Atomic Physics of Strongly Correlated Systems
C. D. Lin

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Department of Physics, Cardwell Hall
Kansas State University, Manhattan, Kansas 66506

This abstract summarizes the programs currently underway in the study of atomic physics of strongly correlated systems. The programs can be divided into three areas:

1. The study of Coulombic 3-body systems in hyperspherical coordinates.

We continue the study of Coulombic 3-body systems in hyperspherical coordinates. A computational procedure has been developed which allows us to treat any three-body systems with arbitrary masses. By using mass-weighted hyperspherical coordinates and adopting the adiabatic approximation, we have calculated the potential curves for Coulombic three-body systems such as ABA where two of the particles are identical. The evolution of potential curves with the mass ratio of $\lambda = m_A/m_B$ have been carried out and the results were published (see pub. #1 listed below). In the last contract period, we have examined the wave functions of the three-body systems for states of different symmetries vs λ . The wave functions allow us to identify the bonding vs anti-bonding nature, as well as the shape, of the states as the mass ratio varies from the small- λ limit like H^- to the large- λ limit of H_2^+ . This work has been finished and the results have been accepted for publications in Phys. Rev. A.

We are continuing more studies along two directions: One is to study the shape of highly excited states of the ABA systems vs λ to examine how the "molecular behavior" emerges. Preliminary calculations indicate that Ps^- in many ways behaves closer to H_2^+ for states which lie below the $n=3$ excitation thresholds. This is different from the lower excited states where Ps^- is much similar to H^- . The other direction is to apply the method for treating Coulombic three-body systems where all the three particles are different. It is known that the electronic structure of H_2^+ is not very different from HD^+ , but if two of the particles are lighter then the system behaves quite differently depending on whether the two lighter particles are identical or not. Hyperpherical coordinates will provide a convenient means for understanding the general properties of these three-body systems.

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2. Further studies of electron correlations in doubly excited states of atoms. Doubly excited states of atoms and ions continue to play major roles in many recent experiments. The advent of slow multiply charged ions from EBIS sources in collisions with surfaces or atoms renders it essential to study the radiative and Auger decays of doubly excited states where the principal quantum numbers of both electrons are quite high. Using the K, T and A quantum numbers, we showed that there are quasi-selection rules for the decay rates. Actual calculations have been carried out for the $6l6l'$ doubly excited states of Ar^{16+} . The results for this study have been published (see Pub. # 2 below). We have also been examining the purity of rotor structure of doubly excited states of atoms and ions. It turns out that the T quantum number, which is understood to be the projection of the total orbital angular momentum along the interelectronic axis, is a better quantum number for system like H^- , than for positive ions. This work was finished in the last few months and a manuscript has been submitted to J. Phys. B for publications.

We are currently developing computational procedures to calculate the properties of doubly excited states of He. Recent high resolution spectra from the photoabsorption of He near the $\text{He}^+(N=5,6)$ thresholds show that the Rydberg states exhibit strong modulations (Domke et al, 1991). It is our goal to achieve ab initio calculations to study such spectra using the hyperspherical approach. To this end, we need to develop procedures for calculating accurate hyperspherical potential curves and to obtain the analytical wave functions for the outer region where the asymptotic potentials are due to the combined Coulomb field and dipole field. We are aiming at developing a multi-channel quantum defect approach for such a calculation.

3. Theoretical studies of ion-atom collisions.

We have studied a number of problems under this general topic. Among the completed projects, we carried out two-electron close-coupling calculations to study the mechanisms of double excitations in collisions of bare ions with helium atoms. The goal is to understand the role of electron-electron interaction vs the double collision mechanism where each electron is excited "separately". This study has been completed and the results are published in Phys. Rev. A (see Pub. #3 below). We have also examined the ejected electron spectra from double capture to doubly excited states in collisions of helium atoms with bare ions of carbon and oxygen. We illustrated the

theoretical analysis needed in order to compare the theoretical results with actual experimental spectra. We emphasize that due to post-collision interaction effects and overlapping resonances, it is not possible to identify individual doubly excited states and deduce the double capture cross sections. Comparison between theory and experiment should be carried out at the ejected electron spectra level. We carried out such calculations using the independent electron approximation and the results will be published in J. Phys. B. We have also studied the limitation of the classical trajectory Monte Carlo (CTMC) method in the prediction of coherence parameters such as the orientation, and dipole moment of excited states formed in atomic collisions. We illustrated that the CTMC method, while predicting results in agreement with experiments and with quantal calculations at times, is not reliable in general. The results from this study will be published in Z. Phys. D.

In the current year, we are performing further calculations on double capture to doubly excited states. Recent experiments from the Berkeley group have obtained the relative cross sections for the populations of $2s^2\ ^1S^e$, $2s2p\ ^1P^o$ and $2p^2\ ^1D^e$ states and their relative M-dependence from double capture in B^{4+} -He collisions. We are carrying two-electron close-coupling calculations by including all the important single and double capture channels. This work is still in progress.

List of Publications

1. BingCong Gou, Z. Chen and C. D. Lin, " Radiative and Auger rates of high-lying doubly excited states of multiply charged helium-like ions," Phys. Rev. A43, 3260 (1991)
2. Z. Chen and C. D. Lin, "Classification of Coulombic three-body systems in hyperspherical coordinates", Phys. Rev. A42, 18 (1990).
3. W. Fritsch and C. D. Lin, "Mechanisms of double excitation in ion-atom collisions at high velocities", Phys. Rev. A41, 4776 (1990)
4. M. Dunn, Z. Chen and C. D. Lin, "Systematic studies of the molecular properties of intrashell and intershell doubly excited states of C^{4+} and He", J. Phys. B23, 2435 (1990).
5. Z. Chen, D. Madison and C. D. Lin, " Calculations of elastic scattering cross sections at large angles between electrons and multiply charged ions in the distorted wave approximation", J. Phys. B24, 3203 (1991)

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