Electron flux distributions in photodetachment of HF^- near an interface: Theoretical imaging method study

Maryam Nawaz Awan and A. Afaq[†]

Centre of Excellence in Solid State Physics, University of the Punjab Lahore-54590, Pakistan

(Received 11 May 2012; revised manuscript received 2 July 2012)

The electron flux distributions in the photodetachment of HF^- near an interface are studied using a two-center model and the theoretical imaging method. An analytical expression for electron flux distributions is derived, which displays oscillations on an observation plane similar to the recent results published by Wang but in the presence of a static electric field. We also discuss the expressions for soft and hard wall cases in detail. A comparison is made with the previous work. The expression is a more general result, and we can deduce from it the electron flux distributions for the photodetachment of H_2^- near an interface. Finally, we show that the expression reveals similar results as those in [Chin. Phys. B **19** 020306 (2010)] when the wall effect is neglected.

Keywords: negative ions, two-center model, electron flux, quantum interference

PACS: 32.80.Gc, 03.65.Sq **DOI:** 10.1088/1674-1056/22/1/013205

1. Introduction

It is a well known fact that the external environment strongly modifies the photodetachment cross section by changing its smooth behavior to having an oscillatory structure.[1–7] The external environment may be a static electric filed, magnetic field, cross electric and magnetic fields, spherical surfaces, or an interface. Near an interface this physical phenomenon has attracted much interest in recent years.[8–17] Recently, Wang[18] studied the photodetachment of HF^- in free space using a two-center model and developed an analytical formula for the electron flux distributions to study the quantum interferences. These interferences are because of the outgoing electron waves originating from the two centers of the system that strongly depend on the laser polarization directions.

Then Wang[19] studied the same problem in the presence of a static electric field using the two-center model and the closed orbit theory. It was shown in that study that the electric field exhibits strong oscillations on the screen in addition to the background oscillations because of two centers. Afaq and Du[4] introduced a new technique known as the theoretical imaging method to study the photo detachment of H^- near a reflecting wall which is straight forward and is different from the closed orbit theory. They have given an argument that the oscillations in the electron flux and cross section are due to the interference of direct and reflected electron waves.

In this article, we use the theoretical imaging method[9] and examine the photodetachment of HF^- in the vicinity of a reflecting wall, taking each center as a coherent source of detached electron waves similar to that in the two-center model.[20] When the z-polarized laser falls on HF^-, which is also on the z axis, electrons are detached. A part of the detached electron wave goes directly away from the system, and the other part of the wave first moves to the interface from which it is bounced and then moves away from the system. The direct wave from the source and the reflected wave interfere with each other, and oscillatory patterns are produced on the screen.

2. Photodetached electron wave function and flux

A schematic illustration of the thought experiment for the photodetachment of HF^- near a reflecting interface is shown in Fig. 1. The HF^- acts as a source (S) placed on the z axis at a distance R from the interface that is placed on the y axis. When the laser beam

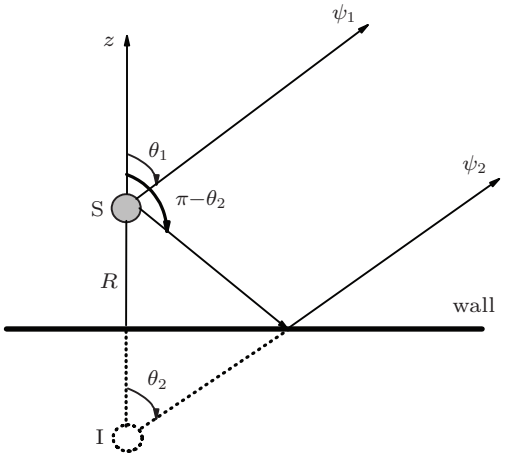


Fig. 1. Schematic diagram for the photodetachment of HF^- (S) near an interface.

[†]Corresponding author. E-mail: aafaq.cssp@pu.edu.pk

© 2013 Chinese Physical Society and IOP Publishing Ltd

interacts with the source, detached-electron waves are produced. Two outgoing detached electron waves Ψ_1 and Ψ_2 are shown, where Ψ_1 is the direct wave emerging from the source, whereas Ψ_2 is the wave reflected from the nearby interface. The reflected wave seems to be originating from an image (I) behind the interface.

Suppose that the bound state of HF^- is the superposition of hydrogen like bound states, i.e, $\phi = (\phi_1 + \phi_2)/\sqrt{2}$, where ϕ_1 and ϕ_2 are the normalized wave functions of H^- and F^-, respectively. After the photodetachment process, the detached electron wave moves a large distance away from the system obeying the semiclassical mechanics. The direct wave Ψ_1 makes an angle θ_1 smaller than $\pi/2$. The second wave first moves towards the interface, from which it is reflected, and then it moves to a large distance away from the system. This second wave makes an angle θ_2 larger than $\pi/2$ with the z axis. When the two waves combine on the screen placed at a distance L from the system, the total outgoing detached electron wave from the system is given by

$$\Psi^+ = \Psi_1 + \Psi_2. \tag{1}$$

The direct wave Ψ_1 can be taken from Ref. [19]

$$\begin{aligned}&\Psi_1(r_1,\theta_1,\phi_1)\\ &= \mathrm{i}\cos\theta_1\left(D_1\,\mathrm{e}^{\frac{\mathrm{i}kd\sin\theta_1\sin\varphi}{2}} + D_2\,\mathrm{e}^{\frac{-\mathrm{i}kd\sin\theta_1\sin\varphi}{2}}\right)\frac{\mathrm{e}^{\mathrm{i}kr_1}}{r_1},\end{aligned} \tag{2}$$

where $D_1 = 4kB_1c_1/(kb_1^2+k^2)^2$, $D_2 = 4kB_2c_2/(kb_2^2+k^2)^2$, $B_1 = 0.31552$ and $B_2 = 0.84$ are the normalization constants of H^- and F^-, respectively, $c_1 = 0.423$ and $c_2 = 0.664$ are the normalization constants of HF^- and can be calculated using the molecular orbit theory.[19] When the second wave is reflected from the interface, it obtains an additional phase of $-\mu\pi/2$, the wave Ψ_2 then is given by

$$\begin{aligned}\Psi_2(r_2,\theta_2,\phi_2) &= -\mathrm{i}\cos\theta_2\left(D_1\,\mathrm{e}^{\frac{\mathrm{i}kd\sin\theta_2\sin\varphi}{2}}\right.\\ &\left. + D_2\,\mathrm{e}^{\frac{-\mathrm{i}kd\sin\theta_2\sin\varphi}{2}}\right)\frac{\mathrm{e}^{\mathrm{i}(kr_2-\mu\pi/2)}}{r_2}.\end{aligned} \tag{3}$$

By substituting Ψ_1 and Ψ_2 in Eq. (1), the total outgoing photodetached electron wave on the screen is

$$\begin{aligned}\Psi^+ &= \mathrm{i}\cos\theta\left(D_1\,\mathrm{e}^{\frac{\mathrm{i}kd\sin\theta_1\sin\varphi}{2}} + D_2\,\mathrm{e}^{\frac{-\mathrm{i}kd\sin\theta_1\sin\varphi}{2}}\right)\\ &\times\left(\frac{\mathrm{e}^{\mathrm{i}kr_1}}{r_1} - \frac{\mathrm{e}^{\mathrm{i}(kr_2-\pi/2)}}{r_2}\right).\end{aligned} \tag{4}$$

Since r_1 and r_2 are large enough compared to the interatomic distance d and the distance of the ion from the interface R, then to simplify the above complicated wave function, the large distance approximation is used, i.e., $r_1 \approx r - R\cos\theta$ and $r_2 \approx r + R\cos\theta$ in the phase terms, while in all other terms, $r_1 \approx r_2 \approx r$ and $\theta_1 \approx \theta_2 \approx \theta$.[9] With these approximations, the above wave function takes the form

$$\begin{aligned}\Psi^+ &= \mathrm{i}\cos\theta\left(D_1\,\mathrm{e}^{\frac{\mathrm{i}kd\sin\theta\sin\varphi}{2}} + D_2\,\mathrm{e}^{\frac{-\mathrm{i}kd\sin\theta\sin\varphi}{2}}\right)\\ &\times\left(\mathrm{e}^{-\mathrm{i}kR\cos\theta} - \mathrm{e}^{\mathrm{i}(kR\cos\theta-\frac{\mu\pi}{2})}\right)\frac{\mathrm{e}^{\mathrm{i}kr}}{r}.\end{aligned} \tag{5}$$

2.1. The soft wall case

For a soft wall, put $\mu = 1$ in Eq. (5), we have

$$\begin{aligned}\Psi^+ &= \mathrm{i}\cos\theta\left(D_1\,\mathrm{e}^{\frac{\mathrm{i}kd\sin\theta\sin\varphi}{2}} + D_2\,\mathrm{e}^{\frac{-\mathrm{i}kd\sin\theta\sin\varphi}{2}}\right)\\ &\times\left(\mathrm{e}^{-\mathrm{i}kR\cos\theta} - \mathrm{e}^{\mathrm{i}(kR\cos\theta-\frac{\pi}{2})}\right)\frac{\mathrm{e}^{\mathrm{i}kr}}{r}.\end{aligned}$$

Solving the above equation using trigonometric relations, we have

$$\begin{aligned}\Psi^+ &= 2\mathrm{i}\cos\theta\left(D_1\,\mathrm{e}^{\frac{\mathrm{i}kd\sin\theta\sin\varphi}{2}} + D_2\,\mathrm{e}^{\frac{-\mathrm{i}kd\sin\theta\sin\varphi}{2}}\right)\\ &\times\cos(kR\cos\theta+\pi/4)\frac{\mathrm{e}^{\mathrm{i}(kr+\pi/4)}}{r}.\end{aligned} \tag{6}$$

The outgoing photodetached electron flux can be evaluated by the following formula:

$$j_r = \mathrm{Re}\left(\Psi^{+*}\frac{1}{\mathrm{i}}\frac{\partial\Psi^+}{\partial r}\right). \tag{7}$$

Using Eq. (6) in Eq. (7), we obtain the outgoing electron flux in the radial direction for the soft wall

$$\begin{aligned}j_r &= \frac{2k\cos^2\theta}{r^2}\left[D_1^2 + D_2^2 + 2D_1D_2\cos(kd\sin\theta\sin\varphi)\right]\\ &\times(1-\sin(2kR\cos\theta)).\end{aligned} \tag{8}$$

If the screen is placed perpendicular to the z axis, then the flux in the perpendicular direction of the plane is

$$\begin{aligned}j_z(r,\theta,\phi) &= \frac{2k\cos^2\theta}{r^2}\left[D_1^2 + D_2^2 + 2D_1D_2\cos(kd\sin\theta\sin\varphi)\right]\\ &\times(1-\sin(2kR\cos\theta))\,\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{n}}.\end{aligned}$$

As $\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{n}} = \cos\theta$, we have

$$\begin{aligned}j_z(r,\theta,\phi) &= \frac{2k\cos^3\theta}{r^2}\left[D_1^2 + D_2^2 + 2D_1D_2\cos(kd\sin\theta\sin\varphi)\right]\\ &\times(1-\sin(2kR\cos\theta)).\end{aligned} \tag{9}$$

2.2. The hard wall case

For a hard wall, put $\mu = 2$ in Eq. (5), we have

$$\begin{aligned}\Psi^+ &= \mathrm{i}\cos\theta\left(D_1\,\mathrm{e}^{\frac{\mathrm{i}kd\sin\theta\sin\varphi}{2}} + D_2\,\mathrm{e}^{\frac{-\mathrm{i}kd\sin\theta\sin\varphi}{2}}\right)\\ &\times\left(\mathrm{e}^{-\mathrm{i}kR\cos\theta} - \mathrm{e}^{\mathrm{i}(kR\cos\theta-\pi)}\right)\frac{\mathrm{e}^{\mathrm{i}kr}}{r},\\ \Psi^+ &= 2\mathrm{i}\cos\theta\left(D_1\,\mathrm{e}^{\frac{\mathrm{i}kd\sin\theta\sin\varphi}{2}} + D_2\,\mathrm{e}^{\frac{-\mathrm{i}kd\sin\theta\sin\varphi}{2}}\right)\\ &\times\cos(kR\cos\theta)\frac{\mathrm{e}^{\mathrm{i}(kr+\pi/4)}}{r}.\end{aligned} \tag{10}$$

Using Eq. (10) in Eq. (7), we obtain the electron flux for the hard wall

$$j_r = \frac{2k\cos^2\theta}{r^2}\left[D_1^2+D_2^2+2D_1D_2\cos(kd\sin\theta\sin\varphi)\right] \times\left(1+\cos(2kR\cos\theta)\right). \quad (11)$$

And the flux in the normal direction will be

$$j_z(r,\theta,\phi) = \frac{2k\cos^3\theta}{r^2}\left[D_1^2+D_2^2+2D_1D_2\cos(kd\sin\theta\sin\varphi)\right] \times\left(1+\cos(2kR\cos\theta)\right). \quad (12)$$

2.3. Spatial distributions of a detached electron flux

In order to find a relationship for the electron flux in the cartesian coordinate system, put $z = L$, $\rho = x^2+y^2$, and then change the spherical coordinates to the cartesian coordinates in Eqs. (9) and (12). We have the flux for the soft wall

$$j_z = \frac{2kL^3}{(\rho^2+L^2)^{5/2}}\left[D_1^2+D_2^2+2D_1D_2\cos\left(\frac{kdy}{\sqrt{(\rho^2+L^2)}}\right)\right] \times\left(1-\sin\frac{2kLR}{\sqrt{(\rho^2+L^2)}}\right). \quad (13)$$

The flux for the hard wall is

$$j_z = \frac{2kL^3}{(\rho^2+L^2)^{5/2}}\left[D_1^2+D_2^2+2D_1D_2\cos\left(\frac{kdy}{\sqrt{(\rho^2+L^2)}}\right)\right] \times\left(1+\cos\frac{2kLR}{\sqrt{(\rho^2+L^2)}}\right). \quad (14)$$

3. Results and discussion

As $L \gg \rho$, then in Eqs. (13) and (14) $L/\sqrt{\rho^2+L^2} \to 1$. So the extra oscillating terms in these equations will produce oscillations in the electron flux due to the interferences of the two detached waves: one direct from the system and the other reflected from the interface, as shown in Fig. 1. The interference may be constructive or destructive when $2kR = n\pi$ with n being an integer or half of integral, respectively. If we take R to be very large so that the wall effect is negligible, then for a particular value of photon energy, the oscillating terms in Eqs. (13) and (14) become zero, and the relationship for electron flux distributions will be similar to that for HF^- in free space.[18] We observe that our results are similar to those in Ref. [18]. So the wall induced oscillations in the spectra would vanish at very large distances. Although this effect is not very clear in the electron flux distribution calculations, we hope it will be prominent in the total cross section calculations. This effect is presented in Fig. 2(d).

In Fig. 2, we have shown the oscillation effect near the interface for fixed photon energy 500 eV by changing the distance between the source and the wall. We can see that the wall effect is visible for small distances, and as the distance R becomes large enough, the wall effect vanishes.

In Fig. 3, a clear picture of our result for $R = 5$ a.u. and $E_{\rm Ph} = 250$ eV is shown. The solid line shows the result for a soft wall, while the dotted line shows the result for the hard wall. These two differ from each other by $\pi/2$. On the other hand, if we put $D_1 = D_2 = D$, $B_1 = B_2 = B$, $k_{b1} = k_{b2} = k_b$, and $c_1 = c_2 = c = \frac{1}{\sqrt{2}}$, then our results may reduce to that of the homo-nuclear diatomic molecular negative ion H_2^- near a reflecting wall, for which we have calculated. So our result for the photodetachment of HF^- near an interface is more general, and one can apply it for any diatomic negative ion.

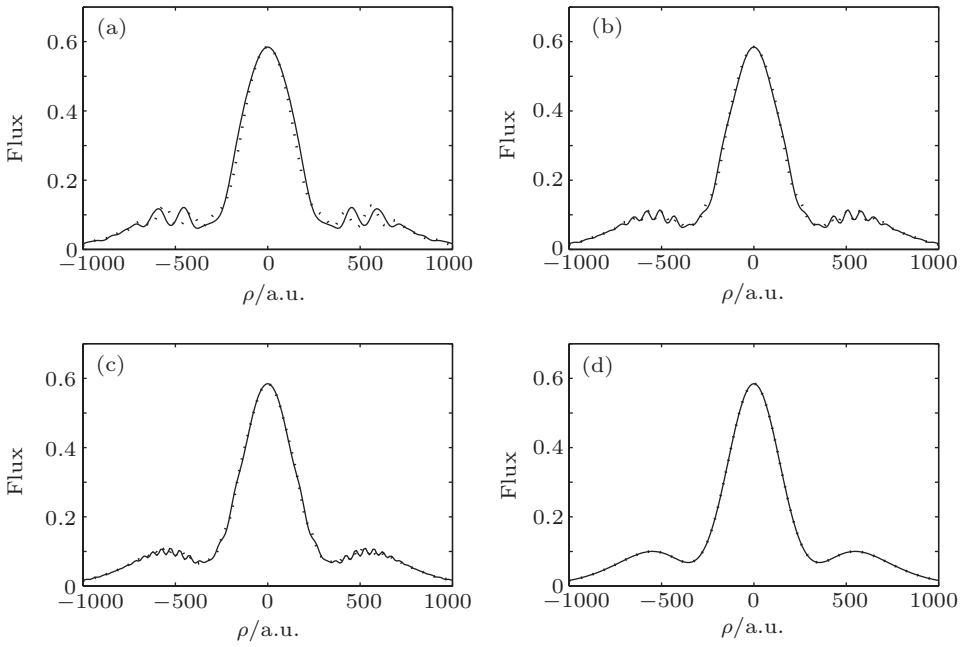


Fig. 2. Photodetached electron fluxes in the photodetachment of HF^- near an interface for (a) $R = 10$ a.u., (b) $R = 20$ a.u., (c) $R = 30$ a.u., and (d) $R = \infty$. Here the photon energy is kept constant at $E_{\rm Ph} = 500$ eV. Dotted lines are for the hard wall case, while solid lines are for the soft wall case.

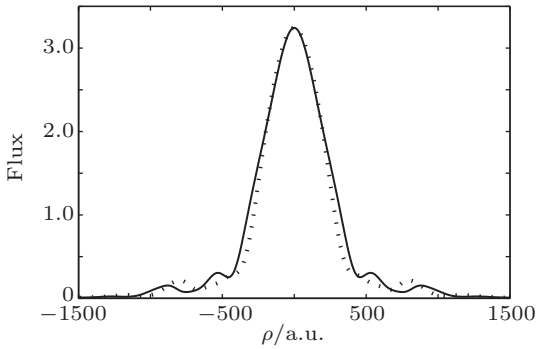


Fig. 3. Photodetached electron fluxes in the photodetachment of HF^- near an interface for $R = 5$ a.u. and $E_{Ph} = 250$ eV. The dotted line is for the hard wall case, while the solid line is for the soft wall case. It is clear that the soft and the hard walls differ form each other by $\pi/2$.

4. Conclusion

In conclusion, we have studied the electron flux distributions in the photodetachment of HF^- anion near an interface. We find that the presence of the interface induces oscillations in the electron flux distribution on an observation plane. We have also shown that our derived formula for electron flux distributions is universal and may be used for any diatomic negative ion to obtain its structural information in molecular photodetachment microscopy experiments.

References

[1] Bryant H C, Mohagheghi A and Stewart J E 1987 *Phys. Rev. Lett.* **58** 2412
[2] Fabrikant I 1980 *Sov. Phys. JETP* **52** 1045
[3] Rau A R P and Wong H 1988 *Phys. Rev.* A **37** 632
[4] Du M L and Delos J B 1988 *Phys. Rev.* A **38** 5609
[5] Du M L 1989 *Phys. Rev.* A **40** 4983
[6] Blondel C *et al.* 2001 *J. Phys.* B **34** L281
[7] Blondel C *et al.* 2001 *Phys. Rev.* A **64** 052504
[8] Yang G, Zheng Y and Chi X 2006 *J. Phys.* B: *At. Mol. Opt. Phys.* **39** 1855
[9] Afaq A and Du M L 2007 *J. Phys.* B: *At. Mol. Opt. Phys.* **40** 1309
[10] Wang D H, Ma X G, Wang M S and Yang C L 2007 *Chin. Phys.* **16** 1307
[11] Wang D H 2006 *Chin. Phys. Lett.* **24** 400
[12] Wang D H, Yu Y J and Wang H R 2009 *Chin. Opt. Lett.* **7** 176
[13] Wang D H and Huang K Y 2010 *Commu. Theor. Phys.* **53** 898
[14] Huang K Y and Wang D H 2010 *J. Chem. Phys.* **114** 8958
[15] Wang D H, Wang S S and Tang T T 2011 *J. Phys. Soc. Jpn.* **80** 094301
[16] Wang D H 2011 *Current Applied Physics* **1** 1228
[17] Wang D H and Huang K Y 2011 *J. Appl. Phys.* **109** 014113
[18] Wang D H 2010 *Chin. Phys.* B **19** 020306
[19] Wang D H 2008 *Chin. Phys. Lett.* **25** 919
[20] Afaq A and Du M L 2009 *J. Phys.* B: *At. Mol. Opt. Phys.* **42** 105101