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Photodetachment in a cavity: From rectangles to parallel plates

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ABSTRACT

Simple analytic formulas are presented for photodetachment cross sections of H^- inside a rectangular cavity using semiclassical closed-orbit theory. The formulas predict oscillations in the spectrum and correlate the oscillations with closed orbits of the system. Explicit fully-quantum-mechanical formulas are also derived. We compare the results from closed orbit theory and quantum-mechanical calculations. We also show how the photodetachment cross section formulas for a rectangular cavity can be reduced to those for a cavity consisting of two plates.

1. Introduction

It is well known that external fields can considerably affect the photodetachment process of negative ions. Many theoretical studies [1–10] and experimental observations [11–14] have revealed the effect in the photodetachment spectra. There are three dominant phenomena in these studies and observations: oscillatory structures above the zero-field threshold, a finite cross-section value at the threshold, and a quantum tunneling effect below threshold.

Yang et al. [15,16] applied closed-orbit theory (COT) [17] to study the photodetachment of H^- near a reflecting surface, which was closely related to photodetachment in external electric and magnetic fields. Subsequently Afaq et al. [18] developed a theoretical imaging method and applied it to study the same system. Then there has been considerable interest in the photodetachment of H^- in different surface environment in recent years, such as in a parallel plate cavity [19,20], in a wedge [21], and in a circular microcavity [22]. The dominant phenomenon which is found in the photodetchment spectra of negative ion in the above cavities is the oscillatory structures above the zero-field threshold.

In this paper we consider the photodetachment in a rectangular cavity with an arbitrary aspect ratio. We apply both closed-orbit theory and quantum approach to calculate the photodetachment cross sections. This system is interesting in that it provides an example that the cross section formulas can be explicitly derived by both the closed-orbit theory and the quantum approach. Furthermore, the rectangular cavity we consider here has an arbitrary aspect ratio. By changing the value of aspect ratio, we can transform the photodetachment cross section formulas in a rectangular cavity into the cross section formulas in a cavity consisting of two parallel plates. Closed-orbit theory provides a clear physical picture and a quantitative tool for analysing the oscillations in the photodetachment. The complete quantum solution can provide all possible knowledge of a system and a different physical picture. Those two approaches are complementary. Here, ions can be placed at any location inside the rectangular cavity, which makes it possible to show the dependence of photodetachment cross sections on the ion position.

The paper is organized as follows. In Section 2, we present the COT formulas of the photodetachment cross sections in a rectangular cavity. In Section 3, we present the quantum derivations of the photodetachment cross sections in a rectangular cavity. In Section 4, we compare the two results and show their connections by extracting closed orbits from the quantum formulas by using the Fourier transform. In Section 5, we demonstrate that the cross section formulas in a rectangular cavity are deduced to those in a cavity consisting two plates.

2. Closed-orbit theory formulas for photodetachment cross sections

We consider the photodetachment of H^- in a tube like cavity with a rectangular intersection. The tube is assumed to be perpendicular to the page. The inner dimension of the rectangular intersection is $a_0 \times b_0$ as shown schematically in Fig. 1. We use a coordinate system such that the negative ion is at the origin. The distance between the negative ion and the left surface is a, and the distance between the negative ion and the lower surface is b. It is convenient to choose the coordinate system

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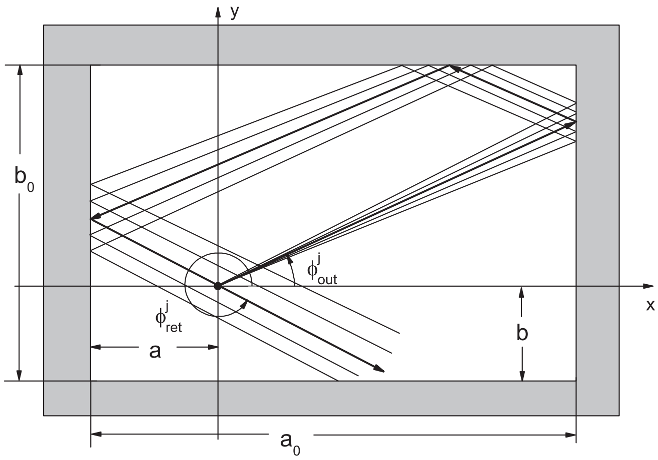

Fig. 1. Schematic illustration of H^- photodetachment inside a tube like cavity with a rectangular intersection. We show a group of trajectories propagating away from the H atom and finally returning to the region of the atom after being reflected three times by the cavity. The center of the group of trajectories is a closed-orbit j (heavy solid line). ϕ^j_{out} and ϕ^j_{ret} denote respectively the azimuthal angles of the outgoing and returning momenta. The quantum interference of the returning detached-electron wave associated with the closed-orbit j leads to an oscillation in the cross section.

such that the z-axis is perpendicular to the intersection. The x-axis is horizontal and parallel to the lower surface in Fig. 1, and the y-axis is vertical and parallel to the left surface.

According to the physical picture of closed-orbit theory (COT) [17], when the active electron is detached by a laser, the active electron and the associated wave propagates out from the negative ion in all directions. The electron trajectories and wave fronts follow straight lines inside the cavity until they are reflected by the surfaces of the cavity. The electron may return to the region of the negative ion after several reflections. Then, the returning electron wave will interfere with the initial outgoing electron and induce oscillations in the total photodetachment cross sections. Closed-orbit theory relates the cross sections to all the closed-orbits of detached-electron and provides a recipe to calculate the cross sections based on the closed-orbits and their associated properties.

The COT formula for photodetachment cross section of H^- in a cavity can be written in the following form [21]

$$\sigma(E)_{COT} = \sigma_0(E) + \sigma_0(E)\frac{3}{\sqrt{2E}} \times \sum_j \frac{f(\theta^j_{out}, \phi^j_{out}; \theta_L, \phi_L) f(\theta^j_{ret}, \phi^j_{ret}; \theta_L, \phi_L)}{L_j} \times \sin\left(\sqrt{2E}L_j - \mu_j \Delta\right), \tag{1}$$

where $\sigma_0(E) = 16\sqrt{2}B^2\pi^2E^{3/2}/3c(E_b+E)^3$ represents the photodetachment cross section of H^- in free space, $B = 0.31522$ is related to the normalization of the initial bound state Ψ_i of H^-, c is the speed of light and its value is approximately 137 a.u., E denotes the energy of the escaping electron, $E_b = 0.754$ eV denotes binding energy of the electron to the negative ion and the photon energy is $E_p = E + E_b$. The summation is over all closed-orbits going out from and returning to the position of the negative ion. (θ_L, ϕ_L) denotes the laser polarization direction. $(\theta^j_{out}, \phi^j_{out})$ and $(\theta^j_{ret}, \phi^j_{ret})$ denote the spherical angles of the outgoing momentum vector $\hbar\mathbf{k}^j_{out}$ and returning momentum vector $\hbar\mathbf{k}^j_{ret}$ of the closed orbit j respectively. $f(\theta, \phi; \theta_L, \phi_L)$ is defined as the form $(\cos\theta\cos\theta_L + \sin\theta\sin\theta_L\ \cos(\phi - \phi_L))$. L_j and μ_j are, respectively, the length and the number of reflections of the closed-orbit j. Δ denotes the phase loss of the wave function accompanying each reflection. In our COT and quantum calculations throughout this paper, we set Δ to π, corresponding to the "hard" wall case [18].

To use the COT formula in Eq. (1), it is necessary to obtain all the closed orbits and their associated properties such as outgoing angle, length, *etc*. Because the trajectories are reflected by the inner surfaces of the cavity, it is clear that all the closed-orbits which go out from the position of the negative ion and later return to the position of negative ion must be in the $x-y$ plane. To find closed-orbits in a cavity, we can launch a large number of trajectories going out from the origin in the $x-y$ plane and keep track of the trajectories as they propagate and get reflected inside the cavity. If a group of nearby trajectories come back to the region of the negative ion, the search can be refined to find the closed-orbit. This procedure has been previously used to find the closed-orbits for an atom in a magnetic field [17]. In Fig. 1 we show a group of trajectories near a closed-orbit (heavy solid line) returning to the region of the negative ion.

For a rectangular cavity, we can apply the image method as demonstrated in Ref. [21] to find all the closed-orbits and get their associated properties. When an object is placed in a rectangular mirror cavity, there are infinite images outside the cavity. These images can be labeled by the two integers (n, m), both n and m counts from negative infinity to positive infinity, but the case that n and m both are zero at the same time should be excluded. Image (n, m) is located at (x_n, y_n), where

$$x_n = (-1)^n\left(a - \frac{a_0}{2}\right) + na_0 + \frac{a_0}{2} - a,$$
$$y_m = (-1)^m\left(b - \frac{b_0}{2}\right) + mb_0 + \frac{b_0}{2} - b. \tag{2}$$

Each image corresponds to a closed orbit, and each closed orbit corresponds to an image. So the index j that specified the closed orbits earlier is replaced by the pair (n, m). The first segment of the closed-orbit before being reflected by the cavity surfaces is given by the straight line connecting the corresponding image and the source.

In what follows, we will use these interpretations to derive the required properties of the closed orbits (n, m). It is conspicuous that the geometrical length of the closed-orbit is equal to the distance between the atom and the image:

$$L_{n,m} = \sqrt{x_n^2 + y_m^2}. \tag{3}$$

The reflection numbers are

$$\mu_{n,m} = |n| + |m|. \tag{4}$$

All the closed-orbits have polar angles $\theta_{out} = \theta_{ret} = \pi/2$. Their outgoing azimuthal angles are given by

$$\phi^{n,m}_{out} = \begin{cases} \arccos\dfrac{x_n}{L_{n,m}}, & (m \geq 0); \\ 2\pi - \arccos\dfrac{x_n}{L_{n,m}}, & (m < 0). \end{cases} \tag{5}$$

The corresponding azimuthal angles of the returning momentum are given by

$$\phi^{n,m}_{ret} = [(-1)^n - 1]\frac{\pi}{2} + (-1)^{(n+m)}\phi^{n,m}_{out}. \tag{6}$$

Using the above properties of the closed orbits, the total cross section for an arbitrary linear laser polarization direction can be written down straightforwardly following Eq. (1). The formulas for an arbitrary laser polarization direction is very efficient for numerical calculations, but it is too long to write down here. If linear laser polarization direction is taken along axes, the formula becomes sufficiently simple. The COT cross section for laser polarization direction along x-axis can be written as

$$\sigma^x_{cot}(E) = \sigma_0(E) + \sigma_0(E)\frac{3}{\sqrt{2E}}\sum_{n,m}\frac{(-1)^m}{L^3_{n,m}}x_n^2\sin\left(\sqrt{2E}L_{n,m}\right), \tag{7}$$

and the COT cross section for y linear polarization can be written as

$$\sigma^y_{cot}(E) = \sigma_0(E) + \sigma_0(E)\frac{3}{\sqrt{2E}}\sum_{n,m}\frac{(-1)^n}{L^3_{n,m}}y_m^2\sin\left(\sqrt{2E}L_{n,m}\right). \tag{8}$$