PHYSICAL REVIEW A **80**, 023408 (2009)

Nonsequential double ionization of Ne in an elliptically polarized intense laser field

XiaoLei Hao, GuanQi Wang, XinYan Jia, and WeiDong Li*
Department of Physics and Institute of Theoretical Physics, Shanxi University, 030006 Taiyuan, China

Jie Liu and J. Chen†
Center for Applied Physics and Technology, Peking University, 100084 Beijing, China
and Institute of Applied Physics and Computational Mathematics, P.O. Box 8009, 100088 Beijing, China

(Received 15 March 2009; published 12 August 2009)

A semiclassical model is developed to investigate the atomic nonsequential double-ionization process in elliptically polarized intense laser field. First, the ellipticity dependence of the ion yield of Ne^{2+} is calculated and a good agreement with the experiment observation is found. Second, the frequency dependence of the ratio of $Ne^{2+}:Ne^{+}$ is investigated for fields with different ellipticities. In the high-frequency regime, the ratio increases rapidly with increasing wavelength and is not dependent on the ellipticity. However, the ratio reaches maximum which decreases with increasing ellipticity and decreases with wavelength in the long-wavelength regime.

DOI: 10.1103/PhysRevA.80.023408 PACS number(s): 33.80.Rv, 34.50.Rk

I. INTRODUCTION

Among the abnormal phenomena in the field of the interaction between atoms and intense laser fields, the nonsequential double-ionization (NSDI) process has attracted more attention and has been intensively investigated in the past two decades [1–16]. Due to its complexity and difficulties in both experimental and theoretical investigations, the rescattering mechanism was established to correctly explain the enhanced double-ionization yield in the NSDI process after quite a long time debate [3–15]. The rescattering process can be understood from a simple quasiclassical notion: when an electron subject to a strong field has undergone a transition into continuum from its initial bound state, its motion is dominated by its interaction with the laser field. In the case of the linearly polarized laser field, when the field reverse its direction, majority of these electrons will be driven back into the vicinity of the ion core and undergo elastic or inelastic scattering, or recombine with the core and emit a high-energy photon [3]. It is commonly accepted that rescattering is responsible for many distinct experimental observations, such as the cutoff in high-order harmonic generation, a plateau formed by high-order above-threshold ionization peaks [17], and the singular angular distributions of the photoelectrons in the plateau regime [18–23].

According to the above rescattering picture, the ellipticity of the polarized field will have significant effect on the NSDI process since its perpendicular component will drive the first tunneled electron away from the nucleus, and then the collision probability with bound electron will be reduced. This picture has been confirmed by the experimental investigation of Dietrich *et al.* in which the NSDI yield decreases fast with increasing ellipticity of the laser field [24]. Watson *et al.* investigated the same problem using a two-dimensional quantum model [25]. Nevertheless, their result is not well consistent with the experimental observation [24] since the diffusion process of the electron might not be correctly described in the limited two-dimensional model [25]. The semiclassical model, first proposed by Corkum *et al.* [3,8], has been developed to study the NSDI and plays an important role in understanding the ion yield, recoil ion momentum distribution, and electron correlation [15]. More recently, it has been also extended to describe the NSDI process of molecules [26]. To our knowledge, the external laser field in the previous semiclassical model is limited to be linearly polarized except the one developed in most recent paper [27] by Shvetsov-Shilovski *et al.* However, this model is based on the strong-field approximation in which the influence of the ion potential on the electron's trajectory is not included, leading to incomplete description of the electrons' dynamics in the double-ionization process. So it is worthy to develop a more comprehensive approach in which the ion potential is explicitly considered to study the electrons' full dynamics in the NSDI process in elliptically polarized field [28]. This effort may also provide a powerful theoretical tool to study the electron dynamics in much wider configuration of external field, e.g., two-color field in which the directions of the fields are not parallel to each other.

II. THEORY

Following the same procedure of the previous semiclassical model [15], the ionization of the first outer electron from the bound state to the continuous state is described by quantum tunneling ionization theory [29]. The subsequent propagation of this ionized electron and the bound electron is governed by the classical dynamics, in which the motions of the two electrons are described by classical Newton equation: the motion of two electrons with different initial conditions in the combined Coulomb potential and the time-dependent intensity laser field. This classical motion equation can be expressed by (in atomic units $e=m=\hbar=1$)

*wdli@sxu.edu.cn
†chen_jing@iapcm.ac.cn

$$\frac{d^2\mathbf{r}_i}{dt^2} = \mathbf{E}(t) - \nabla(V^i_{ne} + V^i_{ee}). \quad (1)$$

where $\mathbf{E}(t)=(E_x(t),0,E_z(t))$ denotes the elliptically polarized intensity 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 tunneling ionized and bounded electrons, with ionization potentials I_{p1} and I_{p2}, are denoted by $i=1,2$, respectively. The Coulomb potentials are

$$V^i_{ne} = -\frac{2}{|\mathbf{r}_i|} \quad \text{and} \quad V^i_{ee} = \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}, \quad (2)$$

where $\mathbf{r}_i$ is the distance between the ith electron and the nucleus.

To solve Eq. (1), we have to know the initial conditions for the two electrons. Assuming the quasistatic approximation is valid for the tunneled electron under the condition that the ellipticity $\varepsilon \ll 1$, we can obtain its initial conditions along with the method in [15]. After rotating the z axis to the direction of the instantaneous external field, the tunneling process can be described by the following Schrödinger equation [29,30]:

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

in parabolic coordinates. Equation (3) describes the tunneling process for a single electron with energy $K=I_{p1}/4$ 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 $U(\eta)=K$ [29]. Its initial position and corresponding velocity are expressed as $x_{10}=-\frac{1}{2}\eta_0\sin\{arctg[\varepsilon tg(\omega t_0)]\}$, $y_{10}=0$, and $z_{10}=-\frac{1}{2}\eta_0\cos\{arctg[\varepsilon tg(\omega t_0)]\}$ and $v_x=v_{per}\cos\theta \times\cos\{arctg[\varepsilon tg(\omega t_0)]\}$, $v_y=v_{per}\sin\theta$, and $v_z=-v_{per}\cos\theta\sin\{arctg[\varepsilon tg(\omega t_0)]\}$ (where v_{per} is the transverse velocity perpendicular to the electric field and θ is the angle between v_{per} and x axis after rotation). The weight of each trajectory is evaluated by $w(t_0,v_{per})=w(0)\overline{w(1)}$ [29], where

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

$$\overline{w(1)} = v_{per}\frac{(2I_{p1})^{1/2}}{E\pi}\exp\left(-\frac{v^2_{per}(2I_{p1})^{1/2}}{E}\right). \quad (5)$$

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 [31].

III. RESULT AND DISCUSSION

A. Comparing with two-dimensional quantum simulation and experiment

First, let us consider the case of experimental observation in [24]. For Ne atom, the ionization potentials are $I_{p1}=0.7928$ a.u. (21.5646 eV) and $I_{p2}=1.506$ a.u. (40.964 eV). The parameters for the corresponding laser field are $I=0.9\times10^{15}$ W/cm^2 and $\omega=0.072\,22$ a.u. ($\lambda=625$ nm). 3×10^5 points are randomly distributed in the parameter volume $-\pi/2<\phi_0<\pi/2$, $v_{per}>0$, and $0<\theta<2\pi$, where $\phi_0=\omega t_0$ so that the weight of the chosen trajectory is large enough. Each trajectories is traced until the electron is actually ionized (e.g., $r_i>300$ a.u.). The double-ionization happened only when the energy of both electrons is greater than zero. The double-ionization cases found in our calculation vary from 30 to 1500, corresponding to the ellipticity of the laser field.

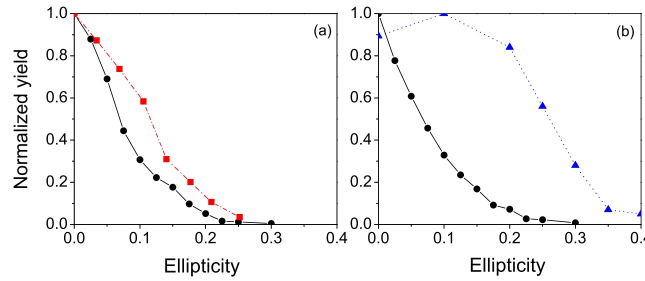

FIG. 1. (Color online) (a) Ellipticity dependence of the ion yield of Ne^{2+}. Dash-dot with square: experimental data of Dietrich [24]. (b) Ellipticity dependence of the ion yield of He^{2+}. Dot with triangle: result of Watson *et al.* [25]. Solid line with circle both in (a) and (b): our semiclassical calculations (the results are normalized).

The profile of the intensive laser pulse is taken as

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

where T is the optical period.

In Fig. 1(a), we show our calculation on the ion yield of Ne^{2+} as a function of the ellipticity of the laser field. The experimental data of Dietrich *et al.* [24] is included for comparison. It is found in Fig. 1(a) that our result is in good agreement with the experimental observation [24]. This result shows that the semiclassical model can be applied to understand the nature of this nonsequential double-ionization process under the elliptically polarized laser field. According to the rescattering picture of the NSDI, the fast drop of ion yield with increasing ellipticity depicted in Fig. 1 can be understood as the following notation: the tunneled electron when it is driven back by the z component of the external field is driven far away from the parent ion by the x component of the laser field, which increases with the increasing ellipticity. Therefore, the probability of the collision between the tunneled electron and its parent ion will be dramatically reduced, resulting in fast decreasing ion yield of Ne^{2+} with increasing ellipticity.

It is interesting to note that the same problem but for different atom (He) had been studied by Watson *et al.* using a two-dimensional quantum model [25]. To compare the current model with this two-dimensional quantum simulation, we take the same parameters as Ref. [25]. For He atom, I_{p1}

=0.905 a.u. (24.59 eV) and I_{p2}=2.004 a.u. (54.468 eV). The intensity of the laser is $I=0.35\times10^{15}$ W/cm^2 and the frequency is ω=0.064 47 a.u.(λ=700 nm). Following the same process as for the Ne atom, we calculate ion yield of He^{2+} as the function of the ellipticity of the laser field in Fig. 1(b). The two-dimensional quantum results are denoted as dot-triangle. It is easy to see that there is a clear difference between our result and the two-dimensional model's [25]. The reason of the difference between current model and the two-dimensional quantum model may be attributed to the fact that, in spite of its classical treatment of the two electrons' evolution, the diffusion of the electron wave packet is emulated in the semiclassical model by launching an assembly in the initial condition of the tunneled electron and the treatment is full dimensional. Nevertheless, the diffusion effect of the first electron when it moves in the external field, which has key importance in the description of the process in the elliptically polarized field, may not be depicted correctly in the two-dimensional approach.

B. Wavelength dependence of NSDI with different ellipticities

It is noteworthy that since the ponderomotive energy $U_p \propto I\lambda^2$, changing the wavelength is an effective way to change U_p, by which the Keldysh parameter $\gamma=\sqrt{I_p/2U_p}$ (where I_p is the ionization potential) is solely determined. In addition, change in the wavelength will also change the number of the photon necessary for ionization (I_p/ω). Therefore, the effect of the electronic structure and the electron-electron correlation should be sensitively probed by studying the wavelength dependence of double ionization, which has been demonstrated in both theoretical and experimental works performed recently [32,33]. In addition, it is worth to be noted that, as shown in the last section, the electron-electron correlation is also sensitive to the ellipticity of the laser field. Hence, it will be interesting to study the wavelength dependence of the NSDI with different ellipticities, from which more insight of the NSDI process may be unveiled, paving the way to control the atomic process via changing the parameters of the external field.

In the following, we study the frequency dependence of the ratio of Ne^{2+}:Ne^{+} with the help of this three-dimensional semiclassical model. The frequency dependence of the ratio of Ne^{2+}:Ne^{+} with different ellipticities is illustrated in Fig. 2. One can read from the Fig. 2 that the ratios first increase, reach a peak, and then drop with increasing wavelength (decreasing frequency). It is noteworthy that the value and position of the peak depend on ellipticity. For $\varepsilon \leq 0.2$, it appears around 200 nm, while for $\varepsilon=0.3$ it appears around 150 nm. The value of the peak decreases with increasing ellipticity.

Our result can be explained using the mechanism used to explain the frequency dependence in linearly polarized laser field [32]. In the view of the rescattering picture, there are two effects that determine the frequency dependence of NSDI [34]. One is the pondermotive energy. It decreases with decreasing wavelength, which will limit the possibility of NSDI for short wavelength. Another one is the diffusion of the electron wave packet, which determines the collision

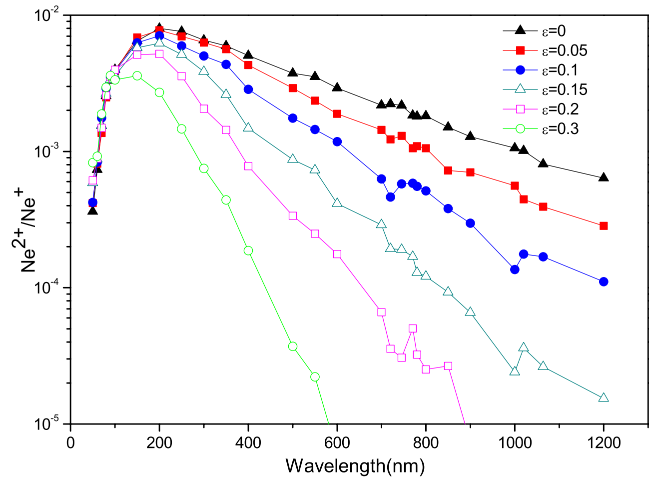

FIG. 2. (Color online) Wavelength dependence of the ratio of Ne^{2+}:Ne^{+} at different ellipticities. $I=1.0\times10^{15}$ W/cm^2.

probability when the tunneled electron returns to the core. In the short-wavelength regime, the quiver radius of the tunneled electron is small and hence the diffusion effect plays an insignificant role. In contrast, the fast increasing kinetic energy of the returned electron ($\sim\omega^{-2}$) increases the probability of excitation of the bound electron (NSDI occurs mainly via the so-called "delayed ionization" in the high-frequency regime [32]). Therefore the double-ionization yield increases fast with the wavelength. In the long-wavelength regime, the width of the wave packet of the first ionized electron at the rescattering moment spread wider since the electron will experience longer time before recollision. The longer the wavelength, the lower the probability of collision between the first electron and the core will be with the same initial condition [32]. In spite of that the kinetic energy of the tunneled electron increases with increasing wavelength, the cross section of the impact excitation and/or ionization of the second bound electron saturates and decreases when the energy of the impact electron is large [8]. Due to the above two effects, the ratio decreases as the wavelength decreases.

Since the pondermotive energy is the dominant aspect to determine the ratio in short-wavelength (high-frequency) regime where it occurs mainly through the so-called delayed ionization [32] and the quiver radius of the electron is small in this regime, resulting in the fact that the diffusion is not strongly influenced by the small ellipticity of the laser field ($\varepsilon \ll 1$ in our case), one can neglect the influence of different ellipticity of the laser field. So the lines with different ellipticities in Fig. 2 coincide with each other in short-wavelength regime. On the other hand, when the wavelength increases to where the quiver radius becomes large and diffusion starts to play important role, the ratio begins to saturate and then decreases with wavelength if the increase in the excitation probability due to the increasing ponderomotive energy cannot compensate the decrease in the collision probability due to the diffusion effect. Obviously, the effect of ellipticity on the decreasing collision probability will add to the diffusion effect. Therefore, the maximal value that the ratio can reach decreases with ellipticity. In addition, when the ellipticity is small ($\varepsilon \leq 0.2$ in our calculation), the ratios still reach peaks at almost the same wavelength. When the ellipticity increases further, the effect of the perpendicular component of the field reduces the recollision probability more significantly and makes the ratio reach a peak at even shorter wavelength as shown in our calculation.

IV. CONCLUSION

In conclusion, we develop a semiclassical model to investigate the NSDI process in elliptically polarized intense laser field. First, the ellipticity dependence of the ion yield of Ne^{2+} is studied. It is found that the results are well consistent with the experiment observation, and it can be satisfactorily explained by the rescattering mechanism of the NSDI process. Calculation for He atom is also performed and obvious discrepancy from a two-dimensional quantum calculation is found. Second, the frequency dependence of the ratio of $Ne^{2+}:Ne^{+}$ is investigated for fields with different ellipticities. In the high-frequency regime, the ratio increases with increasing wavelength and is not dependent on the ellipticity. However, the position and value of the peak in ratio is dependent on the ellipticity of the laser field. When $\varepsilon \leq 0.2$, the ratio reaches maximum at almost the same wavelength as in the linear polarized field but the maximal value decreases with ellipticity. When the ellipticity increases further, the position of the peak shifts to shorter wavelength and the maximal value decreases further. The larger the ellipticity, the shorter wavelength at which the ratio begins to decrease and the lower maximum which the ratio can reach. In the long-wavelength regime, all ratios decrease monotonously with wavelength and the slope of the curves increases with ellipticity. Further examination of our calculations should be made in comparison with future experiments and quantum-mechanical calculations.

ACKNOWLEDGMENTS

This work was supported by the National Natural Science Foundation of China under Grants No. 10574019 and No. 10674087, the National Basic Research Program of China under Grants No. 2006CB806000 and No. 2006CB921603, ICF research fund under Grant No. 2008AA8040022, and CAEP Foundation under Grants No. 2006z0202 and No. 2008B0102007.

[1] A. l'Huillier, L. A. Lompre, G. Mainfray, and C. Manus, Phys. Rev. A **27**, 2503 (1983).
[2] D. N. Fittinghoff, P. R. Bolton, B. Chang, and K. C. Kulander, Phys. Rev. Lett. **69**, 2642 (1992).
[3] P. B. Corkum, Phys. Rev. Lett. **71**, 1994 (1993).
[4] B. Walker, B. Sheehy, L. F. DiMauro, P. Agostini, K. J. Schafer, and K. C. Kulander, Phys. Rev. Lett. **73**, 1227 (1994).
[5] K. C. Kulander, J. Cooper, and K. J. Schafer, Phys. Rev. A **51**, 561 (1995).
[6] D. N. Fittinghoff, P. R. Bolton, B. Chang, and K. C. Kulander, Phys. Rev. A **49**, 2174 (1994).
[7] M. Yu. Kuchiev, J. Phys. B **28**, 5093 (1995).
[8] T. Brabec, M. Y. Ivanov, and P. B. Corkum, Phys. Rev. A **54**, R2551 (1996).
[9] A. Becker and F. H. M. Faisal, J. Phys. B **32**, L335 (1999).
[10] W. C. Liu, J. H. Eberly, S. L. Haan, and R. Grobe, Phys. Rev. Lett. **83**, 520 (1999).
[11] Th. Weber *et al.*, Phys. Rev. Lett. **84**, 443 (2000).
[12] R. Moshammer *et al.*, Phys. Rev. Lett. **84**, 447 (2000).
[13] A. Becker and F. H. M. Faisal, Phys. Rev. Lett. **84**, 3546 (2000).
[14] M. Lein, E. K. U. Gross, and V. Engel, Phys. Rev. Lett. **85**, 4707 (2000).
[15] J. Chen, J. Liu, L. B. Fu, and W. M. Zheng, Phys. Rev. A **63**, 011404(R) (2000); L. B. Fu, J. Liu, J. Chen, and S. G. Chen, *ibid.* **63**, 043416 (2001); L. B. Fu, J. Liu, and S. G. Chen, *ibid.* **65**, 021406(R) (2002); J. Chen and C. H. Nam, *ibid.* **66**, 053415 (2002); D. F. Ye, X. Liu, and J. Liu, Phys. Rev. Lett. **101**, 233003 (2008).
[16] Phay J. Ho, R. Panfili, S. L. Haan, and J. H. Eberly, Phys. Rev. Lett. **94**, 093002 (2005); Phay J. Ho and J. H. Eberly, *ibid.* **95**, 193002 (2005); **97**, 083001 (2006).
[17] J. L. Krause, K. J. Schafer, and K. C. Kulander, Phys. Rev. Lett. **68**, 3535 (1992).
[18] G. G. Paulus *et al.*, J. Phys. B **29**, L249 (1996).
[19] W. Becker, A. Lohr, and M. Kleber, J. Phys. B **27**, L325 (1994).
[20] M. Lewenstein, K. C. Kulander, K. J. Schafer, and P. H. Bucksbaum, Phys. Rev. A **51**, 1495 (1995).
[21] D. Bao, S. G. Chen, and J. Liu, Appl. Phys. B: Lasers Opt. **62**, 313 (1996).
[22] B. Hu, J. Liu, and S. G. Chen, Phys. Lett. A **236**, 533 (1997).
[23] J. Chen, J. Liu, and S. G. Chen, Phys. Rev. A **61**, 033402 (2000).
[24] P. Dietrich, N. H. Burnett, M. Ivanov, and P. B. Corkum, Phys. Rev. A **50**, R3585 (1994).
[25] J. B. Watson, K. Burnett, and P. L. Knight, J. Phys. B **33**, L103 (2000).
[26] J. Chen, J. Fan, Y. Li, and S. P. Yang, Phys. Rev. A **76**, 013418 (2007); Y. Li, J. Chen, S. P. Yang, and J. Liu, *ibid.* **76**, 023401 (2007); J. Liu, D. F. Ye, J. Chen, and X. Liu, Phys. Rev. Lett. **99**, 013003 (2007); D. F. Ye, J. Chen, and J. Liu, Phys. Rev. A **77**, 013403 (2008).
[27] N. I. Shvetsov-Shilovski, S. P. Goreslavski, S. V. Popruzhenko, and W. Becker, Phys. Rev. A **77**, 063405 (2008).
[28] Different from the semiclassical model of Ref. [15], the model of Ref. [16] is a pure-classical theory in which the whole process is described by Newtonian equations, so it can be easily applied to elliptically polarized laser field without further modification. However, the quantum aspect of the process-tunneling ionization of the first electron is not included in this model.
[29] N. B. Delone and V. P. Krainov, J. Opt. Soc. Am. B **8**, 1207 (1991).

[30] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon, New York, 1977).
[31] J. S. Cohen, Phys. Rev. A **26**, 3008 (1982).
[32] J. Chen, J. H. Kim, and C. H. Nam, J. Phys. B **36**, 691 (2003).
[33] P. Kaminski, R. Wiehle, W. Kamke, H. Helm, and B. Witzel, Phys. Rev. A **73**, 013413 (2006).
[34] S. Larochelle *et al.*, J. Phys. B **31**, 1201 (1998).