Double ionization of helium interacting with elliptically polarized laser pulse by classical ensemble simulations*

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This paper uses the classical ensemble method to study the double ionization of a 2-dimensional (2D) model helium atom interacting with an elliptically polarized laser pulse. The classical ensemble calculation demonstrates that the ratio of double to single ionization decreases with the increasing ellipticity of the driving field. The classical scenario shows that there are hardly any e–e recollisions with the circularly polarized laser pulse. The double ionization probability is studied for linearly and circularly polarized laser pulses. The classical numerical results are consistent with the semiclassical rescattering mechanism and in agreement with the experimental results and the quantum calculations qualitatively.

Keywords: classical ensemble method, nonsequential double ionization, ellipticity dependence

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1. Introduction

The multiphoton ionization (MPI) of atoms by strong laser fields can be described by time-dependent quantum mechanical calculations.[1,2] However, the so-called "knee" or "shoulder" structure has been discovered in the ionization yields when helium is exposed to a laser pulse. Two possible mechanisms were suggested in order to explain nonsequential double ionization (NSDI). Fittinghoff *et al.*[3] suggested a "shake-off" effect and Corkum[4] proposed a rescattering mechanism. Entirely quantum calculations[5−11] about NSDI are remarkably good. Other fully quantum-mechanical calculations are based on the S-matrix theory or *ab initio* calculations.[12,13] Eberly and his co-workers[14−17] have studied the NSDI by using classical ensemble simulations. Besides, semiclassical rescattering model[18,19] has also afforded important insights into NSDI.

Experiments have shown that the NSDI rate is greatly reduced in elliptically polarized light.[20,21] Several measurements of the yield of doubly charged ions produced by circular polarization were presented.[22−24] Some numerical quantum simulations under an intense laser field have concentrated on the behaviour of atoms in elliptically polarized laser fields.[25−27]

In this paper, we demonstrate the double ionization in the case of two-dimensional (2D) model helium interacting with elliptically polarized laser pulse by using classical ensemble simulations. Compared with the case of linear polarization, we find that the kinematics caused by an elliptically polarized field are genuinely two-dimensional. Fortunately, the z component does not influence the ionization probability. We also illustrate the double ionization under the influence of elliptically polarized light. The classical ensemble results show the strong ellipticity dependence. The double ionization probability is also studied for linearly and circularly polarized laser pulse.

2. Classical ensemble simulations

In the classical view, helium is considered as a dynamic system which contains three classical particles: one nucleus and two electrons. When a laser field is applied, the motion of each particle depends not only on the laser field but also on the Coulomb field due to the other two particles. In this paper, we consider the 2D model helium. We take the nucleus as the origin of our coordinate system and Newtonian equations are (atomic units are used throughout the paper)

$$\begin{aligned}\ddot{x}_1 &= -E_x(t) - \frac{2x_1}{(x_1^2+y_1^2+\alpha)^{3/2}} \\ &\quad + \frac{(x_1-x_2)}{[(x_1-x_2)^2+(y_1-y_2)^2+\beta]^{3/2}}, \qquad (1)\\ \ddot{y}_1 &= -E_y(t) - \frac{2y_1}{(x_1^2+y_1^2+\alpha)^{3/2}}\end{aligned}$$

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$$+\frac{(y_1-y_2)}{[(x_1-x_2)^2+(y_1-y_2)^2+\beta]^{3/2}}, \quad (2)$$

$$\ddot{x}_2 = -E_x(t)-\frac{2x_2}{(x_2^2+y_2^2+\alpha)^{3/2}} + \frac{(x_2-x_1)}{[(x_2-x_1)^2+(y_2-y_1)^2+\beta]^{3/2}}, \quad (3)$$

$$\ddot{y}_2 = -E_y(t)-\frac{2y_2}{(x_2^2+y_2^2+\alpha)^{3/2}} + \frac{(y_2-y_1)}{[(x_2-x_1)^2+(y_2-y_1)^2+\beta]^{3/2}}, \quad (4)$$

where α and β are the soften parameters, which are used to avoid the singularity in the Coulomb soft-core potential. We choose $\alpha = 0.169$ which made the lowest eigenstate matching the binding energy of He^+. The choice of β is some arbitrary.[5] We choose $\beta = 0.4$. The $E_x(t) = E_0 f(t)\cos(\omega t)$ is the laser pulse along the x axis, $E_y(t) = \epsilon E_0 f(t)\sin(\omega t)$ is a weak perpendicular laser component along the y axis, ϵ is the ellipticity and $f(t)$ is the trapezoidal pulse envelope. We defined that $\epsilon = 0$ represents the linear polarization along the x-axis and $\epsilon = 1$ the circular.

From Legendre transformation, Newtonian equations (1)–(4) can be transformed into Hamiltonian canonical equations whose Hamiltonian function is:

$$H(x_1,y_1,p_{x_1},p_{y_1};x_2,y_2,p_{x_2},p_{y_2};t) = H(p,q,t) = \mathcal{T}(p)+\mathcal{V}(q,t), \quad (5)$$

where the kinetic energy $\mathcal{T}$ and the potential energy $\mathcal{V}$ are given, respectively, as follows:

$$\mathcal{T}(p) = \frac{p_{x_1}^2}{2}+\frac{p_{y_1}^2}{2}+\frac{p_{x_2}^2}{2}+\frac{p_{y_2}^2}{2}, \quad (6)$$

$$\mathcal{V}(q,t) = -\frac{2}{\sqrt{x_1^2+y_1^2+\alpha}}-\frac{2}{\sqrt{x_2^2+y_2^2+\alpha}} + \frac{1}{\sqrt{(x_1-x_2)^2+(y_1-y_2)^2+\beta}} + [(x_1+x_2)E_x(t)+(y_1+y_2)E_y(t)]. \quad (7)$$

In the above equations $q = (x_1, y_1, x_2, y_2)$ stands for the positions of the two electrons, $p = (p_{x_1}, p_{y_1}, p_{x_2}, p_{y_2})$ is the corresponding conjugate momentum.

We choose a set of initial stable states $\{x_i(0), p_{x_i}(0), y_i(0), p_{y_i}(0)\}_{i=1}^2$ by the classical ensemble method.[28−30] We can obtain field-free trajectories by solving the field-free Hamiltonian canonical equations using the symplectic method[30,31] and then pick up a large number of points randomly along the field-free trajectories. For the field-free case, the symplectic method can preserve the energy of the system in time, even for a long time evolution. So these points have the same energy and consist of a microcanonical ensemble and will be served as the initial conditions for the atom-laser interacting system. The Hamiltonian system (5) is a separable system,[30,31] we may use an explicit symplectic scheme to solve it numerically and obtain the classical trajectories of the electron and corresponding momenta $\{x_i(t), p_{x_i}(t), y_i(t), p_{y_i}(t)\}_{i=1,2}$. Here we employ a large microcanonical ensemble (100000 field-free trajectories). For each field-free trajectory, the total energy equals the ground state energy of helium.

We traced the one-particle energies

$$\varepsilon_1 = \frac{p_{x_1}^2}{2}+\frac{p_{y_1}^2}{2}-\frac{2}{\sqrt{x_1^2+y_1^2+\alpha}} + \frac{1}{\sqrt{(x_2-x_1)^2+(y_2-y_1)^2+\beta}}, \quad (8)$$

$$\varepsilon_2 = \frac{p_{x_2}^2}{2}+\frac{p_{y_2}^2}{2}-\frac{2}{\sqrt{x_2^2+y_2^2+\alpha}} + \frac{1}{\sqrt{(x_2-x_1)^2+(y_2-y_1)^2+\beta}}. \quad (9)$$

Each electron is considered to be ionized when $\varepsilon_1 > 0$ or $\varepsilon_2 > 0$, respectively. However, we can also use a distance criterion ($r_d = 6.0$ a.u.)[32] as a threshold to obtain the single- and double-ionization probabilities.

If we choose N initial conditions, then we can obtain N classical trajectories for helium system by using the symplectic method. For each time, we can calculate the number of classical trajectories for the processes of the survival $S_{\rm SUR}$, the single ionization $S_{\rm SI}$, the double ionization $S_{\rm DI}$ according to the criteria mentioned above, respectively. Then we can obtain the corresponding probabilities for these processes at each time as follows:

$$P_{\rm SUR} = \frac{S_{\rm SUR}}{N}, \quad P_{\rm SI} = \frac{S_{\rm SI}}{N}, \quad P_{\rm DI} = \frac{S_{\rm DI}}{N}. \quad (10)$$

3. Results and discussion

The ellipticity dependence of the double ionization is demonstrated in the same wavelength (λ = 775 nm) and the laser peak intensity 8×10^{14} W·cm^{-2} used in the experiment of Dietrich *et al.*[21] The pulse envelope used here is the trapezoidal pulse with a two-cycle linear turn-on followed by twelve cycles of constant and then a two-cycle linear turn-off. Figure 1

shows the ratio of double to single ionization probability as a function of the ellipticity of the driving field. From Fig. 1 we can see that the ratio of the double to single ionization decreases as the ellipticity increases, which is in qualitative agreement with the experimental results[21] and the quantum calculations.[26] As has been pointed out, the result shows the similar tendency with the experimental results obtained by Dietrich *et al.*[21] These phenomena in terms of the recollison model discussed in Ref. [26] can be easily understood. The out electron is driven along polarized axis in the linearly polarized laser pulse, while certain transverse component of the laser field exists for the elliptically polarized laser pulse. When the ellipticity increases, the transverse component of the laser field increases, the recollision probability reduces and hence the NSDI reduces.

Figure 2 shows the sum of kinetic energy, electron-nucleus binding energy, e–e correlation energy, and laser field interaction energy for each of two electrons during the laser pulse. Our classical ensemble calculations represent classical typical processes. From the energy plots of Fig. 2(b), we can easily observe the three NSDI stages (initiation, recollison, ionization) with linearly polarized laser pulse mentioned in Ref. [16]. With the linearly polarized laser pulse, the outer electron escapes, then returns and recollides with the inner electron repeatedly until the inner electron gets enough energy to escape. From Fig. 2(b), we can also observe that after each recollision, the energies of both inner and outer electrons are modified as mentioned in Ref. [33]. But figure 2(a) shows that there are hardly any e–e recollisions in circularly polarized laser pulse. For the linearly polarized laser pulse, the outer electron is driven along the polarized axis, and thus has more chances to recollide with the other electron; while for the circularly polarized laser pulse, which contains a transverse component, the probability of recollisions is smaller.

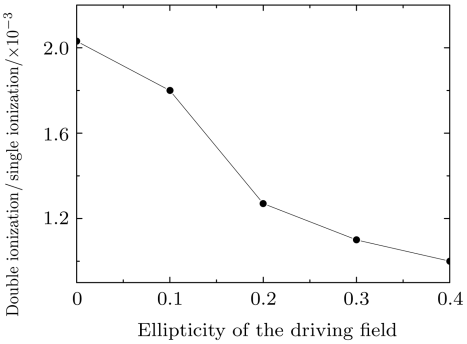


Fig. 1. The ratio of double to single ionization is plotted as a function of the ellipticity of the driving field for a 16-cycle pulse with the laser peak intensity 8×10^{14} W · cm^{-2} and wavelength 775 nm.

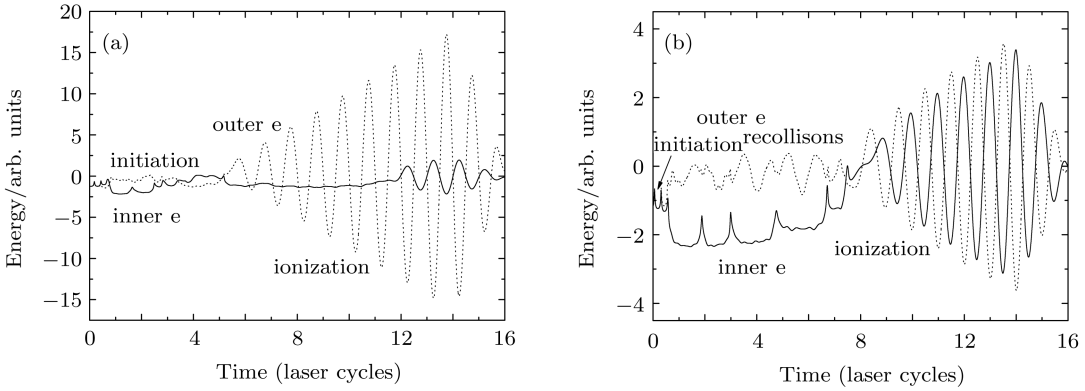


Fig. 2. An example for a pair of two-electron trajectories in terms of the electron energy versus time measured in laser pulse for a 16-cycle pulse with the peak intensity 1.4×10^{15} W · cm^{-2} and wavelength 700 nm, (a) with circularly polarized laser pulse; (b) with linearly polarized laser pulse.

Figure 3 shows the probability of double ionization (DI) with the increasing peak laser intensity for an 8-cycle pulse with wavelength 780 nm for linearly and circularly polarized laser pulse, respectively. From Fig. 3, we can observe that the probability of DI in a linearly polarized field is bigger than that in circularly polarized field. The probability of DI appears to be completely suppressed in circularly polarized pulse. And for linearly polarized pulses the results show enhanced ionization that has been referred to "nonsequential" ionization, but, for circularly polarized pulses the results show no "knee" structure. This may due to the fact that the recollisions seldom occur in a circularly polarized field. These results are in agreement with the experimental results of Walker *et al.*[20] qualitatively.

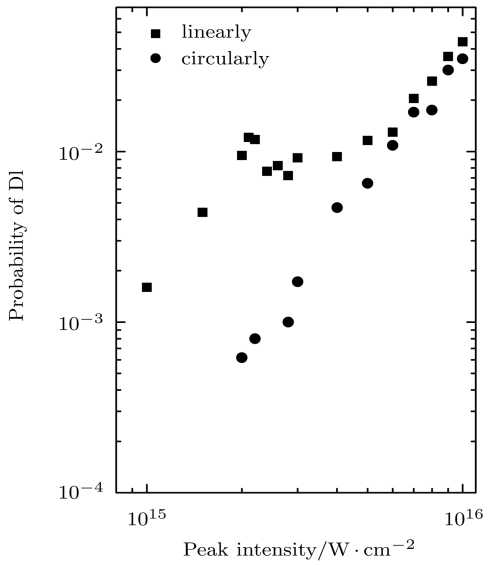


Fig. 3. Probability of double ionization (DI) with the increasing peak laser intensity for an 8-cycle pulse with wavelength 780 nm with linearly and circularly polarized laser pulse, respectively.

4. Conclusions

In summary, we have shown that the ratio of double to single ionization of a 2D model helium atom interacting with an elliptically polarized laser pulse by classical simulations is decreased with the increasing ellipticity of the driving field. The total electron energy-evolution pictures are used to illustrate the three NSDI stages (initiation, recollison, ionization) with linearly and circularly polarized laser pulse. The numerical results show that there are hardly any e–e recollisions in the circularly polarized laser pulse. The probability of DI with the increasing peak laser intensity demonstrates that no "knee" structure for circularly polarized pulses and the probability of DI in a linearly polarized field is bigger than that in the circularly polarized field. The numerical results are in qualitative good agreement with experimental and quantum calculations.

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