

Photodetachment of H^- near two perpendicular metal surfaces

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ABSTRACT

It is a well-known fact that the surfaces can affect the photodetachment of negative ion. In this paper, we focus on how the photodetachment cross-section of H^- is altered when it is placed near two perpendicular metal surfaces. We begin by briefly presenting the electrostatic image potential of the detached electron caused by the metal surfaces, then we study the classical motion of the photo-detached electron near two perpendicular metal surfaces. The photodetachment cross-section of this system has been derived and calculated based on the closed orbit theory. The results show that the cross-section depends on the photon energy and the ion-surface distances sensitively. Compared to the case of the photodetachment of H^- near one metal surface, the oscillatory structure in the cross-section of our system becomes much more complicated. This study provides a new understanding on the photodetachment process of negative ion or atoms in the vicinity of surfaces or cavities.

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1. Introduction

Over the last decade, many researchers have studied the problem of Rydberg atom near a metal surface. As we all know, when a Rydberg atom is closed to a metal surface, the excited electron will interact with the metal surface. Since the interaction of the excited electron with the metal surface take place relatively far from the surface, we can use the electrostatic image method to simulate the atom-surface interaction [1]. Therefore, as a typical theoretical and experimental model system, the photoabsorption of the Rydberg atom near a metal surface can simulate many dynamical effects of atom in strong fields, such as Zeeman-stark effect, diamagnetic effect, instantaneous van der waals interaction, chaotic transport and escape, etc [2–10]. Recently, with the development of the surface physics and photodetachment microscope, the photodetachment of negative ion near surfaces have attracted a lot of interest. Firstly, Yang and Du et al. applied closed orbit theory to study the photodetachment of H^- near an elastic interface [11–14]. In these early studies, the interaction potential between the detached electron and the surface has been neglected and the collision of the electron with the surface is elastic. In fact, the elastic surface is only a simple model, which is different from a real metal surface. For the photodetachment of negative ion near a metal surface, the detached electron is subjected to the potential caused by the presence of image charge in the metal surface; its theoretical analysis is relatively complicate. Considering the interaction of the detached electron and its image, Yang, Zhao and Du

et al. studied the photodetachment of H^- near one metal surface [15–18]. In their studies, they take the laser polarization direction along the z -axis and the metal surface is perpendicular to the z -axis. Therefore, the system has a cylindrical symmetry about z -axis and the angular motion perpendicular to the z -axis can be separated, which reduces the problem to a two-dimensional one and this system is similar to the photodetachment of H^- in a uniform electric field. A meaningful question to ask is how the photodetachment cross-section of H^- is affected by the presence of two metal surfaces? In our last work, we study the photodetachment of H^- near two parallel metal surfaces [19]. Then what will happen if we change the geometric configuration of the two metal surfaces? None has given the report. In this paper, we study the photodetachment of H^- near two perpendicular metal surfaces. In our system, due to the electrostatic image potential caused by the two perpendicular metal surfaces, the cylindrical symmetry is broken, and the Hamiltonian is non-separable in three degrees of freedom, therefore the theoretical treatment of our system is more difficult. Our calculation results suggest that the oscillatory structure in the cross-section of our system becomes much more complicated compared to the case of the photodetachment of H^- near one metal surface. Although no experiments on photodetachment of negative ion near one or two metal surfaces have been carried out presently, our predications show that there are some interesting phenomena here, and we hope that our calculations may guide future experimental measurements.

This paper is organized as follows: In Section 2, we describe the electrostatic image potential and the classical motion of the photo-detached electron near two perpendicular metal surfaces, especially

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discuss the closed orbit of this system. In Section 3, we derive the formula for calculating the photodetachment cross-section. Some numerical results and discussion are presented in Section 4. Finally, Section 5 gives some conclusions of this paper. Atomic units are used throughout this work unless indicated otherwise.

2. Dynamics of the photo-detached electron near two perpendicular metal surfaces

The schematic plot of the system is given in Fig. 1. The H^- ion sits at the origin. As in the previous studies, H^- is regarded initially as a one-electron system loosely bound by a short-ranged, spherically symmetric potential $V_b(r)$ of the hydrogen atom, where r is the distance between the active electron and the nucleus. A z -polarized laser is used for the photodetachment. Two perpendicular metal surfaces are placed in the y - z plane, one is perpendicular to the z -axis and the other is parallel to it. The distances between the ion and the two metal surfaces are denoted as d_1 and d_2 . When a laser is applied to the negative ion, it may absorb a photon, then the active electron is detached and it moves away from the hydrogen atom. According to the electrostatic image method [1], each charge has an image inside the metal but the charge of the image has the opposite sign. The potential acting on the detached electron in the ion-surface system can be described as: $V = V_b + V_c + V_i$. In which V_c is the interaction potential of the electron with the image nucleus, which is also a short-ranged potential. V_i is the interaction potential between the detached electron and its images. In our system, there are two perpendicular metal surfaces and there are three images of the hydrogen atom and the detached electron (see Fig. 1). The detached electron and their images lie on the four vertices of a rectangle.

The image potential V_i between the detached electron and its images can be described as follows:

$$V_i(y,z) = -\frac{1}{4(d_1+y)} - \frac{1}{4(d_2+z)} + \frac{1}{4\sqrt{(d_1+y)^2 + (d_2+z)^2}} \quad (1)$$

In order to show the influence of the electrostatic image potential on the photodetachment of H^- , we plot the three-dimensional potential $V_i(y,z)$ for the ion-surface distance $d_1 = d_2 = 100$ a.u., see Fig. 2. From this figure, we find the image potential between the detached electron and their images can be considered as an attractive potential.

The Hamiltonian of the detached electron near two perpendicular metal surfaces has the following form:

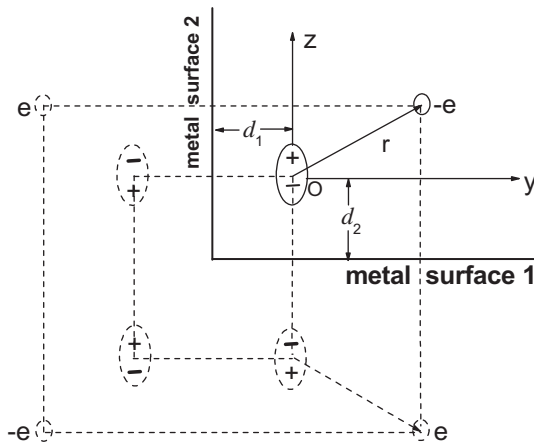


Fig. 1. The schematic plot of a hydrogen atom and a detached-electron and their images near two perpendicular metal surfaces.

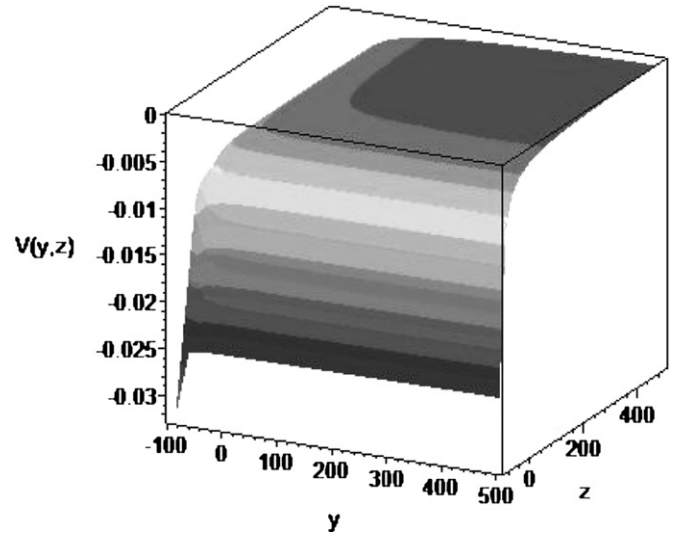


Fig. 2. The three-dimensional plot of the electrostatic image potential of the detached electron and their images, the ion-surface distances $d_1 = d_2 = 100$ a.u.

$$H = \frac{1}{2}(p_x^2 + p_y^2 + p_z^2) - \frac{1}{4(d_1+y)} - \frac{1}{4(d_2+z)} + \frac{1}{4\sqrt{(d_1+y)^2 + (d_2+z)^2}} + \frac{1}{4d_1} + \frac{1}{4d_2} - \frac{1}{4\sqrt{d_1^2 + d_2^2}} + V_b + V_c \quad (2)$$

Here, $(1/4d_1 + 1/4d_2) - 1/4\sqrt{d_1^2 + d_2^2}$ are additional terms to ensure $V(y=z=0)=0$, which has no influence on the photodetachment process. The effect of the short-range potential of the nucleus and the image nucleus V_b and V_c can be ignored after the electron is detached [15]. By solving the Hamiltonian motion equations, we find the motion in the x -direction is free:

$$x(t) = R \sin \theta \cos \phi + k \sin \theta \cos \phi t \quad (3)$$

Here R is the initial spherical radius, (θ, ϕ) is the outgoing angle of the detached electron and $k = \sqrt{2E}$ is the momentum.

The photodetachment process of H^- near surfaces can be described using the closed orbit theory [20]: when H^- absorbs photon energies E_{ph} , outgoing electron waves are generated. These outgoing waves propagate to large distances. Sufficiently far from the origin, the waves propagate according to semiclassical mechanics and they are correlated with classical trajectories. Due to the attractive image potential of the metal surfaces, these waves cannot propagate to infinity and some of the waves are turned back by the surface and return to the origin. Finally, the returning waves overlap with the outgoing source waves to produce the oscillatory structure in the photodetachment cross-section. In all of these classical trajectories of the photo-detached electron emitting from the origin, only those bounced back by image potential to the starting point are called closed orbits. Due to the free motion in x direction, the closed orbits only lie in the y - z plane.

For the system described by the Hamiltonian in Eq. (2), we find that the potential approaches a critical value $E_c = (1/4d_1 + 1/4d_2) - 1/4\sqrt{d_1^2 + d_2^2}$. When the detached-electron energy E is larger than E_c , the electron can travel into infinity and there is no closed orbit. As the detached-electron energy E is above threshold but smaller than E_c , closed orbits can exist. Because of the coupling term $1/\sqrt{4(d_1+y)^2 + (d_2+z)^2}$ in the Hamiltonian, the detached electron's motion along y, z direction cannot be separated. For the sake of

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