From a quantum to a classical description of intense laser–atom physics with Bohmian trajectories

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*New Journal of Physics* 11 (2009) 113035 (10pp)

Received 11 August 2009

Published 20 November 2009

Online at [http://www.njp.org/](http://www.njp.org/)

doi:10.1088/1367-2630/11/11/113035

**Abstract.** In this paper, Bohmian mechanics is applied to intense laser–atom physics. The motion of an atomic electron in an intense laser field is obtained from the Bohm–Newton equation. We find that the quantum potential that dominates the quantum effect of a physical system becomes negligible as the electron is driven far from the parent ion by the intense laser field, i.e. the behavior of the electron smoothly tends towards classical soon after the electron is ionized. Our numerical calculations present direct positive evidence for semiclassical trajectory methods in intense laser–atom physics where the motion of the ionized electron is treated by classical mechanics, while quantum mechanics is needed before the ionization.
1. Introduction

In recent years, intense laser–atom physics has received increasing attention [1], due to nonlinear multiphoton phenomena such as high-order harmonic generation and above-threshold ionization. Without doubt, such multiphoton phenomena could be reproduced by resolving the time-dependent Schrödinger equation. In order to understand these phenomena intuitively, some semiclassical approaches, mixing classical and quantum arguments, have been proposed [2]–[5]. In the semiclassical approaches, the motion of ionized electrons is treated by classical dynamics directly, while quantum mechanics is used before the ionization. These semiclassical approaches have obtained much success in intense laser–atom physics, although there is no explicit evidence for their key assumption that the ionized electron can be treated by classical mechanics directly [6].

Bohmian mechanics (BM) [7]–[9], also called the quantum trajectory method [10], is another version of quantum theory, in which the trajectory concept is used to describe the motion of particles with the Bohm–Newton equation. It has been successfully used to study some fundamental quantum phenomena such as the two-slit experiment [11] and tunneling [12, 13]. Recently, Oriols [14] used BM to simulate the electron transport in mesoscopic systems. Sanz et al [15] applied this theory to atom surface physics. Makowski et al derived some central potentials [16] and two-dimensional noncentral potentials [17] from BM to investigate the exact classical limit of quantum mechanics [18]. BM has also been regarded as a fruitful approach to studying chaos [19, 20], due to its description of trajectories for the quantum system. It has also been successfully applied to intense laser–atom physics to study the dynamics of above-threshold ionization [21] and high-order harmonic generation [22].

The only difference between the Bohm–Newton equation and the Newton equation is that there is an extra term in the Bohm–Newton equation called the quantum potential. When the quantum potential is negligible, the Bohm–Newton equation will reduce to the standard Newton equation and then the motion of the particles can be described by classical mechanics.
In this paper, BM is applied to intense laser–atom physics. We first obtain the electron quantum trajectories of an atomic ensemble from the Bohm–Newton equation. Next, we study how the quantum potentials change as the electrons are driven away from the parent ion by the laser field. We find that the quantum potentials tend to be small and then become completely negligible soon after the electrons are ionized. In this case, the Bohm–Newton equation reduces to the Newton equation. Then the motion of electrons can be described by the classical equation of motion. Thus, our results present direct positive evidence for the previous semiclassical trajectory methods in intense laser–atom physics where the motion of ionized electrons is treated by classical mechanics directly, while quantum mechanics is needed before the ionization. On the other hand, our numerical results clearly show how far the electron is from the core when it is ionized, while the position of the electron at the time of ionization is usually chosen to be 0 (the position of the core) in the semiclassical approaches [2].

2. Quantum trajectory formalism of Bohmian mechanics

BM [7, 8] is derived from a subtle transformation of the time-dependent Schrödinger equation:
\[ i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = (-\frac{\hbar^2}{2m} \nabla^2 + V)\psi(\mathbf{r}, t), \]
where \( V \) is the ordinary potential and \( \psi(\mathbf{r}, t) \) is the time-dependent wavefunction. Firstly, the wavefunction can be written in the polar form \( \psi(\mathbf{r}, t) = R(\mathbf{r}, t)e^{iS(\mathbf{r}, t)/\hbar} \), where \( R \) and \( S \) are real functions. Secondly, the wavefunction is inserted into the time-dependent Schrödinger equation. The real part of the resulting equation has the form
\[
\frac{\partial S}{\partial t} + \frac{V}{2m} + \frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} = 0
\]
and the imaginary part is
\[
\frac{\partial \rho}{\partial t} + \nabla (\rho v) = 0,
\]
where \( \rho(\mathbf{r}, t) = R^2(\mathbf{r}, t) \) and \( v = \nabla S(\mathbf{r}, t)/m \). Equation (1) is similar to the classical Hamilton–Jacobi equation, except that it has an extra term, \( -\frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} \). This term, denoted by \( Q(\mathbf{r}, t) \) in this paper, is usually called the quantum potential. Equation (2) looks like the classical continuity equation. Hence, a Bohm–Newton equation of motion for a Bohmian particle can be constructed as
\[
md\frac{d^2 \mathbf{r}}{dt^2} = -\nabla (V + Q)
\]
from the standpoint of classical mechanics. The motion of a particle is determined by the ordinary potential \( V \) and the quantum potential \( Q \), which plays a crucial role for the appearance of quantum phenomena. Obviously, when the quantum potential \( Q \to 0 \) in equation (3), the Bohm–Newton equation will reduce to the standard Newton equation. Then the motion of particle can be described by classical mechanics.

In fact, the trajectory of the particle can evolve from a much simpler equation of motion than equation (3) [7, 8]:
\[
\frac{d\mathbf{r}}{dt} = \frac{\nabla S(\mathbf{r}, t)}{m}.
\]
To obtain the trajectory of a particle, we need to know its phase \( S(\mathbf{r}, t) \) and its initial position. According to BM, the initial distribution of a particle in an ensemble is given by \( |\psi(\mathbf{r}, 0)|^2 \).
3. Intense laser–atom interaction

The system we consider in this paper is a hydrogen atom in an intense laser field. The Schrödinger equation for the system can be written as (atomic units are used throughout)

\[ i \frac{\partial \psi(r, t)}{\partial t} = [H_0(r) + H_I(r, t)] \psi(r, t). \]  

(5)

Here \( H_0(r) \) is the field-free hydrogen atom Hamiltonian and \( H_I(r, t) \) is the intense laser–atom interaction: \( H_0(r) = -\frac{1}{2} \frac{\partial^2}{\partial r^2} + \frac{\hbar^2}{2m} \frac{l^2}{r^2} - \frac{1}{r} \), \( H_I(r, t) = -r \cdot E(t) = -z E(t) \), where the laser is the linearly polarized field \( (E \parallel z) \) and \( E(t) \) is the laser field profile. Due to the linearly polarized laser field, the magnetic quantum number \( m \) of the atom is a good quantum number, so the three-dimensional atom can be simplified to a two-dimensional model (see figure 1(a)). In our study, we use the grid method and the second-order split-operator technique to numerically solve the time-dependent Schrödinger equation (5), which has been described in detail by Tong and Chu [23]. The laser field profile is

\[ E(t) = \begin{cases} 
    E_0 \sin^2 \left( \frac{\pi t}{6T} \right) \sin(\omega t), & 0 \leq t \leq 3T, \\
    E_0 \sin(\omega t), & t > 3T, 
\end{cases} \]  

(6)
Figure 2. The electron trajectory in the spatial coordinate with the corresponding initial position \( r_0 \). The initial positions \( r_0 \) in the polar coordinate are, from top to bottom: (1.0 au, \( \pi/30 \)), (2.0 au, \( \pi/30 \)), (1.0 au, \( \pi/10 \)) and (1.0 au, 2\( \pi/15 \)), respectively.

where \( T = 2\pi/\omega, E_0 \) and \( \omega \) are the electric field amplitude and angular frequency, respectively (see figure 1(b)). Here, we take \( E_0 = 0.1 \) au and \( \omega = 0.2 \) au. The initial state \( \psi(r, 0) \) of the system is in the ground state of the field-free hydrogen atom.

4. Result

4.1. Electron trajectory from the Bohm–Newton equation

After numerically obtaining the time-dependent wavefunction \( \psi(r, t) \), and then the phase \( S(r, t) \), we can obtain the trajectory of an electron by integrating equation (4) with its initial value at position \( r_0 \) (see appendix A). In this way, we can obtain an ensemble of electron trajectories according to the initial distribution of electrons \( |\psi(r, 0)|^2 \), where \( \psi(r, 0) \) is the ground state of the field-free hydrogen atom. Explicitly, we present four trajectories of electron with the corresponding initial positions in figure 2. Let us take one electron trajectory as an example with \( r_0 = (1.0 \text{ au}, \pi/30) \) in the polar coordinate. The path of the electron has the following characteristic in spatial coordinates: the motion is irregular when the electron is near the parent ion; after the electron has been driven far from the parent ion by the intense laser field, it travels in a straight line with a little oscillation. The reason why the motion of the electron keeps oscillating while the electron is far away from the parent ion is due to the existence of the laser field. The other trajectories with different initial positions have a similar character, as shown in figure 2.

In figure 3, we show the projections of electron trajectory in the \( z \)- and \( x \)-directions as functions of time. In figure 3(a), two curves \( z(t) \) and \( x(t) \) are obtained from the electron trajectory with \( r_0 = (1.0 \text{ au}, \pi/30) \). At the beginning, both \( z(t) \) and \( x(t) \) are near the core. After time \( t \approx 130 \text{ au} \), \( z(t) \) becomes a regular wave curve and \( x(t) \) appears to be a straight
Figure 3. Projections of electron trajectory in the $z$- and $x$-directions as functions of time. The corresponding initial positions of the electrons are from (a) to (d): (1.0 au, $\pi/30$), (2.0 au, $\pi/30$), (1.0 au, $\pi/10$) and (1.0 au, $2\pi/15$), respectively. It is obvious that the motion of the electron in the $x$-direction is uniform, while its motion in the $z$-direction has undulations as the electron is far from the core. The reason for the $z$-undulation is due to the existence of the laser field ($E \parallel z$).

line. Similarly, we have obtained the projections of three other electron trajectories with initial positions $r_0$ (see figures 3(b)--(d)). All of them have a similar character as that in figure 3(a).

4.2. Time-dependent quantum potential in intense laser–atom physics

In section 2, we demonstrated that the quantum potential $Q(r, t)$ together with the ordinary potential $V(r, t)$ dominates the motion of a particle in BM, and the quantum potential plays a crucial role for the appearance of quantum phenomena. If the value of $Q(r, t)$ smoothly becomes negligible ($Q \to 0$), equation (3) will reduce to the Newton equation and then the motion of the electron can be described by classical mechanics.

Now we study the change of quantum potential of an atomic electron as it is driven away from the laser field. After numerically obtaining the time-dependent wavefunction $\psi(r, t)$ and the electron trajectories $r(t)$, we calculate the change of quantum potential $Q(r(t))$ (see appendix B). In figure 4, we show the time-dependent values of the quantum potential $Q(r(t))$ and the ordinary potential $V(r(t)) = -\frac{1}{r} - zE(t)$ with the corresponding electron initial position $r_0$. Here we take the electron with $r_0 = (1.0 \text{ au}, \pi/30)$ as an example (see figure 4(a)). The value of the quantum potential is initially comparable with that of the ordinary potential. After some time, e.g. about 100 au, the quantum potential smoothly decreases and becomes negligible, particularly after $t \approx 133$ au. The changes of quantum potential of three other electrons are presented in figures 4(b)--(d), and they have similar character as that in

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4.3. Classical description after the electron has been ionized

As we have shown above, the Bohm–Newton equation of electron approaches the Newton equation in intense laser–atom physics, as the electron is driven far from the parent ion. In previous semiclassical approaches of intense laser–atom physics, the ionized electron motion is usually treated by classical dynamics, while quantum mechanics applies before the ionization [2]–[5], [24]. Here, we want to verify whether the motion of an electron can be treated by classical mechanics or not, i.e. whether the quantum potential becomes negligible or not, as it becomes ionized.

In figure 5, we show the total energies of electrons (including kinetic energy, Coulomb potential and quantum potential) with different initial positions. When the total energy becomes positive, the electron will be ionized. Here, we take the electron with \( r_0 = (1.0 \text{ au}, \pi/30) \) as an example (see figure 5(a)). Initially, the total energy is less than zero, i.e. the electron is bounded by the core. After time \( t \approx 103 \text{ au} \), the total energy becomes positive but then turns negative at time \( t \approx 120 \text{ au} \). The reason for this again may be that an electron with low energy is not far enough from the core and is recaptured by the parent ion with a photon emitted when the laser field reverses. The total energy becomes positive again and higher than before at
Figure 5. The time-dependent total energies of electrons (including kinetic energy, Coulomb potential and quantum potential) with the initial positions (1.0 au, $\pi/30$), (2.0 au, $\pi/30$), (1.0 au, $\pi/10$) and (1.0 au, $2\pi/15$), respectively.

$t \approx 133$ au and thereafter, i.e. the electron can never be recaptured again by the parent ion. On the other hand, in figure 4(a), we found that the value of the quantum potential of the electron tends to be negligible soon after $t \approx 133$ au. (The corresponding distance between the ionized electron and the core is about 16.2 au; see figure 3). Similarly, in figures 5(b)–(d) and 4(b)–(d), we find that when the electrons are ionized, the corresponding quantum potentials tend to be negligible. Therefore, our numerical solutions show that the quantum potential is negligible as the ionized electron is driven far from the core and thus the motion of the ionized electron is dominated by classical mechanics. In this way, our work presents direct positive evidence for the semi-empirical assumption in the semiclassical approaches of intense laser–atom physics, such as the three-step model [2] and Feynman’s path–integral approach in the strong field approximation [24], in which the motion of an ionized electron is treated by classical mechanics directly. Furthermore, the Bohmian trajectory method can help us to find how far the electron is from the core when it was ionized, while the position of the electron at the time of ionization is usually chosen to be 0 (the position of the core) in the semiclassical approaches [2].

5. Discussion

As has been discussed above, the quantum potential dominates the quantum behavior of a physical system. In previous work on a quasi-static model of strong-field multiphoton ionization [2], a dual procedure is considered to describe the multiphoton phenomena in intense laser–field physics. First a tunneling model is applied to obtain the ionization rate and describes the formation of a sequence of wavepackets. The second part of the quasi-static procedure uses classical mechanics to describe the evolution of an electron wavepacket.
It has been pointed out that if only classical mechanics is considered in the whole process, it cannot give the ionization rate correctly, unless a quantum tunneling process is allowed [25]. This is consistent with our numerical results in this paper: the quantum potential cannot be ignored before the ionization, i.e. quantum mechanics is needed to study the behavior of the electron before the ionization, but the motion of an ionized electron can be described by classical mechanics directly.

6. Remarks

It is interesting that Mahmoudi et al [26] have studied free-electron quantum signatures in intense laser fields by looking for negativities in the Winger distribution. They concluded that the quantum signatures of the free electron get washed away, provided the dipole approximation is made. In this way, their work presents more evidence for the treatment of an ionized electron in the semiclassical approaches of intense laser–atom physics.

Acknowledgments

We thank J B Delos and L You for helpful discussions. This work was supported by National Basic Research Program of China under grant No. 2006CB921203.

Appendix A. Electron quantum trajectory

In this appendix, we show how to obtain the electron quantum trajectory from equation (4). First, equation (4) can be expressed as (atomic units are used)

\[
\frac{dr}{dt} = \nabla S(r, t) = \text{Im} \frac{\nabla \psi(r, t)}{\psi(r, t)},
\]

where \( \psi(r, t) = R(r, t)e^{iS(r, t)} \) and \( \text{Im}(f) \) is the imaginary part of \( f \). In our study, \( \psi(r, t) \) is gained by numerically solving the time-dependent Schrödinger equation (5), using the grid method and the second-order split-operator technique, which has been described in detail by Tong and Chu [23]. Then we use the Runge–Kutta method to evolve equation (A.1) to obtain the electron quantum trajectory.

In our numerical procedure, the range of the variable \( r \) in the radial direction is confined to \((0, 150 \text{ au})\). In the grid method, the numbers of grid points are 350 in the \( r \) direction and 51 in the \( \theta \) direction. The time step for the evolution is 0.01 au.

Appendix B. Time-dependent value of quantum potential

After obtaining the time-dependent wavefunction \( \psi(r, t) \) and the electron quantum trajectory \( r(t) \) with the corresponding initial position \( r_0 \), we can numerically obtain the value of the quantum potential \( Q(r(t)) \) along the trajectory \( r(t) \). First, the quantum potential \( Q(r, t) \) can

\[3\text{ One recent work also concluded that the classical trajectory method should be improved further by including nonclassical effects, see Botheron and Pons [25].} \]
be written as

$$Q(r, t) = -\frac{1}{2} \nabla^2 R(r, t) = -\frac{1}{2} \left[ \text{Re} \left( \frac{\nabla^2 \psi(r, t)}{\psi(r, t)} \right) + \left( \text{Im} \frac{\nabla \psi(r, t)}{\psi(r, t)} \right)^2 \right], \quad (B.1)$$

where $\text{Re}(f)$ is the real part of $f$. Secondly, inserting the quantum trajectory $r(t)$ into equation (B.1), we can numerically obtain the value of quantum potential $Q(r(t))$. 

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