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Quantum and closed-orbit theory Calculations for the photodetachment cross sections of H^- near two perpendicular elastic planes

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Abstract. The photodetachment cross section of H^- near two perpendicular elastic planes is investigated in this paper. Both the traditional quantum approach and closed orbit theory are applied to explicitly derive the formulas of the cross section for different laser polarization direction. We first compared the quantum formulas with closed orbit theory formulas, and then found that the quantum results are shown to be in good agreement with the semiclassical results. Further more, we also found that the cross section depends strongly on the direction of the laser polarization. When the polarization is parallel to the closed orbit, the corresponding oscillation in the cross section is very obvious. However, When the polarization is perpendicular to the closed orbit, the corresponding oscillation is too small for closed-orbit theory formula to describe.

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Key words: photodetachment, closed-orbits theory, elastic planes

1 Introduction

In 1987, Bryant *et al.* found some oscillations occurring among the photodetachment cross section of hydrogen ion in electrostatic field [1]. Rau [2] and Du [3] calculated the photodetachment cross section of hydrogen ion in electrostatic field by using quantum methods in coordinate representation and momentum representation respectively, which is consistent with the experimental results. Another method to calculate photodetachment cross section is closed orbit theory [4,5] which not only can get the results consistent with

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the experiment but also give the clear physical illustration intuitively for the oscillation structure of photodetachment cross section [6].

For decades, the environment around hydrogen ion is more and more complex in recent studies. At first, the researchers pay their main attention to photodetachment in the external field, including uniform field and non-uniform field, such as, the photodetachment in the magnetic field [7,8], in the parallel electromagnetic field and vertical electromagnetic field [9–14], in the electric and magnetic field with any orientation [15–17], in gradient field [18], in non-uniform electric field [19,20], near a repulsive potential [21], near two repulsive potential [22]and near a repulsive potential in the electric field [23]. Later, the photodetachment near the different interfaces aroused the research interests of all either,including near a single elastic interface [24–26], near a inelastic interface [27], near metal nanometer spherical [28], near a metal surface [29–31] and near a deformation spherical [32] and etc. Additionally, the photodetachment in different cavities which are composed by elastic interfaces have also been extensively concerned recently, such as in a parallel plate cavity [33,34], in an open cavity [35], inside a circular microcavity [36] and inside a square microcavity [37], and etc. Some of the above researches use quantum method, some others employ the closed orbit theory method or both.

While in this paper, we will further study the effects of two perpendicular elastic planes on photodetachment of hydrogen anion nearby. The system can be explicitly derived by the quantum approach and has three closed orbit. So we can consider the quantum influence from each one of the closed orbits .

2 Quantum formulas

The hydrogen negative ion is located between two infinitely extending planes which intersect vertically. It is at a distance a in front of one plane and a distance b in front of the other plane. The position of the coordinate system and the dimensions are given in Fig.1.

Then the Hamiltonian describing the detached electron motion of H^- can be given by

$$H=\frac{1}{2}\mathbf{p}^2+V_b(r)+V(\mathbf{r}). \tag{1}$$

where $V_b(r)$ is a short-range potential, and it binds the active electron to the atom. When the electron is far away from the nucleus, the binding potential V_b can be neglected.

The photodetachment cross section is given in terms of the dipole matrix elements by the following expression in atomic units [3]

$$\sigma^{\mathbf{q}}_{quant}=\frac{2\pi^2}{c}\int df 2E_p\left|\langle\Psi_f|\mathbf{q}|\Psi_i\rangle\right|^2\delta(E_f-E), \tag{2}$$

where $\mathbf{q}$ represents either x, y or z for corresponding laser polarizations directions; the speed of light c is approximately 137; the photon energy E_p is equal to the sum of the

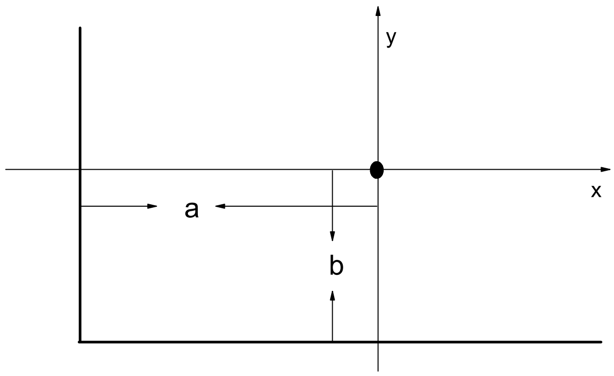

Figure 1: (Color online) Schematic illustration of H^- photodetachment near two perpendicular elastic planes.

binding energy E_b and the final escaping electron energy E. The binding energy of the electron to the negative ion is $E_b = k_b^2/2 \approx 0.754$ eV. Ψ_f is the final wave function and it is normalized according to $\langle \Psi_f | \Psi_{f'} \rangle = \delta(f - f')$. The integral in above function is over all final states. The initial wave function of the electron is given by

$$\Psi_i(\mathbf{r}) = B_0 \frac{e^{-k_b r}}{r}, \tag{3}$$

where the normalization of the initial bound state B_0 is approximately equal to 0.31522.

The final states can be obtained by :

$$\Psi_f(\mathbf{r}) = \frac{1}{\pi^{1/2}} \sin(p_x x + p_x a) \frac{1}{\pi^{1/2}} \sin(p_y y + p_y b) \frac{1}{(2\pi)^{1/2}} e^{i p_z z} \tag{4}$$

Substituting the final wave function (4) and the initial wave function (3) into the module square of the dipole matrix elements and restricting to x, y and z polarization, we obtain

$$|\langle \Psi_f | x | \Psi_i \rangle|^2 = \frac{1}{2\pi} \frac{64 B^2}{(k^2 + k_b^2)^4} \cos^2(p_x a) \sin^2(p_y b) p_x, \tag{5}$$

$$|\langle \Psi_f | y | \Psi_i \rangle|^2 = \frac{1}{2\pi} \frac{64 B^2}{(k^2 + k_b^2)^4} \sin^2(p_x a) \cos^2(p_y b) p_y, \tag{6}$$

$$|\langle \Psi_f | y | \Psi_i \rangle|^2 = \frac{1}{2\pi} \frac{64 B^2}{(k^2 + k_b^2)^4} \sin^2(p_x a) \sin^2(p_y b) p_z. \tag{7}$$

Substituting the module square of the dipole matrix elements into the photodetachment cross section function in Eq. (2), we can obtain the photodetachment cross section for every directions.

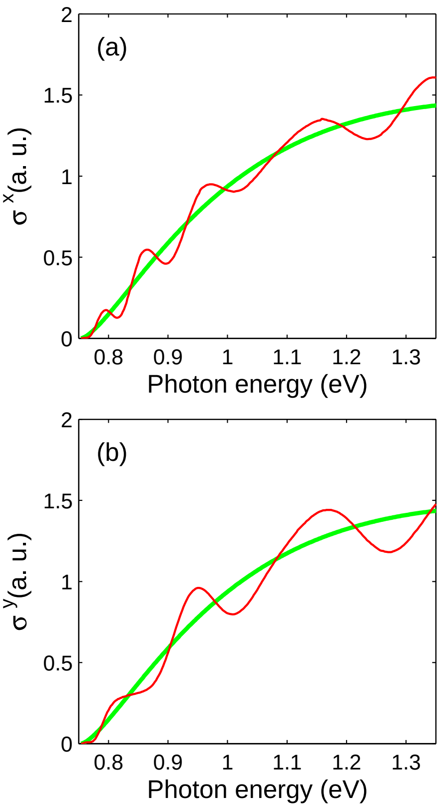

Figure 2: (Color online) Photodetachment cross sections (red and thin lines) as a function of photon energy for H^- near two perpendicular elastic planes. The position of the negative ion is fixed by $a=80$ (a.u.) and $b=60$ (a.u.) The laser is polarized in the x-axis direction (a) and y-axis direction (b). The photodetachment cross section of a negative ion in free space is also given by the green and thick lines for the purpose of comparison.

$$\sigma_q^x = \sigma_0 \frac{3}{\sqrt{2}\pi E^{3/2}} \int_0^{2\pi} d\phi \int_0^{\sqrt{2E}} dp \frac{p^3}{\sqrt{2E-p^2}} \cos^2(ap\cos\phi)\sin^2(bp\sin\phi)\cos^2\phi, \quad (8)$$

$$\sigma_q^y = \sigma_0 \frac{3}{\sqrt{2}\pi E^{3/2}} \int_0^{2\pi} d\phi \int_0^{\sqrt{2E}} dp \frac{p^3}{\sqrt{2E-p^2}} \sin^2(ap\cos\phi)\cos^2(bp\sin\phi)\sin^2\phi, \quad (9)$$

$$\sigma_q^z = \sigma_0 \frac{3}{\sqrt{2}\pi E^{3/2}} \int_0^{2\pi} d\phi \int_0^{\sqrt{2E}} dp p\sqrt{2E-p^2} \sin^2(ap\cos\phi)\sin^2(bp\sin\phi), \quad (10)$$

where $\sigma_0(E) = 16\sqrt{2}B^2\pi^2E^{3/2}/3c(E_b+E)^3$ is the photodetachment cross section of H^- in free space.

We show the photodetachment cross sections as a function of photon energy for the x and y polarization with the negative ion fixed by $a=80$(a. u.) and $b=60$(a. u.). For both x and y polarization, the oscillation patterns appear in the cross sections, but they

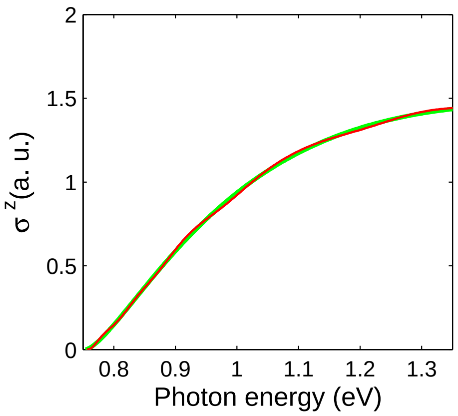

Figure 3: (Color online) Similar to figure 2 but for the z-polarization case.

are absolutely different. For the x-polarization case, the oscillation pattern is dominated by low-frequency oscillations, whereas the oscillation pattern for the x-polarization case is dominated by higher-frequency oscillations. For the z-polarization case, oscillations are still present, but the amplitudes of the oscillations are fairly small.

3 Closed-orbit theory formulas

Assuming the laser polarization is linear and parallel to the $\mathbf{q}$, and according to closed-orbit theory, the detached electron goes into outgoing $p_{\mathbf{q}}$ waves after absorbing a photon. The outgoing waves propagate away from the hydrogen atom in all directions. Sufficiently far from the hydrogen atom, the wave propagates according to semiclassical mechanics. Part of these waves propagate toward the planes and reflected by the planes. The waves then reverse their directions near the surface and and then propagate toward the atom. The interference of the outgoing electron wave and the returning wave in the region of the negative ion leads to the oscillation in the photodetachment cross section.

The COT formula for photodetachment cross section of H^- near elastic planes is generally given by [35]

$$\sigma(E)_{COT} = \sigma_0(E) + \sigma_0(E)\frac{3}{\sqrt{2E}}\sum_j \frac{f(\hat{\mathbf{k}}^j_{out},\hat{\epsilon})f(\hat{\mathbf{k}}^j_{ret},\hat{\epsilon})}{L_j}\sin(\sqrt{2E}L_j - \mu_j\pi), \quad (11)$$

where the summation is over all closed orbits. The closed orbits are the trajectories going out from and returning to the position of the negative ion; $\hat{\epsilon}$ is the direction of the laser polarization; $\mathbf{k}^j_{out}$ and $\mathbf{k}^j_{ret}$ are the outgoing momentum vector and returning momentum vector of the closed orbit j respectively; L_j and μ_j are the length and the number of reflections of the closed-orbit j, respectively. If we use (θ_L,ϕ_L) to denote the laser polariza-

Table 1: Properties of the closed-orbits.

Orbit Label	Length	μ	ϕ_{out}	ϕ_{ret}
1	2a	1	π	2π
2	$2\sqrt{a^2+b^2}$	2	$\pi+\arccos(\frac{a}{\sqrt{a^2+b^2}})$	$\arccos(\frac{a}{\sqrt{a^2+b^2}})$
3	2b	1	$\frac{3\pi}{2}$	$\frac{\pi}{2}$

tion direction and use $(\theta^j_{out},\phi^j_{out})$ and $(\theta^j_{ret},\phi^j_{ret})$ to denote the spherical angles of $\mathbf{k}^j_{out}$ and $\mathbf{k}^j_{ret}$,respectively, we can define $f(\theta,\phi;\theta_L,\phi_L)$ as the form $\cos\theta\cos\theta_L+\sin\theta\sin\theta_L\cos(\phi-\phi_L)$.

There are three closed orbits. All the closed orbits have the same polar angles $\theta^j_{out}=\theta^j_{ret}=\pi/a$. All the three closed orbits and their associated properties are listed in Table I.

The first closed-orbit leaves the emitting atom and is reflected by the right plane, and finally it retraces back to the emitting atom. The second closed orbit is reflected by the corner, then retraces back to the emitting atom. It should be understood that the second closed-orbit is reflected by the bottom or right surface at the point very near the corner, then reflected by the other surface. The third closed closed-orbit leaves the emitting atom downward, and it returns to the atom after being reflected back by the lower cavity surface.

Substituting the properties of the closed-orbits into Eq.(11) and restricting to linear laser polarization direction along axes, we obtain the COT cross sections

$$\sigma^x_{cot}(E)=\sigma_0(E)+\sigma_0(E)\frac{3}{2\sqrt{2E}}[\frac{1}{a}\sin(2a\sqrt{2E})-\frac{a^2}{\sqrt{a^2+b^2}^3}\sin(2\sqrt{a^2+b^2}\sqrt{2E})], \tag{12}$$

$$\sigma^y_{cot}(E)=\sigma_0(E)+\sigma_0(E)\frac{3}{2\sqrt{2E}}[\frac{1}{b}\sin(2b\sqrt{2E})-\frac{b^2}{\sqrt{a^2+b^2}^3}\sin(2\sqrt{a^2+b^2}\sqrt{2E})], \tag{13}$$

$$\sigma^z_{cot}(E)=\sigma_0(E). \tag{14}$$

With z-polarized light, the $x-y$ plane is in the node of outgoing wave, so the closed orbits have no effect [35]. Therefore the cross section for the z-polarization is just the cross section in free space.

4 Results and discussions

In Fig. 4, we compare the cross sections between the quantum results and the COT results and find they agree with each other very well when the polarization is in the closed-orbit plane. When the laser is polarized perpendicular to the closed-orbit plane, the cross sections from quantum approach show oscillations, on the contrary, non-oscillating cross sections obtained from the closed-orbit theory.

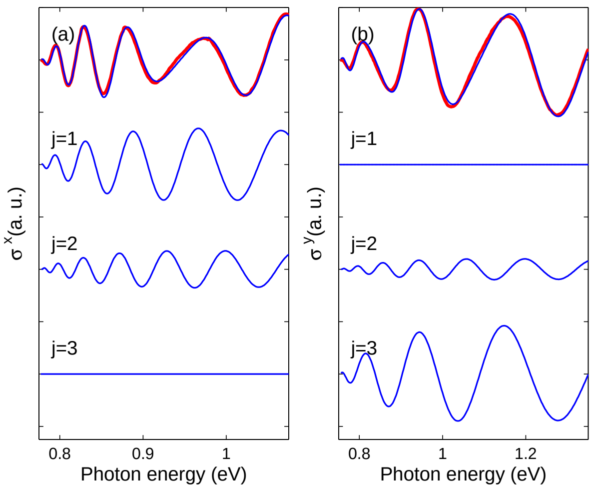

Figure 4: (a) The top panel illustrates the total oscillating part of the cross section for x-polarization. The cross sections between the quantum results and the COT results are compared with each other. The quantum results and COT results agree with each other very well. The oscillatory contributions associated with the three closed-orbits are displayed below. (b) Similar to (a), but the polarization is in the y-axis direction. The negative ion is fixed by $a=80$ (a.u.) and $b=60$ (a.u).

We also show the oscillatory part of the cross sections and the contribution from each closed-orbit in both polarization cases in Fig. 4. It is obvious that in the x-polarization case the largest contribution is made by the first closed orbit. The first closed orbit is the shortest one, and more importantly, the closed orbit lies on the antinode of the out-wave. These two properties are primarily taking responsibilities for the largest contribution. Short closed-orbits are supposed to be associated with low frequency and large amplitude oscillations, and vice versa. In Fig. 4(b) for the y-polarization, we observe the first closed orbit has no contribution to the cross section, because in this case the first closed orbits is on the node of the out-wave. The second closed orbit contributes the same frequency oscillations for both x and y-polarization cases. The second closed orbit contributes larger amplitude for x-polarization than for y-polarization, because for x-polarization the angle between the second closed orbit and antinode of the out-wave is smaller (37°) than for x-polarization (53°).

In summary, we applied traditional quantum mechanic and derived formulas describing the cross sections of H^- near two perpendicular elastic planes. We also derived closed-orbit theory formulas of the same system and compared them with those of the quantum mechanic formulas. We find the photodetachment cross section shows large or small oscillation structure depending on the laser polarization. We find that quantum and closed-orbit theory cross sections agree quite well.

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