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# Multiphoton resonant ionization of hydrogen atom exposed to two-colour laser pulses

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This paper studies the multiphoton resonant ionization by two-colour laser pulses in the hydrogen atom by solving the time-dependent Schrödinger equation. By fixing the parameters of fundamental laser field and scanning the frequency of second laser field, it finds that the ionization probability shows several resonance peaks and is also much larger than the linear superposition of probabilities by applying two lasers separately. The enhancement of the ionization happens when the system is resonantly pumped to the excited states by absorbing two or more colour photons non-sequentially.

**Keywords:** time-dependent Schrödinger equation, multiphoton ionization, ionization probability
**PACC:** 3280F, 3380K, 4250C

## 1. Introduction

The electron ionization is a fundamental problem in the atomic physics. As the simplest atom, the hydrogen atom plays a very important role for understanding this basic dynamics. With the advent of the intense ultrashort laser pulse, the ionization problem attracts much interests in the past several decades. The electron ionization is related to a lot of fascinating subjects, such as high harmonic generation[1−3] and Coulomb explosion.[4] The ionization process can also be used to discover the atomic structures,[5] and the ultrafast dynamics inside the atom and molecule.[6,7] For the application of two-colour field, it has been widely used to enhance the photon-ionization process.[8]

When the laser intensity is higher than $5 \times 10^{12}\,\mathrm{W/cm^2}$, the lowest-order perturbation theory of light–matter interaction is broken down, since the laser electric field can be comparable with the Coulomb field inside the atom. Several nonperturbative theories are developed, such as Floquet theory,[9−11] S-matrix,[12−15] and the numerical solution of the time-dependent Schrödinger equation (TDSE).[16−20] Among these methods, TDSE simulation is very powerful and accurate, though its time cost is expensive in the high dimension calculations.

In this paper, we study the ionization of Hydrogen atom exposed to two-colour laser fields by solving the TDSE numerically. By fixing all parameters of one of the laser fields, and scanning the frequency of another laser field, we find that the ionization probability as the function of second laser frequency shows several resonance peaks and is also much larger than the linear superposition of probabilities by using two lasers separately. Further analysis shows that the enhancement gets the maximum when one of the laser pulse can resonantly pump the electron from the ground state to higher excited states.

## 2. Numerical model

In this section, we give a detailed analysis to the resonance structure of multiphoton ionization of Hydrogen atom. Numerically, we solve the TDSE in 2D (two-dimensional) spacial grids for the hydrogen atom interacting with linearly polarized laser pulses. Due to the same polarizing direction of two laser pulses, the ionization dynamics is effectively confined in the plane including the polarization axes. Although the 3D potential is more accurate, there will be no new results expected which is significantly different from the 2D case. For time saving, we just use 2-D potential to describe system. With this model, the TDSE is written as (Hartree atomic units, $e = m = \hbar = 1$ are used)

$$\frac{\mathrm{i}\partial \Phi(x,y,t)}{\partial t} = [H_0 + V(t)]\,\Phi(x,y,t), \qquad (1)$$

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where $H_0$ is the field-free Hamiltonian

$$H_0 = -\frac{1}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) - \frac{1}{\sqrt{x^2+y^2+a}}, \quad (2)$$

where $a$=0.636 is used to soften the singularity of the Coulomb potential. The time-dependent potential is written in length gauge

$$V(t) = x\sum_{i=1}^{2} E_i f_i \sin\omega_i t, \quad (3)$$

where $f_i$ defines a smooth pulse envelope function as

$$f_i = \begin{cases} \sin^2\left(\dfrac{\pi t}{2T_i}\right), & \text{as } t < T_i, \\ 1, & \text{as } T_i \le t \le \tau_i - T_i, \\ \cos^2\left(\dfrac{\pi(t+T_i-\tau_i)}{2T_i}\right), & \text{as } \tau_i - T_i < t \le \tau_i, \end{cases} \quad (4)$$

where $T_i = 2\pi/\omega_i$, $\tau_i = 3T_i$. In our simulation, the laser parameters of the fundamental laser pulse are fixed at $E_1$=0.02, $\omega_1$=0.057, $\tau_1$=7.95 fs (3 cycles for 800 nm, FWHM (Full width at half maximum)). The parameters of the second laser pulse are tunable.

Due to the time-dependent interaction of two laser pulses, one can get the solution of Eq.(1) numerically by using standard FFT (Fast Fourier Transformation) split-operator algorithm.[21] Note that the initial state $|\Phi(0)\rangle$ is ground state of the system having a binding energy $I_b$=–0.5 a.u.. This can be obtained by the imaginary time relaxation method.[22] Also by subtracting ground wave packets, we can obtain the first excited state with the corresponding binding energy –0.123 a.u.. The sizes of the simulation box are 152 a.u. × 152 a.u. in $x$ and $y$ directions, respectively. The spacial steps $\Delta x = \Delta y$=0.3 a.u., and the time step is $\Delta t$=0.1 a.u.. We use ECS (exterior complex scaling)[23] method to suppress the reflection from the borders of the simulation box. The ionization probability $P$ is defined as ,

$$P = 1 - \text{norm}, \quad (5)$$

$$\text{norm} = \int_{x=-x_R}^{x=+x_R}\int_{y=-y_R}^{y=+y_R} \Phi(x,y,t)^* \times \Phi(x,y,t)|_{t=\infty} \mathrm{d}x\mathrm{d}y, \quad (6)$$

Where $x_R$, $y_R$ is a distant point (typically $x_R = y_R$=60 a.u.) near the box boundary. The ionization probability is integrated at a sufficiently long evolution time over the box inside the boundary where ECS condition has been used.

# 3. Simulation results

When the hydrogen atom is exposed to an intense femtosecond laser pulse, the electron absorbs several photons and liberate from the nucleus bound. If the first laser pulse is switched off (let $E_1 = 0$ in the simulation), then the mechanism of the ionization is quite clear. One can clearly see from the line with box symbol in Fig.1 that the ionization probability reaches the maximum when $\omega_2 = 0.5$, which is the ionization potential. In this case, the electron is resonantly ionized directly from the ground state. Some intriguing phenomena appear if two-colour lasers are applied to the system together. First, the total ionization probability is much larger than the sum of ionization rates getting from the first laser pulse or the second laser pulse separately. Second, there are several peaks when two laser pulses interact with the hydrogen atom together. The first five peaks appear at (from right to left) $\omega_2$=0.3, 0.18, 0.13, 0.099, 0.084 a.u.. In the first peak ($\omega_2 = 0.3$ a.u.), the electron absorbs one photon of the second laser pulse, and jumps to the first excited state, where the electron is much easier to be ionized in the later propagation in the external laser field. The first peak is not exactly equal to the energy gap 0.377 a.u. between the first excited state and the ground state. It is due to the use of 2-D soft core potential, if 3-D soft core potential is applied to calculate the gap, the first peak will be expected to appear at

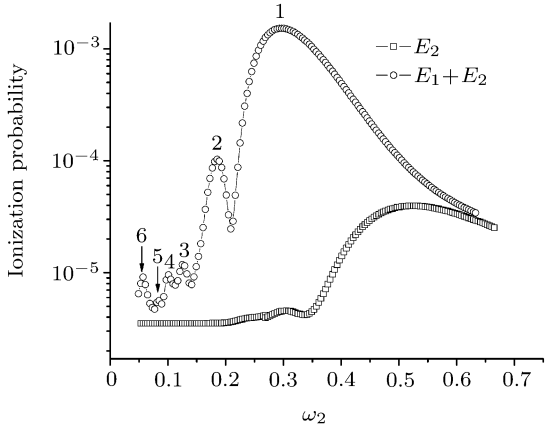



**Fig.1.** The dependence of ionization probability as a function of $\omega_2$ when the hydrogen atom is exposed to two laser pulses (by circle symbol) or only second laser pulse (by box symbol). The fundamental laser parameters are fixed at $E_1$=0.02 a.u., $\omega_1$=0.057, $\tau_1$=7.95 fs (3 cycles for 800 nm, FWHM). The second laser pulse is $E_2$=0.002 a.u.with a duration of 3 cycles and its frequency is tunable.

0.375 a.u.. In the second peak ($\omega_2 = 0.18$), the electron absorbs two photons of the second laser pulse, and is resonantly excited the first excited state (the first excited state is –0.123, the gap with ground state is approximately 0.377), and ionized non-sequentially later. Not surprisingly, the third peak and the fourth peak correspond to resonant excitation by absorbing three and four photons with $\omega_2$. The fifth peak is related to case of five photons. The peaks in the curve with circle symbol in Fig.1 map the resonant excitation. The exceptional case is the sixth peak which locates at $\omega_2 = 0.057$. At this position, the frequency of the fundamental laser and the second laser are same. Both coherent lasers interfere with each other and strongly lead to this high enhancement band.

The ionization probability is much larger when two laser pulses are introduced. We define the enhancement factor to express this amplification of ionization as follows:

$$F = \frac{P_{E_1+E_2} - P_0}{P_0}, \tag{7}$$

where $P_0 = P_{E_1} + P_{E_2}$ and $P_{E_i}$ is the ionization probability when only $E_i$ ($i$=1 or 2) is applied. In our calculation, $P_{E_1} = 3.3210^{-6}$. Figure 2 shows the enhancement factor as a function of the amplitude of the second laser pulse. These five curves correspond to five different $\omega_2$, which satisfy one, two, three, four, five photons resonant pumping. In the multiphoton excitation process, there are a maximum for the enhancement factor. If the intensity of one laser is significantly larger than that of the other, i.e. $E_2 \gg E_1$, the value of $F \to 0$. However, for a specific $E_2$ amplitude, here at $E_2$=0.004 a.u., the biggest enhancement factor larger than 200 for the two photons case is observed. The enhancement in multiphoton ionization by two-colour laser pulses can be understood by a two-step mechanism. First, starting from the ground state, the atom absorbs energy from one laser leading to a excited energy level. In a second step, another laser field causes ionization from the excited states. This is shown in the Fig.2 that Boltzmann-like population of excited energy levels by the first fundamental laser can lead to different enhancements. The enhancement also exhibits a single maximum as the amplitude of $E_2$ is varied. This Maximum suggests an optimum second laser amplitude to achieve the maximum photoionization as the fundamental laser is fixed. We predict that at this optimum laser amplitude, the second colour laser can strongly interfere with the fundamental laser which leads to resonant ionization.

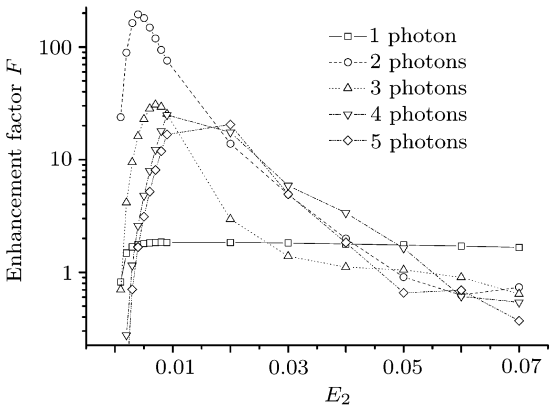



**Fig.2.** The enhancement factor as a function of the amplitude of the second laser pulse as $\omega_2$= 0.5, 0.25, 0.17, 0.125 and 0.1, also marked by 1, 2, 3, 4, 5 photons.

# 4. Conclusion and outlook

In summary, we have studied the ionization of the hydrogen atom exposed to a two-colour laser fields. Our simulation results show that the ionization probability can resolve the multiphoton resonant excitation. The ionization probability can be enhanced a lot when the two-colour laser fields are introduced. If the electron can absorb single or multiphotons and resonantly jump to higher state, then the ionization rate can be much larger than the linear superposition of probabilities by using two lasers separately. Also the enhancement as a function of second laser amplitude shows that there is an optimum amplitude which significantly enhance the ionization probability of system. We conclude that at this optimum laser amplitude, the second colour laser can strongly interfere with the fundamental laser which leads to resonant ionization. Similar effects are expected for other multi-electron atomic systems if they are exposed to two colour laser field. This is an interesting topic needed to be studied further.

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