

# Photodetachment of hydrogen negative ion confined in a magnetic circular nano-cavity

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The photodetachment of hydrogen negative ion confined in a magnetic circular nano-cavity is studied on the basis of the semiclassical closed orbit theory. Firstly, we study the classical movement and find out the closed orbit of the photodetached electron. For each closed orbit, we calculate some geometric parameters like the length, action and amplitude, etc. Using these geometric parameters, we construct the semiclassical wave function of the detached electron. Then we put forward an analytical formula for calculating the photodetachment cross section of this system. Our calculation results suggest due to the interference effects of the returning electron waves traveling along the closed orbit with the outgoing waves, oscillating structure appears in the photodetachment cross section. In addition, our study suggests that the oscillating structure depends on the magnetic field strength and the radius of the nano-cavity sensitively. Our work can provide some reference value for the study of the magnetic ion trap and will be useful in understanding the photodetachment process of negative ions confined in a microcavity in the presence of external fields.

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## 1. Introduction

In the last three decades, various methods have been extensively used to study the photodetachment of negative ions in strong electric and magnetic fields. When a monochromatic laser light is shined on the negative ion, a source of electron wave can be produced if the photon energy is larger than the binding energy of the excess electron. The absence of the long-range interaction between the photodetached electron and the remaining neutral atom means that the motion of the emitted electron wave can be controlled by applying external fields. In early 1978-1979, Blumberg and coworkers first observed the modulations of the photodetachment rate of negative ion in the magnetic field experimentally [1-2]. Greene explained this phenomenon using perturbation theory[3]. Later, Bryant et al observed a ripple like structure in the photodetachment cross section of H<sup>-</sup> ion near threshold, which was caused by the autocorrelation in the wave function of the photoelectron in the presence of electric fields[4]. Du and Delos used a semiclassical theory to analyze these oscillatory structures[5]. They found the electric field profoundly changes the simple spherical wave pattern of a free electron source due to the electric force. Therefore, the oscillatory structure in the photodetachment cross section can be ascribed to the interference of the outgoing detached-electron waves with the waves returning to the emitting ion reflected by the external fields. This physical picture is known as the closed orbit theory[6]. Subsequently, many researches have used this theory to study the photodetachment of

hydrogen negative ion in different external fields, such as in parallel or crossed electric and magnetic fields, etc[7-13]. In contrast, the detached electron wave propagating in the presence of a uniform magnetic field has attracted little attention. Because many people think when the charged particle is put in a homogenous magnetic field, its classical cyclotron motion is very simple and makes no sense for further study. But in reality, propagation of charged particle waves in a uniform magnetic field display an unexpected complex patterns and has been realized in recent photodetachment microscopy experiments [14-16]. In addition, when the charged particle is confined in a circular nano-cavity with the magnetic field, it turns out that the classical trajectory of the charged particle will display a richer variety of structure than the particle moving in a circular nano-cavity without the magnetic field [17-18]. In our previous work, we have studied the photodetachment of H<sup>-</sup> ion in a circular nano-cavity without magnetic field[19]. The detached electron's trajectories consist of a series of straight paths bouncing at the boundary of the nano-cavity and the shapes of the closed orbits are regular polygons. When the magnetic field is added perpendicular to the circular nano-cavity, the detached electron's classical trajectories will bend due to the effect of the Lorentz force and should display any behavior of interest. Besides, strong magnetic field conditions can be imitated in some semiconductors where a small effective electron mass and a large dielectric constant reduce the electric force relative to the Lorentz force[20]. Since many semiconductor devices are circular or semi-circular, then the study of the

detached electron wave propagating confined in a magnetic circular nano-cavity becomes necessary and significant. Although the photodetachment of negative ions in cavity is very simple, but it can simulate many dynamical processes, such as the escape of asteroids or meteors through the solar system [21-22], the ionization of Rydberg atom in external electric and magnetic fields [23], the dynamic escape of a small packet of ultra cold atoms from an optical dipole trap [24], etc.

The outline of this paper is as follows: In section 2, we provide a physical picture description for the classical motion of the photodetached electron confined in a circular nano-cavity plus a perpendicular magnetic field, and then we derive the formula for calculating the photodetachment cross section. In section 3, numerical calculation of the photodetachment cross section and some discussions are given. Some concluding remarks are presented in section 4. Atomic units (which are abbreviated as a.u.) are used throughout this work unless indicated otherwise.

## 2. Theory and quantitative formula

### 2.1 Physical picture description and the classical motion of the detached electron

The schematic of the system is plotted in Fig. 1. The circular nano-cavity is placed in the  $x$ - $y$  plane, with  $x$ -axis along one diameter. The  $H^-$  ion is localized at the origin, which is on the left wall of circular nano-cavity. The external uniform magnetic field  $B$  perpendicular to the circular nano-cavity is added, which is pointing along the  $+z$  axis. After the electron is photodetached by the laser light, it will move in the circular nano-cavity in the form of the electron wave. Due to the effect of the Lorentz force, the detached electron's classical trajectories will bend, with the direction of the curvature depending on the direction of motion with respect to the magnetic field.

The detached electron's Hamiltonian in the presence of the external magnetic field is given by:

$$H = \frac{1}{2} \left[ P + \frac{1}{c} A \right]^2 + V_b(r), \quad (1)$$

where  $V_b(r)$  is the short-range potential between the excess electron and hydrogen atom. As in the previous studies[9-12], this potential can be neglected after the electron is photodetached. In the perpendicular magnetic field, we choose a gauge for the vector potential  $A$  that conforms to the inherent cylindrical symmetry:

$$\mathbf{A} = \frac{1}{2} \bar{B} \times \bar{r} = -\frac{1}{2} B y \bar{i} + \frac{1}{2} B x \bar{j} \quad (2)$$

Then the Hamiltonian governing the detached electron's motion in the  $x$ - $y$  plane is:

$$H = \frac{1}{2} P_x^2 + \frac{1}{2} P_y^2 + \frac{1}{2} \omega_L^2 (x^2 + y^2) + \omega_L L_z, \quad (3)$$

where  $\omega_L = \frac{B}{2c}$  is the cyclotron frequency of the

electron.  $L_z$  is the angular momentum, which is a constant. In our calculation, we take  $L_z = 0$ .

By solving the classical Hamiltonian motion equations, we obtain the detached electron's motion equations in the  $x$ - $y$  plane:

$$\begin{cases} x(t) = \frac{k \sin(\omega_L t)}{\omega_L} \cos \theta & (4a) \\ y(t) = \frac{k \sin(\omega_L t)}{\omega_L} \sin \theta & (4b) \end{cases}$$

Where  $k = \sqrt{2E}$  is the detached electron's momentum.

$\theta$  is the angle of the detached electron's position vector relative to the  $x$ -axis, which is shown in Fig. 1. From the above two equations, we find the detached electron's movement is a cyclotron motion in the  $x$ - $y$  plane. If there is no circular nano-cavity, the detached electron's trajectory in the uniform magnetic field is a circular one, and all the trajectories are closed. But if the detached electron is confined in a circular nano-cavity, it will hit with the surface of the nano-cavity. Then the detached electron's trajectories will be changed. In our study, we still neglect the interaction between the detached electron and the surfaces of the cavity. Then the collision between the electron and the surfaces is elastic[19]. After one or several bounces of the surfaces, the electron may return to the origin of the negative ion. These orbits are called closed orbits. In Fig.1, we plot a group of the detached-electron's closed orbits.

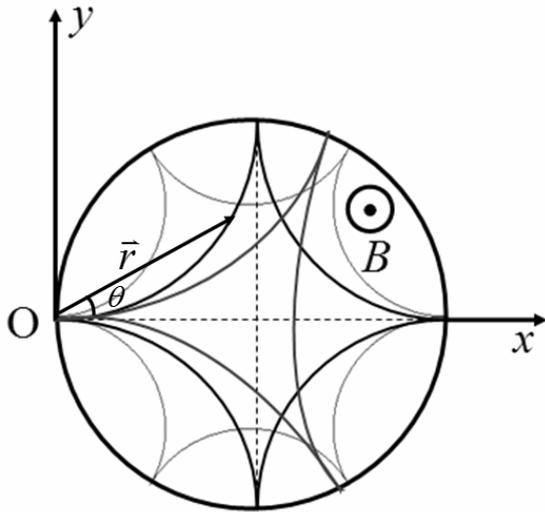


Fig. 1. Schematic illustration of the photodetachment of  $H$  confined in a circular nano-cavity plus a perpendicular magnetic field. The  $H$  lies at the origin. A group of trajectories propagating away from the origin, after being reflected several times by the cavity surfaces and finally return back to the region. Different closed orbits are marked by different lines.

In the following, we show how to search the detached electron's closed orbit confined in the magnetic circular nano-cavity in detail. The schematic is shown in Fig. 2. Suppose the radius of the circular nano-cavity is  $R$  and the electron is emitted from the origin ( $x=0,y=0$ ) along the  $+x$ -axis. The outgoing angle of the detached electron relative to the  $x$ -axis  $\theta_{out}=0$ . The cyclotron radius of the electron in the magnetic field is:  $R_c = k/B$ , and the circular center is denoted as  $O_c$ . For this geometry configuration, the detached electron's closed orbits confined in a circular nano-cavity can be characterized by the angle  $\Theta$ , subtended by the arc between successive bounces with the circular surfaces. Closed orbits appear only if the following condition is satisfied:  $p\Theta = q(2\pi)$ .

Where  $p$  and  $q$  are positive integers and satisfy  $p > 2q$ .  $p$  denotes the number of the bounces between the detached electron and the surface of the nano-cavity,  $q$  is the winding number, which counts how often an orbit wind around the center of the circular nano-cavity[25].

Therefore, we can use a pair of integers  $(p,q)$  to distinguish different closed orbit.

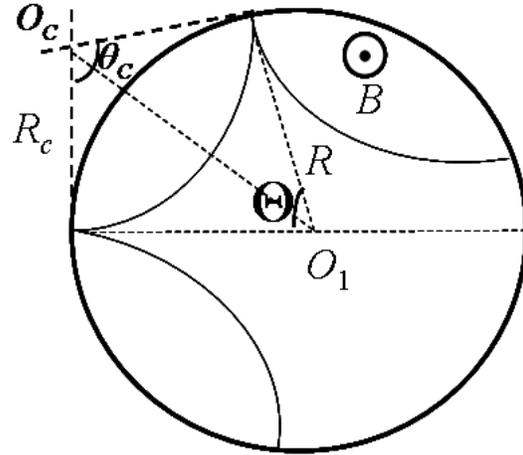


Fig. 2. Geometrical description of the detached electron's closed orbits in a circular nano-cavity plus an external magnetic field. The condition the closed orbit satisfied is  $\Theta=2\pi q/p$ .

The length of the closed orbit is given by:

$$L = 2pR_c\theta_c \tag{5}$$

Where  $\theta_c$  is the central angle corresponding to the arc in the nano-cavity:  $\theta_c = \pi - \Theta$ . The relation between the cyclotron radius  $R_c$  and the circular nano-cavity radius  $R$  is:  $R_c = R \tan(\Theta/2)$ . Some of the closed orbits are given in Fig.3. Fig.3(a) shows the closed orbit with  $p=3,q=1$ , which is denoted as  $(3,1)$ . This orbit leaves the origin along the  $+x$  direction, due to the effect of the Lorentz force, it will bend outward the center of the nano-cavity, after being reflected by the surface of the circular nano-cavity twice, then travels toward to the origin. Similar descriptions can be given to other closed orbits.

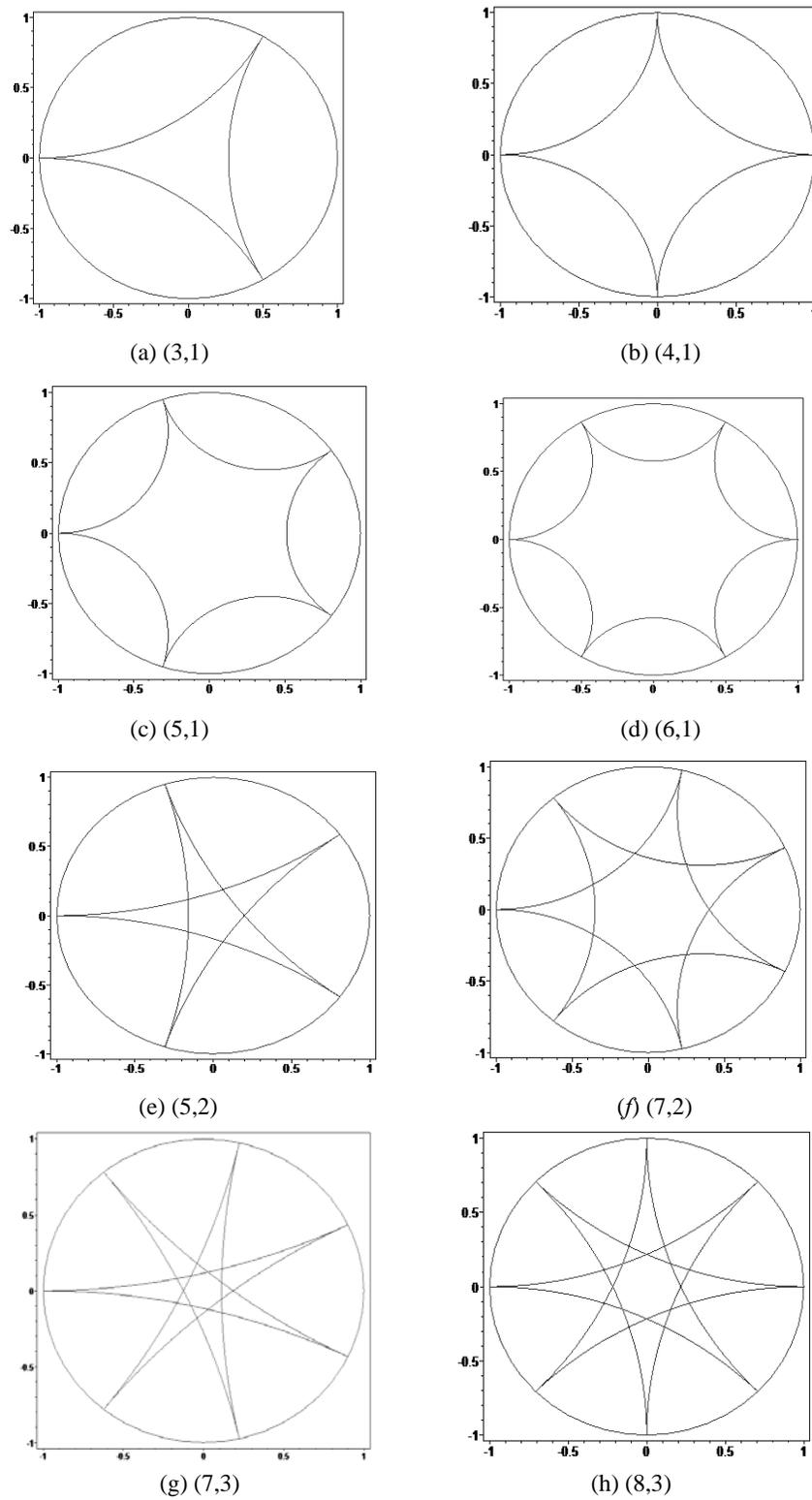


Fig. 3. Some closed orbits of the detached electron inside a magnetic circular nano-cavity. The numbers of  $p$  and  $q$  are given in each plot.

In Table 1, we summarize the collision number  $p$ , wind number  $q$ , the length  $L$  and the geometry feature angle  $\Theta$  of the closed orbit in the circular nano-cavity with

$2 \leq p \leq 10$  and  $1 \leq q \leq 3$ . Suppose the radius of the circular nano-cavity  $R=100\text{a.u.}\approx 5\text{nm}$ .

Table I. Geometry parameters of some closed orbit confined in a magnetic circular nano-cavity.

$(p,q)$	$L(\text{a.u.})$	$\Theta(\text{deg.})$
(3,1)	4353.12	120.00
(4,1)	5026.54	90.00
(5,1)	5478.00	72.00
(6,1)	5804.16	60.00
(7,1)	6051.64	51.43
(8,1)	6246.19	45.00
(9,1)	6403.30	40.00
(10,1)	6532.90	36.00
(5,2)	7735.06	144.00
(7,2)	9454.64	102.86
(9,2)	10544.44	80.00
(7,3)	11011.37	154.29
(8,3)	12135.16	135.00
(10,3)	13836.90	108.00

## 2. 2 Photodetachment cross section

The photodetachment process of H<sup>-</sup> confined in a circular nano-cavity plus a perpendicular magnetic field can be described as follows: when H<sup>-</sup> absorbs photon energies, outgoing electron waves are generated. Due to the effect of the magnetic fields and the confined environment, these waves cannot propagate to infinity, some of the waves are turned back by the surface and return to the origin. The returning waves overlap with the outgoing source wave caused the interference pattern in the photodetachment cross section.

According to the closed orbit theory, the photodetachment cross section of H<sup>-</sup> ion confined in a magnetic circular nano-cavity can be written as:

$$\sigma(E, B) = \sigma_0(E) + \sigma_{osc}(E, B) \quad (6)$$

In which  $\sigma_0(E) = \frac{16\sqrt{2}\pi^2 B_0^2 E^{3/2}}{3c(E_b + E)^3}$  is the smooth

background term of H<sup>-</sup> in free space without external environment[5].  $E$  is the energy of the detached electron,  $E_b=0.754\text{eV}$  is the binding energy of H<sup>-</sup> ion.  $B_0=0.31552$  is a normalization constant.  $\sigma_{osc}(E, B)$  is the oscillating term[26]:

$$\sigma_{osc}(E, B) = -\frac{4\pi}{B_0} (E + E_b) \text{Im} \langle D \psi_i | \psi_{ret} \rangle \quad (7)$$

where  $\psi_i(\vec{r}) = \frac{B_0 e^{i k_b r}}{k_b}$  is the initial wave function of the bound electron,  $k_b = \sqrt{2E_b}$ .  $D$  is the dipole operator. For  $x$ -polarized laser light,  $D = x$ .  $\psi_{ret}$  is the returning wave function of the detached electron.

Inside the circular nano-cavity, the wave function propagates in a manner that is consistent with the semiclassical approximation. The semiclassical method for propagating a wave function goes as follows. An initial curve corresponding to an initial wave front is defined. In our study, the initial curve is a sphere of radius  $R_0$  ( $R_0 \ll R$ ). Then the outgoing wave on the surface of this sphere is[5,19]:

$$\psi_{out}(R, \theta, \varphi) = \frac{4B_0 k i}{(k_b^2 + k^2)^2} \frac{e^{i k R_0}}{R_0} \cos \theta_{out} \quad (8)$$

When this wave propagates out from the surface and travels along the closed orbit, its amplitude and phase are changed. The wave function associated with trajectory  $j$  is:

$$\psi_j(r, \theta, \varphi) = \psi_{out}(r, \theta, \varphi) A_j e^{i[S_j - \mu_j \pi / 2]} \quad (9)$$

In which  $A_j$  is the amplitude, which measures the divergence of adjacent trajectories from the  $j$ -th closed orbit.

$$A_j = \left| \frac{\det J_j^{(2)}(x, y, 0)}{\det J_j^{(2)}(x, y, t_j)} \right|^{1/2} \frac{|x(0)|}{|x(t_j)|} \quad (10)$$

Where  $J^{(2)}(x, y, t)$  is a 2x2 Jacobian matrix, which is given by:

$$J^{(2)}(x, y, t) = \begin{vmatrix} \frac{\partial x}{\partial t} & \frac{\partial y}{\partial t} \\ \frac{\partial x}{\partial \theta} & \frac{\partial y}{\partial \theta} \end{vmatrix} \quad (11)$$

By substituting the electron's motion equations (Eq.(4a) and Eq.(4b)) into the above two formula, we obtain:

$$A_j = \frac{R_0}{k} \left| \frac{\omega_i^2}{\sin^2(\omega_i t) \cos(\omega_i t)} \right|^{1/2}$$

$S_j$  is the action along the  $j$ -th closed orbit. For the present system [17]:

$$S_j = \oint \left( P_j + \frac{A}{c} \right) \cdot dq_j = kL_j + 2\omega_L S_{jc} \quad (12)$$

Where  $L_j$  is the length of the  $j$ -th closed orbit.  $S_{jc}$  is the enclosed areas of the  $j$ -th closed orbit, which is given by:

$$S_{jc} = p \left( \frac{R^2}{2} \sin \Theta - \frac{R_C^2}{2} \theta_C + \frac{R_C^2}{2} \sin \theta_C \right) \quad (13)$$

$\mu_j$  is the Maslov index. After each collision with the surfaces of the nano-cavity, there is a phase loss  $\pi$  of the wave function. Then  $\mu_j = 2(p-1)$ .

The returning wave function associated with  $j$ -th trajectory evaluated on the sphere with radius  $R_0$  is given by:

$$\psi_{ret}^j(r) = 4ikB_0 \frac{\sqrt{4\pi}}{(k^2 + k_b^2)^2} \cos \theta_{out}^j \frac{e^{i\vec{k} \cdot \vec{r}}}{R_0} A_j e^{i[S_j(t_{ret}) - \mu_j \pi / 2]} \quad (14)$$

Inside the sphere, the semiclassical returning wave function can be approximated by a plane wave:

$$\psi_{ret}^j(r) \approx N_j e^{i\vec{k}_{ret}^j \cdot \vec{r}} \quad (15)$$

where  $N_j$  is a matching factor:

$$N_j = 4ikB_0 \frac{\sqrt{4\pi}}{(k^2 + k_b^2)^2 R_0} \cos \theta_{out}^j A_j e^{i[S_j(t_{ret}) - \mu_j \pi / 2]} \quad (16)$$

The whole returning waves are the sum of each returning wave:

$$\psi_{ret} = \sum_j \psi_j^{ret} \quad (17)$$

Using the partial-wave expansion of the returning wave, then substituting Eq.(17) into (7) and calculating the overlap integral of the returning waves with the source wave function  $\langle D\psi_i |$ , we obtain the oscillating term in the photodetachment cross section:

$$\sigma_{osc}(E, B) = -\sum_j \frac{16\pi^2 B_0^2 E}{c(E_b + E)^3} \frac{A_j}{R_0} \cos^2 \theta_{out}^j \sin(S_j - \mu_j \frac{\pi}{2}) \quad (18)$$

Therefore, the total photodetachment cross section for the photodetachment of H<sup>-</sup> ion confined in a circular nano-cavity plus an external magnetic field can be written as:

$$\sigma(E, B) = \sigma_0(E) - \sum_j \frac{16\pi^2 B_0^2 E}{c(E_b + E)^3} \frac{A_j}{R_0} \cos^2 \theta_{out}^j \sin(S_j - \mu_j \frac{\pi}{2}) \quad (19)$$

In this work, all the trajectory of the detached electron are emitted from the origin along the +x-axis, then the outgoing angle of the detached electron relative to the x-axis  $\theta_{out}^j = 0$ .

### 3. Results and discussions

Using Eq.(19), we calculate the photodetachment cross section of H<sup>-</sup> confined in a circular nano-cavity plus an external magnetic field. Firstly, we keep the radius of the circular nano-cavity unchanged,  $R=100a.u.$ , then we show how the photodetachment cross section changed with the magnetic field strength. The results are given in Fig.4. Fig.4(a) is the cross section without the external magnetic field. Under this condition, when the electron is emitted along the +x-axis, only the diameter orbit exist[19], so the photodetachment cross section exhibits a smooth background term plus an oscillating term. The oscillating

amplitude is relatively small. Figs.4(b-f) are the photodetachment cross section with the external magnetic field. From these figures we find when the magnetic field is added, due to the influence of the Lorenz force, the oscillating structure in the cross section becomes complex. Besides, with the increase of the magnetic field strength, the number of the closed orbit is increased and the oscillating amplitude becomes increased obviously. For example, in Fig.4(b), the magnetic field strength  $B=5.0T$ . The cyclotron radius of the detached electron in the

magnetic field is relatively large, thus the number of the closed orbit satisfied the condition in the circular nano-cavity is relatively small. Under this circumstance, the oscillatory structure becomes apparent only in the low energy region. With the increase of the magnetic field strength, the cyclotron radius becomes decreased, and the number of the closed orbit becomes increased, so the oscillating structure becomes complex and the oscillating amplitude becomes enlarged.

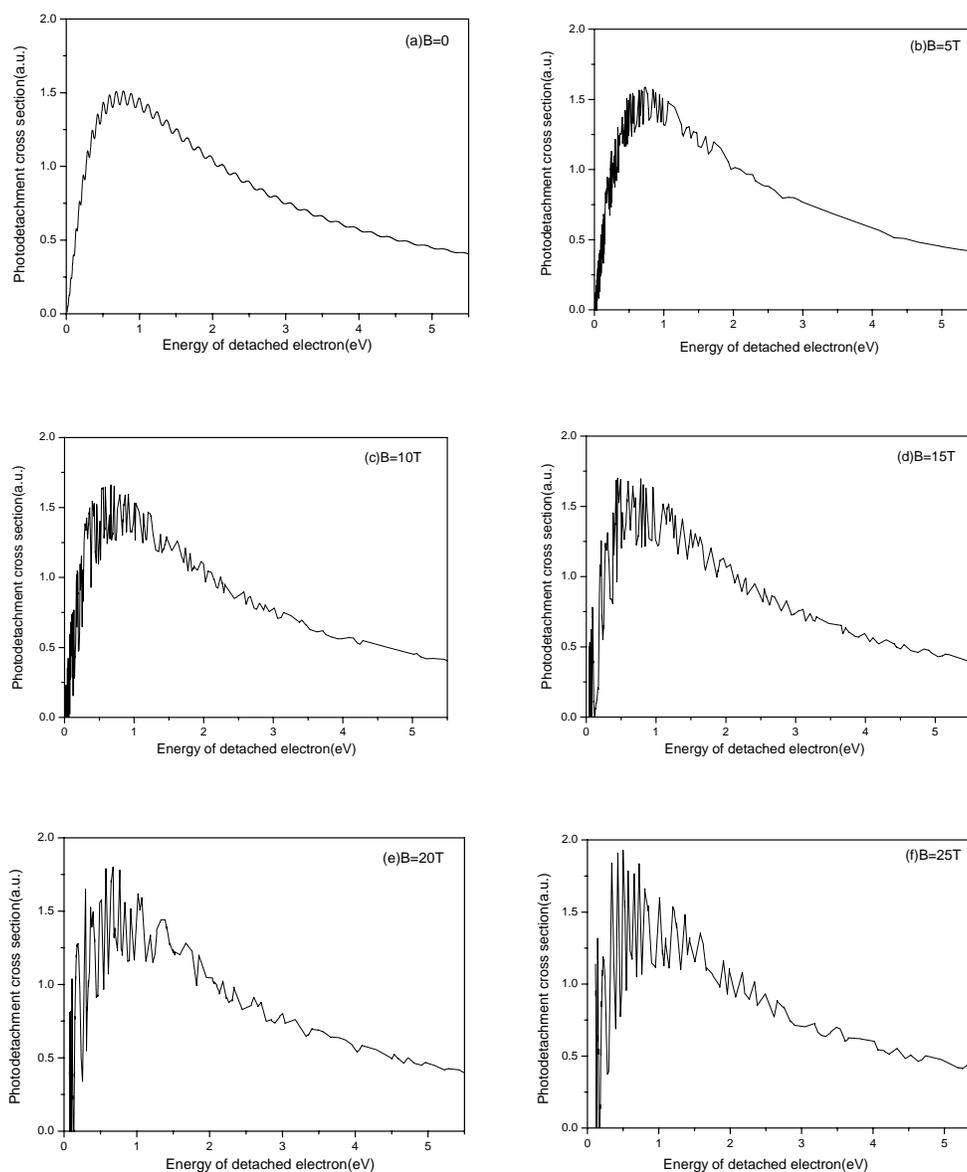


Fig. 4. The photodetachment cross section of  $H$  confined in a circular nano-cavity plus an external magnetic field. The radius of the nano-cavity  $R=100a.u.$ . The magnetic field strength is as follows: (a)  $B=0.0T$ ; (b)  $B=5.0T$ ; (c)  $B=10.0T$ ; (d)  $B=15.0T$ ; (e)  $B=20.0T$ ; (f)  $B=25.0T$ .

In Fig.5, we fix the magnetic field strength,  $B=10.0T$ , and show how the photodetachment cross sections varied with the radius of the circular nano-cavity. In order to show the influence of the external circular nano-cavity on the photodetachment cross sections clearly, we only plot the oscillating part in the total photodetachment cross section. Fig.5(a) shows the cross section with the radius of the circular nano-cavity  $R=100a.u.$ . On this occasion, oscillating structures appear even at very low energy. As the detached electron's energy is high, the cyclotron radius of the detached electron in the magnetic field becomes

large, thus the number of the closed orbit becomes small and the oscillating structure becomes inconspicuous. With the increase of the radius of the circular nano-cavity, the number of the closed orbit satisfied the condition in the circular nano-cavity becomes small. So the oscillating region and the oscillating amplitude become decreased. For example, when  $R=500a.u.$ , the oscillatory structure in the photodetachment cross section appears only in the detached electron's energy larger than  $0.4577eV$  and the oscillating amplitude is decreased obviously.

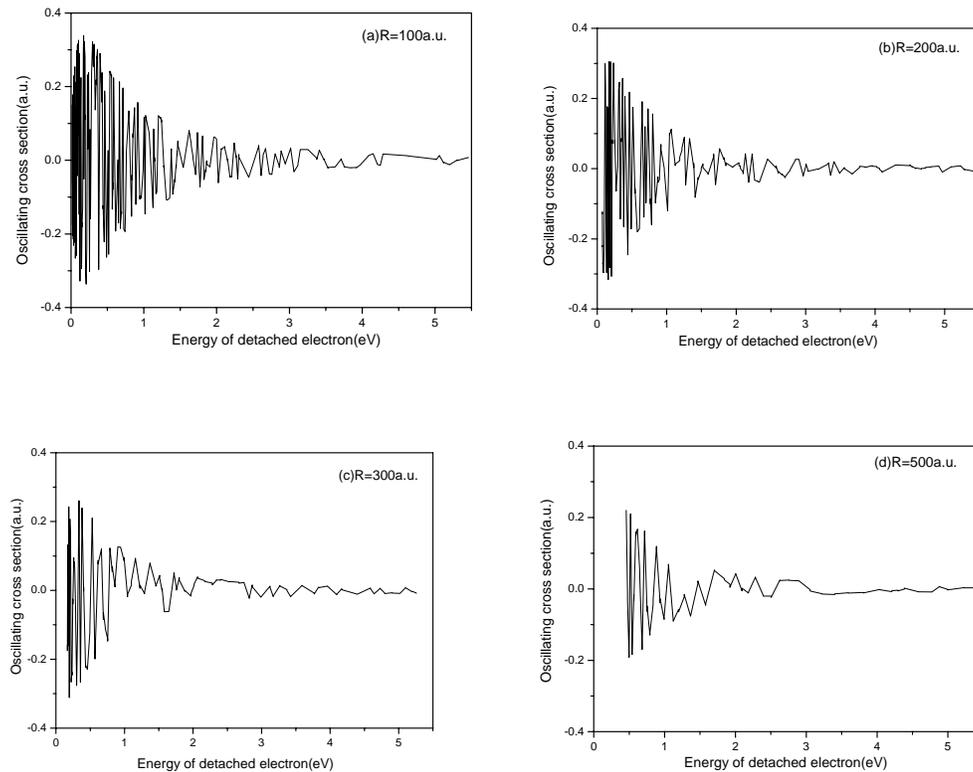


Fig. 5. The oscillating photodetachment cross section of  $H^-$  confined in a circular nano-cavity plus an external magnetic field. The magnetic field strength  $B=10.0T$ . The radius of the nano-cavity is as follows: (a)  $R=100a.u.$ ; (b)  $R=200a.u.$ ; (c)  $R=300a.u.$ ; (d)  $R=500a.u.$ .

#### 4. Conclusions

In conclusion, we have investigated the photodetached electron waves propagating confined in the circular nano-cavity plus an external magnetic field. The classical closed orbits of the detached electron have been found out and an analytical formula for calculating the photodetachment cross section has been put forward. The calculation results suggest that the oscillatory structure in the photodetachment cross section have a strong

dependence on the strength of the magnetic field and the radius of the circular nano-cavity. For a given circular nano-cavity, with the increase of the magnetic field strength, the number of the detached electron's closed orbit moving in the nano-cavity becomes increased. The oscillating structure in the photodetachment cross section becomes complex and the oscillating amplitude becomes enlarged. Recently, studies of the photodetached electron wave propagating in a magnetic circular cavity become increasingly important. It is not only a matter of theoretical

concern but a subject of general interest, owing to their broad area of applications in different research fields, such as in astrophysics and atomic, molecular and condensed matter physics, etc[20]. We hope that our studies will be useful in guiding the future theoretical and experimental research of the magnetic ion trap and the photodetachment processes of negative ions within a confined environment in the presence of external fields.

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