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H^{-}在矩形腔中的光剥离截面

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摘　要:根据半经典闭合轨道理论研究了矩形腔对氢负离子的光剥离进程的影响,利用反射定律分析矩形腔中与光剥离截面相联系的剥离电子运动的闭合轨道,推导出该体系下的光剥离截面公式,在线性极化光的作用下,研究了腔的尺寸对光剥离截面的影响,并将其与麻志君等用量子力学方法研究的结果进行对比.结果表明:矩形腔的存在及其大小对光剥离截面中由闭合轨道相联系的返回波与波源函数发生干涉引起的振荡有很大影响,且振荡曲线随着矩形腔的尺寸变化明显;当激光极化方向沿着 x 轴或者 y 轴时,半经典方法与量子力学方法的结果一致,当激光极化方向沿着 z 轴时,由于矩形腔在 z 轴上对光剥离截面不作用,采用半经典方法光剥离截面与无场的情况相同,但是采用量子力学方法,其结果中却出现振荡,表明半经典方法研究此体系结果更准确.研究结果可对研究负离子光剥离以及外腔中的电子输运问题提供参考.

关键词:原子与分子物理学;光剥离;截面;闭合轨道理论;矩形腔
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Photodetachment of H^{-} in a Rectangular Cavity

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Abstract: On the basis of the semi-classical closed orbit theory, the effect of rectangular cavity on electron photo-detachment from a hydrogen negative ion was studied. Using the law of reflection, the electrons motion of closed orbit associated with photo-detachment cross section in the rectangular cavity was analyzed, and the formula of photo-detachment cross section in the system was deduced. Under the action of linear polarization light, the influence of the size of the cavity on cross section was studied, and the results were compared with that of the quantum mechanics method which MA Zhi-Jun used. It is shown that, the existence and the size of rectangular cavity induces significant oscillation in the photo-detachment cross section owing to the interference effects of the electron wave traveling along closed orbits and source function. The oscillatory structure in the photo-detachment cross section sensitively depends on the size of rectangular cavity. When the laser is linearly polarized in the x-axis or y-axis, quantum mechanics results are in line with the classical results. But when the laser is linearly polarized in the z-axis, rectangular cavity is not function on cross section along z-axis in actual situation, cross section is with the case of no field by semi-classical method, while the volatility is still exist in cross section by quantum mechanics method, which shows that the semi-classical method results are more accurate in this system. The results will be useful in understanding the photo-detachment of negative ions or electron transport in a micro-cavity.

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0 Introduction

Electron detachment from negative ions is one of the most important physical effects. In this process, an electron in a bound state at a negative ion moves into a free state. Photodetachment is probably the most important mechanism because it allows the versatile study of negative-ion systems. Early experiment and theory showed that the photodetachment cross sections of H^- in the presence of external fields display oscillatory structures. In early 1979, Blumberg et al studied the photodetachment of negative ions in a magnetic field, they found the photodetachment cross section of negative ion in magnetic field was shown to have an oscillatory structures related to the photon energy[1]. Later, Bryant et al. observed a ripple like structure in the photodetachment cross section of H^- in the presence of electric fields[2]. Du and Delos developed the closed orbit theory to interpret this "ripple" structure, and discovered that the oscillatory structure is caused by the interference of the detached-electron waves reflected by the external fields and that the outgoing detached-electron waves localized in the regions of the bound state of negative ions[3-5]. Later, photodetachment of H^- in other fields, such as in parallel electric and magnetic fields and in electric and magnetic fields with arbitrary orientations have been also investigated theoretically[6-8]. Recently, much attention has been paid to the photo-induced electronic excitations of adsorbates on metal surfaces[9]. Since H^- has been proposed to use to probe adsorbate state lifetime and charge transfer during back-scattering[10], the photo-detachment of H^- near an interface has attracted much interest. Firstly, Yang et al studied the photo-detachment of H^- near an elastic interface [11-13]. Later, the photo-detachment of H^- near a metal surface has been investigated by Yang, Zhao and Du et al[14-16]. Subsequently, Hansen and coauthors discussed the escape of classical particles from a vase-shaped cavity, which suggested that the fractal structure of the system could affect the escape of the particles[17-18]. Recently, Wang studied the photo-detachment of negative ions inside a closed circular micro-cavity based on closed orbit theory[19-20]. And Ma, Zhao studied the photo-detachment of negative ions inside a micro-cavity using quantum approach[21].

In this research, on the basis of closed orbit theory we study the photo-detachment of H^- in a rectangular cavity and compare the results with the results of Ma. This study can provide a certain basis and validity for the semi-classical theory and quantum mechanics method to study the photo-detachment and will be useful in understanding the photo-detachment of negative ions or electron transport in a micro-cavity. Atomic unit (which is abbreviated as a. u.) is used throughout this work unless indicated otherwise.

1 Derivation of the cross section

1.1 Physical description

In Fig. 1, we show a schematic plot of the system. The H^- ion is assumed to be at the origin. A group of trajectories propagates away from the H^- and finally returns to the region of the atom after being reflected several times by the cavity surfaces. A linearly polarized laser is used for the photo-detachment. The rectangular cavity is placed in the x-y plane, the top and bottom surfaces are perpendicular to the y-axis and the other two surfaces are parallel to it. As in previous studies, H^- is regarded initially as a non-electron system loosely bound by a spherically symmetric, short-range potential of the hydrogen atom. According to the physical picture of the closed orbit theory[5], when a laser is applied to a negative ion, it may absorb a photon, then an active electron is detached. After the electron is detached, the short-range potential of the hydrogen atom can be neglected and the electron can be considered as a free particle. In our discussion, we still consider the surfaces of the cavity as elastic ones and neglect the interaction between the detached electron and the surfaces. Therefore, the electron's trajectories follow straight lines inside the rectangular cavity until they are reflected by the surfaces of the cavity. After one or several reflections at the surfaces, the electron may return to the origin. The returning waves overlap with the outgoing source waves to produce the oscillatory structure in the photo-detachment cross section. In order to search for the closed orbits of an electron in rectangular cavity, we used the procedure that has recently been used to find the closed orbits of an electron inside an open cavity [19]. We launch a large number of trajectories from the origin and keep track of the trajectories as they propagate and are reflected inside the micro-cavity. In all of these classical trajectories of the photo-detached electron emitted from the origin, only those reflected by the surfaces of the micro-cavity to the starting point are called closed orbits. Some of the closed orbits are given in Fig. 1.

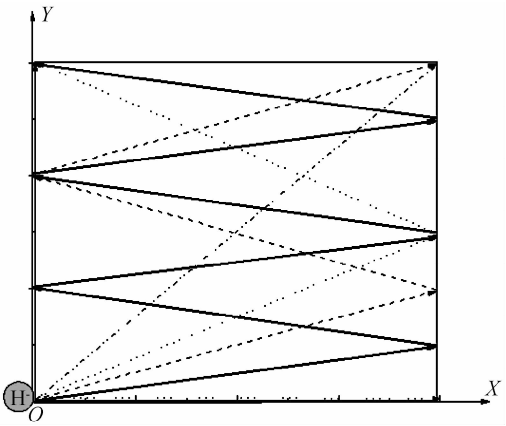


Fig. 1 Schematic illustration of photo-detachment of H$^-$ inside a cavity

1.2 Formula for the photo-detachment cross section

According to the closed orbit theory[5], the photo-detachment cross section of this system can be split into two parts as follows

$$\sigma(E)=\sigma_0(E)+\sum_{j=0}^{j_{\max}}\sigma_{\mathrm{osc}}^{j} \tag{1}$$

$\sigma_0(E)$ is the overlap integral of the direct part with the source function, which is a smooth background term in the cross section as

$$\sigma_0(E)=\frac{16\sqrt{2}B_0^2\pi^2E^{3/2}}{3c(E_{\mathrm{b}}+E)^3} \tag{2}$$

where E is the energy of the detached electron, $E_{\mathrm{b}}=\frac{k_{\mathrm{b}}^2}{2}$ is the binding energy of H$^-$ and approximately 0.754 eV, the normalization constant $B_0=0.315\ 52$.

The second part is the oscillating term which corresponds to the contribution of the returning wave traveling along the closed orbit[19]

$$\sigma_{\mathrm{osc}}(E)=-\frac{4\pi}{c}(E+E_{\mathrm{b}})\mathrm{Im}\langle D\psi_{\mathrm{i}}|\psi_{\mathrm{ret}}\rangle \tag{3}$$

where $\psi_{\mathrm{i}}(r)=\frac{B_0\exp(-k_{\mathrm{b}}r)}{r}$ is the initial wave function of the detached electron. D is the dipole operator, which is the projection of an electron coordinate in the polarization direction of the laser light: $D=a_xx+a_yy+a_zz$[6]. For x-polarized laser light, $a_x=1$, $a_y=a_z=0$. If we adopt a spherical coordinate system, the dipole operator can be written as $D=r\sin\theta\cos\varphi$. Similarly, for y-polarized laser light, $a_y=1$, $a_x=a_z=0$. The dipole operator can be written as $D=r\sin\theta\sin\varphi$.

When a dipole operator acts on the initial state, we obtain $|D\psi_{\mathrm{i}}\geqslant rR(r)\chi(\theta,\varphi)$. Since the initial state is spherically symmetric and we assume that the light is linearly polarized, then the angular factors $\chi(\theta,\varphi)$ are expressed as

$$\begin{cases}\chi_x(\theta,\varphi)=\sin\theta\cos\varphi\\ \chi_y(\theta,\varphi)=\sin\theta\sin\varphi\\ \chi_z(\theta,\varphi)=\cos\theta\end{cases} \tag{4}$$

where ψ_{ret} is the returning part of the detached electron wave function, which represents the electron wave that initially propagates outward into the external region, is reflected back by the rectangular cavity, and finally returns to the vicinity of the negative ion along the closed orbit. In order to obtain the returning wave function associated with each closed orbit, we draw a sphere of radius $R\approx5a_0$ (a_0 is the Bohr radius). Then the outgoing wave on the surface of this sphere is[4]

$$\psi_{\mathrm{out}}(R,\theta,\varphi)=\frac{4\mathrm{i}B_0k}{(k_{\mathrm{b}}^2+k^2)^2}\frac{\exp(\mathrm{i}kR)}{R}\chi(\theta_{\mathrm{out}},\varphi_{\mathrm{out}}) \tag{5}$$

When this wave propagates out of the surface and travels along the closed orbit, it changes its phase and amplitude. After each reflection by the surfaces of the rectangular cavity, a phase loss of the wave function occurs. In the semi-classical approximation, the returning wave ψ_{ret} near the negative ion is a sum of the above outgoing waves

$$\psi_{\mathrm{ret}}(r,\theta,\varphi)=\sum_{j=1}^{n}\psi_{\mathrm{out}}(r,\theta,\varphi)A_j\exp[\mathrm{i}(S_j-\mu_j\pi/2)] \tag{6}$$

where $A_j=|J_j(t_0)/J_j(t)|^{1/2}$ is the amplitude, which measures the divergence of adjacent trajectories from the j-th closed orbit. In which $J_j(t)=\frac{\partial(x,y,z)}{\partial(t,\theta_{\mathrm{out}},\varphi_{\mathrm{out}})}$.

Owing to the classical free motion of the photo-detached electron, the amplitude can be easily worked out and is given by

$$A_j=\frac{R}{R+kT_j}=\frac{R}{R+L_j} \tag{7}$$

where $L_j=kT_j$ is the length of the j-th closed orbit. $S_j=\oint p_j\mathrm{d}q_j$ is the action along the j-th closed orbit. For the present system, we have $S_j=kL_j$[19]. μ_j is the Maslov index, which is the number of collisions of the j-th closed orbit with the rectangular cavity.

Substituting Eq. (6) into Eq. (3) and carrying out the overlap integral, we obtain the oscillatory part of the photo-detachment cross section as

$$\sigma_{\mathrm{osc}}(E)=\frac{16\pi^2B_0^2E}{c(E_{\mathrm{b}}+E)^3}\sum_j\frac{1}{L_j}\chi(\theta_{\mathrm{out}}^j,\varphi_{\mathrm{out}}^j)\cdot\chi^*(\theta_{\mathrm{ret}}^j,\varphi_{\mathrm{ret}}^j)\times\sin\left(kL_j-\frac{\mu_j\pi}{2}\right) \tag{8}$$

Therefore, the total photo-detachment cross section can be written as

$$\sigma(E)=\sigma_0(E)+\frac{16\pi^2B_0^2E}{c(E_{\mathrm{b}}+E)^3}\sum_j\frac{1}{L_j}\chi(\theta_{\mathrm{out}}^j,\varphi_{\mathrm{out}}^j)\cdot\chi^*(\theta_{\mathrm{ret}}^j,\varphi_{\mathrm{ret}}^j)\times\sin\left(kL_j-\frac{\mu_j\pi}{2}\right) \tag{9}$$

where the summation includes all the detached electron′s closed orbit. Since all the closed orbits lie in the x-y plane , the polar angles of the closed orbit are $\theta_{\mathrm{out}}^j=\theta_{\mathrm{ret}}^j=\pi/2$. Thus, the angular factor can be simplified as

$$\begin{cases}\chi_x(\theta_{\mathrm{out}}^j,\varphi_{\mathrm{out}}^j)\chi_x\cdot(\theta_{\mathrm{ret}}^j,\varphi_{\mathrm{ret}}^j)=\cos\varphi_{\mathrm{out}}^j\cos\varphi_{\mathrm{ret}}^j\\ \chi_y(\theta_{\mathrm{out}}^j,\varphi_{\mathrm{out}}^j)\chi_y\cdot(\theta_{\mathrm{ret}}^j,\varphi_{\mathrm{ret}}^j)=\sin\varphi_{\mathrm{out}}^j\sin\varphi_{\mathrm{ret}}^j\\ \chi_z(\theta_{\mathrm{out}}^j,\varphi_{\mathrm{out}}^j)\chi_z\cdot(\theta_{\mathrm{ret}}^j,\varphi_{\mathrm{ret}}^j)=0\end{cases} \tag{10}$$

Using the Eqs. (8) ~ (10), we can write the photo-detachment cross section for different linear polarized lights. For x-polarized light,

$$\sigma_x(E)=\sigma_0(E)+\frac{16\pi^2B_0^2E}{c(E_b+E)^3}\sum_j\frac{1}{L_j}\times \cos\varphi_{\mathrm{out}}^j\cos\varphi_{\mathrm{ret}}^j\sin\left(kL_j-\frac{\mu_j\pi}{2}\right) \tag{11}$$

For y-polarized light,

$$\sigma_y(E)=\sigma_0(E)+\frac{16\pi^2B_0^2E}{c(E_\mathrm{b}+E)^3}\sum_j\frac{1}{L_j}\times \sin\varphi_{\mathrm{out}}^j\sin\varphi_{\mathrm{ret}}^j\sin\left(kL_j-\frac{\mu_j\pi}{2}\right) \tag{12}$$

For z-polarized light,

$$\sigma_z(E)=\sigma_0(E) \tag{13}$$

From the Eq. (13), we find that for the z-polarized light, there is no outgoing wave in the x-y plane, so the returning waves have no effect on the cross section, and the cross section has no oscillations.

2 Results and discussion

In order to calculate the photo-detachment cross section of H^- inside a rectangular cavity, we must find all the closed orbits of the photo-detached electron. Since the shape and length of the closed orbits are related to the size of rectangular cavity, we firstly assume that the size of the rectangular cavity is $a=80$ a. u. and $b=60$ a. u. we calculate the cross section with different length of the closed orbit, and the laser is linearly polarized in the x-axis. Since the electron′s motion in the rectangular cavity is the same as a particle in a rectangular billiard[22], we can use the same method as finding the period orbits in the rectangular billiard to find the closed orbits of the detached electron. We assume negative ion lying at the vertex of the rectangular cavity, the length of the closed orbit can be written as

$$L=2\sqrt{q^2a^2+p^2b^2} \tag{14}$$

where p and q are non-negative integers, $2p$ and $2q$ are the numbers of collisions of the electron with the horizontal and vertical surfaces of the rectangular cavity, respectively. The outgoing angle of the electron relative to the x-axis is $\tan\varphi_{\mathrm{out}}=pb/(qa)$. The corresponding returning angles of each closed orbit are given by $\varphi_{\mathrm{ret}}=\pi-\varphi_{\mathrm{out}}$.

Some of the closed orbits are given in Fig. 2. Fig. 2(a) shows that the closed orbit leaves the atom in a direction at an outgoing angle $\varphi_{\mathrm{out}}=36.87°$, is reflected once by the right and left surface, and returns back to the atom. Fig. 2(b) shows that the closed orbit leaves the atom at an outgoing angle $\varphi_{\mathrm{out}}=20.56°$, is reflected once by the right surface, then travels toward the top left corner and returns back to the atom. Similar descriptions can be given to the other four closed orbits. In Table 1, we summarize the numbers of collisions p and q, the length L, and the outgoing angle of the closed orbits with length $L<1\,000$ a. u..

Using Eq. (11) and Eq. (14) for the length L and outgoing angle of the closed orbit, we calculate the photodetachment cross section of H^- with a negative ion lying at the vertex of rectangular cavity for the laser polarized along the x-direction. The results are given in Figs. 3. Fig. 3(a) shows the cross section with a length of the closed orbit $L<500$ a. u. An oscillatory structure appears in the cross section in contrast to the smooth curve in free space. However, the oscillating amplitude and frequency are relatively small. With an increase in the length of the closed orbit, the effect of the rectangular cavity becomes significant. Both the amplitude and frequency of the cross section increased, shown in Figs. 3(b)~3(d). The reasons for this are as follows: With an increase in the length of the closed orbit, the number of closed orbits increases correspondingly. For example, as a length of the closed orbit $L<500$ a. u., there are only ten closed orbits; with the increase of L to 1000 a. u., the number of the closed orbits increases to 30. According to the closed orbit theory, the oscillation in the photodetachment cross section is caused by the effect of interference between the outgoing and the returning waves traveling along the closed orbits. The more closed orbits there are, the more the returning waves are reflected by the micro-cavity; therefore, the contribution of the closed orbits to the cross section becomes significant.

Table 1 Geometric parameters of the closed orbits inside a rectangular cavity

p,q	L/(a. u.)	φ_{out}/(°)	p,q	L/(a. u.)	φ_{out}/(°)
0,1	160	0	3,1	393.95	66.04
0,2	320	0	3,2	481.66	48.37
0,3	480	0	3,3	600	36.87
0,4	640	0	3,4	734.30	29.36
0,5	800	0	3,5	877.27	24.23
1,1	200	36.87	4,1	505.96	71.55
1,2	341.76	20.56	4,2	576.89	56.31
1,3	494.77	14.04	4,3	678.82	45.00
1,4	651.15	10.62	4,4	800.00	36.87
1,5	808.95	8.53	4,5	932.95	30.96
2,1	288.44	56.31	5,1	620.97	75.07
2,2	400.00	36.87	5,2	680.00	61.93
2,3	536.66	26.56	5,3	768.37	51.34
2,4	683.52	20.56	5,4	877.27	43.15
2,5	835.22	16.70	5,5	1000.00	36.87

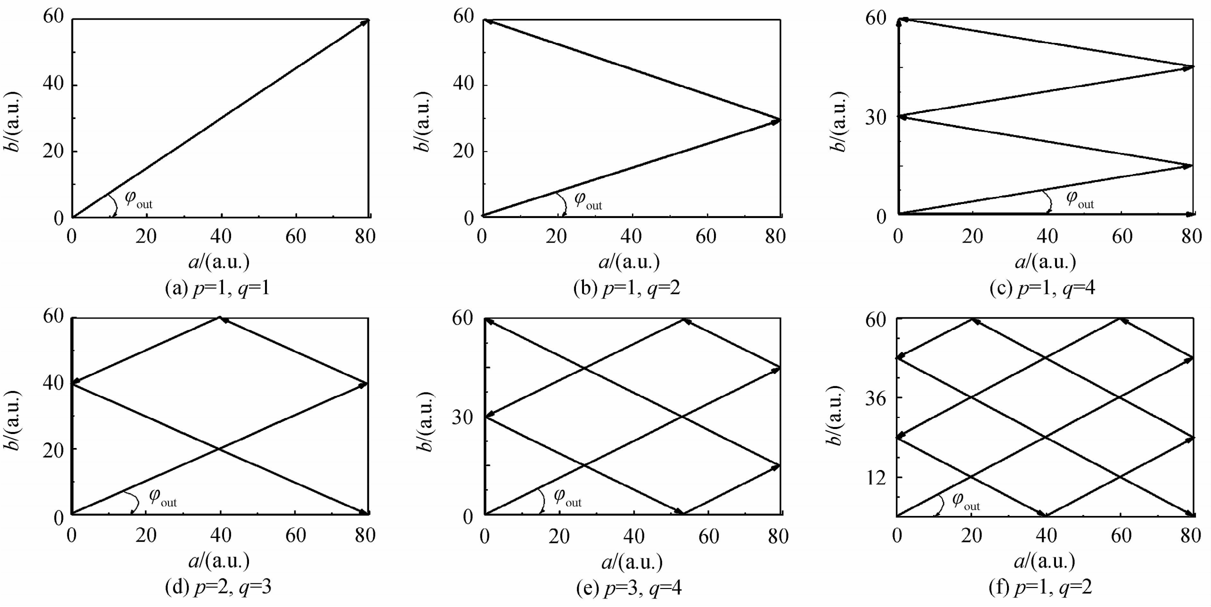


Fig. 2 Some closed orbits of the detached electron in a rectangular cavity

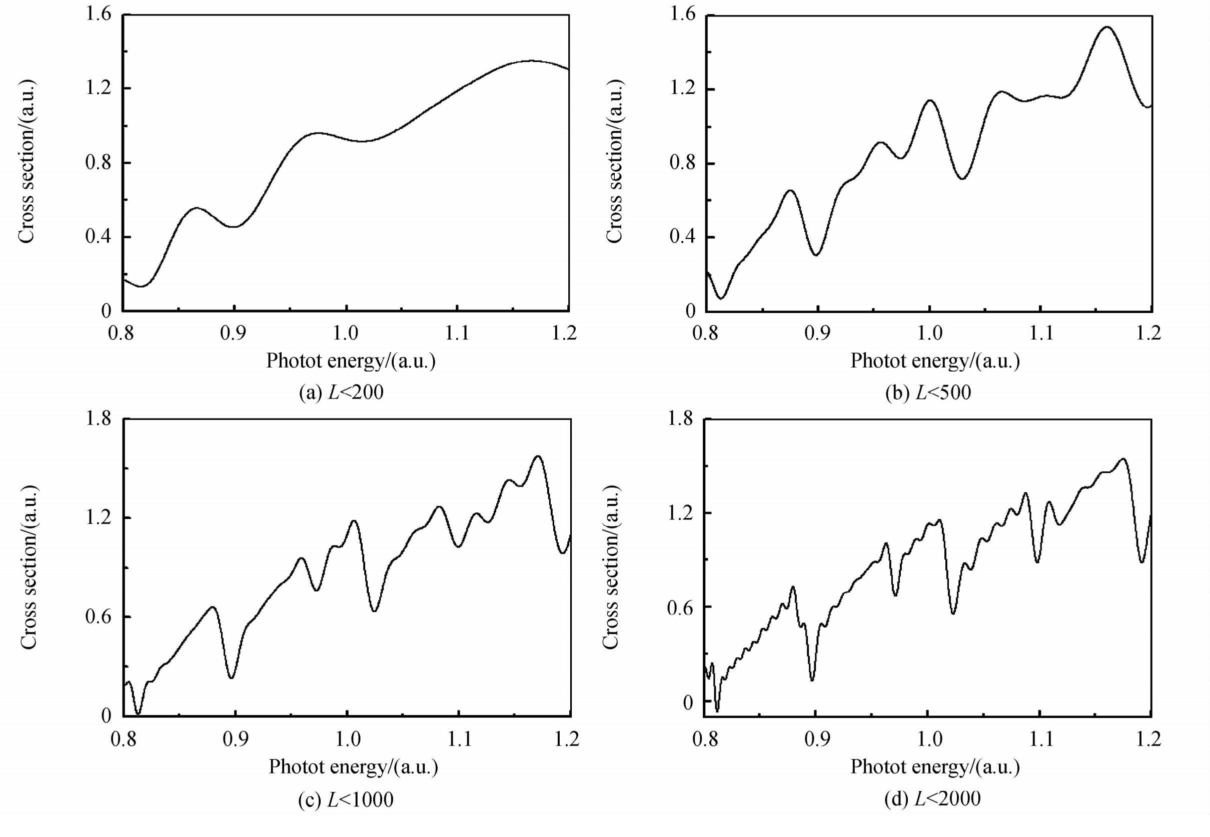
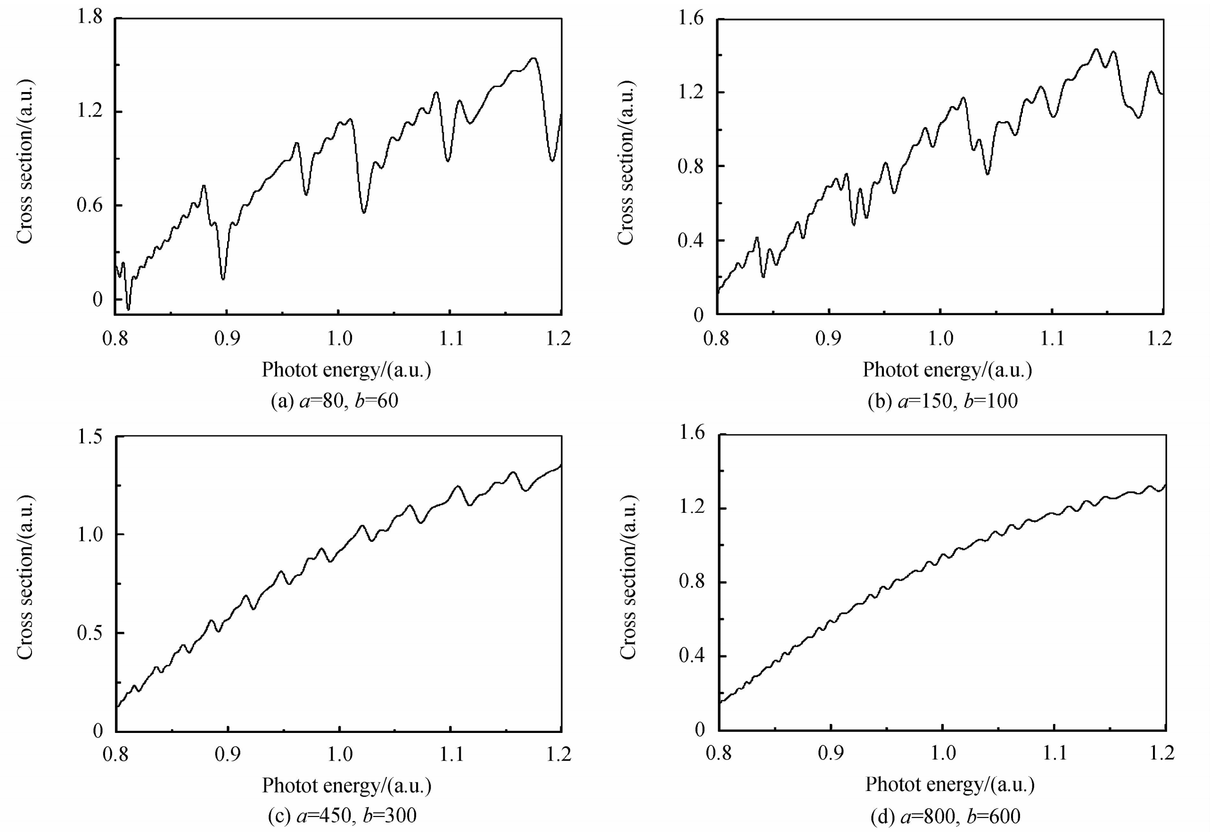


Fig. 3 Photodetachment cross section of H^- in a rectangular cavity with different lengths of the closed orbit

We calculate the photodetachment cross section of H^- in different rectangular cavity under given length of the closed orbit $L=2\ 000$ a. u. in Fig. 4. Fig. 4(a) shows the cross section with rectangular cavity of $a=80$ a. u. and $b=60$ a. u.. Oscillatory structure appears in the cross section relatively acute, and the oscillating amplitude and frequency are large. With the increase of the size of the rectangular cavity, the amplitude and frequency of the cross section decrease, shown in Figs. 4(b)～4(c). When the rectangular cavity size increased to $a=800$ a. u. $b=600$ a. u., the cross section is similar to the case of in free space, and then the effect of rectangular cavity can be neglect. The reasons for this are as follows: With the increase of the rectangular cavity size, the number of closed orbits decreases correspondingly. According to the closed orbit theory, the less closed orbits there are, the less the returning waves are reflected by the cavity ; so the contribution of



(a) a=80, b=60

(b) a=150, b=100

(c) a=450, b=300

(d) a=800, b=600

Fig. 4 Photodetachment cross section of H$^-$ in different rectangular cavity with length of the closed orbit $L=2\ 000$a. u.

the closed orbits to the cross section becomes small.

3 Comparisons

In Ref. [21], authors use quantum mechanics method to study this topic, when the laser is linearly polarized in the x-axis or y-axis, they conclude that with the increase of the rectangular cavity size, the oscillation in the cross section become less, finally the oscillation vanish and the cross section tend to smooth curve. The influence of the rectangular cavity is more and more weak until vanish. These quantum mechanics results are in line with the classical results. But when the laser is linearly polarized in the z-axis, semi-classical theory conclusion is that cross section is a smooth curve, and no oscillation in the cross section. This case is consistent with the case of no external field. The quantum mechanics results show that volatility is still exist in the cross section. However rectangular cavity is not function on cross section along z-axis in actual situation, when the laser polarization direction along the z-axis, cross section should be with the case of no field, so the semi-classical method results are more accurate to study this system. We think the reasons of drawing different conclusion results are that we use different approximation in the study.

4 Conclusions

We studied the photodetachment of H$^-$ in rectangular cavity using the closed orbit theory. An analytical formula of the cross section is derived. The photodetachment cross sections show two main features. First, they have a strong dependence on the photon energy; second, they are related to the size of rectangular cavity. In our calculation, we assume that a negative ion lies at the vertex of the cavity. Similar calculations can be carried out by assuming that a negative ion lies at an arbitrary position in the microcavity. A change in the rectangular cavity size will lead to some changes in the cross section of detached electron. At present, studies of ion-microcavity interactions are becoming increasingly important in ion source development, surface chemistry and analysis, reactive ion etching, photodetachment microscopy experiments, and other fields. We hope that our studies will be useful in guiding future theoretical and experimental research on photodetachment processes of negative ions or on electron transport in a microcavity.

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