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Investigation of invisible oscillation on the photodetachment cross-section of H_2^- near a hard surface

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Abstract. Induced effects in the photodetached electron spectra from a diatomic negative ion (H_2^-) near a hard surface are investigated. A z-polarized laser is used to knock off electrons from H_2^- in the vicinity of a hard surface. Theoretical imaging method is used to derive a generalized modulation function for the total photodetachment cross-section, which describes invisible oscillation. It is found that the hard surface strongly affects the detached electron flux as well as total photodetachment cross-section. There exists strong dependence on the distance of H_2^- from the hard surface and also on the separation of atomic centres of H_2^-. Unlike the detached electron flux, no visible oscillations are noted in the photodetachment cross-section.

Keywords. Invisible oscillation; hard surface; photodetachment cross-section.

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1. Introduction

Negative ions have many applications in plasma physics, atomic physics and atmospheric physics. The induced effects of uniform fields and plane walls on the photodetached electron spectrum have been intensively investigated [1–8]. The study of photoelectron detached from a negative ion in the presence of magnetic field or electric field or gradient electric field or metallic surface is important for understanding negative ions dynamics and surface physics [5,9–21].

Almost two decades ago, Gibson *et al* [22] have performed an experiment related to the photodetachment of Au^- in a static electric field by using pulsed dye-laser beam (perpendicular to the field). They have reported laser polarization-dependent electric field oscillations in the p-wave detachment cross-section of Au^- near the threshold. The experiment support the theory for laser polarizations both parallel and perpendicular to the static electric field. The simultaneous effect of electric and magnetic fields on the photodetachment of H^- is reported in ref. [23]. The modulation in the cross-section is caused by the static electric field and is enhanced by the magnetic field.

In recent years, theoretical imaging technique has been used by many authors and all of them have reported that surfaces, walls and interfaces induce oscillations in the cross-section just like a static electric field [24,25]. Overall, much attention has been paid to the effects of walls, uniform electric and magnetic fields in the photodetachment of negative ions. Haneef *et al* have reported photodetachment of monoatomic negative ion near a hard spherical surface [1,3]. In a recent study, we have reported oscillatory behaviour of the photodetachment cross-section of H_2^- near a surface, where the laser polarization direction is assumed perpendicular to the surface [2]. The same problem is revisited in the present article. This time we assume a laser polarized parallel to the hard surface and report that no visible oscillations are induced in the photodetachment cross-section. Our results also predict that unlike the photodetachment cross-section, the detached electron flux is oscillatory. Therefore, a laser polarization can be used to control the oscillation in the photodetachment cross-section of negative ions near a hard surface. Our research will guide future structural investigation of diatomic negative ions near the surfaces and ion traps.

2. Schematic description

Figure 1 is a schematic representation of a theoretical model describing photodetachment of diatomic negative hydrogen ion (H_2^-) near a hard reflecting surface. Similar to the case of hard wall of ref. [25], a hard reflecting surface may be modelled by a potential barrier of infinite height. The hard surface is positioned at the origin in such a manner that its norm vector is parallel to the y-axis as shown in the figure. A negative hydrogen ion (H_2^-) is placed on the y-axis at a distance R from the surface. An observing screen is placed at a very large distance r compared to distance R, i.e. $r \gg R$. It is clear from the figure that a reflecting surface like a plane mirror forms the image at the same distance behind the surface.

A plane-polarized laser which has polarization direction parallel to the z-axis is used for the detachment of electron. A single photon, which is absorbed by H_2^- if the photon energy is high enough, can lead to the emission of photodetached electron. Quantum mechanically, infinite numbers of matter waves are associated with the photodetached electron. Once the photodetached electron waves are generated, they propagate to large distances [26]. In the present thought experiment, H_2^- acts as a source of infinite numbers of detached electron waves propagating in all directions.

Spherical polar coordinates are used to characterize the emission vectors of the electron detached from H_2^-. In the absence of the surface the waves emitted from the centre of H_2^- is denoted by ψ_1 and termed as direct waves. The direct electron wave at a large distance from H_2^- is obtained by using the superposition of detached electron waves generated

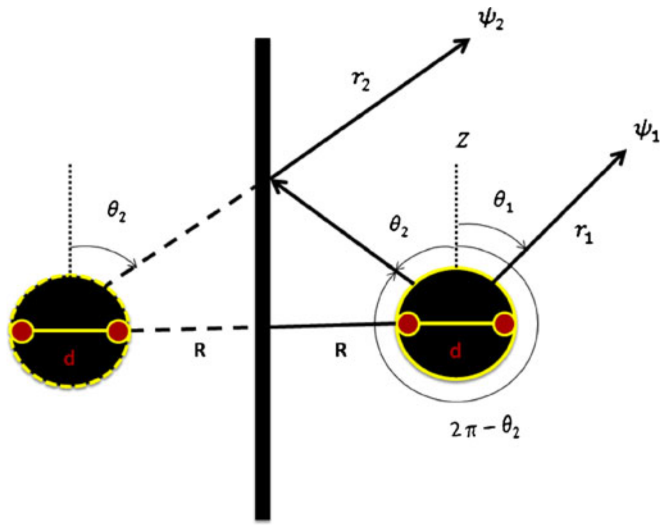

Figure 1. The schematic representation of the photodetachment of H_2^- near a surface. The yellow solid line circle and yellow dashed line circle represent H_2^- and its image respectively. The distance of H_2^- and its image from the hard surface is R (atomic units). The screen is considered to be placed at a distance r away that is large compared to R, i.e., $r \gg R$. The direct wave is represented by ψ_1. The reflected wave is represented by ψ_2, which appears as originated from the image behind the surface.

from the two centres [27]. Let ψ_1^+ and ψ_2^+ be the two coherent electron waves of the two centres of H_2^-, then the direct detached electron wave ψ_1 from the centre of H_2^- can be written as a linear combination $\psi_1 = (1/\sqrt{2})(\psi_1^+ + \psi_2^+)$ [27]. Assume that ψ_1^+ represents the outgoing detached electron wave function produced in the detachment of H^- in the absence of external agencies. The outgoing wave ψ_1^+ satisfies the Schrödinger equation

$$(H - E)\psi_1^+ = D(r)\psi_i. \tag{1}$$

Here $H = (p^2/2) + V_b(r)$ is the Hamiltonian which governs the motion of the detached electron. $D(r) = r\varepsilon$ is the dipole operator which defines the projection of electron position on the laser polarization direction (ε). For a z-polarized laser light $D(r) = r\varepsilon = r\cos\theta = Z$. The wave function $\psi_i = B\exp(-k_b r)/r$ is the initial bound wave function with $B = 0.31552$ and k_b is related to the binding energy E_b of H^- by $k_b = \sqrt{2E_b}$ [28]. As in ref. [28], H^- can be regarded as a one-electron system, with the active electron loosely bound by a short-range spherically symmetric potential $V_b(r)$ of the hydrogen atom, where r is the position of the electron with respect to the hydrogen atom. When the electron is photodetached from the hydrogen atom and moves far away from the origin, the short-range potential $V_b(r)$ can be omitted. In other words, the initial state of the active electron is an s state and after the detachment near the nucleus the electron carries one angular momentum, and at this stage it is a good approximation to neglect $V_b(r)$ [29]. To find solution of eq. (1) near the nucleus, the procedure of closed orbit theory [29–33] is used in the absence of the external agencies. In spherical polar coordinates the required detached electron wave function for H^- is given as

$$\psi_1^+ = \frac{4ikB\cos\theta_1^+}{(k_b^2+k^2)^2}\left[\frac{\exp(ikr_1^+)}{kr_1^+}\right].$$

A similar wave function, if the electron is assumed to detach from the second centre of the diatomic H_2^-, can be written as [28]

$$\psi_2^+ = \frac{4ikB\cos\theta_2^+}{(k_b^2+k^2)^2}\left[\frac{\exp(ikr_2^+)}{kr_2^+}\right].$$

Here $k=\sqrt{2E}$ is the momentum (in atomic units) of the detached electron having energy E. As given in ref. [27], we use large-distance approximation $r_1^+ = r_1 + (d\sin\theta\sin\phi)/2$ and $r_2^+ = r_1 - (d\sin\theta\sin\phi)/2$ for the phase terms and in all other places we use $r_1^+ = r_2^+ = r_1$ and $\theta_1^+ = \theta_2^+ = \theta_1$. With these approximations and substitutions the direct wave function ψ_1, originated from the centre of H_2^- in the absence of the surface is given below [27].

$$\psi_1(r_1,\theta_1,\phi_1) = \frac{4\sqrt{2}kBi}{(k_b^2+k^2)^2}\cos\left(\frac{kd\sin\theta\sin\phi}{2}\right)\cos\theta_1\frac{\exp(ikr_1)}{kr_1}. \tag{2}$$

The wave ψ_1 travels a distance r_1 and directly reaches the screen. In the presence of the surface, the detached electron wave ψ_2 is supposed to propagate in the direction $2\pi-\theta_2$. Furthermore, when ψ_2 is reflected from the surface it appears as it is originated from the image behind the surface and covers distance r_2. The reflected wave ψ_2 can be written as

$$\psi_2(r_2,\theta_2,\phi_2) = \frac{4\sqrt{2}kBi}{(k_b^2+k^2)^2}\cos\left(\frac{kd\sin\theta\sin\phi}{2}\right) \times\cos(2\pi-\theta_2)\frac{\exp(i(kr_2-\pi))}{kr_2}. \tag{3}$$

The additional phase shift $(-\pi)$ in the wave function ψ_2 is produced by the hard surface [25]. As given in ref. [26] photodetachment is a two-step process. In the first step an electron wave is generated while in the second step the electron wave propagates to large distance. Similarly, in the given schematic representation the two waves are propagating to large distances. Hence, by large-distance approximation these waves can be considered as propagating parallel to the screen. The total wave function from the system can be obtained by the linear superposition of ψ_1 and ψ_2.

$$\psi_T = \psi_1 + \psi_2. \tag{4}$$

The total wave function of the system can be obtained by substituting eqs (2) and (3) in eq. (4).

$$\psi_T = \frac{4\sqrt{2}kBi}{(k_b^2+k^2)^2}\cos\left(\frac{kd\sin\theta\sin\phi}{2}\right)\left[\cos\theta_1\frac{\exp(ikr_1)}{kr_1} - \cos\theta_2\frac{\exp(ikr_2)}{kr_2}\right]. \tag{5}$$

Using the large-distance approximations the wave function in eq. (5) can be simplified by substituting $r_1 \approx r - R\sin\theta\sin\phi$, $r_2 \approx r + R\sin\theta\sin\phi$ in the phase terms and $\theta_1 \approx \theta_2 \approx \theta$; $r_1 \approx r_2 \approx r$ in all other places. The total wave function reduces to

$$\psi_{\mathrm{T}} = \frac{8\sqrt{2}ikB}{(k_{\mathrm{b}}^2 + k^2)^2}\cos\theta\cos\left(\frac{kd\sin\theta\sin\phi}{2}\right)\sin\left(kR\sin\theta\sin\phi\right)\frac{\exp(ikr)}{kr}. \quad (6)$$

This is the total wave function of the detached electron at a screen from the system. The wave function carries all the information about the system which can be extracted using quantum mechanical tools.

3. Results and discussion

The total wave function obtained in eq. (6) is used to calculate the detached electron flux. The detached electron flux in the radial direction is calculated using the flux formula:

$$\vec{j}(r,\theta,\phi) = \frac{i}{2}\left(\psi_{\mathrm{T}}\vec{\nabla}\psi_{\mathrm{T}}^{*} - \psi_{\mathrm{T}}^{*}\vec{\nabla}\psi_{\mathrm{T}}\right) \quad (7)$$

$$j_{\mathrm{r}}(r,\theta,\phi) = j_0(r,\theta)[1 + \cos(kd\sin\theta\sin\phi) - \cos(2kR\sin\theta\sin\phi) - \cos(kd\sin\theta\sin\phi)\cos(2kR\sin\theta\sin\phi)]. \quad (8)$$

The first term, $j_0(r,\theta) = 32k^3B^2\cos^2\theta/r^2(k_{\mathrm{b}}^2 + k^2)^4$ represents the flux of monoatomic negative ion in the free space. The middle term represents oscillation induced by separation of the centres. The last term describes the oscillation induced by the surface. In figure 2 the detached electron flux given in eq. (8) is plotted in spherical polar coordinates (r,θ,ϕ), where $R = 150$ a.u., $d = 25$ a.u., $E_{\mathrm{ph}} = 2$ eVnversely with the square of the coordinate r. Oscillation can be seen in the figure with the variation in θ. For clear understanding of the oscillation the detached electron flux in eq. (8) is to be expressed in Cartesian coordinate system. To observe the spatial distribution of the detached electron flux, an observation screen is assumed to be placed perpendicular to the y-axis at a distances L from the surface, where L is much larger than the distance R ($L \gg R$). In the

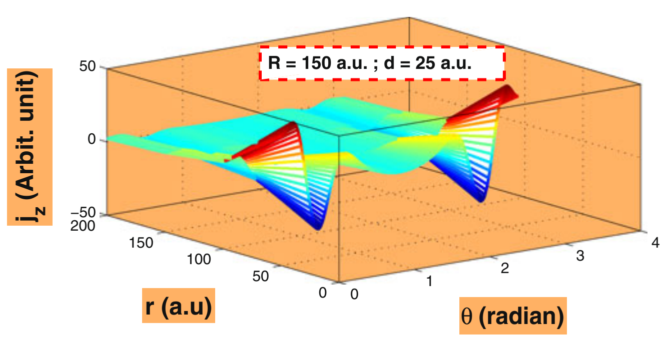

Figure 2. The detached electron flux using eq. (8) is plotted for distance $R = 150$ a.u., $d = 25$ a.u., $\phi = \pi/3$ and $E_{\mathrm{ph}} = 2$ eV.

photodetachment microscopy experiments, L is generally equal to thousands of atomic units [34,35]. Hence the electron flux at any point ($x = 0$, $y = L$, z) on the screen is given by

$$j_y(z) = \frac{32k^3 B^2 z^3}{(k_b^2 + k^2)^4 (L^2 + z^2)^{5/2}} \left[1 + \cos\left(\frac{kdL}{(L^2 + z^2)^{1/2}}\right)\right] \times \left[1 - \cos\left(\frac{2kRL}{(L^2 + z^2)^{1/2}}\right)\right]. \quad (9)$$

In figure 3 the detached electron flux vs. distance z is plotted for fixed values of photon energy $E_{ph} = 3$ eV, $d = 20$ a.u. and different values of R. The value of $R = 50$ a.u. for figure 3a, the value of $R = 250$ a.u. for figure 3b and the value of $R = 450$ a.u. for figure 3c. In the figure the result is compared with the detached electron flux of H^- in free space. The frequency of oscillations increases for increasing distance R. Hence it can be concluded that the surface induces oscillations in the detached electron flux which can be seen in the figure.

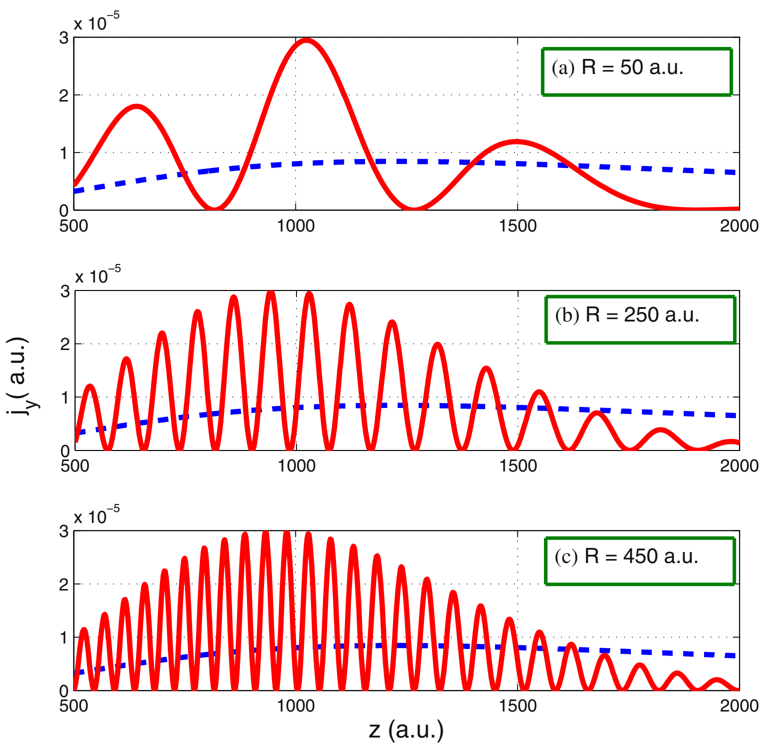

Figure 3. Comparison of the detached electron flux from H_2^- placed near a surface (solid line) and H^- (dashed line) is shown. The photon energy $E_{ph} = 3$ eV and $d = 20$ a.u., for (**a**) $R = 50$ a.u., (**b**) $R = 250$ a.u. and (**c**) $R = 450$ a.u.

To observe the general behaviour of the total photodetachment cross-section, an imaginary semispherical surface Γ enclosing the system is considered. The generalized differential cross-section can be defined as the electron flux crossing an infinitesimal area $\mathrm{d}s = r^2 \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi$ on this surface [28].

$$\frac{\mathrm{d}\sigma(q)}{\mathrm{d}s} = \frac{2\pi E_{\mathrm{ph}}}{c} \vec{j}_r \cdot \hat{n}. \tag{10}$$

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 atomic units. The total cross-section can be derived by integrating the differential cross-section over the surface (Γ).

$$\sigma(q) = \int_{\Gamma} \frac{\mathrm{d}\sigma(q)}{\mathrm{d}s} \mathrm{d}s. \tag{11}$$

Solving eqs (8), (10) and (11) simultaneously, we obtain

$$\sigma(E_{\mathrm{ph}}) = \sigma_0(E_{\mathrm{ph}}) H(k, d, R), \tag{12}$$

$$\sigma_0(E_{\mathrm{ph}}) = \frac{16\pi^2 B^2 \sqrt{2}(E_{\mathrm{ph}} - E_{\mathrm{b}})^{3/2}}{3c(E_{\mathrm{ph}})^3}, \tag{13}$$

$$H(k, d, R) = [1 - A(kd) + A(2kR) + A(kd - 2kR) + A(kd + 2kR)], \tag{14}$$

where $A(kd)$, $A(2kR)$, $A(kd - 2kR)$ and $A(kd + 2kR)$ are as given below.

$$A(kd) = \left(3\frac{\cos(kd)}{(kd)^2} - 3\frac{\sin(kd)}{(kd)^3}\right), \tag{15}$$

$$A(2kR) = \left(\frac{3}{2}\frac{\cos(2kR)}{(2kR)^2} - 3\frac{\sin(2kR)}{(2kR)^3}\right), \tag{16}$$

$$A(kd - 2kR) = \left(\frac{3}{2}\frac{\cos(kd - 2kR)}{(kd - 2kR)^2} - \frac{3}{2}\frac{\sin(kd - 2kR)}{(kd - 2kR)^3}\right), \tag{17}$$

$$A(kd + 2kR) = \left(\frac{3}{2}\frac{\cos(kd + 2kR)}{(kd + 2kR)^2} - \frac{3}{2}\frac{\sin(kd + 2kR)}{(kd + 2kR)^3}\right). \tag{18}$$

$\sigma_0(E_{\mathrm{ph}})$ is the photodetachment cross-section of H^- in the free space and $H(k, d, R)$ is a generalized modulation function describing invisible oscillations in the photodetached electron spectra. Generalized modulation function is also responsible for the change in peak height of the photodetachment cross-section in low-energy region.

The photodetachment cross-section given in eq. (12) is plotted in figure 4 for $R = 15$ a.u. and $d = 4$ a.u.. The photodetachment cross-section of H^- in free space (dashed line) is given for comparison. It is noted from the figure that the result of eq. (12) and that of H^- in free space is different. For the given values of R and d, the photodetachment cross-section of eq. (12) (solid line) in the low-energy region is almost twice that of the

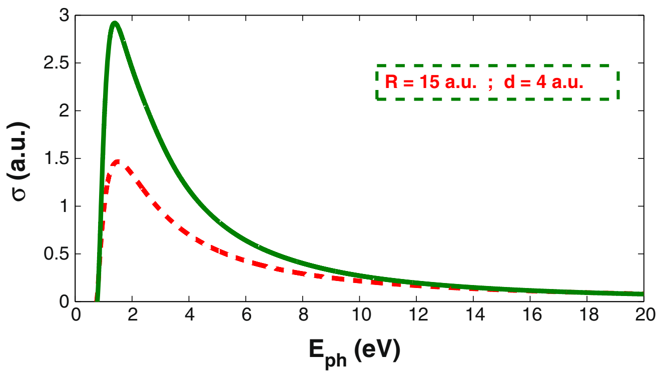

Figure 4. The photodetachment cross-section in eq. (12) is plotted for a fixed value of $R = 15$ a.u. and $d = 4$ a.u. The cross-section of H^- in free space (dashed line) is shown for comparison.

cross-section of H^- in free space, whereas in the high-energy region the cross-section approaches the cross-section of H^- in free space.

The photodetachment cross-section obtained in eq. (12) is also compared (figure 5) with the cross-section of ref. [2]. The parameters $R = 300$ a.u. and $d = 100$ a.u. are kept fixed. The cross-section of eq. (12) (dashed line) is smooth, whereas the cross-section of ref. [2] (solid line) is oscillatory. The smooth behaviour of the cross-section is attributed to the laser polarization parallel to the surface. In general, a surface oriented parallel to the laser polarization direction, cannot induce visible oscillation in the photodetachment cross-section.

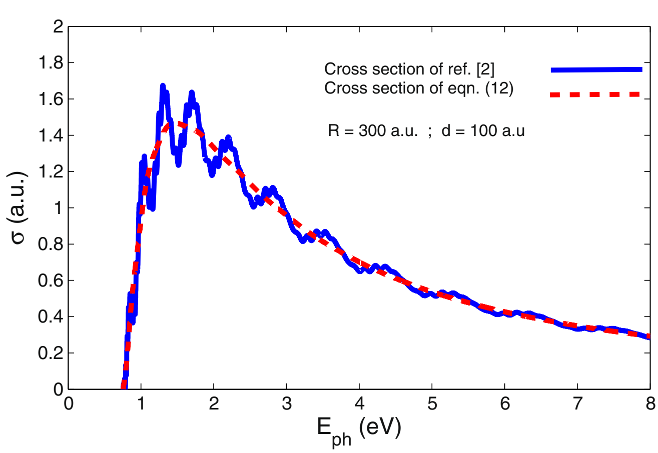

Figure 5. A comparison of the photodetachment cross-section of eq. (12) and that of ref. [2] is shown.

4. Conclusions

In conclusion, theoretical imaging method is used to investigate invisible oscillations in the spectra of diatomic negative ion (H_2^-) near a hard surface. Strong interference pattern in the detached electron flux is observed in the presence of the hard surface. The photodetachment cross-section of H_2^- in the presence of hard surface is larger than that of the H^- in free space. Furthermore, unlike the cross-section of ref. [2] the present cross-section is smooth. Hence it is concluded that when laser polarization is parallel to the hard surface, no visible oscillation can be induced in the photodetachment cross-section of a negative diatomic molecule. This work can help in the dynamics and structural investigations of diatomic negative ions. We hope that our results will be useful for guiding future experimental work related to the photodetachment of negative ions in the vicinity of hard surfaces, cavities and ion traps [36,37].

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