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ABSTRACT

This report presents the progress made in our continuing study of strongly correlated atomic systems within the last year. We have examined the shape of three-body systems in hyperspherical coordinates by studying the evolution of the density functions with the mass ratio of the particles in the system. We have calculated the ejected electron spectra from the autoionizing states formed in double capture processes in collisions of multiply charged ions with atoms. We have investigated the systematics and the propensity rules of radiative and Auger decay rates of high-lying doubly excited states. We have also studied ion-atom collisions for processes which pose great challenges to detailed theories, by looking into processes where the cross sections are small such as the excitation process in $\text{He}^{++} + \text{H}$ collisions, or by looking into fine details such as the orientation parameters in excitation and charge transfer processes.

Progress Report

This report summarizes the progress we have made in the study of strongly correlated atomic systems. In this report we first summarize the progress made in the last three years. We then present specific progress made in the last ten months of this reporting period.

1. Progress Report for the period of August 1989-January 1992

In this period we have published 20 refereed articles. We have also published a review article in Phys. Rept. under the title "The Semiclassical Close-Coupling Description of Atomic Collisions: Recent Developments and Results", co-authored with W. Fritsch. This review partly summarizes what we have contributed to the subject of theoretical studies of ion-atom collisions in the past decade under the support of this grant. We have also been asked by the editor of the same journal to contribute another review article on "Hyperspherical Coordinate Approach to Atomic and Other Coulombic three-Body Systems", scheduled to be completed by the end of 1992.

We group this progress report into two sections: one on the general Coulombic three-body systems and the other on theoretical studies of ion-atom collisions. A list of the publications in the last three years are given in Appendix A and each article will be referred by A_i ($i=1-21$) in the following.

(A). Atomic and other Coulombic three-body systems

In the last three years, we published six papers related to doubly excited states (A_2 , A_3 , A_4 , A_{12} and A_{14}) of atoms and ions. We presented formulas for extracting energies of intrashell doubly excited states along the isoelectronic sequence and quantum-defect formulas for intershell doubly

excited states (A2). Energies of doubly excited states of Berylliumlike ions were calculated by treating the four-electron systems as two excited electrons in a model-potential core (A3). The calculated energies were compared to those of helium-like systems. It was shown that, unlike heliumlike systems, the energy levels of Berylliumlike ions do not have the rotor structure. We have also examined the systematics of autoionization widths of doubly excited states along the rotor series (A4). It was found that the widths are essentially constant along the rotor series except near the end of the series where the last member was found to be always very broad and the one next to the last always very narrow. No simple interpretation has been provided yet. In view of the interest by experimentalists in doubly excited states where both electrons have rather large principal quantum numbers, we have undertaken the calculation of the radiative and Auger widths of such states (A14). These states are produced in ion-atom or ion-surface collisions. We used the configuration-interaction method to calculate the energies and wave functions of many states. It was found that among the many possible decay channels there exist simple quasi-selection rules. In terms of the bending vibrational quantum number v , it was shown that v_i and v_f should be identical for the dominant channels. This is true for both the radiative and the Auger decay channels. In our continuing studies of the properties of the rovibrational structure of doubly excited states, we examined other "molecular" properties such as the averaged angle between the two electrons with respect to the nucleus and the averaged $\mathbf{p}_1 \cdot \mathbf{p}_2$ which is proportional to the mass polarization term or to the momentum correlation (A12). Such studies established the degree of deviations of doubly excited states from the traditional molecules.

We have also been studying Coulombic three-body systems where the masses of the system are arbitrary. By solving the Schrödinger equation in mass-

weighted hyperspherical coordinates and treating the hyperradius as the adiabatic parameter, we have shown how the adiabatic potential curves vary with the mass ratio $\lambda = m_A/m_B$ for the ABA three-body systems (A10). This allows us to relate the similarity between the traditional atomic system such as H^- ($\lambda \rightarrow 0$) to the conventional molecular system ($\lambda \rightarrow \infty$). This generalization allows us to treat all the three-body systems in a unified fashion and to understand the equivalence of different classification schemes for doubly excited states of atoms. Additional progress in understanding the nodal structure of these wave functions and how they vary with λ is addressed in section 2A below.

B. Theoretical studies of one- and two-electron processes in ion-atom collisions

Our studies of ion-atom collisions have been based on the close-coupling method where the time-dependent wave functions are expanded in terms of atomic orbitals on the target and the projectile centers. Over the years we had calculated dominant charge transfer cross sections for a number of collision systems where experimental data were available, or where such data were needed for applications in thermonuclear fusion studies. In the last three years, we have been focused on processes where the cross sections are smaller. For such weaker channels the convergence of the close-coupling calculations is more questionable, especially at lower energies. We have examined the excitation to $H(n=2)$ and $H(n=3)$ states in $He^{++} + H$ collisions and found that a relatively large set of basis functions is needed to achieve good convergence (A21).

We have also examined a number of two-electron transitions in ion-atom collisions. In particular, we studied double excitation processes at high energies using a two-electron close-coupling code to calculate double excitation cross sections to $2\ell 2\ell'$ states in collision of bare ions with helium

atoms. The calculations were carried out to assess the role of electron-electron interaction in relation to the double collision mechanism for two-electron processes. It was found that the relative importance of the two mechanisms depends on the specific doubly excited states studied and that a complete study of double excitation requires a proper treatment of the ejected electron spectra where interference with the single ionization continuum has to be included (A9). We have also examined the ejected electron spectra from doubly excited states formed in double capture processes in collisions between multiply charged ions and helium atoms. Such studies pose a great challenge theoretically since not only the scattering amplitudes to each doubly excited state have to be calculated, but also the Auger decay branching ratios and amplitudes have to be calculated for each state. These amplitudes have to be added, weighted with models for post-collision interactions, to derive the ejected electron spectra. We have carried out such a study for the ejected electron spectra for C^{6+} -He and O^{8+} -He collisions where the double capture amplitudes were calculated using an independent electron model, and doubly excited states were calculated using configuration-interaction wave functions (A15, A16). The calculated electron spectra were compared to experimental measurements at specific angles. This double electron capture work was presented in the Hot Topics session of the XVIIth International Conference on the Physics of Electronic and Atomic collisions, held in Brisbane, Australia, July 10-16, 1991.

We have also examined the orientation and alignment parameters of excited states formed in ion-atom and electron-atom collisions. First, we established the general properties of these parameters between electron-atom and ion-atom collisions to show that the sign of the incident charge is important in determining the sign of the orientation parameters (A1). We further compared these parameters as calculated by the close-coupling method

to those obtained from the classical trajectory Monte-Carlo method (A17) to show that the CTMC predictions for such parameters are questionable in general.

For ionization processes, we have been testing some simpler models, especially for inner-shell ionization of heavy atoms by light ions. Using the distortion approximation, we showed (A7, A8) that both excitation and ionization cross sections calculated using the distortion approximation are in general in good agreement with experiments.

We have also examined the elastic scattering of electrons with positive ions at large angles in connection with measurements of Binary-Encounter Electrons (BEE) measured at zero degrees. It was found that the elastic cross sections at large angles increase with increasing number of electrons for a fixed nuclear charge. It turns out that this can be easily interpreted even with a potential scattering model (A13), but exchange effect or higher order effects should be considered to achieve good agreement with experimental data (A19).

Refereed Articles Published (1989-1991)

PUBLICATIONS:

- A21. W. Fritsch, R. Shingal and C. D. Lin, "Close-coupling Study of Electron Excitation in 1-300 keV/u He^{++} -H collisions", Phys. Rev. **A44**, 5686 (1991)
- A20. X. H. Liu, Z. Chen and C. D. Lin, "Demonstration of Molecule-like Normal Modes of Coulombic Three-body Systems in Hyperspherical Coordinates", Phys. Rev. **A44**, 5468 (1991)
- A19. 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).
- A18. W. Fritsch and C. D. Lin, " Theory of ion-atom collisions- Coupled Channel Methods,", Rept. Prog. Phys. **202**, 1 (1991)
- A17. N. Toshima and C. D. Lin, "Coherence Parameters of Atomic Excited States: Comparison of Results from the CTMC and the Quantal Calculations.", Z. Phys. **D21**, 227 (1991).
- A16. Z. Chen and C. D. Lin, "State-Selective Double Capture in Collisions of Bare Ions with Helium Atoms at Low Energies: II. Ejected Electron Spectra. " J. Phys. **B24**, 4231 (1991).
- A15. Z. Chen, R. Shingal and C. D. Lin, "State-Selective Double Capture in Collisions of Bare Ions with Helium Atoms at Low Energies: I. Total Cross Sections. " J. Phys. **B24**, 4215 (1991).
- A14. 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).

- A13. R. Shingal, Z. Chen, K. R. Karim, C. D. Lin and C. P. Bhalla, " Charge state dependence of elastic scattering cross sections at large angles between electrons and multiply charged ions," J. Phys. B23, L637 (1990).
- A12. 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).
- A11. Z. Chen and C. D. Lin, " Reply to 'Comment on Calculations of energies of intrashell doubly excited states of beryllium-like ions", J. Phys. B23, L87 (1990)
- A10. Z. Chen and C. D. Lin, "Classification of Coulombic three-body systems in hyperspherical coordinates", Phys. Rev. A42, 18 (1990).
- A9. W. Fritsch and C. D. Lin, "Mechanisms of double excitation in ion-atom collisions at high velocities", Phys. Rev. A41, 4776 (1990)
- A8. T. Mukoyama and C. D. Lin, " Calculations of K-shell ionization cross sections by charged particles in the distortion approximation using pseudostates", Phys. Rev. A40, 6886 (1989).
- A7. T. Mukoyama and C. D. Lin, "Target atomic number dependence of projectile excitation cross sections of He-like iron ions", Phys. Lett. A141, 138 (1989)
- A6. M. Kimura, N. F. Lane and C. D. Lin, " Current status of theoretical studies of ion-atom collisions at low to intermediate collision energies", Chinese J. Phys. 27, 22 (1989).
- A5. T. Mukoyama and C. D. Lin, "Calculations of cross sections for excitation and ionization of inner shells of atoms by heavy ions in the distortion approximation", Chinese J. Phys. 27, 117 (1989).
- A4. Z. Chen and C. D. Lin, " Novel systematics of autoionization widths of doubly excited states of atoms," Phys. Rev. A40, 6712 (1989).

- A3. Z. Chen and C.D. Lin, "Calculations of Energies of Doubly Excited States of Berylliumlike Ions," J. Phys. **B22**, 2875 (1989).
- A2. C. D. Lin, "Systematics of Energies of Double Excited States of Heliumlike Ions," Phys. Rev. **A39**, 4355 (1989).
- A1. C. D. Lin, R. Shingal, A. Jain and W. Fritsch, " Orientation and Alignment of Collisionally Excited States," Phys. Rev. **A39**, 4455 (1989).

2. Progress Report for the period March 1, 1991-January 15, 1992

This section reports the progress made since the last report which was submitted in March, 1991. It covers a brief summary of the published papers within this period (listed as B1-B8 below) and conclusions from the preprints accepted or submitted for publications (C1-C6).

A). Summary of published results in 1991.

In the last year we have published eight papers covering a number of subjects. We have calculated the radiative and Auger rates of doubly excited states in the $6l6l'$ manifolds and examined the relative strengths of various decay channels to establish the quasi-selection rules for both processes (B8). The selection rules are then established in terms of the correlation quantum numbers derived from our previous studies.

We have also calculated the ejected electron spectra from doubly excited states which were formed from double capture to these states in collisions between bare ions such as C^{6+} and O^{8+} on He. To calculate double capture probabilities, we have used an independent electron approximation (B7) where single capture amplitudes are calculated using the close-coupling method expanded in terms of atomic orbitals. These amplitudes are combined, properly weighted with configuration-interaction coefficients, to form double capture amplitudes to each doubly excited state. In order to compare with experimental ejected electron spectra, it was necessary to calculate the amplitudes for the electron emission coherently from each state and take into account the post-collision interaction. Such calculations were carried out for the $2l3l'$ doubly excited states of C^{4+} and $3l3l'$ doubly excited states of O^{6+} and the results were compared to experimental measurements (B6). The calculations were in reasonable agreement with experiments, but

experimental data at a few different angles are needed for further test of the theory.

We have also published one paper comparing the orientation and alignment parameters of excited states formed in collisions of atoms with electrons, positrons, protons and antiprotons (B5). Our goal was to examine whether the classical trajectory Monte Carlo method (CTMC), which has been widely used in the literature, is capable of predicting quantities which are related to the scattering amplitudes in quantum scattering theory. Our results indicate that the CTMC calculations in general are not in agreement with the close-coupling results.

Together with Don Madison, we have also examined the importance of exchange in the distorted wave Born approximation for calculating elastic scattering cross sections at large angles (B3). This was carried out in connection with the experimental studies of Binary Encounter Electrons of positive ions in collisions with H_2 targets by Richard's group at the J. R. Macdonald Laboratory. It was found that inclusion of electron exchange can improve substantially the agreement between theoretical calculations and experiments.

In this period we have also shown how the density function of a three-body system varies with the relative masses of the three particles (B2). This was carried out by displaying the modulus of the wave functions in proper hyperspherical coordinates and follow their variations with the mass ratios. Such investigations established the relation between the traditional atomic and molecular three-body systems.

At the request of the fusion community, we have also calculated cross sections for excitations to $n=2$ and $n=3$ states of H in He^{++} collisions with H from 1-50 keV/amu (B1). We have found that a relatively large basis set is needed in order to obtain reliable cross sections.

B). Summary of results from preprints accepted or submitted for publications

In the last year we initiated a program toward calculating accurate atomic parameters of doubly excited states of atoms using hyperspherical coordinates. The goal was to calculate photoabsorption spectra of H^- and He in the energy region where the inner electron is also excited to a state of large principal quantum number. Experimental photoabsorption data for both H^- and He near the $N=5-8$ excited thresholds have been measured and interesting structures were observed [1,2]. The conventional methods are not expected to be very efficient for treating such problems since the number of channels that has to be included in the calculation is quite large. We thus approach this problem from the hyperspherical viewpoint where qualitative results have been established by us over the years, and it has been shown that many channels are not excited and these channels probably can be omitted in the theoretical calculation. To carry out such calculations, there are a number of problems that have to be solved first. To describe the outer region of doubly excited states, an outer electron sees a combined Coulomb field and a permanent dipole field, i.e., the potential takes the form $-1/r - A/r^2$. The general quantum defect theory for such a combined field has been discussed previously by Greene et al [3], but was never implemented. In preprint (C2) we described the quantum defect theory for such a combined Coulomb and dipole field and calculated the quantum defect in a single hyperspherical channel approximation. The accuracy of the one-channel results gives us an estimate whether other weaker channels can be eliminated in later calculations.

To obtain a single-channel potential from potential curves which were calculated adiabatically, a procedure for obtaining diabatic curves in the avoided crossing region is needed. Although such a procedure has been

discussed in the literature [4], these methods rely on accurate values of the nonadiabatic coupling terms in the avoided crossing region and the coupling terms throughout the whole range of the adiabatic parameter R . We have developed a new procedure for determining diabatic curves by interpolating the wave functions in the avoided crossing region by requiring that all the coupling terms be small. The method has been applied to the avoided crossing in the $+$ and $-^1P^o$ hyperspherical potential curves of He (C1).

We have also examined the "purity" of the quantum number T in the classification of doubly excited states of atoms. Recall that T was interpreted as the projection of L along the interelectronic axis, it is similar to the Λ quantum number of a diatomic molecule which is the projection of L along the internuclear axis. For a given L , the range of T is $0, 1, \dots, L$. To examine the "purity" of T for a given doubly excited state, we project the wave functions which were calculated using configuration-interaction method onto the body-frame with the interelectronic axis chosen as the quantization axis (see C6). We examine the purity of T along the rotor series. For example, for each $(K,T)^A$ rotor series, if T is a good quantum number, the purity should be 100%. We found that the purity decreases with increasing L . For each rotor series, we also found that the purity decreases with increasing nuclear charge Z . This study establishes the "goodness" of the approximate quantum number T , and it is important to recognize that the "goodness" depends on the states addressed.

In the last year we also have performed a careful calculation on double capture to $2\ell 2\ell'$ doubly excited states in B^{4+} -He and Be^{4+} -He collisions. The calculations were initiated by the experiments being carried out by the Berkeley's group where the angular distributions of the ejected electrons from these doubly excited states were measured [5]. Such experiments provide information about the magnetic substate distribution of each doubly excited

state formed in the collision, and thus provide a more stringent test of the theoretical models. We performed a careful close-coupling calculation by solving the two-electron time-dependent Schrödinger equation where the wave function is expanded in terms of correlated atomic basis functions. In other words, we included important configuration interaction in the basis functions. From such calculations, we obtained both the single and double capture cross sections. For double capture cross sections, we showed that our results were in good agreement with experiments (C5). We also showed that single capture cross sections obtained were also in good agreement with earlier measurements.

In our earlier study of the orientation and alignment parameters, we examined the excitation and electron capture to 2p states in collisions such as electrons, positrons, protons and antiprotons with atomic hydrogen (A1, A17). We showed that these parameters calculated using the CTMC method are not in agreement with those obtained by the close-coupling or distorted wave approximations. We were concerned whether the discrepancy is somehow related to the small excitation probabilities in such collisions. We thus decided to examine one more system: electron capture to 2p states in $\text{He}^{++}\text{-H}$ collisions. In this case the electron capture probabilities are of the order of 10-50 % for incident energies in the range of 10-50 keV/amu. We examined the orientation parameter and the effective dipole moment of the $n=2$ states calculated using CTMC and using the close-coupling method. It was shown (C3) that the CTMC results again in general do not agree with the quantal calculations. We have also found that the CTMC results depend sensitively on the ensemble average chosen for the initial state.

Our work on the ejected electron spectra from double capture to doubly excited states were chosen in the "hot topics" session in the International Conference on the Physics of Electronic and Atomic Collisions (ICPEAC) at

Brisbane, Australia, July 1991. A written report of this report will be published (C4) in the next year.

- [1] M. Domke et al, Phys. Rev. Lett. 66, 1306 (1991).
- [2] Harris et al, Phys. Rev. Lett. 65, 309 (1990).
- [3] C. H. Greene, A. R. P. Rau and U. Fano, Phys. Rev. A26, 2441 (1982); C. H. Greene, U. Fano and G. Strinati, Phys. Rev. A19, 1485 (1979).
- [4] T. G. Heil, S. E. Butler and A. Dalgarno, Phys. Rev. A23, 1100 (1981).
- [5] M. Prior, private communications.

B. Journal Publications

- B1. W. Fritsch, R. Shingal and C. D. Lin, "Close-coupling Study of Electron Excitation in 1-300 keV/u He^{++} -H collisions", Phys. Rev. **A44**, 5686 (1991)
- B2. X. H. Liu, Z. Chen and C. D. Lin, "Demonstration of Molecule-like Normal Modes of Coulombic Three-body Systems in Hyperspherical Coordinates", Phys. Rev. **A44**, 5468 (1991)
- B3. 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).
- B4. W. Fritsch and C. D. Lin, " Theory of ion-atom collisions- Coupled Channel Methods," , Rept. Prog. Phys. **202**, 1 (1991)
- B5. N. Toshima and C. D. Lin, "Coherence Parameters of Atomic Excited States: Comparison of Results from the CTMC and the Quantal Calculations.", Z. Phys. **D21**, 227 (1991).
- B6. Z. Chen and C. D. Lin, "State-Selective Double Capture in Collisions of Bare Ions with Helium Atoms at Low Energies: II. Ejected Electron Spectra. " J. Phys. **B24**, 4231 (1991).
- B7. Z. Chen, R. Shingal and C. D. Lin, "State-Selective Double Capture in Collisions of Bare Ions with Helium Atoms at Low Energies: I. Total Cross Sections. " J. Phys. **B24**, 4215 (1991).
- B8. 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).

C. Articles accepted and submitted

- C1. J. Q. Sun and C. D. Lin, "Diabatic States in the avoided-crossing region", J. Phys. B. (accepted)
- C2. J. Q. Sun and C. D. Lin, " A single channel quantum defect theory for the description of doubly excited states of helium", Phys. Rev. A (submitted)
- C3. N. Toshima, R. Shingal and C. D. Lin, " Orientation parameters and dipole moments of $\text{He}^+(n=2)$ states in $\text{He}^{++}+\text{H}$ collisions: Comparison of CTMC and close-coupling results", J. Phys. B. (accepted)
- C4. C. D. Lin, Z. Chen and R. Shingal, " Ejected electron spectra of doubly excited states from double capture in collisions of bare ions with helium atoms", to be published by Institute of Physics, UK.
- C5. W. Fritsch and C. D. Lin, " One- and two-electron capture in collisions of slow B^{4+} and Be^{4+} with helium", Phys. Rev. A. (submitted)
- C6. Z. Chen, C.-G. Bao and C. D. Lin, " Analysis of the Projection of the Total Orbital Angular Momentum along the Interelectronic Axis for Doubly Excited States of Atoms", J. Phys. B. (accepted)

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