ATOMIC PHYSICS OF STRONGLY CORRELATED SYSTEMS

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Our work in the last year and a half has been devoted to the understanding of strongly correlated atomic systems. Two types of problems are investigated: (1) electron correlations of doubly-excited electrons in hyperspherical coordinates; (2) differential and total electron transfer cross sections in fast ion-atom collisions. The theoretical work in the latter category is closely related to the experimental studies at Kansas State University in the effort of understanding inelastic processes in ion-atom collisions. Our methods of studies in these problems differ significantly from the traditional ones: we use atomic eigenfunction expansion method in ion-atom collisions while most of the traditional works have been using molecular orbital expansion; we use adiabatic expansion in understanding electron correlations in doubly-excited states while most of the traditional approaches use close-coupling expansion using unrelaxed target states. These different approaches provide new insights to the problems under investigation.

I) Electron Correlations Studied in Hyperspherical Coordinates

A) Radial and angular correlations of doubly-excited electrons:

Perturbation theories and configuration mixing methods are often used to study electron correlations, but the nature of electron correlations, particularly for doubly-excited states, are not revealed by these traditional approaches. Using hyperspherical coordinates in the adiabatic approximation, we have been able to map out the charge-density distributions for doubly-excited states belonging to different channels. Suitable surface plots of the charge-density distributions will be used to illustrate the
pattern of electron correlations between two doubly-excited electrons in $H^-$ and in He. These plots will be presented at the meeting.

B) Two-valence electron systems studied in hyperspherical coordinates:

Electron correlations are known to play important roles in alkali negative ions and in alkaline earth atoms. To extend hyperspherical coordinates to these systems we adopt the model two-electron Hamiltonians of Victor, Dalgarno and Laughlin. Their model potentials have been fitted to reproduce the low-lying bound states of the one-electron ions. We solve these model two-electron problems in hyperspherical coordinates to examine the similarities and differences of these systems as compared with the "true" two-electron atoms, $H^-$ and He. The more accurate potentials used here also will allow us to extend the works of Greene where simpler model potentials were adopted. This study is possible because of the availability of the recently developed approximate analytical channel functions in hyperspherical coordinates. Initial results for Li$^-$ and Be will be presented.

II) Charge Transfer in Fast Ion-Atom Collisions

In this area of research we are interested in understanding the dynamics of electron transfer in ion-atom or atom-atom collisions. In the model studies, the basic problem consists of an electron and two nuclei of charge $Z_A$ and $Z_B$. By changing the collision velocity $v$, we investigate the mechanism of electron transfer from target atom $A$ to projectile $B$ with a vast range of $Z_A$ and $Z_B$. Unlike collisions at very low velocities where dynamical models based upon molecular-orbital expansion are believed to be valid, dynamical models for collisions at higher velocities are not well established. Our work has been mainly in studying the dynamics of charge transfer in a model three-body system.
A) Simple two-center, two-state atomic expansion model for K-K charge transfer:

The region of validity of this simple model was established in our earlier works. Recent measurements of differential electron transfer cross sections for H⁺ + H and H⁺ + He at the University of Missouri, Rolla, and for F⁺⁺ + Ne at Kansas State University compare favorably with our calculations. The double K-K charge transfer cross sections measured at Kansas State University and at Brookhaven are also well predicted by our calculations.

B) Three-center atomic expansion method:

The simple model in (IIA) is not valid for low-velocity collisions at small impact parameters. It is expected that united-atom orbitals will play a big role in this new regime. In the test study for H⁺ + H(ls) → H(ls) + H⁺, we add to the two-center expansion in (IIA) the united-atom orbital, He⁺(ls), placed at the center of the charges. Importance of united-atom orbitals in our calculations are noticed at small impact parameters. The results will be shown in the oral presentation.

C) Including pseudostates in a two-center expansion:

Because of the numerical difficulties of (IIIB), we also consider putting united-atom orbitals in the two collision centers. By including a few such pseudostates, we showed that the normal MO regime can be reached in our extended AO model. Comparison with MO calculations will be presented.