Exploration of nonsequential-double-ionization dynamics of Mg atoms in linearly and circularly polarized laser fields with different potentials

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Exploration of non-sequential double ionization dynamics of Mg atom in linearly and circularly polarized laser fields with different potentials

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The non-sequential double ionization (NSDI) of Mg atom is investigated in both linearly and circularly polarized laser fields with different kinds of potentials. The numerical results indicate that the "knee" structure still exist in circularly polarized laser fields in 800 nm case with different potentials, which can be well explained by the corresponding momentum and position distribution of electrons. Moreover, the ionized electron energy of Mg atom at the end of pulse also shows the behavior of rescattering electrons is different between linearly and circularly polarized cases. Besides, we also look into the angular distribution at the end of pulse with different kind of potentials to illustrate the difference of double ionization mechanism between linearly and circularly polarized case.

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I. INTRODUCTION

The nature of strong-field ionization processes has both practical and fundamental interest [1–3]. Dynamics of simple systems has been studied thoroughly both theoretically and experimentally, such as helium [4, 5]. In earlier studies, Fittinghoff *et al.* [6] suggested a "shake-off" model that one electron is thought to ionize very fast and then the second electron ionizes due to the sudden change of the binding potential and consequently "shake-off" the atom. Corkum [7] proposed a rescattering model that one electron ionizes first and revisits the core to let the second electron free by collision, which is widely accepted to explain the NSDI. In general, NSDI seldom occur in circularly laser fields for most atoms such as He, Li, et al, that's because the perpendicular part of the laser field will force the electron move away from the core, thus the recollision can't occur. But the numerical calculations and experimental research show that for Mg atom the NSDI still occur in circularly laser fields at the wavelength of 800 nm [8, 9], which attracts much interest to study the ionization dynamics of Mg in intense laser fields [10]. On the other hand, with the development of ultrafast laser technology, the tracing of electron motion in atoms in strong-field also have been a hot topic recently but the dynamical origin of the NSDI in circularly polarized fields still needs further exploration [11, 12].

In principle, the treatment of laser-matter interaction involving an atom or molecule needs full quantum theory. However, it turns out that semi-classical or classical simulations are useful to treat the strong-field ionization with very strong two-electron correlation, such as NSDI and non-sequential triple ionization (NSTI) [13–17].

In this paper, we will investigate the double ionization mechanism of Mg in linearly and circularly polarized laser fields by the classical ensemble method with different kinds of potentials, and compared them together. We will illustrate how non-sequential double ionization happens at 800 nm circularly laser fields. Particularly, we will investigate the corresponding momentum and position distribution of doubly ionized electrons to study the classical cutoffs for laser-induced NSDI. Besides, we will also look into the dynamical signature of ionization dynamics by a specific form of electron yield and angular distribution.

II. THEORETICAL METHOD

We use the classical ensemble method to explore the ionization dynamics of 3D Mg atom in intense laser fields. Since it consists of 1s, 2s, 2p and 3s orbitals, and we just consider the electrons of 3s orbital of Mg atom. It is a simplified model for Mg atom indeed. The electrons in 3s orbital is much easier to ionize than others, and also have the greatest contribution to double ionization process. This model of Mg atom have already been used before[8, 10]. The classical Hamiltonian of 3D Mg in an intense laser field can be given by (atomic units are used throughout unless otherwise stated):

$$H(\mathbf{r}_1, \mathbf{r}_2; \mathbf{P}_1, \mathbf{P}_2; t) \;=\; \mathcal{T}(p) + \mathcal{V}(q, t) \qquad (1)$$

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where the kinetic energy $\mathcal{T}$ and the potential energy $\mathcal{V}$ are given respectively by

$$\mathcal{T}(p) = \frac{\mathbf{P}_1^2}{2} + \frac{\mathbf{P}_2^2}{2}, \quad (2)$$

$$\mathcal{V}(q,t) = -\sum_{i=1}^{2} \frac{2}{|\mathbf{r}_i|} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} + (\mathbf{r}_1 + \mathbf{r}_2)E(t). \quad (3)$$

In the above equations, $q = (\mathbf{r}_1, \mathbf{r}_2)$ stands for the positions of the two electrons, $p = (\mathbf{P}_1, \mathbf{P}_2)$ is for their corresponding conjugate momenta, $E(t)$ is the laser field. Here we use the complex error function to get the exact Coulomb potential [18], and compared with the corresponding results using soft core potentials [8]. The use of soft Coulomb potentials is to move the singularity of Coulomb potentials, and avoid the auto-ionization states. The parameter is a=2.4 a.u., b=1.0 a.u..

The canonical system of equations for Mg atom is

$$\frac{dp}{dt} = -\frac{\partial \mathcal{V}(q,t)}{\partial q}, \quad (4)$$

$$\frac{dq}{dt} = \frac{\partial \mathcal{T}(p)}{\partial p}. \quad (5)$$

We choose a set of initial stable states $\{\mathbf{r}_i(0), \mathbf{P}_i(0)\}_{i=1}^2$ by the monte-carlo method and solve the above canonical equations numerically by symplectic method in order to obtain the time evolutions of the corresponding electron position and momenta $\{\mathbf{r}_i(t), \mathbf{P}_i(t)\}_{i=1}^2$. Since the Hamiltonian system (1) is a separable Hamiltonian system in the sense that q and p are contained separately in $\mathcal{V}(q,t)$ and $\mathcal{T}(p)$. Also, the Hamiltonian function contains the time variable, we may use an explicit symplectic scheme [19]to solve it so that we can obtain the classical trajectories of Mg in an intense laser field.

We propagate in time the dynamical response of the electron pairs in each of a large number N of atoms and interpret the result in a statistical manner. One particular atom's two-electron motion will be referred to as a trajectory. In our calculation, we assume the initial condition has the same energy approximately equal to the sum of first and second ionization energy [8].

Once the initial conditions for the participating pairs are obtained, the field is turned on and all trajectories are propagated in intense laser field. We defined the energy of each electron as $E_1(t)$ and $E_2(t)$, respectively. where $E_i = P_i^2/2 - 1/|R_i|$, i=1,2, If both $E_1(t)$ and $E_2(t)$ greater than zero at the end of the laser pulse, the double ionization occurs.

III. RESULTS AND DISCUSSION

In the present work, we choose an linearly polarized laser pulse $(E(t),\ 0,\ 0)$ with $E(t) = E_0 f(t)\sin(\omega_0 t)$, where the frequency $\omega_0 = 0.057$ a.u. (800 nm in wavelength) and the pulse shape $f(t)$ is sin square, the pulse duration $T = 8T_0$ with $T_0 = 2\pi/\omega_0$ being the period of the pulse, and E_0 is the peak intensity. The circularly polarized electric fields chosen in this paper can be written as $(E_x(t)/\sqrt{2},\ E_y(t)/\sqrt{2},\ 0)$, where $E_x(t) = E_0 f(t)\cos(\omega_0 t)$, $E_y(t) = E_0 f(t)\sin(\omega_0 t)$. In this work, we utilize a micro-canonical ensemble which consists of 1×10^5 two-electron "trajectories" and the time step is 0.05 a.u..

Fig. 1 shows the double ionization probability of Mg as a function of laser intensity in linearly and circularly polarized laser fields with different kinds of potentials. We can see from Fig.1(a) that the "knee" structure occurs in circularly polarized laser fields at the laser intensity 1×10^{14} TW/cm^2, which is in agreement with the corresponding experimental results and numerical calculations [8, 9]. This means the non-sequential double ionization of Mg occurs in circularly case. In general, the recollision mechanism of non-sequential double ionization is suppressed in circularly polarized laser fields because the returning electron is unlikely to encounter the core. But under special conditions, especially in lower energy cases, the ionized electron can reach the core and collides with the inner one, leading to an appreciable amount of NSDI and its characteristic "knee" structure. From Fig.1 (a) and (b) we can see there exist a big difference between the double ionization probability with different potentials and the "knee" structure occurs earlier in Fig.1(b), but they presents similar tendency. It is also shown in Fig.1 that there is no "knee" structure in linearly polarized cases with both potentials.

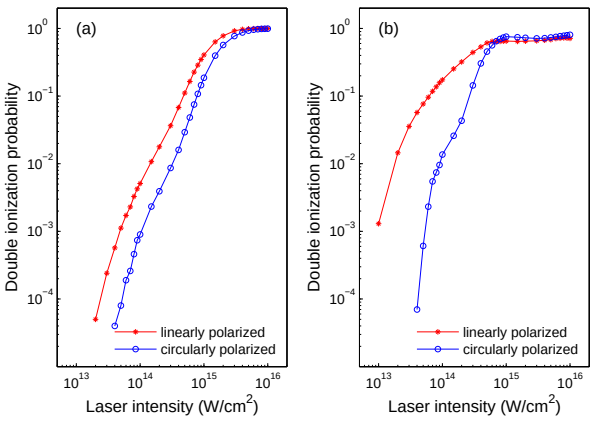

FIG. 1: (Color online) The double ionization probability of Mg as a function of the laser intensity in linearly (red asterisk)and circularly(blue circle) polarized laser fields with (a) exact potential and (b) soft core potential, respectively.

In order to further understand or identify the non-sequential double ionization mechanism of Mg atom in circularly polarized laser fields, we calculated the corresponding momentum and position distribution of correlated electrons of Mg atom in double ionization processes as follows. We first presents the momentum distribution of Mg atom in linearly and circularly polarized laser fields with the increasing laser intensity in Fig. 2. The circle presents the value of $2\sqrt{U_p}$. Fig.2(a) and (c) shows in

linearly polarized case at first the momentum of two electrons distributed around the core and the value of momentum distribution is no larger than $2\sqrt{U_p}$ [20] which means NSDI is seldom occur. As the intensity increases, the momentum distribution looks like a slim cross shape, which is the signature of RESI [11] (recollision excitation with subsequent tunnelling ionization). We also can see from Fig.2(b) and (d) that in circularly polarized case the momentum distribution presents the same tendency which transfer from a "V" shape [21] (Fig.2(d2)) to a cross structure (Fig.2(d4)) with the increasing laser intensity. At the beginning the electron momentum are mainly distributed in second and fourth quadrant and in Fig.2(b2)and (d2) the momentum distribution beyond the $2\sqrt{U_p}$ range which indicates the NSDI occur, as the laser intensity increases, the cross shape occurs in circularly polarized case which means the RESI is predominant. When the laser intensity increases even larger, the cross shape become thinner, in other words, the momentum of one electron is large and the other is small, which indicates the SDI is predominant in these circumstance. Interestingly, This momentum distribution is similar with the Ar case in Ref.[12]. We can also compared from Fig.2 that the cross shape is more symmetric and thinner with the exact potential than soft potential, which is probably due to the fact that the soft parameter can screen some interaction between electron and nuclear so that the tunnelling process is more likely to occur in exact potential case.

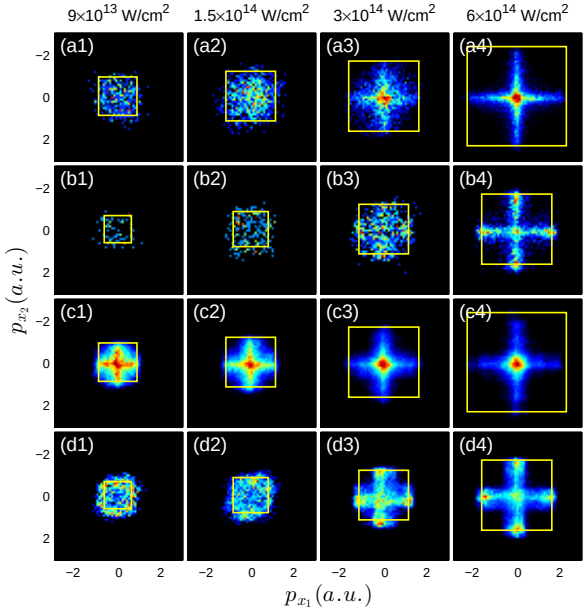

FIG. 2: (Color online) The momentum distribution of 3D Mg at the end of laser pulse with the increasing laser intensity in linearly ((a) and (c)) and circularly ((b) and (d)) polarized laser fields with exact potential((a) and (b) and soft core potentials ((c) and (d)). The laser wavelength is 800 nm.

Recent research illustrate that both CI and RESI has contribution to the NDSI process of Ar ionization in few-

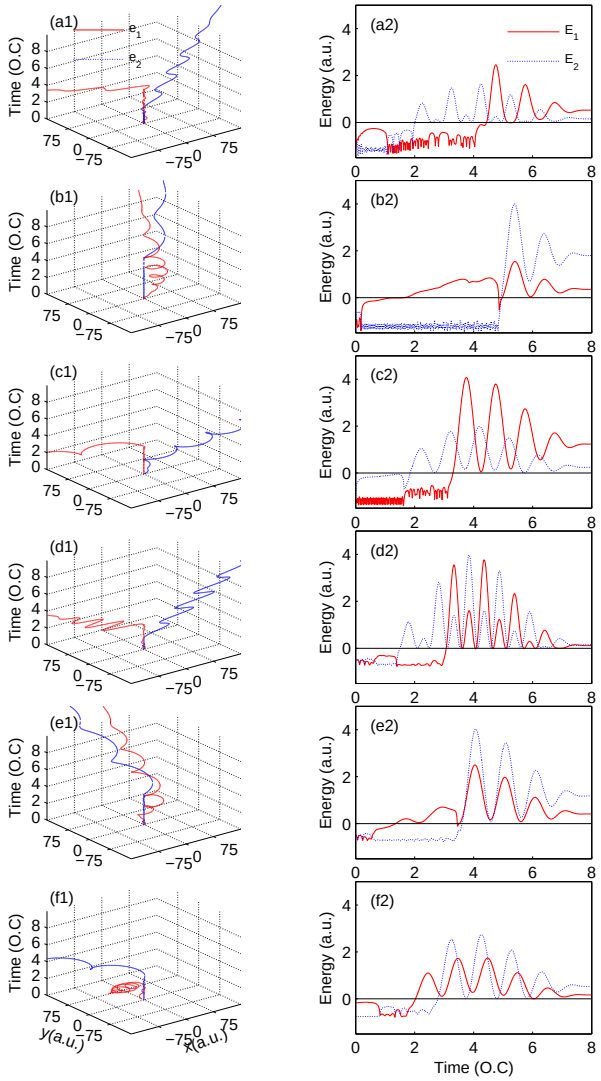

FIG. 3: (Color online) The position and energy distribution of 3D Mg as a function of time with exact potential ((a),(b) and (c)) and soft potential ((d),(e) and (f)) in linearly and circularly polarized laser fields. (a) and (d) is linearly polarized case, (b),(c),(e) and (f) is circularly polarized case. The red solid and blue dashed line represents two electrons, respectively. The laser intensity is 200 TW/cm^2, wavelength is 800 nm.

cycle laser fields [22], and it is comparable in Mg atom case. To further investigate this phenomenon, similar as Ref.[23], we calculate the 3D trajectories and corresponding energy distribution of electrons in Mg atom as a function of time in linearly and circularly polarized laser fields in Fig.3. Fig.3(a1) and (a2) shows a typical SDI two-electron trajectory that one ionizes after another in linearly polarized laser fields, Fig.3(b1) and (b2) shows a typical CI two-electron trajectory in circularly polarized laser fields, which is composed of one electron close to the core and another one further away, then come back to the core and share energy with the another one quickly.

Fig.3(c1) and (c2) shows a typical RESI trajectory in circularly polarized laser fields, we can see that one electron ionizes and come back to the core and collides with the other one and share energy, which let it transit to the excited states, and then ionizes in laser fields after time interval. Fig.3(c),(d) and (e) presents the similar phenomenon with soft potentials. Above phenomenon illustrated that even the perpendicular part of the circularly polarized lasers can force the electron move away and miss the core more often, but it can still recollide with the inner electron at a suitable moment which can lead to NSDI in Mg atom case.

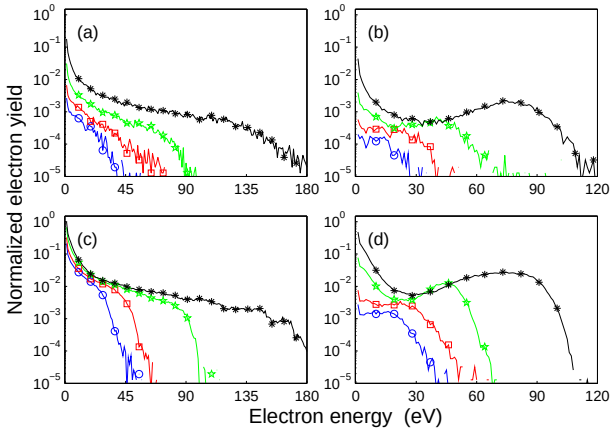

FIG. 4: (Color online) The kinetic energy of ionized electrons of 3D Mg atom at the end of laser pulse in linearly and circularly polarized laser fields with exact potential ((a) and (b)) and soft potentials((c) and (d)), respectively. where (a) and (c) are linearly polarized case, and (b) and (d) are circularly polarized case, where the blue (circle), red (square), green (pentagram) and black(asterisk) line corresponding to 90 TW/cm^2, 150 TW/cm^2, 300 TW/cm^2 and 600 TW/cm^2, respectively.

Fig. 4 shows the kinetic energy of ionized electrons of 3D Mg atom at the end of laser pulse in linearly and circularly polarized laser fields. The results show that the probability of kinetic energy of ionized electrons become larger with the increasing intensity, Corresponding to Fig.4, the exact value of U_p with increasing intensity is 5.3568 eV, 8.928 eV, 17.856 eV and 35.712 eV, respectively. In Fig.4 we can see there are several electrons which energy are greater than 2 U_p, which indicates that there still exist rescattering electrons. Compared Fig.4(a) with Fig.4(b), the greatest energy of electron can obtain is larger in linearly polarized cases than in circularly polarized cases, that's because the horizontal part of circular polarized case is smaller than linearly polarized case, But the probability of electrons in the high-energy regime is larger in circularly polarized case than in linearly polarized case, which also indicates due to the perpendicular part of circular polarized case there are more electrons returning back to the core and rescattering, the RESI is more easier to occur than that in the linearly polarized case.

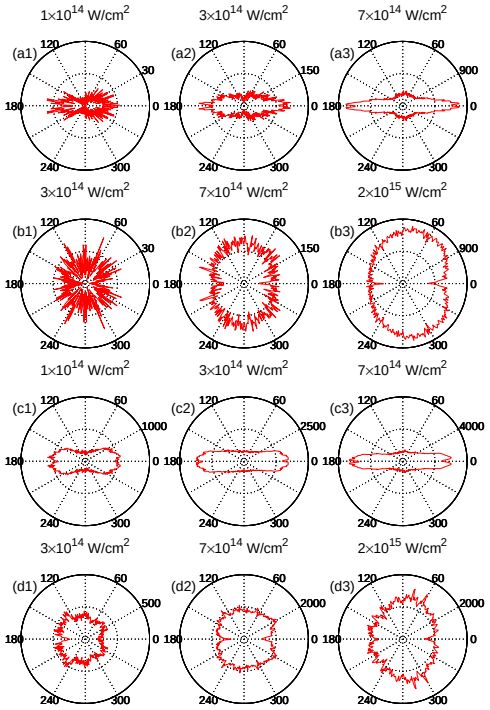

FIG. 5: (color online) The angular distribution of 3D Mg atom at the end of laser pulse using exact potential ((a) and (b)) and soft potential ((c) and (d)) in linearly ((a) and (c)) and circularly ((b) and (d)) polarized laser fields with the increasing laser intensity.

At last, since it is a 3D case, we wonder the difference of the angular distribution in linearly and circularly polarized case. Fig. 5 shows the angular distribution of double ionized electrons of 3D Mg atom at the end of laser pulse in linearly and circularly polarized laser fields with increasing laser intensity. We can see from Fig.5(a) and (c) in linearly polarized case that the angular distribution becomes thinner and closer to the x axis, which indicates that in the multi-photon ionization is predominant in lower intensity whereas the tunnelling ionization is more important in higher intensity. But it is not necessary in circularly polarized case. Compared with different potentials, in linear case the angular distribution is more closer to the x-axis with exact potentials; in circularly polarized cases, the angular distribution is more symmetric and the value is larger with exact potentials. From Fig.5(b) and (d) we can see that the multi-photon process is still predominant even for higher intensity case, and the emission time of electrons is not the same with different potentials. This may due to the fact that in circularly polarized case the electron has a transverse momentum, so the electron is not likely to emit along the x axis anymore. Moreover, with different emission time of half cycle or a quarter cycle of laser pulse, the angular distribution is turn to right or left, respectively[24],

which can give us some useful information in angular distribution of double ionized electrons.

IV. CONCLUSIONS

In summary, we investigated the ionization dynamics of Mg atom in linearly and circularly polarized laser fields with different kinds of potentials, and compared them together. The non-sequential double ionization of Mg atom occurs in circularly polarized laser fields. To explain this phenomenon, we calculated the corresponding momentum distribution of electrons and the results shows that the momentum distribution presents the same tendency which transfer from a "V" shape to a cross structure with the increasing laser intensity in circularly polarized case. The corresponding double ionized NSDI and SDI trajectories are also presented. Moreover, the energy of ionized electron of Mg is investigated which also indicates there exsits the scattering of electrons. In addition, we also investigated the angular distribution of electrons in linearly and circularly polarized case with different potentials, and compared them together. The result shows the multi-photon process is still predominant even for higher intensity case, and the emission time of electrons is not the same with different potentials.

Acknowledgments

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