PHOTO-DETACHMENT OF H^-

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ABSTRACT: A simple analytical formula for photo-detachment cross section of H^-in free space is re-derived using basic concepts of quantum mechanics. Our expression is identical to the results derived by T. Ohmara and H. Ohmara [Phys. Rev. ***118****, 154 (1960)] many years ago using effective range theory. The expression derived by them was in terms of wave number, whereas we present in terms of detached-electron energy. Similar smooth behavior of total cross section of H^-inabsence of any external environment has been depicted. One can obtain binding energy, electron affinity, and atomic size of $H^-$by observing the cross section spectra. The threshold value in the spectra is main characteristic that plays important role to find electron affinity of a negative ion. The Wigner lawis used to describe this threshold behaviorin our result.*

1. INTRODUCTION

A negative ion is an atom with an extra electron thatgives the whole system a net negative charge. It is a fragile quantum system with some striking properties distinguishing it from other atomic or molecular neutral systems.The preferred method for exploring such systems is photo-detachment process. In this process, electromagnetic radiations are made incident upon a negative ion to detach an extra electron that can be written symbolically as;

$$H^- + hv \rightarrow H + e^-.$$

In 1953, $H^-$was the first negative ion to be studied by photo-detachment in an ion-beam experiment [1]. It is unique among all negative ions because its photo-detachment cross section was observed in free space before it was discovered in the laboratory [2].Also it is the main source of opacity in solar atmosphere as suggested by Wildt in 1939 and has large concentration in transition region of planetary nebulae that becomes practically important in the field of Astrophysics, Physics and Chemistry involving weakly ionized gases and plasmas [3–6].

Photo-detachment is possible by virtue of energy conservation: “a minimum energy of photon hv, equal to the electron affinity, required to detach an electron from the negative ion obeying law of conservation of energy that is$\boldsymbol{hv = E + \frac{\hbar^2 k^2}{2m}}$where, $\hbar\boldsymbol{k}$is the linear momentum of free electron and **E** is its detached-energy [7]. Conservation of parity and conservation of total angular momentum ($\Delta L = 0, \Delta S = 0, \Delta J = 0$) leads to the electric dipole selection rules, that severely limits the number of accessible final states [8].

Cross section is a measure of probability. How a negative ion interacts with electromagnetic radiation and how it varies with photon energy, requires one to determine the magnitude of the cross section [9]. Generally, cross section of single electron detachment starts at zero threshold, rises to maximum, and then asymptotically decreases towards higher photon energies [3].

This paper is organized as follows. In section**1.1** a brief review of cross section measurement of H^- in free space is addressed. A rough idea about the structure of photo-detachment cross section is given in section **1.2**. In this section the Wigner law, reason of resonances, and asymptotic behavior are also presented briefly. In section **2**, we present a simple analytical theory and a formula for photo-detachment cross section of H^- in free space re-derived on the basis of simple rules of quantum mechanics.

1.1. HISTORICAL REVIEW

The behavior of cross section just above threshold has been an interesting subject for experimentalists and theoreticians. The absorption by H^- in determining the opacity of our solar atmosphere had opened a new door for scientists in calculation of photo-detachment cross section of H^-. In particular, Chandrasekhar and co-workers havedone a series of calculations of the cross section using various refinements of wave functions of the bound and unbound states. He was the first scientist who proved the cross section spectra of H^- in free space is smooth. Chandrasekhar and Elbert used dipole velocity matrix elements, Hart and Herzberg's 20-parameter ground-state wave function, and a Hartree approximation for the free-state wave function to calculate cross section [10]. Such calculationshavealso been carried out by Geltman [11]. T. Ohmara and H.Ohmara discussed the photo-detachment spectra of H- on the basis of effective range theory (also called ”loosely bound ” approximation) and a formula was derived for bound free coefficient of continuous absorption for photon frequency [12].Marco A. C. Nascimento and William A. Goddard also computed photoionization cross section of hydrogen negative ion by using a discrete-basis-set expansion to represent both the ground and continum states of the system. They proposed a smooth cross section behavior for H^- ion that had good agreement with experimental and theoretical results [13]. In 1989 Farley proposed an analytical model based on zero-core-contribution (ZCC) approximation to calculate photodetachment cross section of negative hydrogen ion near threshold [7]. In 1997 Andreas E. Klinkmuller discussed this characteristic of negative ion with the help of an analytical model in which three simplifying assumptions were made to calculate the photo-detachment cross section. The cross section behavior based on this model agreed qualitatively with experimental results [8].

Experimental results bearing on this subject have been slender. The first detailed experimental study of photo-detachment cross section was undertaken by Branscomb and his co-workers by using tungsten lamp and a crossed ion beam of H$^-$ [1]. By using this technique the same authors measured the first photo-detachment threshold of O$^-$ [14]. The first precise measurement of the wavelength dependence of the photo-detachment cross section of the negative atomic hydrogen ion was reported by Stephen J. Smith and David S. Burch [15]. Feldmann employed a 3-KeV H$^-$ion beam crossed by laser to determine the photo-detachment threshold [16].

1.2. PHOTOTETACHMENT CROSS SECTION

After photo-detachment process, according to a standard approach, detached-electron and residual atom are treated as one dimensional problem with an effective potential $\boldsymbol{V_{eff} = V(r) + \frac{\hbar^2}{2\mu r^2} l(l+1)}$,where second term iscentrifugal barrier term. Here,**μ** is the reduced mass, and **r** is distance between the electron and the core of the neutral atom[17]. The assertion of Wigner photo-detachment law is that the interaction between detached-electron and neutral atom falls off faster than r^{-2}for large **r**. Therefore in $\boldsymbol{V_{eff}}$ the dominant term is centrifugal barrier at largest [7].

Wigner law is known as threshold law because it holds near threshold. In 1948, Wigner theory has predicted that the cross section near threshold depends only on the angular momentum of the final state [18]. The energy dependence of the cross section for the formation of two particles with angular momentum$l\hbar$ is given by$\boldsymbol{\sigma(E) \propto k^{2l+1}\sigma(E) \propto \Delta E^{l+1/2}}$, where ΔE is the energy above threshold and$\boldsymbol{l}$is the orbital angular momentum of the detached electron.

In contrast with photoionization, the photo-detachment cross section starts with zero threshold [8]. Staring at zero, it rises with increasing photon energy as density of states raises and as the electron is able to cross the centrifugal barrier [18].

The general structure ofphoto-detachment cross section is classified in three main region (i) threshold region, (ii) peak point, and (iii) asymptotic region. This behavior is shown schematically below in Fig. (1).

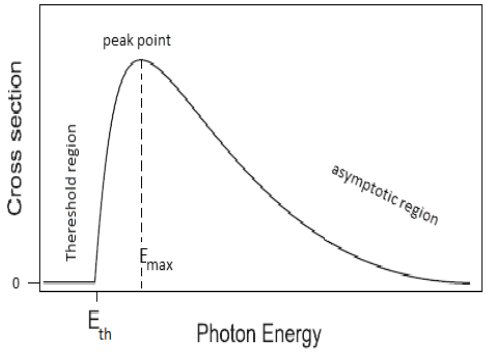

Fig.1: General behavior of cross section over a wide range of photon energy.

Near threshold, commonly the cases $l = 0{,}1$, also known as s-wave and p-wave respectively, are important[8]. When an electron is removed from H$^-$, the outgoing electron has$l = 1$. This behavior is called p-wave threshold. The cross section rises with $\Delta E^{3/2}$ dependence and slope will be zero at threshold [2]. Photo-detachment from the s orbital leads to p-wave threshold, and if the photo-detachment occurs due to a p orbital then the final state will be either s-wave or d-wave [7].

Sometime some sharper structures occur in this smooth photo-detachment cross section. These structures are either resonances or Wigner cusps. Resonances occur due to the auto-detaching states of the negative ions while wigner cusp located at the threshold of s-wave detachment channels is a discontinuity in scattering cross section.

The wave function of escaping electron oscillates rapidly as the photon energy increases. Overlap of this oscillating wave function with fixed initial wave function leads to an asymptotic decrease in cross section [8].

2. **An analytical Expression.** The H$^-$ will be considered as an effectively one electron system. Let $\Psi_i = \frac{Be^{-k_b r}}{r}$be the initial bound state of H$^-$.Where B=0.31522 is related to the normalization constant of initial bound state of H$^-$ and $k_b = \sqrt{2E_b}$, $E_b$is the binding energy and it is approximately equal to 0.754eV.

Let a z polarized laser light with photon energy $E_{ph} = E + E_b$ is used to detach the loosely bound electron from H$^-$ ion. In quantum mechanics an infinite number of waves are attached with escaping electron, which propagates away from the source in all possible directions in spherical mannersas there is no external field is involved. The schematic diagram of this phenomenon is given below in Fig.(2):

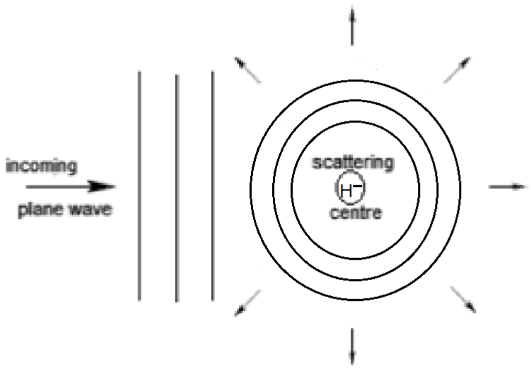

Fig.(2) Scattering geometry of photo-detachment of H$^-$ ion.

The outgoing detached-wave function is written as[19]:

$$ {}_f(r) = U(k,\theta,\varphi)\frac{e^{ikr}}{kr}. \qquad (1)$$

Where$U(k,\theta,\varphi) = \frac{4ik^2B}{({k_b}^2+k^2)^2}cos\theta$ is the laser polarization factor for z-polarized laser light. If the factor $\frac{4kB}{({k_b}^2+k^2)^2}$ is replaced by another constant C then ${}_f$ will be modified as:

$$ {}_f = \mathrm{iCcos\theta}\frac{\mathrm{e^{ikr}}}{\mathrm{r}}. \qquad (2)$$

Electron flux of these outgoing waves can be derived by using $\boldsymbol{\nabla}_f$ in the simple formula of quantum mechanicsi.e.,$\boldsymbol{j}(r,\theta,\varphi) = \frac{i}{2}\left({}_f\boldsymbol{\nabla}_f{}^* - {}_f{}^*\boldsymbol{\nabla}_f\right)$.

The electronic flux of the detached outgoing electron will be

$$\boldsymbol{j}(r,\theta,\varphi) = \frac{kC^2cos^2\theta}{r^2} \equiv \boldsymbol{j_0}(r,\theta,\varphi). \qquad (3)$$

Electron flux on the surfaceof screen is obtained by projecting it in radial direction for one system in the direction normal to the screen. If the screen is placed normal to z-direction then flux in z direction will be;

$$\mathrm{j_z(r,\theta,\varphi)} = \frac{\mathrm{kC^2cos^2\theta}}{\mathrm{r^2}}\hat{\boldsymbol{r}}.\hat{\boldsymbol{n}}. \qquad (4)$$

With the help of this simplified electronic flux one can easily find the generalized cross section i.e.

$$\frac{d\sigma}{dS}(q) = \frac{2\pi}{c}\,E_{ph}\,(\mathbf{j}\cdot\hat{\boldsymbol{r}}) \qquad (5)$$

Where **q**is the generalized coordinates on surface**,** in our case generalized coordinates are energy, and $\hat{\boldsymbol{r}}$is exterior norm vector at **q**, anddS is the differential area of the surface. By integrating this generalized differential cross section over the whole surface we get total cross section i.e.

$$\sigma(E) = \frac{8\pi^2}{3c}E_{ph}kC^2\,. \qquad (6)$$

Where c= 137is the speed of light in a.u.By putting values of $E_{ph}$and $C = \frac{4kB}{({k_b}^2+k^2)^2}$, we can get the background cross section

$$\sigma(E) = \frac{16\sqrt{2}\pi^2B^2(E_{ph}-E_b)^{3/2}}{3c(E_b+E)^3}, \qquad (7)\text{or}$$

$$\sigma\left(E_{ph}\right) = \frac{16\sqrt{2}\pi^2B^2(E_{ph}-E_b)^{3/2}}{3c\left(E_{ph}\right)^3}$$

$$\equiv \sigma_0\left(E_{ph}\right). \qquad (8)$$

Eq. (8) represents the total cross section of H$^-$ ion in free space. It would be smooth with the variation of laser photon energy. Using standard values for B=0.31522 a. u. , c=137 a. u. and E$_b$ =0.745 a. u., we plot Eq. (8) in Fig. 3. This smooth curve starts from the threshold value of H$^-$ ion and then increases to a maximum value by increasing the photon energy. This smooth curve is in accordance with the general behavior of the cross section as shown in Fig. 2.

3. COMPARISION AND DISCUSSION

In the calculation, we have used the simple thoughts of quantum mechanics and study a main feature of hydrogen negative ion, total cross section.

We have used the above result of Eq. (8) and developed the photo-detachment cross section spectra of H$^-$ ion with the help of Matlab technique setting photon energy range 0-10 eV.

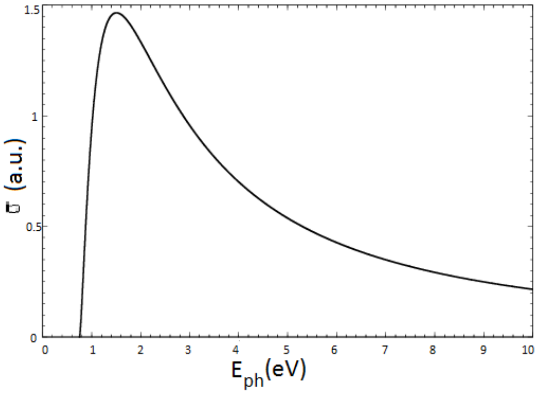

Fig.3.The Photo-detachment cross section of H$^-$ ion versus Photon energy (eV) in Eq. (9) by using Matlab technique is illustrated.

Figure 3 demonstrates the steep rise in curve just above threshold that reaches to a maximum and then asymptotically falls as $E^{3/2}$.Photo-detachment cross section of H$^-$ has p-wave threshold, it is also clear from Eq. (8), because the total cross section has$E^{3/2}$ dependence according to Wigner threshold law.

T. Ohmara and H.Ohmara [12] derived a formula for bound free coefficient of continuous absorption for photon frequency, i.e.

$$K_v = \frac{6.8475\times10^{-18}\gamma k^3}{(1-\gamma\rho)(\gamma^2+k^2)^3}cm^2. \qquad (9)$$

Where, k is wave number of ejected electron in atomic units. This formula was derived based on effective range approximation and has accordance with our output. This “loosely bound” approximation has good agreement with experimental work [12]. The results of Chandrashekar [20], S. J. Smith and D.S. Burch [15], and T. Ohmara and H.Ohmara agree and curves of cross section also have same smooth behavior [12].

Andreas E. Klinkmuller [8] discussed the photo-detachment cross section behavior with the help of an analytical model in which three simplifying assumptions were made to calculate the photo-detachment cross section. These assumptions are: (I) a hydrogen-like orbital for the bound outermost electron; (II) the detached electron is approximated as a plane wave, and (III) attractive zero range potential. The solution for this model in a.u. is given as:

$$\sigma(\omega) = \frac{16\pi}{3c}\sqrt{E_D}\,\frac{\sqrt{(\omega-E_D)^3}}{\omega^3}\,, \qquad (10)$$

withE$_D$ being the detachment limit. The effect of Eq. (10) is also same as discussed in Eq. (8); only cross section variation is taken with respect to frequency. The cross sectional spectra obtained from Eq. (9) and Eq. (10) confirms our result shown in Fig.3. Wigner law also holds for all these cross section curves near threshold.

CONCLUSION

A formula of total cross section for photo-detachment of H$^-$ in free space is re-derived by using the basic concepts of quantum mechanics.This formula facilitates us to determine the structure of H^- ion. The result obtained in Eq. (8) confirms that in the absence of external environment, the total photo-detachment cross section is always smooth which is in accordance to the previous theoretical and experimental predictions. One can find the threshold value using this result and then electron affinity that may further be related to the binding energy of negative ion. Also the peak value of curve may be utilized to find atomic radius of hydrogen negative ion. We hope that our review work may help to the researchers and students who are working in this field.

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