceleration in the laser field, i.e., the outer electron has to tunnel out later, and if not it will move out directly without returning to the core. On the other hand, with non-zero initial longitudinal velocity, the tunnelled electron will experience a longer time before being brought back by the laser field to collide with the core. In our calculation, the average travel time increases from 0.6 cycle to 0.64 cycle after considering non-zero initial longitudinal velocity. Moreover, this increase of the travel time leads to increasing diffusion of the wave packet and hence reduces the probability of collision,

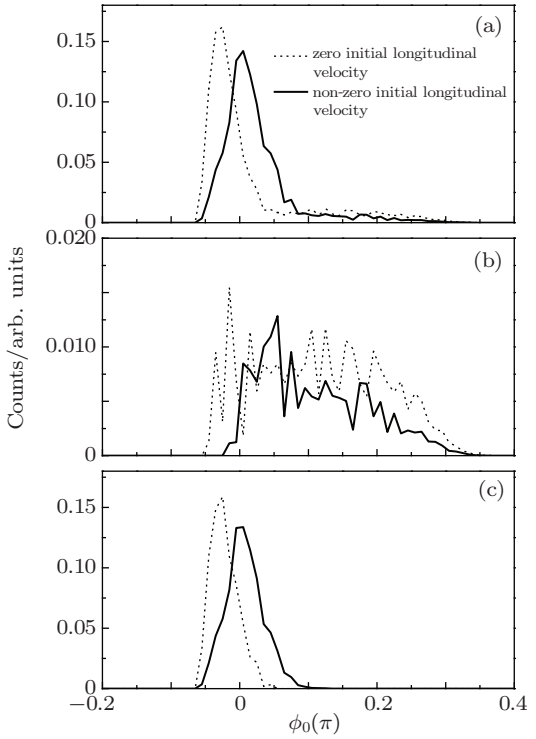


Fig. 3. (a) Distribution of the initial phase ϕ_0 of the tunnelled electron in an elliptical polarization field, (b) distributions of ϕ_0 for SRC events, and (c) MRC events.

especially the hard collision which leads to CI, between two electrons. Therefore, the CI is significantly suppressed compared with CEI as shown in Fig. 2(b).

3.2. Correlated momentum distribution in the direction of the minor polarization axis (x axis)

Then we show the correlated electron momentum distribution in the direction of the minor polarization axis (x axis) in Fig. 4 and we also present the distribution in a linear polarization field with zero initial longitudinal velocity in Fig. 4 for comparison. In the case of linear polarization, the electrons mainly distribute around the origin (Fig. 4(a)), which directly results from the Gaussian initial transverse velocity distribution in the semiclassical model; while in the case of an elliptically polarized field, because the electric field in the direction of the x axis is very weak in our case, the distribution still mainly locates in the center part. However, there are some differences in details: the distribution of the MRC is enhanced and becomes broader while that of the SRC is reduced. These differences can be attributed to the effects of the field in the x direction. One is that the x direction field will reduce the probability of recollision between the first electron with the core and hence reduce the probability of DI. Another one is that the x-direction field will accelerate the two ionized electrons and result in greater momentum in the x direction at the end of the laser pulse. Compared with SRC, the MRC, in which the Coulomb focus effect plays an important role, will not be reduced so much because the Coulomb focus effect will partly cancel out the effect of the x direction laser field. Therefore, for the case of SRC, the main effect of the field in the x direction is to reduce the probability of DI; while for the case of MRC, the main effect of the x-direction field is to accelerate the ionized electrons in the x direction, which results in the broader momentum distributions.

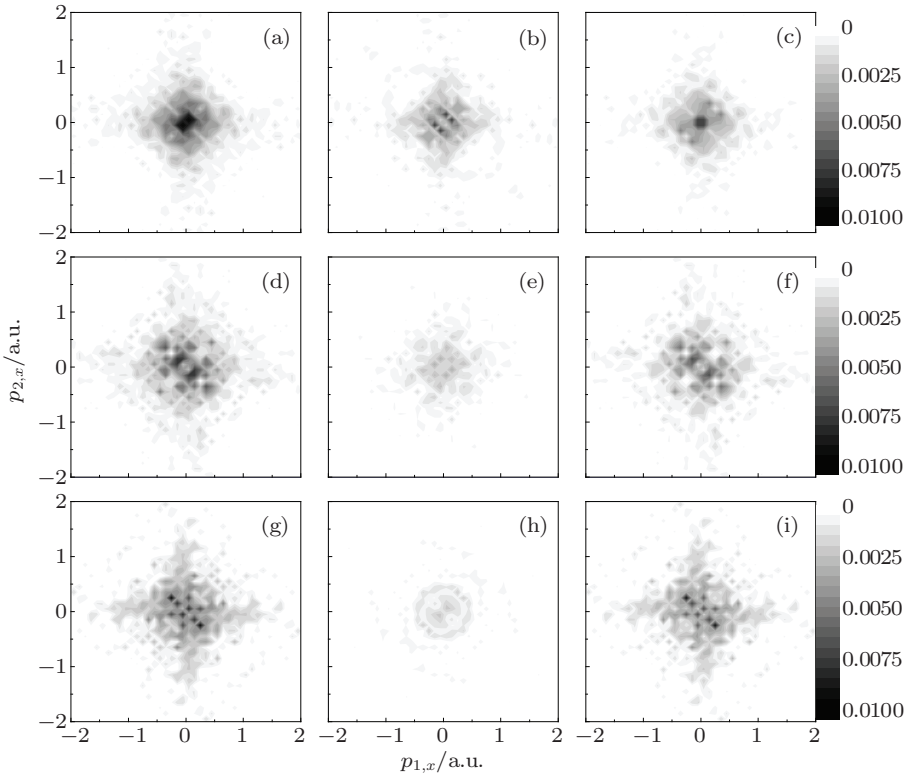


Fig. 4. The correlated electron momentum distributions in x-axis direction. Panels 4(a), 4(b), and 4(c) are linear polarization with zero initial longitudinal velocity; panels 4(d), 4(e), and 4(f) are elliptical polarization with zero initial longitudinal velocity; panels 4(g), 4(h), and 4(i) are elliptical polarization with non-zero initial longitudinal velocity; panels 4(a), 4(d), and 4(g) for total events; 4(b), 4(e), and 4(h) for only SRC events; 4(c), 4(f), and 4(i) for only MRC events.

Also, if we consider non-zero initial velocity, the momentum distributions are similar to the zero initial velocity case, except that the distribution of the SRC is reduced and becomes narrow. We believe that this change also results from the strong suppression of the first peak in Fig. 2(b). Different from the case of z direction, in which the first peak in Fig. 2(b) corresponds to the center part in correlation momentum distribution, it corresponds to a relative higher momentum in the case of x direction. This is because the formula of the field in x direction is sine but not cosine and hence the acceleration of the field in x direction decreases with increasing DI time for SRC, whose DI time is mainly in the region of 0.5 cycle$< t_{\rm i} <$1 cycle. In our calculation the first peak in Fig. 2(b), peaks around 0.55 optical cycle, corresponds to an acceleration of 0.58 a.u. in x direction, which just corresponds to the disappearing distribution in Fig. 4(h) compared with Fig. 4(e).

4. Conclusion

In conclusion, the semiclassical rescattering model is used to investigate the effect of non-zero initial longitudinal velocity of a tunnelled electron on the NSDI process in an elliptically polarized laser field. We have studied the correlated electron momentum distributions of double ionization in the direction of the major polarization axis (z axis) and the minor polarization axis (x axis), respectively. We find that the non-zero initial longitudinal velocity has a suppressing effect on SRC events in the DI process. For correlated momentum distribution in the direction of z axis, the non-zero initial longitudinal velocity will result in a significant reduction of distribution in the center part; and for correlated momentum distribution in the direction of x axis, the distribution of the SRC becomes narrower if we consider non-zero initial longitudinal velocity. The above effect originates from the fact that the CI peak (the first peak) in the double ionization time distribution, which is responsible for the center part of the correlation momentum distribution in z direction but corresponds to the relative high momentum in x direction, almost disappears after considering non-zero initial longitudinal velocity. The disappearance of the CI peak results from the delay of the tunnelling time and the increasing travel time of the first electron.

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