Photodetachment of negative ion in a gradient electric field near a metal surface*

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Based on closed-orbit theory, the photodetachment of H^- in a gradient electric field near a metal surface is studied. It is demonstrated that the gradient electric field has a significant influence on the photodetachment of negative ions near a metal surface. With the increase of the gradient of the electric field, the oscillation in the photodetachment cross section becomes strengthened. Besides, in contrast to the photodetachment of H^- near a metal surface in a uniform electric field, the oscillating amplitude and the oscillating region in the cross section of a gradient electric field also become enlarged. Therefore, we can use the gradient electric field to control the photodetachment of negative ions near a metal surface. We hope that our results will be useful for understanding the photodetachment of negative ions in the vicinity of surfaces, cavities, and ion traps.

Keywords: photodetachment, metal surface, gradient electric field, closed orbit theory

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1. Introduction

Following a detailed experimental study of the photodetachment of H^- in the presence of a strong electric field,[1] many theoretical studies about the oscillating structures in the photodetachment cross section of H^- in various external fields have been carried out.[2−12] Among them, Du and Delos' closed orbit theory has attracted a lot of interest.[3] They pointed out that the oscillation in the cross section is caused by the interference between two pathways for the detached electrons, one is directly along the escape direction and the other is in the direction of reflection of an oppositely moving wave from the static field barrier. Recently, much attention has been paid to the photo-induced electronic excitations of adsorbates on metal surfaces.[13] Since H^- was proposed to use to probe the adsorbate state lifetime and the charge transfer during backscattering,[14] the photodetachment of H^- near a metal surface has aroused much interest. Firstly, Zhao and Du,[15] and Rui and Yang[16] studied the photodetachment of H^- in the presence of a metal surface. In their work, the photodetachment cross sections are changed a little only in a small energy region above the threshold. Therefore how to control the photodetachment of H^- near a metal surface is an interesting research subject. It is shown that the photodetachment cross section of H^- near a metal surface can be modified by an external electric field.[17−21] In these early studies, only the influence of a uniform electric field on the photodetachment of negative ions was studied. However, the effect of an inhomogeneous electric field, such as a gradient electric field on the photodetachment of negative ions, has been studied relatively little. In 1999, Yang *et al.*[22] studied the photodetachment of H^- in a gradient field for the first time. As to the influence of a gradient electric field on the photodetachment of H^- near a surface, no reports have been given to the best of our knowledge. However, there is a need to carry out this study. In many ion trap experiments the ions are set to be in an inhomogeneous field, however in many cases the inhomogeneous field can be simplified as a gradient field.[22,23]

In this paper, we study the influence of a gradient electric field on the photodetachment of H^- near a metal surface based on the closed orbit theory. Our studies suggest that in contrast to the photodetachment of H^- near a metal surface in a uniform electric field, the oscillating amplitude and the oscillating region in the cross section of a gradient electric field

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becomes enlarged. Therefore, we can use the gradient electric field to control the photodetachment of negative ions near a metal surface. We hope that our studies will guide the future experimental studies of the photodetachment of negative ions in the vicinity of surfaces and ion traps.

This paper is organized as follows. In Section 2, we discuss the classical motion of the detached electron in a gradient field near a metal surface. Then we describe the closed orbits of the detached electron and give the formula of the photodetachment cross section. In Section 3, we calculate the photodetachment cross sections of this system under different gradient electric fields. In particular, we discuss the difference in the photodetachment of H^- near a metal surface between in the gradient electric field and in a uniform electric field. Section 4 is devoted to some conclusions drawn from the present study in this paper. Atomic units are used throughout this work unless otherwise noted.

2. Theory and method

2.1. Hamiltonian and closed orbits

A schematic diagram is shown in Fig. 1. Take the direction of electric field as the z axis and use the cylindrical coordinates (ρ, z, ϕ). Suppose that the applied electric field is in the z direction: $F = \alpha z$. Here α is the electric field gradient in the z direction. In our work, we assume it to be positive. A hydrogen negative ion H^- sits at the origin and a z-polarized laser is used for the photodetachment. A metal surface perpendicular to the z axis is set to be at $z = -d$, where d is the ion–surface distance. As in the previous study,[11] H^- can be regarded as a one-electron system, with the active electron loosely bound by a short-range potential $V_{\rm b}(r)$ 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 $V_{\rm b}(r)$ can be omitted.

According to the electrostatic image method,[24] the Hamiltonian governing the motion of the detached electron in cylindrical coordinates can be described as

$$H = \frac{1}{2}(P_\rho^2 + P_z^2) - \frac{1}{4(d+z)} + \frac{1}{4d} + \frac{1}{2}\alpha z^2. \quad (1)$$

The first four terms on the right-hand side in the above equation describe the motion of the detached electron near a metal surface, while the last term represents the interaction between the electron and the gradient electric field.

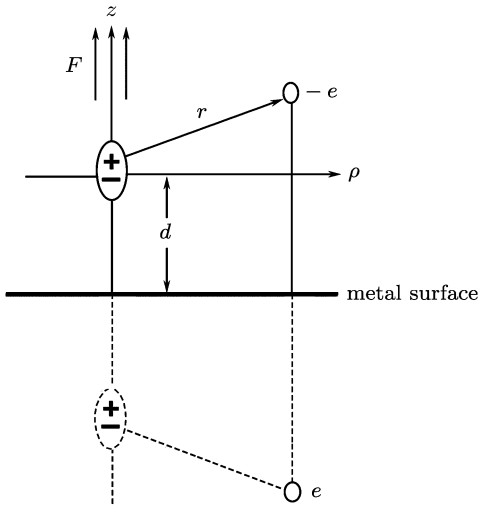


Fig. 1. Schematic representation of H^- in a gradient field near a metal surface, with the gradient electric field being along the $+z$ axis.

Closed orbit theory gives a prescription for calculating the oscillations in the photodetachment cross section from the closed orbits once we have all the closed orbits of the detached electron. Assuming that the detached electron is initially on the sphere of radius R centred at the nucleus and emanated with velocity k in the direction of the outgoing angle θ, by solving the Hamiltonian motion equation, we find that the motion in the ρ direction is free:

$$\rho(t) = R\sin\theta + kt\sin\theta. \quad (2)$$

The motion equation along the z direction cannot be given by a simple expression, but we can simulate the detached electron's trajectories using the numerical method. Some of the detached electron trajectories are shown in Fig. 2(a). From this figure we find that due to the free motion in ρ direction, the only closed orbit is along the $+z$ axis. This orbit leaves the origin and moves along the positive direction of z axis. Then it is slowed down, stopped and attracted back to the origin under the action of the electric field and the metal surface. This case is like the classical motion of the detached electron in a uniform electric field near a metal surface,[17] which is shown in Fig. 2(b) for comparison. The closed orbit is marked by the darker line in each plot.

The period T and the action S of the closed orbit can be calculated as follows. According to Eq. (1), the momentum of the outgoing detached electron along the closed orbit can be written as

$$P_z = \sqrt{2\left(E - \frac{1}{4d} - \frac{1}{2}\alpha z^2 + \frac{1}{4(d+z)}\right)}. \quad (3)$$

When the detached electron reaches the top ($z = z_{\rm top}$) of the closed orbit, its z-momentum $P_z = 0$. By setting P_z to be zero, we obtain the turning point of the closed orbit $z_{\rm top}$. The period of each closed orbit is given by

$$T = 2\int_0^{z_{\rm top}} \frac{1}{P_z}\,{\rm d}z. \tag{4}$$

The action of the closed orbit is given by

$$S = 2\int_0^{z_{\rm top}} P_z\,{\rm d}z. \tag{5}$$

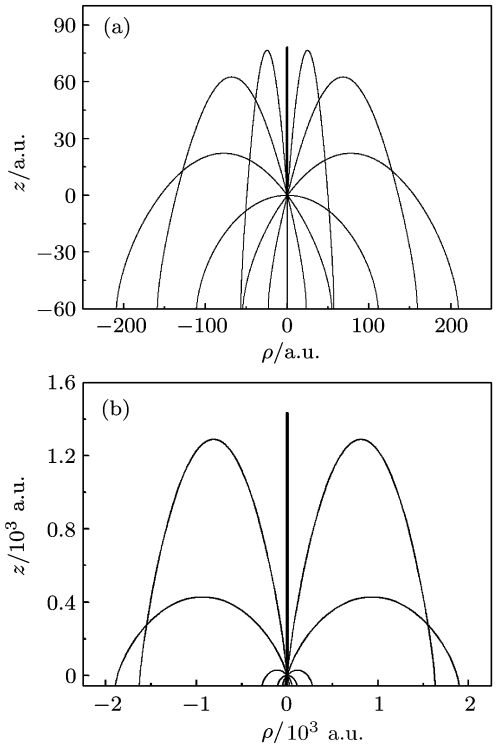


Fig. 2. (a) Some trajectories of the detached electron in a gradient electric field near a metal surface. The gradient of the electric field is $\alpha = 10^{-6}$ a.u. (atomic unit). (b) Some trajectories of the detached electron in a uniform electric field near a metal surface. The electric field strength is $F = 10^{-6}$ a.u. The closed orbit is marked by the vertical thicker line in each plot. The distance between the ion and the metal surface is $d = 60$ a.u. and the electron energy is $E = 0.15$ eV.

2.2. Formulae for photodetachment cross section

According to the closed orbit theory, the photodetachment cross section of H^- in an electric field near a metal surface can be divided into two parts:

$$\sigma(E, F, d) = \sigma_0(E) + \sigma^{\rm osc}(E, F, d). \tag{6}$$

The first part is the photodetachment cross section of H^- without any external field or metal surface:[11]

$$\sigma_0(E) = 16\sqrt{2}B^2\pi^2E^{3/2}/3c(E_{\rm b} + E)^3,$$

where E is the energy of the detached electron, $E_{\rm b}$ is the binding energy of H^- and it is approximately equal to 0.754 eV. $B = 0.31552$ is a normalization function constant, and c is the speed of light. The second part is the oscillating term, which corresponds to the contribution of the returning wave traveling along the closed orbit.[11] Since the classical motion of the detached electron is similar to the case in a uniform electric field, therefore the derivation of the oscillating part in the cross section is also the same as the photodetachment cross section of H in a uniform electric field near a metal surface.[17] For simplicity, we only give the final expression as

$$\sigma^{\rm osc}(E, F, d) = \frac{8\pi^2B^2\sqrt{2E}}{c(E_{\rm b} + E)^3T}\cos(S), \tag{7}$$

in which T and S are the period and the action of the closed orbit, which are given by Eqs. (4) and (5).

3. Results and discussion

Using Eq. (7), we calculated the photodetachment cross sections of H^- near a metal surface in different gradient electric fields. The results are given in Fig. 3. In our calculation, we keep the ion–surface distance $d = 100$ a.u. Figure 3(a) shows the result in the case with the electric field gradient being very small, $\alpha = 10^{-9}$ a.u. Under this condition, the influence of the electric field is very small, and the present system recovers to the photodetachment cross section of H^- near a metal surface without the electric field.[15] The oscillation is limited only in a small region above the threshold and the oscillating amplitude is relatively small. With the increase of the gradient of the electric field, the influence of the electric field becomes significant. The oscillation in the photodetachment cross section becomes strengthened and the oscillating amplitude of the cross section increases apparently, as we can see from Figs. 3(b)–3(d). The reason can be analyzed as follows. With the increase of the gradient of the electric field strength, the electric field force acting on the detached electron becomes strong. When the

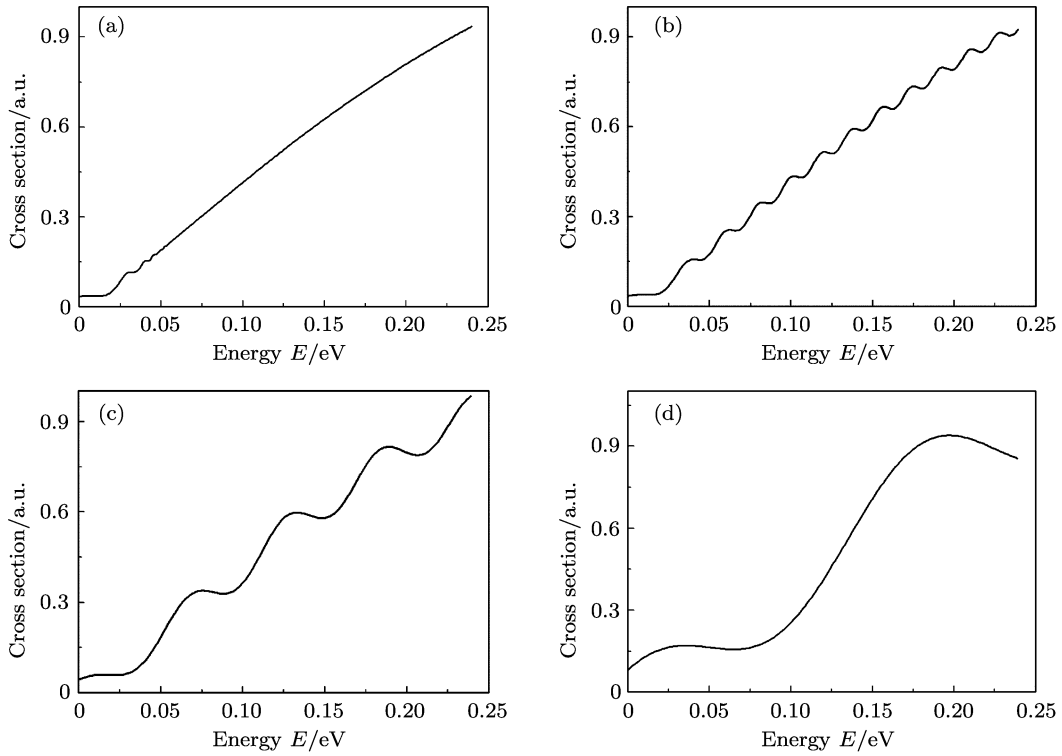


Fig. 3. Photodetachment cross sections of H^- in different gradient electric fields near a metal surface. The distance between the ion and metal surface is $d = 100$ a.u. The gradients of the electric field are (a) $\alpha = 10^{-9}$ a.u., (b) $\alpha = 10^{-7}$ a.u., (c) $\alpha = 10^{-6}$ a.u., (d) $\alpha = 10^{-5}$ a.u.

detached electron leaves the origin and moves along the $+z$ axis, it will be attracted back to the origin by the electric field and the metal surface in a short period of time. Thus the bigger the electric field gradient, the shorter the period of the closed orbit becomes. From Eq. (7), we can see that as the period T of the closed orbit is short, its contribution to the photodetachment cross section becomes significant.

Next, we compare the photodetachment cross section of H^- near a metal surface in a gradient electric field with that in a uniform electric field.[17] The result is given is Fig. 4. In our calculation, we keep the ion-surface distance $d = 60$ a.u. The electric field gradient $\alpha = 10^{-6}$ a.u. and the strength of the uniform electric field F is also equal to $F = 10^{-6}$ a.u. From this figure, we find that the oscillating amplitude in the cross section of a gradient electric field is much larger than that in a uniform electric field and the oscillating region in the cross section becomes enlarged. The reason can be interpreted as follows. When the gradient electric field is applied, the motion of the detached electron is limited to a small region near the hydrogen atom (see Fig. 2(a)), and the period of the closed orbit is short. However, in a uniform electric field, the range that the detached electron can reach is very far (see Fig. 2(b)), and the period of the closed orbit is large.

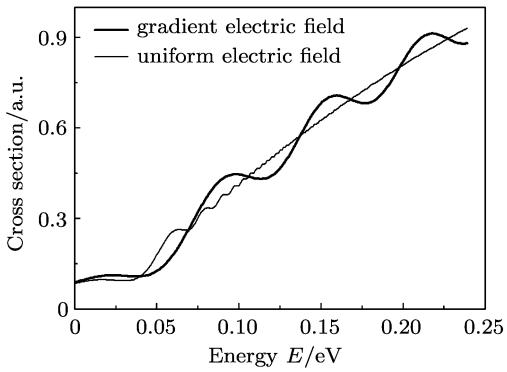


Fig. 4. Comparison of the photodetachment cross section of H^- near a metal surface between in a gradient electric field and in a uniform electric field. The distance between the ion and the metal surface is $d = 60$ a.u. The gradient and the strength of the electric field are both equal to 10^{-6} a.u.

In Fig. 5, we plot the periods of the electron closed orbit for comparison. Figure 5(a) shows the period of the electron closed orbit in a gradient electric field. From this figure we find that the period of the closed orbit increases monotonically with the increase of the detached electron energy. Figure 5(b) indicates the period of the electron closed orbit in a uniform elec-

tric field. We find that as the electron energy varies between 0 and 0.01 eV, the change of the period is very small. But as the energy is above 0.01 eV, the period increases very quickly and its value becomes very large. According to the closed orbit theory, the larger the period of the closed orbit, the smaller its contribution to the photodetachment cross section becomes.

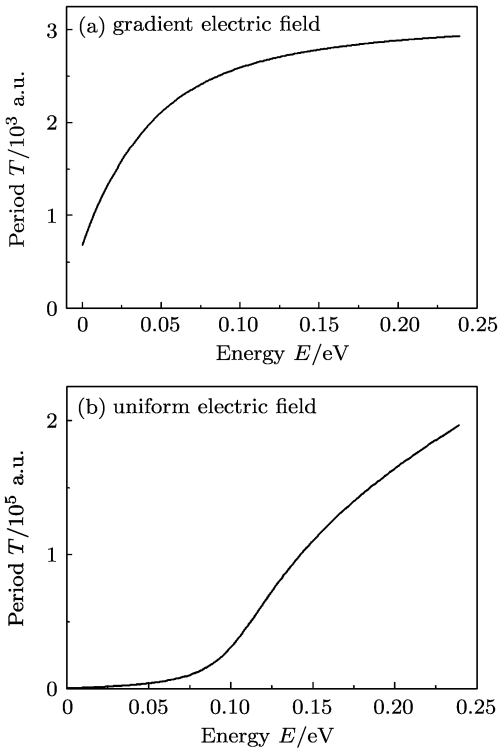


Fig. 5. (a) The period of the detached electron closed orbit in a gradient electric field near a metal surface, with the gradient of the electric field being $\alpha = 10^{-6}$ a.u. and (b) the period of the detached electron closed orbit in a uniform electric field near a metal surface, with the electric field strength being $F = 10^{-6}$ a.u. The distance between the ion and metal surface is $d = 60$ a.u.

4. Conclusions

By using the closed-orbit theory, we investigated the influence of a gradient electric field on the photodetachment of H^- near a metal surface. The results suggest that as the electric field gradient is very small, the influence of the electric field is very small and the photodetachment cross section is nearly the same as the photodetachment of H^- near a metal surface. With the increase of the electric field gradient, the oscillation in the photodetachment cross section becomes strengthened. In addition, the oscillating amplitude and the oscillating region in the cross section of a gradient electric field are larger, in contrast to the photodetachment of H^- near a metal surface in a uniform electric field. Therefore, we can change the electric field gradient to control the photodetachment of H^- near a metal surface. At present, no experiments on this system are available for comparison. We hope that our results will be useful for guiding the future experimental research of the photodetachment processes of ions in the vicinity of surfaces, cavities, and ion traps.[25,26]

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