Classical trajectory Monte Carlo investigation for Lorentz ionization of H (1s)*

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Lorentz ionization of H(1s) is investigated by classical trajectory Monte Carlo (CTMC) simulation. The effect of the transverse magnetic field on the considered process is analyzed in terms of the time evolution of interactions in the system, total electron energy, and electron trajectories. A classical mechanism for the ionization is found, where the variation of the kinetic energy of the nuclei is found to be important in the process. Compared with the results of tunneling ionization, the classical mechanism becomes more and more important with the increase of the velocity of the H-atom or the strength of the magnetic field.

Keywords: Lorentz ionization, tunneling ionization, classical trajectory Monte Carlo

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1. Introduction

If an atom moves into a region of space where there is a constant magnetic field which is perpendicular to the atom velocity, a constant electric field appears in the reference frame in which the atom or ion is at rest (we call it the atom frame) as a result of the Lorentz transformation. The atom would be ionized by the electric field, which has been known as Lorentz ionization.[1,2] In the study of magnetic confinement fusion, Lorentz ionization of atoms at high excited states is an important mechanism to trap neutral beam atoms.[3] It may happen in astrophysics where magnetic fields as strong as 10^2 T–10^5 T (white dwarfs), or even 10^7 T–10^9 T (neutron stars) can be found.

So far, people have made many discussions about the atomic structure in a strong magnetic field[4,5] and have much more understanding about the ionization under an electric field than about Lorentz ionization. Numerous investigations have been carried out into the ionization of atoms under the applied electric fields,[6–8] which include laser pulses, microwave fields, electro-static fields, and so on. Usually, if an electric field is applied, the applied field provides energy for the electron to overcome the Coulomb potential barrier[6] and the electron becomes free through some mechanisms, such as tunnel, photon, multiphoton, and over-barrier ionization. As for Lorentz ionization, as far as we know, Popov *et al.*[1,2] have studied it based on their results about the ionization of atoms in combined electric and magnetic fields. They obtained some semi-classical results for ionization rate, considering the mechanism of tunnel ionization (TI) caused by the constant electro-static field in the atom frame. To our knowledge, if the applied field is the magnetic field, the electron cannot get kinetic energy from the field and the Coulomb potential cannot be influenced by the magnetic field since the Lorentz force does not influence the atom. It is interesting to ask where does the energy for the electron to be free come from in Lorentz ionization and whether the motion of the nuclei plays an important role in the process. In addition, it is still not well understood whether some other mechanisms besides tunnel ionization operate in Lorentz ionization. In this paper, we explore these problems.

The classical trajectory Monte Carlo (CTMC) simulation is known to be a good method to simulate the ionization of the atom or molecule under the applied fields, by which good results can usually be obtained in many cases.[9–12] In this work, CTMC is used to investigate the Lorentz ionization of H (1s) in the lab frame where the energy conservation of the system can be kept very well. The effect of the transverse magnetic field in the process is analyzed in terms of trajectories, such as the electron energy and the kinetic energy of the proton. Though TI is a quantum effect which CTMC cannot describe, our simulation gives a quite different mechanism. It is a classical one where the variation of the kinetic energies of the nuclei is found to be important, which enhances the electron kinetic energy relative to the proton high enough to overcome the Coulomb potential and make the electron free. Compared with the TI results in Ref. [1], it is found that the mechanism competes with TI and becomes more and more important with the increase of the atom velocity or the applied magnetic field strength.

This paper is organized as follows: we present a brief description of the CTMC method in the next section. In Section 3, the results for the ionization time distribution are presented and the comparison with TI result in Ref. [1] is made.

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Section 4 presents some trajectories to analyze the classical ionization mechanism. The distribution for the variation of the proton kinetic energy and the momentum distributions of the ionized electrons are given in Section 5. Finally, some conclusions are presented. Atomic units ($e = m_e = \hbar = 1$) are used in this work unless otherwise explicitly indicated.

2. Brief description of CTMC

In CTMC, a coordinate system needs to be established and both the initial coordinates and the momenta of the proton and electron should be fixed first. In the simulation, the origin of the coordinate system is at the initial position of the proton of H(1s) atom. We use v_p to denote the initial velocity of the proton, which is along the z direction. The initial electron coordinates and momenta relative to the proton are determined by the usual field-free micro-canonical distribution.[13] The applied magnetic field B is along the x direction. Then, the atom enters the region of the magnetic field with an initial velocity v_p, and the evolution of the system under the magnetic field and the Coulomb field is obtained by solving the classical motion equations of the proton and electron. For simplicity, we use v_e and v_t to denote the electron and proton velocities at time t, respectively, and define the total energy of the system E and the electron energy relative to the proton E_{et} as $E = v_e^2/2 + m_p v_t^2/2 - 1/R_{et}$ and $E_{et} = (v_e - v_t)^2/2 - 1/R_{et}$, respectively. Here R_{et} is the distance between the electron and the proton, and m_p is the mass of the proton. The integration of motion equations is carried out (from time $t = 0$) up to time when $t = 10^6$ for unionized trajectories ($E_{et} < 0$) or $R_{et} > 10^5$ for ionized trajectories ($E_{et} > 0$). Without the magnetic field, the conservation of the total energy E is well done with a variation about 10^{-4}. However, sometimes, it will become quite different if the transverse magnetic field is applied. The electron motion will be distorted so intensely that sometimes the electron is very close to the proton, for example, $R_{et} < 10^{-3}$. For such a short distance, the Coulomb force becomes very strong and the electron velocity is very high, which may induce a high error in numerical calculations. To get reliable results, 10^5 trajectories are calculated for each B and v_p with soft Coulomb potential chosen to ensure that $|\Delta E| < 10^{-4}$ where $\Delta E = E_0 - E_f$ with E_0 and E_f being the total energy E at initial and final time, respectively. This ensures $|\Delta E| \ll E_{ion}$, where E_{ion} is the ionization energy of H(1s). In the simulation it is found that E_{et} oscillates with time, which will be explained later. Furthermore, E_{et} is always positive after a long time when it first becomes positive at some time. We define t_{ion} as the first time when $E_{et} > 0$.

3. Ionization time distribution and the comparison with TI

First, we present the t_{ion} distribution of the ionization event number for different values of v_p at $B = 0.149$ in Fig. 1. Similar results are observed for $B = 0.0106$, which are not shown here. Figure 1 indicates that more ionization events are produced and the ionization happens earlier with v_p increasing. Besides this, there is always a peak corresponding to each v_p. Although it is not clear why there is a peak in the time distribution, we can make a comparison of the peak position t_{peak} of the distribution with the TI time t_{TI}, which is the reciprocal of the ionization rate in Ref. [1]. All these are listed in Table 1 together with those for $B = 0.0106$. In Table 1, the classical ionization probability P_{ion} is defined as the ratio of the event number with the total trajectory number, and the t_{TI} with the symbol star is obtained by extrapolating the curve in Fig. 1 of Ref. [1] and the others from Table IV or Eq. (14) in Ref. [1]. The table indicates that there are two mechanisms responsible for ionization: one is tunnel ionization and the other is classical since our simulation is classical. The two mechanisms are complementary and competitive with each other. Usually, t_{peak} is shorter than t_{TI} and P_{ion} rises up rapidly with v_p increasing, which indicates that more electrons can be ionized in a classical way before the tunneling ionization occurs with higher v_p. This means the classical ionization mechanism becomes more and more important than tunneling ionization when v_p becomes higher and higher.

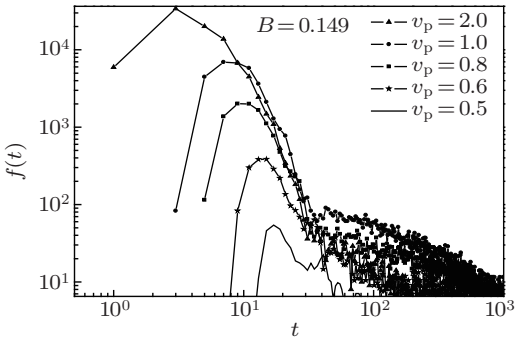


Fig. 1. Time distribution of the ionization event number.

Table 1. Classical ionization probability P_{ion}, peak position t_{peak}, and ionization time t_{TI} for different v_p and B.

	v_p	P_{ion}	t_{peak}	t_{TI}
$B = 0.0106$	20	74%	3.64	10.15
	15	47%	7.0	12.0
	10	13.6%	13.6	53.2
	9	7.7%	16.5	67.8
	8	3.0%	18.4	137.6
$B = 0.149$	2	94.3%	3.0	4.65
	1	46.0%	7.0	18.8
	0.8	24.0%	9.4	21.5
	0.6	8.2%	14.5	101.3
	0.5	2.5%	16.5	1200

4. Ionization trajectories

In order to know more about the classical mechanism, many ionization trajectories are analyzed and two typical cases are found, which are corresponding to the increasing or decreasing of the proton kinetic energy and plotted in Figs. 2 and 3, respectively. Figure 2(a) shows the evolution of E_{et} and ΔE_{kT} for a trajectory where E_{kT} is decreased finally. Here, ΔE_{kT} is defined as $m_{\rm p}(v_t^2 - v_{\rm p}^2)/2$, which is the increment of the proton kinetic energy. Figure 2(b) gives the evolution of the electron kinetic energy E_{ke} and $1/R_{et}$ for the same trajectory. Figure 2 indicates that both E_{ke} and E_{kT} are decreased in the process, and R_{et} becomes larger and larger gradually although it oscillates with time. In the process, the Coulomb potential overcomes and the electron is ionized at last. This mainly corresponds to the case of slow $v_{\rm p}$ or small B. In Fig. 3, ΔE_{kT} is always positive, and E_{ke} becomes smaller and smaller with time evolution. Meanwhile, $(v_{\rm e} - v_t)^2/2$ is increased high enough to overcome the Coulomb potential and the electron becomes free finally. This kind of trajectories mainly corresponds to the case of rapid $v_{\rm p}$, for example, $v_{\rm p} = 2.0$ and $B = 0.149$. Those trajectories with E_{kT} decreased and E_{ke} increased are also observed, which are not shown here.

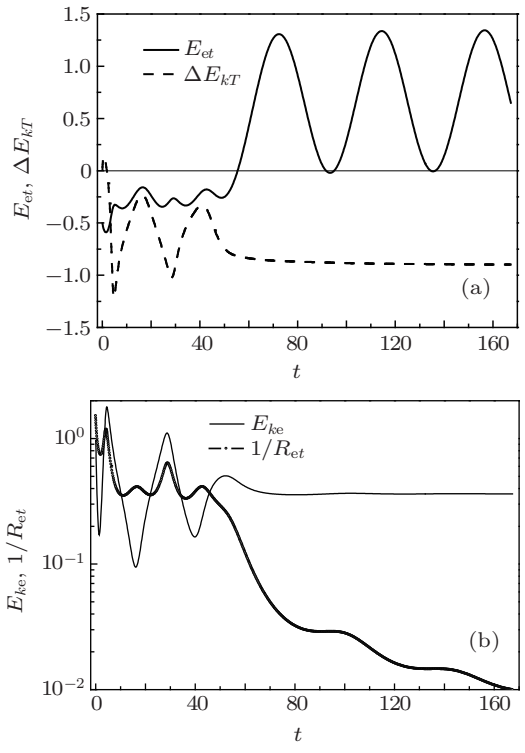


Fig. 2. A trajectory with E_{kT} decreased. Time evolution of E_{et} and ΔE_{kT} (a), and E_{ke} and $1/R_{et}$ (b).

In addition, all the trajectories indicate that E_{et} may be negative after the first time when it becomes positive. It remains oscillating with time although its minimum rises up gradually and becomes positive at last. The behavior of such oscillations is due to the longitudinal-Lorentz force. From the definition of E_{et}, we know that

$$E_{et} = \frac{1}{2}(v_{\rm ex}^2 + v_{\rm ey}^2 + v_{\rm ez}^2 + v_{\rm p}^2) - v_{\rm ez}v_{\rm p} - \frac{1}{R_{et}}.$$

Because of the transverse magnetic field, both $v_{\rm ey}$ and $v_{\rm ez}$ always oscillate with time, which results in the change of E_{et}. This is more understandable in the proton frame if we notice that the applied constant electro-static field accelerates and decelerates the electron since the electron moves back and forth in the field.

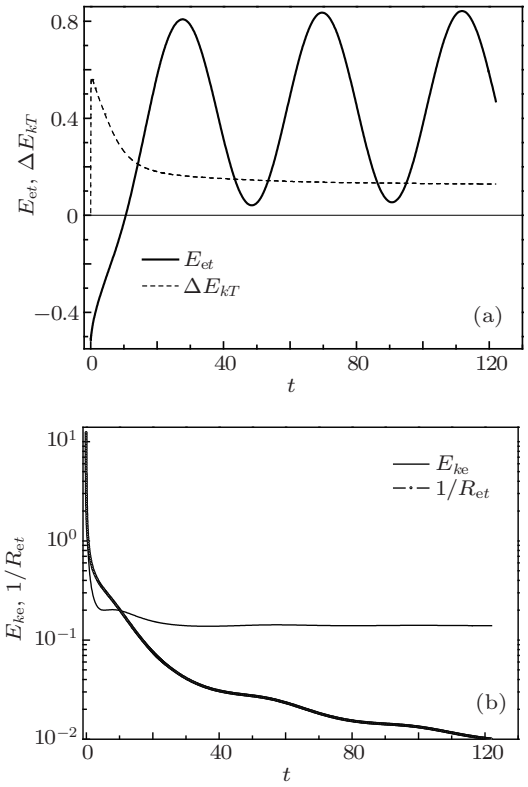


Fig. 3. A trajectory with E_{kT} increased. Time evolution of E_{et} and ΔE_{kT} (a), and E_{ke} and $1/R_{et}$ (b).

5. Distribution for ΔE_{kT} and the electron momentum

Since the variation of E_{kT} is important for Lorentz ionization, which is different from the case in which only the electric field is applied, figure 4 plots the distribution of ΔE_{kT} for each $v_{\rm p}$ with $B = 0.149$. Obviously, the distribution becomes wider and wider with the increase of $v_{\rm p}$, which is due to the wider and wider distribution for the initial kinetic energy of the electron. From the figure, it is seen that when $v_{\rm p}$ is small, for example, $v_{\rm p} = 0.6$, the proton kinetic energy is always decreased ($\Delta E_{kT} < 0$). However, with the increase of $v_{\rm p}$, more and more events with $\Delta E_{kT} > 0$ appear. To find this, we define α_T as the ratio of the number of those ionization events for $\Delta E_{kT} < 0$ to the total ionization event number. A similar definition of $\alpha_{\rm e}$ is made for electrons. Table 2 gives the results of α_T and $\alpha_{\rm e}$ for different values of $v_{\rm p}$ and B.

The value of B is given in the parentheses in the first column of Table 1. From this table we can obtain

i) When v_p is small or $v_p^2/2 << E_{ion}$, for example, $v_p = 0.5$, both α_T and α_e are equal to 1.0. This is understandable since the electron kinetic energy is not sufficient to overcome the Coulomb potential energy barrier. In this case, both electron and proton must lose a part of their kinetic energies for the ionization.

ii) With the increase of v_p, $v_p^2/2$ gradually becomes close to or even greater than E_{ion}. In this case, both α_T and α_e obviously become lower than 1.0, for example, $\alpha_T = 0.80$ and $\alpha_e = 0.72$ when $v_p = 1.0$ and $B = 0.149$. This is because the electron can become free at the cost of a part of its kinetic energy. Meanwhile, another part of the electron kinetic energy is lost to enhance the proton kinetic energy by Lorentz force. This results in more and more ionization events being produced with v_p increasing, where the proton kinetic energy is increased.

iii) When v_p is very high, for example, $v_p^2/2 \gg E_{ion}$, both the values of α_T and α_e are close to 0.5 at $v_p = 20.0$. It can be understood because the loss of a small part of the electron or proton kinetic energy is sufficient to overcome the Coulomb potential in this case. This results in the proton kinetic energy being reduced in about one half of the ionization events and increased in the other half.

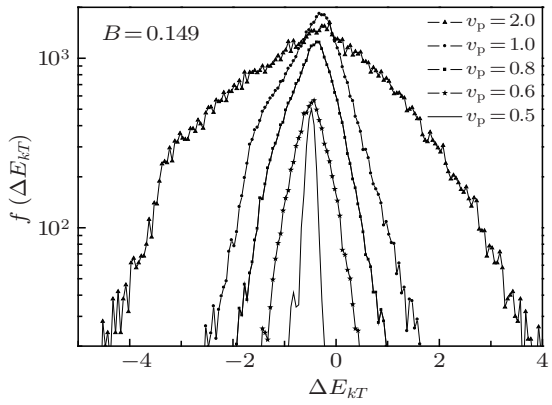


Fig. 4. Distribution for the change of the proton kinetic energy E_{kT}.

Table 2. The results α_T and α_e for different v_p and B.

$B = 0.0106$			$B = 0.149$		
v_p	α_T	α_e	v_p	α_T	α_e
20	0.49	0.53	2	0.63	0.61
15	0.52	0.52	1	0.80	0.72
10	0.54	0.52	0.8	0.86	0.80
9	0.56	0.54	0.6	0.90	0.88
8	0.60	0.53	0.5	1.0	1.0

It is interesting to see whether an ionization event would happen for a very small v_p and a very high B, so that the total energy of the system E is negative but with a very strong constant electro-static field in the atom frame. For this problem, some simulations with $v_p = 0.01$ and $B = 50.0$ have been performed and no ionization events are observed. In this case, the Coulomb potential cannot be overcome by the full loss of the total kinetic energy of the system so that no ionization occurs. But the electron becomes ionized if the simulation is done in the atom frame. This means that it is not suitable to study the problem in the atom frame if v_p is very small.

Since different ionization mechanisms may lead to different momentum distribution for the ionized electrons, the momentum distributions obtained from our simulation are presented in Fig. 5 for $v_p = 2.0$ and $B = 0.149$, where v_{ex} is the electron velocity in x direction and $v_{normal} = \sqrt{v_{ey}^2 + v_{ez}^2}$. Similar results can be found for $v_p \geq 1.0$. The final kinetic energy of the electrons is found to be mainly distributed around $0.5v_p^2$. It is easy to see that v_{ex} and v_{normal} are distributed around 0.0 and v_p, respectively. This is because the electron can move away from the proton either along the magnetic field or in the opposite direction. Also, the electron is ionized around $v_{ey} = 0$ and $v_{ez} = v_p$, which turns out to be the observed v_{normal} distributed by Lorentz force. It is different with $v_{ex} = 0$, $v_{ey} = 0$, and $v_{ez} = v_p$, which is converted from the atom frame to the lab frame according to the TI results in Ref. [1].

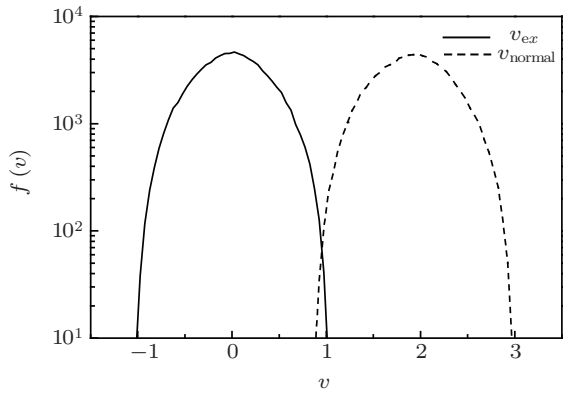


Fig. 5. Momentum distribution of the ionized electrons for v_{ex} and v_{normal} in arbitary units.

In addition, some comparisons are made for the simulation results in the atom frame between the classical Lorentz ionization and the ionization caused by the constant electrostatic field, which is equal to v_pB and in y direction according to Lorentz transformation. Almost the same t_{ion} distributions are obtained but with much more ionization events caused by the constant electro-static field especially for a low v_pB case. Under such an electric field, the ionized electron certainly can be accelerated without limitation. But for Lorentz ionization, the final kinetic energy of the ionized electron will be a constant. This can be seen from the motion equation of an electron

$$\frac{dv_{ex}}{dt} = 0, \quad \frac{dv_{ey}}{dt} = -v_{ez}B - v_pB, \quad \frac{dv_{ez}}{dt} = -v_{ey}B,$$

where Coulomb potential is ignored if R_{et} is large enough. It is easy to see that $v_{ex}^2 + v_{ey}^2 + (v_{ez} + v_p)^2$ is a constant.

In summary, a classical mechanism is found for Lorentz ionization, which is quite different from the usual tunneling

ionization. In the mechanism both the variations of the kinetic energy of the electron and proton, which is caused by the longitudinal Lorentz force, are important to the ionization. This mechanism becomes increasingly essential with the increase of the atom velocity or the strength of the transverse magnetic field.

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References

[1] Popov V S, Karmakov B M and Mur V D 1999 *J. Exp. Theor. Phys.* **88** 902
[2] Popov V S, Karmakov B M and Mur V D 1998 *J. Exp. Theor. Phys.* **86** 860
[3] Futch J R A H and Damm C C 1967 *Plasmas Physics* **9** 423
[4] Zhao J J, Wang X F and Qiao H X 2011 *Chin. Phys. B.* **20** 053101
[5] Pilón H O 2012 *Phys. Lett. A* **376** 1608
[6] Landau L D and Lifshitz E M 1977 *Quantum Mechanics* (Problem 1) (Pergamon: Oxford)
[7] Keldysh L V 1960 *Sov. Phys. JETP* **20** 1307
[8] Ammosov M V, Delone N B and Krainov V P 1986 *Sov. Phys. JETP* **64** 1435
[9] Hansen J P, Lu J, Madsen L B and Nilsen H M 2001 *Phys. Rev. A* **64** 033418
[10] Villeneuve D M, Ivanov M Yu and Corkum P B 1996 *Phys. Rev. A* **54** 736
[11] Cohen J S 2001 *Phys. Rev. A* **64** 043412
[12] Liu J, Ye D F, Chen J and Liu X 2007 *Phys. Rev. Lett.* **99** 013003
[13] Abrines P and Percival I C 1966 *Proc. Phys. Soc. London* **88** 861
[14] Olson R E and Salop A 1977 *Phys. Rev. A* **16** 531