Photodetachment of hydrogen negative ion inside a circular microcavity*

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The photodetachment of a hydrogen negative ion inside a circular microcavity is studied based on the semiclassical closed orbit theory. The closed orbit of the photo-detached electron in a circular microcavity is investigated and the photodetachment cross section of this system is calculated. The calculation result suggests that oscillating structure appears in the photodetachment cross section, which is caused by the interference effects of the returning electron waves with the outgoing waves traveling along the closed orbits. Besides, our study suggests that the photodetachment cross section of the negative ions depends on the laser polarization sensitively. In order to show the correspondence between the cross section and the closed orbits of the detached electron clearly, we calculate the Fourier transformation of the cross section and find that each peak corresponds to the length of one closed orbit. We hope that our results will be useful for understanding the photodetachment process of negative ions or the electron transport in a microcavity.

Keywords: photodetachment, circular microcavity, closed-orbit theory

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1. Introduction

The photodetachment of negative ions in external fields has aroused a lot of interest over the last three decades. Electron detachment from a negative ion represents one of the most important physical effects. When a negative ion is irradiated by a laser, it provides a coherent source of electrons at the position of the negative ion. Since H^- is the simplest negative ion, many researchers have studied the photodetachment of H^- in different external fields or environments both theoretically and experimentally. Early experiment and theory showed that the photodetachment cross section of H^- in the presence of external fields displays oscillatory structures.[1–8] Du and Delos[9] used closed orbit theory to analyze these oscillatory structures. They discovered that the oscillatory structure was caused by the interference between the detached-electron waves reflected by the external fields and the outgoing detached-electron waves localized in the region of the bound state of the negative ion.[9,10] The correspondence of their closed orbit theory results in the exact quantum-mechanical results for the same system suggests the correctness of this theory.[4,10] Recently, with the development of the surface physics, closed orbit theory has been used to study the photodetachment of the negative ion near surfaces.[11–25] In 2006–2007, Yang *et al.*,[11,12] Wang,[13] and Afag and Du[14] used the closed orbit theory to study the photodetachment of H^- near an elastic interface. Later, the photodetachment of H^- near metal surfaces was studied.[15–25] Very recently, Zhao and Du[26] studied the photodetachment of H^- in an open wedge cavity. In these previous studies, they all studied the photodetachment of a negative ion near surfaces or inside an open cavity. As to the photodetachment of a negative ion inside a closed microcavity, the study is relatively little. In our recently published work,[27] we studied the photodetachment of a negative ion inside a square microcavity. Since the motion of the detached electron is related to the configuration of the cavity, then what will happen if a negative ion is inside a circular microcavity? As to the photodetachment of a negative ion inside a circular or semi-circular microcavity, no report has been given to the best of our knowledge.

In this paper, we study the photodetachment of H^- inside a closed circular microcavity for the first time. In our discussion, we still consider the surfaces of the microcavity as elastic ones and ignore the interaction between the detached electron and the surface. The electrons follow straight lines inside the microcavity until they are reflected by the surface of the microcavity.[27] Therefore, the electron moving in the circular microcavity can be considered as a particle in a circular billiard.[28,29] Our study shows that when a H^- ion is photodetached inside a circular microcavity, oscillating structure appears in the photodetachment cross section and the oscillating structure in the photodetachment cross section depends on the laser polarization sensitively.

The rest of this paper is organized as follows. In Section 2, we first give a physical picture describing the classical motion of the photo-detached electron inside a circular microcavity, then we give the formula for calculating the photode-

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tachment cross section. In Section 3, we calculate the total photodetachment cross section and the Fourier transformed cross section of a negative ion inside a circular microcavity. Finally, some conclusions of this paper are given in Section 4. Atomic units are used throughout this paper unless otherwise indicated.

2. Derivation of the photodetachment cross section

2.1. Physical picture and the closed orbits of the detached electron

In Fig.1, we show the schematic plot of the system. The H^- ion is assumed to be at the origin. A linearly polarized laser is used for the photodetachment. The circular microcavity is placed in the x–y plane, with x axis being along a diameter. H^- can be regarded as a one-electron system, with the active electron loosely bound by a short-ranged, spherically symmetric potential of the hydrogen atom. According to the physical picture of closed orbit theory (COT),[9] when the active electron is photo-detached by a laser, it is detached and the associated wave propagates out from the negative ion in all directions. After one or several bounces of the surface, the electron may return to the origin of the negative ion, in which case the returning electron waves will interfere with the outgoing source waves to produce the oscillatory structure in the photodetachment cross section. The COT relates the oscillations in the photodetachment cross sections to the closed orbits of the detached electron. Therefore, in order to calculate the photodetachment cross section, we must find out the closed orbits of the photodetached electron. To search for the closed orbits of the electron in a circular mirocavity, we launch a large number of trajectories going out from the origin and keep track of the trajectories as they propagate and reflect inside the microcavity. In all of these classical trajectories of the photodetached electron emitting from the origin, only those that are bounced back by the surface of the microcavity to the starting point are called closed orbits. In Fig. 1, we plot a group of the detached-electron trajectories near a closed orbit.

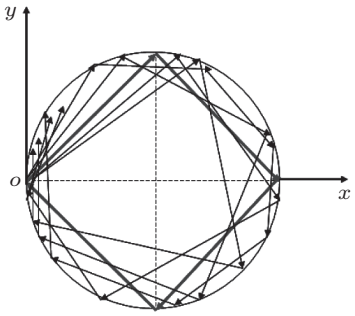


Fig. 1. Schematic illustration of H^- photodetachment inside a circular microcavity. The H^- lies at the origin. A group of trajectories propagate away from the H atom and finally return to the region of the atom after being reflected several times by the microcavity surface. The closed orbit is marked by the thick black line.

Since the electron motion in the circular microcavity is the same as in a circular billiard,[28,29] we can use the same method to find the closed orbits of our system. Suppose that the radius of the circular microcavity is R and the electron is emitted from the origin ($x = 0$, $y = 0$). For this geometric configuration, the closed orbits in a circular microcavity can be characterized by angle Θ, subtended by the chord between successive bounces with the circle containing surfaces.[28] See Fig. 2. Closed orbits appear when an integer number of such bounces bring the particle back to the origin. This condition can be written as $p\Theta = q(2\pi)$, where p and q are non-negative integers, $p \geq 2q$ with p denoting the number of the bounces on the surface of the microcavity and q being the number of rotations made by the particle before returning to the origin in phase space.[28] Therefore, we use a pair of integers (p, q) to distinguish different closed orbits. The outgoing angle of the electron relative to the x axis is $\varphi_{\text{out}} = (\pi - \Theta)/2$. The corresponding returning angles of each closed orbit are given by $\varphi_{\text{ret}} = \pi - \varphi_{\text{out}}$.

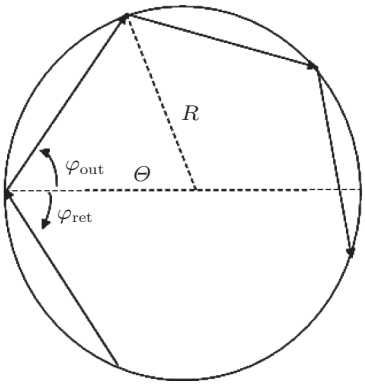


Fig. 2. Geometry leading to closed orbits in a circular microcavity. The length between two successive bounces is given by $2R\sin(\Theta/2)$ and the condition for closed orbits is $\Theta = 2\pi q/p$.[28]

The length of the primitive closed orbit is given by[28]

$$L = 2pR\sin\left(\frac{\pi q}{p}\right). \tag{1}$$

Repetitions of these closed orbits are possible so that integer multiples of these values are also possible. If p and q are relatively primes, the labels of the closed orbits using$p$ and q are distinct. However, if p and q share a common factor n, $p = n\tilde{p}$, $q = n\tilde{q}$, then orbits labeled by $(p,q) = n(\tilde{p},\tilde{q})$ can be considered as an n-fold repetition of the primitive orbit $(\tilde{p},\tilde{q})$.[28] Some of the closed orbits are given in Fig. 3. Figure 3(a) shows the closed orbit with $p = 2$, $q = 1$, which is denoted as (2,1). This orbit leaves the atom along the diameter direction with the outgoing angle $\varphi_{\text{out}} = 0$, after being reflected by the right surface, it then retraces back to the atom. This orbit is called the diameter orbit.[28] For $q > 2$, the shapes of the closed orbit are polygons. For example, figure 3(b) shows the (3,1) closed orbit, which is a trigon. This orbit emits

from the origin with the outgoing angle $\varphi_{\rm out} = 30^0$, after being reflected by the surface of the circular billiard twice, then travels toward the origin. Similar descriptions can be given to other closed orbits.

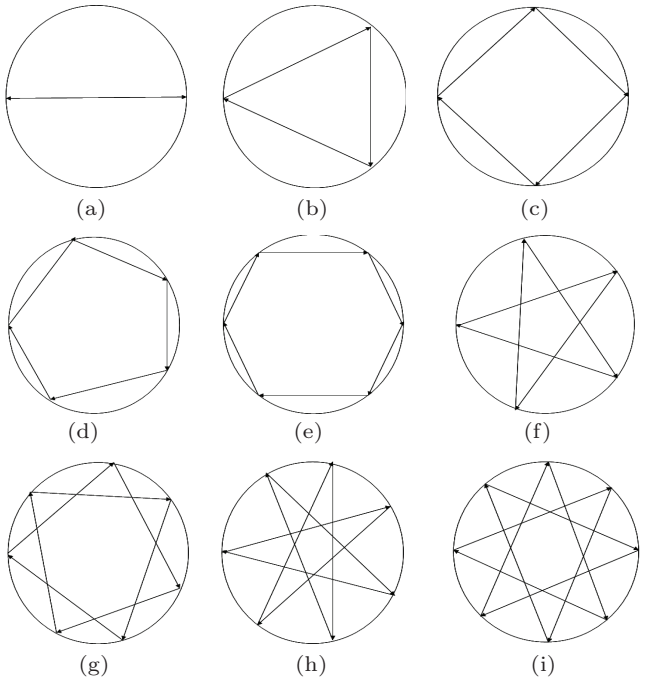


Fig. 3. Some closed orbits of the detached electron inside a circular microcavity. The p and q are (a) (2,1), (b) (3,1), (c) (4,1) (d) (5,1), (e) (6,1), (f) (5,2), (g) (7,2), (h) (7,3), and (i) (8,3) respectively.

Table 1. Geometry parameters of the closed orbits inside a circular microcavity.

(p,q)	L/a.u.	$\varphi_{\rm out}/(^\circ)$
(2,1)	400.00	0.00
(3,1)	519.62	30.00
(4,1)	565.69	45.00
(5,1)	587.79	54.00
(6,1)	600.00	60.00
(7,1)	607.44	64.29
(8,1)	612.29	67.50
(9,1)	615.64	70.00
(10,1)	618.03	72.00
(4,2)	800.00	0.00
(5,2)	951.06	18.00
(6,2)	1039.23	30.00
(7,2)	1094.56	38.57
(8,2)	1131.37	45.00
(9,2)	1157.02	50.00
(10,2)	1175.58	54.00
(6,3)	1200.00	0.00
(7,3)	1364.90	12.86
(8,3)	1478.21	22.50

In our calculation, we suppose the radius of the circular microcavity $R = 100$ a.u.(atomic units). In Table 1, we summarize the values of collision number p, rotation number q, length L and outgoing angle $\varphi_{\rm out}$ of the closed orbit in the circular microcavity with $2 \le p \le 10$ and $1 \le q \le 3$. The length of the closed orbit $L \le 1500$ a.u. Due to the symmetry of the circular microcavity, we only give the closed orbits with the outgoing angle $0 \le \varphi_{\rm out} \le 90^0$. The length, collision and rotation number of those closed orbits with $-90^0 < \varphi_{\rm out} \le 0^0$ are the same as the ones with $-\varphi_{\rm out}$.

2.2. Photodetachment cross section

According to the closed orbit theory,[10] the derivation of the photodetachment cross section of H^- in a circular microcavity is similar to the one given by Zhao and Du,[26] and Wang *et al.*[27] for the derivation of the photodetachment cross section of H^- in an open or in a square microcavity. Therefore, we only briefly summarize the main results. The total photodetachment cross section can be written as

$$\sigma(E) = \sigma_0(E) + \sigma_{\rm osc}(E), \tag{2}$$

where $\sigma_0(E) = 16\sqrt{2}\pi^2 B^2 E^{3/2}/3c(E_{\rm b}+E)^3$ is the smooth background term of H^- in free space without microcavity,[11] and $\sigma_{\rm osc}(E)$ is the oscillating term, which is given by[26,27]

$$\sigma_{\rm osc}(E) = \frac{16\pi^2 B^2 E}{c(E_{\rm b}+E)^3} \sum_j \frac{1}{L_j} \chi(\theta^j_{\rm out}, \varphi^j_{\rm out}) \chi^*(\theta^j_{\rm ret}, \varphi^j_{\rm ret}) \times \sin(kL_j - \mu_j \pi/2). \tag{3}$$

Here, the summation includes the closed orbits of all the detached electrons, L_j is the length of the closed orbit, which is given by Eq. (1), μ_j the Maslov index, $\theta^j_{\rm out}$ and $\varphi^j_{\rm out}$ are the polar and outgoing angles, while $\theta^j_{\rm ret}$ and $\varphi^j_{\rm ret}$ are the polar and returning angles of the j-th closed orbit. Since all the closed orbits lie in the x–y plane, the polar angles of the closed orbit $\theta^j_{\rm out} = \theta^j_{\rm ret} = \pi/2$.[26] $\varphi_{\rm out} = (1/2 - q/p)\pi$ and $\varphi_{\rm ret} = \pi - \varphi_{\rm out}$. $\chi(\theta^j_{\rm out}, \varphi^j_{\rm out})\chi^*(\theta^j_{\rm ret}, \varphi^j_{\rm ret})$ is an angular factor, which is related to the laser polarization. If we assume that the light is linearly polarized and we adopt a spherical coordinate system, then the angular factor for x-polarized laser light can be written as[26,27]

$$\chi_x(\theta^j_{\rm out}, \varphi^j_{\rm out})\chi^*_x(\theta^j_{\rm ret}, \theta^j_{\rm ret}) = \cos\varphi^j_{\rm out} \cos\varphi^j_{\rm ret}. \tag{4}$$

For the y-polarized laser light

$$\chi_y(\theta^j_{\rm out}, \varphi^j_{\rm out})\chi^*_y(\theta^j_{\rm ret}, \theta^j_{\rm ret}) = \sin\varphi^j_{\rm out} \sin\varphi^j_{\rm ret}. \tag{5}$$

Therefore, the total photodetachment cross section of H^- in a circular microcavity for the x-polarized light is given by[26,27]

$$\sigma_x(E) = \sigma_0(E) + \frac{16\pi^2 B^2 E}{c(E_{\rm b}+E)^3} \times \sum_j \frac{1}{L_j} \cos\varphi^j_{\rm out} \cos\varphi^j_{\rm ret} \sin(kL_j - \frac{\mu_j \pi}{2}). \tag{6}$$

For the y-polarized light

$$\sigma_y(E) = \sigma_0(E) + \frac{16\pi^2 B^2 E}{c(E_{\rm b}+E)^3} \times \sum_j \frac{1}{L_j} \sin\varphi^j_{\rm out} \sin\varphi^j_{\rm ret} \sin(kL_j - \frac{\mu_j \pi}{2}). \tag{7}$$

2.3. Fourier transformed photodetachment cross section

In order to show the correspondence between the cross section and the detached electron closed orbits, we perform the Fourier transformation (FT) of the photodetachment cross section. The Fourier transformation of the cross section is defined as[27,30]

$$F(L') = \int_{k_1}^{k_2} [\sigma(E) - \sigma_0(E)] \exp(-ikL')\,dk, \tag{8}$$

where L' is the geometric length of the closed orbit. Therefore, the Fourier transformation of the photodetachment cross section will show the features at value of L' corresponding to the length of classical closed orbit. For a finite length of the closed orbit, $F(L')$ is a complex number. In our calculations, we calculate $|F(L')|^2$.

3. Results and discussion

Using Eqs. (6) and (7) and the formulas for the length L and the outgoing angle of the closed orbit, we calculate the photodetachment cross sections of H^- in a circular microcavity for different laser polarizations. The results are given in Figs. 4 and 5. Figure 4 shows the total photodetachment cross sections for the laser light polarized along the x direction. Figure 4(a) is the cross section with a length of the closed orbit $L \leq 500$ a.u. Oscillatory structure appears in the cross section in contrast to the smooth curve in the free space. Under this condition, only the diameter closed orbit (2,1) contributes to the cross section, as we can see from Table 1. Therefore, the oscillating amplitude and frequency are both relatively small. With the increase of the length of the closed orbit, the number of the closed orbits increases correspondingly and the amplitude and the frequency of the cross section also increase apparently, as we can see from Figs. 4(b)–4(f). They can be interpreted using the closed orbit theory: the oscillation in the photodetachment cross section is caused by the interference effect between the outgoing waves and the returning waves traveling along the closed orbits. The more the closed orbit, the more the returning waves bounced back by the microcavity are. Therefore, their contributions to the cross section become significant.[10]

Figure 5 shows the total photodetachment cross sections for the laser light polarized along the y direction. The lengths of the closed orbit are the same as the ones given in Fig. 4.

By comparing Fig. 5 with Fig. 4, we find that there are some similarities and dissimilarities in both cases. The similarities are that with the increase of the length of the closed orbit, the oscillation in the cross section becomes complex. However, the oscillatory structures are different. For example, in Fig. 5(a), there is no obvious oscillatory structure in the cross section and the cross section is the same as the one in free space. The reason is as follows. When the length of the closed orbit $L \leq 500$ a.u., only the diameter closed orbit (2,1) with the outgoing angle $\varphi_{\text{out}} = 0$ contributes to the cross section. From Eq. (7), we find when $\varphi_{\text{out}} = 0$, the factor $\sin\varphi_{\text{out}} = 0$ the oscillating cross section is also 0, therefore, its contribution to the cross section disappears. Besides, in Fig. 5(a), the oscillating structure is dominated by high-frequency oscillations, whereas in Fig. 5(b), the oscillating structure is dominated by low-frequency oscillations. This result is similar to the one given by Du and Zhao.[26] From the above two figures, we conclude that the photodetachment cross section of H^- in a circular microcavity is not only related to the length of the closed orbits, but also depends on the laser polarizations.

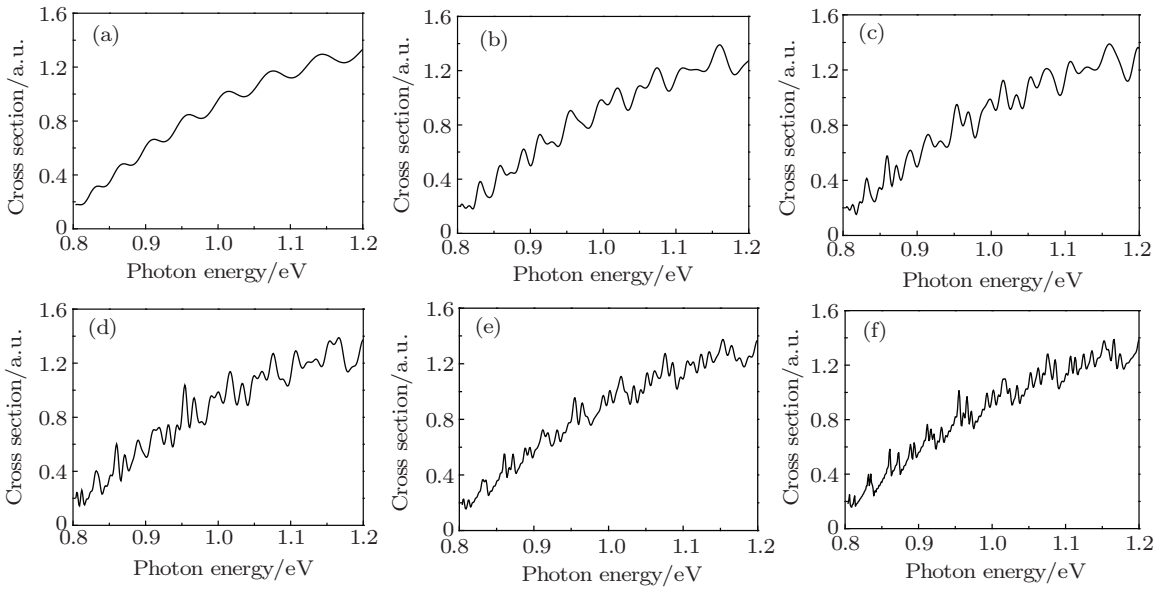


Fig. 4. Photodetachment cross sections of H^- in a circular microcavity with different lengths of the closed orbit: (a) $L \leq 500$ a.u., (b) $L \leq 1000$ a.u., (c) $L \leq 1500$ a.u., (d) $L \leq 2000$ a.u., (e) $L \leq 3000$ a.u., and (f) $L \leq 5000$ a.u. The laser is linearly polarized in the x-axis direction.

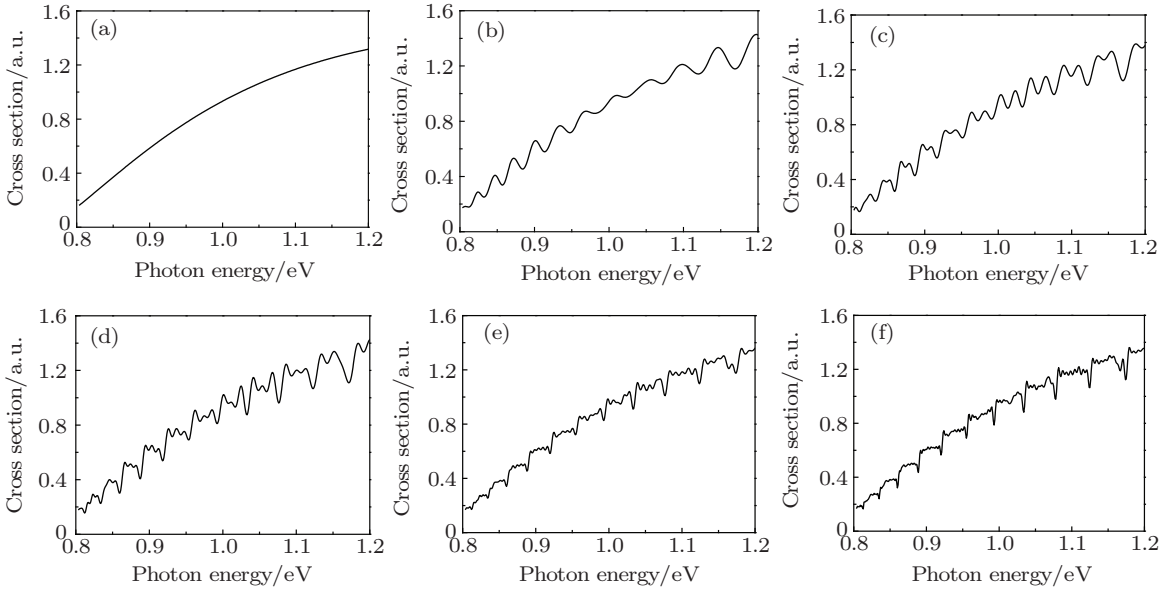


Fig. 5. Photodetachment cross section of H^- in a circular microcavity with different lengths of the closed orbit: (a) $L \leq 500$ a.u., (b) $L \leq 1000$ a.u., (c) $L \leq 1500$ a.u., (d) $L \leq 2000$ a.u., (e) $L \leq 3000$ a.u., and (f) $L \leq 5000$ a.u. The laser is linearly polarized in the y-axis direction.

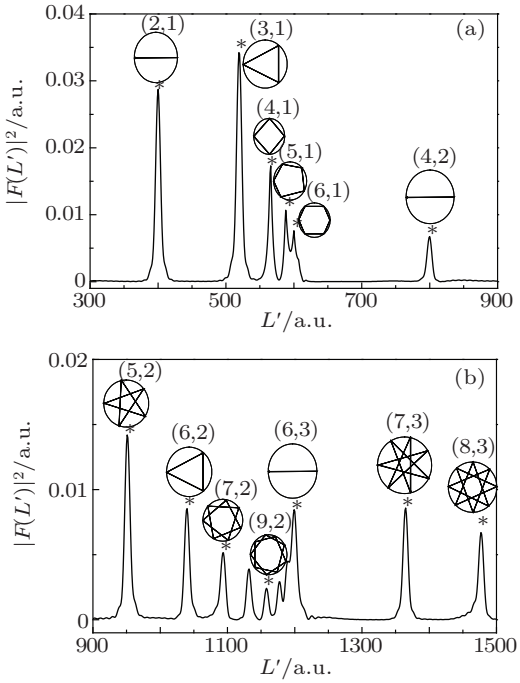


Fig. 6. Fourier transformed cross sections of H^- in a circular microcavity with different lengths of the closed orbit: (a) $L \leq 900$ a.u. and (b) $900 \leq L \leq 1500$. Some typical closed orbits are shown beside the peaks.

Finally, in order to show the correspondence between the cross section and the detached electron closed orbits clearly, we calculate the Fourier transformation of the cross section with laser polarization along the x axis. The calculation is carried out using $k_1 = 0.027a_0^{-1}$, $k_2 = 0.86a_0^{-1}$, and a step size $\Delta k = 0.001a_0^{-1}$. The result is given in Fig. 6. In our calculation, we did not include all of the possible orbit length formulas in order to let plots be distinguishable. We include only those closed orbits with $2 \leq p \leq 10$ and $1 \leq q \leq 3$. Figure 6(a) is the case with the length of the closed orbit L≤900 a.u., while figure 6(b) is the case with the length of the closed orbit 900 a.u.$\leq L \leq$ 1500 a.u. A series of sharp peaks appear and each peak corresponds to the length of one closed orbit and all the lengths of the closed orbits can be found in Table 1. Some closed orbits are plotted beside each peak. For example, the first peak in Fig. 6(a) at $L' = 400$ a.u. corresponds to the diameter orbit (2,1), the second peak at $L' = 519.60$ a.u. corresponds to the (3,1) closed orbit, etc.

4. Conclusions

In this paper, we investigate the photodetachment of H^- in a circular microcavity by using the closed orbit theory for the first time. The calculation results suggest that the amplitude and frequency of photodetachment cross section strongly depend on the length of the closed orbit and the laser polarization. In this work, we perform the calculation on the assumption that the negative ion lies inside the circular microcavity. Similar calculations can be carried out on the assumption that the negative ion lies inside the quasi-circular microcavity.[28] The variation in the shape of the microcavity will lead to some changes in the details of the classical motion of the detached electron but should not change the main conclusions. In this paper, we study the photodetachment of H^- in the circular microcavity based on the semiclassical closed orbit theory. Closed orbit theory provides a clear physical picture and a quantitative tool for the photodetachment of a negative ion in the microcavity. However, a complete quantum soulution can provide all possible knowledge of a system and propably give a more exact result. Those two perspectives are complementary.[32] In the next work, we will carry

out the quantum mechanics calculation using the method given by Hu *et al.*[31] and compare our semiclassical closed orbit theory result with the quantum result. At present, studies of ion-microcavity interaction become increasingly important in the development of ion sources, surface chemistry and analysis, reactive ion etching, photodetachment microscopy experiments, etc. We hope that our studies will be useful for guiding one in doing the future theoretical and experimental research of the photodetachment processes of negative ions or the electron transport in a microcavity.

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