

An Introduction to Multiphoton Ionization and Study of Ionization Rate of Hydrogen Atom:

N. Shrestha, J. J. Nakarmi and L. N. Jha

Central department of Physics, Tribhuvan University, Kirtipur, Kathmandu

Correspondence: nilamstha@yahoo.com

Abstract

We have discussed the problems of non linear interaction between electromagnetic radiations with atoms from semi-classical point of view. Time dependent Schrödinger equation for single electron system is solved by using perturbative technique to obtain transition probability. Higher order perturbation is also discussed which is used in multiple processes, in which two or more quanta are emitted instead of a single photon. The theory is based on assumption that the perturbation is small. From this transition probability ionization rate and absorption cross-section of hydrogen atom is calculated. Its variation with photon energy and field strength is analyzed which agrees very well with experimental observations.

Keywords: non linear interaction, perturbative technique, multiple processes, absorption cross-section.

Introduction

An atom can be ionized by photons with energy $h\nu$ much less than ionization energy, if the photon flux is strong enough, which, from a practical point of view can only be achieved with laser radiation [1]. This process is designated as Multiphoton Ionization and results from the simultaneous absorption of a number N-photons defined as[2].

$$N h \nu + X = X^*$$

The first lasers in the early 1960s equipped physicists with extraordinary tool. It became possible to study not only multiphoton transitions between bound states, but also between bound free multiphoton transition i.e. Multiphoton ionization [3]. The multiphoton excitation and ionization processes have received an increasing interest, both from the experimental as well as from the theoretical side.

When photons, meets the atom, the atomic electron(s) can take up the energy of one or many photons [4]. If the electron is released by absorption of only one single photon then the ionization probability will be proportional to the number of photons which interacts with the atom. Hence in one-photon ionization the probability linearly depends on the number of interacting photons (photon flux) [5,6].

$$\text{N-photon Ionization rate} \propto \sigma_N I^N,$$

Where, σ_N generalized cross-section and I^N laser intensity numerically equal to photon flux, for N photons.

Ionization Rate of Hydrogen Atom

We now calculate the probability of ionization of a hydrogen atom initially in its ground state [7], when it is placed in a harmonically time varying electric field [8].

The perturbation

$$H^1 = 2eE_0 r \cos \omega t \quad (\text{Electric dipole approximation})$$

Fermi-Golden rule for the transition rate, [9]

$$\Gamma_{i \rightarrow f} = \frac{2\pi}{\hbar} \left| \langle f | H^1 | i \rangle \right|^2 \delta(E_f - E_i - \hbar\omega)$$

Taking the incoming wave to be an electromagnetic field having vector potential

$$\vec{A}(\vec{r}, t) = \vec{A}_0 \cos(\vec{k} \cdot \vec{r} - \omega t)$$

Hence the interaction Hamiltonian is given by replacing the electron kinetic energy term

$$\begin{aligned} H^1 &= \frac{e}{m} \cos(\vec{k} \cdot \vec{r} - \omega t) \vec{A}_0 \cdot \vec{p} \\ &= \left[H^{10} e^{-i\omega t} + (H^{10})^* e^{i\omega t} \right] \cdot \vec{p} \end{aligned}$$

(Under dipole approximation)

Density of states (DOS)

We make the assumption that the final state is the plane wave state, $|\vec{k}_f\rangle \propto e^{i\vec{k}_f \cdot \vec{r}}$ [10] which has to be confined into a box of side L and use the boundary conditions. The normalized plane wave state becomes:

$$|\vec{k}\rangle = \frac{1}{\sqrt{V}} e^{i\vec{k} \cdot \vec{r}} = \frac{1}{L^{3/2}} e^{i\vec{k} \cdot \vec{r}}$$

Thus, DOS becomes,

$$\rho(E)\Delta E = 4\pi k^2 \left(\frac{L}{2\pi}\right)^3 \frac{m}{\hbar^2 k} \Delta E$$

Matrix Element for hydrogen atom:

The ground state wave function for hydrogen is

$$|100\rangle = \left(\frac{1}{\sqrt{\pi a_0^3}}\right) e^{-r/a_0}$$

Here, the interaction Hamiltonian matrix for the hydrogen atom is [11]

$$H_f^1 = \langle f | H^1 | i \rangle$$

$$= \left[\left(\frac{1}{L}\right)^{3/2} \left(\frac{e}{2m}\right) \sqrt{\frac{1}{\pi a_0^3}} \right] \int d^3r e^{-i\vec{k}_f \cdot \vec{r}} \vec{A}_0 \cdot (-i\hbar\nabla) e^{-r/a_0}$$

Integrating by parts gives the gradient operator acting on the plane wave states,

Solving the integration, and using Fermi-Golden Rule:

$$\Gamma_{i-f} = \frac{2\pi}{\hbar} |\langle f | H^1 | i \rangle|^2 \delta(E_f - E_i - \hbar\omega)$$

$$= \frac{2\pi}{\hbar} \left[\left(\frac{1}{L}\right)^{3/2} \left(\frac{e}{2mc}\right) \sqrt{\frac{1}{\pi a_0^3}} (\vec{A}_0 \cdot \vec{p}_f) \left(\frac{8\pi/a_0}{(a_0^{-2} + k_f^2)^2}\right) \right]^2 \delta(E_f - E_i - \hbar\omega)$$

Here δ - function measures the density of possible outgoing states. The ejected electrons are measured by a sensitive detector to some small solid angle $d\Omega$.

Hence,

$$\Gamma_{i-f} = \frac{2\pi}{\hbar} |\langle f | H^1 | i \rangle|^2 \rho(k, d\Omega)$$

$$= \frac{2\pi}{\hbar} \left[\left(\frac{1}{L}\right)^{3/2} \left(\frac{e}{2m}\right) \sqrt{\frac{1}{\pi a_0^3}} (\vec{A}_0 \cdot \vec{p}_f) \left(\frac{8\pi/a_0}{(a_0^{-2} + k_f^2)^2}\right) \right]^2 (L/2\pi)^3 k_f (m/\hbar^2) d\Omega$$

Here, $(\vec{A}_0 \cdot \vec{p}_f)^2 = A_0^2 p_f^2 \cos^2 \vartheta$ ejection is most likely to be parallel to the electric field. The total ionization rate is given by the integrating the rate over all angles, and on the unit sphere $\cos^2 \vartheta = z^2 = 1/3$, thus,

$$(\vec{A}_0 \cdot \vec{p}_f)^2 d\Omega = 4\pi A_0^2 p_f^2 / 3$$

The total ionization rate is, Γ_{i-f}

$$= \frac{2\pi}{\hbar} \left[\left(\frac{1}{L}\right)^{3/2} \left(\frac{e}{2m}\right) \sqrt{\frac{1}{\pi a_0^3}} \left(\frac{8\pi/a_0}{(a_0^{-2} + k_f^2)^2}\right) \right]^2 \frac{4\pi}{3} A_0^2 p_f^2 (L/2\pi)^3 k_f (m/\hbar^2)$$

$$\Gamma_{i-f} = \frac{16e^2 A_0^2 p_f^3}{3mc^2 \hbar^4 a_0^5 (a_0^{-2} + (p_f/\hbar)^2)^4}$$

Ionization Cross-section

The area of the disc equivalent to one atom is the ionization cross-section. Since during ionization an atom takes energy of $\hbar\omega$ from the incident beam, the rate of energy absorption is just $\hbar\omega \Gamma_{i-f}$ [12], hence,

$$\hbar\omega \Gamma_{i-f} = c \langle E_p(\omega) \rangle \times \text{Cross-section}(\sigma(\omega))$$

Energy density is given by,

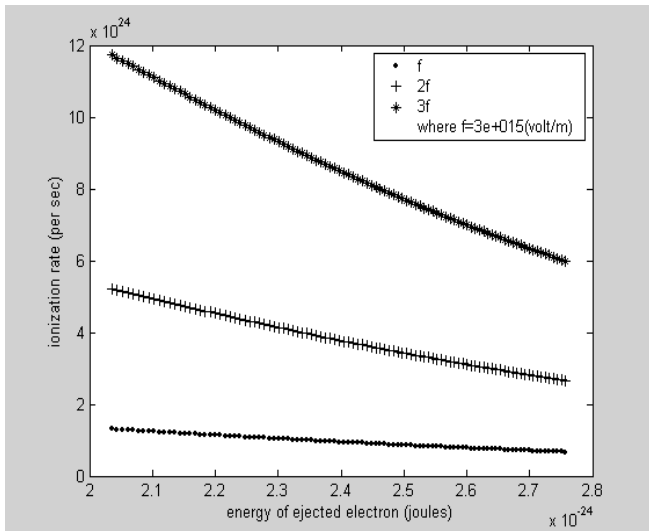
$$E_p(\omega) = \frac{1}{8\pi} (|\vec{E}|^2 + |\vec{B}|^2) = \frac{1}{8\pi} \left(2 \frac{\omega^2}{c^2} A_0^2 \sin^2(k \cdot r - \omega t) \right)$$

Averaging over $\sin^2(k \cdot r - \omega t)$, gives the energy absorption density,

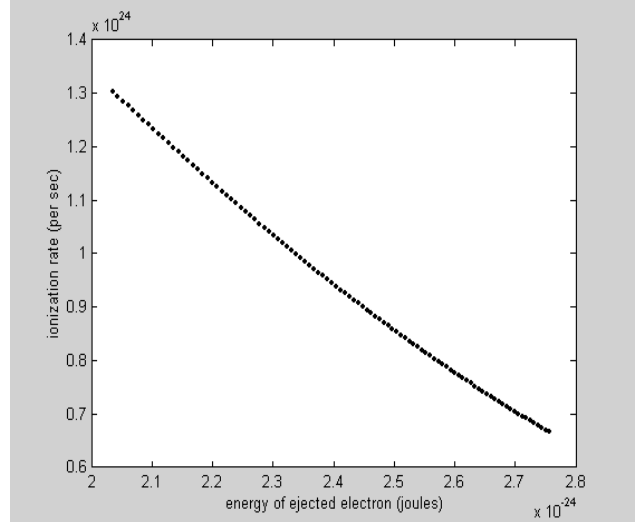
$$\langle E_p(\omega) \rangle = \frac{A_0^2 \omega^2}{8\pi c^2}$$

Hence, the absorption cross section is

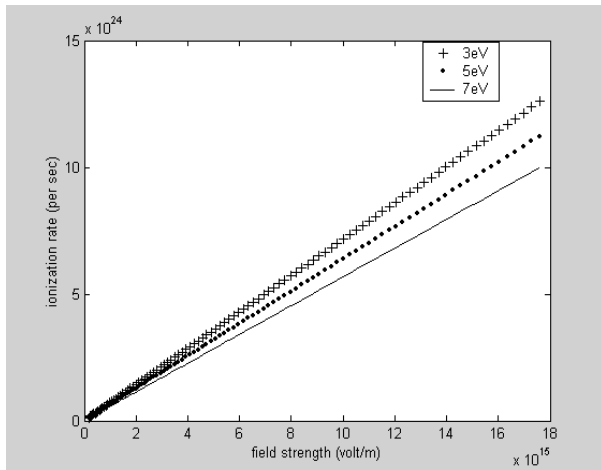
$$= \frac{128}{\omega} \frac{e^2}{a_0^5 \hbar^3} \frac{\pi p_f^3}{3m} \left(\frac{1}{a_0^{-2} + (p_f/\hbar)^2} \right)^4$$



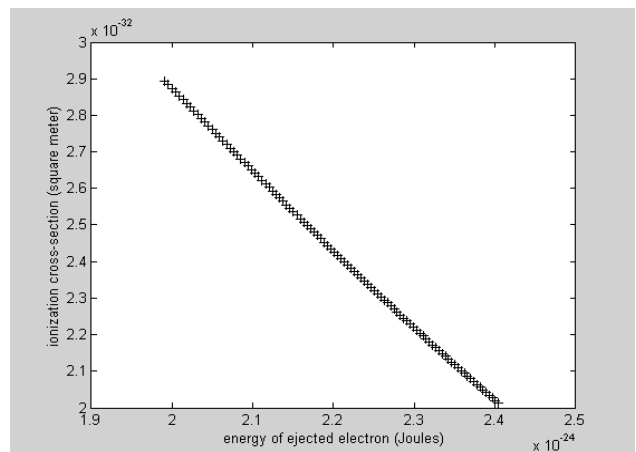
Plot (1)



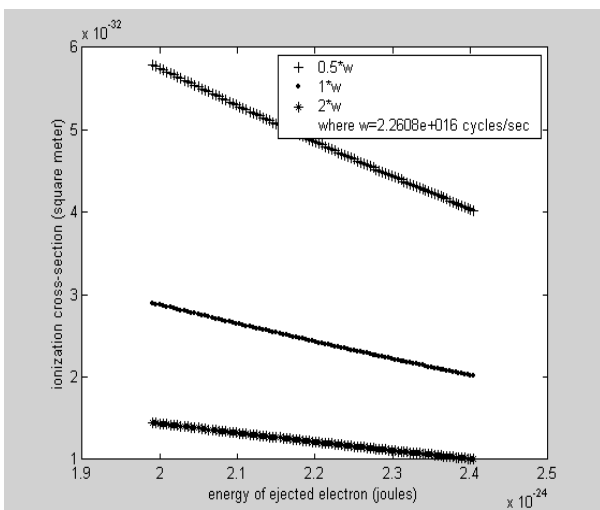
Plot (2)



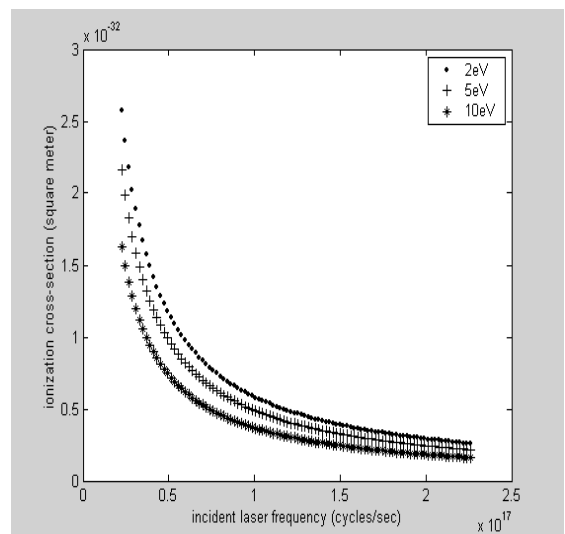
Plot (3)



Plot (4)



Plot (5)



Plot (6)

Results and Discussion

The results are presented in the various plots: in the plot (1) and (2) we have shown that ionization rate decreases with energy of ejected electron. In plot (3), ionization rate increases with increase of field strength for three different values of energy of ejected electron. From plot (4) to (6), it shows that ionization cross-section is independent of field strength; it depends inversely to energy of ejected electron for fixed value and three different values of photon energy, but in plot(6), it gradually decreases with incident photon frequency.

Conclusion

We have solved the time dependent Schrödinger equation and calculated ionization rate and cross-section of the simplest atom like hydrogen by using perturbative technique.

Acknowledgement

It is my pleasure to acknowledge National Science Council, Taiwan for the financial support for the paper presentation on 3rd IUPAP, ICWIP 2008 in Seoul, South Korea and in parts by grants from University of Grant Commission, Sanathimi, Bhaktapur, Nepal.

References

- [1] G. Mainfray and C. Manus 1980. Resonance Effects in multiphoton Ionization of atoms, *Applied Optics*, 19, 3934 -3940.
- [2] Charles K. Rhodes 1985, Multiphoton ionization of atoms, Vol 229, No. 4720 , www.sciencemag.org
- [3] G. Mainfray and C. Manus, 1991, Multiphoton Ionization of Atoms, *IOP publishing Ltd, Phys. 54*, 1333-1372.
- [4] L. D. Landau and E.M. Lifshitz, 1965, Quantum Mechanics, Pergamon Press, pp 136.
- [5] N. B. Delone and V. P. Krainov, 1999, Multiphoton processes in Atoms, 2nd edition, Springer Berlin, pp 187.
- [6] Von Peter Koval,2004, Two- Photons ionization of atomic inner-shells, Ph. D. Dissertation., University Kassel.
- [7] E. Merzbazcher,, 2004 Quantum Mechanics, John Wiley and Sons, Inc., pp 509.
- [8] N. F. Mott, 1962, Elements of Wave Mechanics, Cambridge University Press, pp 121.
- [9] Kenneth Krane, 1998, Modern physics, John wiley and sons, Inc., NY, pp 146
- [10] L. I. Schiff, 1968, Quantum Mechanics, McGraw-Hill International editions, pp 287.
- [11] Michael Fowler, 2007, *Photoelectric effects in Hydrogen atom e-net*
- [12] B. H. Bransden and C. J. Joachain,1983, *Physics of Atoms and Molecules*, Longman Inc., NY, pp 521, and pp 552 .