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

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The nonsequential double ionization (NSDI) of Mg atoms is investigated in both linearly and circularly polarized laser fields with different kinds of potentials. The numerical results indicate that the “knee” structure still exists in circularly polarized laser fields in the 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 atoms at the end of the pulse also shows that 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 the pulse with different kind of potentials to illustrate the difference in the double-ionization mechanism between the linearly and circularly polarized cases.

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I. INTRODUCTION

The nature of strong-field ionization processes is of both practical and fundamental interest [1–3]. The dynamics of simple systems, such as helium, has been studied thoroughly both theoretically and experimentally [4,5]. In earlier studies, Fittinghoff et al. [6] suggested a “shake-off” model where 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 where one electron ionizes first and revisits the core to set the second electron free by collision, which is widely accepted to explain nonsequential double ionization (NSDI). In general, NSDI seldom occurs in circular laser fields for most atoms, such as He and Li, because the perpendicular part of the laser field forces the electron to move away from the core and thus the recollision can’t occur. But numerical calculations and experimental research show that for Mg atoms the NSDI still occurs in circularly polarized laser fields at wavelengths of 800 nm [8,9], which attracts much interest in the study of the ionization dynamics of Mg atoms 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 has also been a hot topic recently but the dynamical origin of the NSDI in Mg atoms is 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 semiclassical or classical simulations are useful for treating strong-field ionization with very strong two-electron correlations, such as NSDI and nonsequential triple ionization (NSTI) [13–17].

In this paper, we investigate the double-ionization mechanisms of Mg in linearly and circularly polarized laser fields using the classical ensemble method with different kinds of potentials, and we compare them. We illustrate how NSDI happens in 800-nm circularly polarized laser fields. In particular, we investigate the corresponding momentum and position distribution of doubly ionized electrons to study the classical cutoffs for laser-induced NSDI. In addition, we also look into the dynamical signature of ionization dynamics with a specific form of electron yield and angular distribution.

II. THEORETICAL METHOD

We use the classical ensemble method to explore the ionization dynamics of a three-dimensional (3D) Mg atom in intense laser fields. Since it consists of 1s, 2s, 2p, and 3s orbitals and we consider only the electrons of the 3s orbital of the Mg atom, it is a simplified model for the Mg atom indeed. The electrons in the 3s orbital are much easier to ionize than others and also have the greatest contribution to the double-ionization process. This model of a Mg atom has 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)

$$H(r_1,r_2;P_1,P_2,t) = T(p) + V(q,t),$$

where the kinetic energy $T$ and the potential energy $V$ are given, respectively, by

$$T(p) = \frac{P_1^2}{2} + \frac{P_2^2}{2};$$

$$V(q,t) = -\sum_{i=1}^{2} \frac{2}{|r_i|} + \frac{1}{|r_1 - r_2|} + (r_1 + r_2)E(t).$$

In the above equations, $q = (r_1,r_2)$ stands for the positions of the two electrons, $p = (P_1,P_2)$ is for their corresponding conjugate momenta, and $E(t)$ is the laser field. Here we use the complex error function to get the exact Coulomb potential [18].
and we compare this with the corresponding results using soft core potentials [8]. The purpose of the soft Coulomb potentials is to move the singularity of the Coulomb potentials and avoid the autoionization states. The parameters are $a = 2.4$ a.u. and $b = 1.0$ a.u.

The canonical system of equations for the Mg atom is

$$\frac{dp}{dt} = -\frac{\partial V(q,t)}{\partial q},$$  \hspace{1cm} (4)

$$\frac{dq}{dt} = \frac{\partial T(p)}{\partial p}.$$  \hspace{1cm} (5)

We choose a set of initial stable states $\{\mathbf{r}_i(0),\mathbf{p}_i(0)\}_{i=1}^2$ using the Monte Carlo method and solve the above canonical equations numerically by the symplectic method in order to obtain the time evolutions of the corresponding electron positions 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 $V(q,t)$ and $T(p)$, and 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 results in a statistical manner. One particular atom’s two-electron motion is referred to as a trajectory. In our calculation, we assume the initial condition has the same energy approximately equal to the sum of the 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 the intense laser field. We define the energy of each electron as $E_i(t) = E_i + T_i$, where $E_i = \frac{p_i^2}{2m} - V(\mathbf{r}_i)$, and $T_i = \frac{p_i^2}{2m}$ is the kinetic energy. 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 $E_x(t) = E_0 f(t) \cos(\omega t)$ and $E_y(t) = E_0 f(t) \sin(\omega t)$. In this work, we utilize a microcanonical ensemble which consists of $1 \times 10^5$ two-electron “trajectories” and the time step is 0.05 a.u.

Figure 1 shows the double ionization probability of Mg as a function of laser intensity in linearly and circularly polarized laser fields with (a) the exact potential and (b) the soft core potential.

**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) the exact potential and (b) the soft core potential.

In order to further understand or identify the NSDI mechanism of Mg atoms in circularly polarized laser fields, we calculated the corresponding momentum and position distribution of the correlated electrons of Mg atoms in double-ionization processes as follows. We first present the momentum distribution of Mg atoms in linearly and circularly polarized laser fields with increasing laser intensity in Fig. 2. The Square presents the value of $2\sqrt{U}/p$. Figures 2(a) and 2(c) show in the linearly polarized case at first the momentum of two electrons distributed around the core and the value of the momentum distribution is no larger than $2\sqrt{U}/p$ [20], which means NSDI seldom occurs. As the intensity increases, the momentum distribution looks like a slim cross shape, which is the signature of RESI [11] (recollision excitation with subsequent tunneling ionization). We also can see from Figs. 2(b) and 2(d) that in the circularly polarized case the momentum distribution presents the same tendency, which transitions 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 is mainly distributed in the second and fourth quadrant, and in Figs. 2(b2) and 2(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 the circularly polarized case which means the RESI is predominant. When the laser intensity increases even more, the cross shape becomes thinner; in other words, the momentum of one electron is large and the other is small, which indicates that sequential double ionization is predominant in these circumstances. Interestingly, this momentum distribution is similar to that of the Ar case in Ref. [12]. We can also see from Fig. 2 that the cross shape
with the exact potential is more symmetric and thinner than that with the soft potential, which is probably due to the fact that the soft parameter can screen some interaction between the electrons and nucleus so that the tunneling process is more likely to occur in the exact potential case.

Recent research illustrates that both collision ionization (CI) and RESI have contributed to the NDSI process of Ar ionization in few-cycle laser fields [22], and their contributions are comparable to the Mg atom case. To further investigate this phenomenon, similar to Ref. [23], we calculate the 3D trajectories and corresponding energy distribution of electrons in the Mg atom as a function of time with exact potentials [(a) and (b)] and soft core potentials [(c) and (d)]. The laser wavelength is 800 nm.

Figure 4 shows the kinetic energy of ionized electrons of the 3D Mg atom at the end of the laser pulse in linearly and circularly polarized laser fields. The results show that the probability of the kinetic energy of ionized electrons becomes larger with the increasing intensity. Corresponding to Figs. 4(a)–4(d), the exact value of $U_p$ with increasing intensity is 5.3568, 8.928, 17.856, and 35.712 eV, respectively. In Fig. 4 we can see there are several electrons whose energy is greater than $2U_p$, which indicates that rescattering electrons still exist. Comparing Figs. 4(a) with 4(b), the greatest energy electrons can obtain is larger in linearly polarized cases than in circularly polarized cases, because the horizontal part of the...
FIG. 4. (Color online) The kinetic energy of ionized electrons of the 3D Mg atom at the end of the laser pulse in linearly and circularly polarized laser fields with exact potentials [(a) and (b)] and soft potentials [(c) and (d)]. Panels (a) and (c) show the linearly polarized case, and panels (b) and (d) show the circularly polarized case. The blue (circles), red (squares), green (pentagrams), and black (asterisks) lines correspond to 90, 150, 300, and 600 TW/cm², respectively.

circularly polarized case is smaller than that of the linearly polarized case. The probability of electrons in the high-energy regime is larger in the circularly polarized case than in the linearly polarized case, which also indicates that due to the perpendicular part of the circularly polarized case there are more electrons returning back to the core and rescattering, and the RESI more easily occurs in the circularly polarized case than in the linearly polarized case.

At last, since it is a 3D case, we wonder what is the difference of the angular distribution in the linearly and circularly polarized cases. Figure 5 shows the angular distribution of double-ionized electrons of the 3D Mg atom at the end of the laser pulse in linearly and circularly polarized laser fields with increasing laser intensity. We can see from Figs. 5(a) and 5(c) in the linearly polarized case that the angular distribution becomes thinner and closer to the x axis, which indicates that in the multiphoton process ionization is predominant at lower intensities whereas tunneling ionization is more important at higher intensities. However, this is not necessarily so in the circularly polarized case. Compared with different potentials, in the linear case the angular distribution is closer to the x axis with exact potentials; in the circularly polarized cases, the angular distribution is more symmetric and the value is larger with exact potentials. From Figs. 5(b) and 5(d) we can see that the multiphoton process is still predominant even for the higher intensity case, and the emission time of electrons is not the same with different potentials. This may be due to the fact that in the 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 times of a half cycle or a quarter cycle of the laser pulse, the angular distribution is turned to the right or the left, respectively [24], which can give us some useful information on the angular distribution of double-ionized electrons.

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

IV. CONCLUSIONS

In summary, we investigated the ionization dynamics of the Mg atom in linearly and circularly polarized laser fields with different kinds of potentials and compared them. The DSDI of Mg atoms 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 transitions from a “V” shape to a cross structure with the increasing laser intensity in the circularly polarized case. The corresponding NSDI and SDI trajectories are also presented. Moreover, the energy of ionized electrons of Mg is investigated which also indicates there exists the scattering of electrons. In addition, we also investigated the angular distributions of electrons in linearly and circularly polarized cases with different potentials and compared them. The results show the multi-photon process is still predominant even for the higher intensity case and the emission time of electrons is not the same with different potentials.
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