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Photodetachment of H^- in an electric field between two parallel interfaces*

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By using the closed orbit theory, the photodetachment cross section of H^- in a static electric field between two parallel elastic interfaces is derived and calculated. It is found that the photodetachment cross section depends on the electric field and the distance between the ion and the elastic interface. The oscillation of the cross section becomes more complicated than in the case of H^- near one elastic interface. The results show that near the detachment threshold, the influence of the additional interface can be neglected. But with the increase of the energy, its influence becomes great. At some energies, the cross sections display sharp peaks, contrasting with the staircase structure when only one interface exists. This study provides a new understanding of the photodetachment process of H^- in the presence of external field and interfaces.

Keywords: closed-orbit theory, photodetachment cross section
PACC: 3450D, 3280F, 0365S

1. Introduction

It is well known that the environment such as potential walls or cavities can have a significant influence on the photodetachment cross section of ions and the photoabsorption spectra of atoms. Early experiment and theory showed the total photodetachment cross section of H^- in the presence of a static field to have oscillatory structures.[1,2] The oscillations in the photodetachment cross section can be interpreted by Du and Delos' closed orbit theory.[3] They found that the oscillations were caused by the interference between the detached-electron waves reflected by the potential barrier of the electric field and the outgoing detached-electron waves localized in the regions of the bound state of H^-. Later, photodetachment of H^- in other fields, such as in parallel electric and magnetic fields,[4] cross electric and magnetic fields,[5] electric and magnetic field with arbitrary orientations have also been studied theoretically.[6]

Recently, a lot of attention has been paid to the photo-induced electronic excitations of adsorbates on metal surfaces.[7−10] Since it was proposed that H^- be used to probe the adsorbate state lifetime and the charge transfer during the backscattering,[11] the photodetachment of H^- near an interface has attracted much interest. In Refs.[12, 13], Yang *et al* applied an elastic wall model to the electron scattering interface. They derived and calculated the photodetachment cross section of H^- near an interface, separately, without and with a static electric field by using the closed orbit theory. Afaq and Du *et al*[14] discussed the photodetachment of H^- near a reflecting interface using a theoretical imaging method. Wang *et al*[15] studied the photodetachment of H^- near two parallel interfaces without the electric field. As to the photodetachment of negative ion in a static electric field near two interfaces, nobody has carried out its study. In this paper, by using the closed orbit theory, we study the photodetachment of H^- in a static electric field between two parallel interfaces. For simplicity, we still consider the interface as an elastic reflecting wall. The results show that the photodetachment cross section of H^- in a static electric field between two parallel interfaces oscillates in a much more complicated manner than in the case in which there exists only one interface, which suggests that two interfaces have a great influence on the photodetachment of H^-. Near the electron detachment threshold, our result is identical to the one given by Yang *et al.*[13] But with the increase of the energy, our results come to differ from theirs. Atomic units are used in the present paper unless otherwise indicated.

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2. The classical motion

The schematic plot of the system is shown in Fig.1. The electric field is along the z axis. A hydrogen negative ion sits at the origin, and a z-polarized

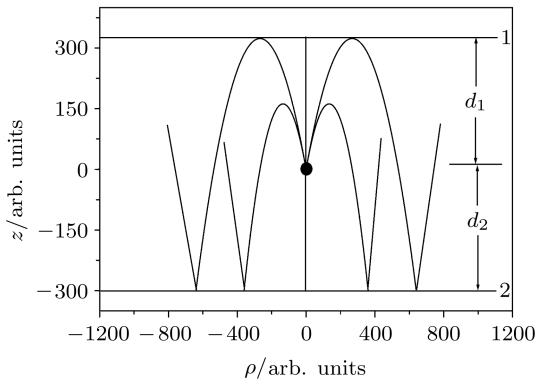


Fig.1. Schematic of the classical trajectories of the detached electron of H^- in a static electric field between two parallel elastic interfaces. The electric field is along the $+z$ axis. H^- is denoted by a black dot at the origin. d_1 and d_2 represent the distances between the H^- and the elastic interfaces 1 and 2.

laser is applied for the photodetachment. Two parallel elastic interfaces perpendicular to the z axis are located at $z = d_1$ and $z = -d_2$. So the photodetachment electron can be reflected by the electric field and the interfaces. We still consider the H^- as a one-electron system, with the active electron loosely bound by a short-range, spherically symmetric potential $V_b(r)$.[15] In the cylindrical coordinates (ρ, z, ϕ), the Hamiltonian of a detached electron is

$$H = \frac{1}{2}(P_\rho^2 + P_z^2) + Fz + V(z) + V_b(r), \qquad (1)$$

in which $V(z)$ is the interaction between the electron and the interfaces, and it can be described as

$$V(z) = \begin{cases} 0, & -d_2 < z < d_1, \\ \infty, & z \leqslant -d_2 \text{ or } z \geqslant d_1. \end{cases} \qquad (2)$$

Owing to the cylindrical symmetry of the system, the component for ϕ motion has been separated and the z component of the angular momentum is a constant of motion, which has been set to be zero. When the electron is far away from the nucleus, the short-range potential $V_b(r)$ can be neglected. By solving the Hamiltonian motion equation, we obtain the classical motion of the electron between two parallel interfaces:

$$\begin{aligned} \rho(t,\theta) &= k\sin\theta t, \\ z(t,\theta) &= k\cos\theta t - \frac{1}{2}Ft^2, \end{aligned} \qquad (3)$$

where k is the momentum of the detached electron and θ is the emission angle between the momentum and the z axis. Because the elastic interfaces are perpendicular to the z direction, they have no influence on the ρ motion. For $0 < \theta < \pi$, the electron trajectory is a parabola before hitting the interface. However, when an electron hits the wall, it bounces back and changes the sign of the momentum in the z direction but keeps its magnitude. Figure 1 shows the classical trajectories of the photo-detached electron. From this figure we can see that only the orbit emitting up along the z axis can be drawn back by the electric field or bounced back by the elastic interface to the origin. There are only four fundamental closed orbits and the others are their repetitions, which is similar to the case given by Wang *et al.*[15] From Fig.1 we find not all the electrons can hit the upper interface, which depends on the initial momentum of electron and the electric field strength. The maximum distance the electron can reach along the $+z$ axis is $d_{\max} = k^2/(2F)$. Given F, with the increase of the initial momentum k, $d_{\max}$ is increased. When $d_{\max} < d_1$, the electron cannot hit the upper interface before it pulls back by the electric field. Under this condition, the closed orbits are the same as the ones given in Ref.[13], the upper elastic interface has no influence on the photodetachment of the negative ion. On the other hand, if $d_{\max} \geqslant d_1$, the electron can hit the upper interface. Therefore, considering the influence of the upper interface, there can exist the four fundamental closed orbits of the detached electron as follows: (i) The electron goes up along the $+z$ direction and hits the upper interface before reaching its maximum point, then bounces back by the upper interface and returns to the origin. (ii) The electron comes down in the $-z$ direction and hits the second interface, then bounces back and finally returns to the origin, this orbit is always the same as the one given in Ref.[15]. (iii) The electron completes the first orbit and then passes through the origin, and continues to complete the second orbit. (iv) This orbit is similar to the one of (iii) but in a reverse order, the electron completes the second orbit and then the first orbit.

The periods of these four fundamental closed orbits are

$$\begin{aligned} T_1 &= \frac{2k - 2\sqrt{k^2 - 2Fd_1}}{F}, \\ T_2 &= \frac{-2k + 2\sqrt{k^2 + 2Fd_2}}{F}, \\ T_3 &= T_4 = T_1 + T_2 \end{aligned}$$

$$= \frac{2\sqrt{k^2+2Fd_2}-2\sqrt{k^2-2Fd_1}}{F}. \quad (4)$$

The length and action of these orbits, respectively, are

$$L_1 = 2d_1, \quad L_2 = 2d_2, \quad L_3 = L_4 = 2(d_1+d_2), \quad (5)$$

$$S_1 = \frac{1}{12}F^2T_1^3 - \frac{1}{2}FkT_1^2 + k^2T_1,$$
$$S_2 = \frac{1}{12}F^2T_2^3 + \frac{1}{2}FkT_2^2 + k^2T_2,$$
$$S_3 = S_4 = S_1 + S_2. \quad (6)$$

Maslov indices of these orbits can be found by counting the returning points,[3] and we have $\mu_1 = \mu_2 = 1$, $\mu_3 = \mu_4 = 2$. For simplicity, we denote $T_3 = T_4 = T$, $L_3 = L_4 = L$, and $S_3 = S_4 = S$.

The period, length, action and Maslov index of all the other closed orbits consisting of these four fundamental orbits can be written as

$$T_{jn} = T_j + nT, \quad L_{jn} = L_j + nL,$$
$$S_{jn} = S_j + nS, \quad \mu_{jn} = \mu_j + 3n, \quad (7)$$

in which $j = 1, 2, 3, 4$ and $n = 0, 1, 2, 3, \cdots, +\infty$. The indices jn refer to the nth repetition of the jth closed orbits.

3. The photodetachment cross section

The photodetachment process of H^- in a static electric field between two parallel interfaces can be described as follows: when H^- absorbs photon energy $E_{\rm ph}$, outgoing electron waves are generated. These outgoing waves propagate a long distance. Due to the effects of the electric field and the interface, these waves cannot propagate to infinity, some of them turn back by the electric field or the interfaces and return to the origin. Finally, the returning waves overlap with the outgoing source waves to give the interference pattern in the photodetachment cross section. According to the closed orbit theory, the photodetachment cross section can be split into two parts:

$$\sigma(E) = \sigma_0(E) + \sigma^{\rm osc}(E), \quad (8)$$

where $\sigma_0(E)$ is the smooth background term without the external field;[6] the second part on the right-hand side of expression (8) is the oscillating term which corresponds to the contribution of the returning wave travelling along the closed orbit:

$$\sigma^{\rm osc}(E) = -\frac{4\pi}{c}(E+E_{\rm b}){\rm Im}\langle D\psi_i|\psi_{\rm ret}\rangle, \quad (9)$$

where $\psi_i = B{\rm e}^{-k_b r}/r$ is the initial wave function of the detached electron; D is the dipole operator,[6] and for the z-polarized light, $D = z$; $\psi_{\rm ret}$ is the returning part of the detached electron wave function. In fact, not all the outgoing waves return to the nucleus. Only the returning waves travelling along the closed orbits can overlap with the steadily-producing outgoing spherical wave, thus producing the oscillation in the cross section. The returning wave associated with the closed orbit jn is written as $\psi_{jn}^{\rm ret} = A_{jn}{\rm e}^{{\rm i}[S_{jn}-\mu_{jn}\pi/2]}$, where A_{jn} is the amplitude of the returning wave and given by[13]

$$A_{jn} = \left|\frac{1}{T_{jn}^2[k^2+(-1)^j FkT_{jn}]}\right|^{1/2}. \quad (10)$$

When the electron returns near to the nucleus, the electron motion is approximated by a free motion, i.e. the wave function is approximately an incoming plane wave. Therefore, the returning semiclassical wave should be proportional to the incoming plane wave: $\psi_{jn}^{\rm ret} = N_{jn}{\rm e}^{{\rm i}kr\cos\theta_j^{\rm ret}}$, where $\theta_j^{\rm ret}$ is the returning angle of the jth orbit and N_{jn} is the proportional constant, given by[13]

$$N_{jn} = (-1)^{\mu_j-1}\frac{4{\rm i}Bk^2}{(k_b^2+k^2)^2}A_{jn}{\rm e}^{{\rm i}[S_{jn}-\mu_{jn}\pi/2]}. \quad (11)$$

The whole returning waves are the sum of each returning wave and expressed as

$$\psi_{\rm ret} = \sum_{jn}\psi_{jn}^{\rm ret}. \quad (12)$$

The overlap integral of the returning waves with a source wave function $\langle D\psi_i|$ gives the oscillation in the photodetachment cross section. Buy substituting Eq.(12) into Eq.(9), we obtain

$$\sigma^{\rm osc}(E) = \sum_{jn}C_{jn}\sin(S_{jn}-\mu_{jn}\pi/2), \quad (13)$$

where

$$C_{jn} = (-1)^{\mu_j-1}\frac{16B^2\pi^2E}{c(E_b+E)^3}A_{jn}. \quad (14)$$

Therefore, the total photodetachment cross section is

$$\sigma(E) = \frac{16\sqrt{2}B^2\pi^2E^{3/2}}{3c(E_b+E)^3} + \sum_{jn}C_{jn}\sin(S_{jn}-\mu_{jn}\pi/2). \quad (15)$$

4. Results and discussion

Using Eq.(15), we calculate the photodetachment cross section of H^- in a static electric field between two parallel elastic interfaces for different values of the distance between the ion and the elastic interface and different electric field strengths (see Figs.2–4).

In our calculation, the energy of detached electron varies between 0 and 0.4 eV. In Fig.2, we keep the electric field F at 200 kV/cm and the second interface at $d_2 = 300$ arb. units, then we change the distance between the ion and the first interface. Under this condition, the maximum height the electron can reach along the $+z$ axis is $d_{\max} = E_{\max}/F = 379.06$ arb. units. The results show that when $d_1 > d_{\max}$, the electron cannot hit the upper interface. Therefore, the upper interface has no influence on the photodetachment cross section. The results should return to the case where only one interface exists. Take $d_1 = 1000$ arb. units as an example, the calculated cross section is shown in Fig.2(a). This result is the same as the one given by Yang *et al.*[13] With the decrease of d_1, the influence of the upper interface becomes significant. Fig.2(b) shows that the result, with $d_1 = 300$ arb. units, has only a little difference from that in Fig.2(a). But with $d_1 = 200$ arb. units, the cross section changes greatly when the photon energy $E_p = E + E_b$ is larger than 0.965 eV. With $d_1 = 120$ arb. units, the cross section oscillates in a much more complicated manner above the photon energy 0.881 eV. The reasons are as follows: the closer to the ion the upper interface moves, the more the returning waves bounced back by this interface, therefore, their contribution to the cross section becomes great. This figure also suggests that near the detachment threshold, the influence of the upper surface can be neglected. But with the increase of the energy, its influence becomes important. The sharp peak in this figure can be explained by using Eqs.(15) and (10). At some energy, the denominator in Eq.(10) approaches zero, which makes the amplitude of the closed orbit in Eq.(15) infinite, thus its contribution to the cross section is great. As to this problem, we will modify it by using the uniform semiclassical approximation method in the future work.[16]

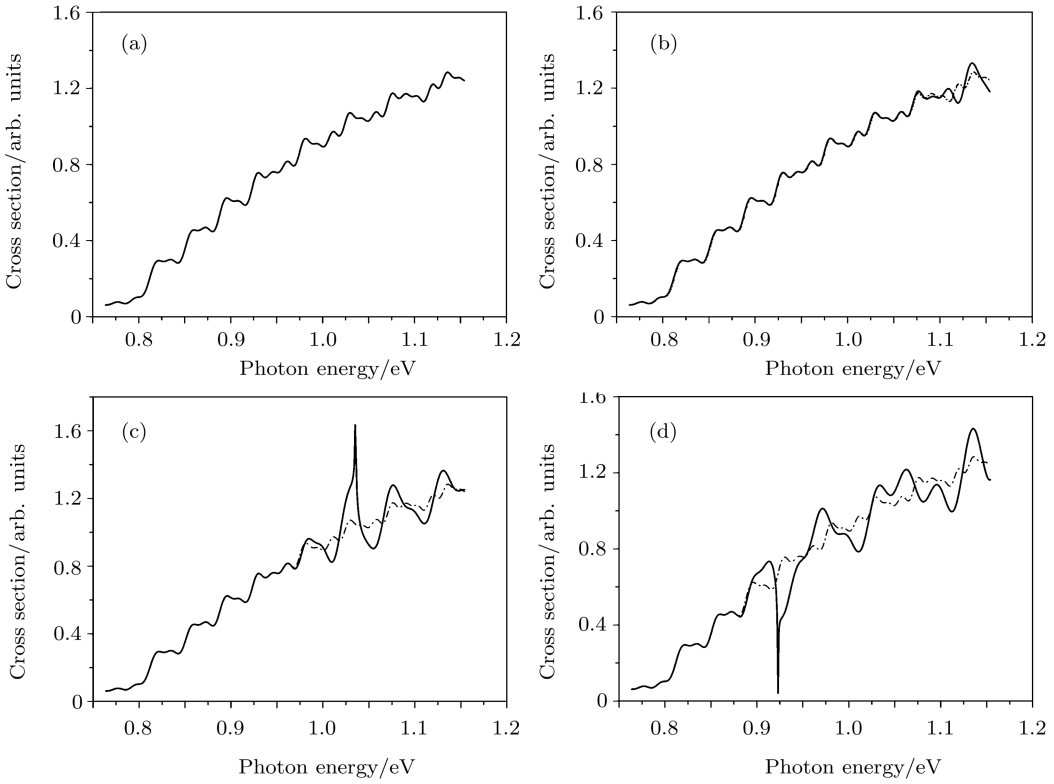


Fig.2. The photodetachment cross section of H^- in a static electric field between two parallel elastic interfaces. The electric field $F = 200$ kV/cm and the second interface is located at $d_2 = 300$ arb. units. The values of distance d_1 between the H^- and the first interface are: 1000 arb. units. (a), in which the photodetachment cross section of H^- amounts to that in a static electric field near one elastic interface;[13] 300 arb. units. (b); 200 arb. units. (c); and 120 arb. units. (d). The solid lines represent the cross section near two elastic interfaces and the dashed line refers to the result in the case where only one elastic interface 2 exists, which amounts to $d_1 \to \infty$, and $d_2 = 300$ arb. units.

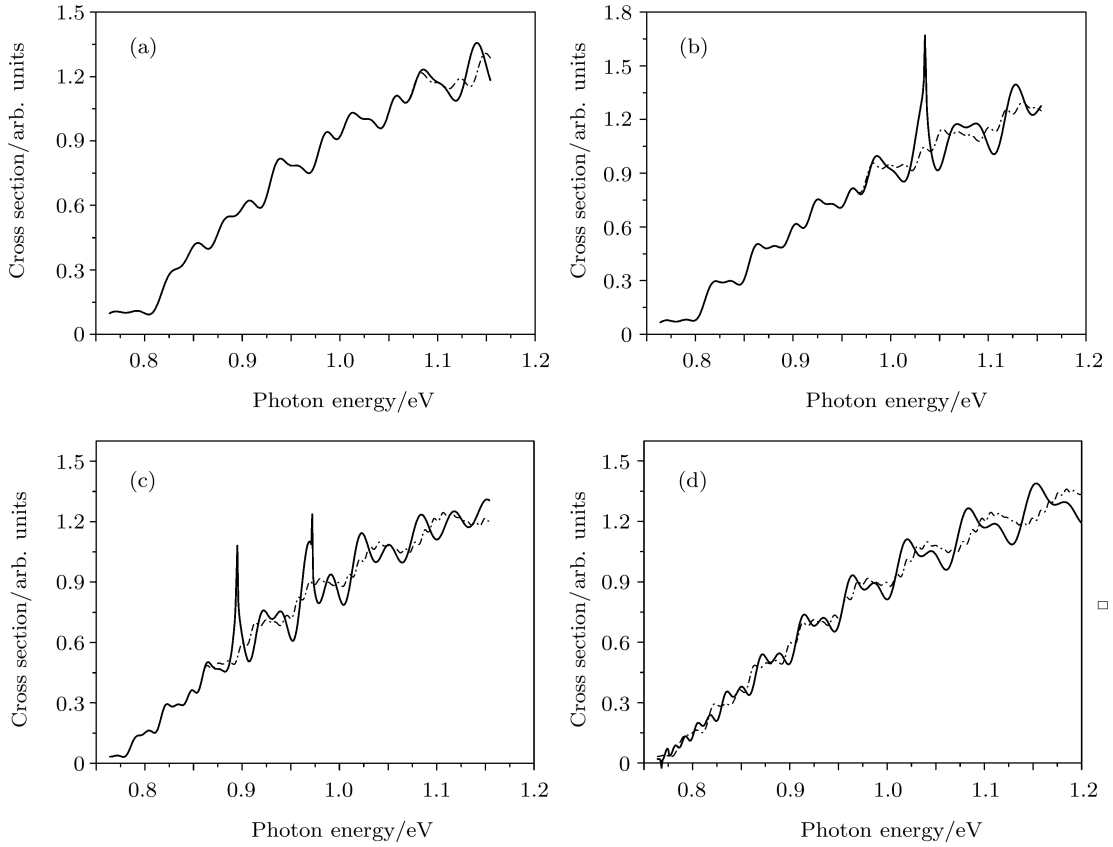


Fig.3. The dependence of the photodetachment cross section on the electric field. The two interfaces are fixed at $d_1 = d_2 = 200$ arb. units and the values of electric field (F) are: 300 (a), 200 (b), 100 (c), and 10 kV/cm (d). The solid lines represent the result with two elastic interfaces existing, and the dashed lines refer to the results with only one elastic interface 2 existing.

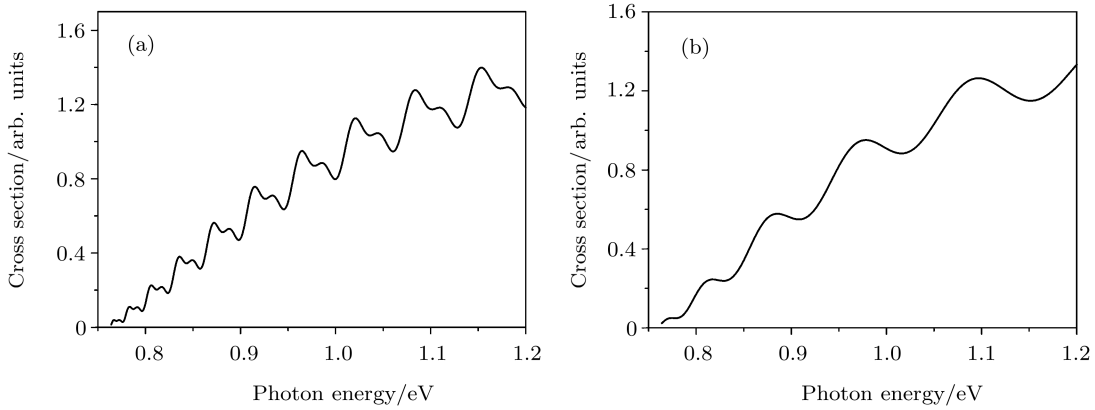


Fig.4. Photodetachment cross section of H^- in a static electric field between two parallel elastic interfaces as $F \to 0$. (a) The solid line represents the result with $F = 1$ V/cm, $d_1 = 200$ arb. units, and $d_2 = 300$ arb. units, and the dashed line refers to the result without electric field, which amounts to the photodetachment cross section of H^- between two parallel elastic interfaces.[15] (b) The photodetachment cross section with $F = 1$ V/cm, $d_1 \to \infty$, and $d_2 = 100$ arb. units. The solid line represents the result obtained from our closed orbit theory and the dashed line refers to the result obtained by using the imaging method.[14]

In Fig.3, we show how the electric field influences the photodetachment cross section for a fixed distance between the ion and the interface. We keep $d_1 = d_2 = 200$ arb. units, and the electric field decreases from 300 to 10 kV/cm. From Figs.3(a)–3(c), we find that with the decrease of the electric field, the oscillation of the cross section becomes much more complicated. This can be interpreted as follows: with

the decrease of the electric field, the maximum height the electron can travel along the $+z$ axis is high. The probability with which the electron hits the upper interface becomes large. Thus the influence of the upper interface is significant, which amounts to putting the upper interface closer to the ion. If we further reduce the electric field (F), for example, to a value of 10 kV/cm, i.e. $F = 10\,\mathrm{kV/cm}$, the cross section displays a multi-periodical oscillation structure. Under this condition, the cross section is different from that with only one interface even near the detachment threshold (see Fig.3(d)).

When F is very small, for example, $F = 1\,\mathrm{V/cm}$, in atomic units this value is much less than 1 and close to 0. Under this condition, the influence of the electric field can be neglected. The photodetachment cross section approximates that in the case of H^- near two parallel elastic interfaces.[15] Figure 4 shows the photodetachment cross section of H^- between two parallel elastic interfaces, separately, with and without electric field. The solid line in Fig.4(a) represents the photodetachment cross section with an electric field $F = 1\,\mathrm{V/cm}$, while the dashed line refers to the cross section without the electric field. They are nearly the same, which suggests that the influence of the electric field can be neglected. Furthermore, if we locate one interface at infinity ($d_1 \to \infty$), the cross section returns to that in the case of H^- near one interface without the electric field.[12] In Fig.4(b), we plot the cross section by using our formula and the one given by Afraq and Du, they are in correspondence with each other, which suggests that our analysis is correct.

5. Conclusion

In summary, we have studied the photodetachment of H^- in a static field near two parallel interfaces by using the closed orbit theory. We find that the elastic interfaces and the electric field have a significant influence on the photodetachment process. The calculated photodetachment cross section oscillates in a much more complicated manner than the case in which there exists only one elastic interface. This study provides a general framework for an understanding of the photodetachment process of H^- in the presence of electric field and two interfaces. At present, no experimental results on this system are available for comparison. In the future work, we will carry out the quantum calculation and compare the result obtained from our semiclassical closed orbit theory with the quantum result. We hope that our results will be useful for guiding the experimental study of the photodetachment of negative ions in the vicinity of interfaces.

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