**THEORETICAL ATOMIC COLLISION PHYSICS
PROGRESS 1990-91
N.F. Lane, Rice University and Rice Quantum Institute**

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I ABSTRACT

The theoretical atomic physics program at Rice University focuses on obtaining a better understanding of the mechanisms that control inelastic collisions between excited atoms and atoms, molecules and ions. Particular attention is given to systems and processes that are of potential importance to advanced energy technologies. In the current year, significant progress has been made in quantitative studies of: quenching of low-Rydberg Na atoms in thermal energy collisions with He, Ne and Ar atoms; selective excitation resulting from charge transfer in collisions of highly stripped ions of He, Li, C, and with Li, Na and He atoms and H₂ molecules at keV energies; differential elastic and single, and double electron transfer in He⁺⁺ collisions with He at keV energies; inelastic electron-transfer in ultra-low-energy-energy (T=8 to 80K) collisions between ³He⁺ and ⁴He and ⁴He⁺ and ³He; a formalism for ionization by electron impact of ions in dense, high-temperature plasmas.

II BACKGROUND AND INTRODUCTION

(Please note that this section and the following section on progress in the current grant year are essentially identical to the respective sections of the renewal proposal for 1991-94)

The theoretical atomic and molecular physics program at Rice University has addressed a wide range of basic atomic collision and radiative phenomena of possible importance to advanced energy technologies, e.g. controlled fusion, and applicable to research in astrophysics, atmospheric physics, plasma physics, and other physical sciences.

Specifically, in the 1970's the Rice theory program emphasized studies of: electron-molecule scattering;¹ slow ion, atom, and molecule collisions;² Penning ionization of atoms and molecules;³ charge-transfer;⁴ ion-surface interactions;⁵ and excited atoms in quantum liquids.⁶ In the early part of the 1980's the program stressed: electron and ion collisions in dense, hot, plasmas;^{7,8} radiative (emission and absorption) charge transfer in slow ion-atom collisions;⁹ approximate exchange/correlation potentials for electron scattering and photoionization processes;¹⁰ classical studies of collisions of high-Rydberg atoms with polar molecules;¹¹ model threshold study of vibrational excitation of CO₂.¹² In the grant period 1984-87, the emphasis of the Rice program continued to shift toward heavy-particle collisions at low-to-intermediate energies including: excitation and charge-transfer¹³⁻¹⁹; Rydberg atom collisions^{20,21}; Penning ionization^{22,23} and collisions processes in plasmas.^{24,25} Dr. Mineo Kimura joined the group in 1984-85, when the PI's research group was located at JILA (University of Colorado), as a postdoctoral Research Associate. Dr. Kimura moved to Argonne National Laboratory in 1986, when the PI returned to Rice University; however many research projects launched at JILA were continued in subsequent years and new collaborative projects were initiated. This collaboration has brought new expertise, techniques and insights to the program and has made it possible for this group to move into some new areas of atomic collisions research.

The past three years, 1987-90, have been particularly productive. Quantum mechanical and semi-classical methods were used to obtain information, some of which has been reported,²⁶⁻⁶⁸ in several areas:

- alignment and orientation in Li^+/He , Na^+/He , Li/He , Na/He , H/He , H^+/He and He^+/H collisions 26, 37, 38, 52, 58
- differential elastic and charge-transfer cross sections for He^{2+}/H , He^{2+}/He , H^+/He , H^+/H_2 collisions 29, 53, 60, 61
- charge-transfer cross sections for collisions of fully stripped ions ($Z=6-9$) and selected partially stripped ions with H and H_2 27, 66
- charge-transfer cross sections for collisions of He^{2+} , He^+ , C^{4+} , C^{6+} , N^{7+} and O^{6+} ions with He atoms and for He^+/Na collisions 32, 34, 39, 49
- selective state charge transfer in He^{2+}/Na , Li^{2+}/H , and Li^{3+}/Li collisions 42, 54, 55
- low-energy radiative and non-radiative charge transfer in He^+/H and H^+/He collisions 48, 65
- very-low-energy charge-transfer collisions of He^+ with H_2 molecules and the slightly non-resonant $^3\text{He}^+/\text{}^4\text{He}$ and $^4\text{He}^+/\text{}^3\text{He}$ collisions 63, 64
- Penning ionization cross sections and electron-energy distributions in collisions of $\text{He}(2^1,3\text{S})$ atoms with Na and K at thermal energies 30, 45, 46
- Penning and associative ionization and ion-pair formation in collisions of $\text{He}(2^1,3\text{S})$ atoms with Li at low and intermediate energies 57
- quenching cross sections for collisions between low-Rydberg $\text{Na}(\text{ns})$ atoms and rare-gas atoms at thermal energies 47, 62
- state-changing cross sections for collisions between Rydberg $\text{Rb}(\text{nl})$ atoms with HF and HCl molecules over a range of energies and initial quantum numbers 28, 56
- momentum transfer in electron collisions with polyatomic molecules 40, 58a
- ionization rates in dense, high-temperature ICF plasmas 68

This list includes several projects that involved visiting scientists who were at Rice for short periods and some of whom received modest support from the grant.^{31, 32, 40-43, 49, 58a, 66, 67} Other papers mentioned above that are not co-authored by the PI report work initiated or performed by Dr. Kimura when he was supported by the grant.^{33-36, 39} Also, a number of articles of a general nature were published during this period.^{38, 44, 50, 51}

For the next proposed grant period 1991-94, we plan a much more focused program of research. The proposal also anticipates less direct involvement of Dr. Kimura, who has a very active independent research program and a number of collaborations. It is anticipated, however, that Dr. Kimura will continue some level of interaction with the PI and his group and with others.

We continue to be influenced by the experimental activities at the Rice Quantum Institute (RQI), particularly the groups of G.K. Walters, R.F. Stebbings and F.B. Dunning, at JILA (Univ. of Colo. and NIST), and at the DOE national laboratories. We also benefit from collaborations with theoretical colleagues at Rice and at other institutions.

III PROGRESS IN CURRENT GRANT YEAR

This section contains only a very brief account of progress, so far, under the current one-year grant; essentially, it is an updated and revised version of the text included in Abstracts of the 1990 DOE Contractors Workshop.⁶⁹ Some of this work is a continuation of research begun under the earlier three-year grant covering the period July 1, 1987 - June 30, 1990 and briefly summarized in Sec. II and reported in detail in the Progress Report that accompanied last year's renewal proposal.⁷⁰ Progress has been made in several areas:

RYDBERG ATOM COLLISIONS (A. Kumar, B. Saha, M. Kimura, N. Lane)

We have extended our earlier study of quenching of Rydberg Na atoms in thermal-energy collisions with He atoms⁴⁷ to the cases of Ne and Ar targets, in order to investigate several trends, e.g., the variation in the s-to-f (and $L>3$) propensity rule, for different electron-atom interactions. As in the earlier studies, multi-state, semi-classical, impact-parameter close coupling calculations are performed using as a basis, the adiabatic molecular orbitals obtained from a one-electron CI calculation, in which the Ne and Ar atoms and the alkali-atom core are represented by pseudopotentials. Rydberg states having $L>3$ are not included; we assume that $L=3$ states mix readily with $L>3$ states at large separations.

Briefly, we have found that for Na(9s) in thermal-energy collisions with Ne and Ar atoms, downward transitions dominate, as observed in the measurements;⁷⁴ the cross sections for upward transitions are seen to increase with increasing velocity. The s-to-f and ($L > 3$) propensity rule is not found to be present for 9s, where the transition to 8p dominates both for Ne and Ar, but is expected at higher values of n , perhaps 10 or 11. The comparison with measured quenching rates (at 425K) for Ar are similar to those for He, viz. the calculated rates are about two to three times larger than the measured values. The ratio of the calculated rates for Ar/He is 1.22 in excellent agreement with the experimental ratio of 1.26. We are not aware of any measurements for the Ne target, where we find the corresponding ratio for Ar/Ne to be 2.18 and He/Ne to be 1.79. As found in many physical circumstances, Ne is a more weakly interacting collision partner than either He or Ar due to the strong cancellation of exchange and polarization in the electron-Ne interaction in contrast with that of He, which is dominated by the former, and Ar, which is dominated by the latter.

In addition, we have applied the same approach to thermal collisions of Rydberg Li atoms with He in order to examine the significance of a different ordering and spacing of the Rydberg levels (Li and Na have quite different quantum defects) and the corresponding differences in avoided crossings and coupling matrix elements. We find that downward transitions still dominate and that the s-to-f (and $L>3$) propensity rule holds, e.g. for initial states 6s and higher, but the dominant transition is from ns to $(n-1)f$, rather than to $(n-2)f$ as is the case with Na Rydberg collisions. The explanation lies in the ordering of the relevant adiabatic energy curves and the nature of the coupling. We also performed selected two-state quantum mechanical calculations to establish a degree of confidence in our semi-classical results. A paper reporting these results is in preparation for publication.⁶²

In the future we plan to extend the Rydberg atom collision research to explore several areas, including: oriented and aligned initial Rydberg states; intracollisional interference effects; very low collision energies, where quantum collision effects are important; ion-pair formation in collisions with electron-attaching targets; interference between Rydberg state-changing and Penning ionization and ion-pair formation; and charge transfer in collisions with ions.

ION-ATOM (MOLECULE) COLLISIONS (A. Kumar, B. Saha, C. Dutta, M. Kimura, N. Lane)

We are in the process of completing a series of semi-classical close-coupling calculations of partial cross sections for selective excitation, via charge transfer, in collisions of highly stripped ions with rare-gas and alkali atoms and with H_2 . These processes are of possible importance to advanced short-wavelength laser systems. In addition to our published studies of He^{2+}/Na and Li^{3+}/Li collisions^{54,55}, we have obtained results, in a few cases preliminary, for collision energies in the range of 0.1 to 10 keV/amu for the systems: C^{6+}/Na , C^{4+}/Na , N^{7+}/Na , N^{5+}/Na , He^{2+}/H_2 , and C^{4+}/H_2 , with work underway on C^{4+}/He , which may provide some insight into the process of double charge transfer in C^{5+}/He collisions, for which experimental results are available.⁷⁵ The dominant mechanism for charge transfer in these systems is an avoided crossing with a state correlating asymptotically with an excited-state manifold of the final ion, $C^{5+}(n=4)$, $C^{3+}(n=3)$, etc. The outermost crossings (with the highest energetically accessible states) are often diabatic; these are routinely examined to insure that their contributions are indeed small. In all cases, the molecular orbitals used as the collision basis set are determined by means of a CI calculation in which all closed shells are represented by pseudopotentials. We intend to complete most of these studies in the current grant year, and are preparing papers for publication.⁷¹⁻⁷³ Limited extensions of studies of this type will be proposed in the future for systems and processes of particular importance. There is a clear need to refine the model e- H_2 potential so that it can be used at small internuclear separations, say $R < 1$ a.u., where some important interactions leading to charge-transfer can occur. We are interested in pursuing this in future years.

In order to help with the interpretation of the beautiful high resolution measurements made by Stebbings' group at Rice of differential cross sections for elastic scattering and single, and double charge transfer in He^{++}/He collisions (keV range), we have performed a number of quantum mechanical calculations. The agreement between the calculated and measured differential cross sections for elastic and double charge transfer is good, provided that a diabatic potential is selected for the gerade symmetry, as one would expect. Structure in the differential cross sections arises from rainbow scattering (very small angles), diffraction (larger angles) and g-u interference (still larger angles). The measurements resolve all features except the very subtle rainbows. Because we limited the single-electron-transfer study to two states, only fair agreement is obtained with the measurements. A paper is in preparation for publication.⁶¹

We have completed calculations of cross sections and rates for quasi-resonant charge transfer in very low-energy collisions, e.g. $T=8K$ to $80K$, of $^3He^+ + ^4He$ (endothermic) and $^4He^+ + ^3He$ (exothermic), using the theory of Thorson and Delos^{76,77} In comparison

with the recent experiments of Schauer et. al.,⁷⁸ we obtain good agreement with the individual measured rates and excellent agreement with the independently measured ratios of the rates.

IONIZATION IN DENSE HIGH-TEMPERATURE PLASMAS (J. Weisheit and N.F. Lane)

Progress continues to be made in the development of high-power lasers and in the efficiency with which this power is coupled to implosion targets: plasma densities N_e in excess of 10^{24} electrons/cm³ recently have been reported.^{79,80} Atomic ions must be strongly perturbed by such an environment, in which the mean inter-electron separation is less than a Bohr radius. Because spectroscopy provides the most detailed information on these implosion experiments, the understanding of how a dense plasma modifies atomic collisional and radiative processes remains an important subject of research.

For the past several years we have carried out a series of studies of dense plasma effects on atomic collisions. These focussed first on bound-state excitations by ion and by electron impact.^{7,24,25} The present focus is on electron-impact excitations to the continuum, i.e., ionization. As in the case of bound-bound transitions, one key issue is how to handle the simultaneous interactions of a target ion with a large number of plasma electrons. Here, we have decided to extend the formalism recently developed for *excitation* via plasma fluctuations⁸¹ to treat ionization too. In this theory, the traditional concept of a cross section (which is eventually averaged with respect to a distribution of collision speeds to produce a rate coefficient) is dropped in favor of a direct calculation of the probability of a transition due to stochastic changes in the plasma's local electric field. These changes are fully characterized by the dynamic structure factor S_{ee} , which is the Fourier transform of the autocorrelation function of plasma density fluctuations.^{82,83} The general, first-order expression we have derived for the probability of ionizing an electron bound in state "n" by an amount I is

$$W_n = (8\pi\alpha a_0^2 c N_e) \int_1^\infty \frac{dE}{E} \int_0^\infty dk S_{ee}(k, \omega_E) [df_n(k, E)/dE],$$

where the constants multiplying the iterated integral have their usual meanings, $E = \hbar\omega_E$ is the energy transferred to the bound electron, and df_n/dE is the generalized oscillator strength per unit (continuum) energy interval.⁸⁴ At present, we are carrying out numerical calculations for a variety of approximations to the plasma structure factor -- weak or strong Coulomb coupling, dynamic or static response, plus a variety of approximations to the oscillator strength density, including the binary encounter formula,⁸⁵ and Fock's plane-wave formula⁸⁶ for hydrogenic states.

The main result we intend to establish is the extent to which high plasma density modifies the rate of ionization of excited ionic levels, especially those near the continuum. Also of importance is a determination of the accuracy of the several approximations listed above. And, finally, we hope to make a formal connection between this work and recent studies of the enhancement of three-body recombination rates by collective effects (plasmon emission) in dense, cool plasmas.⁸⁷⁻⁸⁹

This project completes a series of collaborative investigations involving the PI and Dr. Jon Weisheit, begun when Dr. Weisheit was at the Lawrence Livermore National Laboratory. Dr. Weisheit received some support from the grant during the summer of 1990. The PI does not propose extension of this work, at least in the near future.

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V. PROJECT PERSONNEL

A. LIST OF PERSONNEL WORKING ON PROJECT (from July 1, 1990)

The research personnel working on the project this year include:

Bidhan Saha
Research Associate- full time
Department of Physics
Rice University
(partially supported by the Robert A. Welch Foundation)

Chizuko Dutta
Research Associate- part time
Department of Physics
Rice University

Mineo Kimura
Research Scientist
Argonne National Laboratory
(no salary from this grant)

Jon Weisheit
Professor of Space Physics and Astronomy
Rice University
(worked on project part of summer 1990)

Neal Lane, Principal Investigator

B. CHANGES IN PERSONNEL DURING GRANT PERIOD (from July 1, 1990)

The only significant personnel change was the departure of Dr. Anil Kumar, who was a Research Associate on the project and who returned to his university in India in the summer of 1990.

C. TIME DEVOTED TO PROJECT BY PRINCIPAL INVESTIGATOR

Neal Lane devoted 20% time to the grant during the academic year 1989-90 and 50% time during each of the summer periods.

VI. PUBLICATIONS ARISING FROM GRANT

A. PUBLISHED IN 1990 OR ACCEPTED

A. Kumar, N.F. Lane and M. Kimura, "Selective-state charge transfer in a collision between an alpha particle and ground-state Na: a molecular-states approach," Phys. Rev. A **42**, 3861 (1990).

A. Kumar, N.F. Lane and M. Kimura, "Selective-state charge transfer in a collision between a Li^{3+} ion and a ground-state Li atom: a molecular state approach," Phys. Rev. A **42**, xxxx (1990).

M. Kimura and N. F. Lane, "Semi-Classical Study of the Collision of a Highly Excited Rydberg Atom with the Molecules HF and HCl," *Phys. Rev.* **42**, 1258 (1990)

M. Kimura and N.F. Lane, "Theoretical Study of Ion Pair Formation and Penning and Associative Ionization in Low-to-Intermediate energy $\text{He}^*(2^1,3\text{S}) + \text{Li}$ Collisions," *Phys. Rev.* **41**, 5938 (1990).

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H. Tanaka, L. Boesten, H. Sato, M. Kimura, M.A. Dillon and D. Spence, "Elastic and Vibrational Differential Cross Sections for Collisions of Low- and Intermediate-energy Electrons with Silane", *J. Phys. B* **23**, 577 (1990).

(Dr. Sato was a summer visitor who received a small amount of support from the grant)

B. SUBMITTED OR IN ADVANCED STAGES OF PREPARATION

Some of the following papers are co-authored by Dr. H. Sato and Dr. N. Shimakura, who visited Rice for short periods during the summers and received very modest support from the grant. These papers acknowledge the DOE OBES Division of Chemical Sciences.

L.K. Johnson, R.S. Gao, G.J. Smith, C.L. Hakes, K.A. Smith, N.F. Lane, R.B. Stebbings and M. Kimura, "Absolute Differential Cross Sections for Small-Angle Direct, Single-, and Double-Charge-Transfer Scattering of Protons from H_2 ," (in preparation).

B. Saha, A. Kumar, N.F. Lane, and M. Kimura, "Quenching of low-lying Rydberg states of Li and Na induced by thermal-energy collisions with rare-gas atoms: a comparative study," (in preparation).

M. Kimura and N.F. Lane, "Theoretical study of charge transfer in $\text{He}^+ + \text{H}_2$ collisions in the meV regime," (submitted for publication).

C. M. Dutta, M. Kimura, and N.F. Lane, "Theoretical Study of Non-resonant Charge Transfer in the Region of the Threshold to 60K for $^3\text{He}^+ + ^4\text{He} \rightarrow ^4\text{He}^+ + ^3\text{He}$," (submitted for publication).

M. Kimura, N.F. Lane, A. Dalgarno, and R.G. Dixon, "Inelastic Processes in collisions of H^+ with He," (in preparation).

N. Shimakura and M. Kimura, "Electron capture in collisions of N^{5+} ions with H atoms from the meV to keV energy regions," (submitted for publication).

M. Kimura, H. Sato, and N.F. Lane, "Two-electron excitation in low-energy collision of Li^+ with He," (in preparation).

J. C. Weisheit and N.F. Lane, "Ionization by electron impact in dense, high-temperature plasmas" (in preparation).

A. Kumar, B. Saha, C. Dutta, M. Kimura, and N.F. Lane, "Selective-state charge transfer in collisions of highly stripped ions of C and N with Na" (in preparation).

B. Saha, M. Kimura, and N.F. Lane, " Selective-state charge transfer in collisions of He^{2+} and C^{4+} ions with H_2 " (in preparation).

C. Dutta, M. Kimura, and N.F. Lane, "Double charge transfer in a collision between C^{4+} and He" (in preparation for submission).

R.S. Gao, C.M. Dutta, N.F. Lane, K.A. Smith, R.F. Stebbings and M. Kimura, "Theoretical and experimental studies of $\text{He}^{2+} + \text{He}$ system: Cross sections for direction elastic and single-, and double charge transfer scattering of KeV energies," (in preparation).

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