# Photodetachment of $H^-$ near an elastic surface in a magnetic field*

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This paper investigates the photodetachment of the negative hydrogen ion $H^-$ near an elastic wall in a magnetic field. The magnetic field confines the perpendicular motion of the electron, which results in a real three-dimensional well for the detached electron. The analytical formulas for the cross section of the photodetachment in the three-dimensional quantum well are derived based on both the quantum approach and closed-orbit theory. The magnetic field and the elastic surface lead to two completely different modulations to the cross section of the photodetachment. The oscillation amplitude depends on the strength of the magnetic field, the ion-wall distance and the photon polarization as well. Specially, for the circularly polarized photon-induced photodetachment, the cross sections display a suppressed $(E-E_{\rm th})^{1/2}$ threshold law with energy $E$ in the vicinity above Landau energy $E_{\rm th}$, contrasting with the $(E-E_{\rm th})^{-1/2}$ threshold law in the presence of only the magnetic field. The semiclassical calculation fits the quantum result quite well, although there are still small deviations. The difference is attributed to the failure of semiclassical mechanics.

**Keywords:** negative hydrogen ion, photodetachment, elastic surface, magnetic field

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## 1. Introduction

In this decade, much attention has been paid to the photodetachment of a negative hydrogen ion $H^-$ near a surface since $H^-$ projectile is proposed to probe adsorbate state lifetime and charge transfer during backscattering.[1] The photodetachment of $H^-$ near an elastic interface has been studied at quantum and semiclassical levels.[2,3] Its photodetachment spectrum is modulated by the elastic surface and is superposed of a smooth background and sinusoidal oscillations. These oscillations are formed due to the interference between the outgoing wave promoted by the laser and the returning electronic waves reflected by the elastic surface. This physical picture can be formulated quantitatively by closed-orbit theory. The elastic surface acts as an infinite potential wall, making it an ideal model to study the classical dynamics of the photodetached electron and its quantum correspondence.

Photodetachment of $H^-$ near an elastic surface in a static electric field has also been studied. The linear potential well, made up of the barrier of electric field and the elastic surface, leads to the quantization of the energy in the $z$ direction (perpendicular to the elastic surface) so that the photodetachment spectrum displays an irregular staircase structure.[4] Recently, photodetachments of $H^-$ in other 'quantum wells' formed by two elastic surfaces,[5−7] a metal surface and the image potential[8] or two metal surfaces,[9] have also been investigated theoretically. In these studies, however, the 'quantum wall' or 'quantum well' are only in the $z$ direction, keeping the motion in the surface $(\rho,\phi)$ free. What happens if we locate $H^-$ in a three-dimensional quantum well?

In the present work, we investigate the photodetachment of $H^-$ in a three-dimensional configuration by applying a magnetic field perpendicular to the elastic surface. Instead of being free, in this case, the motion in the plane $(\rho,\phi)$ is confined by the magnetic field. In addition to the quantum wall located in the $z$ direction, a quantum system in a three-dimensional well is built up. Using the frame transformation method, we derive an analytical formula of photodetachment cross sections of $H^-$ in quantum approach. At the same time, we also perform a semiclassical calculation based on the closed-orbit theory. The results are compared with the quantum calculations.

## 2. Theory

To investigate the photodetachment of $H^-$ near an elastic wall in a magnetic field, we fix a negative

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ion $H^-$ at the coordinate origin. A elastic wall perpendicular to $z$-axis is put at $z = z_0$ ($z_0 < 0$) and the magnetic field is along the $z$-axis. If we use a laser to excite the ion to a certain high Rydberg state, the electron attached to the H atom will escape the attractive potential and a photodetachment process occurs.

The photodetachment cross section in the presence of magnetic field $B$ and an elastic wall at $z_0$, is given in terms of dipole matrix elements by the expression[10]

$$\sigma = \left(\frac{4\pi^2 E_{\rm p}}{c}\right)\sum_n |\langle f_{E,n}|D|i\rangle|^2 , \tag{1}$$

where $c$ is the speed of light, $E_{\rm p}$ the photon energy, $|i\rangle$ the initial state of the wave function of $H^-$, and $|f_{E,n}\rangle$ is the final-state wave function after the detachment, labeled by energy $E$ and quantum number $n$. Here $n$ is used to distinguish the discrete energy band in which $E$ falls. The final-state wave function is normalized according to

$$\langle f_{E,n}|f_{E',n'}\rangle = \delta(E - E')\delta_{n,n'}. \tag{2}$$

Additionally, the symbol $D$ in Eq. (1) is the dipole operator and its form depends on the polarization of photons. For photons polarized along the $z$ direction, the dipole operator is taken as $D = z$; for circularly polarized photons, $D = (x + {\rm i}\, y)/\sqrt{2}$.

The scanty effect of the magnetic field on the initial bound state of $H^-$ is not considered. In the one-electron approximation, the initial state wave function is given by $\psi_i(r) = C{\rm e}^{-k_{\rm b}r}/r = R(r)/\sqrt{4\pi}$, where $C = 0.31552$, $k_{\rm b} = \sqrt{2E_{\rm b}} = 0.2355883$.[11,12]

Just after the electron is detached, the effects of the short-range potential of the atomic core on it can be neglected. So the final wave functions describing electron motion after detachment can be approximated to be the wave functions of an electron in a magnetic field with the boundary condition $\Psi(z_0) = 0$. It can be obtained by solving the Schrödinger equation in cylindrical coordinates

$$\Psi_{E,n,m}(r) = \phi^B_{n,m}(\rho, \Phi)\phi_{q_n}(z), \tag{3}$$

where

$$\begin{aligned}\phi_{q_n}(z) = {} & \frac{1}{\sqrt{\pi q_n}}(\sin(qz_0)\cos(qz) \\ & + \cos(qz_0)\sin(qz))\end{aligned} \tag{4}$$

is the normalized wave function of an electron in the $z$-direction[3] and

$$\begin{aligned}\phi^B_{n,m}(\rho, z, \Phi) = {} & (2\pi)^{-1/2}{\rm e}^{{\rm i}\, m\Phi}N_{nm}{\rm e}^{-\alpha\rho^2/2}(\alpha\rho^2)^{|m|/2} \\ & \times L_n^{|m|}(\alpha\rho^2)\end{aligned} \tag{5}$$

is the normalized wave function of an electron in a magnetic field. Here the normalization factor is

$$N_{nm} = [2\alpha n!/(n + |m|)!]^{1/2}, \tag{6}$$

where $2\alpha$ is the cyclotron frequency $B/c$. The parameters in Eqs. (3)–(6) are constrained by the energy relation

$$\begin{aligned}E = {} & \frac{k^2}{2} = E_n^m + \frac{q_n^2}{2} \\ = {} & \alpha(2n + m + |m| + 1) + \frac{q_n^2}{2}.\end{aligned} \tag{7}$$

In a region where $\rho$ is too large and $\alpha^2\rho^2/2 \ll E_n^m$, the wave function $\phi^B_{n,m}(\rho, \Phi)$ is proportional to zero field wave function $\phi^{B=0}_{n,m}(\rho, \Phi)$

$$\phi^B_{n,m}(\rho, \Phi) = P(n, m, B)\phi^{B=0}_{n,m}(\rho, \Phi) \tag{8}$$

with

$$\phi^{B=0}_{n,m}(\rho, \Phi) = (2\pi)^{-1/2}{\rm e}^{{\rm i}\, m\Phi}J_m(k_\rho, \rho), \tag{9}$$

where

$$k_\rho = (2E_n^m)^{1/2} = [2\alpha(2n + m + |m| + 1)]^{1/2}. \tag{10}$$

To compute the dipole matrix elements in Eq. (1), we transform the final wave function from cylindrical coordinates to spherical coordinates with the frame transformation method developed by Fano,[13] Harmin[14] and Greene[15]

$$\begin{aligned}\phi_{E,n,m}(r) = {} & \sin(q_n z_0)\sum_l{}' P(n, m, B) \\ & \times U_{q_n,l}(n, m)f_{lm}(r) \\ & + \cos(q_n z_0)\sum_l{}'' P(n, m, B) \\ & \times U_{q_n,l}(n, m)f_{lm}(r),\end{aligned} \tag{11}$$

where the summation $\sum_l{}'$ includes all the $l$s such that $(-1)^l = (-1)^m$, and the summation $\sum_l{}''$ includes all the $l$s such that $(-1)^l = (-1)^{m+1}$. The expansion coefficients are given by Greene[15] as

$$P(n,m,B)U_{q_n,l}(n,m) = \left(\frac{2l+1}{kq_n}\right)^{1/2}\left[\frac{(l-m)!}{(l+m)!}\right]^{1/2}(-1)^{[(l-1-m)/2]}P_{lm}(q_n/k) \times [2\alpha n!/(n+|m|)!]^{1/2}\left[\frac{(2n+m+|m|+1)}{2}\right]^{1/2}, \quad (12)$$

where $[x]$ in the phase factor $(-1)^{[x]}$ denotes the smallest integer greater than or equal to $x$.

Substituting $\phi_{E,n,m}(r)$ for the final states $f_{E,n}$ in Eq. (1), the photodetachment cross sections can be calculated. According to the dipole transition selection rule, only the $l = 1$ terms in Eq. (11) contribute to the cross sections. When the photons are polarized along the field direction, the $l = 1$ term in the $\sum_l''$ of Eq. (11) contributes to the cross section. Finally, we can express the cross section as

$$\sigma_z(E,B) = H_z(E,B)\sigma_0(E), \quad (13)$$

where

$$H_z(E,B) = \sum_n \cos(q_n z_0)^2\left(\frac{6\alpha q_n}{k^3}\right) \quad (14)$$

and $\sigma_0(E)$ is the field-free cross section[10]

$$\begin{aligned}\sigma_0(E) &= \left(\frac{4\pi^2 E_{\rm p}}{c}\right)|\langle f_{10}|z|\psi_i\rangle|^2 \\ &= \left(\frac{4\pi^2 E_{\rm p}}{c}\right)\left|\langle f_{11}|\frac{1}{\sqrt{2}}(x+{\rm i}\,y)|\psi_i\rangle\right|^2 \\ &= 0.05408\frac{E^{3/2}}{(E_{\rm b}+E)^3}a_0^2. \end{aligned} \quad (15)$$

The summation in Eq. (14) includes all the Landau levels defined in Eq. (7) in which $m$ is set to 0 or 1, respectively.

For circularly polarized photons, the $l = 1$ term in the $\sum_l'$of Eq. (11) contributes to the cross section. Then the cross section is rewritten as

$$\sigma_+(E,B) = H_+(E,B)\sigma_0(E), \quad (16)$$

where

$$H_+(E,B) = \sum_n \sin(q_n z_0)^2\left(1-\frac{q_n^2}{k^2}\right)\left(\frac{3\alpha}{kq_n}\right) \times \left[1+\frac{1}{2(n+1)}\right]. \quad (17)$$

The photodetachment of $H^-$ near an elastic wall or in external fields can also be understood in the framework of closed-orbit theory.[16,17] In semiclassical theory, the photodetachment cross section can be written as

$$\sigma(E) = \left(\frac{4\pi^2 E_{\rm p}}{c}\right){\rm Im}\left|\langle D\psi_i|\hat{G}^+|D\psi_i\rangle\right|, \quad (18)$$

where $\hat{G}^+$ denotes the outgoing Green's function. Equation (18) has the following physical meaning: the dipole operator related to the incident laser field acts on the initial state to create a source wave, this wave will propagate outward by the Green's function and, finally, it overlaps with itself to give the absorption spectrum. According to the closed-orbit theory developed by Du and Delos,[16,17] the photodetachment cross section can be reduced to a simple formula

$$\sigma(E) = \sigma_0(E) + \sum_j C_j(E)\sin\Phi_j(E), \quad (19)$$

where $\sigma_0(E)$ is the photodetachment cross section in the absence of fields according to Eq. (15). Other terms arise from the returning orbits and contribute to an oscillation structure for the cross section. This summation includes all closed orbits which begin and end at the nucleus. The phase $\Phi_j(E)$ of the oscillation term is given by

$$\Phi_j(E) = S_j(E) - \mu_j\frac{\pi}{2} - \phi_j, \quad (20)$$

where $S_j(E)$ is the classical action for the closed orbit, $\mu_j$ the Maslov index which counts the total number of singular points through which the electron passes on its journey, and $\phi_j$ the additional phase shift introduced by the joint of the semiclassical wave with the quantum wave near the origin. In the case of magnetic fields, $\phi_j$ has the value of $\pi/4$.[18]

The recurrence amplitudes $C_j(E)$ in Eq. (19) are given by[18]

$$C_j(E) = \sigma_0 6\chi(\theta_{\rm out}^j)\chi^*(\theta_{\rm ret}^j)\,|R_j|\,, \quad (21)$$

where $\chi(\theta,\Phi)$ represents the angular distribution of outgoing waves. The angle $\theta_{\rm out}^j$ and $\theta_{\rm ret}^j$ are the initial and final directions of the $j$th closed orbit, respectively. The $|R_j|$ is defined as $|R_j| = \frac{\left|f_{\rm out}^{(+)j}\right|}{\left|f_{\rm ret}^{(-)j}\right|}\frac{|J_j(t_0)|^{1/2}}{|J_j(t_{\rm ret})|^{1/2}}$,[18] where $J_j(t_0)$ is the Jacobian with the form

$$J_j(t_0) = \frac{\partial(x,y,z)}{\partial(t,\theta_{\rm out},\Phi_{\rm out})}. \quad (22)$$

When the electron travels away from the origin and enters the outer region, the short-range potential $V_{\rm b}(r)$ can be negligible. Then the motion of the electron is followed by

$$\rho(t) = \frac{1}{\omega_{\rm l}} k \sin(\theta_{\rm out}) \left|\sin(\omega_{\rm l} t)\right|, \tag{23a}$$

$$z(t) = k \cos(\theta_{\rm out})\, t. \tag{23b}$$

The $z$-motion is free and the motion in $\rho$ is a cyclotron motion with the Larmor frequency $\omega_{\rm l} = B/2c$. Considering the effect of the elastic surface, we can classify the closed orbits as follows:

(I) The parallel closed orbits along the $z$-axis. The electron goes down in the negative $z$-direction, hits the surface, then bounces back and, finally, returns to the origin. The corresponding parameters for these orbits are

$$T = \frac{2z_0}{k\cos(\theta)}, \tag{24a}$$

$$S = 2z_0 k, \tag{24b}$$

$$\mu = 2, \tag{24c}$$

$$R_j = \frac{\pi\omega_{\rm l}}{E\left|\sin(\omega_{\rm l} T)\right|}. \tag{24d}$$

(II) The perpendicular closed orbits in $\rho$. The motion in $\rho$ is cyclotron motion in the magnetic field with cyclotron period $T_{\rm c} = \pi/\omega_{\rm l}$. For this kind of orbits, we have

$$T_j = jT_{\rm c}, \tag{25a}$$

$$S_j = \frac{jE\pi}{\omega_{\rm l}}, \tag{25b}$$

$$\mu_j = 2j - 1, \tag{25c}$$

$$R_j = (2\pi)^{3/2} \frac{1}{k\sqrt{T_j}}. \tag{25d}$$

(III) The closed orbits off the $z$-axis. The electron is emitted from the origin with a certain initial angle $\theta_j$, and reaches the surface at $t_{\rm f} = z_0/k\cos(\theta)$. After bouncing back by the surface, the direction of the electron's velocity is changed, it will travel along the reverse direction before it collides with the surface. If $t_{\rm f} = jT_{\rm c}$ $(j = 1, 2, \ldots)$, the detached-electron reaches the $z$-axis and hits the surface at the same time. In this case, after the same time $t_{\rm f}$, it will return to the origin and form a closed orbit.[19] The initial angle of this kind of orbits is given by $\cos(\theta_j) = -z_0\omega_{\rm l}/j\pi k$. In this case, we have

$$T_j = 2t_{\rm f} = 2j\pi/\omega_{\rm l}, \tag{26a}$$

$$S_j = 2E\frac{j\pi}{\omega_{\rm l}}[\cos(\theta_j)^2 + 1], \tag{26b}$$

$$\mu_j = 4j, \tag{26c}$$

$$R_j = 2\pi\left(\frac{\omega_{\rm l}}{E}\right)(2j)^{-1/2}. \tag{26d}$$

In this way, Eqs. (20) and (21) can be numerically evaluated. Substituting Eqs. (20) and (21) into Eq. (19), we can obtain the semiclassical photodetachment cross section $\sigma(E)$.

## 3. Results and discussion

Using Eqs. (14), (16) and (19), we can calculate the photodetachment cross sections for different values of magnetic field and distance between ion and elastic wall. The zero-field cross section $\sigma_0(E)$ defined in Eq. (15) is a smooth function of energy $E$ so that the $H$ function defined in Eqs. (14) and (17) contains almost all the structures that occur in the photodetachment cross sections $\sigma_z(E,B)$, $\sigma_+(E,B)$ of $H^-$ near an elastic surface in magnetic field. In Figs. 1 and 2, we plot $H_z(E,B)$ and $H_+(E,B)$ as a function of $E$ for various combinations of magnetic field and distance between ion and elastic wall in solid lines, respectively.

In Fig. 1 the excitation photon is polarized along the field direction while in Fig. 2, the photon is circularly polarized. The magnetic field and elastic surface lead to two completely different modulations of the $H$ function. In the parameter range we consider that, as in Figs. 1 and 2, the magnetic field effect is much smaller than that for the distance parameter. This is a consequence of the angular distribution of the outgoing wave. In this case, waves propagate down and then are reflected up by the surface in $z$ direction. Their interference produces large amplitude oscillations. When the distance between the ion and surface decreases, as shown in Figs. 1(a)–1(c) and Figs. 2(a)–2(c), the cross section induced by the elastic surface will predominate although it will no longer strongly oscillate. In this case, more electron waves will be reflected by the elastic wall and interfere with the outgoing source waves, resulting in a predominant surface effect. Especially, at $z_0 = 1500$ a.u. in Fig. 1(a) and Fig. 2(a), the oscillation amplitude caused by the magnetic field and that caused by the elastic surface are comparable and it is not possible to identify the contributions of the magnetic field and the surface effect, which are shown in solid lines. This is very different from the cases in Figs. 1(b)–1(d) and Figs. 2(b)–2(d). It can be seen that when the distance decreases to 150 a.u., as shown in Fig. 1(c) and Fig. 2(c), the overall pattern of the spectrum is similar to the pattern

in the presence of only the elastic surface except for some fine oscillation structures induced by the magnetic field. As shown in Figs. 1(b), 1(d) and Figs. 2(b), 2(d), if we take the same distance value $z_0 = 300$ a.u. but decrease the magnetic field intensity from $B = 2$ T to $B = 1$ T, the total cross section will oscillate less.

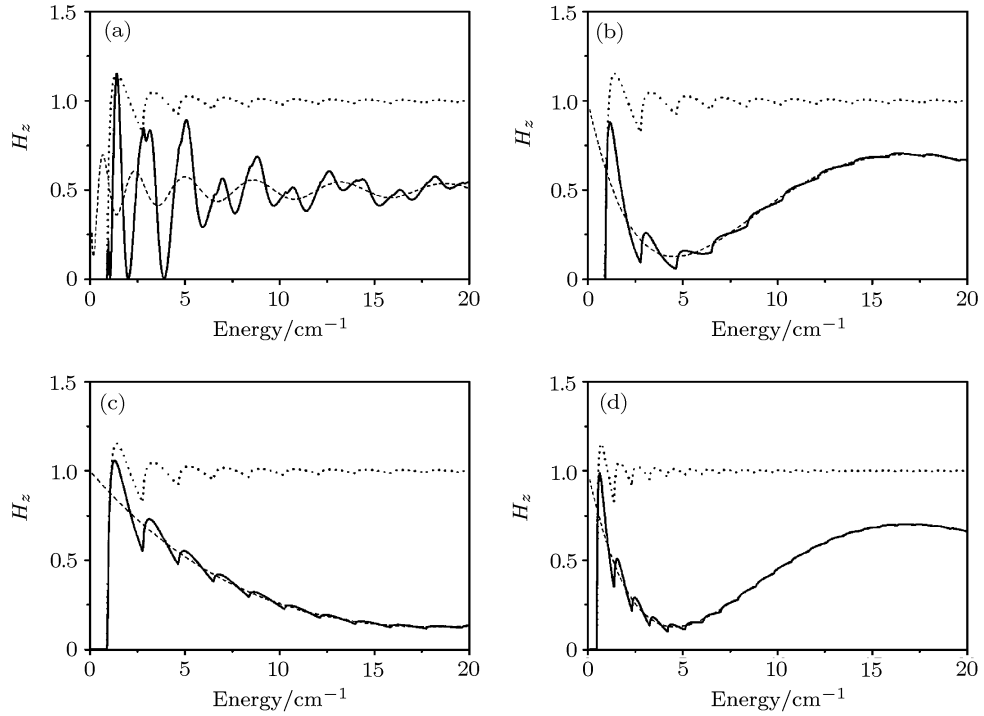



**Fig. 1.** The factor $H_z(E, B)$ as a function of $E$ under different conditions. The factor $H_z(E, B)$ defined in Eq. (14), for only magnetic field and for only elastic surface is plotted in solid line, dotted line and dashed line, respectively, for comparison. The excitation photon is polarized along the filed direction. (a) $B = 2$ T, $z_0 = 1500$ a.u.; (b) $B = 2$ T, $z_0 = 300$ a.u.; (c) $B = 2$ T, $z_0 = 150$ a.u.; (d) $B = 1$ T, $z_0 = 300$ a.u.

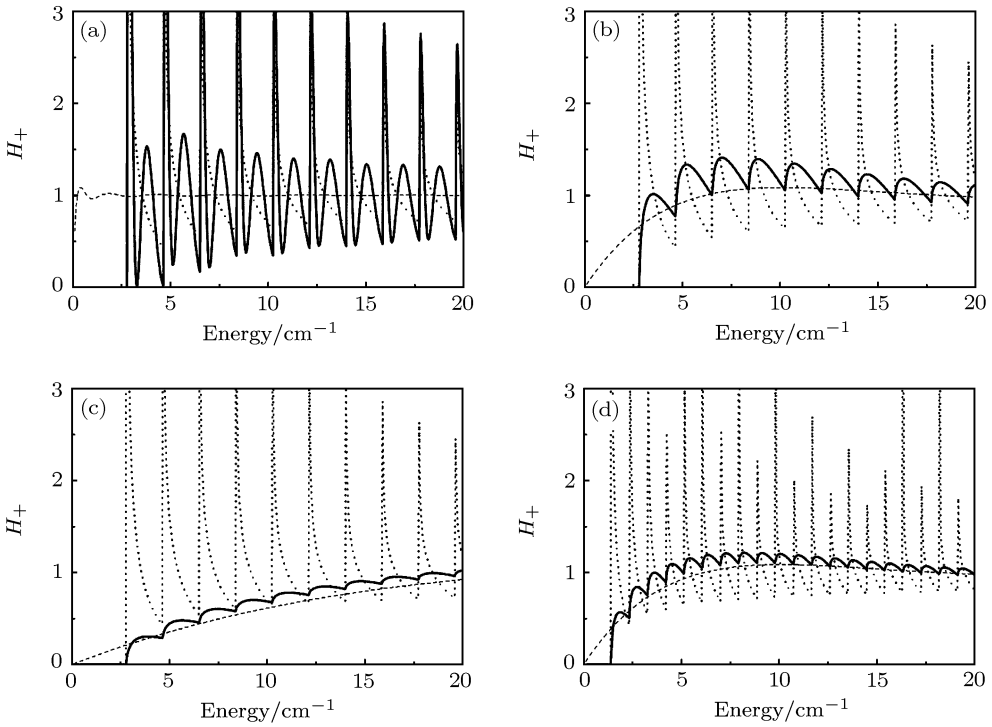



**Fig. 2.** The factor $H_z(E, B)$ as a function of $E$ under different conditions. The factor $H_z(E, B)$ defined in Eq. (17), for only an elastic surface and for only magnetic field is plotted in solid line, dashed line and dotted line, respectively, for comparison. The excitation photon is polarized. (a) $B = 2$ T, $z_0 = 1500$ a.u.; (b) $B = 2$ T, $z_0 = 300$ a.u.; (c) $B = 2$ T, $z_0 = 150$ a.u.; (d) $B = 1$ T, $z_0 = 300$ a.u.

Comparing the calculations for linearly polarized photons as shown in Fig. 1 and for circularly polarized photons as shown in Fig. 2, we can notice that the magnetic field effect is much stronger for circular polarization but the oscillation structure is also predominated by the elastic surface. In Figs. 2(a)–2(d), the $H$ functions for the case of only the magnetic field show equally spaced Landau levels and threshold law in the vicinity above each levels $E_{\rm th}$, i.e., $\Delta H \propto (E-E_{\rm th})^{-1/2}$.[10,20] However, the introduction of elastic surface suppresses the character of infinity at each Landau level, where $\Delta H \propto (E-E_{\rm th})^{1/2}$ for $(E-E_{\rm th}) \to 0$. The dependence of the $H_+$ on the distance between the ion and surface, and on the strength of magnetic field is similar to the case of linear polarization.

We add a brief postscript to our calculations for two extreme cases: the photodetachment in pure elastic surface potential and in pure magnetic field potential, which are shown in dotted lines and dashed lines in Figs. 1 and 2. In the first case, the $H$ function for the $H^-$ near an elastic surface can be obtained by taking the magnetic field to be zero in Eqs. (13) and (16). In the zero-magnetic field limit, the summation in Eqs. (13) and (16) will be replaced by an integral

$$H_z = \int \cos(q_n z_0)^2 \left(\frac{6\alpha q_n}{k^3}\right) {\rm d}n. \tag{27}$$

Using the relationship $E = \alpha(2n+m+|m|+1)+q_n^2/2$ in Eq. (7), we find that

$$\begin{aligned} &\sigma(E, B=0) \\ &= \frac{16\sqrt{2}B_0^2\pi^2}{3c}\frac{E^{3/2}}{(E_{\rm b}+E)^3} \\ &\quad + \frac{2\pi^2}{c}\frac{4B_0^2 E}{z_0(E_{\rm b}+E)^3}\sin\left(2\sqrt{2E}z_0\right), \end{aligned} \tag{28}$$

which is exactly the same result as that in the case for the $H^-$ near an elastic surface obtained by Yang *et al.*[2,3]

The photodetachment of $H^-$ in an pure magnetic field has been studied by Greene[8] and Crawford.[21] The $H$ function for the linear and circular polarizations are shown in Figs. 1 and 2, respectively, with a dotted line. The cross section formulas in the presence of only the magnetic field can be obtained by directly setting the surface-dependent factor $\sin(q_n z_0)$ and $\cos(q_n z_0)$ in Eqs. (14) and (17) to unity for Landau level below $E$ and to zero for Landau level above $E$.

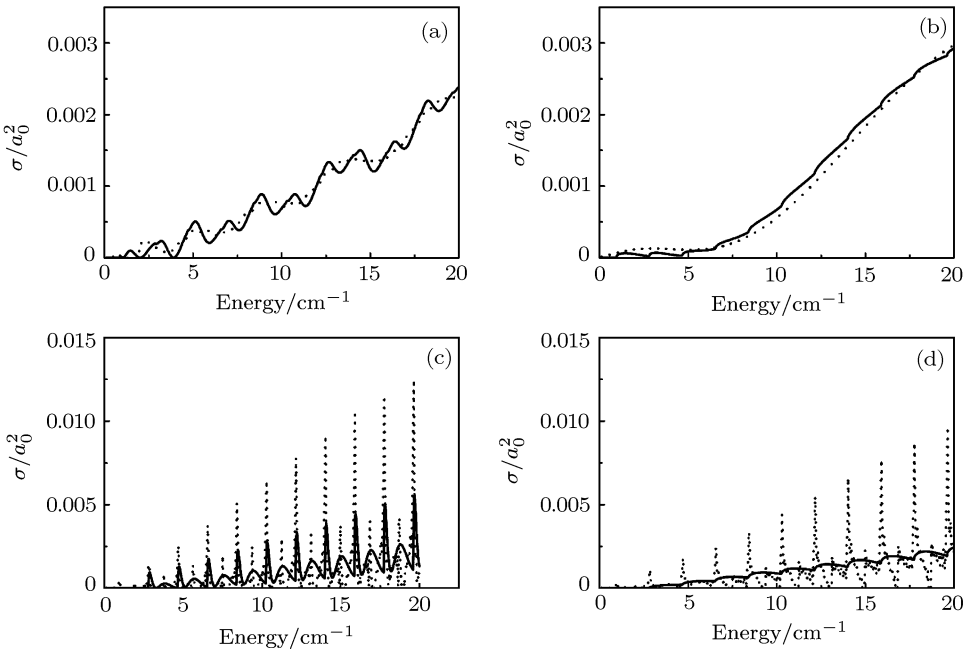



**Fig. 3.** The photodetachment cross section of the negative hydrogen ion near an elastic wall in magnetic field with different methods. Solid lines correspond to the result of quantum approach while dotted lines are for the closed orbit theory. (a) and (b) correspond to the photons polarized along the field direction while (c) and (d) correspond to the case of circularly polarized photons. (a), (c) $B = 2$ T, $z_0 = 1500$ a.u.; (b), (d) $B = 2$ T, $z_0 = 300$ a.u.

The photodetachment cross sections calculated with the frame transformation method are compared with the closed-orbit theory result as shown in Fig. 3. Figures 3(a) and 3(b) represent linear polarization. The semiclassical cross sections fit the quantum results quite well. The main difference between them is that the quantum cross sections have some ripples while the semiclassical ones go up more smoothly. This is the result of the quantization of the energy in the direction perpendicular to the magnetic fields, the limited quantum number violates the large quantum number approximation in semiclassical theory.[4,16] Figures 3(c) and 3(d) are for the circularly polarized photons, from which we can notice that the quantum cross sections show smooth oscillation structures while the semiclassical cross sections show singularity at some thresholds. This derivation can be attributed to the breakdown of the semiclassical mechanics in the bifurcated point where new orbit is born at these energies.[16,17]

# 4. Conclusion

In summary, we have analysed the photodetachment of $H^-$ near an elastic wall in a magnetic field and have derived analytical formulas for the cross section based on both a quantum approach and the closed-orbit theory. The magnetic field and elastic surface lead to two completely different modulations to the cross section of the photodetachment although oscillation strength depends on the distance between the ion and the elastic wall, and the strength of the magnetic field. For the photodetachment by a circularly polarized photon, the cross sections display the $(E-E_{\rm th})^{1/2}$ threshold law, instead of the $(E-E_{\rm th})^{-1/2}$ threshold law in presence of only the magnetic field. The semiclassical results fit the quantum result quite well and the remaining deviations can be attributed to the failure of the semiclassical mechanics. Beside the quantum wall in the $z$ direction, the magnetic field traps the motion of the electron in $(\rho, \phi)$, and the Landau levels in the magnetic field create another factor to modulate the photodetachment spectrum of $H^-$, which demonstrates a photodetachment in a real three-dimensional well.

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