Invisible oscillations in the photodetachment cross section of H⁻ near a surface

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Abstract. The photodetachment of H⁻ near a surface is investigated. A laser polarized parallel to the surface is used for the detachment of the electron. Analytical expressions for the detached-electron flux and total photodetachment cross section are derived. The detached electron flux displays strong interference pattern on the screen. Unlike the detached electron flux no visible oscillations are found in the photodetachment cross section. The photodetachment cross section in low energy limits is double of the cross section of H⁻ in free space.

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Key words: photodetachment, invisible oscillation, theoretical imaging method

1 Introduction

Interference phenomenon of quantum particles, like electrons and photons, has played vital role in the development of quantum mechanics [1]. Interest in the photodetachment process and photodetachment spectroscopy is shown in the recent years [2]. The photodetachment cross section for hydrogen negative ion (H^-) has been investigated experimentally [3,4] and theoretically [5–11].

External fields and surfaces significantly manipulate the photodetachment process of negative ions [12–14]. The induced effects of external fields and walls in the photodetached electron spectra is an interesting topic of investigation in quantum interference.

Effects of laser polarizations relative to the static electric field direction have been studied by closed orbit theory [15,16]. Yang *et al.* applied closed orbit theory to study the

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photodetachment of H⁻near a wall. The derived formula has two parts, one for smooth background term and second for oscillatory term. Their result shows some deviation from the one in static electric field. In another study Yang *et al.* [17] applied closed orbit theory and quantum approach to study the photodetachment of H⁻in a static electric field near a wall. They found that the cross section displays irregular staircases. Theoretical imaging method [18] and the closed orbit theory [7, 19] have provided a useful theoretical frame-work to understand the oscillations in the absorption spectra of H⁻near a reflecting surface. In the present work we use theoretical imaging method and study the photodetachment of electron from H⁻near a surface in a laser field polarized parallel to the surface, it induces invisible oscillations in the photodetachment cross section of H⁻. Atomic units are used throughout the article or mentioned otherwise.

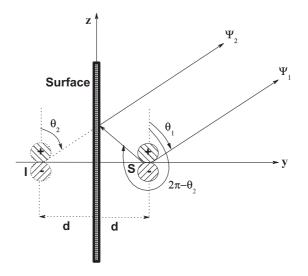


Figure 1: Schematic diagram of the photodetachment of hydrogen negative ion (H⁻) near a hard reflecting surface. The surface is orientated parallel to z-axis. The H⁻ which acts as a source (S) of the detached electron waves is placed at a distance (d) in front of the surface. The surface like a plane mirror forms image of the H⁻behind the surface. A z-polarized laser is used to shine the system. The two component waves are indicated by Ψ_1 and Ψ_2 . The component wave Ψ_1 is the direct outgoing wave and the component wave Ψ_2 appears as originated from the image (I) of H⁻behind the surface. The two adjacent circles in front of the surface represent the p-symmetry of the outgoing detached electron wave. The observing screen is assumed to be placed at a large distance from our system.

2 Theory

The schematic diagram for the photodetachment of H^- near a reflecting surface is shown in Fig. 1. The surface is placed at origin perpendicular to the *y*-axis. The hydrogen

ion (H⁻) is placed on *y*-axis at a distance (*d*) from the surface. The surface is assumed as a plane mirror which forms image of H⁻at the same distance behind the surface. A *z*-polarized laser of sufficient energy shines the system and knock off the electron from the H⁻. Quantum mechanically infinite component waves are associated with the detached electron, which propagate in all possible directions. Only two components waves are shown in figure which reach to the screen. In the figure Ψ_1 is the direct component wave moving along the trajectory r_1 making angle θ_1 with *z*-axis. The component wave Ψ_2 initially propagates towards the surface with an angle $2\pi - \theta_2$, then after reflection propagates along the trajectory r_2 . The reflected wave appears to be originating from the image of H⁻ behind the surface. The total detached electron wave at a large distance r (r >> d) from the surface is given by

$$\Psi^{+} = \frac{1}{\sqrt{2}} [\Psi_{1} + \Psi_{2}] \tag{1}$$

The direct component wave Ψ_1 in the absence of the surface is [8]

$$\Psi_1 = C \cos\theta_1 \frac{exp(ikr_1)}{r_1} \tag{2}$$

where $C = \frac{4kBi}{(k_b^2 + k^2)^2}$, $k = \sqrt{2E}$ (E is the detached electron energy), k_b is related to the binding energy E_b of H⁻ by $E_b = \frac{k_b^2}{2}$ and *B* is normalization constant having value 0.31552 [6]. The reflected component wave Ψ_2 can be obtained by propagating the detached electron wave from the source in the direction $(2\pi - \theta_2)$ followed by a reflection from the surface, which contributes an additional phase $-\mu \frac{\pi}{2}$ to the wave Ψ_2 ,

$$\Psi_2 = Ccos(2\pi - \theta_2) \frac{exp(i(kr_2 - \mu \frac{\pi}{2}))}{r_2}$$
(3)

where μ is constant and depends upon the nature of surface. In the present case we consider a hard surface for which $\mu = 2$. Ideal hard surface is the one which reflects all detached electron waves falling on it and hence it can be assumed as a potential barrier of infinite height [18].

Let (r, θ, ϕ) be the spherical polar coordinates of the total detached electron wave relative to the origin of the coordinate system. Then the total detached electron wave is

$$\Psi^{+}(r,\theta,\phi) = \frac{C}{\sqrt{2}} \left[\cos\theta_1 \frac{\exp(ikr_1)}{r_1} + \cos\theta_2 \frac{\exp(i(kr_2 - \pi))}{r_2} \right]$$
(4)

As in Ref. [7,19,20] the photodetachment occurs in two steps. In the first step a detached electron wave is generated while in the second step the detached electron wave propagates to large distance. Similarly we assume the two component waves propagate to large distance, hence r_1 and r_2 are very large as compared to the distance (*d*) between

H⁻ and the surface. The total detached electron wave is simplified by using large distance approximation and substituting $r_1 \approx r - dsin\theta \sin\phi$ and $r_2 \approx r + dsin\theta \sin\phi$ in the the phase terms, while in all other parts $r_1 \approx r_2 \approx r$ and $\theta_1 \approx \theta_2 \approx \theta$. With these approximations Ψ^+ reduces to

$$\Psi^{+}(r,\theta,\phi) = \sqrt{2}C\cos\theta\cos\left(kd\sin\theta\sin\phi - \frac{\pi}{2}\right)\frac{\exp(i(kr - \frac{\pi}{2}))}{r}$$
(5)

As the electron flux is defined as

$$\overrightarrow{j}(r,\theta,\phi) = \frac{i}{2} (\Psi^+ \overrightarrow{\nabla} \Psi^{+*} - \Psi^{+*} \overrightarrow{\nabla} \Psi^+)$$
(6)

Solving Eqn. 5 and Eqn. 6 simultaneously, we can evaluate the electron flux in the radial direction, i.e.

$$j_r(r,\theta,\phi) = \frac{kC^2 cos^2\theta}{r^2} \left(1 - cos(2kdsin\thetasin\phi)\right)$$
(7)

Finally a screen is placed perpendicular to the z-axis at a distance z = L, where L is much greater than d and in photodetachment microscopy experiments its value is several thousand atomic units [10, 11]. For simplicity, the spherical polar coordinates (r, θ, ϕ) are replaced by Cartesian coordinates (x, y, z). After simplification the detached electron flux can be written as

$$j_z(x,y) = \frac{kC^2L^3}{(x^2 + y^2 + L^2)^{5/2}} \left[1 - \cos(\frac{2kdy}{(x^2 + y^2 + L^2)^{1/2}}) \right]$$
(8)

To observe the general behavior of the total photodetachment cross section, an imaginary semi-spherical surface (Γ) enclosing the system is considered. The generalized differential cross section can be defined as the electron flux crossing an infinitesimal area $ds = r^2 \sin\theta d\theta d\phi$ on this surface [8]

$$\frac{d\sigma(q)}{ds} = \frac{2\pi E_{ph}}{c} \vec{j}_r \cdot \hat{n}$$
⁽⁹⁾

where 'q' is the coordinate on the surface, \hat{n} is the exterior normal unit vector of the infinitesimal area at coordinate 'q' and c is the speed of light in a.u. The total cross section can be derived by integrating the differential cross section over the surface (Γ).

$$\sigma(q) = \int_{\Gamma} \frac{d\sigma(q)}{ds} ds \tag{10}$$

The total photodetachment cross section is obtained by solving Eqn. 7, Eqn. 9 and Eqn. 10 simultaneously

$$\sigma = \sigma_0 H(kd) \tag{11}$$

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where $\sigma_0 = \frac{8\pi^2 k C^2 E_{ph}}{3c}$ is the cross section of H⁻in the absence of the surface and

$$H(kd) = 1 - 3\frac{\sin(2kd)}{(2kd)^3} + 3\frac{\cos(2kd)}{(2kd)^2}$$
(12)

The calculated cross section in Eqn. 11 is greater than the cross section of H⁻ in the absence of surface [6]. The function H(kd) is induced by the surface, which is responsible for the increase in the cross section and represents invisible oscillations.

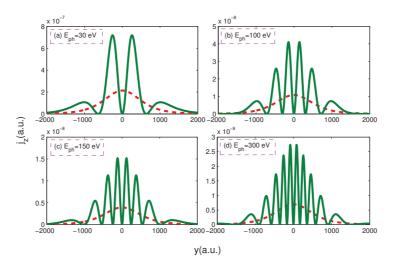


Figure 2: The detached electron flux in Eqn. 8 is plotted at x = 0 for different values of photon energies (a) $E_{ph} = 30$ eV, (b) $E_{ph} = 100$ eV, (c) $E_{ph} = 150$ eV, (d) $E_{ph} = 300$ eV. The distance of H⁻from the surface is kept fixed(d=4 a.u.). The screen is placed at a distance L=1000 a.u. from the surface. The flux of H⁻in the absence of surface (dotted line) is given for comparison.

3 Results and discussion

The detached electron flux (Eqn. 8) is plotted (for x = 0) in Fig. 2. The flux of H⁻in the absence of the surface (dotted line) is given for comparison. We have fixed d = 4a.u. and L = 1000 a.u. whereas the values of photon energy is varied for each plot, i.e. for Fig. 2(a) $E_{ph} = 50$ eV, Fig. 2(b) $E_{ph} = 100$ eV, Fig. 2(c) $E_{ph} = 150$ eV and Fig. 2(d) $E_{ph} = 300$ eV respectively. It is clear from the plots that the surface has induced oscillations in the detached electron flux. For the increasing values of photon energy the amplitude of oscillations fall down while its frequency increases. In Fig. 3 the detached electron flux is compared with the result of Ref. [18] for different values of distance (*d*), i.e. (a) d = 117 a.u., (b) d = 123 a.u., (c) d = 129 a.u. and (d) d = 135 a.u.. Here we have fixed the photon energy at $E_ph = 1$ eV. The detached electron flux (solid line) is different from the flux (dashed line) of Ref. [18].

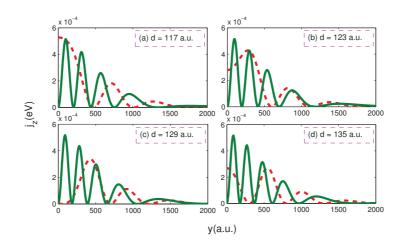


Figure 3: The detached electron flux in Eqn. 8 is compared with the detached electron flux of Ref. [18]. Here the values of photon energy E_{ph} =1eV and L=1000 a.u. are kept fixed. The value of the distance d is varied for each plot, i.e.; (a) d=117 a.u., (b) d=123 a.u., (c) d=129 a.u. and (d) d=135 a.u.. The difference between the two results is due to the direction of laser polarization relative to the orientation of the surfaces.

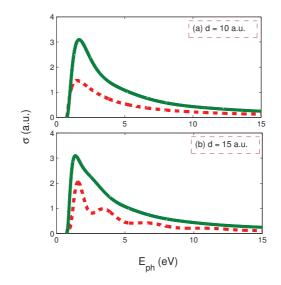


Figure 4: In 4(a) the cross section of Eqn. 11 is plotted verses photon energy. The cross section is also compared with the cross section of H⁻ in the absence of the surface (dashed line). In the low photon energy limits the cross section is two times of the cross H⁻ in the absence of the surface. In the high photon energy limits the cross sections are almost equal. In the plot 4(b) the cross section in Eqn. 11 (solid line) is compared with the cross section of Ref. [18] (dotted line). No oscillations can be seen in our cross section (solid line) where as the cross section of Ref. [18] is oscillatory.

In Fig. 4a the photodetachment cross section is plotted versus photon energy for a fixed distance (d = 10 a.u.) of H⁻from the surface. The figure shows that the photodetachment cross section (Eqn. 11) is greater than the cross section of H⁻ in the absence of the surface. The photodetachment cross section is two times of the cross section of H⁻ in the absence of the surface. A comparison plot of Eqn. 11 and the cross section derived in Ref. [18] is shown in Fig. 4b. The cross section (solid line) is greater than the cross section of Ref. [18]. It is clear from the figure that, no visible oscillations are found in the photodetachment cross section (solid line). On the other hand the photodetachment cross section of Ref. [18] (dashed line) is oscillatory.

4 Conclusion

In summery, theoretical imaging method is used to explore the induced effects of hard surface in the photodetachment spectra of a hydrogen negative ion (H⁻). The surface is oriented in such a fashion that the laser polarization direction is parallel to the surface. Strong oscillations are observed in the plots of detached-electron flux. With the increase in photon energy the amplitude and frequency of the observed oscillations were decreasing and increasing respectively. In low energy limits the peak of the photodetachment cross section is two times of the cross section of H⁻ in the absence of the surface, while the cross sections overlap in the high energy limits. Unlike the detached electron flux, no visible oscillations are found in the photodetachment cross section, whereas the cross section of Ref. [18] is oscillatory. Hence we concluded that when the laser polarization is parallel to the orientation of the surface, invisible oscillations are induced in the photodetachment cross section.

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