Vol 18 No 12, December 2009
1674-1056/2009/18(12)/5291-05

Chinese Physics B

© 2009 Chin. Phys. Soc.
and IOP Publishing Ltd

Multiphoton ionization of the hydrogen atom exposed to circularly or linearly polarized laser pulses

Wang Pei-Jie(王培杰)[a)†] and He Feng(何 峰)[b)]

[a)] *The Beijing Key Laboratory for Nano-Photonics and Nano-Structure, Capital Normal University, Beijing* 100048, *China*

[b)] *James R. Macdonald Laboratory, Department of Physics, Kansas State University, Manhattan, Kansas* 66506-2604, *USA*

(Received 18 March 2009; revised manuscript received 13 May 2009)

This paper studies the multiphoton ionization of the hydrogen atom exposed to the linearly or circularly polarized laser pulses by solving the time-dependent Schrödinger equation. It finds that the ratio of the ionization probabilities by linearly and circularly polarized laser pulses varies with the numbers of absorbing photons. With the same laser intensity, the circularly polarized laser pulse favors to ionize the atom with more ease than the linearly polarized laser pulse if only two or three photons are necessary to be absorbed. For the higher order multiphoton ionization, the linearly polarized laser pulse has the advantage over circularly polarized laser pulse to ionize the atom.

Keywords: time-dependent Schrödinger equation, multiphoton ionization, ionization probability

PACC: 3280F, 3380K, 4250C

1. Introduction

The ionization is a fundamental problem in atomic physics.[1] Several major aspects, such as above-threshold ionization, high harmonic generation, molecular photon-dissociation, photoelectron spectroscopy, and attosecond pulse generation are derived directly or indirectly from the electron ionization.[2−5] An interesting aspect of multiphoton ionization concerns the role of circular and linear polarization in atomic system[6,7] and even in dielectric systems.[8] Early experiments[9] on two- and three-photon ionization of atoms have shown that circularly polarized laser pulse gives larger ionization probability than the linearly polarized light, which is consistent with the perturbation theory. For the high order multiphoton ionization, Klarsfeld and Maquet[10] predicted that the atom is also more easily ionized by the circularly polarized laser pulse. However, Reiss[11] gave an opposite proposal that the linearly polarized laser pulse favors to ionize the electron if four or more photons are necessarily to be absorbed. Later, LaGattuta[12] argued that the linearly polarized laser pulse has the advantage on the circularly polarized pulse to ionize the electron in very high laser intensities. We here want to numerically clarify the efficiency of photon ionization of different orders by shining these two polarized laser pulses with the same intensity separately.

If we consider the physical process where the laser intensity is higher than 5×10^{12} 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,[13−15] S-matrix,[16−18] and the numerical solution of the time-dependent Schrödinger equation (TDSE).[3,19−23] Among these methods, TDSE simulation is very powerful and accurate, though its time cost is expensive in the high dimensional calculations.

As the simplest atom, hydrogen atom plays a very important role for understanding this basic ionization mechanism. In this paper, we study the ionization of hydrogen atom exposed to linearly and circularly polarized laser fields by solving the TDSE numerically, and calculate the multiphoton ionization (including 1−5 photons ionization) probabilities. Our conclusion is consistent with the analytical results by Reiss.[11]

2. Numerical model

In this Section, we give a detailed analysis to the different ionization probabilities of hydrogen atom by two different polarized laser fields. Numerically, we solve the TDSE in two-dimensional (2D) Cartesian coordinate for the hydrogen atom interacting with the

†Corresponding author. E-mail: peijiewang@mail.cnu.edu.cn

linearly and circularly polarized laser pulses. The 2D model is proper because no dynamics evolves in the third dimension except for the spread of wavepacket, which does not change the ratio of the ionization probabilities by linearly and circularly polarized laser pulses. Within this model, the TDSE is written as ($e = m = \hbar = 1$)

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

with the field-free Hamiltonian

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

where a is used to soften the singularity of the Coulomb potential. The Hartree atomic units are used through this paper. The time-dependent potential is written in the length gauge,

$$V(t) = \begin{cases} xfE_0\sin(\omega t), & \text{linearly,} \\ \dfrac{f}{\sqrt{2}}(xE_0\cos(\omega t) + yE_0\sin(\omega t)), & \text{circularly,} \end{cases} \tag{3}$$

where f defines a smooth pulse envelope function as

$$f = \sin^2(t\pi/\tau), \tag{4}$$

where $\tau = 3T$, and $T = 2\pi/\omega$. We use the standard fast Fourier transformation (FFT) split-operator algorithm[24] to solve the TDSE. The initial state is the ground state of the hydrogen atom, which is obtained by using the imaginary time relaxation method.[25] By tuning the soft core parameter as 0.636, the simulation model yields the exact ionization potential $I_\mathrm{b} = -0.5$ a.u. By projecting out the obtained ground state in the imaginary time propagation, we achieve the first excited state with the corresponding binding energy 0.123 a.u. The sizes of the simulation box are 152 a.u. $\times$ 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)[26] method to suppress the reflection from the borders of the simulation box, and the absorbing length is 5 a.u. in each dimension. The ionization probability P is defined as,

$$P = 1 - P_\mathrm{b}, \tag{5}$$

where the probability of the bound states,

$$P_\mathrm{b} = \int_{x=-x_R}^{x=+x_R}\int_{y=-y_R}^{y=+y_R} \mathrm{d}x\mathrm{d}y\Phi(x,y,t)^*\Phi(x,y,t)|_{t=\infty}, \tag{6}$$

which is defined as that probability remaining in the area $|x| < x_R$ and $|y| < y_R$, $x_R = y_R = 62$ a.u. We propagate the wavepacket for some additional time after the laser pulse till P_b is stable.

3. Simulation results

From Figs.1–5, we show the ionization probability as a function of the laser intensity when the laser pulse is linearly or circularly polarized with the frequency $\omega = 0.5$ a.u. (Fig.1), 0.25 a.u. (Fig.2), 0.1667 a.u. (Fig.3), 0.125 a.u. (Fig.4), and 0.1 a.u. (Fig.5) respectively. In these five pictures, the minimum Keldish parameter is $\gamma = 1.45$. Concerning the definition of tunneling and multiphoton ionization[2,27] in our study, we find that the multiphoton ionization is always dominant.

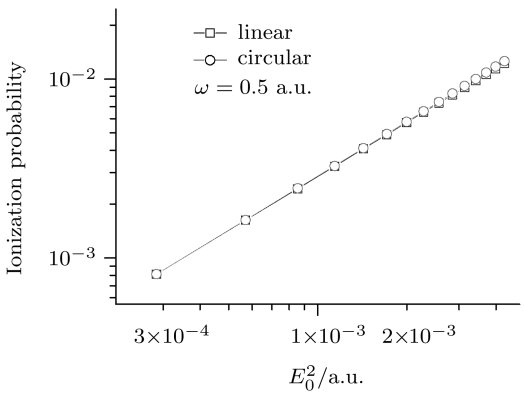


Fig.1. The ionization probability as a function of laser intensity when the hydrogen atom is exposed to linearly polarized laser pulses (box symbol) or circularly polarized laser pulses (circle symbol). The laser frequency is fixed at $\omega = 0.5$ a.u. with a duration of 3 cycles.

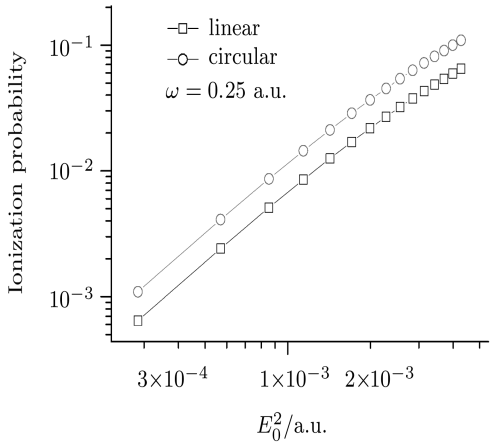


Fig.2. Same as Fig.1 but with the laser frequency $\omega = 0.25$ a.u.

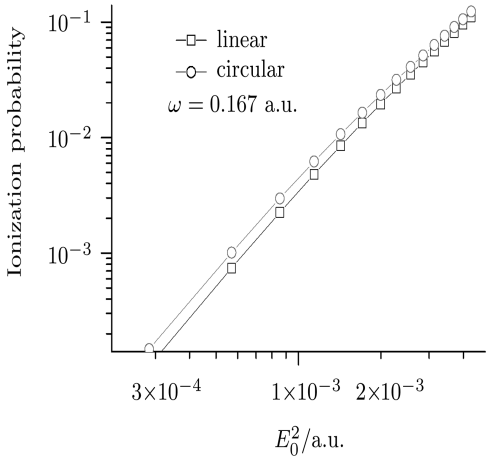


Fig.3. Same as Fig.1 but with the laser frequency $\omega = 0.167$ a.u.

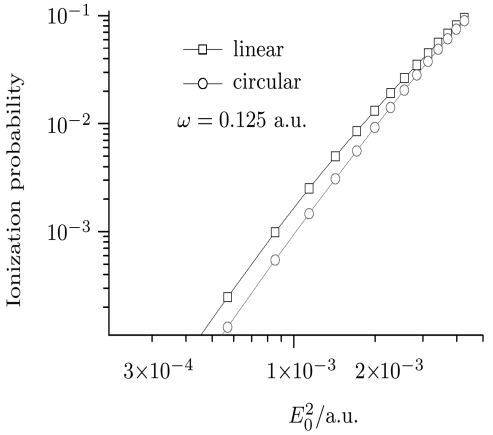


Fig.4. Same as Fig.1 but with the laser frequency $\omega = 0.125$ a.u.

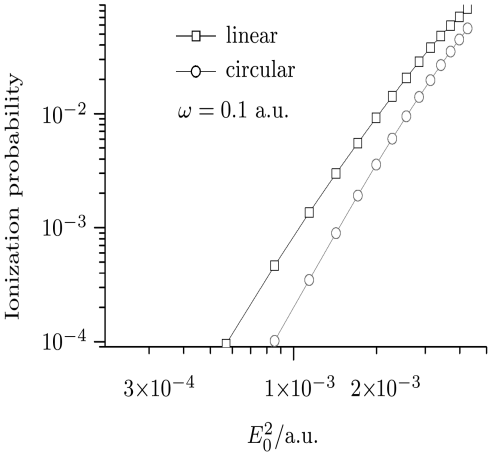


Fig.5. Same as Fig.1 but with the laser frequency $\omega = 0.1$ a.u.

When the laser frequency ω is 0.5 a.u. (Fig.1), the ionization probabilities are the same for both polarized laser fields. Recalling that the ionization yield is proportional to I^N for N-photon ionization, we get the slope of N if the ionization yield is plotted as a function of peak intensity in the log–log scale. The slopes of the two curves are exactly 1, which indicates that it is single photon ionization. For smaller frequencies, the ionization probabilities become different when linearly and circularly polarized laser pulses are used. For two-photon ionization (Fig.2), the atom is more easily ionized by the circularly polarized laser pulse than linearly polarized laser pulse. The same phenomenon also happens in the three-photon ionization (as shown in Fig.3). However, for the higher order of multiphoton ionization, such as four photons (Fig.4), five photons (Fig.5), or even more photons (not shown), the linearly polarized laser pulse has advantage on the circularly polarized laser pulse to ionize the atom.

Figure 6 shows the ionization ratio by using linearly and circularly polarized laser pulses with the same laser intensity $I = E_0^2 = 0.0023$ a.u. The arrows with different N mark the resonant multiphoton ionization. Here we define the ionization ratio $R = P_{\rm lin}/P_{\rm cir}$. We change the laser frequency continuously from 0.1 a.u. to 0.5 a.u. It is clearly seen that $R = 1$ where single photon is enough to ionize the

atom, and $R < 1$ as 0.15 a.u. $< \omega <$ 0.5 a.u., where at least two or three photons have to be absorbed to ionize the atom. With even more photons ionization, the advantage of the linearly polarized laser pulse is more and more obvious.

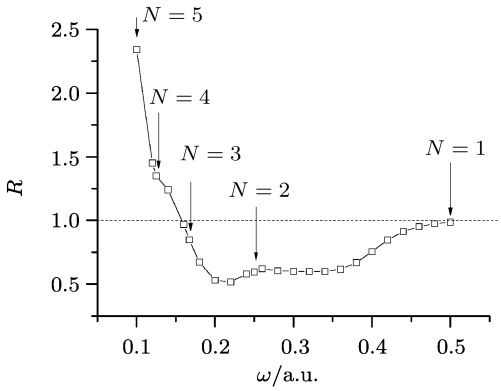


Fig.6. The ratio of the ionization probability $R = P_{\rm lin}/P_{\rm cir}$ at $I = E_0^2 = 0.0023$ a.u. with different laser frequencies. The arrows with different N mark the resonant ionization.

Generally, the ionization amplitude can be written as

$$P = \left| \int \mathrm{d}t \left\langle \sum_l \Phi_{\mathrm{f},l} | \boldsymbol{d} | \Phi_{\mathrm{i}} \right\rangle \right|^2 , \qquad (7)$$

where l is the angular momenta, Φ_{i} and Φ_{f} are the initial and final wave functions respectively, the dipole $\boldsymbol{d}$ is $-[xE_x(t)+yE_y(t)]$ or $-xE_x(t)$ for the case of circularly and linearly polarized laser pulse, where E_x and E_y are the components of the laser field along x and y directions. The ionization probability is the competition of the two factors: (i) the allowed channels of choosing angular momenta for the ionized electron; (ii) the overlap between $\Phi_{\mathrm{f},l}$ and $\boldsymbol{d}\Phi_{\mathrm{i}}$. The allowed l is generally decided by the dipole selection rules.[28] Figure 7 shows the allowed angular momenta in the ionization by absorbing different photons when (a) linearly, and (b) circularly polarized laser pulses are used, respectively. In this figure, the solid lines represent the transition satisfying the selection rule, and the circles represent final states absorbing certain photons. When the circularly polarized laser pulses are used, we can only choose $l = N$ for the final angular momentum, where N is the photon number absorbed. However, during the interaction of the linearly polarized laser pulse and hydrogen atom, the angular momentum of the ionized electron can be $1+N/2$ or $(N+1)/2$, corresponding to an even or odd N, respectively. The ionization yield is benefited from the more allowed angular momenta, but lost due to the less overlap between $\Phi_{\mathrm{f},l}$ and $\boldsymbol{d}\Phi_{\mathrm{i}}$ as the angular momentum changes. In the lower-photon ($N \leq 3$) ionization, the simulations show that the circularly polarized laser pulse has the advantage over linearly polarized laser pulse to ionize the atom. In this case, the electron can choose two (linearly) or one (circularly) angular momenta, which does not differ much and the linearly polarized laser pulse does not favor a lot by the first factor. If more than three photons are needed to ionize the atom, the electron can choose more and more angular momenta if it is shined by linearly polarized laser pulse, then the first factor is dominated and more ionization probability is obtained. Our numerical results are consistent with the prediction of Reiss.[11]

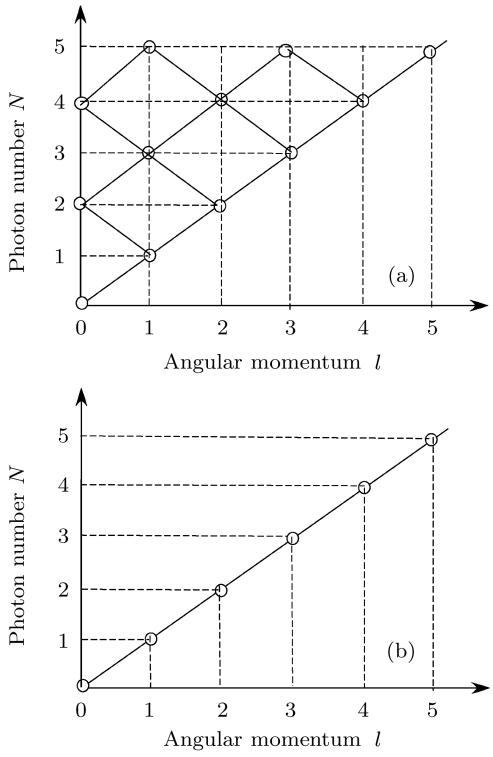


Fig.7. The angular momentum transition during the ionization induced by (a) linearly polarized, and (b) circularly polarized laser pulses.

4. Conclusion

In summary, we have studied the multiphoton ionization of the hydrogen atom exposed to two different polarized laser fields. Numerically, we solved the TDSE in 2D spacial grids for the hydrogen atom interacting with different polarized laser pulses and got

the multiphoton ionization probability. Our simulation results show that the ratio of linearly to circularly polarization ionization probability is 1 for single photon resonant ionization. For the low order, double- or triple-photon ionization, the ratio is less than 1. However, the ratio is larger than 1 for higher order ($N \geq 4$) photon ionization. The twist of the ionization ratio is explained quantitatively by analyzing the transition matrix, namely, the competition of the allowed angular momenta and the wave function overlap caused by the dipole interaction.

Acknowledgments

We gratefully acknowledge the supports by the Beijing Key Laboratory for Nano-Photonics and Nano-Structure.

References

[1] Mainfray G and Manus G 1991 *Rep. Prog. Phys.* **54** 1333
[2] Brabec T and Krausz F 2000 *Rev. Mod. Phys.* **72** 545
[3] He F, Ruiz C and Becker A 2007 *Phys. Rev. Lett.* **99** 083002
[4] Liao Q, Lu P X, Lan P F, Cao W and Li Y H 2008 *Phys. Rev.* A **77** 013408
[5] Liao Q, Lu P X, Lan P F, Yang Z Y and Li Y H 2008 *Opt. Express* **16** 6455
[6] Wang P J and Fang Y 2008 *Chin. Phys.* B **17** 3668
[7] Zhang J T and Takashi N 2007 *Phys. Rev.* A **75** 043403
[8] Temnov V V, Sokolowski T K, Zhou P, El-Khamhawy A and von der Linde D 2006 *Phys. Rev. Lett.* **97** 237403
[9] Fox R A, Kogan R M and Robinson E J 1971 *Phys. Rev. Lett.* **26** 1416
Kogan R M, Fox R A, Burnham G T and Robinson E J 1971 *Bull. Am. Phys. Soc.* **16** 1411
[10] Klarsfeld S and Maquet A 1972 *Phys. Rev. Lett.* **29** 79
[11] Reiss H R 1972 *Phys. Rev. Lett.* **29** 1129
[12] LaGattuta K J 1990 *Phys. Rev.* A **41** 5110
LaGattuta K J 1991 *Phys. Rev.* A **43** 5157
[13] Shakeshaft R, Potvliege R M, Dörr M and Cocke W E 1990 *Phys. Rev.* A **42** 1656
[14] Burke P G, Franken P and Joachain C J 1991 *J. Phys.* B **24** 761
[15] Dimou L and Faisal F H M 1992 *Phys. Lett.* A **171** 211
[16] Keldysh L V 1964 *Zh. Eksp. Teor. Fiz.* **47** 1945
[17] Faisal F H M 1973 *J. Phys.* B **6** L89
[18] Reiss H R 1980 *Phys. Rev.* A **22** 1786
[19] Kulander K C 1987 *Phys. Rev.* A **35** 445
[20] Krause J L, Schafer K J and Kulander K C 1992 *Phys. Rev.* A **45** 4998
[21] Muller H G 1999 *Phys. Rev.* A **60** 1341
[22] Nurhuda M and Faisal F H M 1999 *Phys. Rev.* A **60** 3125
[23] Zhang X M, Zhang J T, Gong Q H and Xu Z Z 2009 *Chin. Phys.* B **18** 1014
[24] Fleck, Moris J R and Feit M D 1976 *Appl. Phys.* **10** 126
[25] Protopapas M, Keitel C H and Knight P L 1997 *Rep. Prog. Phys.* **60** 389
Javanainen J, Eberly J H and Su Q 1988 *Phys. Rev.* A **38** 3430
[26] He F, Ruiz C and Becker A 2007 *Phys. Rev.* A **75** 053407
[27] Keldysh L V 1965 *Sov. Phys. JETP* **20** 1307
[28] Nakajima T and Buica G 2006 *Phys. Rev.* A **74** 023411