

Resonance States of Hydrogen Atoms Near Metal Surfaces

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Abstract

Resonant charge transfer between a metal surface and a single ion is investigated. A combination of the complex-absorbing potential (CAP) method and the basis splines method is used to calculate energy shifts and lifetimes of a one-dimensional (1D) hydrogen atom located in the vicinity of an Al metal surface. This method can be easily extended to the three-dimensional case.

Keywords:

resonant charge transfer, ion-surface interaction, numerical calculation

1. Introduction

Resonant charge transfer process between metal surfaces and ions plays an important role in a number of surface-diagnostic methods such as Auger electron spectroscopy, ion neutralization spectroscopy and secondary-ion-mass spectroscopy. Several computational schemes have been developed for calculating resonance-energy positions and widths associated with charge exchanges between metal surfaces and one-electron ions. The coupled-angular mode (CAM) method was employed by Borisov *et al.* [1] to calculate such resonance parameters, while Deutscher *et al.* [2] used the complex rotation method. A two-center basis set expansion scheme was also developed by Kürpick and Thumm [3].

In this work, we use a combination of the complex-absorbing potential (CAP) method and the basis splines method. A simple system of a one-dimensional hydrogen atom located near an Al metal surface is used to test the efficiency of our numerical scheme. However, our approach can be easily extended to the realistic, three-dimensional case. This paper is organized as follows. In Sec. 2, we explain briefly our method. Results of our calculations are shown in Sec. 3. A summary is given in Sec. 4.

2. Method

The complex absorbing potential (CAP) was introduced by Jolicard and Austin [4], and has been applied previously to studies of photodissociation processes [5]. This method deals with a CAP Hamiltonian containing a coordinate-dependent complex potential which consists of a real physical potential $V(\vec{q})$ and an imaginary

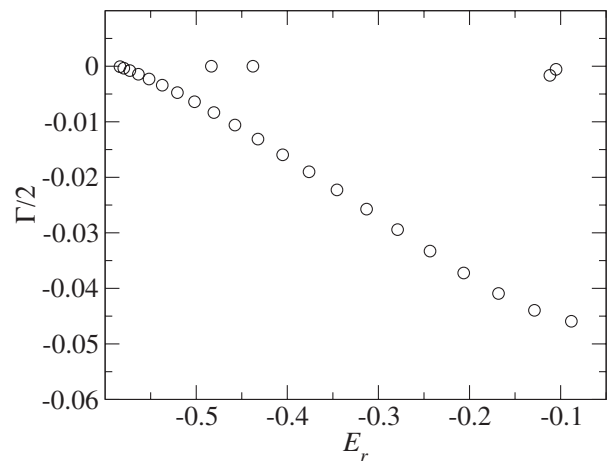


Fig. 1 Diagram for positions E_r and half-widths $\frac{\Gamma}{2}$ of energies in the complex energy plane for resonance states with a CAP Hamiltonian.

one $iW(\vec{q})$, where $W(\vec{q})$ is a slowly increasing potential different from zero only in the asymptotic region. With a CAP Hamiltonian, resonance states appear, where resonance energies $E = E_r - i\Gamma/2$ are obtained as discrete complex eigenvalues of the Hamiltonian (see Fig. 1).

The CAP Hamiltonian of a one-dimensional hydrogen atom located at the origin of the x coordinate in the vicinity of a metal surface is written in atomic units as

$$\hat{H} = -\frac{1}{2} \frac{d^2}{dx^2} + V(x) - iW(x). \quad (1)$$

In the present work, we adopt a following quadratic potential for $W(x)$,

$$W(x) = \begin{cases} 0, & x \leq x_0 \\ \gamma(x - x_0)^2, & x > x_0 \end{cases}, \quad (2)$$

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where γ is a strength parameter and the semi-infinite domain $[x_0, \infty)$ represents the asymptotic region of the x coordinate.

As a finite basis for representing state vectors and operators we choose a set of fifth-order basis splines [6]. In such a basis, the Hamiltonian in Eq. (1) is represented as a complex symmetric matrix. This Hamiltonian matrix is diagonalized to determine a set of complex eigenvalues.

3. Calculations

The method described above is applied here to a one-dimensional hydrogen atom (located at the origin) near an Al metal surface. The potential is given as a sum of three interaction potentials for an atomic electron:

$$V = V_{e-i} + V_{e-s} + \Delta V_{e-s}, \quad (3)$$

where V_{e-i} is a pure Coulomb potential due to the nucleus of the atom, given in atomic units by

$$V_{e-i} = -\frac{1}{|x|}. \quad (4)$$

V_{e-s} is an electron-surface potential and ΔV_{e-s} is a correction for V_{e-s} , due to the presence of the atomic nucleus. To describe the electron-surface interaction we use the local potential by Jennings, Jones and Weinert [7]. It contains three parameters that we took from [7] corresponding to the Al surface: The first parameter is the bottom of the metal conduction band $V_0 = 0.585$ a.u. and the second one the size of the surface region $\lambda = 1.0$. The third parameter, giving the position of the reference image plane, is incorporated in the definition of the ion-surface distance. This distance D is measured from the image reference plane. The third term ΔV_{e-s} in Eq. (3) is taken so as to describe an interaction of the

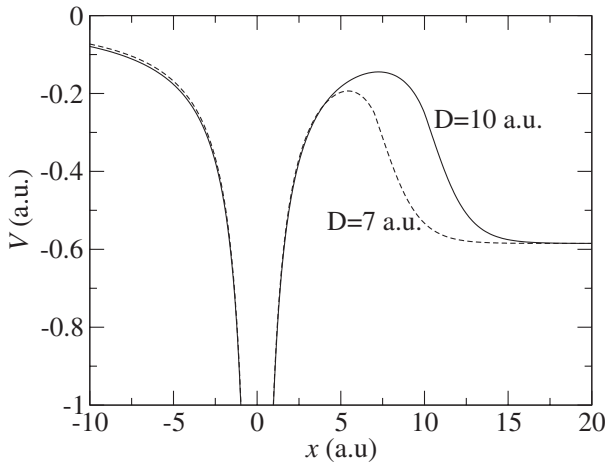


Fig. 2 Potential $V(x)$ of the 1D hydrogen atom near the Al surface for $D=7$ a.u. and 10 a.u.

electron with the classical image charge of the nucleus of the atom:

$$\Delta V_{e-s} = \frac{1}{|2D - x|}. \quad (5)$$

The above expressions for $V(x)$ in Eq. (3) correspond to the case where the electron is outside the metal. On the surface, the two potentials V_{e-i} and ΔV_{e-s} cancel each other and they vanish inside the metal. $V(x)$ for the 1D hydrogen atom near the Al surface is shown in Fig. 2. It is seen in Fig. 2 that this potential is characterized by a potential barrier leading to resonance states.

Figs. 3 and 4 present the resonance positions and widths of energies for the four lowest states of the system under consideration. They are plotted as functions of the distance D between the hydrogen atom and the image reference plane. Except the third lowest state, the resonance positions become high as the ion approaches the surface and the resonance widths increase as D de-

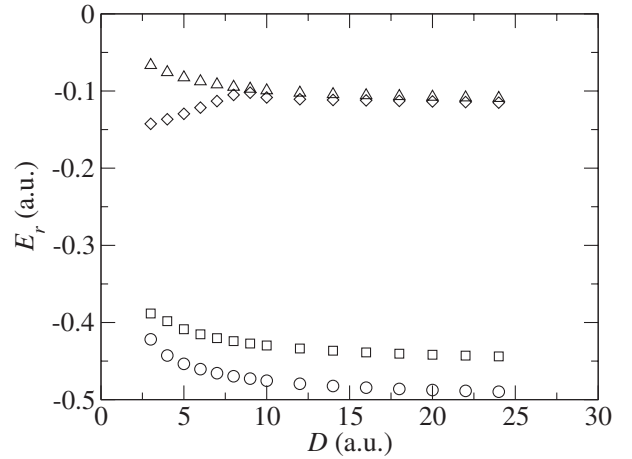


Fig. 3 Resonance positions of the four lowest states as functions of D .

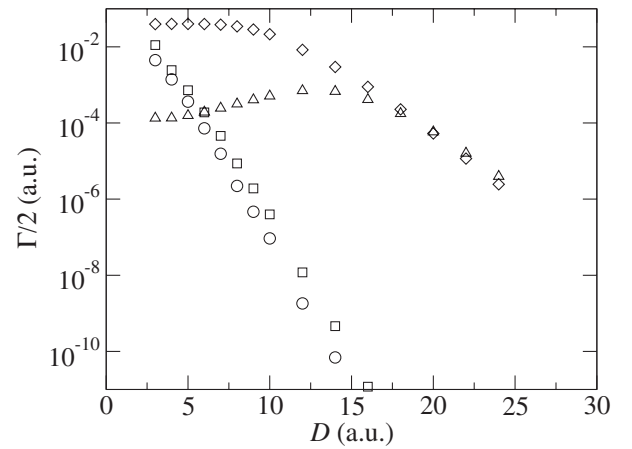


Fig. 4 Resonance widths of the states shown in Fig. 3 as functions of D . The symbols used to indicate numerical data for corresponding resonance states in Fig. 3 are also used in the same manner in the figure.

ceases. The reason for this is due to an enhancement of the tunneling effect through the potential barrier. The above behaviors are similar to those found in the 3D case in Refs. [1,2,3,8].

4. Summary

In this work, we have performed model calculations of the resonance positions and widths of energies in a one-dimensional hydrogen atom near an Al surface. We have used a combination of the complex absorbing potential method with the basis splines method. Although we have focused only on the 1D case, our approach can be also extended to the 3D case. For the 3D case, we expect to obtain qualitatively similar results and they will serve as applications to realistic problems such as surface-diagnostic methods.

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