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Resonance-enhanced two-photon ionization of hydrogen atom in intense laser field investigated by Bohmian-mechanics*

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Resonance enhanced two-photon ionization process of hydrogen atom via the resonant laser pulse is studied by Bohmian mechanics (BM) method. By analyzing the trajectories and energies of Bohmian particles (BPs), we find that under the action of high frequency and low intensity multi-circle resonant laser pulses, the ionized BPs first absorb one photon completing the excitation, and then absorb another photon, completing the ionization after staying in the first excited state for a period of time. The analysis of work done by the forces shows that the electric field force and quantum force play a major role in the whole ionization process. At the excitation moment and in the excitation-ionization process, the effect of the quantum force is greater than that of the electric field force. Finally, we discuss the principle of work and energy for BPs, and find that the electric field force and quantum force are non-conservative forces whose work is equal to the increment of mechanical energy of the system. In addition, it is proved that the quantum potential energy actually comes from the kinetic energy of the system and the increment of kinetic energy is equal to that of the kinetic energy of the system.

Keywords: Bohmian mechanics, quantum force, resonance-enhanced two-photon ionization

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1. Introduction

The rapid development of high-power laser makes it possible to discover the electrodynamic behavior of atoms and molecules. Resonance enhanced multiphoton ionization (REMPI) technology is one of the important research methods which has important application values in the field of molecular spectroscopy, isotope separation, photodissociation kinetics,[1–3] and so on. Presently, the main research methods of multiphoton ionization are low-order perturbation theory,[4] numerically solving the time-dependent Schrödinger equation (TDSE), and rate equation theory. However, these theories can not directly describe the trajectory of electrons, making it difficult to obtain the dynamic process of electrons in multiphoton ionization. Under this circumstance, Bohmian mechanics (BM) method has been developed to solve this problem. BM, also known as de Broglie Bohm theory, differs from orthodox quantum mechanics (Copenhagen school) in its description of microscopic particles.

In orthodox quantum mechanics, probability density is used to describe the kinematic state of microscopic particles, however, due to the uncertainty principle, there is no concept of orbit for microscopic particles, making it difficult to describe the motion of microscopic particles. In the view of the BM, microscopic particles have the concept of orbit. As long as the initial state and position of microscopic particles are determined, the motion position of the microscopic particles in the external field can be calculated, obtaining the trajectories of the particles, which makes the description of microscopic particles' motion more clear and intuitive. Due to the uncertainty of the initial positions of microscopic particles, there are many possibilities for the trajectories of microscopic particles, for this reason, the BM does not violate the uncertainty principle. Results consistent with those of orthodox quantum mechanics can be obtained by the BM. Recently, the BM has become a powerful tool in dealing with strong field physics.[5–22] For the single electron case, it can be used to describe the excitation and ionization process.[13,14] Therefore, we speculate that the resonance enhanced two-photon ionization process can also be analyzed in detail by using this theory, and we attempt to analyze it from the perspective of trajectory, energy of BPs, and the work done by the resultant force on BPs.

2. Theoretical method

Under the dipole approximation in the length gauge, the TDSE describing the interaction between intense laser and hy-

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drogen atom is (atomic units are used throughout this paper)

$$\mathrm{i}\frac{\partial}{\partial t}\psi(x,t)=\left[-\frac{\partial^2}{2\partial x^2}+V(x)+E(t)x\right]\psi(x,t), \tag{1}$$

where $V(x)$ is the atomic potential function. In this paper, the softening Coulomb potential $V(x)=-q/\sqrt{x^2+A}$ is adopted whose parameters are $A=0.367$ and $q=0.561$, and the corresponding energies of the ground state and the first excited state are $E_0=-0.4996$ and $E_1=-0.1249$, respectively. Firstly, the ground state electron probability density function $|\psi(x,0)|^2$ is sampled according to the acceptance–rejection sampling method and these random numbers are used as the initial positions of the BPs to denote the possible initial positions of the electron. After the positions of these particles are determined, the probability of electrons appearing in the position is the same, i.e., $1/N$ (N is the number of selected particles). Secondly, we use the splitting operator method to calculate the evolution of the wave-function in the external field, and then use the wave-function obtained to calculate the velocity of each BP according to the BM theory,

$$v^k(t)=\mathrm{Im}\left[\frac{1}{\psi(x,t)}\frac{\partial}{\partial x}\psi(x,t)|_{x=x^k(t)}\right],\quad (k=1,2,\ldots,N_{\mathrm{tra.}}). \tag{2}$$

By integrating Eq. (2), the position of the k-th BP at moment t can be obtained as

$$x^k(t)=x^k(t=0)+\int_0^t v^k(t')\,\mathrm{d}t'. \tag{3}$$

The total energy of each particle is equal to

$$E_{\mathrm{total}}(x^k,t)=-\frac{1}{2}\mathrm{Re}\frac{\nabla^2\psi(x^k,t)}{\psi(x^k,t)}+V(x^k). \tag{4}$$

Using the total energy of BPs, we can monitor the states of electrons, such as excitation and ionization.

The quantum potential of each BP is

$$Q(x,t)=-\frac{1}{2}\left[\mathrm{Re}\frac{\nabla^2\psi(x,t)}{\psi(x,t)}+\left(\mathrm{Im}\frac{\nabla\psi(x,t)}{\psi(x,t)}\right)^2\right]_{x=x^k(t)}, \tag{5}$$

and the quantum force is

$$\begin{aligned}F_{\mathrm{Q}}&=-\frac{\partial Q}{\partial x}\\&=\frac{1}{2}\frac{\partial}{\partial x}\left[\mathrm{Re}\frac{\nabla^2\psi(x,t)}{\psi(x,t)}+\left(\mathrm{Im}\frac{\nabla\psi(x,t)}{\psi(x,t)}\right)^2\right]_{x=x^k(t)}.\end{aligned} \tag{6}$$

To obtain the quantum force, we need to take the third derivative of the wave-function, which brings about large errors. Alternatively, we can first calculate the resultant force via the derivation of BPs' velocity

$$F_{\mathrm{R}}=\frac{\partial v^k}{\partial t}, \tag{7}$$

then we can obtain the quantum force

$$F_{\mathrm{Q}}=F_{\mathrm{R}}-F_{\mathrm{C}}-F_{\mathrm{E}}, \tag{8}$$

where $F_{\mathrm{C}}=-\frac{\partial V}{\partial x}\Big|_{x=x^k}$ is the Coulomb force, and $F_{\mathrm{E}}=qE(t)$ is the electric field force.

By integrating the forces with respect to displacement, we can obtain the work done by the resultant force, electric field force, Coulomb force, and quantum force, respectively,

$$\begin{aligned}A_{\mathrm{R}}&=\int_{x_1}^{x_2}F_{\mathrm{R}}\,\mathrm{d}x,\quad A_{\mathrm{E}}=\int_{x_1}^{x_2}-E(t)\,\mathrm{d}x,\\A_{\mathrm{C}}&=\int_{x_1}^{x_2}F_{\mathrm{C}}\,\mathrm{d}x,\quad A_{\mathrm{Q}}=\int_{x_1}^{x_2}F_{\mathrm{Q}}\,\mathrm{d}x.\end{aligned} \tag{9}$$

3. Results and discussion

We use low intensity multi-circle resonant frequency laser pulses to realize the resonant enhanced two-photon ionization process, because this kind of laser pulses can make the electron transition to the first excited state sufficiently, which increases the probability of ionization. As shown in Fig. 1, the peak amplitude, central frequency, and duration of laser pulse are 0.1 a.u., 0.3747 a.u., and 20 optical cycles, respectively.

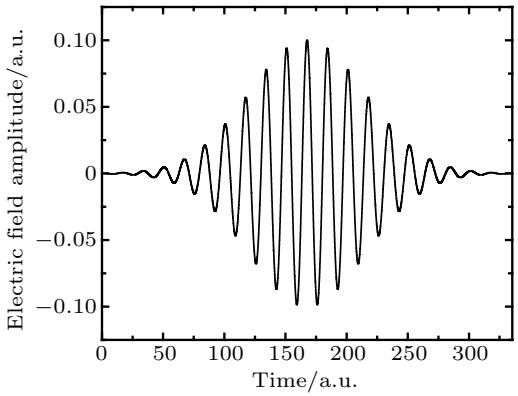


Fig. 1. Time evolution of laser field whose peak amplitude, central frequency, and duration are 0.1 a.u., 0.3747 a.u., and 20 optical cycles, respectively.

Figure 2 shows the 100 Bohmian trajectories and the probability density image of electron obtained by numerically solving the TDSE. We can see that the picture of Bohmian trajectories (Fig. 2(a)) is in good agreement with the probability density obtained by solving the TDSE (Fig. 2(a)), indicating that the motion of the electronic wave packet can be described by the Bohmian trajectories accurately. In order to explore the dynamical process of resonance ionization of BPs in an external field in detail, we select one typical trajectory of BP for analysis, as shown by the bold blue curve in Fig. 2(a), and it can be seen that this BP gradually moves away from the nuclear region and then is ionized by the external field.

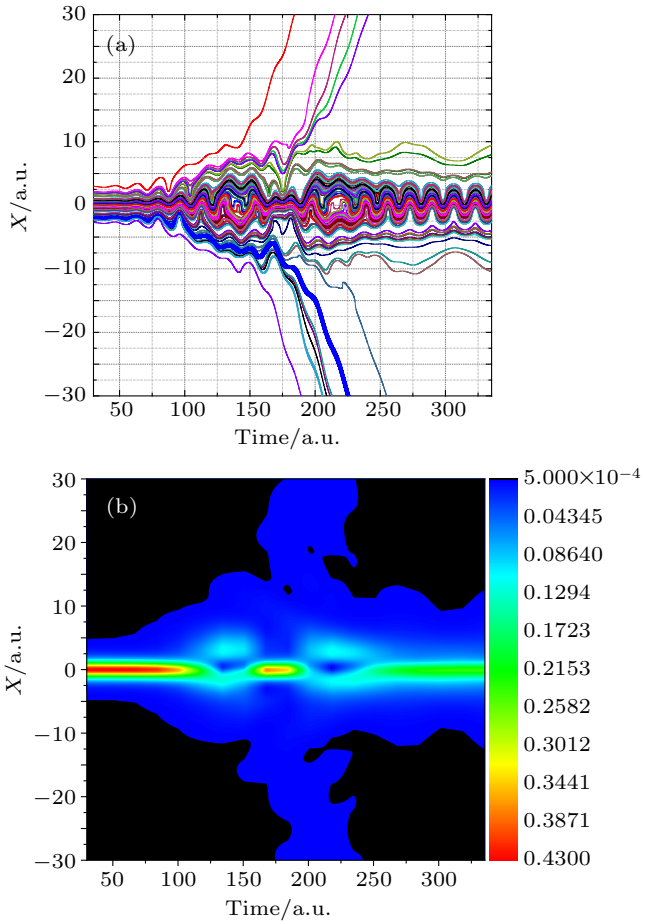


Fig. 2. Ionization process of electron irradiated by the laser pulse whose duration is 60 optical cycles. (a) Bohmian trajectories calculated by the BM and (b) probability density of the electron obtained by numerically solving the TDSE.

To study the state of motion of the BP at different time, we present the time-evolution of its trajectory and energy, as shown in Fig. 3. It can be seen from Fig. 3(b) that at $t = 0$, the total energy of the BP in the ground state is 0.5 a.u. With the increase of time, the electric field strength increases, the BP's total energy changes due to the absorption of the electric field energy, and its value oscillates around the energy of ground state with increasing amplitude. After $t = 100$ a.u., the BP stays near the first excited state whose energy is around 0.1249 a.u., and the fluctuation of its energy decreases rapidly and its state becomes relatively stable. The above process suggests that at the period from $t = 0$ a.u. to $t = 100$ a.u., the BP absorbs the energy of one photon with resonance frequency and completes the excitation process.

After staying in the first excited state for a period of time (from $t = 100$ a.u. to $t = 166$ a.u.), the BP re-absorbs energy being ionized. After the ionization, its total energy is 0.2 a.u., and the difference between this total energy and the energy of the first excited state is $\Delta E = 0.2$ a.u. $+ 0.1249$ a.u. $=$ 0.3249 a.u., which is close to the energy of the second photon (0.3747 a.u.), indicating that the BP re-absorbs one photon being ionized. In the following part, we will discuss the physical mechanism of the above process by analyzing the influence of the work done by the forces acting on the BP.

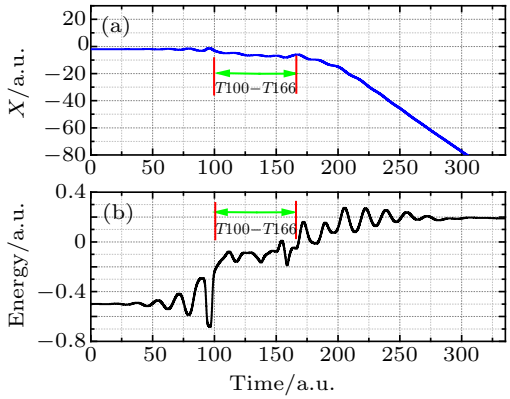


Fig. 3. Time evolution of (a) trajectory and (b) energy of the typical BP.

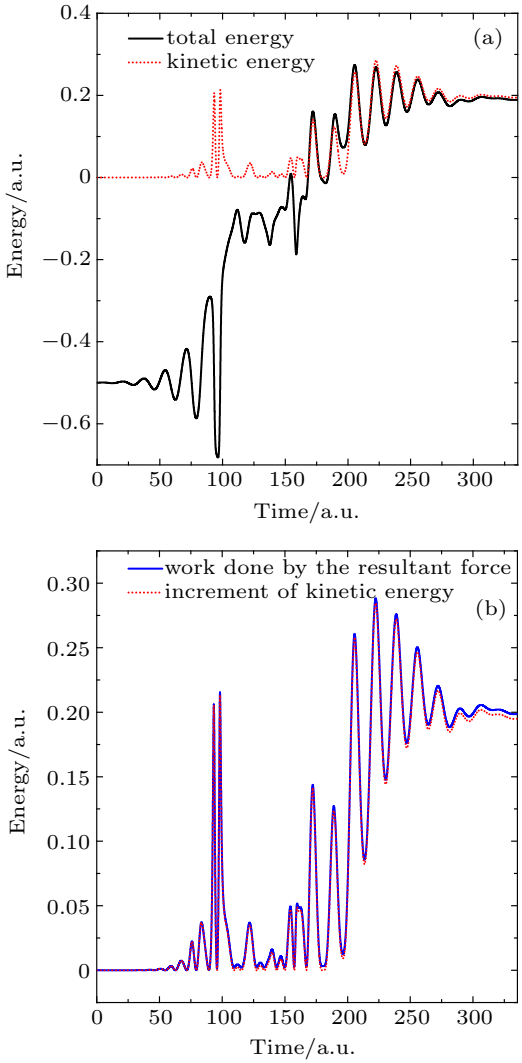


Fig. 4. (a) Time evolution of the total energy (solid black curve), and kinetic energy (dotted red curve) of BP, (b) the work done by the resultant force acting on BP (solid blue curve), and the increment of kinetic energy (dotted red curve).

According to the BM theory, the motion of BPs in the external field is affected by the electric field force, the Coulomb force of atomic nucleus, and the quantum force. At the same time, since the BM theory emphasizes the particle nature of microscopic particles, their motion should have the dynamic

characteristics of particles and the kinetic energy theorem should be satisfied. In order to verify that the Bohmian theory satisfies the kinetic energy theorem, we calculate the work done by the resultant force of the three forces and the increment of kinetic energy, as shown in Fig. 4(b). It can be seen from the figure that the work done by the resultant force and the increment of kinetic energy are in good agreement, and thus it is feasible to use the principle of work and energy to discuss the contribution of the forces.

From Fig. 4(a), we can see that when the BP is in the ground state ($t < 96$ a.u.) and the first excited state (107.8 a.u. $< t <$ 166 a.u.), its kinetic energy is very small, which is almost negligible. The change of the total energy is actually dominated by that of the potential energy. When the total energy of the BP is larger than zero, the potential energy of the BP decreases rapidly, and the change of the total energy is dominated by that of the kinetic energy. When the BP is pumped to the first excited state (from $t = 96$ a.u. to $t = 107.8$ a.u.) and undergoes the excitation-ionization process (from $t = 166$ a.u. to $t = 300$ a.u.), its kinetic energy increases rapidly, which provides the needed energy for excitation and ionization transitions.

To analyze the contribution of the work done by the forces to the whole ionization process, the excitation (from $t = 96$ a.u. to $t = 107.8$ a.u.), and the excitation-ionization process (from $t = 166$ a.u. to $t = 300$ a.u.), we present the work done by the resultant forces and its component forces in Figs. 5 and 6. Figure 5 presents the work done by the forces in the whole ionization process. Figure 6 presents the work done by the forces at the excitation moment (from $t = 96$ a.u. to $t = 107.8$ a.u.), and in the excitation-ionization process (from $t = 166$ a.u. to $t = 300$ a.u.).

In Fig. 5, from the viewpoint of the excitation process of the BP absorbing a photon (from $t = 0$ a.u. to $t = 107.8$ a.u.), we can see that when the BP is in the first excited state ($t = 107.8$ a.u.), the absorption of the first photon is completed. At this moment, the work done by the quantum force is very small, which is close to zero, and the work done by the Coulomb force is equivalent to that done by the electric field force, but their signs are opposite, resulting in the fact that the total work is close to zero and the kinetic energy is also close to zero. From the view point of the entire ionization process in which BP absorbs two photons ($t = 335$ a.u.), the work done by the electric field force and the quantum force in the whole ionization process is positive which is an important factor to realize resonance enhanced two-photon ionization. The Coulomb force from atomic nucleus always does negative work after the BPs are excited, as shown in Fig. 5.

Next, we discuss the contribution of work done by the resultant force and its component forces at the excitation moment and in the excitation-ionization process. In Fig. 5, the green and yellow parts represent the excitation moment (from $t = 96$ a.u. to $t = 107.8$ a.u.) and excitation-ionization process (from $t = 166$ a.u. to $t = 300$ a.u.) of the BP, respectively. In the following part, we only study the work done by the resultant force and each component force at these two periods, and present it in Fig. 6. It should be noted that at the excitation moment (in the excitation-ionization process), the starting and ending positions to calculate the work done by the forces correspond to the BP's positions at $t = 96$ a.u. and $t = 107.8$ a.u. ($t = 166$ a.u. and $t = 300$ a.u.), respectively. It can be seen from Fig. 6(a) that the positive work done by the quantum force (dotted magenta curve) is significantly greater than that done by the electric field force (dashed red curve). In the excitation-ionization process of the BP, as shown in Fig. 6(b), the work done by the electric field force fluctuates around zero, and its contribution to the overall positive work is not obvious, and most of the positive work done by the resultant force comes from the quantum force. It suggests that the quantum force plays a more important role at the excitation moment and in the excitation-ionization process.

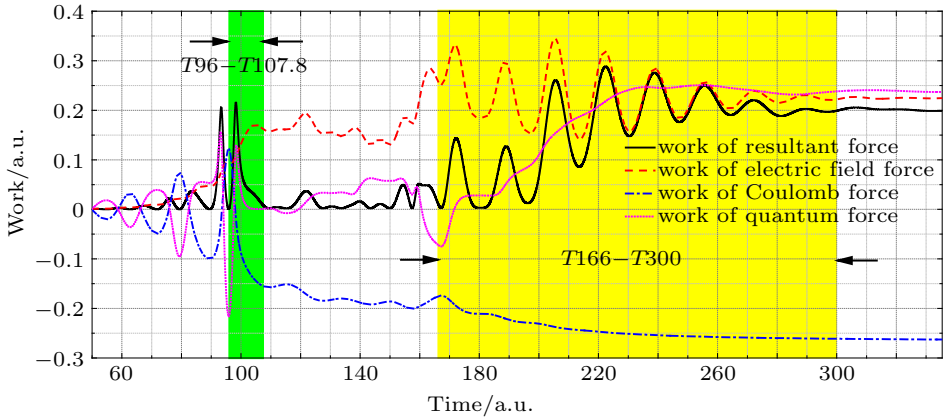


Fig. 5. Work done by the resultant force (solid black curve) and its component forces, i.e., electric field force (dashed red curve), Coulomb force (dash-dotted blue curve), and quantum force (dotted magenta curve).

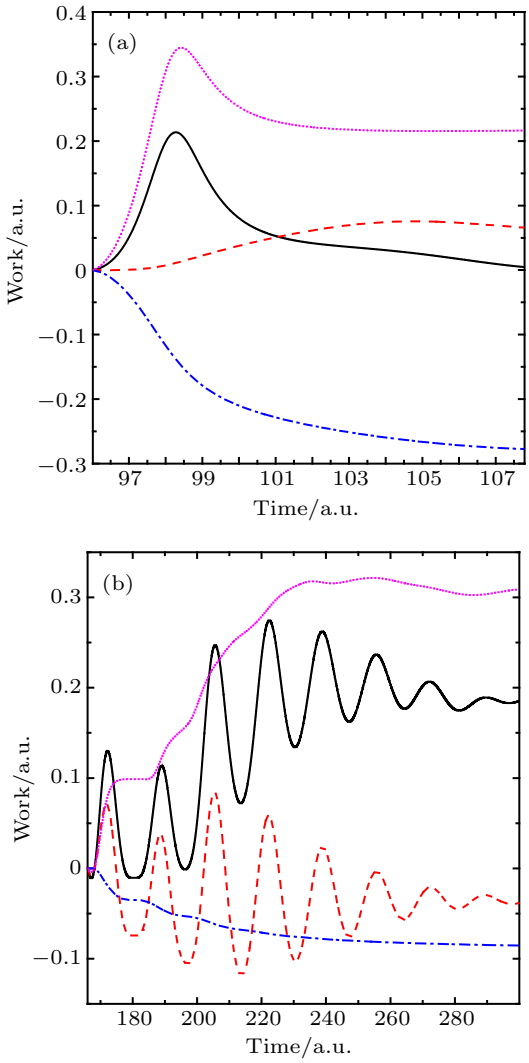


Fig. 6. Work done by the resultant forces (solid black curve) and its component forces, i.e., electric field force (dashed red curve), Coulomb force (dash-dotted blue curve), and quantum force (dotted magenta curve) (a) at excitation moment (from $t = 96$ a.u. to $t = 107.8$ a.u.) and (b) in the excitation-ionization process (from $t = 166$ a.u. to $t = 300$ a.u.).

Finally, we discuss the principle of work and energy for the three forces. According to the theorem of kinetic energy, the work done by the resultant force is equal to the increment of kinetic energy, i.e.,

$$A_{\rm Q} + A_{\rm C} + A_{\rm E} = \Delta E_{\rm K}, \tag{10}$$

where $\Delta E_{\rm K}$ represents the increment of kinetic energy. Therefore, the work done by the Coulomb force is

$$-A_{\rm C} = A_{\rm Q} + A_{\rm E} - \Delta E_{\rm K}. \tag{11}$$

Since the Coulomb force is a conservative force, the negative value of the work done by it is equal to the increment of the Coulomb potential energy,

$$-A_{\rm C} = \Delta V_{\rm C} = V_{\rm Cf} - V_{\rm Ci}, \tag{12}$$

where $V_{\rm Ci}$ and $V_{\rm Cf}$ are the Coulomb potential energies of the BP at the initial and arbitrary time, respectively. From Eqs. (11) and (12), we can obtain

$$A_{\rm Q} + A_{\rm E} = \Delta E_{\rm K} + \Delta V_{\rm C}. \tag{13}$$

Inspired by Eq. (13), we introduce the total energy of BP to conduct the analysis. Since the strength of the electric field is zero at the initial moment, and the initial kinetic energy of BP is zero, therefore,

$$\Delta E_{\rm K} = E_{\rm Kf} - E_{\rm Ki} = E_{\rm Kf} - 0 = E_{\rm Kf}, \tag{14}$$

where $E_{\rm Ki}$ and $E_{\rm Kf}$ are the kinetic energies of the BP at the initial and arbitrary time, respectively. The total energy of BP at arbitrary time is

$$E_{\rm total} = E_{\rm Kf} + V_{\rm Cf} + Q. \tag{15}$$

Combining Eqs. (11), (12), (13), and (15), we can obtain

$$\begin{aligned} E_{\rm total} &= E_{\rm Kf} + V_{\rm Cf} + Q \\ &= E_{\rm Kf} + A_{\rm Q} + A_{\rm E} - \Delta E_{\rm K} + V_{\rm Ci} + Q \\ &= A_{\rm Q} + A_{\rm E} + V_{\rm Ci} + Q, \end{aligned} \tag{16}$$

$$\begin{aligned} A_{\rm Q} + A_{\rm E} &= E_{\rm total} - V_{\rm Ci} - Q \\ &= E_{\rm Kf} + V_{\rm Cf} + Q - V_{\rm Ci} - Q \\ &= E_{\rm Kf} + V_{\rm Cf} - V_{\rm Ci} \\ &= \Delta E_{\rm K} + \Delta V_{\rm C}. \end{aligned} \tag{17}$$

From Eqs. (13) and (17), we find that the work done by the quantum force and electric field force is equal to the increment of kinetic energy and Coulomb potential energy, and the work done by non-conservative force is equal to the increment of mechanical energy of the system. Therefore we can arrive at the conclusion that the quantum force belongs to non-conservative force, and $\Delta E_{\rm K}$ in Eqs. (13) and (17) is equal to the increment of kinetic energy of the system. However, $\Delta E_{\rm K}$ is the increment of kinetic energy. Here comes the question: what is the relationship between it and the increment of kinetic energy of the system? We can define the kinetic energy of the system as (it is proved detailedly in Appendix A)

$$E_{\rm system\ kinetic} = E_{\rm Kf} + Q. \tag{18}$$

Therefore, the total energy in Eq. (15) can be written as the sum of the kinetic energy and potential energy of the system

$$E_{\rm total} = E_{\rm Kf} + V_{\rm Cf} + Q = E_{\rm system\ kinetic} + V_{\rm Cf}. \tag{19}$$

Consequently, equation (17) can also be written as

$$\begin{aligned} A_{\rm Q} + A_{\rm E} &= E_{\rm total} - V_{\rm Ci} - Q \\ &= E_{\rm Kf} + V_{\rm Cf} + Q - V_{\rm Ci} - Q \\ &= (E_{\rm Kf} + Q) - (E_{\rm Ki} + Q) + V_{\rm Cf} - V_{\rm Ci} \\ &= \Delta E_{\rm system\ kinetic} + V_{\rm Cf} - V_{\rm Ci} \\ &= \Delta E_{\rm system\ kinetic} + \Delta V_{\rm C} \\ &= \Delta E_{\rm K} + \Delta V_{\rm C}. \end{aligned} \tag{20}$$

It should be noted that the initial kinetic energy is zero, i.e., $E_{\rm Ki}=0$, and thus we can arrive at the conclusion that the increment of kinetic energy equals to that of the kinetic energy of the system

$$\Delta E_{\rm K}=\Delta E_{\text{system kinetic}}, \tag{21}$$

and the quantum potential energy actually comes from the kinetic energy of the system.

4. Conclusions

The resonance enhanced two-photon ionization process of hydrogen atom in intense laser field is studied by the BM method. We study the trajectory, energy of the BPs, and the work of the forces acting on the BPs in the ionization process over time. By monitoring the energy of the BP, it is found that the ionization process absorbs the energy of two photons, and the electric field force and quantum force play a major role. At the excitation moment and in the excitation-ionization process, the contribution of the quantum force is greater than that of the electric field force. We also discuss the principle of work and energy for BPs, and find that the electric field force and quantum force are non-conservative forces, and their work is equal to the increment of kinetic energy and Coulomb potential energy of the BPs. In addition, we also prove that the quantum potential energy actually comes from the kinetic energy of the system and the increment of kinetic energy equals to that of the kinetic energy of the system.

Appendix A

The total energy of the system is expressed by the Hamiltonian H, where $\langle\hat{T}\rangle$ is the mean value of the kinetic energy operator, and $\langle\hat{V}_{\rm Cf}\rangle$ is the mean value of the Coulomb potential energy. The wave-function can be written as $\psi(x,t)=R(x,t)\exp[{\rm i}S(x,t)]$ and the Hamiltonian can be expanded as

$$\begin{aligned}
E=\langle\hat{H}\rangle&=\langle\hat{T}+\hat{V}_{\rm Cf}\rangle=\langle\hat{T}\rangle+\langle\hat{V}_{\rm Cf}\rangle\\
&=\int\psi^*\hat{T}\psi{\rm d}V=\int\psi^*\left[-\frac{1}{2}\nabla^2\psi\right]{\rm d}V+\int R^2V_{\rm Cf}(x){\rm d}x\\
&=\int R{\rm e}^{-{\rm i}S/\hbar}\left[-\frac{1}{2}\nabla^2(R{\rm e}^{{\rm i}S})\right]{\rm d}V+\int R^2V_{\rm Cf}(x){\rm d}x\\
&=\int R{\rm e}^{-{\rm i}S}\left[-\frac{1}{2}\nabla\cdot\left(\nabla R{\rm e}^{-{\rm i}S}+\frac{\rm i}{\hbar}R\nabla S{\rm e}^{-{\rm i}S}\right)\right]{\rm d}V\\
&\quad+\int R^2V_{\rm Cf}(x){\rm d}x\\
&=\int R\left[-\frac{1}{2}\left(\nabla^2R+2{\rm i}\nabla R\cdot\nabla S+{\rm i}R\nabla^2S-{\rm i}R(\nabla S)^2\right)\right]{\rm d}V\\
&\quad+\int R^2V_{\rm Cf}(x){\rm d}x\\
&=\int R^2\left(-\frac{1}{2}\frac{\nabla^2R}{R}\right){\rm d}V-\frac{\rm i}{2}\int\nabla\cdot(R^2\nabla S){\rm d}V\\
&\quad+\int R^2\left(\frac{1}{2}(\nabla S)^2\right){\rm d}V+\int R^2V_{\rm Cf}(x){\rm d}x.
\end{aligned}\tag{A1}$$

The first, third, and fourth terms on the right side of Eq. (A1) are the mean values of quantum potential energy $\langle Q\rangle$, kinetic energy $\langle p^2\rangle/2m$, and Coulomb potential energy $\langle V_{\rm Cf}\rangle$, respectively. For the second term, according to the divergence theorem,

$$\int\nabla\cdot(R^2\nabla S){\rm d}V=\oint(R^2\nabla S)\cdot\boldsymbol{n}{\rm d}\boldsymbol{S}=0, \tag{A2}$$

we find that the mean value of the kinetic energy operator corresponds to that of the classical kinetic energy and quantum potential[23]

$$\langle\hat{T}\rangle=\frac{\langle p^2\rangle}{2m}+\langle Q\rangle. \tag{A3}$$

Therefore, the mean value of the total energy of the system can be expressed as

$$E=\langle\hat{H}\rangle=\langle\hat{T}+\hat{V}_{\rm Cf}\rangle=\frac{\langle p^2\rangle}{2m}+\langle Q\rangle+\langle V_{\rm Cf}\rangle. \tag{A4}$$

According to the relationship between the position and probability density of BP $|\psi(x,t)|^2=R(x,t)^2=\lim_{N\to\infty}\frac{1}{N}\sum_{k=1}^{N}\delta[x-x^k(t)]$,[23] we find that the mean value of the total energy of the system is equal to that of the energy of all BPs,[14]

$$\begin{aligned}
E=\langle\hat{H}\rangle&=\langle\hat{T}+\hat{V}_{\rm Cf}\rangle=\frac{\langle p^2\rangle}{2m}+\langle Q\rangle+\langle V_{\rm Cf}\rangle\\
&=\int R^2(\frac{1}{2}(\nabla S)^2){\rm d}x+\int R^2\left(-\frac{1}{2}\frac{\nabla^2R}{R}\right){\rm d}x+\int R^2V_{\rm Cf}(x){\rm d}x\\
&=\int_{-\infty}^{+\infty}\lim_{M\to\infty}\frac{1}{M}\sum_{k=1}^{M}\delta(x-x^k(t))(\frac{1}{2}(\nabla S)^2){\rm d}x\\
&\quad+\int_{-\infty}^{+\infty}\lim_{M\to\infty}\frac{1}{M}\sum_{k=1}^{M}\delta(x-x^k(t))\left(-\frac{1}{2}\frac{\nabla^2R}{R}\right){\rm d}x\\
&\quad+\int_{-\infty}^{+\infty}\lim_{M\to\infty}\frac{1}{M}\sum_{k=1}^{M}\delta(x-x^k(t))V_{\rm Cf}(x){\rm d}x\\
&=\lim_{M\to\infty}\sum_{k=1}^{M}\frac{1}{M}(\frac{1}{2}(\nabla S)^2)\Big|_{x=x^k(t)}\\
&\quad+\lim_{M\to\infty}\sum_{k=1}^{M}\frac{1}{M}\left(-\frac{1}{2}\frac{\nabla^2R}{R}\right)\Big|_{x=x^k(t)}\\
&\quad+\lim_{M\to\infty}\sum_{k=1}^{M}\frac{1}{M}V_{\rm Cf}(x)\Big|_{x=x^k(t)}\\
&=\lim_{M\to\infty}\frac{1}{M}\sum_{k=1}^{M}\left[\frac{1}{2}(\nabla S)^2-\frac{1}{2}\frac{\nabla^2R}{R}+V_{\rm Cf}(x)\right]\Big|_{x=x^k(t)}\\
&=\lim_{M\to\infty}\frac{1}{M}\sum_{k=1}^{M}E_k,
\end{aligned}\tag{A5}$$

where

$$\begin{aligned}
E_k&=\left[\frac{1}{2}(\nabla S)^2-\frac{1}{2}\frac{\nabla^2R}{R}+V_{\rm Cf}(x)\right]\Big|_{x=x^k(t)}\\
&=E_{\rm KF}+Q+V_{\rm Cf}=E_{\text{system kinetic}}+V_{\rm Cf}
\end{aligned}\tag{A6}$$

is the total energy of the k-th BP. In brackets, the first term is the kinetic energy of the BP, the second one is the quantum potential, and the third one is the Coulomb potential. Compared with Eq. (A1), the sum of the first two terms of Eq. (A6) is still equal to the kinetic energy of the system, that is to say, for a single BP, the quantum potential still belongs to the kinetic energy of the system.

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