國立交通大學

物理研究所

碩士論文

古典蒙地卡羅方法探討強雷射與原子系統的交互作用

Classical Trajectory Monte Carlo Method Study of Atomic Dynamics under Intense Laser Pulse

研 究 生 ： 楊政道

指導教授 ： 江進福 教授

中 華 民 國 九 十 八 年 六 月

古典蒙地卡羅方法探討強雷射與原子系統的交互作用

Classical Trajectory Monte Carlo Method Study of Atomic Dynamics under Intense Laser Pulse

研 究 生：楊政道　　Student：Cheng-Tao Yang

指導教授：江進福 教授　　Advisor：Tsin-Fu Jiang

國 立 交 通 大 學

物 理 研 究 所

碩 士 論 文

A Thesis

Submitted to institute of Physics

College of Science

National Chiao Tung University

in partial Fulfillment of the Requirements

for the Degree of

Master

in

Physics

June 2009

Hsinchu, Taiwan, Republic of China

中華民國九十八年六月

古典蒙地卡羅方法探討強雷射與原子系統的交互作用

研 究 生：楊政道　　　　　　　　　　　　　　指導教授：江進福

國立交通大學物理研究碩士班

摘要

在這篇論文中我們利用古典蒙地卡羅方法來探討原子系統與強快速雷射的交互作用及雷射中磁場效應的貢獻。一般原子再高強度雷射的照射下會產生 High Harmonic Generation 現象。此現象在高強度快速雷射下及考慮雷射磁場下所造成的影響，將是我們探討的問題。

Classical Trajectory Monte Carlo Method Study of Atomic Dynamics under Intense Laser Pulse

Student : Cheng-Tao Yang **Advisor :** Tsin-Fu Jiang

Institute of physics
National Chiao Tung University

ABSTRACT

In this thesis, we use Classical Trajectory Monte Carlo method to study the atomic dynamics under short intense pulse and magnetic effect. When an atom is exposed to an intensity laser pulse, it develops a time-dependent dipole moment and radiates a series of odd harmonics of incident laser frequency. This phenomenon of harmonic generation has been observed over wide ranges of laser intensity (e.g. $10^{13} \sim 10^{16}\, {}^{W}\!/_{cm^2}$). However, current laser systems can produce very short (femtoseconds) and high intensity pulses stronger than $10^{17}\, {}^{W}\!/_{cm^2}$. Under such high-intensity and short time laser, the dynamics of atom and the effect of the magnetic filed component are important, and not yet well studied.

致謝

首先我要感謝我的指導教授江進福老師，帶領我去學習研究並給予我許多幫助及指導。感謝研究室的徐煥鈞學長及鄭世達學長，在我每次有問題的時候耐心與我討論並分享自身的經驗，在我需要的時候給予協助及及建議並分享自身的經驗。也感謝研究室的同學陳明輝、張繼允、吳明軒、鄭玉書，謝謝他們的情義相挺，最後要感謝家人與女友的信任及肯定，謝謝大家。

Index

Index of Figure

Chapter 1

Introduction

In atomic physics, the strong laser is defined when its intensity is in the range of $10^{13} \sim 10^{16}\ \mathrm{W}\!\!\big/_{cm^2}$, i.e. the electric field of the laser is approaching the order of electric field of nucleus exerting on the electron. Atoms driven by an strong laser pulse can produce a series spectrum at odd multiples of the incident laser frequency. This process, known as high harmonic generation, has been thoroughly studied over above laser intensity. Recently developed laser systems can produce very short and high intensity pulses, for example some as short as a few to tens of femto-seconds with intensities up to $10^{17}\ W\!\!\big/_{cm^2}$. An atom under such strong laser, the Lorentz force on an electron is given by

$$\vec{F} = q\vec{E} + \frac{q}{c}\vec{v} \times \vec{B} \tag{1}$$

It shows that the force on an electron due to the magnetic field $\vec{B}$ has an effect reduced by the ratio $v\!\big/_c$ compare to the electric field. In such high-intensity laser fields, the electrons may gain velocities of the order of the velocity of light. In this regime magnetic field forces is comparable to electric field forces. In this thesis we study the femto-seconds pulse and the effect of magnetic field in intense pulse on a hydrogen atom simulated by Classical Trajectory Monte Carlo method.

We will first briefly introduce the background of high harmonic generation (HHG) in chapter 2, and in chapter 3 we will use Classical Trajectory Monte Carlo method (CTMC) to approach the high harmonic generation phenomenon of hydrogen atom, in chapter 4, we use the CTMC to study classical hydrogen atom interact with femto-seconds pulse, and in chapter 5 we study the effect of magnetic in the femto-seconds intense pulse, finally we summary the result in chapter 6.

Chapter 2

High Harmonic Generation

High harmonic generation (HHG) is an intriguing and experimentally well-confirmed phenomenon which results from the nonlinear response of a microscopic system to a strong laser field. There are two striking features have been identified, namely, the occurrence of a "plateau", i.e., the almost constant intensity of the harmonics over a wide range of orders N, and sharp "cutoff" at a certain maximum order $N_{\max}$ of harmonics.

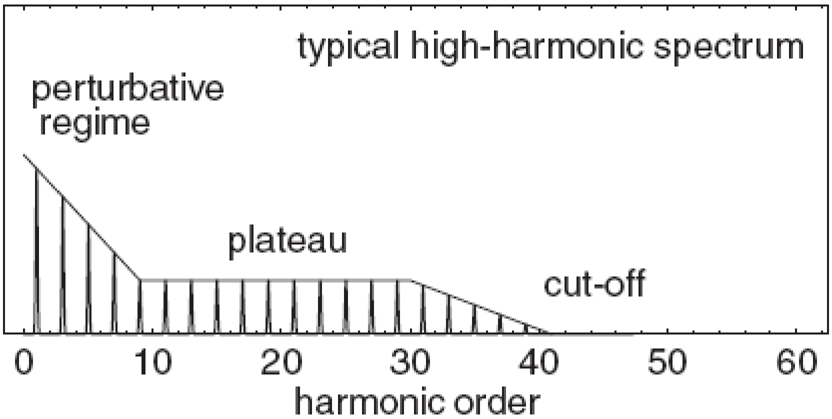


Fig.2-1 typical high-harmonic spectrum

The basic generation mechanism for high harmonics can be explained using semi-classical so-called "Simple-man model" or "Three–step model" by Corkum(1993) and Kulander(1993) et al.

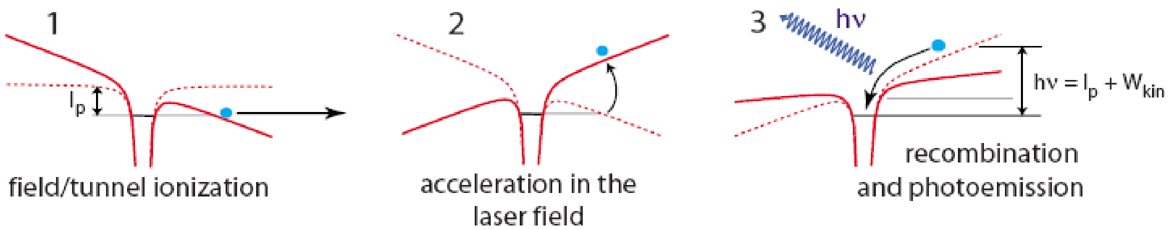


Fig.2-2 three-step model

In the strong field of high-intensity laser pulse, bound electrons from atoms or molecules are field ionized close to maximum of the laser field and set free with zero initial velocity. There are then accelerated away from their nucleus by the same electric field and move on classical electron trajectories in a laser field. When the electric field reverses, electron accelerated back to nucleus, and photon emitted if electron-ion recombination occur.

The energy of photon is determined by the ionization potential of atom and kinetic energy of the electron, i.e.,

$$\hbar\omega = I_p + E_{kin}(\phi)\,, \tag{2}$$

where I_p is the ionization potential of atom, $E_{kin}(\phi)$ is kinetic energy of the electron, and ϕ is the phase of the electric field at the moment of ionization. The high frequency cutoff at a certain maximum order $N_{\max}$ of harmonics radiation can be determined by the maximum photon energy. i.e.,

$$E_{cutoff} = \hbar w_{\max} = I_p + 3.17U_p\,, \tag{3}$$

where U_p is the ponderomotive energy, i.e., the average quiver energy of the electron in the laser field,

$$U_p = \frac{\mathrm{e}^2 E_0{}^2}{4m_e w^2} \propto I\lambda^2\,. \tag{4}$$

An electron ionized by tunneling at $\phi \approx 17^{\circ}, 197^{\circ}$,etc., will arrive at the ion with maximum kinetic energy ($3.17U_p$) .

The region where the high–order harmonics have been found in experiments corresponds to the onset of strong ionization. In other word ionization and high order harmonics generation are closely linked.

The HHG phenomenon has been studied over wide ranges of laser intensity (e.g. $10^{13} \sim 10^{16}\ \mathrm{W}/_{cm^2}$). In high intensity laser field electrons may gain velocities of the order of the velocity of light, and in this region magnetic field force becomes comparable to electric force. When the laser intensity is larger than $10^{17}\ W/_{cm^2}$, the effect of the magnetic filed component is important, and if the intensity is too high, one may also have to consider relativistic effect, but the true relativistic effects, are $(v/_c)^2$, and the magnetic effect from Lorentz force

$$\vec{F} = e(\vec{E} + \frac{\vec{v}}{c} \times \vec{B}) \tag{5}$$

is $(v/_c)$ only. There is, however, an intensity region between non-relativistic and fully relativistic domains, and the influence of the magnetic field is required.

We can use the ratio of the ponderomotive energy of the electron to its rest energy, this can help us to determine the intermediate regime,

$$U_p = \frac{\mathrm{e}^2 {E_0}^2}{4m_e w^2} = \frac{m_e c^2}{4} \left(\frac{e^2 {E_0}^2}{m_e w^2}\right) \frac{1}{m_e c^2} = \frac{m_e c^2}{4} \left(\frac{eE_0}{m_e wc}\right)^2 \tag{6}$$

$$\frac{U_p}{m_e c^2} = \frac{1}{4} \left(\frac{eE_0}{m_e wc}\right)^2 \tag{7}$$

$$U_p \approx \frac{1}{2} m_e v^2 \tag{8}$$

from (7) and (8) we have

$$\left(\frac{v}{c}\right)^2 \approx \frac{1}{2} \left(\frac{eE_0}{m_e wc}\right) \tag{9}$$

The relativistic effect is significant only for the ratio of the ponderomotive energy of the electron to its rest energy approach unit, and for a laser with a wavelength 800nm, the magnetic effect can occur at $\sim 10^{15}\ W/_{cm^2}$, whereas true relativistic effects become important until $\sim 10^{17}\ W/_{cm^2}$.

Chapter 3

Classical Trajectory Monte Carlo Method

The magnitude of the electric field of the laser radiation is comparable to the field binding an electron to an atom, and perturbation theory breaks down.

The high harmonic generation is widely studied by direct solve time dependent $Schrödinger - Equation$ (TDSE)

$$i\frac{\partial}{\partial t}\psi(\vec{r},t)=\left(-\frac{1}{2}\nabla^{2}-\frac{1}{r}+\vec{r}\cdot\vec{E}(t)\sin(wt)\right)\psi(\vec{r},t). \tag{10}$$

But there are many numerical problems.

First of all, the time step for integration is very small because the electron's ionization may occur rapidly over a relatively small number of laser cycles. Second the singular point of Coulomb potential. Usually it is approximated by soft core potential. Third, when solve the partial differential equation the numerical method is limited by the numerical boundary value. In this project, we use Classical Trajectory Monte Carlo method to study the atomic dynamics under short intense pulse and magnetic effect.

In this paper, we consider a classical hydrogen atom, with an infinite mass nucleus fixed at the origin of the coordinates, interacting with a highly intense laser field that is linearly polarized along z axis, and with the electric field component $E(t)$. For multi-electron atoms, one generally has to limit the calculations to that for a single electron in effective potentials as represent, the influence of the remaining atomic electrons. This approach is called the single active electron approximation.

CTMC method for a classical hydrogen-atom

The assumption of the classical Monte Carlo method is that the atom can be represented by an ensemble of electron in a micro-canonical distribution with an energy distribution function $\rho(E)$ given by

$$\rho(E) \propto \delta(E - E_0)\,, \tag{11}$$

where E_0 denotes the internal energy of the hydrogen atom,

$$E_0 = (-0.5/n)^2\, a.u\,, \tag{12}$$

with n being the principal quantum number.

The CTMC method consists for three steps:

1. Set up classical electron distribution to quantum distribution of hydrogen atom with quantum number “n”.
2. The numerical integration of Hamilton’s equations of motion
3. Calculate the mean value of length dipole approximation

Generation of the initial condition

To describe the quantum system by classical mechanics, it is important to generate a set of electron’s position and momentum distribution. It is possible to use Kepler’s equation of planetary motion to represent classical hydrogen atom initial conditions. It can be specified by the binding energy of the electron, and five additional parameters $\varepsilon, \xi, \theta, \phi, \eta$ randomly distributed in the following range:

$$0 \le \varepsilon^2 \le 1,\ 0 \le \theta_n \le 2\pi,\ -\pi \le \eta \le \pi,\ -\pi \le \phi \le \pi,\ -1 \le \cos\theta \le 1\,. \tag{13}$$

Here ε is eccentricity, and θ_n is a parameter of the orbital proportional to time, and θ, ϕ, η are Euler angles. A random distribution of θ_n corresponds to equal probability of the atom having any phase in its periodic motion. The eccentric angle ξ is more geometrically useful than θ_n and is determined by solving Kepler’s equation $\theta_n = \xi - \varepsilon \sin\xi$.

The atomic initialization can be completed by following step. (1) for a given quantum state, $|n\rangle$ is specified by the binding energy E_0 ; (2) choosing the eccentricity ε and placing the orbit in some arbitrary orientation; (3) locating the "electron" at the eccentric angle ξ on the orbit; the position and momentum of electron can be fixed by a solution of Kepler's equation; and (4) performing the rotation specified by the Euler angles θ, ϕ, η .

Hence the initial coordinates and momentums are given by $\vec{C}^0 = A\vec{C}_0^0$ and $\vec{P}^0 = A\vec{P}_0^0$, where

$$\vec{C}_0^0 = \begin{bmatrix} 0 \\ a(1-\varepsilon^2)^{1/2}\sin\xi \\ a(\cos\xi - \varepsilon) \end{bmatrix},\ a = \frac{Z}{2E_0}\ ,)^{1/2} \tag{14}$$

$$\vec{P}_0^0 = \begin{bmatrix} 0 \\ b(1-\varepsilon^2)^{1/2}\cos\xi/(1-\varepsilon\cos\xi) \\ -b\sin\xi/(1-\varepsilon\cos\xi) \end{bmatrix},\ b = (2mE_0 \tag{15}$$

$$A = \begin{bmatrix} -\sin\phi\cos\eta + \cos\phi\cos\theta\cos\eta & -\sin\phi\cos\eta - \cos\phi\cos\theta\sin\eta & \cos\phi\sin\theta \\ \cos\phi\sin\eta + \sin\phi\cos\theta\cos\eta & \cos\phi\cos\eta - \sin\phi\cos\theta\sin\eta & \sin\phi\sin\theta \\ -\sin\theta\cos\eta & \sin\theta\sin\eta & \cos\theta \end{bmatrix} \tag{16}$$

In the above, Z is the nuclear charge of the atom, and m is the mass of electron in the atom.

In practice, we need five random parameters to generate a set of initial condition, and there are three most important criteria for a good uniform random number generator we need to know. First, a good generator should have a long period, which should be close to the range of the integers on the computer. Second, a good generator should have good randomness. There should be only a very small correlation among all the numbers generated. One way to illustrate the behavior of the n-data point correlation is to plot x_n and x_{n+1} in an x-y plane, a good random number generator will have a very uniform distribution of the points. Finally, a good generator has to be very fast. In fact, one may need a lot of random numbers in order to have good statistical result. At this point, the speed of the generator is very important factor.

The numerical integration of equations of motion

In order to use classical mechanics to describe the evolution of an electron's wave packet, we need to solve the set of Hamilton's equation of motion, and calculate the expectation value. For simplicity, we shall consider the electric field of laser first, and check the result in CTMC method. Next consider the magnetic field of laser, and check HHG result.

After preparing the initial condition of electron, the motion of the electron under intense laser field is determined via the Hamiltonian. For classical hydrogen atom with electric field in z-direction, with dipole approximation,

$$H = \frac{p^2}{2m} - \frac{e^2}{r} + eE_0 z f(t)\sin(wt+\phi), \tag{17}$$

let $f(t)=1$ first, and there are six coupled Hamilton's equation of motion,

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i},\ \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \tag{18}$$

$$\begin{aligned} \frac{dp_x}{dt} &= -\frac{x}{r^3}\ , & \frac{dx}{dt} &= p_x \\ \frac{dp_y}{dt} &= -\frac{y}{r^3}\ , & \frac{dy}{dt} &= p_y \\ \frac{dp_z}{dt} &= -\frac{z}{r^3} - E_0\sin(wt+\phi)\ , & \frac{dz}{dt} &= p_z \end{aligned} \tag{19}$$

For each set of initial conditions, the Bulirsch-Stoer method is applied to calculate the classical trajectories of the electron's motion. The Bulirsch-Stoer method is applied here, because it can obtain high-accuracy solutions to ordinary differential equations with minimal computational. In Bulirsch-Stoer method, a single Bulirsch-Stoer step takes us from t to $t+\Delta$, where Δ is supposed to be quite large, not at all infinitesimal distance. A large interval Δ is spanned by different sequences of finer and finer sub-steps. Their results are extrapolated to an answer that is supposed to correspond to infinitely fine sub-steps, and the integrations are done by the modified midpoint method.

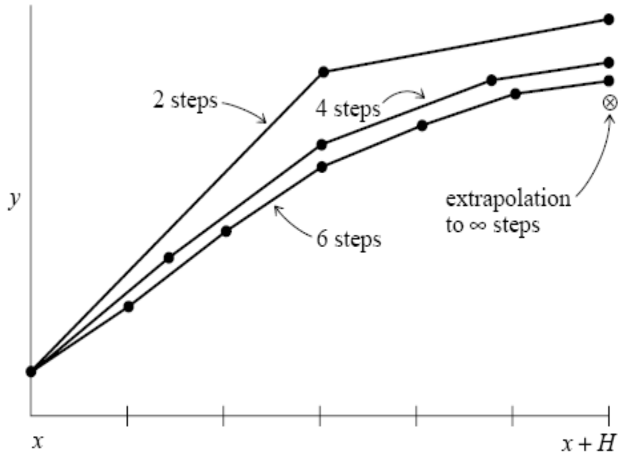


Fig.3-1 Bulirsch-Stoer method: 1. A large interval H is spanned by different sequence of finer and finer sub-steps 2.Integrations are done by the modify midpoint method 3.Extrapolation technique is rational function or polynomial extrapolation.

The mean value of length dipole approximation

To obtain the harmonic spectra requires the evaluation of the time dependent dipole moment of the atom .Length dipole,

$$\langle \psi | z | \psi \rangle = \bar{z}(t) = \frac{1}{N} \sum_{k=1}^{N} z_k(t), \tag{20}$$

and its power spectrum,

$$I(w) = \frac{1}{T} \left| \int_0^T e^{iwt} \bar{z}(t) dt \right|^2 . \tag{21}$$

For a set of trajectories, if the distance of motion from nucleus is greater than 50a.u. and electron’s energy is greater than zero, then these trajectories are treated as free electrons under laser field, i.e., the electron is ionized. Only trajectories with no-ionization are used to calculate the mean value of length dipole.

Note that if one follows an ionization trajectory over the large number of laser cycle, the corresponding spectrum is dominated by the continuous background which ultimately washed out the harmonics. This observation supports the view that harmonics generation is more efficient for bounded trajectories or, more precisely, when the electronic motion is close to the nucleus that is sufficient acceleration to generate the harmonics. For classical hydrogen atom with electric field in z-direction, over 30-cycle laser pulse with $w = 0.057a.u.\, E_0 = 0.15a.u.$,

$$H = \frac{p^2}{2m} - \frac{e^2}{r} + ezE(t) \tag{22}$$

In Fig.4 and Fig.5, there are three harmonics spectrum feature. The spectrum can be divided into three parts: the perturbative regime at low orders, the plateau for intermediate order, and the cut-off at the high orders. In this result, we can use CTMC method to approach HHG phenomenon very well.

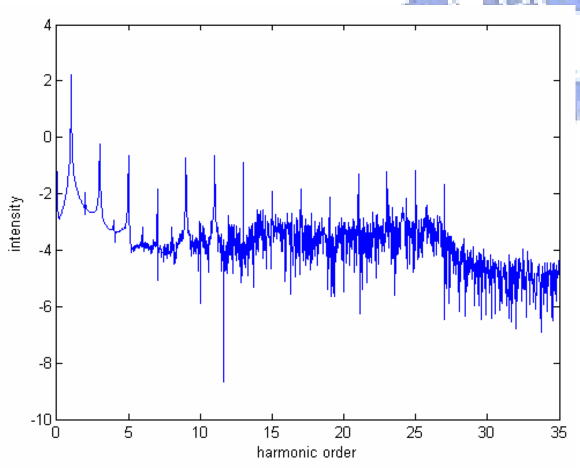


Fig.3-2 high harmonic generation spectrum

$E(t) = E_0 \sin(wt + \phi)$

$E_0 = 0.15a.u.\;\; w = 0.043a.u. t = 30T_{laser}$

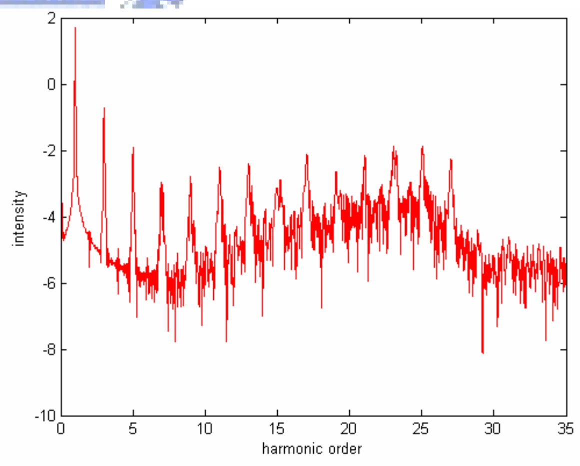


Fig.3-3 HHG spectrum

$$E(t) = E_0 (\sin(\frac{\pi t}{30T_{laser}}))^2 \sin(wt + \phi)$$

$E_0 = 0.15a.u.\;\; w = 0.043a.u.\;\; t = 30T_{laser}$

Chapter 4

Short pulse

Here, in order to use Classical Trajectory Monte Carlo method to study the atomic dynamics under intense pulse, the laser intensity will be very high, and this can let electrons have very strong ionizations, and the HHG spectrums are washed out by strong ionizations. To avoid the total electron ionizations, we focus our attention on the short intense pulse.

For the laser with $w = 0.057 a.u. E_0 = 0.15 a.u.$ interacts with a ground state hydrogen atom over 4-cycle laser pulses. From Fig.4-1, Fig.4-2, and Fig.4-3, for short intense pulses, the high harmonic generation's spectrum resolution is not very well, and the periodicity is gone for high order radiations, and the intensity is lower than 30-cycles. From Fig. 4-4, we also find that for short pulses the high harmonic generation spectrums depend on laser phase ϕ strongly. For same conditions but with different phase, the spectrums can be totally unlike.

For short pulses, the high-harmonic spectrums are generated by a single electron trajectory close to the peak, so that the periodicity of the high harmonic generation process is completely suppressed, and for short pulses the different phase corresponds to different laser forms. In this result, if the electron wants tunnel the potential, i.e., ionization, it must fit it's the max velocity and position on the laser field maximum, then it may be free and driven by field to generate HHG radiation, but for long pulse, the field action time is long enough that the phase doesn't pay a role on the duration. The low harmonic spectrums are generated by a single electron close to nuclear, i.e., the electron's motions are strongly controlled by the nucleus, and periodicity of the high harmonic generation is still kept. From above results, we find for short pulse such as few-cycle laser, the high harmonic generation is governed directly by the intense pulse evolution.

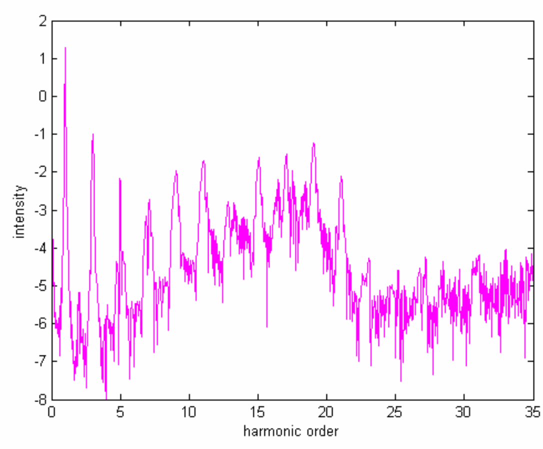


Fig.4-1 HHG spectrum

$$\vec{E}(t) = E_0(\sin(\frac{\pi t}{30T_{laser}}))^2 \sin(wt+\phi)\hat{z}$$

$$E_0 = 0.15a.u. \quad w = 0.057a.u. \quad t = 30T_{laser} \quad \phi = 0$$

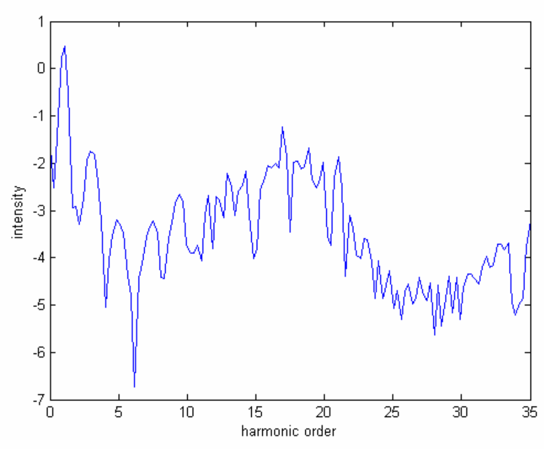


Fig.4-2 HHG spectrum for short pulse

$$\vec{E}(t) = E_0(\sin(\frac{\pi t}{4T_{laser}}))^2 \sin(wt+\phi)\hat{z}$$

$$E_0 = 0.15a.u. \quad w = 0.057a.u. \quad t = 4T_{laser} \quad \phi = 0$$

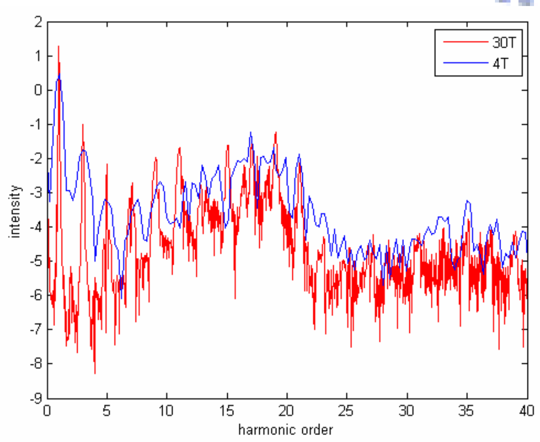


Fig.4-3 spectrum for 30-cycle and 4-cycle

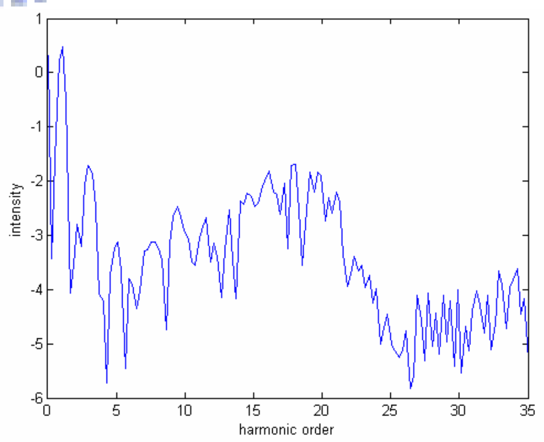


Fig.4-4 HHG spectrum with different phase

$$\vec{E}(t) = E_0(\sin(\frac{\pi t}{4T_{laser}}))^2 \sin(wt+\phi)\hat{z}$$

$$E_0 = 0.15a.u. \quad w = 0.057a.u. \quad t = 4T_{laser} \quad \phi = \frac{\pi}{2}$$

Here, we also change the ionization criterion to study the spectrum. We have try different criterion, for instance, the electron's energy is positive and the distance to the nucleus $r > 50a.u.$, $r > 100a.u.$, and $r > 200a.u.$ in Fig.4-5. We find that the high-harmonic generation spectrum is depend on ionization criterion, this result supports that only for the electronic motion is close to the nucleus that is sufficient acceleration to generate the harmonics.

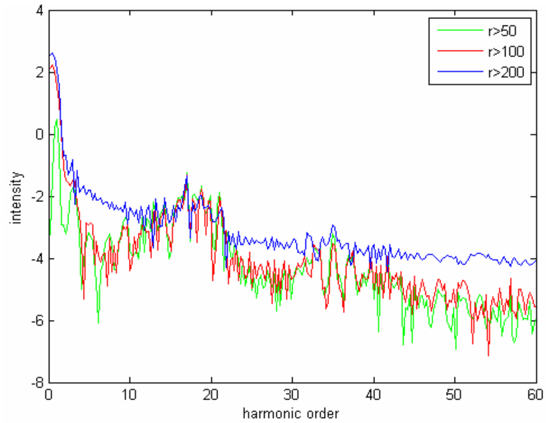


Fig.4-5 HHG spectrum with different ionization criterions

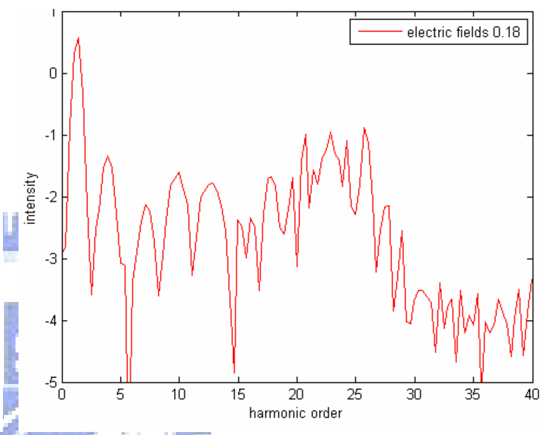


Fig.4-6 HHG spectrum with $w = 0.057a.u.$ $E_0 = 0.18a.u.$ over 4-cycle

Now for the intense laser with $w = 0.057a.u.$ $E_0 = 0.18a.u.$ over 4-cycles, In Fig.4-6, high harmonic generation's spectrum resolution is still not very well. The low order spectrums are still controlled by the nucleus, but for high-order harmonic, the high intense pulses can let electrons velocities become very high, and ionizations are very strong. i.e., electrons radius are far from the core and the coulomb potential effect is small for these electrons. Under such conditions, the magnetic effect can be important in high-order harmonic, i.e., plateau regime.

Chapter 5

Magnetic field effect

In atomic physics, electromagnetic fields of optical frequencies are usually quite adequately described in terms of the dipole approximation, base on the inequality

$$a_0 / \lambda << 1 , \tag{23}$$

where a_0 is the Bohr radius, and λ is the wavelength of the radiation. This means that the phase of a traveling plane wave can be approximated as $wt - \vec{k} \cdot \vec{r} \approx wt$. In order to study the magnetic effect, an atom is subjected to a sufficiently intense fields, the dipole approximation may not valid, because the full relativity effect the spatial dependence is strong. To study the regime in which the effect of the magnetic field should be account for, but where the full relativity is not required. We need an electromagnetic gauge in which both electric and magnetic fields are present, and where both are retained only within the dipole approximation.

Electric and Magnetic fields in dipole approximation

In classical electrodynamics the scalar potential can be written as

$$\Phi = -\vec{r} \cdot \vec{E}(\varphi), \quad \varphi \equiv wt - \vec{k} \cdot \vec{r} , \tag{24}$$

in addition, there is a vector potential of very similar appearance, given by

$$\vec{A} = -\hat{k}\left[\vec{r} \cdot \vec{E}(\varphi)\right], \ \hat{k} \equiv \frac{\vec{k}}{wc} \tag{25}$$

That is, $\hat{k}$ is a unit vector in the direction of propagation. These potential describe completely the electric and magnetic field with full $wt - \vec{k} \cdot \vec{r}$ phase dependence,

$$\vec{E} = -\nabla\Phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}, \ \vec{B} = \nabla \times \vec{A} \tag{26}$$

The vector potential $\vec{A}$ above contains spatial dependence in the

$\vec{r}\cdot\vec{E}(\varphi)$ combination as well as in the phase $\varphi \equiv wt - \vec{k}\cdot\vec{r}$. This means that even in the dipole approximation limit $\varphi \to wt$, the vector potential retains important spatial dependence. Now we take the dipole limit of the above potentials,

$$\Phi = -\vec{r}\cdot\vec{E}(wt),\ \ \vec{A} = -\hat{k}\left[\vec{r}\cdot\vec{E}(wt)\right] \tag{27}$$

we obtain

$$\vec{E} = -\nabla\Phi - \frac{1}{c}\frac{\partial\vec{A}(wt)}{\partial t} = \vec{E}(wt) + \vec{k}\left[\vec{r}\cdot\frac{d\vec{E}(wt)}{d(wt)}\right] \tag{28}$$

The extra term is seen to drop out in the dipole approximation, since

$$\left|\frac{d\vec{E}(wt)}{d(wt)}\right| = O(|\vec{E}|),\ \ |\vec{k}|\cdot|\vec{r}| = O(2\pi\frac{a_0}{\lambda}) << 1 \tag{29}$$

the magnetic field follows directly from the curl of vector potential,

$$\vec{B}(wt) = \hat{k}\times\vec{E}(wt)\,. \tag{30}$$

These potential provide both electric and magnetic fields of a plane wave in the correct phase, amplitude, and vector relationships, but within the dipole approximation.

Interaction Hamiltonian

The Hamiltonian for a hydrogen atom in a plane-wave field is now,

$$H = \frac{1}{2m}\left[\vec{p} - \frac{\hat{k}}{c}e\vec{r}\cdot\vec{E}(wt)\right]^2 - \frac{e^2}{r} - e\vec{r}\cdot\vec{E}(wt)\,. \tag{31}$$

Here, we consider ground state hydrogen under electric field in z-direction and magnetic field in x-direction, over 4-cycle laser pulse with $w = 0.057a.u.\, E_0 = 0.17a.u.$

$$\begin{aligned}\vec{E}(t) &= E_0(\sin(\frac{\pi t}{4T_{laser}}))^2\sin(wt+\phi)\hat{z}\\ \vec{B}(t) &= \frac{E_0}{c}(\sin(\frac{\pi t}{4T_{laser}}))^2\sin(wt+\phi)\hat{x}\end{aligned} \tag{32}$$

The blue line is the electric field only, and the red line is electric and magnetic fields

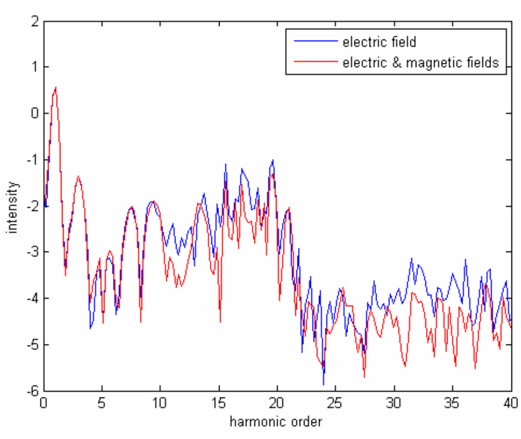


Fig.5-1 $CTMC$ trajectories = 10000

ionization = r > 50 and energy > 0

$E_0 = 0.17 a.u.$

$w = 0.057 a.u.$

$t = 4T_{laser}$

$\phi = 0$

(1) Electric field

ionization = 6981

(2) Electric and Magnetic fields

ionization = 6974

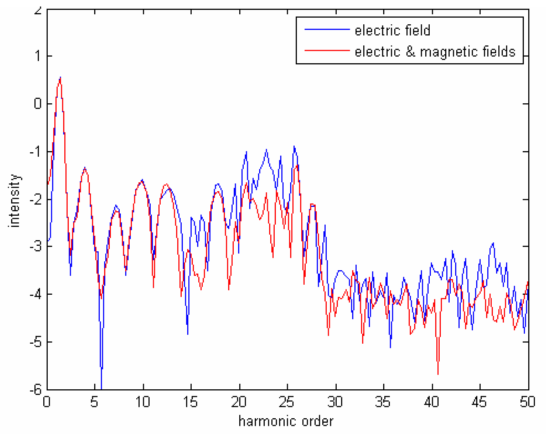


Fig.5-2 $CTMC$ trajectories = 10000

ionization = r > 50 and energy > 0

$E_0 = 0.18 a.u.$

$w = 0.057 a.u.$

$t = 4T_{laser}$

$\phi = 0$

(1) Electric field

ionization = 8713

(2) Electric and Magnetic fields

ionization = 8684

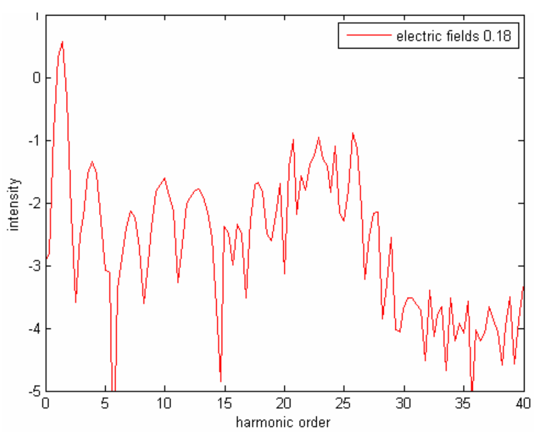


Fig.5-3 HHG spectrum with

$E_0 = 0.18 a.u.$ $w = 0.057 a.u.$ $t = 4T_{laser}$ $\phi = 0$

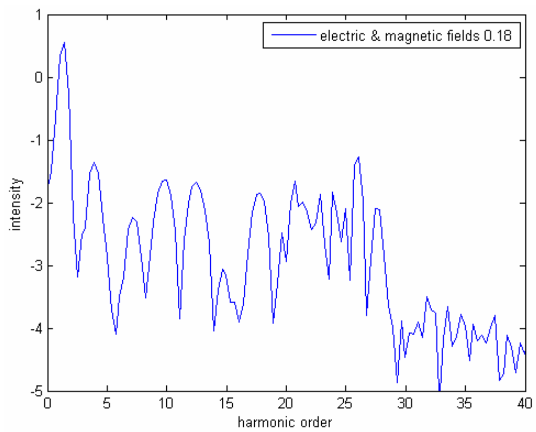


Fig.5-4 HHG spectrum with magnetic effect

$E_0 = 0.18 a.u.$ $w = 0.057 a.u.$ $t = 4T_{laser}$ $\phi = 0$

We can see from these figures, when the magnetic effects have to take into account, harmonics in the high radiation spectrum are changed strongly, but small for low order harmonic frequency. The intensities of plateau are lower than spectrum for electric field only, there are some peak intensity gone, the number of ionization is reduced by magnetic field, and the total spectrums also depend on laser phase.

Magnetic effect

In order to study the magnetic effects of atomic dynamics under intense laser pulse, we note that a free electron moving in a plane wave field follows a figure-8 motion caused by the combined action of the electron and magnetic field.

The free electron in plane wave

$$\begin{aligned} \vec{E}(t) &= E_0 e^{i(wt+\phi)}\hat{z} \\ \vec{B}(t) &= \frac{E_0}{c} e^{i(wt+\phi)}\hat{x} \end{aligned} \tag{33}$$

the Lorentz force is

$$\vec{F} = q\vec{E} + \frac{q}{c}\vec{v}\times\vec{B} \tag{34}$$

For $v << c$ we can use the perturbation theory, and the motion is in the y-z plane, i.e.

$$\vec{v}\times\vec{B} = v_z B\hat{y} - v_y B\hat{z} \tag{35}$$

$$m\frac{d}{dt}\begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -eE_0 e^{i(wt+\phi)}) \end{bmatrix} + \frac{e}{c}\begin{bmatrix} 0 \\ -v_z E_0 e^{i(wt+\phi)} \\ v_y E_0 e^{i(wt+\phi)} \end{bmatrix} \tag{36}$$

zero order,

$$\frac{dv_x^{(0)}}{dt} = \frac{dv_y^{(0)}}{dt} = 0 \tag{37}$$

$$\frac{dv_z^{(0)}}{dt} = -\frac{e}{m} E_0 e^{i(wt+\phi)}$$

$$v_z^{(0)}(t) = i\frac{e}{mw} E_0 e^{i(wt+\phi)} + v_z(0) \Rightarrow U_p = \frac{1}{2} m\langle v_z^2 \rangle = \frac{e^2 E_0^2}{4mw^2} \tag{38}$$

first order,

$$\frac{dv_y^{(1)}}{dt} = -\frac{ev_z^{(0)}}{mc} e^{i(wt+\phi)} = -\frac{e^2 E_0^2}{2m^2 wc} e^{i2(wt+\phi)}$$

$$v_y^{(1)}(t) = -\frac{e^2 E_0^2}{4m^2 w^2 c} e^{i2(wt+\phi)} + v_y(0) \tag{39}$$

We are interested in the excursion only, we let $v_z(0) = v_y(0) = 0$, and use atomic unit to simplify the problem, then we gain the trajectories,

$$y(t) = \int v_y dt = -\frac{E_0^2}{8w^3 c} e^{i2(wt+t)}$$

$$z(t) = \int v_z dt = \frac{E_0}{w^2} e^{iwt} \tag{40}$$

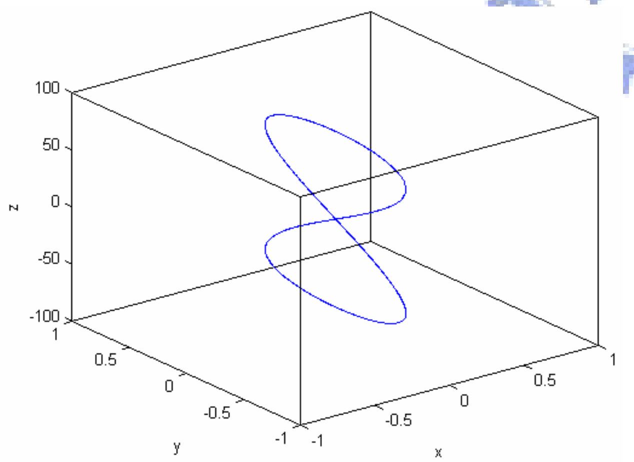


Fig.5-5 free electron's trajectory under intense laser driven by electric and magnetic field with $w = 0.057 a.u.\ E_0 = 0.25 a.u.$ over 4-cycle

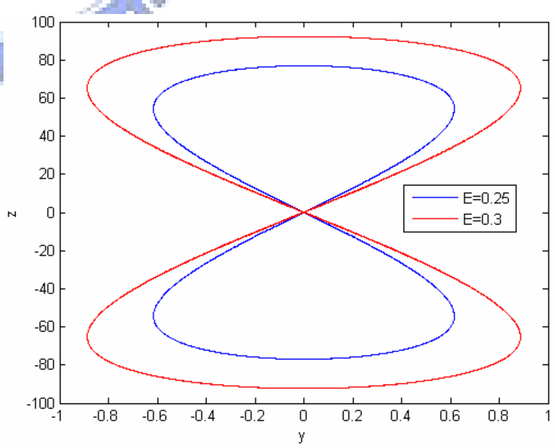
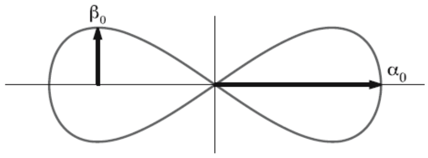


Fig.5-6 the 8-motion for $w = 0.057 a.u.\ E_0 = 0.25 a.u.$ and $w = 0.057 a.u.\ E_0 = 0.3 a.u.$

The 8-motion induced by the coupling of the electric and magnetic fields in a plane wave. The amplitude α_0 is in the direction of the electric field, and β_0 is in the direction of the propagation vector $\vec{k}$ perpendicular to the electric and magnetic fields.



$$\alpha_0 = \frac{E_0}{w^2} \qquad \beta_0 = \frac{E_0^2}{8w^3c} \tag{41}$$

Fig.5-7 the 8-motion

The magnetic component of the Lorentz force is perpendicular to the direction of motion $\vec{v}$, it can do no work on the electron. That is the magnetic field of laser does not insert field energy into the electron, it couples to the electric field in such fashion as to distort the linear oscillatory motion.

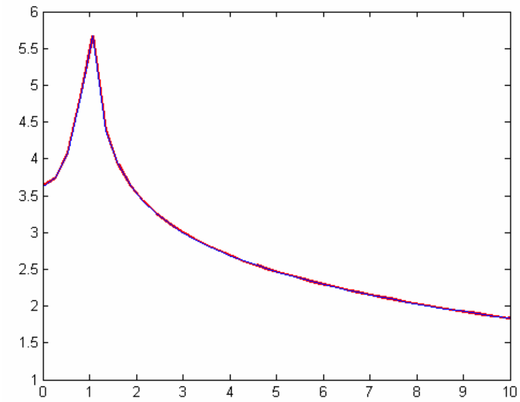


Fig.5-8 The spectrum of free electron under electric field (blue line) and the free electron under both magnetic and electric fields (red line)

The spectrum of electric field and both electric and magnetic fields are identicalness. That is there is no another frequency added by magnetic fields such as cyclotron frequency. From another point, the interaction Hamiltonian

$$H = \frac{1}{2m}\left[\vec{p} - \frac{\hat{k}}{c} e\vec{r} \cdot \vec{E}(wt)\right]^2 - \frac{e^2}{r} - e\vec{r} \cdot \vec{E}(wt)\,, \tag{42}$$

it can be rewrite into

$$H = \frac{|\vec{p}|^2}{2m} - \frac{e^2}{r} - e\vec{r} \cdot \vec{E}(wt) - \frac{\vec{p} \cdot \hat{k}}{mc} e\vec{r} \cdot \vec{E}(wt) + \frac{(e\vec{r} \cdot \vec{E}(wt))^2}{2mc^2}. \tag{43}$$

The equation can be divided into three parts:

$$\begin{aligned} H_{atom} &= \frac{|\vec{p}|^2}{2m} - \frac{e^2}{r} \\ H_{electric} &= -e\vec{r} \cdot \vec{E}(wt) \\ H_{magnetic} &= -\frac{\vec{p} \cdot \hat{k}}{mc} e\vec{r} \cdot \vec{E}(wt) + \frac{(e\vec{r} \cdot \vec{E}(wt))^2}{2mc^2} \approx -\frac{\vec{p} \cdot \hat{k}}{mc} e\vec{r} \cdot \vec{E}(wt) \end{aligned} \tag{44}$$

The first one is the Hamiltonian of hydrogen atom, second one is the Hamiltonian due to the electric field of laser, and third one is the Hamiltonian from the magnetic field of laser, in third one the second term's magnitude is about $(v/c)^2$, where should be dropped. The magnetic Hamiltonian, it roles as a v/c addition to electric field effect and coupling into the propagation direction $\hat{k}$ of the laser. This coupling underlies 8-motion.

The number of ionization is reduced by magnetic field, this is because the magnetic force changes the electron's direction of motion and electrons are trapped by the magnetic effect. Even thought the number of trapped electron increase, some HHG plateau spectrum still gone. This can be treat as the consequence, that the magnetic force prevent the electron goes back to or near to their parent core, i.e., there is less interaction with the nucleus, the spectrum occurs only when the electronic motion is close to the nucleus that is sufficient acceleration to generate the harmonics. In other hand, for lower harmonic orders there are no huge changes, because the electrons with lower velocity the magnetic effects are small, also the motions are strongly controlled by the nucleus, This results seen that the magnetic field serves reduce the high harmonic generation phenomenon. For the intensity drop in plateau regime, the electrons with high velocity have strong magnetic force on them, and magnetic force change the direction of motion, it let electron's motion more close to the nucleus than the electric force does, i.e., the dipole moment is decreased by magnetic force. After Fourier transform the intensity drop in plateau regime.

Chapter 6

Conclusion

In this thesis we use intense pulse on a classical hydrogen atom, and simulated it by Classical Trajectory Monte Carlo method to study atomic dynamic under intense short pulse and the magnetic effect. We find that for short pulse the total spectrum is phase dependence is strong, and the periodicity of the high harmonic generation process is completely suppressed, but kept for low order harmonic. From the above results, we find that for short pulse such as few-cycle laser, the high harmonic generation is governed directly by the intense pulse evolution. The magnetic part in laser field can trap the electrons in the region near to their parent core, and in high harmonic generation plateau regime, i.e., the high frequency, there are some intensity peaks were gone, also the intensity of plateau are lower than spectrums that caused by electric field only. Magnetic force can let electron miss their core and trap electron's motion close to their core. For low order harmonic spectrum, i.e., perturbative regime, the spectrums are dominated by Coulomb potential, and the magnetic effect is small so that the spectrums don't change too much. The magnetic effect serves to change high harmonic generation in plateau.

Reference

[1] P. B. Corkum, "Plasma Perspective on Strong-Field Multiphoton Ionization", PRA, 71, 13, 1993.

[2] H. R. Reiss, "Dipole-approximation magnetic fields in strong laser beams", PRA, 63, 013409, 2000.

[3] James S. Cohen, "Comment on the classical-trajectory Monte Carlo method for ion-atom collisions", PRA, 26, 5, 1982.

[4] J. Cooper, "Harmonic generation by a classical hydrogen atom in the presence of an intense radiation field", PRA, 41, 3, 1990.

[5] Thomas Brabec and Ferenc Krausz, "Intense few-cycle laser fields: Frontiers of nonlinear optics", Reviews of Modem Physics, Vol. 72, No. 2, 2000

[6] Carsten Winterfeldt, Christian Spielmann, and Gustav Gerber, "Colloquium: Optimal control of high-harmonic generation", Reviews of Modem Physics, Vol. 80, No. 1, 2008

[7] William H. Press, Saul A. Teukolsky, William T. Vetterling, Brian P. Flannery, Numerical Recipes in Fortran 77 The Art of Scientific Computing , Second Edition, Cambridge, Cambridge, 2001

Appendix A

Simple man model

In this model, the electron first tunnels from the ground state of atom through the barrier formed by the Coulomb potential and the laser field. Its subsequent motion can be treated classically, electron with initial conditions of velocity and position equal zero at the time of tunneling and primarily consists of oscillatory motion in phase with the laser field in dipole approximation.

In order to see the photon energy maximum is

$$\hbar w_{\max} = I_p + 3.17 U_p \tag{45}$$

let we consider linear polarization electric field

$$\vec{E}(t) = E_0 \cos(wt)\hat{z} \tag{46}$$

in this case, the motion is given by the well known equations

$$\begin{aligned} z(t) &= -\frac{qE_0}{mw^2}\cos(wt) - \frac{qE_0}{mw} t\sin(wt') + \frac{qE_0}{mw^2}\cos(wt') + \frac{qE_0}{mw} t'\sin(wt') \\ \frac{dz}{dt} &= \frac{qE_0}{mw}\left[\sin(wt) - \sin(wt')\right] \end{aligned} \tag{47}$$

where we assume initial conditions are

$$\begin{aligned} z(t') &= 0 \\ \left(\frac{dz}{dt}\right)_{t=t'} &= 0 \end{aligned} \tag{48}$$

i.e., the velocity and position after tunneling is zero, and t' is the tunneling moment. From this solution we can find the energy distribution for the electron that does come back.($z(t) = 0, \ \text{for } t > t'$)

$$\begin{aligned} U_p &= \frac{q^2 E_0^2}{4mw^2} \\ E_k &= 2U_p\left[\sin(a+x) - \sin(a)\right]^2 \end{aligned} \tag{49}$$

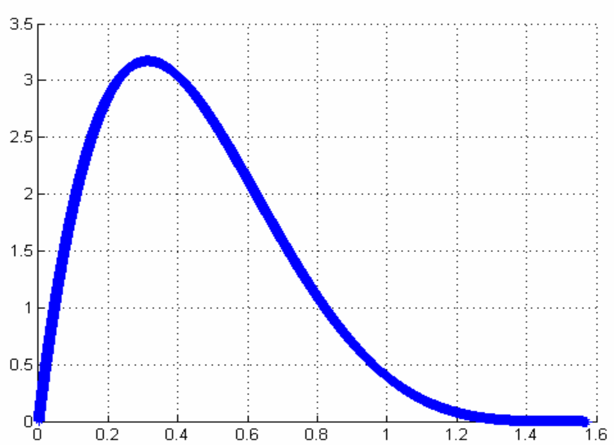


Fig. A-1 the graph of ionization phase from 0 to $\pi/2$ (x-axis) with electron energy divided by U_p (y-axis), the maximum energy occurs at 18° with $E_k = 3.1731U_p$

The energy distribution over wt' form 0 to $\pi/2$, and energy divided by U_p.

Hence, the cut-off formula

$$E_{cutoff} = \hbar w_{\max} = I_p + 3.17U_p. \tag{50}$$

It is very successful.

Appendix B

Atomic units

Atomic units are used for convenience, as by setting the fundamental constants $\hbar = m = e^2 = 1$, $\alpha = e^2/\hbar c = 1/137.037$, to simplify the calculations.

(1) 1 atomic charge unit = e = charge of the electron = $1.602\times10^{-19}\,C$

(2) 1 atomic mass unit = m = mass of electron = $9.109\times10^{-31}\,kg$

(3) 1 atomic length unit = a = radius of the first Bohr orbit =

$$\hbar^2/me^2 = 5.2917\times10^{-11}\,m$$

(4) 1 atomic velocity unit = v_0 = electron velocity in the first Bohr orbit =

$$e^2/\hbar^2 = 2.1877\times10^{6}\,m/s$$

(5) 1 atomic momentum unit = p_0 = electron momentum in the first Bohr orbit =

$$me^2/\hbar^2 = 1.9926\times10^{-24}\,kg\ m/s$$

(6) 1 atomic energy unit = twice the ionization potential of hydrogen =

$$e^2/a = me^4/\hbar^2 = p_0^2/m = 4.359\times10^{-18}\,J$$

(7) 1 atomic time unit = $a/v_0 = \hbar^3/me^4 = 2.4189\times10^{-17}\,s$

(8) 1 atomic frequency unit = $v_0/a = me^4/\hbar^3 = 4.1341\times10^{16}\,s^{-1}$

(9) 1 atomic unit of electric potential = $e/a = me^3/\hbar^2 = 27.210\,V$

(10) 1 atomic unit of electric field strength =

$$e/a^2 = m^2e^5/\hbar^4 = 5.142\times10^{11}\,V/m$$

Appendix C

Fourier Transform

In discrete Fourier Transform

$$F(w) = \int_a^b f(t) e^{-iwt} dt \tag{51}$$

the integral can be write into Riemann sum

$$F(w_\mu) = \frac{\Delta t}{\sqrt{2\pi}} \sum_{j=0}^{N-1} f(t_j) e^{-iw_\mu t_j} \tag{52}$$

with

$$t_j = a + j\Delta t\,, \quad j = 0,1,2,3,4..........N-1$$
$$\Delta t = \frac{b-a}{N} \tag{53}$$

$f(t_j)$ is periodic in $(N\Delta t)$

and

$$w_\mu = \frac{-\pi}{\Delta t} + \mu\Delta w\,, \quad \mu = 0,1,2,3,4......N-1$$
$$\Delta w = \frac{2\pi}{N\Delta t} \tag{54}$$

The discrete Fourier Transform can be rewrite into,

$$F(w_\mu) = \frac{\Delta t}{\sqrt{2\pi}} e^{-i\theta_\mu} \sum_{j=0}^{N-1} (-1)^j f(t_j) e^{-i\frac{2\pi j\mu}{N}} \tag{55}$$

with $\theta_\mu = \mu\Delta w a - \frac{\pi a}{\Delta t}$.