Complex Absorbing Potential Method to Study the Stark Effect in Low-lying States of Hydrogen and Lithium

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In an attempt to develop a convenient computational technique for locating resonance states we have made an extensive study of the Complex Absorbing Potential (CAP) method [1] in resonant scattering problem. Resonant effects in electron-atom scattering can be explored theoretically by the exact quantum mechanical methods, but the computation of the scattering wavefunction is a difficult task because of their non L^2 -nature. To reduce the computer requirements with slow convergence of these algorithms, several approximation techniques have been developed and tested. Feshbach projection techniques, the stabilization method of Hazi and Taylor, and the complex coordinate rotation method are the big steps forward in the development of the scattering theory. Despite their formal beauty these methods give rise to problems concerning its use[2], especially for a many-electron atomic system. On the other hand the CAP method is a handsome alternative, rather a powerful method having some advantages over the others [1, 3].

The CAP method introduces an artificial complex absorbing potential that makes all eigenfunctions L^2 [2]. If one chooses a suitable form of the complex absorbing potential it generates an absorbing region where the wavepackets are damped. As a result, the resonance wavefunctions become square integrable. By the introduction of the complex potential $(-i\eta W)$, the physical Hamiltonian (H) leading to an effective Hamiltonian$(H(\eta) = H - i\eta W)$ becomes complex symmetric. A variational method can be applied and the eigenvalues can be computed by diagonalization of the complex symmetric matrix that represents $H(\eta)$ in a real square integrable basis.

As an illustrative example we have employed the method to a model problem described by the one-dimensional model potential of Bain *et.al.* [4]

$$V(r) = 7.5r^2e^{-r},$$

and demonstrated that the CAP method is very much reliable. In order to apply the CAP method we choose a spherically absorbing potential $W = r^6$. The energy of the lowest S-wave resonance in our calculation turns [3] out to be

$$E = 3.42639031 - 0.01277448i \text{ a.u.},$$

which is well documented in the literature [1, 4].

In an attempt to determine the feasibility of the CAP method in a real system, we first perform calculations to study the Stark effect in the hydrogen atom. Inspection of the results

of our calculation reveals that a satisfactory account of resonance energy and width of H atom ground state in the weak and strong DC electric field can be made by using the CAP method with a well defined estimated uncertainity [3]. Then we have made a more severe test of this method, in an application to the Stark effect in the degenerate $n = 2$ and $n = 3$ sublevels of hydrogen. The results confirm prior expectations for the widths of the split states [5]. The advantage of the present method is that like the method of complex co-ordinate rotation, the resonance positions and widths can be determined by straightforward eigenvalue calculations without impositions of the usual scattering boundary conditions. In the hydrogen atom case this is not the enormous advantage, as there are large number of methods suitable for finding the resonances in hydrogen atom under the external DC fields. A more complex case is the resonance calculations for many-electron atomic systems. It is the purpose of the present work to go beyond the existing theories with regard to the Stark problem in a many-electron system and additionally, to present some new results in this area.

A major advantage of the CAP procedure is that the unperturbed Hamiltonian operator $H(0)$ and the perturbed complex absorbing potential can be treated seperately. This is very interesting aspect of the method which allows to make an important progress in the area of resonance calculations for the many-electron systems. In a step forward, we have applied the method to calculate the resonance paramteters of Li atom in DC electric field. A model potential [6] is used to represent the interaction between the core and the outer electron. We focus our attention to the lowest $2S$ state and excited $2P, 3P, 3D$ and $4S$ states. Results for the electric field effects on such states will be presented at the meeting.

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