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Photodetachment cross-section of H^- ion in a three-dimensional cubical microcavity

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Abstract. The photodetachment of negative ions inside a two-dimensional microcavity has been studied by many researchers. As to the photodetachment of negative ions in the three-dimensional microcavity, the research is relatively little. In this paper, we study the photodetachment cross-section of H^- ion inside a three-dimensional cubical microcavity for the first time. We have observed the classical dynamics of the photodetached electron inside the cubical microcavity and found out its closed orbits. Then we calculate the photodetachment cross-section of this system. It is shown that owing to the interference effects of the electron wave travelling along various closed orbits, oscillatory structures appear in the photodetachment cross-section. And the oscillatory structures depend on the laser polarization sensitively. Compared to the photodetachment of H^- ion inside a square microcavity, in photodetachment of H^- ion in cubical cavity the number of the closed orbits is increased and the oscillatory structure in the photodetachment cross-section becomes much more complex. Through our study, researchers can gain a deep understanding on the correspondence of the classical dynamics and the quantum mechanics. Our study may guide future experimental research in the field of the photodetachment electron dynamics inside a three-dimensional microcavity.

Keywords. Photodetachment; spectrum; cubical microcavity; negative ion.

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1. Introduction

In the past several decades, many experimental and theoretical researchers have studied the photodetachment processes of negative ions under various environments, such as in the external fields, near a surface or in a microcavity. Early experiments and theory showed that oscillatory structures appear in the photodetachment cross-section of negative ions after they are subjected to external fields [1–6]. Du and Delos put forward a semiclassical closed orbit theory to explain the oscillatory structures in the photodetachment cross-section. They discovered that the oscillatory structure is caused by the interference of the detached electron waves reflected by the external fields with the outgoing electron waves localized in the sources of negative ions [7,8]. The predictions of closed orbit theory have also been verified by the photodetachment microscopy experiments of negative ions [9,10]. Since H^- ion is a very simple system and has been proposed as a probe to investigate the lifetime of the adsorbate and charge transfer mechanism in the backscattering process [11], the photodetachment of H^- ion near the surfaces has attracted much interest. First, Yang *et al* investigated the photodetachment cross-section of H^- ion near an elastic interface on the basis of the closed orbit theory [12–14]. Subsequently, Afaq and Du put forth a theoretical imaging method to re-study this system and found that the oscillations in the cross-section are similar to that of Yang *et al* [15]. Later, Zhao *et al* studied the photodetachment of H^- ion near metal surfaces [16–26]. Recently, many researches have studied the photodetachment of H^- ion from a surface to a microcavity. In the research of the escape or transport process of the electron in the semiconductor microjunctions, in the billiard system, or in the photodetachment microscopy, the photodetachment of electron from an ion within a microcavity would be encountered. In 2011, Zhao and Du studied the escape of a particle from an open wedge-shaped cavity [27]. In their work, the particle was obtained from the photodetachment of H^- ion. Hansen and Novick *et al* discussed the escape of classical particles from a vase-shaped cavity [28–30].

Our group and Zhao *et al* have studied the photodetachment of H^- ion inside a closed square, circular or an equilateral triangle microcavity [31–34]. Most of these previous studies were concentrated on the photodetachment of H^- ions inside a two-dimensional microcavity. As to the photodetachment of H^- ions inside a three-dimensional microcavity, the reports are very little to the best of our knowledge. But it is necessary to carry out this study, because in the study of escape and transport process of electron through semiconductor microjunctions, the shapes of many devices are usually cubical or spherical. In this work, we study the photodetachment of H^- ion inside a three-dimensional microcavity for the first time. In order to calculate the photodetachment cross-section of this system, we find out the closed orbits of the detached electron inside the cubical microcavity. Compared with the photodetachment of H^- ion inside a square microcavity [31], the number of orbits of the detached electron is increased and the oscillations in the photodetachment cross-section become much more complex. The microcavity presented in this study for the physical system is very useful to understand the photodetachment of negative ions. We hope that our work may guide future photodetachment microscopy experiments inside a microcavity.

This paper is planned as follows: In §2, we discuss the classical motion of the detached electron inside a cubical microcavity and find out the closed orbits of the detached electron. Then we obtain an analytical formula for calculating the photodetachment cross-section of this system. In §3, we calculate the photodetachment cross-section of this system. The dependence of the cross-section on the laser polarization is discussed in detail. Conclusions and perspectives are given in §4. Atomic unit (which is abbreviated as a.u.) is used in this work unless indicated otherwise.

2. Derivation of the photodetachment cross-section

2.1 *The classical motion of the detached electron*

A schematic plot of the photodetachment of H^- ion inside a cubical microcavity is shown in figure 1. We put H^- ion at the origin, while a cubical microcavity is placed in the x–y–z plane. The side length of the cubical microcavity is a. As in previous studies, H^- ion can be regarded as a one-electron system. The binding potential between the active electron and the hydrogen atom is a short-ranged, spherically symmetric one. Based on the physical picture of the closed orbit theory [7], when a laser light irradiates H^- ion inside a cubical microcavity, the active electron may absorb a photon. If the photon energy is larger than the binding energy between the electron and hydrogen atom, the active electron will be photodetached. The detached electron may move away from the negative ion in all possible directions. Due to the influence of the microcavity, the detached electron cannot move to infinity. When the electron hits the surfaces of the microcavity, it will be reflected. In this work, we still neglect the interaction between the detached electron and the surfaces. So the surfaces of the microcavity can be considered as elastic ones [27]. After several reflections by the surfaces of the microcavity, the electron may return to the origin, thus forming closed orbits. The interference between the returning electron waves with the outgoing source waves causes oscillating structures in the photodetachment cross-section. In order to calculate the photodetachment cross-section of H^- ion inside a cubical microcavity, we must find out all the closed orbits of the detached electron. The motion of the detached electron inside a cubical microcavity is similar to a cubic billiard [35,36]. Suppose the electron is emitted from the origin, we use three non-negative integers (p, q, m) to distinguish different closed orbits, where $2p$, $2q$ and $2m$ denote the number of hits on the surfaces along x, y, z directions, respectively. Then the length of the detached electron's closed orbit is

$$L(p, q, m) = 2a\sqrt{p^2 + q^2 + m^2}. \tag{1}$$

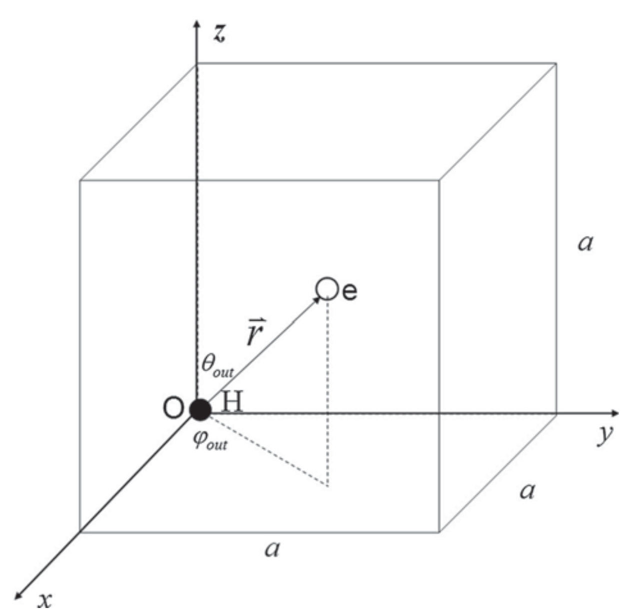

Figure 1. Schematic plot of the photodetachment of H^- ion inside a cubical microcavity. The H^- ion lies at the origin, a cubical microcavity is placed in the $x-y-z$ plane. The length of the side of the cubical microcavity is a. The direction of the outgoing electron is denoted by two spherical angles θ_{out} and φ_{out}.

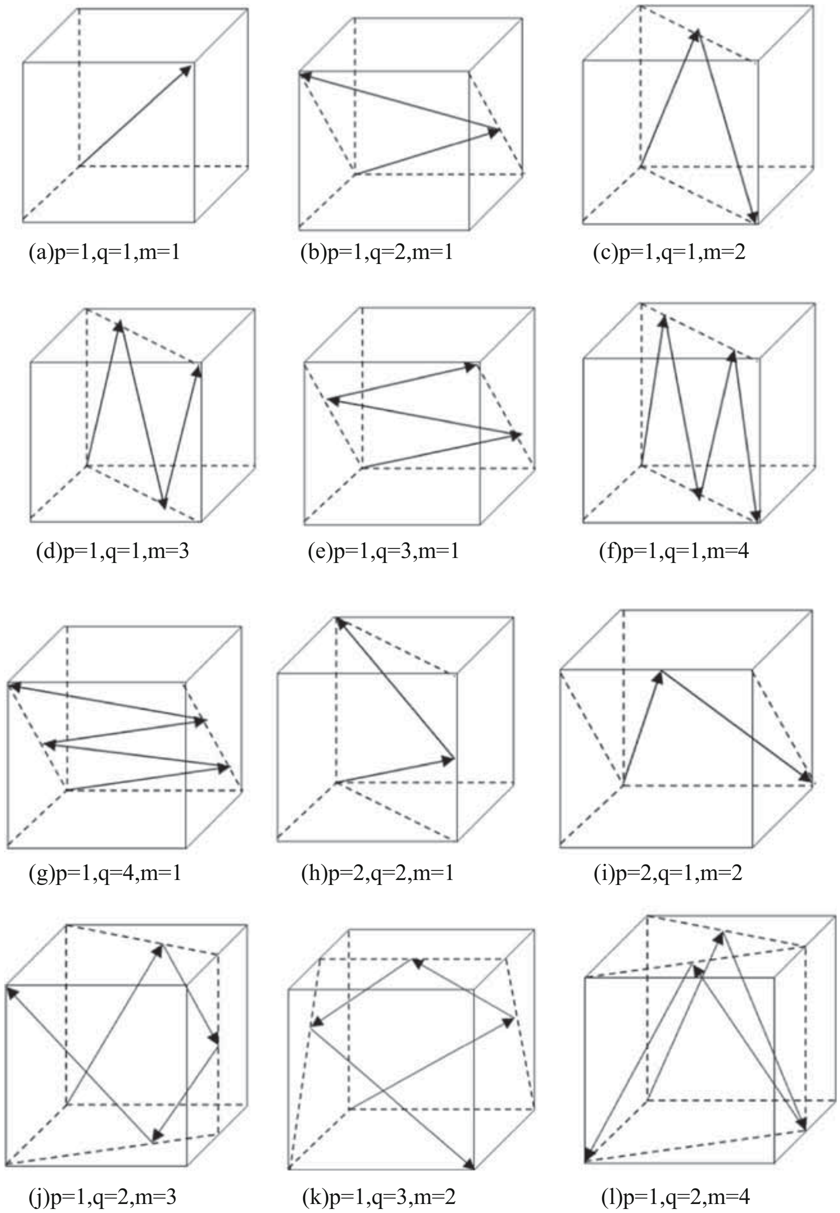

Figure 2. Some closed orbits of the detached electron inside a cubical microcavity. The values of p, q and m for different closed orbits are given in each plot.

If we use spherical angles $\theta_{\text{out}}, \varphi_{\text{out}}$ to denote the outgoing directions of the electron, then

$$\tan\theta_{\text{out}} = \frac{\sqrt{p^2+q^2}}{m}, \quad \tan\varphi_{\text{out}} = \frac{q}{p}.$$

Some of the closed orbits are given in figure 2. Figure 2a shows that the closed orbit leaves the origin in a direction with the spherical angles $\theta_{\text{out}} = 54.73°$, $\varphi_{\text{out}} = 45°$, which is denoted as (1,1,1) closed orbit. After emitting from the origin, it travels toward the top corner of the microcavity and then returns back to the origin. Figure 2b shows the (1,2,1) closed orbit, which leaves the origin at the outgoing angle $\theta_{\text{out}} = 65.90°$, $\varphi_{\text{out}} = 63.43°$, reflects by the right surface once, it then travels toward the left top corner of the microcavity and returns back to the origin. Similar descriptions can be given to the other closed orbits. Suppose the side length of the cubic microcavity $a = 100$ a.u. In table 1, we summarize the numbers of collisions p, q, m, the length L, and the outgoing angle $\theta_{\text{out}}, \varphi_{\text{out}}$ of the closed orbits with length $L \leq 1000$ a.u.

Table 1. The geometry parameters of some closed orbits inside a cubical microcavity.

(p, q, m)	L (a.u.)	θ_{out} (deg.)	φ_{out} (deg.)
(1,1,1)	346.41	54.73	45.00
(1,1,2)	489.90	35.26	45.00
(1,2,1)	489.90	65.90	63.43
(2,1,1)	489.90	65.90	26.56
(1,2,2)	600.00	48.19	63.43
(2,1,2)	600.00	48.19	26.56
(2,2,1)	600.00	70.53	45.00
(1,1,3)	663.32	25.24	45.00
(1,3,1)	663.32	72.45	71.56
(3,1,1)	663.32	72.45	18.43
(2,2,2)	692.82	54.73	45.00
(1,2,3)	748.33	36.70	63.43
(1,3,2)	748.33	57.69	71.56
(2,1,3)	748.33	36.70	26.56
(2,3,1)	748.33	74.50	56.31
(3,1,2)	748.33	59.69	18.43
(3,2,1)	748.33	74.50	33.69
(2,2,3)	824.62	43.31	45.00
(2,3,2)	824.62	60.98	56.31
(3,2,2)	824.62	60.98	33.69
(1,1,4)	848.53	19.47	45.00
(1,4,1)	848.53	76.37	75.96
(4,1,1)	848.53	76.37	14.04
(1,3,3)	871.78	46.51	71.56
(3,1,3)	871.78	46.51	18.43
(3,3,1)	871.78	76.73	45.00
(1,2,4)	916.51	29.21	63.43
(1,4,2)	916.51	64.12	75.96
(2,1,4)	916.51	29.21	26.56
(2,4,1)	916.51	77.40	63.43
(4,1,2)	916.51	64.12	14.03
(4,2,1)	916.51	77.39	26.56
(2,3,3)	938.08	50.24	56.31
(3,2,3)	938.08	50.24	33.69
(3,3,2)	938.08	64.76	45.00
(2,2,4)	978.80	35.26	45.00
(2,4,2)	978.80	65.90	63.43
(4,2,2)	978.80	65.90	26.56

2.2 *Photodetachment cross-section of H^- ion inside a cubical microcavity*

According to the closed orbit theory [8], the total photodetachment cross-section of H^- ion inside a microcavity can be written as a smooth background term $\sigma_0(E)$ plus an oscillating term, which can be written as follows:

$$\sigma(E) = \sigma_0(E) + \sigma^{\text{osc}}(E), \tag{2}$$

where

$$\sigma_0(E) = \frac{16\sqrt{2}\pi^2 B^2 E^{3/2}}{3c(E_b + E)^3}$$

represents the photodetachment cross-section of H^- ion in a free space, which is independent of the microcavity [8]. $B = 0.31552$ is a constant, which is related to the normalization of the initial bound state of H^- ion. c is the speed of the light, which is approximately 137 a.u. $E_b = k_b^2/2$ is the binding energy of the electron with the hydrogen atom, $E_b = 0.754$ eV.

$\sigma^{\text{osc}}(E)$ is the oscillating photodetachment cross-section, which is related to the shape of the microcavity. For our system, this term corresponds to the contribution of the returning wave travelling along various detached electron's closed orbits in the cubical microcavity [27]:

$$\sigma^{\text{osc}}(E) = -\frac{4\pi}{c}(E + E_b)\text{Im}\langle D\psi_i|\psi_{\text{ret}}\rangle, \tag{3}$$

where $\psi_i(\vec{r})$ is the initial bound-state wave function of H^- ion, $\psi_i(\vec{r}) = B\text{e}^{-k_b r}/r = R(r)$. $|D\psi_i\rangle$ is the modified wave function due to operation of D. D is the dipole operator, which is equal to the projection of an electron coordinate along the polarization direction of the laser light: $D = a_x x + a_y y + a_z z$ [5]. For different polarization light, the parameters a_x, a_y, a_z are different. For x-polarized laser light, $a_x = 1, a_y = a_z = 0$; for y-polarized laser light, $a_x = 0, a_y = 1, a_z = 0$; for z-polarized laser light, $a_x = a_y = 0, a_z = 1$. If we adopt the spherical coordinate system, then the dipole operator for x-polarized laser light is: $D = r\sin\theta\cos\varphi$. For y-polarized laser light, $D = r\sin\theta\sin\varphi$. For z-polarized laser light, $D = r\cos\theta$. When a dipole operator D acts on the initial-state wave function $\psi_i(\vec{r})$, we get

$$D|\psi_i\rangle = rR(r)\chi(\theta,\varphi), \tag{4}$$

where $\chi(\theta,\varphi)$ is the angular factor, which can be expressed as [5]

$$\begin{aligned} &\chi_x(\theta,\varphi) = \sin\theta\cos\varphi, \\ &\chi_y(\theta,\varphi) = \sin\theta\sin\varphi \\ &\chi_z(\theta,\varphi) = \cos\theta. \end{aligned} \tag{5}$$

ψ_{ret} in eq. (3) is the returning detached electron wave function near the negative ion, which is related to the initial outgoing detached electron wave $\psi_{\text{out}}(R,\theta,\varphi)$ as

$$\psi_{\text{ret}}(r,\theta,\varphi) = \sum_j \psi_{\text{out}}(R,\theta,\varphi)A_j \text{e}^{i[S_j - \mu_j\pi/2]}, \tag{6}$$

where the sum runs over all the electron's closed orbits going out from and later returning to the origin, A_j, S_j and μ_j are the amplitude, action and the Maslov index of the jth closed orbit. The initial outgoing electron wave from the negative ion can be written as [31]

$$\psi_{\text{out}}(R,\theta,\varphi) = \frac{4Bki}{(k_b^2 + k^2)^2}\frac{\text{e}^{ikR}}{R}\chi(\theta,\varphi) \tag{7}$$

in which R is the radius of a small sphere, $R \approx 5.0$ a.u. $k = \sqrt{2E}$ is the momentum of the detached electron.

The amplitude A_j in eq. (6) measures the divergence of adjacent trajectories from the jth closed orbit:

$$A_j = \left| \frac{J_j(t_0)}{J_j(T_j)} \right|^{1/2}.$$

$J_j(t)$ is the Jacobian, which is defined as

$$J_j(t) = \frac{\partial(x, y, z)}{\partial(t, \theta_{\text{out}}, \varphi_{\text{out}})}.$$

T_j is the period of the jth closed orbit. Owing to the classical motion of the detached electron in the cubical microcavity, by a careful derivation, we get

$$A_j = \frac{R}{R + kT_j} = \frac{R}{R + L_j} \tag{8}$$

in which $L_j = kT_j$ denotes the length of the jth closed orbit.

The classical action along the jth closed orbit is defined as: $S_j = \oint \vec{k} \cdot \mathrm{d}\vec{l}$. For our system, $S_j = kL_j$. The Maslov index μ_j equals the number of collisions of the jth closed orbit with the surfaces of the microcavity.

The returning wave travelling along the jth closed orbit is given by

$$\psi_{\text{ret}}^j(r, \theta, \varphi) = \frac{i4Bk\chi\left(\theta_{\text{out}}^j, \varphi_{\text{out}}^j\right)}{\left(k_b^2 + k^2\right)^2} \frac{1}{L_j} \mathrm{e}^{i(S_j - \mu_j \pi/2)} \mathrm{e}^{i\vec{k}_{\text{ret}}^j \cdot \vec{r}}, \tag{9}$$

where $\vec{k}_{\text{ret}}^j$ is the momentum of the returning electron near the nucleus. When the returning wave returns inside the small sphere of radius R, it can be approximated by an incoming plane wave:

$$\psi_{\text{ret}}^j(r, \theta, \varphi) = N_j \mathrm{e}^{i\vec{k}_{\text{ret}}^j \cdot \vec{r}} \tag{10}$$

where N_j is a matching factor, which can be obtained by matching eqs (10) and (9):

$$N_j = \frac{i4Bk\chi\left(\theta_{\text{out}}^j, \varphi_{\text{out}}^j\right)}{\left(k_b^2 + k^2\right)^2} \frac{1}{L_j} \mathrm{e}^{i(S_j - \mu_j \pi/2)}. \tag{11}$$

To calculate the overlap of the returning wave with the source function $\langle D\psi_i | \psi_{\text{ret}} \rangle$, we use the partial wave expansion of the plane wave [5]:

$$\psi_{\text{ret}}^j(r, \theta, \varphi) = 4\pi N_j \sum_{l,m} (-i)^l j_l\left(k_{\text{ret}}^j r\right) Y_{l,m}(\theta, \varphi) Y_{l,m}^*\left(\theta_{\text{ret}}^j, \varphi_{\text{ret}}^j\right), \tag{12}$$

where $(\theta_{\text{ret}}^j, \varphi_{\text{ret}}^j)$ are angles of the returning electron wave.

Substituting the above equations into eq. (3) and carrying out the overlap integral, we get

$$\langle D\psi_i | \psi_{\text{ret}} \rangle = -\frac{4\pi B^2 E}{(E_{\text{b}} + E)^4} \sum_j \frac{1}{L_j} \chi\left(\theta_{\text{out}}^j, \varphi_{\text{out}}^j\right) \times \chi^*\left(\theta_{\text{ret}}^j, \varphi_{\text{ret}}^j\right) \mathrm{e}^{i(kL_j - \mu_j \pi/2)}. \tag{13}$$

With the help of the above integral, we obtain the oscillatory part of the photodetachment cross-section:

$$\sigma^{\text{osc}}(E) = \frac{16\pi^2 B^2 E}{c(E_{\text{b}} + E)^3} \sum_j \frac{1}{L_j} \chi\left(\theta_{\text{out}}^j, \varphi_{\text{out}}^j\right) \times \chi^*\left(\theta_{\text{ret}}^j, \varphi_{\text{ret}}^j\right) \sin(kL_j - \mu_j \pi/2). \tag{14}$$

Therefore, the total photodetachment cross-section can be written as

$$\sigma(E) = \sigma_0(E) + \frac{16\pi^2 B^2 E}{c(E_{\text{b}} + E)^3} \sum_j \frac{1}{L_j} \chi\left(\theta_{\text{out}}^j, \varphi_{\text{out}}^j\right) \times \chi^*\left(\theta_{\text{ret}}^j, \varphi_{\text{ret}}^j\right) \sin(kL_j - \mu_j \pi/2). \tag{15}$$

Using the angular factor given by eq. (5), we can easily get the photodetachment cross-section of H^- ion in a cubical microcavity for different polarized laser lights.

For x-polarized light,

$$\sigma_x(E) = \sigma_0(E) + \frac{16\pi^2 B^2 E}{c(E_{\text{b}} + E)^3} \sum_j \frac{1}{L_j} \sin\theta_{\text{out}}^j \cos\varphi_{\text{out}}^j \times \sin\theta_{\text{ret}}^j \cos\varphi_{\text{ret}}^j \sin(kL_j - \mu_j \pi/2). \tag{16}$$

For y-polarized light,

$$\sigma_y(E) = \sigma_0(E) + \frac{16\pi^2 B^2 E}{c(E_{\text{b}} + E)^3} \sum_j \frac{1}{L_j} \sin\theta_{\text{out}}^j \sin\varphi_{\text{out}}^j \times \sin\theta_{\text{ret}}^j \sin\varphi_{\text{ret}}^j \sin(kL_j - \mu_j \pi/2). \tag{17}$$

For z-polarized light,

$$\sigma_z(E) = \sigma_0(E) + \frac{16\pi^2 B^2 E}{c(E_b + E)^3} \sum_j \frac{1}{L_j} \cos\theta_{\text{out}}^j \cos\theta_{\text{ret}}^j \times \sin(kL_j - \mu_j \pi/2). \tag{18}$$

2.3 *Fourier-transformed photodetachment cross-section*

According to the closed orbit theory, the oscillatory structure in the photodetachment cross-section is related to the closed orbits of the detached electron. In order to show the correspondence between the oscillation in the cross-section with the closed orbits of the detached electron in the cubical microcavity clearly, we perform the

Fourier transformation of the photodetachment cross-section. The Fourier transformation of the cross-section is defined as

$$F(L') = \int_{k_1}^{k_2} [\sigma(E) - \sigma_0(E)] \exp(-ikL') \mathrm{d}k, \qquad (19)$$

where L' is the geometric length of the closed orbit of the detached electron. Through the calculation, we shall show the correspondence between the length of the closed orbit L' in the cubical microcavity and the peak in the Fourier-transformed photodetachment cross-section. Since $F(L')$ takes complex values, we take $|F(L')|^2$ in our calculation.

3. Results and discussion

Using eqs (16)–(18), we calculate the total photodetachment cross-section of H^- ion inside a cubical microcavity for different polarization laser light as a function of photon energy $E_p = E + E_b$. The results are shown in figures 3, 4 and 5. Compared with the smooth photodetachment cross-section without the microcavity, oscillatory structures appear in the cross-section inside the cubical microcavity. Figure 3 shows the total photodetachment cross-sections for different lengths of the closed orbits. The laser light is polarized along the x-direction. In figure 3a, we calculate the photodetachment cross-section by including only those closed orbits with the length $L \leq 500$ a.u. Oscillatory structures appear in the cross-section, but the oscillating amplitude and frequency are relatively small. As we increase the length of the closed orbit, the oscillatory structures in the total photodetachment cross-section become much more complex. Both the oscillating amplitude and the oscillating frequency in the cross-section become enlarged, the effect of the cubical microcavity becomes significant, as we can see from figures 3b and 3d clearly. The reasons can be interpreted as follows: From table 1, we find that as the length of the closed orbit $L \leq 500$ a.u., closed orbits of only four detached electrons have contributions to the photodetachment cross-section. As we increase the length of the closed orbit, the number of closed orbits in the cubical microcavity increase correspondingly. As the length of the closed orbit L is increased to 1000 a.u., the number of the closed orbits of the detached electron is increased to 38. According to the closed orbit theory, each closed orbit contributes one oscillating term to the photodetachment cross-section. The more the number of closed orbits, the more oscillating terms appear in the cross-section, which makes the oscillatory structures in the total photodetachment cross-section become much more complex.

Figures 4 and 5 show the total photodetachment cross-sections for the laser light polarized along y and z directions, respectively. We choose the lengths of the

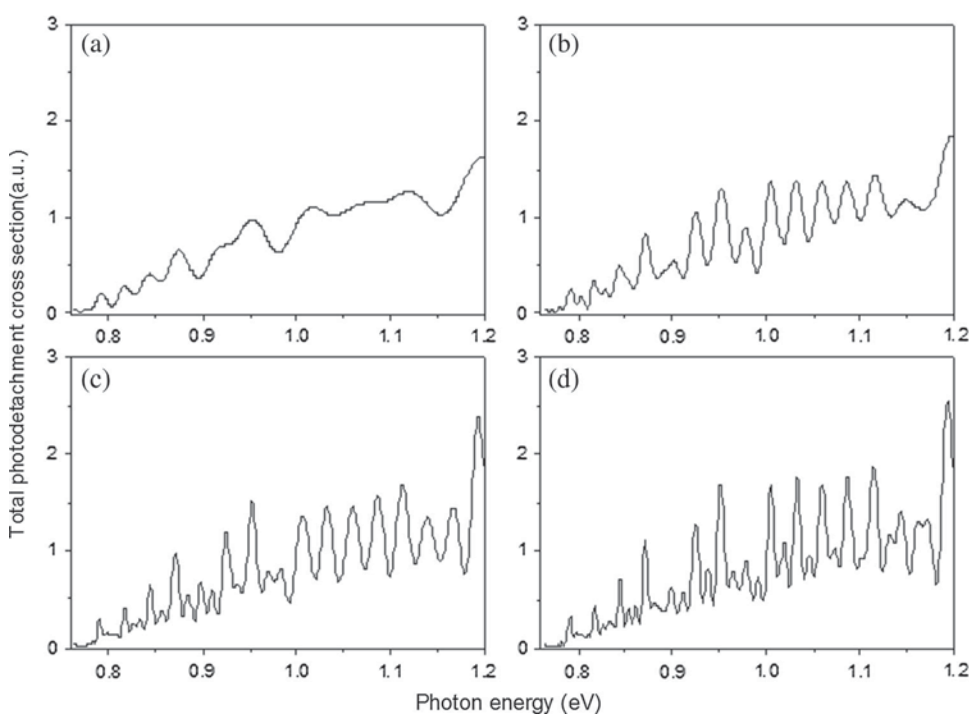

Figure 3. Photodetachment cross-section of H^- ion inside a cubical microcavity with different lengths of the closed orbit. The laser light is polarized along x-axis. (**a**) $L \leq 500$ a.u., (**b**) $L \leq 1000$ a.u., (**c**) $L \leq 1500$ a.u. and (**d**) $L \leq 2000$ a.u.

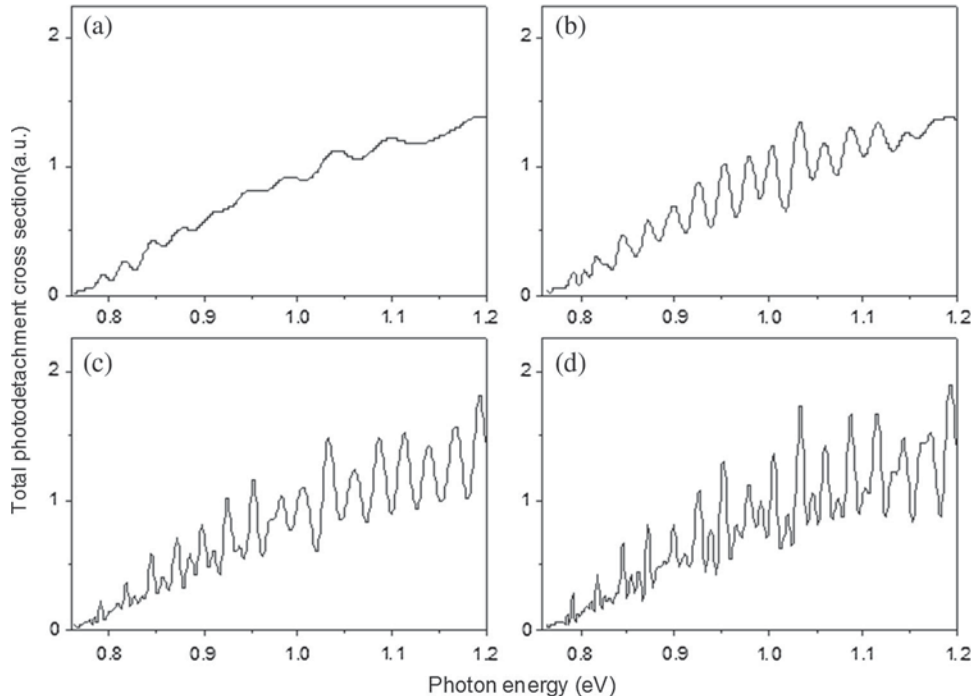

Figure 4. Photodetachment cross-section of H^- ion inside a cubical microcavity with different lengths of the closed orbit. The laser light is polarized along y-axis. (**a**) $L \leq 500$ a.u., (**b**) $L \leq 1000$ a.u., (**c**) $L \leq 1500$ a.u. and (**d**) $L \leq 2000$ a.u.

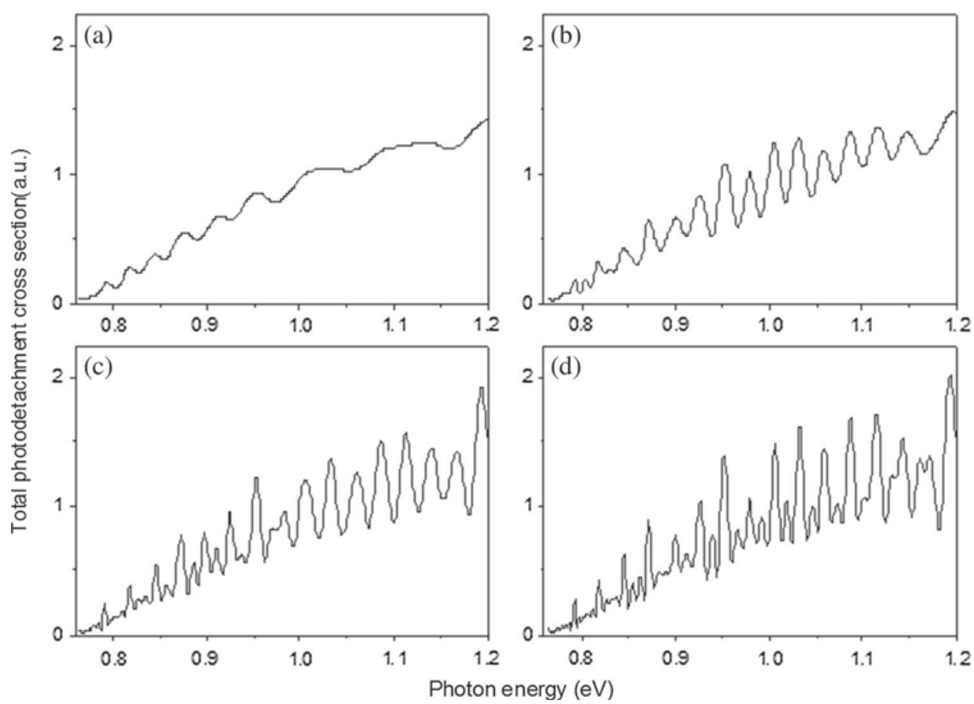

Figure 5. Photodetachment cross-section of H^- ion inside a cubical microcavity with different lengths of the closed orbit. The laser light is polarized along z-axis. (**a**) $L \leq 500$ a.u., (**b**) $L \leq 1000$ a.u., (**c**) $L \leq 1500$ a.u. and (**d**) $L \leq 2000$ a.u.

closed orbit the same as those given in figure 3. From these two figures, we still find that the oscillatory structures in the cross-section become complicated with the increase of the length of the closed orbit. However, by comparing figures 3, 4 and 5, we find that even though the closed orbits are the same for different polarized laser light, the oscillatory patterns are different in the x-polarization, y-polarization and z-polarization. Both the oscillating amplitude and the oscillating frequency in the cross-section are different. This suggests that

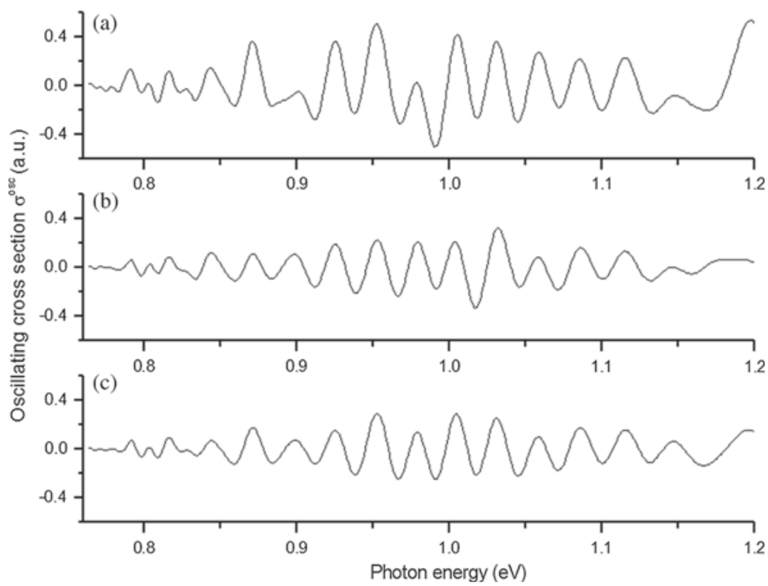

Figure 6. The oscillating cross-section of H^- ion inside a cubical microcavity with the length of the closed orbit $L \leq 1000$ a.u. (**a**) The laser light is polarized along x-axis, (**b**) the laser light is polarized along y-axis and (**c**) the laser light is polarized along z-axis.

the photodetachment cross-sections of H^- ion inside a cubical microcavity depend strongly on the laser polarization. In order to show the dependence of the cross-section on the laser polarization clearly, we display only the oscillatory part of the cross-section for different polarized laser light. The results are shown in figure 6. We choose the length of the closed orbit $L \leq 1000$ a.u. This figure suggests that the oscillating structure in the cross-section for x-polarized laser light is quite different from those cases for the y- and z-polarized laser light. The amplitude in the oscillating cross-section during x-polarization is relatively larger than during y- and z-polarizations. Besides, in figure 3a, the oscillation pattern is dominated by low-frequency oscillations; however, in figures 3b and 3c, for the y-polarization and z-polarization, the oscillation structure appears to be dominated by high-frequency oscillations.

Next, we compare the photodetachment cross-section of H^- ion inside a cubical microcavity with the case of the photodetachment inside a square microcavity [31]. We choose the length of the closed orbit $L \leq 3000$ a.u., with the laser light polarized along x-direction. The result is given in figure 7. From this figure, we find that the oscillating structure of the cross-section in the cubical microcavity is more complex than in the square microcavity. Both the oscillating amplitude and frequency are larger than in the case of the photodetachment inside a square microcavity. The reason can be analysed as follows: For the photodetachment of H^- ion inside a square microcavity, the movement of the detached electron is only limited in a two-dimensional plane, the closed orbit of the electron is denoted by two non-negative integers (p, q). However, for the photodetachment of H^- ion inside a cubical microcavity, the movement of the detached electron is expanded to six planes, we use three non-negative integers (p, q, m) to denote the closed orbit of the electron. If $m = 0$, the movement of the detached electron is similar to the case of the square microcavity. As $m > 0$, the movement of the detached electron is extended to the three-dimensional space. Therefore, the number of closed orbits in cubical microcavity is much larger than in square microcavity. The more closed orbits there are, the more the returning waves are reflected by the microcavity. Thus, the interference effect between the returning waves travelling along the closed orbits with the outgoing waves becomes strong, which causes large oscillating amplitude and frequency for the photodetachment cross-section inside a cubical microcavity.

Finally, we calculate the Fourier-transformed photodetachment cross-section for the laser light polarized along the x-axis. In our calculation, we do not include all the possible orbits in order for the plot to remain distinguishable. We include only those closed orbits with $1 \leq p \leq 10$, $1 \leq q \leq 10$ and $1 \leq m \leq 10$, the length of the closed orbit $L \leq 1000$ a.u. The result is given in figure 8. A series of peaks appear in the Fourier-transformed photodetachment cross-section and each peak corresponds to the length of one close orbit of the detached electron. From table 1, we find that as $L \leq 1000$ a.u., there are altogether 38 closed orbits of

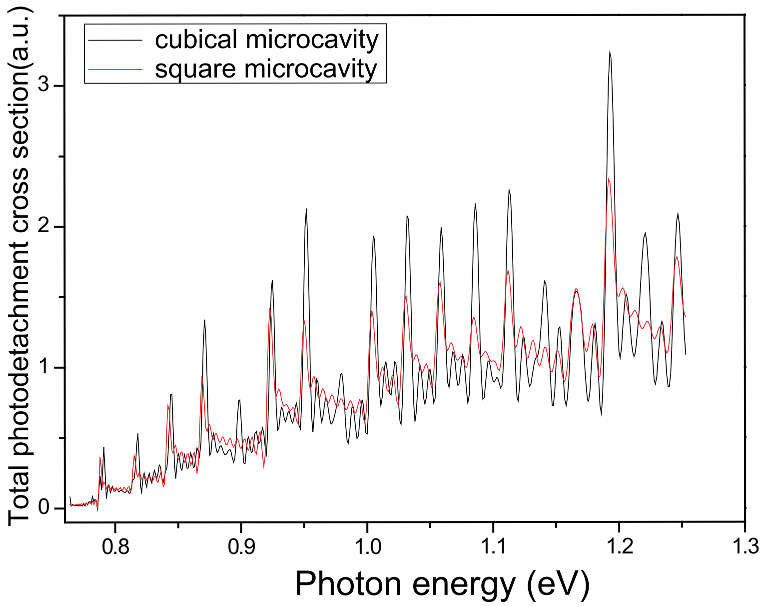

Figure 7. Comparison of the photodetachment cross-section of H^- inside a cubical microcavity with the case of the photodetachment inside a square microcavity. The length of the closed orbit $L \leq 3000$ a.u. and the laser light is polarized along x-direction. The black line denotes the photodetachment cross-section of H^- inside a cubical microcavity, while the red line denotes the photodetachment cross-section inside a square microcavity.

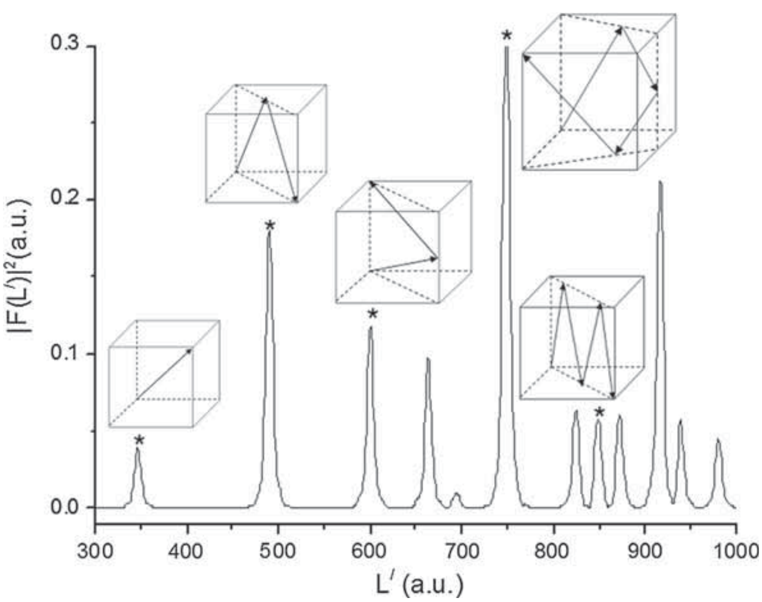

Figure 8. Fourier-transformed cross-section of H^- inside a cubical microcavity. Some typical closed orbits are shown beside the peaks.

the detached electron. However, some closed orbits have the same length, and there are only 12 closed orbits with different lengths. Correspondingly, there are 12 peaks in the Fourier-transformed cross-section corresponding to the length of the closed orbits of the detached electron. For example, the first peak at $L' \approx 346$ a.u. corresponds to the length of the (1,1,1) closed orbit; the second peak at $L' \approx 490$ a.u. corresponds to the length of the (1,1,2), (1,2,1) or the (2,1,1) closed orbit, etc. Some typical closed orbits are shown beside each peak.

4. Conclusions

We have studied the photodetachment of H^- ion inside a three-dimensional cubical microcavity by means of the closed orbit theory. An analytical formula for calculating the photodetachment cross-section of this system for different polarized laser light is put forward. Then we calculated the photodetachment cross-section of this system. Results of our calculation suggest that the photodetachment cross-section has a strong dependence on the length of the closed orbit and the laser polarization. In order to show the correspondence between the oscillating cross-section and the detached electron's closed orbits clearly, we calculated the Fourier-transformed cross-section. We found that each peak corresponds to the length of one closed orbit. At present, studies of ion–microcavity interactions have much practical interest in the fundamental scientific research and technology, such as in the ion source development, adsorbate dynamics, electron transportation, microelectronics, photodetachment microscopy experiments, etc. We hope that our studies may guide the future researches on the photodetachment processes of negative ions inside a three-dimensional microcavity.

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