V-LIKE STRUCTURE IN THE CORRELATED ELECTRON MOMENTUM DISTRIBUTION FOR NONSEQUENTIAL DOUBLE IONIZATION OF HELIUM

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ABSTRACT

We investigate the nonsequential double ionization process of He atom by using classical three-dimensional ensemble model. The result shows that a pronounced V-like structure is exhibited in the two-electron momentum distribution along the laser polarization axis. At high laser intensity, this structure which was observed experimentally [Phys. Rev. Lett. ***99****, 263003 (2007)] can be explained by the asymmetric energy sharing of two electrons at recollision process.*

Keywords: He atom, recolliding electron, bound electron, nonsequential double ionization.

TÓM TẮT

Cấu trúc chữ V trong phân bố động lượng tương quan electron đối với quá trình ion hóa kép không liên tục của He

Chúng tôi khảo sát quá trình ion hóa kép không liên tục của nguyên tử He bằng mô hình tập hợp ba chiều. Kết quả cho thấy cấu trúc chữ V trong phân bố động lượng tương quan của hai electron dọc theo trục phân cực của laser được thể hiện rõ nét. Đối với laser cường độ cao, cấu trúc này đã được quan sát bằng thực nghiệm [Phys. Rev. Lett. ***99****, 263003 (2007)] và có thể được giải thích dựa vào sự phân bố năng lượng bất đối xứng giữa hai electron khi xảy ra quá trình tái va chạm.*

Từ khóa: nguyên tử He, electron tái va chạm, electron liên kết, ion hóa kép không liên tục.

1. Introduction

When an atom or a molecule is exposed to the laser field, the electron can be ionized, after some moment the second electron can be set free from its parent ion, this is double ionization (DI) process. Strong-field DI process can be classified into two different mechanisms: sequential DI and nonsequential DI (NSDI). In case of linear polarized and sufficiently high intensity laser field, DI is dominated by the nonsequential process. NSDI of atoms and molecules by intense laser field has drawn extensive study for more than three decades since it provides a profound understanding

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of laser-matter interaction [1] and a uniquely clean example of electron-electron (*e-e*) correlation [8] (see also [2] for a full review). Most of the experimental findings indicate that the NSDI process can be well understood by the quasiclassical rescattering model [3]. In this model, the first electron is dislodged near the peak of the oscillating electric field, then is driven back to its parent ion when the field changes its sign, and ionizes the second electron through recollision process. Although the recollision model describes the NSDI process clearly, the details of recollision remain obscure. Throughout this paper we refer the first and second ionized electron as recolliding and bound electron, respectively.

We are aware of the experiment done by A. Rudenko *et al.* in 2007 [8] on NSDI of He by 25 fs 800 nm laser pulses at 1,5 PW/cm^2. In this experiment, a V-like structure was observed in the correlated two-electron momentum distribution (CTEMD) which is in contrast with earlier experimental results, but in agreement with various theoretical predictions [5, 9]. For relatively low laser intensity, these theoretical studies considered the nuclear attraction [5] and final-state electron repulsion [9] as the root of this V-like structure. However, for sufficiently high laser intensity, it is questionable whether the responsible microscopic dynamics for the V-like structure is similar to that at the relatively low laser intensity.

For understanding the origin of such V-like structure at sufficiently high laser intensity, in this paper we use the classical three-dimensional ensemble model proposed by S. L. Haan in 2001 [6]. The advantage of the classical calculation over the full-quantum consideration is that it can provide the intuitive picture for the trajectory of individual electron evolving in the laser field [4]. Our simulation well reproduces the V-like structure in the CTEMD along the laser polarization direction. We found that for sufficiently high intensity, means 2 PW/cm^2 and 5 PW/cm^2, neither the Coulomb attraction nor the final-state electron repulsion is responsible to the V-like structure. It is the asymmetric energy sharing between recolliding and bound electrons during the recollision process that plays decisive role in forming such structure in CTEMD. For deeply investigate the microscopic dynamics for the V-like shape, the back analysis for individual electron's trajectory is needed also in the transverse plane with respect to the direction of the laser field. However, this investigation is tedious, thus we postpone it to the future study.

The paper is organized as follows. In section 2, we introduce the classical ensemble model. In section 3, we present and discuss the numerical results for the CTEMD for NSDI of He by 800nm, 2PW/cm^2 and 5PW/cm^2. Section 4 concludes the paper.

2. The classical ensemble model

Since being introduced from 2001 [6], the three-dimensional ensemble model is considered to be a powerful approach in studying strong-field DI. The reliability of this method versus full quantum calculation is introduced in [4, 6]. Within the classical model, the evolution of the two-electron system is governed by Newton's classical equations of motion (atomic units are used throughout this paper)

$$\frac{d^2\vec{r}_i}{dt^2} = -\vec{\nabla}\left[V_{ne}\left(r_i\right) + V_{ee}\left(r_1, r_2\right)\right] - \vec{E}\left(t\right), \tag{1}$$

where subscript i is the label of the two electrons, and $\vec{E}(t)$ is the electric field, which is chosen to be linearly polarized along the x axis and has a trapezoidal pulse shape with ten optical cycle including two-cycle turn on, six cycle at full strength, and two-cycle turn off. Here $V_{ne}\left(r_i\right)$ is the ion-electron attractive potential

$$V_{ne}\left(r_i\right) = -\frac{2}{\sqrt{r_i^2 + a}}, \tag{2}$$

and the *e*-*e* repulsive potential has the form

$$V_{ee}\left(r_1, r_2\right) = \frac{1}{\sqrt{\left(r_1 - r_2\right)^2 + b}}. \tag{3}$$

Note that in classical calculation, the real Coulomb potential of the nucleus makes the calculation much more challenging since our model is unstable against autoionization [4]. Thus the soft-core Coulomb potential is considered. This potential is widely used in study of strong-field ionization without loss of physical properties [4, 6, 7, 10]. In our calculation, the soft parameter a is set to 0,75 for avoiding autoionization and b is set to 0,01 [4, 10].

To solve equation (1), we need to specify the initial conditions. In classical model, atom is characterized solely by the ionization energy. Thus we set the whole ensemble be populated at a classically allowed position for the helium ground-state energy of -2,9035 a.u. The available kinetic energy is randomly distributed between the two electrons in momentum space. Then these electrons are allowed to evolve in sufficiently long time without the influence of the laser field to obtain the stable positions and momentum distributions [10]. This is the required initial condition. After determining the initial condition, we solve the above equation for each atom independently in the existence of laser field. Such ordinary differential problem (equation (1)) can straightforwardly be solved using Runge-Kutta method [11]. At the end of the pulse, the energies of two electrons in each atom are calculated and analyzed as

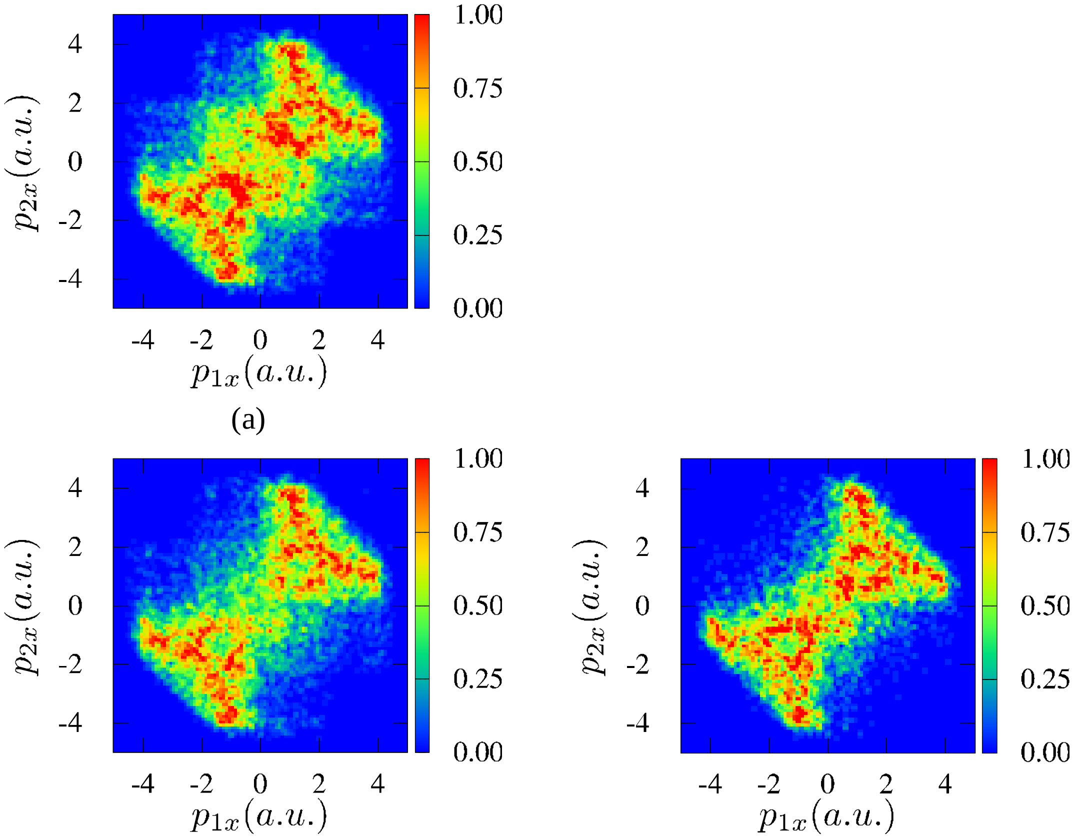
$$E_1 = \frac{v_{x1}^2}{2} + \frac{v_{y1}^2}{2} + \frac{v_{z1}^2}{2} - \frac{1}{\sqrt{x_1^2 + y_1^2 + z_1^2 + a}} + \frac{1}{2\sqrt{(\mathrm{x}_1 - \mathrm{x}_2)^2 + (\mathrm{y}_1 - y_2)^2 + (\mathrm{z}_1 - \mathrm{z}_2)^2 + b}}, \tag{4a}$$

$$E_2 = \frac{v_{x2}^2}{2} + \frac{v_{y2}^2}{2} + \frac{v_{z2}^2}{2} - \frac{1}{\sqrt{x_2^2 + y_2^2 + z_2^2 + a}} + \frac{1}{2\sqrt{(\mathrm{x}_1 - \mathrm{x}_2)^2 + (\mathrm{y}_1 - y_2)^2 + (\mathrm{z}_1 - \mathrm{z}_2)^2 + b}}, \tag{4b}$$

where x_i, y_i, z_i and v_{xi}, v_{yi}, v_{zi} are the drift positions and velocities of electron i in Cartesian coordinates, respectively. The atom is considered to be doubly ionized only if the energies of both electrons are positive [4, 10]. We note that in the framework of classical consideration, both electrons are ionized by over-the-barrier mechanism and no tunneling ionization occurs. In order to obtain statistically stable results, we use ensemble sizes as millions of atoms.

3. Illustrative results and discussion

We proceed to illustrate the numerical results for the correlated electron momentum distribution in the DI process of He. The lasers used in this paper have wavelength of 800 nm. We consider high intensity laser pulses in two cases: 2.10^{15} W/cm^2 and 5.10^{15} W/cm^2.



(a)

(b)

(c)

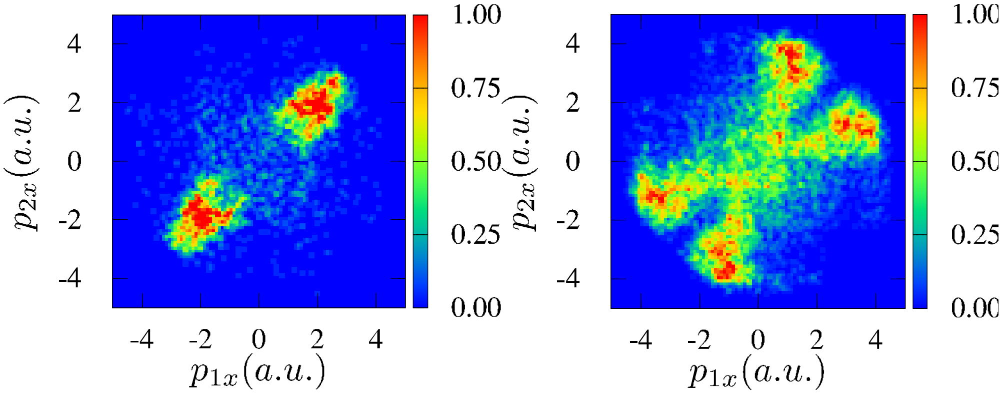
Figure 1. *Correlated electron momentum distributions along the laser's polarization axis for 800 nm, 2 PW/cm^2 laser pulse: (a) for total DI events, (b) for DI events excluding those occur at the turn-on stage of the trapezoidal pulse, (c) for DI events when neglecting the final state e-e repulsion. The ensemble sizes are 10^6 atoms.*

Figure 1 shows the CTEMD in the direction parallel to the laser polarization, where the laser intensity is 2.10^{15} W/cm^2. Figure 1(a) presents the obviously overall V-like shape observed experimentally in [8]. Nevertheless, a cluster of distribution around the origin which is different from experimental data is clearly seen. This fact is straightforwardly understood. Back analysis [4] indicates that these signals stem from the trajectories where DI events occur at the turn-on stage of the laser field. For the soft parameters used in our calculation, the first electron can be ionized easily at the turn-on stage of the pulse, it also returns to recollide with the parent ion leading to the second ionization at this stage. This effect results in unexpected contribution to the CTEMD as stated above. In order to focus on the high intensity regime, we exclude the events in which DIs occur at the early stage of the laser pulse and present in figure 1(b). The CTEMD now well coincides with the experimental data in [8]. Note that the V-like shape is obvious even though the soft parameter *a* used in calculation is as large as 0,75. We attempted to execute the calculations for smaller *a*, there is no noticeable discrepancy can be observed. For that reason, we bypass to present such results in this paper. This fact states that the nuclear attraction plays no role in forming the V-like shape in CTEMD which is in contrast with the previous conclusion in [5, 8, 9] for the relatively low intensity laser pulse.

For investigating the role of final state *e-e* repulsion in forming V-like shape at high intensity laser field, we performed additional calculation in which the final state *e-e* interaction in equation (3) is replaced by the screening Yukawa interacting potential as

$$V'_{ee}\left(r_1,r_2\right)=\frac{1}{\sqrt{\left(r_1-r_2\right)^2+b}}\exp\left(-\lambda\sqrt{\left(r_1-r_2\right)^2+b}\right), \qquad (4)$$

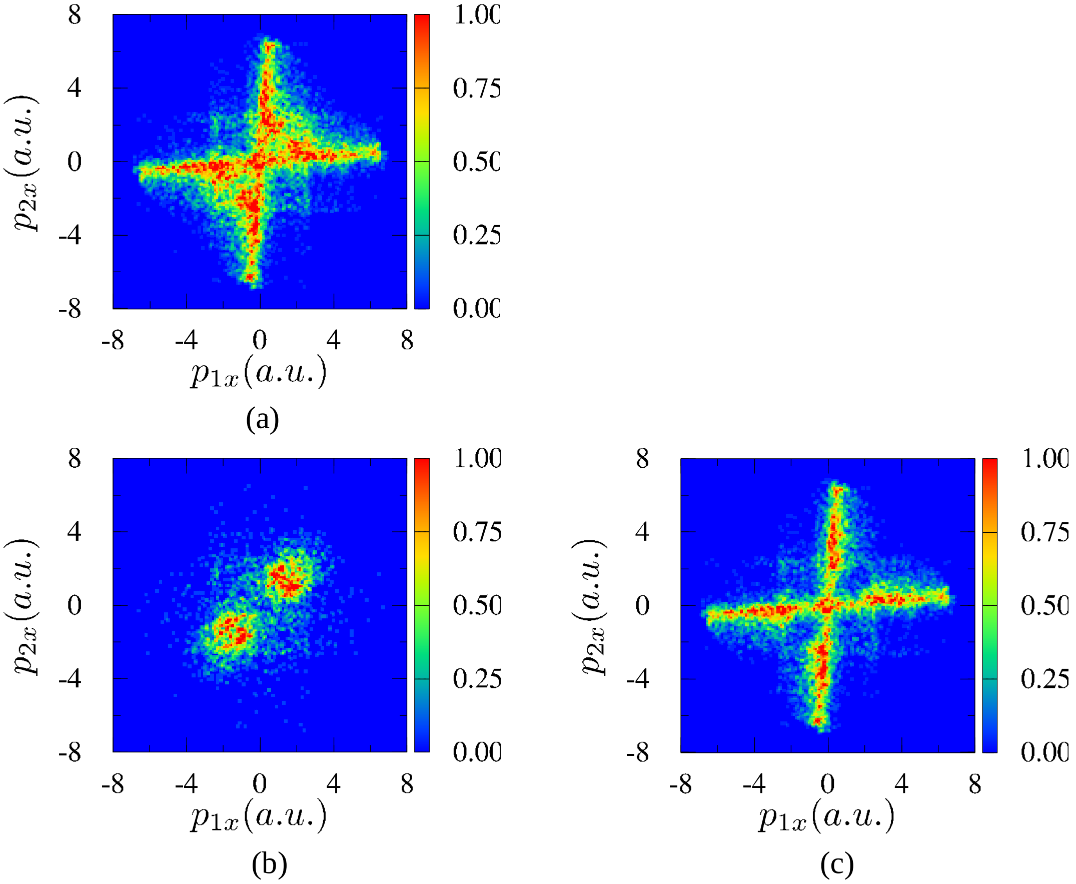
here the screening factor $\lambda=5$ is large enough to make the effective interaction between two electrons rapidly decreases [10]. As can be seen in figure 1(c), the V-like shape still exists and there is almost no different from figure 1(b). This is convincing evidence showing that for sufficiently high intensity laser field, the final state *e-e* interaction is not responsible to V-like structure in CTEMD.



(a) (b)

Figure 2. *Correlated longitudinal electron momentum distributions for the trajectories where the energy different between two electrons just after recollision is (a) smaller than 1 a.u. and (b) larger than 1 a.u.*

In order to explore the root of V-like structure. We again use back analysis technique to trace the evolution of electrons in the influence of laser field. Tracing process allows us to determine all essential quantities of the DI process such as the recollision time and the energy exchange between recolliding and bound electrons [4, 10] during recollision. Note that the recollision time is defined as the instant when the distance between first ionized electron and its parent ion approach to minimum. Here we separate the trajectories into two different mechanisms: symmetric and asymmetric energy sharing and introduce in figure 2. We set the critical energy discrepancy equal to 1 a.u. which is sufficiently small to classify these two mechanisms. Figure 2(a) and 2(b) portray the CTEMD of the trajectories where two electrons have approximately similar and much different energy after recollision, respectively. They correspond to symmetric and asymmetric energy sharing, respectively. It is clear that in case of symmetric energy sharing (SES), the ionized electrons have similar drift momenta, thus the events are clustered on the main diagonal as in figure 2(a). In contrast, the final momenta of these two electrons are much different when asymmetric energy sharing (AES) happens, and off-diagonal features can be obviously observed in figure 2(b). Based on these results, we can conclude that the AES during recollision is the decisive reason for the V-like shape in the CTEMD. The root of AES in high intensity laser regime is obvious. According to the simple-man model [3], at the relatively low laser intensity, due to the lower recolliding energy, the recolliding electron passes the core with a small velocity, thus the time of the *e-e* interaction is long enough for the recolliding electron to transfer a considerable part of its energy to the bound electron through *e-e* interaction. Therefore the contribution of SES to the V-like structure is noticeable. However, at the high laser intensity, the short *e-e* interaction time leads to the low-energy exchange efficacy at recollision, which makes AES plays important role in forming such finger-like shape in the CTEMD.



(a)

(b)

(c)

Figure 3. *Correlated electron momentum distributions along the laser's polarization axis for 800 nm, 5 PW/cm^2 laser pulse: (a) for DI events excluding those occur at the turn-on stage of the trapezoidal pulse, for the trajectories where the energy different between two electrons just after recollision is (b) smaller than 1 a.u. and (c) larger than 1 a.u.*

We proceed to similar investigation for higher intensity laser field in order to reconfirming our finding. Figure 3 shows the result for CTEMD using laser intensity of 5.10^{15} W/cm^2. Note that in figure 3(a) the DI events at the turn-on stage of the laser are excluded. Obviously, we can observe the more pronounced V-like structure in the CTEMD. The events in the present case are clustered nearer to ray $p_{1x}=0$ or $p_{2x}=0$ in compare to those in case of 2.10^{15} W/cm^2 (See figure 1(b)). It indicates that the final momenta of two ionized electrons are much more different. Since under the influence of stronger electric field, the recolliding electron passes the core with larger velocity in comparison to that of previous calculation, and thus the time of *e-e* interaction is shorter leading to the lower-energy exchange at the recollision. That also makes AES play dominant role in forming the V-like structure in the CTEMD. Figures 3(b) and 3(c) show identical analysis as in figure 2 and reconfirm our conclusion in the above discussion.

4. Conclusion

In this paper, we introduce the three-dimensional classical ensemble model in the study of DI process. By using this method, we can reproduce the V-like structure in the CTEMD observed experimentally [8]. Back analysis indicates that neither nuclear attraction nor final state *e-e* repulsion is the origin of this V-like shape. Indeed these features are important in case of sufficiently low intensity laser pulse [4, 9]. For high intensity fields used in this paper, our analysis demonstrates that the origin of such V-like structure is the asymmetric energy sharing between recolliding and bound electrons during recollision process. It is instructive to note that in order to deeply study the dynamic of recollision process, one needs more analysis also for the perpendicular momenta with respect to the direction of the laser polarization axis. As stated in the Introduction part, such analysis is time-consuming, thus we let it for the next project.

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(Received: 20/3/2015; Revised: 14/5/2015; Accepted: 18/5/2015)