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Ionization of two-electron atom (xenon) studied by Bohmian mechanics theory*

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The ionization dynamics of two-electron atom in an intense laser field is studied by the Bohmian mechanics (BM) theory, and the xenon atomic potential function is used as a model. The single ionization process and double ionization process are calculated by the BM theory and their results are in good agreement with those calculated by numerically solving the time-dependent Schrödinger equation. The analyses of the types, trajectories, and forces of Bohmian particles (BPs) undergoing the single and double ionizations indicate that the re-collision process accounts for a considerable proportion in the singly ionized cases. Furthermore, the analysis of the work done by the external force acting on the BPs shows that the quantum force plays an important role in the re-collision process. This work is helpful in understanding the ionization of two-electron atom in an intense laser field.

Keywords: Bohmian mechanics, quantum force, atomic ionization, re-collision process

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1. Introduction

The study of the interaction between intense ultrashort laser pulse and atom/molecule can help us understand in depth the dynamical process of extranuclear electrons.[1–5] The ionization of two-electron atom has attracted extensive attention in the study of strong-field physics,[6–8] especially the non-sequential double ionization,[9–13] for the two-electron system contains the important correlation effect. A great many methods have been developed to describing the dynamical process of two-electron system, including numerically solving the time-dependent Schrödinger equation (TDSE), S-matrix theory, classical and semi-classical ensemble model, *etc*. Of these methods, numerically solving the TDSE is the most accurate one,[14–16] however, it is difficult to obtain the information about the dynamical process of electrons. The S-matrix theory imposes an artificial phase on different excited states,[17,18] which lacks a solid theoretical basis. Although the classical and semi-classical ensemble model methods can also be used to calculate ionization,[19–23] they will inevitably lose a lot of quantum information and bring great errors to the calculated results. To overcome the above difficulties, Bohmian mechanics (BM) method has been developed to deal with the two-electron problems. The BM is a causal interpretation of quantum mechanics. Bohmian particles (BPs) represent the possible positions of electrons, and Bohmian trajectories represent the possible trajectories of electrons. Once the initial positions and initial state of electrons are determined, the trajectories will be uniquely determined. From a methodological point of view, there are two main types of BM. The first one can be called "synthetic BM", and in the "synthetic" approach, the quantum trajectory ensemble is solved over time as a whole, without prior knowledge about the TDSE solution;[24–26] The second one can be called "analytic BM", and in the "analytic" approach, the TDSE is numerically solved by conventional means, and then the ex post facto is used to extract Bohmian trajectories.[27] In this paper, the second approach is adopted. By analyzing the paired Bohmian trajectories, we try to study the effect of the re-collision process on single and double ionization.

In recent years, the BM method has been widely used to study strong-field physical phenomena.[28–41] Since the computational cost increases significantly as the dimension of the calculation increases, in this paper, we use the one-dimensional model to study the dynamics of two-electron system. Although the one-dimensional model magnifies the effect of Coulomb force, it can still present the essential physical mechanism in the interaction between laser and atom.[42] As for the ionization, we judge it by dividing the region of the electron space, which will be introduced in detail later.

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2. Theoretical method

According to the BM theory,[43,44] the dynamics of the two electrons in a xenon atom in an external field can be described by the one-dimensional TDSE (atomic units are used throughout this paper):

$$\mathrm{i}\frac{\partial}{\partial t}\psi(x_1,x_2,t) = \left[-\frac{1}{2}\frac{\partial^2}{\partial x_1^2}-\frac{1}{2}\frac{\partial^2}{\partial x_2^2}+V_a(x_1,x_2) + (x_1+x_2)E(t)\right]\psi(x_1,x_2,t), \quad (1)$$

where

$$V_a(x_1,x_2) = -\frac{2}{\sqrt{x_1^2+4.26}}-\frac{2}{\sqrt{x_2^2+4.26}} + \frac{1}{\sqrt{(x_1-x_2)^2+6.5}}$$

is the Coulomb potential energy of the two-electron atom (the first and second term correspond to the Coulomb attraction between the nucleus and electrons 1 and 2, and the third term refers to mutual Coulomb repulsion of the two electrons);

$$E(t)=E_0\exp\left[-2\ln 2\frac{(t-0.35T)^2}{\tau^2}\right]\cos[\omega(t-0.5T)+\phi]$$

is the expression of laser electric field, where $E_0 = 0.17$ a.u., $T = 110.23$ a.u., $\tau = 31.49$ a.u., $\phi = 3.15\pi$, and $\omega = 0.057$ a.u.. The two-electron wave-function that the BP follows can be expressed as

$$\psi(x_1,x_2,t) = R(x_1,x_2,t)\exp\left[\mathrm{i}S(x_1,x_2,t)\right], \quad (2)$$

where R and S are both the real numbers. Substituting Eq. (2) into Eq. (1), and extracting imaginary and real parts on both sides of the equation, we can obtain the following equations:

$$\frac{\partial R^2(x_1,x_2,t)}{\partial t}+\sum_{i=1}^{2}\frac{\partial}{\partial x_i}\left[\frac{\partial S(x_1,x_2,t)}{\partial x_i}R^2(x_1,x_2,t)\right]=0, \quad (3)$$

$$-\frac{\partial S(x_1,x_2,t)}{\partial t} = \sum_{i=1}^{2}\frac{1}{2}\left[\frac{\partial S(x_1,x_2,t)}{\partial x_i}\right] + Q(x_1,x_2,t)+V_a(x_1,x_2)+(x_1+x_2)E(t). \quad (4)$$

Equation (4) is the quantum Hamilton–Jacobian equation, where the subscript i denotes the i-th electron. The term on the left-hand side of Eq. (4) refers to the total energy, and the first, second, third, and last terms on the right-hand side of Eq. (4) are the kinetic energy of the two electrons, quantum potential energy, classical Coulomb potential energy, and electric potential energy, respectively. The expression of quantum potential is

$$Q(x_1,x_2,t) = \sum_{i=1}^{2}-\frac{1}{2}\frac{\partial^2 R(x_1,x_2,t)}{\partial x_i^2}\Big/R(x_1,x_2,t). \quad (5)$$

From the kinetic term in Eq. (4), the velocity of the i-th electron is obtained as follows:

$$v_i(t) = \left[\frac{\partial S(x_1,x_2,t)}{\partial x_i}\right]\Big|_{x_1=x_1(t),\,x_2=x_2(t)}. \quad (6)$$

According to Eq. (2), the velocity of the i-th electron can also be expressed by the wave-function

$$v_i(t) = \mathrm{Im}\left[\frac{1}{\psi(x_1,x_2,t)}\frac{\partial}{\partial x_i}\psi(x_1,x_2,t)\right]\Big|_{x_1=x_1(t),\,x_2=x_2(t)}. \quad (7)$$

Therefore, we can obtain the position of the i-th electron at any time as given by

$$x_i(t) = x_i(0)+\int_0^t v_i(t')\,\mathrm{d}t'. \quad (8)$$

Firstly, the probability density function of the ground state of xenon atom at an initial instant $|\psi_0(x_1,x_2,0)|^2$ is derived by the imaginary time evolution method. Then, the initial spatial positions of N pairs of BPs are given at random by sampling $|\psi_0(x_1,x_2,0)|^2$ through the acceptance–rejection sampling method and used to denote the possible initial positions of two electrons, *i.e.*, $x_1^k(t=0)$ and $x_2^k(t=0)$ ($k = 1,2,3,\ldots,N$ denotes the k-th BP). Next, the time-evolution of wave-function $\psi(x_1,x_2,t)$ of one-dimensional xenon atom in the laser field is calculated by the second-order symmetric difference method. The initial state of the wave-function satisfies the spatial exchange symmetry. The velocities and trajectories of paired particles are calculated according to the multi-body BM as follows:

$$v_1^k(t) = \frac{\mathrm{d}x_1^k(t)}{\mathrm{d}t} = \mathrm{Im}\left[\frac{1}{\psi(x_1,x_2,t)}\frac{\partial\psi(x_1,x_2,t)}{\partial x_1}\right]\Big|_{x_1=x_1^k(t),x_2=x_2^k(t)}, \quad (9)$$

$$v_2^k(t) = \frac{\mathrm{d}x_2^k(t)}{\mathrm{d}t} = \mathrm{Im}\left[\frac{1}{\psi(x_1,x_2,t)}\frac{\partial\psi(x_1,x_2,t)}{\partial x_2}\right]\Big|_{x_1=x_1^k(t),x_2=x_2^k(t)}, \quad (10)$$

$$x_1^k(t) = x_1^k(0)+\int_0^t v_1^k(t')\,\mathrm{d}t',$$

$$x_2^k(t) = x_2^k(0)+\int_0^t v_2^k(t')\,\mathrm{d}t'. \quad (11)$$

According to the BM theory, the forces acting on each BP are as follows:

The resultant force acting on each BP: $F_{\mathrm{R}} = \mathrm{d}v_i^k(t)/\mathrm{d}t$.

Coulomb force from nucleus acting on the k-th BP of the i-th electron:

$$F_{\text{nucleus Coulomb}} = -\frac{\partial}{\partial x_i}\left[-\frac{2}{\sqrt{(x_i)^2+4.26}}\right]\Big|_{x_i=x_i^k(t)}.$$

Coulomb force from the k-th BP of the j-th electron acting on the k-th BP of the i-th electron:

$$F_{\text{e–e Coulomb}} = -\frac{\partial}{\partial x_i}\left[\frac{1}{\sqrt{(x_i-x_j)^2+6.5}}\right]\Big|_{x_i=x_i^k(t),\,x_j=x_j^k(t)}.$$

Quantum force acting on each BP: $F_{\rm Q} = F_{\rm R} - F_{\rm nucleus\ Coulomb} - F_{\rm e-e\ Coulomb} - F_{\rm E}$.

Electric field force acting on each BP: $F_{\rm E} = -E(t)$.

By integrating the forces with respect to displacement, we can obtain the work done by the above forces:

$$A_{\rm R} = \int_{x_i^k(0)}^{x_i^k(t)} F_{\rm R}\,{\rm d}x,$$

$$A_{\rm nucleus\ Coulomb} = \int_{x_i^k(0)}^{x_i^k(t)} F_{\rm nucleus\ Coulomb}\,{\rm d}x,$$

$$A_{\rm e-e\ Coulomb} = \int_{x_i^k(0)}^{x_i^k(t)} F_{\rm e-e\ Coulomb}\,{\rm d}x,$$

$$A_{\rm E} = \int_{x_i^k(0)}^{x_i^k(t)} F_{\rm E}\,{\rm d}x, \quad A_{\rm Q} = \int_{x_i^k(0)}^{x_i^k(t)} F_{\rm Q}\,{\rm d}x. \tag{12}$$

The total energy of the k-th BP of the i-th electron is equal to

$$E_i^k(x_i,x_j,t) = \left[-\frac{1}{2}{\rm Re}\left(\frac{\partial^2\psi(x_i,x_j,t)}{\partial x_i^2}\Big/\psi(x_i,x_j,t)\right) - \frac{2}{\sqrt{(x_i)^2+4.26}} + \frac{1}{\sqrt{(x_i-x_j)^2+6.5}}\right]\Bigg|_{x_i=x_i^k(t),x_j=x_j^k(t)}. \tag{13}$$

3. Results and discussion

Figure 1(a) shows the time-evolution of laser field selected in this paper. It can be seen from the figure that the laser electric field is asymmetric: the peak amplitude in the negative direction (0.1060 a.u.) is slightly higher than that in the positive direction (0.0836 a.u.). The purpose of this setting is to allow the ionized electron to acquire enough energy in the electric field to return to the nuclear region and collide with the electron in the nuclear region, so that the re-collision process can be easily observed. In this paper, the initial state is the two-electron ground state and satisfies the spatial exchange symmetry as shown in Fig. 1(b).

In order to verify the reliability of the BM method in calculating single and double ionization, $N_{\rm total}$ (where $N_{\rm total}$ is set to be 200 and 1×10^6, separately) pairs of BPs are selected to calculate the ionization. In the calculation, we judge the ionization by the method of dividing the region of the electron space. For the selected BP pairs, we judge the ionization according to their positions: in the case of $x_1^k \le 10$ a.u., $x_2^k \le 10$ a.u., no ionization occurs, which takes place N_1 times; in the case of $x_1^k > 10$ a.u., $x_2^k \le 10$ a.u. or $x_1^k \le 10$ a.u., $x_2^k > 10$ a.u., single ionization occurs, which takes place N_2 times; in the case of $x_1^k > 10$ a.u., $x_2^k > 10$a.u., double ionization occurs, which takes place N_3 times. Thereby, the probability of being unionized, singly and doubly ionized can be calculated by $P_1(t) = N_1(t)/N_{\rm total}$, $P_2(t) = N_2(t)/N_{\rm total}$, and $P_3(t) = N_3(t)/N_{\rm total}$, respectively.

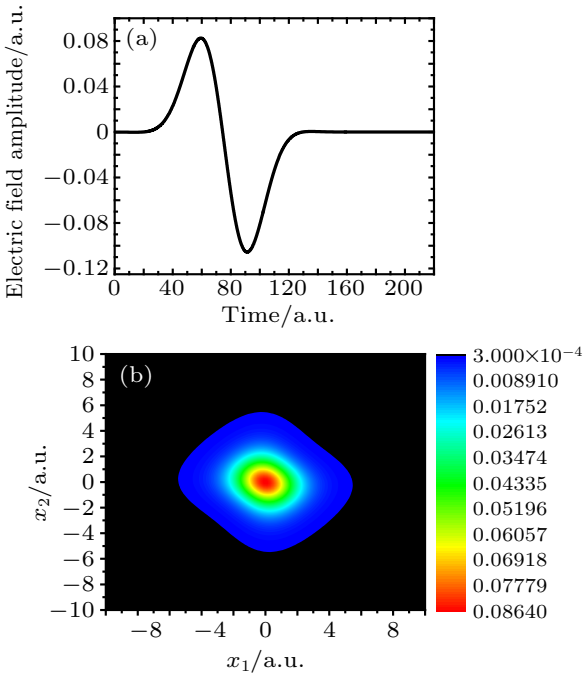


Fig. 1. (a) Time-evolution of laser field whose central frequency and duration are 0.057 a.u., and 2 optical cycles, respectively. (b) Probability density image of ground state wave-function.

For the TDSE method, the probability that both electrons are in the bound states is

$$P_1(t) = \int_{-10\ {\rm a.u.}}^{10\ {\rm a.u.}}\int_{-10\ {\rm a.u.}}^{10\ {\rm a.u.}} |\psi(x_1,x_2,t)|^2\,{\rm d}x_1\,{\rm d}x_2. \tag{14}$$

The probability of being singly ionized is

$$P_2(t) = \int_{-\infty}^{-10\ {\rm a.u.}}\int_{-10{\rm a.u.}}^{10\ {\rm a.u.}} |\psi(x_1,x_2,t)|^2\,{\rm d}x_1\,{\rm d}x_2 + \int_{10\ {\rm a.u.}}^{\infty}\int_{-10\ {\rm a.u.}}^{10\ {\rm a.u.}} |\psi(x_1,x_2,t)|^2\,{\rm d}x_1\,{\rm d}x_2 + \int_{-\infty}^{-10\ {\rm a.u.}}\int_{-10\ {\rm a.u.}}^{10\ {\rm a.u.}} |\psi(x_1,x_2,t)|^2\,{\rm d}x_2\,{\rm d}x_1 + \int_{10\ {\rm a.u.}}^{\infty}\int_{-10\ {\rm a.u.}}^{10\ {\rm a.u.}} |\psi(x_1,x_2,t)|^2\,{\rm d}x_2\,{\rm d}x_1. \tag{15}$$

The probability of being doubly ionized is

$$P_3(t) = 1 - P_1(t) - P_2(t). \tag{16}$$

Figure 2 shows the time-evolution of ionization probability of xenon atom calculated by the BM method and TDSE method. It can be seen from the figure that the ionization probabilities calculated by the two methods are in good agreement with each other, and the more the BPs selected, the better the agreement will be as shown in Figs. 2(a) and 2(b), indicating that the BM method can accurately describe the single and double ionization process.

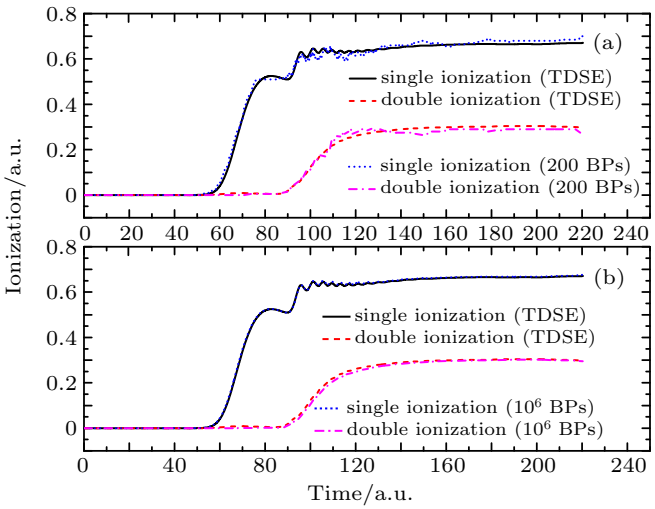


Fig. 2. Variation of single and double ionization probability of xenon atom with time for (a) 200 and (b) 1×10^6 pairs of BPs, with solid black and dotted blue (dashed red and dash-dotted magenta) curves denoting single (double) ionization probability calculated by TDSE and BM methods, respectively.

In order to distinguish between the singly ionized BP pair and the doubly ionized BP pair and analyze their dynamical processes, the 200 BP pairs are selected, for 200 BP pairs can accurately describe the ionization process as shown in Fig. 2(a). Figure 3 shows the time-evolution of trajectories of 200 BP pairs in an external field. Obviously, re-collision behaviors can be seen in the single ionization process as shown in Figs. 3(a) and 3(b), indicating that most of the re-collisions occur in the single ionization process. It should be noted that our conclusion does not mean that the double ionization is independent of the re-collision process, for the Coulomb potential of xenon atoms selected in this paper is relatively small, thereby making the electrons weakly bound to nucleus, and consequently double ionization is prone to occur. In our work, the re-collision process is rarely observed in the double ionization process (see Figs. 3(c) and 3(d)), which indicates that most of the double ionization that occurs under this laser and atomic parameters is sequential double ionization rather than non-sequential one, for the re-collision process must be involved in the non-sequential double ionization.

For the single ionization, we find that quite a few BP pairs undergo the re-collision process. Therefore, the question now arises: how do the particles exchange energy and momentum to fulfill the ionization? In the following, we will discuss the underlying physical mechanism.

We select a pair of BPs that undergo single ionization from Figs. 3(a) and 3(b), and present their trajectories and energy varying with time in Figs. 4(a) and 4(b), respectively. It can be seen from Fig. 4(a) that the first BP (solid black curve) is ionized by the external field and returns to the vicinity of the nuclear region after the direction of laser field has reversed. After it interacts with the second BP (dash-dotted red curve) near the nuclear region, the second BP is "knocked" out of the nuclear region, thus being ionized and the first BP stays in the nuclear region due to the energy loss during the collision. In Fig. 4(b), we can see that the two colliding BPs exchange energy at about 110 a.u. However, the energy exchange process does not occur instantaneously, but is completed in a period of time. Next, we will discuss the physical mechanism leading the energy to exchange between the two BPs through the force analysis.

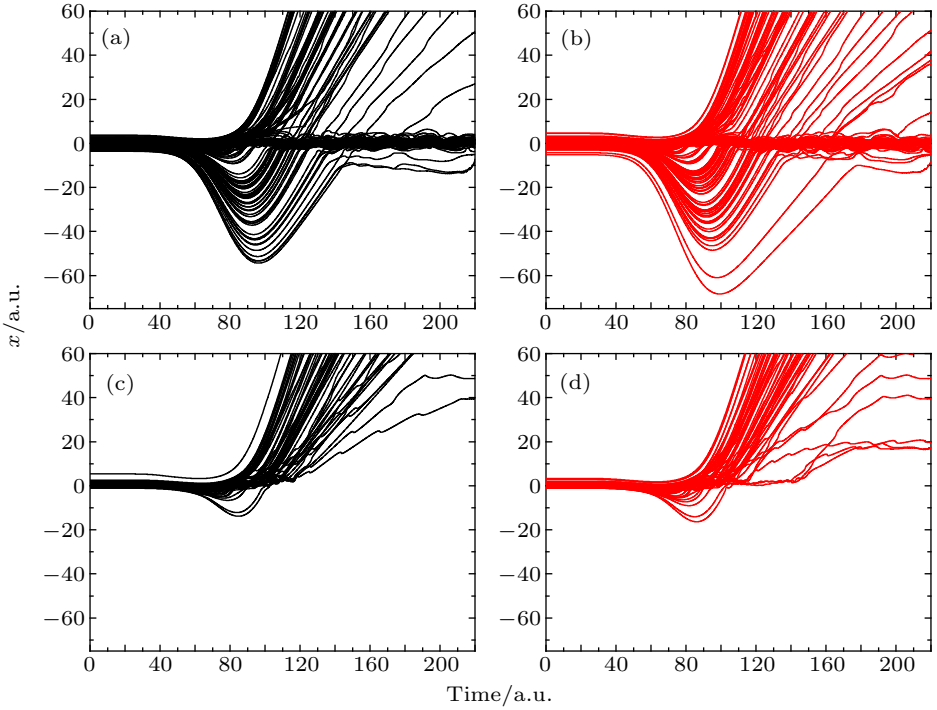


Fig. 3. Time-evolution of trajectories of 200 BP pairs in external field, showing [(a), (b)] singly, and [(c), (d)] doubly ionized BP pairs' trajectories. Panels (a) and (c) refer to trajectories of the first BP and panels (b) and (d) refer to trajectories of the second one.

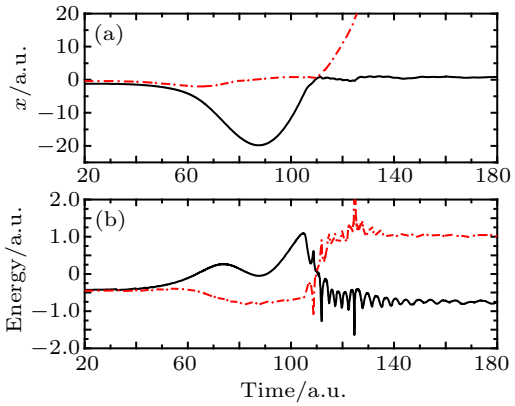


Fig. 4. Time-evolution of typical BP pair in Figs. 3(a) and 3(b) showing (a) trajectories and (b) energy of the first (solid black curve) and second (dash-dotted red curve) BPs.

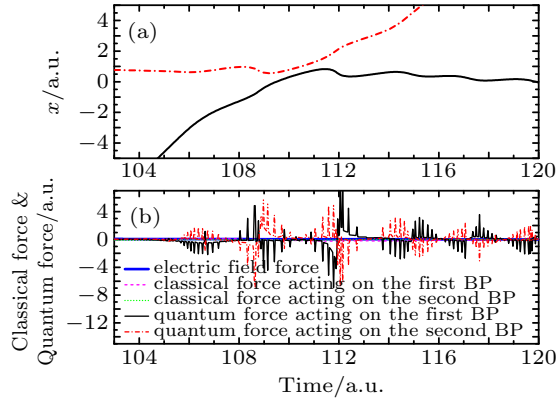


Fig. 5. Time-evolution of trajectories and the force acting on the BP pair in Fig. 4(a) within recombination time: (a) trajectories of the first (solid black curve) and second (dash-dotted red curve) BPs from $t = 103$ a.u. to $t = 120$ a.u.; (b) quantum force acting on the first (solid black curve) and second (dash–dotted red curve) BPs, classical force acting on the first BP (sum of the Coulomb attraction from the nucleus and Coulomb repulsion from the second BP) (dashed magenta curve), and classical force acting on the second BP (dotted green curve), with bold solid blue curve denoting electric field force.

Figure 5 shows the time-evolution of the trajectories and the force acting on the BP pair in Fig. 4(b) within the recombination time. From Fig. 5(a), we can see that the re-collision process takes place near the nuclear region, and the two BPs separate from each other after oscillating several times. The Coulomb force acting on the BP near the nucleus is mainly the Coulomb attraction from nucleus and the Coulomb repulsion from the other BP. In order to distinguish it from quantum force and study the problem conveniently, we call the sum of these two forces the classical force as shown by the dashed magenta and dotted green curves in Fig. 5(b). Obviously, during the recombination (from $t = 103$ a.u. to $t = 120$ a.u.), the classical force is very small and can be neglected compared with the quantum force (solid black and dash-dotted red curves). Especially, in the period from $t = 108$ a.u. to $t = 112.7$ a.u., the quantum force plays a key role in the energy exchange between two BPs. We find that although the collision process takes place in the nuclear region, it is different from the commonly known elastic collision process. In the classical case, the elastic collision process of two electrons occurs when two electrons approach to each other, the coulomb repulsion force between them increases sharply, and consequently they exchange their momenta. However, it can be seen from Fig. 5 that though the two BPs are very close to each other in the recombination process, the distance between them is still relatively large, as a result, the Coulomb repulsion between them is small. Instead, the quantum forces with equal value and opposite directions, which are much larger than the Coulomb force and external electric field force, make the two BPs undergo the "elastic collision".

In the following, we will analyze the re-collision process of the two BPs in Fig. 4(a) from the perspective of work done by the forces,as shown in Fig. 6. Firstly, we analyze the work done by the external force acting on the first BP (solid black curve). In the period from $t = 0$ a.u. to $t = 105$ a.u., the work done by the external forces mainly comes from the electric field force, the Coulomb attraction force from atomic nucleus, and the Coulomb repulsion force from the other BP. The BP is ionized in the external field, and gradually moves to the nuclear region after direction of the electric field has reversed. From $t = 105$ a.u. to $t = 110$ a.u., the BP turns closer to the nucleus, and the negative work done by the quantum force increases rapidly; from $t = 110$ a.u. to the end, the negative work done by the quantum force changes little, which is balanced by the positive work done by the electric field force. At the same time (from $t = 105$ a.u. to the end), the work done by the classical force rapidly decays to zero, making the work done by the resultant force rapidly decrease to zero, and thus the kinetic energy of the first BP rapidly decreases to zero. It can be seen from the time-evolution of trajectory and energy in Fig. 4 (solid black curve) that the BP returns to the nuclear region and stays in the ground state after the recombination.

Then, the work done by the external force acting on the second BP (dash-dotted red curve in Fig. 4(a)) is analyzed. In the period from $t = 0$ a.u. to $t = 108$ a.u., the work done by each component is basically balanced, and thus the work done by the resultant force is almost zero. From $t = 108$ a.u. to $t = 125$ a.u., the positive work done by the quantum force acting on the BP increases rapidly, making it quickly acquire kinetic energy and gradually leave the nuclear region; from $t = 125$ a.u. to the end, the positive work done by the quantum force changes little. At the same time (from $t = 108$ a.u. to the end), the positive work done by the electric field force and the Coulomb force from the first BP exactly balances the negative work done by the Coulomb force from the nucleus, which makes the work done by the resultant force that completely comes from quantum force. In combination with the trajectories and energy in Fig. 4 (dash–dotted red curve), we can see that after the recombination process, the BP leaves the nuclear region and acquires a certain kinetic energy, whose value is about 1 a.u.

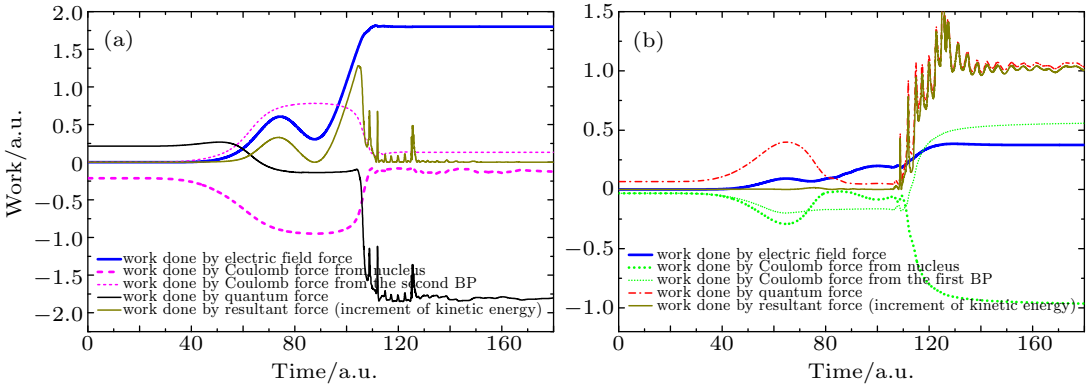


Fig. 6. (a) Work done by resultant force acting on the first BP (solid dark yellow curve) and its component forces, *i.e.*, electric field force (bold solid blue curve), Coulomb force from the nucleus (bold dashed magenta curve), Coulomb force from the second BP (dashed magenta curve), and quantum force (solid black curve). (b) Work done by the resultant force acting on the second BP (solid dark yellow curve), and its component forces, *i.e.*, electric field force (bold solid blue curve), Coulomb force from the nucleus (bold dotted green curve), Coulomb force from the first BP (dotted green curve), and quantum force (dash-dotted red curve).

4. Conclusions

The calculation results of single and double ionizations show that the BM theory can accurately describe the dynamical process of one-dimensional two-electron system in the external field. Taking xenon atomic model for example, we classify the trajectories of 200 pairs of BPs. It is found that the re-collision process dominates the dynamical behaviors of singly ionized BP pairs. For the single ionization, by analyzing the work done by the external force acting on the typical BP pair that undergo the re-collision process, we find that quantum force plays a key role in decelerating the recombined BP and accelerating the collided BP. This work suggests that the BM can be used to analyze the dynamical process of the two-electron system in an external field, and can fully reflect the quantum behaviors caused by the correlation between two electrons.

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