Hyperspherical Approach for Ion-Atom Collisions at Low Energies

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Single electron transfer and excitation processes in slow collisions of singly/multiply charged ions with hydrogenic atoms/ions is one of the most basic reactions in a three-body Coulomb system. For such collisions, a variety of quantum mechanical approaches have been proposed in the past. One of the well-developed approaches is the hyperspherical close-coupling method. This method has been used extensively for the collisions of electrons and positrons with atomic hydrogen as well as collisions involving muons [1]. The method, however, has never been applied to ion-atom collisions until recently [2,3].

In references [2,3], the two-channel adiabatic hyperspherical method has been applied to calculate the elastic and charge transfer reactions in simple collision systems at low energies. To extend the method to excitation and charge transfer to excited states, however, one must include higher channels. To avoid treating the sharp avoided crossings in the adiabatic approach, the so-called 'diabatic-by-sector' method has been employed previously. However, this method has its limitations [4]. An alternative hyperspherical formulation [5] has been developed, also within the spirit of the diabatic approach. This method is adopted here for treating ion-atom collisions at low energies.

Consider a system described by variables (R,Ω), where R is the hyperradius and Ω denotes all the other angular coordinates. Starting with the time independent Schrodinger equation in the body-frame

$$\left[T(R) + H_{ad}(R;\Omega) - E\right]\Psi(R,\Omega) = 0 \qquad (1)$$

where $T(R)$ is the kinetic energy operator for motion in R and H_{ad} is the adiabatic Hamiltonian in Ω which depends parametrically on R. We seek solutions of (1) in the form

$$\Psi(R,\Omega) = \sum_{j,I,v} a^{j}_{vI}\, u_j(R)\Phi_{vI}(R_j;\Omega)\ , \qquad (2)$$

where $u_j(R)$ is a B-spline basis function and $\Phi_{vI}(R_j,\Omega)$ denotes the channel function. The index j represents the radial grid, I is the absolute value of the projection of total angular momentum J along the body frame quantization axis, and v denotes the adiabatic channel number. Substituting (2) into (1), we obtain a generalized algebraic eigenvalue problem for the coefficients a^{j}_{vI} .

The method has been tested for bound states. For instance, the HD^+ system, with 1 channel calculation, we obtained the binding energy of the lowest state at 21515.056 cm^{-1}, which is to be compared with the exact value of 21515.981 cm^{-1}. In combination with the **R**-matrix propagation technique, this method is being extended to scattering calculations to obtain cross sections for excitation and charge transfer in ion-atom collisions at low energies.

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