

THEORETICAL INVESTIGATION OF ELECTRON- POSITIVE ION/ATOM INTERACTIONS

Progress Report

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MASTER

INTRODUCTION

Photoionization cross sections and matrix elements for ground and excited states are important in Resonance Ionization Spectroscopy¹ and one-atom detection. Some transitions in Na and K are important in studies of chemically driven visible laser amplifiers using fast near-resonant energy transfer.² On the fundamental side, van der Waals forces and the Casimir force represent the limiting cases of cavity QED and the resonance lines of Na and Rb may be studied in the laboratory to test QED.³ Also, the atomic physics of multicharged and many-electron ions and their behavior under different plasma conditions is needed to search for new X-ray laser active media, particularly to reach the "water window"⁴ where the highest difference between the absorption coefficients of O and C occurs.

COMPLETED RESEARCH

For the period covered by this report we investigated and accomplished the following:

A. Electron Scattering from Atomic K.

Electron impact elastic, excitation and total cross sections for K have been investigated¹⁰ using elaborate CI target wave functions in the close-coupling approximation. Coupling effects have been studied by comparing 7CC and 5CC results. The 7CC calculation coupled the states $4s\ ^2S$, $5s\ ^2S$, $3d\ ^2D$, $4p\ ^2P^0$, $4d\ ^2D$, $5p\ ^2P^0$ and $6s\ ^2S$ while the 5CC consisted of the 7CC states less the $4d\ ^2D$ the $6s\ ^2S$ states. We found the important result that the cross section for the dipole-forbidden transition $4s\ ^2S \rightarrow 3d\ ^2D$ is large due to the virtual double-dipole mechanism.⁵ For the total cross section, σ_T there is a large discrepancy near threshold between the Kwan et. al.⁶ measurement on the one hand and other data on the other hand.

Our⁷ calculation indicates that near threshold the elastic cross section, σ_e dominates the resonance cross section, σ_R and the sum of excitation cross sections other than σ_R , σ_0 . This dominance by σ_e near threshold explains the underestimation of σ_T by the Kwan et. al. measurement since it measures σ_e inaccurately near threshold. Furthermore, the Phelps et. al.⁸ measured σ_R shows a minimum in the electron energy interval $2 \leq E \leq 10$ eV, while other data, including the Chen and Gallagher⁹ one, do not. Consequently, the Walters-Phelps⁶ curve may be improperly constructed by Kwan et. al.

B. Photoionization of Na near the $2s^2 2p^5 3s$ and $2s 2p^6 3s$ Innershell Thresholds

Photoionization cross sections from ground state Na have been measured^{10,11} and calculated¹² near the $2s^2 2p^5 3s$ and $2s 2p^6 3s$ inner-shell thresholds. Also, the

photoionization cross sections of excited $3p\ ^2P^0$ and $3d\ ^2D$ states have been calculated¹³ using the R-matrix Methodology¹⁴ near the $2s2p^63s$ thresholds. In this energy region, the ground and excited state photoionization cross sections are characterized by reach resonance structures converging to the various ionic thresholds. The calculated results are found to be very sensitive to the initial and final state wave functions.

C. Charge Transfer Matrix Elements

Charge transfer is important in ion-atom (ion) collisions to understand inter alia chemical reactions. The proton-hydrogen collision problem is quantum mechanically a three-body problem. However, in the approximation of straight-line trajectories for the protons, the problem simplifies considerably; it reduces to the solution of the one-electron time-dependent Schrödinger equation. In the coupled channel calculation of one electron in the field of two classically moving nuclei, the evaluation of one-electron, two-center, three-dimensional integrals is most troublesome. Various approaches have been employed over the years, depending upon the nature of the particular problem.

Recently, we¹⁵ have developed a numerical approach to calculate the charge transfer matrix elements and used the proton-hydrogen collision problem as illustration. The procedure involves reducing the initial integrals to one-dimensional integrals by using a Feynman integral technique and modified spherical Bessel function of the third kind. A special routine which uses continuation in the complex plane has been designed to evaluate the integrals in the region far away from the target to remove their rapid oscillation in this region. This analytic continuation is then computed using the Gauss-Laguerre method. The resultant coupled differential equations are solved by the Runge-Kutta method. Charge transfer cross sections for proton-hydrogen scattering have been compared with those of Cheshire and of Rapp to check the calculation.

The method will be extended so that it is valid also for low energy ~ 5 keV through the use of molecular orbitals.

D. Other Accomplishments

- (i) Conceived and wrote the proposal to establish the NSF-MRCE Center for Theoretical Studies of Physical Systems at Clark Atlanta University. Dr. Carlos Handy and myself are the associate director and director, respectively.
- (ii) Selected to evaluate for the Junior Engineering Technical Society at the 43rd International Science and Engineering Fair, Nashville, Tennessee, May 13-16, 1992.

- (iii) Became a member of the Board of Directors of the National Association of Research Centers of Excellence. The Centers are funded by NSF.

E. Graduate Students Supported (Partially or Fully)

Ms. Sheryl Good; G. Ndow and Stephen Hiamang.

PROPOSED RESEARCH

We propose the following:

- Construction of an elaborate CI target wave function for K for use in the R-matrix method¹⁴ to investigate the behavior of σ_R in the energy range $2 \leq E \leq 15$ eV. We hope to give a definite answer to the question; Is the measured⁸ minimum in σ_R real and due to the formation of K⁻?
- Investigation of electron impact excitation cross sections for the core-excited quartet levels of Na and K which are metastable against autoionization. These are important for understanding atomic spectroscopy and the construction of XUV lasers.
- Continuation of investigation of the photoionization of Na, both ground and excited states, in the region of the $2s2p^63s$ inner-shell thresholds to determine the most important correlation terms. Our cross sections are sensitive to the type and number of correlation terms on both the initial and final states as well as the excited orbitals employed.
- Continue the investigation of the photoionization of K near the $3s^23p^54s$ and $3s3p^64s$ inner-shell thresholds. The R-matrix will be used to study shake-up and conjugate shake-up satellite lines associated with the $3p^55s$ (or $3s3p^65s$) and with the $3p^54p$ (or $3s3p^64p$) final ionic configurations, respectively.
- Obtain electron impact excitation cross sections for some of the K-like and Na-like ions to determine where coupling and wave function effects become unimportant and to establish trends for cross sections as a function of Z.
- Revise the e-Cr⁵⁺ paper for resubmission for publication to Phys. Rev. A. as well as complete the publication of the e-N²⁺ paper.

- Study the variation of the d^{-1} multi-minima in photoionization of Na and K to establish its behavior as the principal quantum number, n and the nuclear charge, Z increase.
- Continue the delineation of correlation and coupling effects in the various shake up ($\Delta l = 0$) satellites and conjugate shake-up ($\Delta l = \pm 1$) satellites for both Na and K photoionization.

PRESENTATIONS

- A. Division of Atomic, Molecular and Optical Physics Annual Meeting, Chicago, May 20-22, 1992.**
- "A Numerical Method for the Calculation of Two Center Integrals", Z. Chen, D. Bessis and A.Z. Msezane.
- "Calculation of Charge Transfer Cross Sections in Proton-Hydrogen Scattering", Z. Chen, A.Z. Msezane and J.F. Reading.
- "Photoionization of Sodium in the Ground and Excited States", S.S. Tayal, A.Z. Msezane and S.T. Manson.
- B. XVII ICPEAC, Brisbane, Australia, July 10-16, 1991**
- "Correlation Effects in Photoionization of Atomic K", W. Armstrong-Mensah, F. Nyandeh and A.Z. Msezane, Book of Abstracts of Papers, page 24.
- "Photoionization of Na Atoms in the Vicinity of the 2s Thresholds", A.Z. Msezane, S. Tayal and S.T. Manson, Book of Abstracts of Papers, page 23.
- "Electron Impact Excitation of Atomic Potassium", P. Awuah and A.Z. Msezane, Book of Abstracts of Papers, page 155.

PUBLICATIONS

- "A Numerical Method for the Calculation of Two Center Integrals", Zhifan Chen, Daniel Bessis and, Alfred Z. Msezane, J. Phys. B. (Submitted) (1992).
- "Differential and Integral Cross Sections for Electron Collisional Excitation of $^3P - ^1D$ and $^3P - ^1S$ Transitions in Atomic Oxygen", S.S. Tayal, J. Phys. B (in press) (1992).

"Cross Sections for Electron Scattering by Atomic Potassium", Alfred Z. Msezane, Paul Awuah, Stephen Hiamang, and F.K.A. Allotey, Phys. Rev. A (Resubmitted) (1992).

"Photoionization of excited Na near the $2s2p^53s$ and $2s^22p^53s$ Thresholds", S.S. Tayal, A.Z. Msezane and S.T. Manson, Phys. Rev. A (submitted) (1992)

REFERENCES

1. G.S. Hurst, M.G. Payne, S.D. Kraner and J.P. Young, Rev. Mod. Phys. 51, 767 (1979).
2. K.K. Shen, C. Winshead and J.L. Gole, Bull, Am. Phys. Soc. 35, 2359 (1990).
3. E.A. Hinds and Sandoghdan, Abstracts of Papers, ICAP-12, Ann Arbor, MI, eds W.E. Baylis et. al. (1990) p. 1-27.
4. O.I. Tolstikhin and A.V. Vinogradov, Appl. Phys. B 50, 213 (1990).
5. K.H. Winters, and Vanderpooten, J. Phys. B 15, 3945 (1982).
6. C.K. Kwan, W.E. Kauppila, R.A. Lukaszew, S.P. Parikh, T.S. Stein, Phys. Rev. A, 44, 1620 (1991).
7. A.Z. Msezane, P. Awuah, S. Hiamang and F.K.A. Allotey, Phys. Rev. A. (Resubmitted) (1992).
8. J.O. Phelps, J.E. Solomon, D.F. Korff, C.C. Lin and E.T.P. Lee, Phys. Rev. A 20, 1418 (1979).
9. S.T. Chen and A.C. Gallagher, Phys. Rev. A 17, 551 (1978).
10. H.W. Wolff, K. Radler, B. Sonntag and R. Haensel, Physik 257, 353 (1972).
11. D. Cubaynes, J.M. Bizau, M. Richter and F.J. Wuilleumier, Europhys. Lett 14, 747 (1991).
12. A.Z. Msezane, W. Armstrong-Mensah, and J. Niles, Phys. Rev. A 42, 1286 (1990); A.Z. Msezane, F. Nyandeh and J. Niles, J. Phys. B 23, L691 (1990).
13. S.S. Tayal, A.Z. Msezane and S.T. Manson, Phys. Rev. A (submitted) (1992).
14. K.A. Berrington, P.G. Burke, M. Le Dourneuf, W.D. Robb, K.T. Taylor and Vo Ky Lan, Computer Phys. Commun. 14, 367 (1978).
15. Z. Chen, D. Bessis and A.Z. Msezane, J. Phys. B. (submitted) (1992).

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