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

TRUONG DANG HOAI THU[*], PHAM NGUYEN THANH VINH[**]

ABSTRACT

In this paper, we deeply investigate the evolution of the ionized electrons of He in laser field by trajectory-analysis method to understand the physical dynamics of the asymmetric energy sharing process. The results show that the discrepancy in transverse momentum spectra of the recolliding and bound electrons not only serves as a signature of this process, but provides insight into the attosecond three-body interactions.

Keywords: nonsequential process, double ionization, classical ensemble model, asymmetric energy sharing, transverse momentum distribution.

TÓM TẮT

Phép phân tích quỹ đạo cho việc giải thích cấu trúc chữ V trong phân bố động lượng tương quan electron đối với quá trình ion hóa kép không liên tục của Heli

Trong bài báo này, chúng tôi khảo sát sâu hơn vào quá trình chuyển động của các electron ion hóa của He trong trường laser bằng phương pháp phân tích quỹ đạo nhằm hiểu hơn về vấn đề động học vật lí của quá trình phân bố năng lượng bất đối xứng. Kết quả cho thấy sự khác nhau trong phân bố động lượng vuông góc của electron tái va chạm và electron liên kết không chỉ đóng vai trò như dấu hiệu nhận biết của quá trình này mà còn cung cấp cái nhìn sâu hơn về quá trình tương tác ba vật thể trong khung thời gian 10^{-18} giây.

Từ khóa: quá trình không liên tục, ion hóa kép, mô hình tập hợp cổ điển, phân bố năng lượng bất đối xứng, phân bố động lượng vuông góc.

1. Introduction

In recent years, the non-linear phenomena induced by intense laser field have drawn extensive interests since they provide a striking understanding of laser-matter interaction [1]. Among them, nonsequential double ionization (NSDI) process is considered as a complementary for clean scenery of electron-electron (*e*-*e*) correlation [8] (see also [2] for further information). This process is well understood by the quasiclassical rescattering model known as so-called three-step model. In this model,

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the first electron escapes the atom by quantum tunneling through a finite barrier induced by the external electric field, then is forced by the laser away from and then back to the core where a recollision process liberates both electrons at once. There are several approaches to this problem. The first one is quantum consideration using the exact solutions from solving the time-dependent Schrödinger equation, the second approach is based on classical model in which the individual particle is propagated under solely the influence of the oscillating laser field. Haan *et al.* indicated that under specific ranges of laser fields, the results from classical model are in good consistency to those using quantum calculations [6]. The advantages of the classical calculation over the full-quantum consideration are: (i) the entire process of double ionization can be easily calculated from beginning to the end of the pulse, and (ii) at any time, individual double ionization trajectories can be back analyzed to extract insight into their dynamic. [5]

By using the classical ensemble model proposed by Haan *et al.* [6], recently we can reproduce the experimentally observable V-like structure [9] in the correlated two-electron momentum distribution (CTEMD) which is in contrast with earlier experimental results [8]. Our study indicated that in case of sufficiently high laser intensity, the root of V-like structure is the asymmetric energy sharing (AES) between recolliding and bound electrons during recollision process. Indeed, for relatively low laser intensity, the nuclear attraction [5] and final-state electron repulsion [10] play dominant role in forming V-like structure. Note that in [9] we used linearly polarized laser at high intensity of 2 PW/cm^2 for avoiding the contamination from sequential ionization process where two electrons are dislodged from the ion core without any recollision. Although the origin of V-like structure in CTEMD was thoroughly discussed in [9], the microscopic dynamics of the AES process still deserve further consideration. Thus in this paper we provide the trajectory analysis to deeply understand the physics beneath the AES process which forms the V-like structure in CTEMD. We figure out that the AES leaves footprints on the transverse momentum distribution (TMD) spectra which also provide insight into the attosecond three-body interactions.

The paper is organized as follows. In section 2, we briefly introduce the classical ensemble model. More details of this model can be referred to our previous article [9]. In section 3, we present and discuss the numerical results from the trajectory analysis to deeply understand the dynamic of AES for NSDI of He by 800nm, 2PW/cm^2. Section 4 concludes the paper.

2. Three-dimension classical ensemble model

The classical model has been successfully used for understanding NSDI in high intensity regime since being proposed in 2001 [6]. The validity of this approach was discussed previously in [5, 6]. In the classical model, the evolution of the two-electron system is determined by the classical equation of motion (atomic units are used throughout this paper)

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

where subscript i is the electron label running from 1 to 2, and $\mathbf{E}(t)$ is the electric field chosen to be linearly polarized along the x axis. In order to focus on the NSDI process induced by high intensity regime of laser field, we also use trapezoidal pulse shape of laser field with ten optical cycles including two-cycle turn on, six cycles at full strength, and two-cycle turn off. The potentials are

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

and

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

representing ion-electron and electron-electron interaction, respectively. Note that the soft-core Coulomb potential widely used in study of strong-field ionization [5, 6, 7, 11] is considered for avoiding autoionization made by the infinitely deep Coulomb potential of the nucleus. In this paper, the soft parameters *a* and *b* are set to 0,75 and 0,01, respectively, in consistent with our previous study [9] to avoid autoionization. [5, 11]

To obtain the initial value, the ensemble is populated starting from a classically allowed position for the helium ground-state energy of -2,9035 a.u. The available kinetic energy is distributed between the two electrons randomly in momentum space. Then the electrons are allowed to evolve a sufficient long time (100 a.u.) in the absence of the laser field to obtain stable position and momentum distribution [11]. Having this initial condition, we numerically solve equation (1) for individual atom in the influence of the laser field by using well-known Runge-Kutta method [12]. Then the energies of two electrons in each atom are analyzed at the end of the pulse. The atom is considered to be double ionization only if the energies of both electrons are positive [5, 11] (read [9] for more details). We note that in the framework of the classical model, no tunneling ionization occurs; the electrons are ionized by over-the-barrier mechanism.

3. Numerical results and discussion

It is instructive to recall in figure 1 the V-like structure in CTEMD (top panel) together with the CTEMD for two cases: symmetric energy sharing (SES) (bottom left panel) and AES (bottom right panel) during recollision process for demonstration the role of AES in forming such structure. We note that at high laser intensity used in this paper (i.e. 2PW/cm2), to obtain the CTEMD which is symmetry with respect to the secondary diagonal, we operate two calculations using two laser pulses whose carrier envelope phases are π different, then do the superposition of these data. Since in case of trapezoidal laser pulse, the first electron is too easy to be ionized, thus most of the double ionization events occur at the first half cycle of the platform of laser pulse.

For classifying SES and AES mechanisms, we set the critical energy discrepancy just after recollision equal to 1 a.u. which is sufficiently small. Note that in [11], the authors claimed that critical energy to be 2 a.u. for such classification which is not appropriate to separate the signals from SES and AES in our opinion. Indeed we have checked and confirmed that the discrepancy between SES and AES (figures 1(b) and 1(c)) is not obvious by using the suggested value in [11]. Thus we come to the decision to use critical energy as 1 a.u.

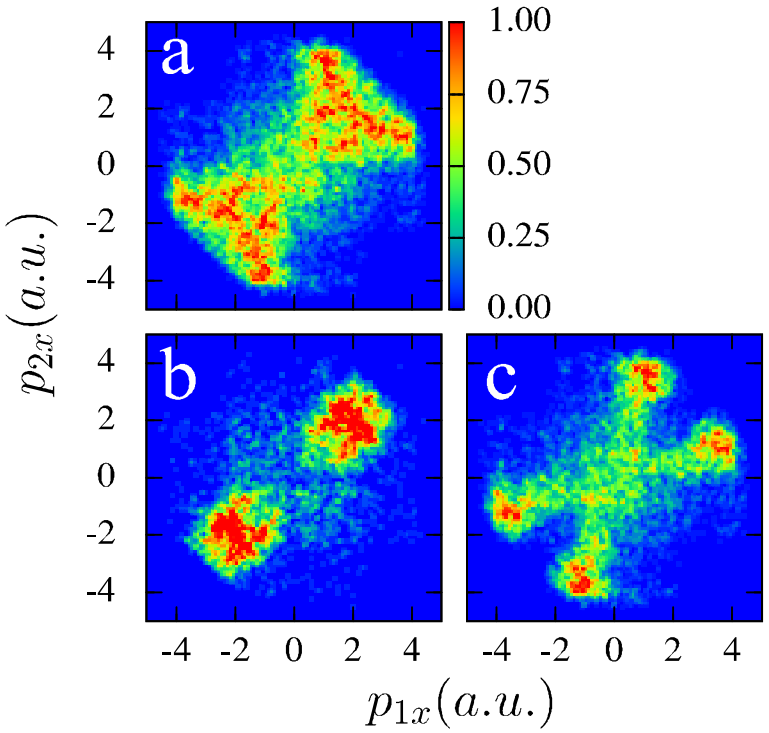

Fig 1. *CTEMD along the laser's polarization axis for 800 nm, 2 PW/cm^2 laser pulse: for all DI events (a), for the trajectories where the energy different between two electrons just after recollision is smaller than 1 a.u. (b) and larger than 1 a.u. (c)*

It is clear that in case of SES, the ionized electrons have similar drift momenta, thus the signals are concentrated to the main diagonal as in figure 1(b). In contrast, the final momenta of these two electrons are much different when AES happens resulting in off-diagonal distribution in figure 2(b).

In order to further understand the AES, we present in figure 2 the count of DI trajectories with respect to the laser phase at recollision by using trajectory back analysis [5]. The results show that for SES (figure 2(a)), recollisions occur close to the extremum of the field, while for AES (figure. 2(b)), recollisions happen around the zero crossing of the field. According to the simple-man model [4], the electrons with the maximal recolliding energy return to the ion core near the zero crossing of the laser field, while those returning to the core near the extremum of the field have much lower recolliding energy. Thus our results are in good agreement with this model. We found that in case of high intensity used in our calculation, more than 75% of DI trajectories are favorable to the AES situation. The percentage of electrons corresponding to AES situation grows with the increasing in laser intensity. In AES case, the returning electron has large energy and passes the core so quickly, thus the *e-e* interaction time is so short that the recolliding electron can transfer only a small part of its energy to the bound electron, resulting in the AES at high laser intensity. Note that for sufficiently low laser intensity, the recolliding electron has much lower energy, and the *e-e* interaction time is long enough, hence AES is no longer dominant in forming the V-like shape in CTEMD. [5, 8, 10]

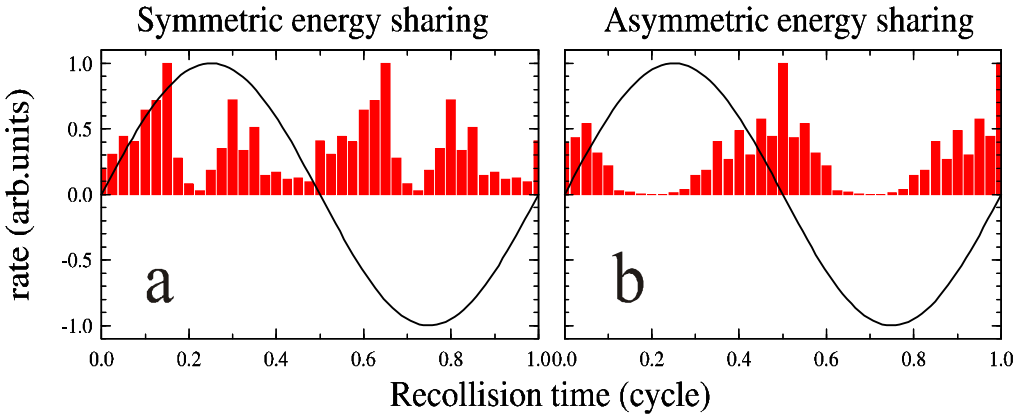

Fig 2. *DI yield with respect to the laser phase at recollision for the events corresponding to SES (a) and AES (b). The solid black curves represent laser field.*

More details of recollision can be obtained by investigating the behavior of TMDs. Since in the transverse plane perpendicular to the polarization direction of the laser field, there is no external force, thus the TMD becomes stable as the electrons recede from the atoms. In addition, in the transverse directions, the electron feels solely the Coulomb interaction of the nuclear core. Hence the TMD can provide pure information of the Coulomb focusing effect of the core. In figures 3(a) and 3(b), we show the drift transverse momentum ($p_{i\perp} = \sqrt{p_{iy}^2 + p_{iz}^2}$) spectra of the recolliding (solid red curve) and the bound (dashed blue curve) electrons for SES and AES, respectively. Obviously, for the SES situation, the final TMD of these two electrons are similar. Nevertheless, in AES case, the recolliding and bound electrons exhibit remarkably different TMDs, the spectrum of bound electron peaks near 0,2 a.u., while that of recolliding electron has a maximum at 1,2 a.u. At higher intensity which is not shown in this paper, the TMD of bound electron still has maximum around the origin, while that of recolliding electron's TMD shifts to larger transverse momentum $P_\perp$. That shift originates from the larger energy of recolliding electron induced by higher laser intensity just before the recollision process. The difference in TMD between SES and AES implies different three-body interaction, which can be explored by inspecting the history of the whole DI events.

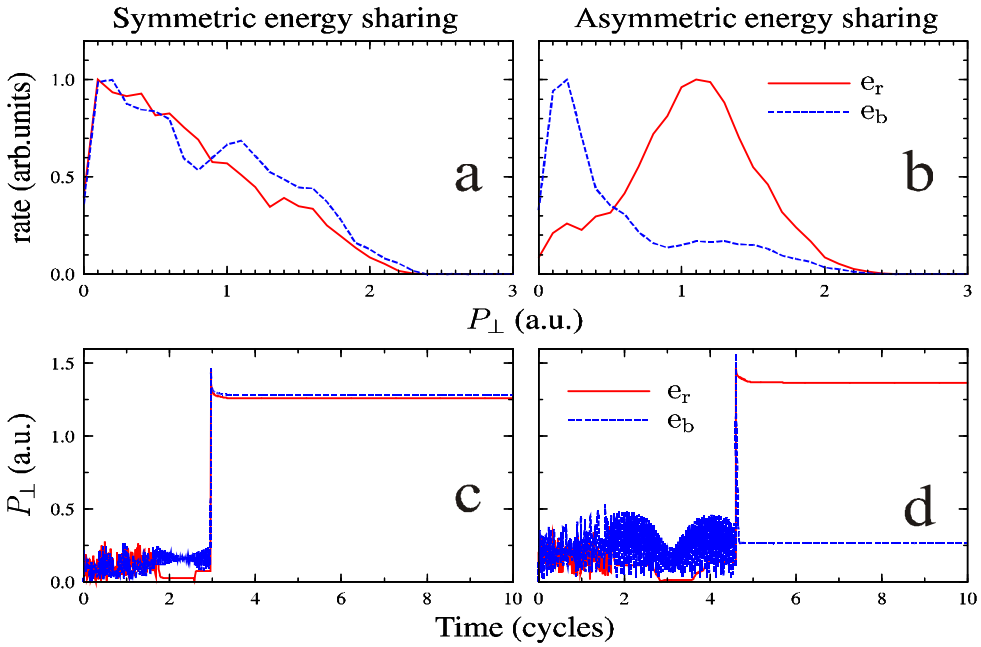

Fig 3. *Final transverse momentum spectra for recolliding and bound electrons in cases of SES (a) and AES (b). Time evolution of TMD for recolliding and bound electrons taken from two sample trajectories corresponding to SES (c) and AES (d).*

As shown in the bottom of figure 3, two electrons in both trajectories attain similar TMD upon recollision. Note that this representation implies the opposite directions of transverse momenta in transverse directions (i.e. k_y and k_z) with respect to the direction of the laser polarization axis. Just after recollision, both the bound and recolliding electrons experience a sudden decrease in TMD for SES trajectory (see figure 3(c)). For AES trajectory, the bound electron suffers a much larger sudden decrease in TMD while the transverse momentum of the recolliding electron does not change much after recollision (see figure 3(d)). We ascribe the sudden decrease of the transverse momenta to the nuclear attraction between electrons and core in the transverse plane. For the SES trajectory, the nuclear attraction plays similar role in the decreasing the transverse momenta since the two electrons leave the core with similar momentum. For the AES trajectory, the recolliding electron leaves the core with a very fast initial momentum, so nucleus almost does not affect its transverse momentum. However, the bound electron takes a longer time to leave the core, so its initial momentum is small leading to the largely sudden decrease of the transverse momentum. Note that the TMDs for both two electrons commonly become stabilized as they move away from the ion core as expected since there is no external force in the transverse plane. Indeed, while carefully looking insight into the stabilizing TMD, we observe small fluctuation which cannot be seen in this representing scale. Such fluctuation, in our understanding, is due to the numerical errors.

Although the trajectory-analysis method in this paper as well as in reference [11] provides us unambiguously microscopic dynamics of the AES process, it is impossible to observe those features experimentally since the recolliding and bound electrons cannot be distinguished in experiment. Thus it is instructive to implement in figure 4 the correlated momentum distribution of two ionized electrons in transverse plane. In this figure we show the transverse momentum spectra from different parts of the parallel momentum distributions without tracing back the trajectories. Figures 4(a) and 4(b) correspond to the data around and apart from the principle diagonal in figures 1(b) and 1(c), respectively. This procedure can be considered in experiment, thus we believe that such analysis is meaningful. In SES situation (figure 4(a)), the discrepancy in transverse momenta of two ionized electrons is not large so that the data cluster around the principle diagonal. Meanwhile this difference is much more noticeable in case of AES as expected (see figure 4(b)). We can conclude that the two-electron correlated transverse momentum distribution contains the imprint of AES process.

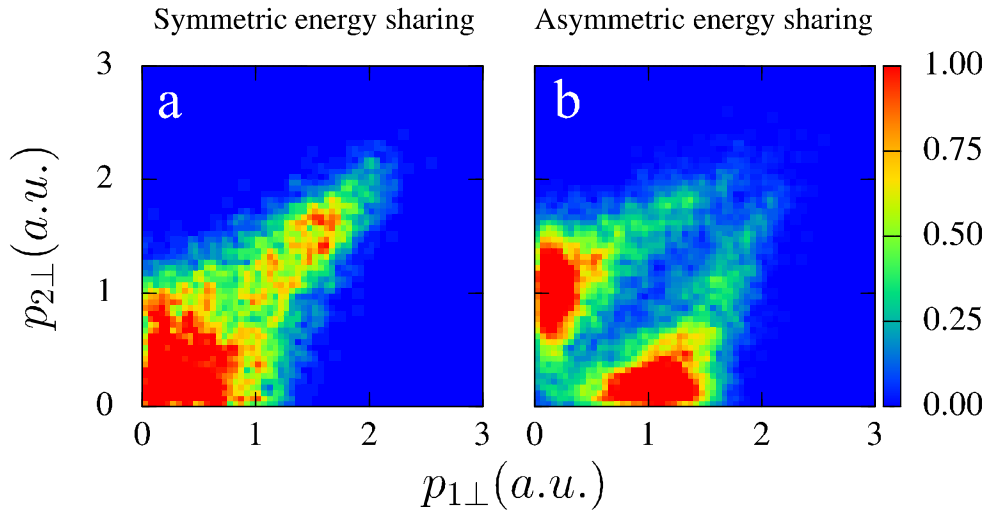

Fig 4. *Two-electron correlated momentum distribution in transverse plane: for SES (a) and AES (b).*

4. Conclusion

In conclusion, we have provided a deep insight into the evolution of the electrons in laser field by trajectory-analysis method to further understand the physical dynamics of the process. The results show that the different transverse momentum spectra of the recolliding and bound electrons originate the asymmetric energy sharing at recollision. Because of the asymmetric energy sharing, the bound electrons leave the nucleus with a very small initial momentum and thus its transverse momentum is strongly focused by the nuclear attraction when they move away from the core. Meanwhile, the recolliding electrons leave the core with a very fast initial momentum thus the nuclear attraction almost does not affect its transverse momentum. The difference in the transverse momentum spectra of the recolliding and bound electrons provide a clear scenario of the attosecond three-body dynamics among nucleus and two ionized electrons.

REFERENCES

1. Becker A. and Faisal F. H. M. (2000), "Interpretation of momentum distribution of recoil ions from laser induced nonsequential double ionization", *Physical Review Letter*, 84, 3546.
2. Becker A., DörnerR., and MoshammerR. (2005), "Multiple fragmentation of atoms in femtosecond laser pulses", *Journal of Physics B*, 38, S753.
3. Brabec T., Ivanov M.Y., and Corkum P.B. (1996), "Coulomb focusing in intense field atomic processes", *Physical Review A*, 54, R2551.

4. Corkum P. B. (1993), "Plasma perspective on strong field multiphoton ionization", *Physical Review Letters*, 71, 1994.
5. Haan S. L., Breen L., Karim A., and Eberly J. H. (2006), "Variable time lag and backward ejection in full-dimensional analysis of strong-field double ionization", *Physical Review Letter*, 97, 103008.
6. Panfili R., Eberly J. H., and Haan S. L. (2001), "Comparing classical and quantum dynamics of strong-field double ionization", *Optics Express*, 8, 431.
7. Pham Vinh N. T., Tostikhin Oleg I., and Morishita Toru (2014), "Molecular Siegert states in an electric field. II. Transverse momentum distribution of the ionized electrons", *Physical Review A*, 89, 033426.
8. Rudenko A., De Jesus V. L. B., ErglerTh., ZrostK., Feuerstein B., SchröterC. D., MoshammerR., and UllrichJ. (2007), "Correlated two-electron momentum spectra for strong-field nonsequential double ionization of He at 800 nm", *Physical Review Letter*, 99, 263003.
9. Truong Thu D. H., Huynh Son V., and Pham Vinh N. T. (2015), "V-like structure in the correlated electron momentum distribution for nonsequential double ionization of helium", *Journal of Science of Ho Chi Minh University of Education*, 5(70), 26.
10. Ye D. F., Liu X., and Liu J. (2008), "Classical trajectory diagnosis of a fingerlike pattern in the correlated electron momentum distribution in strong field double ionization of Helium", *Physical Review Letter*, 101, 233003.
11. Zhou Yueming, Liao Qing and Lu Peixiang (2010), "Asymmetric electron energy sharing in strong-field double ionization of helium", *Physical Review A*, 82, 053402.
12. William H. P, Teukolsky A., Vetterling W. T., and Flannery B. P. (1992), "Numerical Recipes in FORTRAN", Cambrigde University Press, Cambridge.

(*Received: 17/7/2015; Revised: 06/8/2015; Accepted: 24/9/2015)*