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TITLE: "STRUCTURE AND DYNAMICS OF ATOMS, IONS, MOLECULES, AND SURFACES"

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[Section numbers in text refer to the numbering in the original Renewal Proposal]

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Structure and Dynamics of Atoms, Ions, Molecules, and Surfaces: Atomic physics with ion beams and synchrotron radiation

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The goals of this aspect of the JRML program are (1) to explore the dynamics of photoelectron emission from and the structure of small molecules, (2) to identify and explain basic mechanisms whereby electrons are removed from simple systems in capture and ionization processes.

Recent progress and future plans (refer to three-year proposal for further detail):

A.1.1 COLTRIMS measurements of electron spectra from low energy ionization of atomic H and He targets *E. Edgu and C. L. Cocke* The goal of this project is to identify and characterize the process whereby a slow charged projectile promotes into the continuum an electron from a neutral target. The projectile velocity is sufficiently low that direct kinematic ionization is forbidden, and saddle-point electron promotion, in some form, is expected to the major process. The electron momentum distributions show clear patterns that are much more definitive in determining the ionization mechanism than are total cross sections. Several theoretical treatments of this problem have been made, but the agreement between theory and experimental momentum space distributions of the continuum electrons is at best qualitative. The purpose of this experiment is to provide bench-mark data for the electron distributions for a *true one-electron system* (bare nuclei on atomic hydrogen), under conditions such that the collision plane and the transverse momentum transfer to the projectile are controlled. We use COLTRIMS techniques to image the momenta of the recoil ion and electron in coincidence. The major technical problem has been to develop a (semi-) cold target of atomic hydrogen. During the past year, we have attempted to do this using a Slevin atomic hydrogen source. The effort has failed, and we have replaced this with a 2.43 GHz microwave discharge source. In the meanwhile, a paper on ionization of He at proton energies between 25 and 100 keV is in preparation. Future work on this project will focus on making the experiment work. This project is the Ph.D. thesis work of Erge Edgu.

A.3.2. Complete Multi-Particle Measurememt of the Double Ionization of D_2, *A.Landers, E.Wells, Timur Osipov,C.L.Cocke.* Two runs at the LINAC on this project have been carried out. The data are under analysis.

A.5.1. Electron capture from H_2^+ by doubly charged projectiles *I. Reiser, H.Braeuning(U.Giessen) ,C.D.Lin, E.Sidky and C.L.Cocke*. To what extent can a single electron capture from a two-center target be treated in terms of interfering amplitudes for capture from two separate atomic centers? The purpose of this experiment is to address this question with a true one-electron molecule, namely H_2^+. The experiment is thus electron capture from H_2^+ by singly charged projectiles (Ar^{2+} , N^{2+} and He^{2+}, and is being carried out both on the JRML ion-ion collision facility (differential cross sections) and on the Univ. of Giessen Ion-Ion facility (total cross sections). Total cross section measurements have been completed; the results agree well with a simple model calculation. These results have been published. Differential cross sections for N2+ (a nearly resonant capture) have been completed, and measurements for the other ions are underway. Strong differential structure is observed, not in agreement with the model calculation. During the coming year these measurements will be completed. This project is the Ph.D. thesis work of Ingrid Reiser (Pub. # 29,30).

A.6.Interaction of fs laser pulses with ion beams and neutral targets: A Major Research Instrumentation grant from the NSF was approved. This is being used to acquire the necessary laser facility to carry out this work. During the coming year, the first stage of the laser will be installed, beamlines and target chambers will be constructed/modified to allow the study of the interaction of fs laser pulses with neutral systems, both atomic and molecular, and with ion beams from the KSU ECR source. The former setup will be located at the COLTRIMS chamber presently used at the LINAC, and the latter will replace the present ion-ion collision chamber. See contribution of Z.Chang for further detail.

A.6. Photoelectron diffraction from light molecules fixed in space *A.Landers (Western Mich.Univ.), R.Doerner, Th.Weber, M.Hattass, O.Jagutzki, A.Nauert, A.Staudte, H.Schmidt-Boecking(U.Frankfurt), M.H.Prior(LBL), A.Cassimi(CIRIL), T.Osipov, I.Ali, C.L.Cocke (KSU)*. We have measured the diffraction patterns of photoelectrons issuing from core photoionization of fixed-in-space light molecules . This work is carried out at the ALS using COLTRIMS imaging techniques. The alignment/orientation of the molecule at time of photoionization is determined from the momentum of the fragments and the vector momentum of the photoelectron is measured in coincidence. Target molecules studied to date are CO, N_2 and C_2H_n (n=2,4,6).

For CO, N_2 , from the photoelectron angular distributions the amplitudes and phases of the partial waves, including the relative phases between sigma and pi amplitudes, can be extracted. The results are in good agreement with theoretical calculations carried out by several groups. The data show at most very weak non-dipole contributions in the photoelectron spectra. For low kinetic-energy-release channels, the photoelectron spectra wash-out, indicating that the intermediate fragment lifetime is long enough that the orientation of the molecule with respect to the initial axis is lost to rotational motion prior to fragmentation. One letter and two full articles have been published on these systems. This work is being extended to circular polarization, which will allow us to determine the relative phase of sigma and pi amplitudes, not available by other methods (Pub. # 33).

For the C_2H_n sequence, full photoelectron spectra have been taken on and off the calculated position of the resonance for C_2H_2, C_2H_4 and C_2H_6. A clear indication of f-wave structure is seen on resonance, and a partial wave analysis is underway. For the case of acetylene (C_2H_2) an unexpected two-body breakup channel of the dication was observed, resulting in the fragments C^+ and CH_2^+. This is attributed to the rearrangement of the molecule from the acetylene to the vinylidene configuration after photoelectron emission but prior to fragmentation. The vinylidene and acetylene configurations are populated with similar probabilities. Preliminary analysis of the data indicates that, while a very marked f-wave structure is seen in the photoelectron spectra in the acetylene channel, this structure is partially lost in the vinylidene channel. This suggests that the lifetime of the vinylidene configuration may be longer than characteristic rotation times. This project is the Ph.D. project of Timur Osipov at KSU. Near-future work on this project will include obtaining complete data on and analysis of the C_2H_n data. More long range plans include attempting to extend these techniques to time-dependent probes of molecular structure.

Structure and Dynamics of Atoms, Ions, Molecules, and Surfaces: Atomic Physics with High Velocity, Highly Charged Ion Beams

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The goals of this part of the JRML program are 1) to study the dynamics of the dominant processes by which electrons from bound neutral target states are brought to the continuum and to bound states of high velocity, highly-charged ions and 2) to study resonant reactions in high velocity, highly charged ion–neutral target collisions.

Study of Two-Electron Processes in Ion-Atom Collisions: Transfer Ionization (A.2.1) *R. Unal, P. Richard, I. Ben-Itzhak, C. L. Cocke, and C. D. Lin*

Recent progress: We have measured transfer ionization, TI, and single electron capture, SC, for high velocity highly charged ions bombarded on a collimated supersonic He jet target by the method of recoil ion momentum spectroscopy. The main goals of this study are to understand projectile charge and projectile energy dependences of the TI/SC ratio and to measure the electron emission spectra in TI.

In the recent past we have measured the TI/SC ratio for O^{q+}, F^{q+}, Cl^{q+}, and Ti^{q+} beams at a projectile energy of 2-MeV/u. We observed a huge increase in the TI/SC ratio with increasing q from values near 1 for q ~ 9 to values near 15 for q ~ 18. This trend greatly exceeds the perturbative q^2 scaling predictions, which was very surprising in view of the fact that even higher q data existed in the literature with smaller TI to SC ratios. A coupled channel prediction however agreed fairly well with our observations and therefore put the higher q data in question.

We installed a new improved recoil spectrometer system since these original measurements were performed. This year we have completed several new measurements with this system to address the issues described above. 1) We performed measurements of q-dependences for O and F projectiles at several energies. For the few electron projectiles we find that the data follows the perturbative q^2 dependences, whereas the many electron projectiles show antiscreening effects. 2) We added Si^{q+}, Ti^{q+} and Cu^{q+} data to our systematics. The previous Ti^{q+} data suffered from large error bars. The new data, which has much smaller error bars, still show an increasing trend in the TI/SC ratio but not quite as steep as the original data. 3) Very recently we extended the data set to I^{q+} beams. This allowed us to overlap with some of the existing data in the literature. It should be pointed out that none of the published data on this subject previous to our work uses recoil momentum spectroscopy and thus suffers from systematic errors due to impurity beam issues, which were not properly addressed. We observed a very steep energy dependence in the I^{q+} data. These data are in the process of being analyzed. We anticipate that several papers describing the results of this research will be published during the next year. One paper describing a small part of the work has been published this year (Pub #24). This project is the Ph. D. thesis of R. Unal.

Future plans: We plan to complete the high velocity high q experiments during the next year and begin the measurement of the electron distribution in the TI process. Manpower issues may impede our progress towards completing all of our goals in the next year.

Doubly and Triply Excited Resonance States in High Z Few Electron Ions (A.2.2)

H. Aliabadi, E. Benis, C. P. Bhalla, P. Richard, M. Zamkov, and T. J. M. Zouros (U Crete, Greece)

Recent progress: We have studied resonant electron elastic, inelastic and superelastic scattering in the last few years. A summary of our resonant elastic scattering work (the $2p^2\,{}^1D$ resonance in C^{4+}, N^{5+}, O^{6+} and F^{7+}) was published this year (Pub #22). The results of our one case study of electron inelastic scattering (the $3l3l'$ manifold in F^{7+}) were published last year. The results of our discovery of superelastic electron scattering in highly charged ion-atom collisions has just been published in Physical Review Letters (Pub #27). We constructed a new high vacuum, high voltage double zero-degree electron spectrometer with capabilities that allow us to extend our data to high q ions (Pub #19). Our goal, to measure the $2p^2\,{}^1D$ resonances in Mg^{10+}, Al^{11+} and Si^{12+} and the $3\ell 3\ell'$ resonances in Mg^{10+} with this spectrometer, has been frustrated this year due to the difficulty in getting all of the LINAC resonators to operate at their highest field levels, which is required by this experiment. The LINAC system is presently shut down for a one-month repair of the faulty resonators, which will hopefully allow the LINAC system to operate at full energy.

Another one of our projects in electron scattering has been completed and published in two recent papers (Pub #16 and Pub #17). This project was the measurement of the ionization of atomic hydrogen, molecular hydrogen and helium by high velocity, highly charged ions and the comparisons with the latest CDW theory.

The other area of proposed work is the study of hollow ion, triply excited resonance states. We have demonstrated that electron elastic scattering from two-electron metastable ion beams can form these states. Two conference proceedings have been published on this work. We have made great strides on this subject during the last year, having done a complete study of the production mechanisms for forming $1s2s\,{}^3S$ metastable ion beams in gas vs. thin foils and having established a model for predicting these results. These are the first measurements of the energy dependence of metastable ion production in gas and thin foil media. A preliminary paper on this subject has been published (Pub #18) and a paper has been accepted in Phys. Rev. A for the November issue. A Phys. Rev A paper on obtaining absolute cross sections for triply excited states using these results has been submitted for publication.

Future Plans: During the next year we will attempt to reach the beam energies necessary to form the $2p^2\,{}^1D$ resonance in Mg^{10+}, $A\ell^{11+}$, and Si^{12+}. We will measure the $1s2s\,{}^3S$ metastable fractions in C^{4+}, N^{5+}, O^{6+} and F^{7+} beams and test our model for calculating the ratio of the metastable fraction in gas vs. solid targets. These metastable fractions are needed to obtain absolute cross sections for the formation of triply excited states in high velocity, highly charged ion-atom collisions. We will then be able to measure triply excited state cross sections in these systems. We anticipate no problems in reaching these goals. However the LINAC must perform at its highest voltages in order to excite the $2p^2\,{}^1D$ and the **$3\ell 3\ell'$** resonances in Mg^{10+}.

Other publications include work on low velocity highly charged ions (Pub #15).

Structure and Dynamics of Atoms, Ions, Molecules, and Surfaces: Multi-Particle Dynamics in Ion-Molecule Collisions

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Recent progress and future plans:

Ground state dissociation of HD^+ (Section A.3.4)

The fast removal of one electron from a hydrogen molecule is followed by very slow dissociation if the vibrational continuum of the electronic ground state is populated in the vertical transition. We name this process ground state dissociation (GSD). For the HD isotope of hydrogen the dissociation favors H^+ + D(1s) over H(1s) + D^+ production due to the small, 3.7 meV, energy gap between these two dissociation limits[4,13]. We have used this slow dissociation process of hydrogen to probe the following reaction mechanisms:

1. Charge transfer and elastic scattering in very slow H^+ + D(1s) "half" collisions -- *E. Wells, I. Ben-Itzhak, K.D. Carnes, B.D. Esry in collaboration with H. Sadeghpour*

We have studied charge transfer and elastic scattering in the H^+ + D(1*s*) collision system. This system provides an interesting case study for theorists, since scattering calculations for this system depend in turn on HD^+ structure calculations, which must correctly account for the difference in nuclear mass[12]. Our aim was to study the collision at energies from about 1 eV down to the charge transfer threshold at 3.7 meV, and below for the elastic channel. To accomplish this goal we used ground state dissociation (GSD) of HD^+ to measure electron transfer from the 1sσ to the 2*p*σ state. Charge transfer occurs at an internuclear separation of about 12 a.u., around the avoided crossing resulting in the D^+ + H(1*s*) final state. In contrast, H(1*s*) + D^+ is the final state of elastic scattering. The energy of the resulting H^+ or D^+ fragment is typically less than 300 meV and is determined for each fragment by imaging its momentum vector using a COLTRIMS-style apparatus.

The measured relative yields of H^+ and D^+ fragments as a function of kinetic energy in the HD^+ center of mass frame provide a direct measure of the electron transfer probability from the initial 1sσ to the final 2pσ state for very slow "half" collisions. Our recently published experimental results[43] are in good agreement with our half collision calculations except near the charge transfer threshold where better resolution and subtraction of the H_2 contamination are needed. Better subtraction of the H_2^+ contamination extended our agreement with theory down to about 12 meV. Further improvements of the experimental setup are underway in an attempt to probe the threshold behavior of charge transfer and the resonances in the elastic channel. We hope to reach 1 meV or better resolution in the near future.

2. Separating the momentum transfer to a hydrogen molecule as a whole from the momentum transfer to the internal motion of its nuclei in the CM frame -- *I. Ben-Itzhak, C.L. Cocke, M.A. Abdallah, M. Stöckli in collaboration with W. Wolff and H.E. Wolf*

In a collision, momentum can be transferred either to the CM motion of the molecule or to the internal motion of its nuclei in the CM frame. We have used the GSD process to probe and separate these two contributions from each other for slow He^+ + H_2 (or D_2) collisions (~v= 0.25 a.u.). The GSD fragments are very sensitive probes of small amounts of momentum transfer because of their small dissociation speed. It was found that for these collisions most of the momentum is transferred to the molecule as a whole for both electron capture and ionization processes. However, we observed some transverse momentum transfer to the motion of the nuclei in the CM system for the ionization process and none for electron capture. It is suggested that direct scattering off one nucleus is the cause of this momentum transfer. We are planning to use the same technique to probe angular alignment effects in other reactions such as single ionization and single capture.

Collision induced dissociation and dissociative capture (Sections A.3.5 and A.3.6) -- *D. Hathiramani, I. Ben-Itzhak, K.D. Carnes*

Collision induced dissociation (CID) and Dissociative capture (DC) are defined by the reactions

$$AB^+ + He \rightarrow A + B^+ + He \quad \text{or} \quad A^+ + B + He \qquad (1)$$

and

$$AB^+ + He \rightarrow A + B + He^+, \qquad (2)$$

respectively, for a generic AB^+ molecular ion. At collision energies of a few keV the molecular fragments will continue their flight forward at the beam velocity, while moving away from each other in the center of mass frame. The kinetic energy released (KER) upon dissociation can be determined from the measured impact position and time difference between the two hits on a multi-hit detector placed on the beam axis. An apparatus for such measurements has been constructed and tested to have a 0.3 mm spatial resolution and 0.5 ns timing resolution. Minor improvements of the new experimental setup are underway and we hope to conduct the first experiments before the end of this year. The first of these measurements will focus on the isotopic effects seen in the CID of HD^+. This system will be, later, combined with one of the in-house COLTRIMS jets to enable studies of DC reactions. In the near future the system will be merged with a CRYEBIS beam line where studies of molecular breakup caused by slow highly charged ions will be conducted.

High intensity lasers (Section A.6) -- *I. Ben-Itzhak, in collaboration with R. Jones and E. Wells*

In order to improve my understanding of the interaction of atoms and molecules with intense laser fields and even more to learn the difficulties faced when conducting such experiments I have spent a few weeks working with Professor Jones at UVA on population trapping of Rydberg ions. This experience will hopefully help us make better progress in the development of our new initiative in this field.

Formation and decay mechanisms of doubly charged molecular ions (Sections A.3.7) -- *I. Ben-Itzhak, B.D. Esry, in collaboration with: A. Bar-David, I. Gertner, B. Rosner*

The measured mean lifetime of $^3He^4He^{2+}$ molecular ions has been attributed to high angular momentum states. It has been suggested that the source of this angular momentum is the creation mechanism of the $^3He^4He^+$ parent molecular ions in the ion source. Using a 3D-imaging technique[41] the mean lifetime and KER of long-lived $^3He^4He^{2+}$ molecular ions were determined to be τ=164±20 ns and $9.8\pm^{0.2}_{0.4}$ eV, respectively, in nice agreement with the calculated values for a distribution of states around the ν=1 and l=14,15 states. In order to determine if these high angular momentum states were measured just because they matched the range of high experimental sensitivity or because He_2^+ formation really peaks at high l values, we have recently conducted similar measurements of the homonuclear $^4He_2^{2+}$ dimers. For this isotope low l-states as well as high l-states are within the high sensitivity range of our experimental setup. Preliminary results suggest that high angular momentum states are preferred but more detailed data analysis is still needed.

Structure and Dynamics of Atoms, Ions, Molecules, and Surfaces: Ion-Atom Collisions with Laser Prepared Targets

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A.1.2 Charge Transfer in Extremely Slow Collisions Between Highly Charged Ions and Helium (B. D. DePaola, C. W. Fehrenbach, K. Okuno, and C. Verzani)

In the last progress report we described our octopole ion beam guide (OPIG) low energy collisions apparatus. At that time, charge state analysis was done through the use of an electrostatic retardation system, which placed limits on how much deceleration was possible with the OPIG. Nevertheless, useful measurements of single and double charge capture cross sections were measured and published [Pub. # 15] for Si^{q+}, q=3-5, down to collision energies of a few hundred eV. Since that time we modified the OPIG system in several ways. First of all, a pair of electric quadrupole lenses were added downstream of the OPIG in order to better control the exiting ion beam. Most importantly, we have replaced the electro-static charge-state analysis system with one consisting of an electromagnet and a position sensitive detector. With these improvements we have been able to extend the range of our collisions measurements to below 10 eV/u Ar^{9+}, with the possibility of going even lower. After making these improvements we have measured the absolute cross sections for single and double charge transfer as a function of collision velocity.

A.4.3 COLTRIMS with a Laser-Cooled Target: MOTRIMS (B. D. DePaola, C. L. Cocke, C. W. Fehrenbach, X. Flechard, and H. Nguyen)

Since the last report on this project, we have designed constructed, tested and implemented the entire MOTRIMS apparatus. The various components which have been added include the momentum spectrometer, two position-sensitive detectors, and the beamline and ion source. The data were of extremely high quality, having a momentum resolution of 0.03 a.u., a factor of two better than the best reported in the literature for conventional COLTRIMS, and an order of magnitude better than that reported in other MOTRIMS experiments. We have made studies of charge transfer cross sections for singly charged ions on rubidium in the ground state (5s) and in the excited states 5p and 4d. Throughout the range of collision energies studied (from 2 keV to 7 keV) all of the final state charge transfer channels were resolved, and cross sections, differential in scattering angle, were obtained with a resolution of roughly 25 μradians. Some of these results have been published [Pub. # 34] while other results are being prepared for publication. One of the important results coming from these studies was the realization that with our complete state selectivity and our complete control of the timing (both photon control and ion times of flight) in the experiments we have the capability of measuring both the cross sections and relative populations of ground and excited states of the rubidium *at the same time* and *independently of excitation models*. Thus, in addition to working as well as expected for the measurement of charge transfer cross sections, the apparatus has demonstrated utility in the measurement of the time-dependent dynamics in a magneto-optical trap.

STUDY OF HIGH HARMONIC GENERATION

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1. High harmonic generation with an OPA

Many nonperturbative laser-matter interactions (including high harmonic generation) are sensitive to the wavelength of the laser. It is therefore highly desirable to perform such studies with optical parametrical amplifiers (OPAs) that provide tunable wavelengths. Very recently, we have developed an OPA that is able to produce high intensity, $2x10^{14}$ W/cm^2. With it we demonstrated the first nonperturbtive OPA-noble gases interaction. We plan to upgrade the OPA for studying high harmonic generation. The x-ray spectrometer and detection system needed for this study exist in our lab.

1. *Upgrade of the high intensity OPA*. We will upgrade this OPA to produce intensities higher than 10^{15} W/cm^2. Our previous OPA intensity is limited by the laser energy, 1.2 mJ, that pumped the OPA. A 6 mJ, 20 fs kHz laser is currently under development in our lab. With this laser as the pump, we should be able to reach the 10^{15} W/cm^2 with a tunable wavelength from 1.1-1.6 μm (signal) and 1.6 to 2.6 μm (idler).

2. *HHG study with the OPA.* Much effort has been devoted to extend HHG into the keV x-ray regime, which will enable x-ray spectroscopy studies of the inner shell electrons and diffraction/absorption studies of solids with sub-femtosecond resolution. Recently we demonstrated that by using a long wavelength (~1.5 μm) infrared pump pulse, the cut-off photon energies were increased by a factor of two or more compared to that by conventional 800nm pump laser. It also shows that a harmonic wavelength can be easily tuned to cover any wavelength from the 5th order to the cutoff by changing the OPA wavelength. We will extend this study to gases that have larger ionization potentials and much higher saturation intensities. Our calculation shows that by changing the driving field wavelength from 0.8 μm to 1.6 μm, the cut-off of helium is extended from ~ 0.5 keV to ~ 2 keV. This will lead us to develop a tunable, coherent, ultrashort keV x-ray source. One of the major microscopic factors that affects that efficiency is the quantum diffusion of the electron wave packet in the laser field. Since quantum diffusion is sensitive to the change of the excitation wavelength, we will study this effect qualitatively by tuning the wavelength of the OPA.

2. High harmonic generation from ions

We have shown before that the mJ level pulses from a kHz laser can be focused to 10^{18} W/cm^2. Such an intensity is high enough to produce high harmonic generation from ionized noble gases. Since the cutoff photon energy is strongly dependent upon the ionization potential of the target, we expect to produce much more energetic photons from ions compared to neutral gases. This provides another way to produce keV x-rays through high harmonic generation. We intend to interact with pure ions instead of plasma to obtain clean results. The main difficulty is to create an ion target with enough numbers of ions for interaction with laser pulses. The JRM lab has developed a variety of ion sources in the past. We will combine our ion source expertise with our laser expertise to solve this problem.

Theoretical studies of interactions of atoms, molecules and surfaces

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B.1. Ejected-Electron Momentum Distributions in Time-Dependent Atomic Systems

***Progress last year*:**

The main focus of this project is to study the mechanism of ion impact ionization of atoms at low energies. We have adopted a semiclassical approach by expanding the wavefunctions in momentum space. In the last year, we finished the calculations for He^{2+} +H collisions. The results showed that it is possible to identify a saddle point mechanism for ionization if one looks for the change of longitudinal momentum distributions. This work has now been published (see pub. #39). Another relevant publication is #10.

We have also investigated the total ionization cross sections for the basic H^++H collisions in the 15-100 keV region. It turns out that there are large discrepancies among the many theoretical calculations and many experiments for this basic collision system. Our results support the other most sophisticated calculations by other methods, and the ionization cross sections are 20-40% higher than the experimental data. This work is completed and the paper has been accepted for publication in Phys. Rev. A. The previous postdoc Emil Sidky has left to take on a new job elsewhere.

***Current year plan*:**

We are not continuing the ion-atom ionization project at this time. We have recognized the limitation of the current theoretical model and the computer codes, which would not allow us to extend the calculation to large internuclear separation to extract the momentum distributions of the ionized electron. A new propagation technique was introduced by Brett Esry. Currently his postdoc Dr. Gou is working on this problem. We have shifted our research direction in this area to laser-atom interactions, with the aim of interacting with the experiments to be done by Dr. Zenghu Chang's group. We are using the scaled coordinates method to solve the time-dependent laser-atom interaction Hamiltonian. My graduate student Mr. Z. X. Zhao is working on this project. The scaled coordinates method has been applied to one-dimensional problems and the method has been shown to work well. A paper on this work has been submitted to Phys. Rev. A. He is generalizing the method to 2D and 3D and will concentrate on short-pulse lasers by working closely with the in-house experimental group once the code is debugged.

We will devote our major effort to laser-atom interactions in the coming years. A new postdoc, Dr. X. M. Tong, will join us at the end of October. He has plenty of experience in his area, and I expect him to make major contributions in this area.

In adopting scaled coordinates method we got extensive help from Brett Esry. On the other hand, we expect to assist him in his low-energy ion-atom ionization project in due time after the code is developed.

An alternative method for doing laser-atom collisions has been reported in Pub. # 1.

B2. Hyperspherical Approach to Ion-atom Collisions at Low Energies

Progress last year

The major thrust of this project is to perform benchmark calculations for cross sections in ion-atom collisions at low energies without the ambiguity of electron translational factors. There are three steps involved in order to carry out the calculations. First we need to obtain adiabatic hyperspherical potential curves and coupling terms. Second we need efficient ways to integrate the hyperradial equations. Third, we need to be able to carry out the 2D matching at a large hyperradius. The first step was done earlier but we faced many problems in step 2 and step 3 for a few months in the last year. (A simple two-channel calculation was reported in Pub. #11)

Current year plan:

Early this year I put the postdoc Chiennan Liu on this project. He has since succeeded in completing step 2 and step 3 for the test cases. More precisely, he has a code working, which allows him to calculate the inelastic scattering cross sections for any three-body systems, calculated within the framework of hyperspherical coordinates. To generalize the code to ion-atom collisions specifically, additional coding has to be done so that calculations involving thousands of partial waves can be carried out. On the other hand, when time is available we may start doing some atom-diatom collisions at low energies. I expect that we will be able to finish all the computer codes within the next six months to start carrying out actual calculations.

B3. Analysis of Electron Correlations of Triply Excited States of Atoms

Progress last year:

In the last year we have succeeded in identifying all the normal modes of the sixty-four 3l3l’3l” triply excited states of a model atom. With these normal modes identified we were able to classify all the 64 states into manifolds according to their inherent normal modes, and showed that states in each manifold form a rotational multiplet similar to that of a symmetric top. We showed that intrashell triply excited states of real atoms, such as those calculated for N^{2+} and N^{4+}, can indeed be grouped according to the manifolds of the model atom. Thus we can claim *that the classification of intrashell triply excited states has been completed*. A paper describing this work has been submitted and accepted by Phys. Rev. A. (A shorter report on this work is in Pub. #40)

Current year plan:

After the classifications of intrashell triply excited states are completed, we are working on the classification of intershell triply excited states. We are focusing on the 2l2l’3l” triply excited states. We have now identified the best way to visualize the wavefunctions of these states, and several new normal modes have emerged for the intershell states. We expect to finish this project within the coming grant period.

B4. Weakly Bound Molecular Systems

Progress last year

We have carried out an investigation of the rotational excited states of Helium trimers. This work has been completed and published (see pub. #36).

Current year plan:

No new projects in mind at present.

B5. Electron Capture and Excitations in ion-atom collisions and other systems

***Progress last year*:**

We have performed some calculations for transfer ionization cross sections for collision systems studied by Richard's group. For protons on He, we carried out two-electron model calculations. For more complex systems such as F^{9+} on He, we have to use the independent electron model. In connection with the experiments of DePaola's group, we are also performing calculations for electron capture from laser-cooled alkali atoms.

Last year we also completed the investigation of the radiative decay rates of He doubly excited states below the $He^{+}(N=2)$ threshold. Our timely investigations have stimulated additional experimental measurements. This work has now been published; see Pub. #37. There is no new plan on this particular subject.

Other publications, mostly with experimentalists, are in Pub. #2,7,8,9,29,38.

***Current year plan*:**

Mr. Teck Lee is the graduate student working on ion-atom collisions now. We expect to examine the collision systems studied by the experimentalists carefully. This includes total electron capture cross sections from the ground state and the excited states, as well as the differential cross sections, for the in-house MOTRIMS experiments. The experimentalists are expected to obtain very accurate relative total cross sections, which can be tested by our calculations.

7. B.9. Interactions of Atoms and Ions with Surfaces, Clusters, and Thin Films

Uwe Thumm

7.1 (B.9.1.) Electron Capture from Thin Metallic Films

Recent progress: Based on the self-energy method for charge transfer in ion--surface collision, we are investigating the broadening of atomic levels near thin metallic films. Size quantization in the growth direction of the film gives rise to characteristic structures in level widths, atomic occupation probabilities, and transition distances as a function of the film thickness [1]. The large variation of the calculated transition distances with the film thickness may result in observable effects in atomic interactions with thin films.

Future plans: We plan to calculate the full electronic self-energy of hydrogenic atoms interacting with thin metallic films and layered nano--structures. Adiabatic resonance states generated from the self-energy for thin film targets will serve as basis states in time-dependent close-coupling calculations for the electronic dynamics in atom-film interactions, in close analogy to the semi-infinite case of a metal surface [2].

7.2 (B.9.2.) Charge--Transfer Dynamics Near Metal Surfaces

Recent progress: Within a new two-center close-coupling expansion, we solved the time-dependent Schrödinger equation for an active electron interacting with a slow projectile and a metal surface. The continuum of metal conduction band states is discretized in terms of wave packets.

Future plans: The efficient discretization of (ionization or conduction band) continua is an outstanding problem that requires the (often neglected) careful analysis of convergence, dephasing, and recurrence effects [3]. We intend to streamline our code and to increase the number of states that represent the discretized conduction band continuum in order to fully eliminate recurrence effects, even at very slow projectile velocities.

7.3 (B.9.3.) Wave-Packet Propagation Techniques Applied to Ion-Surface Interactions

Recent progress: Apart from contributing to the qualitative understanding of the interaction mechanisms, e.g., through computer animations, the direct propagation of the wave function on a numerical grid also enables the quantitative assessment of (one--electron) charge transfer. The wave function at any time *t* is given by (in atomic units)

$$\Psi(\vec{r},\vec{D},t) = \exp\{-iH(\vec{r},\vec{D})t\}\,\Psi_0(\vec{r},\vec{D}), \quad H = T + V_{\mathrm{surface}} + V_{\mathrm{atom}}. \tag{1}$$

The ion--survival probability is obtained by following the reflected projectile until the integrated probability density around the projectile has reached a stable value. So far, our calculations are based on the corrugated surface potential

$$V_{\mathrm{surface}}(\vec{r}) = 0.5[\Theta(z)-1][1+0.5\cos(x)\cos(y)\cos(z)], \quad \Theta(z) = \mathrm{atan}(z)/\pi + 0.5. \tag{2}$$

Θ is a smeared--out step function. The effective potential for H^- was modeled by regularizing

$$V_{atom}(r_p) = -(1+\frac{1}{r_p})\exp(-2r_p) - \frac{\alpha}{r_p^4}\exp(-\frac{r_0^2}{r_p^2}) \qquad (3)$$

at the origin. r_p measures the distance from the projectile center, $\alpha = 2.25$ is the atomic polarizability of H, and $r_0^2 = 2.547$. The projectile is led along a broken—straight--line trajectory, starting at t=0 at a distance of 30 a.u. from the jellium edge of the surface with an incident velocity $(v_x,v_z)=(0.1,-0.1)$ and with $d_{min}=2$. Boundary conditions at the edge of the grid were imposed by a suitable absorptive complex potential. The ion--survival probability, obtained by integration over the atomic probability density at t=600 amounts to 0.07 [4].

Future plans: We intend a detailed investigation of the influence of crystal orientation, surface states, and image states of the substrate on the transfer of charge to and from a projectile.

7.4 (B.10.) Ionization in Intense Laser Fields: Distribution of Emitted Electron Momenta

Recent progress: The basic features of single ionization by a strong, short laser pulse can be studied within the restricted dimensionality of a 1D (soft-core Coulomb) model atom. We expose the atomic ground state $\psi_0(x)$ to a laser pulse of the form $V_L(x,t) = E_0 f(t)\sin(\omega t)x$, with a Gaussian envelope function f(t) of width of 500. We further assume a laser wavelength of 780 nm and an intensity of I=10^{15} W/cm^2 = 0.0285. The Keldysh parameter $\gamma = \sqrt{\varepsilon_i/(2U_p)} = 0.4$ is < 1 which favors tunneling as the most likely ionization mechanism. Due to the interaction of the atom with the laser pulse, the electronic wave function evolves according to

$$\psi(x,t) = \exp\{-i\int^{i} dt' H(x,t')\}\psi_0(x), \quad H(x,t) = T + V_{1D}(x) + V_L(x,t). \qquad (4)$$

T is the electron's kinetic energy. We obtain the time-dependent wave function $\psi(x,t)$ by numerically propagating ψ_0 using the split-operator, Cranck-Nicholson method.

In order to extract momentum-differential emission probabilities from our calculation, we introduce small `detection intervals' to the right and to the left of the atom that lie outside the classical excursion range x_{exc} of the electron. We choose these intervals at I_L = [-250, -225] and I_R = [225, 250]. Next, we define a momentum grid $\{p_j\}$ with step size $\delta p = 0.04$.

The probability $dP_R(p_j,\delta p)$ for emission of an electron with momenta in the interval $I(p_j,\delta p) = [p_j - \delta p/2, p_j + \delta p/2]$ an now be related to the 1D released current $j_R = \mathrm{Re}[\int_{I_R} dx\,\psi^* p \psi\}$ and the momentum expectation value in the interval I_R, $<p>_R$, according to $dP_R(p_j,\delta p) = \int dt\; j_R\; \Theta(p_j,\delta p)$ where $\Theta(p_j,\delta p) = 1$ if $<p>_R \in I(p_j,\delta p)$ and $\Theta(p_j,\delta p) = 0$ for all other $<p>_R$. For emission to the left, j_L,dP_L,$<p>_L$ are obtained in the same way. The sum of dP_R and dP_L shows a dip around momenta $p = 0$, in qualitative agreement with the double-hump momentum distribution found in recent single ionization measurements.

Future plans: We intend to investigate the Fourier transform of $C(t) = \int dx\, \psi(x,t)^* \psi_0(x)$ in an attempt to identify and characterize field—induced resonances. We have started to investigate double ionization of 2D model atoms.

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B.D. Esry

(Section numbers correspond to the original proposal)

Program Scope

The goal of this research program, begun in the last year, is to explore the few-body problem in a variety of circumstances including bound states, collisions, and in external fields. A major component of this program is to develop novel theoretical tools required for this effort. In the last year, special emphasis has been placed on developing a general method for treating time-dependent wave functions in scaled coordinates. This scaling method promises considerable computational savings, thus making a larger class of systems amenable to time-dependent calculations. Applications of this new approach and plans for other projects are also addressed.

B.6 New Initiative: Time-Dependent Treatment of Continuum Phenomena

Recent progress

After many years of investigation, the theory for ion-atom collisions is well developed and can handle bound-bound transitions quite reliably. Bound-free processes, on the other hand, are much less reliably treated, but progress is being made | largely with time-dependent methods. One problem that continues to plague current theoretical treatments is the inability to integrate the Schrödinger equation to large internuclear separations. Such long-time propagation is necessary to make the final state analysis less ambiguous, especially for low-energy collisions. The final momentum distribution of the ionized electron can then be extracted and compared with both experimental results and existing theory. It is hoped that with a cleaner asymptotic analysis we can help resolve the discrepancies remaining between them. We have developed a representation for the time-dependent Schrödinger equation that simplifies the problem considerably [14]. The new representation, a combination of a coordinate and a wave function transformation, removes nearly all of the effects of kinetic energy from the wave function. This "scaling" representation eliminates the necessity of absorbing boundaries, allowing essentially boundary-free propagation of the wave function. It is then only necessary to propagate the relatively smooth envelope of the continuum wavepacket. In collaboration with C.D. Lin, the scaling method has since been applied to the model problem of an intense laser interacting with a one-dimensional atom. It was found there that the scaling does indeed reduce the computational burden by roughly an order of magnitude on average. My postdoc, Wei Guo, arrived in August and has begun to apply the scaling method to the standard one-electron, straightline nuclear trajectory problem. While the transformed three-dimensional Schrödinger equation has been derived, he has begun coding and testing a one-dimensional model of the collision. The motivation for beginning with such a model is, in part, to give him some experience with the time-dependent techniques which are new for him. Also, it gives us the opportunity to explore the scaling method for this application in an efficient manner since the one-dimensional model already contains all of the elements peculiar to the scaling method.

Future plans

Once we understand scaling for the one-dimensional model, we will proceed to the full three-dimensional calculation. The first system we will study is *p*+H(1*s*); this is the most fundamental system to understand and there are a number of other studies to compare with. There appear to be few obstacles to a successful implementation of the method, but even within the scaling approach we are considering different schemes whose relative efficiency must be evaluated. The scaling method has the potential to allow integration to very large times and thus unambiguous analysis, but remains to be explored for ion-atom collisions.

B.7 New Initiative: Rearrangement Processes in Asymmetric Three-Body Systems

Recent progress

The vast majority of problems of current interest in atomic physics are described by a Schrödinger equation that is not separable in any coordinate system. Adiabatic approximations, such as the Born-Oppenheimer approximation, are convenient and powerful tools for dealing with such equations. Unfortunately, at the very points where the physics gets interesting | near the avoided crossings | the numerical treatment gets difficult. It follows that a representation that does not have avoided crossings would be desirable. Such representations are generically called diabatic, but it is difficult in general to generate a diabatic representation that includes as much physics as compactly as the adiabatic representation. I have recently finished developing one possible diabatization scheme with Hossein Sadeghpour that is a mixed representation. Standard, strict diabatic transformations are well known and require the nonadiabatic derivative coupling. Since our representation is based upon the same equation but with only part of the nonadiabatic coupling included, we have dubbed it the \split diabatic representation". No approximations are made, however, since the remaining coupling is retained in its adiabatic form. The new representation can thus be considered a mixed representation since it is neither purely diabatic nor purely adiabatic, but the avoided crossings are eliminated. The split diabatic representation also avoids one of the problems of the strict diabatic representation, namely the unphysical behavior of the diabatic potentials at large distances. It turns out that because of long range nonadiabatic coupling | present for both the Born-Oppenheimer and the adiabatic hyperspherical representations | the strict diabatic potential curves oscillate sinusoidally at large distances. The long range portion of the nonadiabatic coupling need not be included in the definition of the split diabatic representation, though, so the asymptotic potential curves coincide precisely with the physically appealing adiabatic potentials.

Future plans

We intend to explore applications of the split diabatic representation. In particular, one advantage of adiabatic representation is the ability to selectively include or exclude individual channels. The advantage begin that including only physically important channels can greatly improve the computational efficiency. While the split diabatic representation produces physical potential curves and has the potential to reduce the number of channels, it is not suitable for automatic application to a large number of channels because someone must decide what part of the coupling to use in the definition. We will thus also seek diabatic representations that are suitable for large problems.

B.8 New Initiative: Hyperspherical Approach to Four-Body Systems

Recent progress

The extension of the hyperspherical approach to arbitrary mass Coulomb four-body problem promises all of the benefits it has provided for the study of the three-body problem. It also promises to be a significant computational challenge. I have started writing the computer code to solve the problem of the Ps_2\molecule", i.e. two electrons and two positrons.

Future plans

I will continue to develop the four-body code as time permits - this project is a lower priority than the two described above. I do not plan to assign any postdoc or student to this project at this time.

Contributions to other JRML efforts

I have long maintained collaborations with experimentalists in our program. The publications that have resulted and appeared in the last year are Refs. [4,12,13,36,43] from the publication list. I have also been working closely with C.D. Lin's group on very low energy ion-atom collisions in hyper-spherical coordinates.

FINANCIAL REPORT

It is anticipated that there will be no unexpended funds for the current funding period.

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