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13. ABSTRACT (Maximum 200 words)  This grant has contributed to the establishment of a strong group in Theoretical Atomic and Molecular Physics at Clark Atlanta University. The general thrust of the group has been: 1) the development of novel theoretical methods for application to electron scattering at small-scattering angles which is important inter alia to spacecraft propulsion technologies and planetary atmospheres; 2) the calculation, using extensive configuration-interaction wave functions in sophisticated methodologies of energy levels, optical oscillator strengths, effective collision strengths for use in plasma modeling and photoionization cross sections; and 3) the support of minority students who are underrepresented in the physical and mathematical sciences. The acquisition through the AFOSR research grant of the powerful IBM RISC 6000/590 workstation and attendant software as well as the support of a Post-Doctoral Fellow and students have improved the research environment at the Center for Theoretical Studies of Physical Systems (CTSPS) and impacted the training of students in the Atlanta University Center, the largest consortium of private HBCUs in the nation. National and international visitors and collaborators have been attracted to CTSPS, creating an excellent environment for research, thereby advancing the field of small-angle electron scattering to a level that has never been attained before.  The project has been very productive. Twenty-five publications have been generated with an additional six publications submitted for publication in refereed journals. Additionally, 31 papers have been presented at national and international conferences over the past three years. Three students in Physics, two M.S. and one undergraduate, have been supported.					
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**THEORETICAL STUDIES OF ELECTRON AND PHOTON  
INTERACTIONS WITH ATOMS AND IONS**

**FINAL REPORT**

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The funding provided by the Air Force Office of Scientific Research under Grant: F49620-94-1-0302 P00001 has contributed to the establishment of a strong group in **Theoretical Atomic and Molecular Physics** at Clark Atlanta University. The general thrust of the group has been: 1) the development of novel theoretical methods for application to electron scattering at small-scattering angles which is important **inter alia** to spacecraft propulsion technologies and planetary atmospheres; 2) the calculation, using extensive configuration-interaction wave functions in sophisticated methodologies of energy levels, optical oscillator strengths, effective collision strengths for use in plasma modeling and photoionization cross sections; and 3) the support of minority students who are underrepresented in the physical and mathematical sciences. The acquisition through the AFOSR research grant of the powerful IBM RISC 6000/590 workstation and attendant software as well as the support of a Post-Doctoral Fellow and students have improved tremendously the research environment at the Center for Theoretical Studies of Physical Systems (CTSPS) and impacted the training of students in the Atlanta University Center, the largest consortium of private HBCUs in the nation. National and international visitors and collaborators have been attracted to CTSPS, creating an excellent environment for research, thereby advancing the field of small-angle electron scattering to a level that has never been attained before.

Dr. Alfred Msezane, Professor of Physics and director of CTSPS, has been responsible for the overall direction of the Atomic and Molecular Physics Group, the portion of the research concerned with small-angle electron scattering and some aspect of photoionization of atomic states. Dr. Tayal, Associate Professor of Physics, has been responsible for the calculation of energy levels, oscillator strengths and collision strengths for use in plasma modeling. Dr. Tayal has now developed capabilities in studies of astrophysical plasmas and has received funding from the National Science Foundation and NASA. Dr. Zineb Felfli, Post-Doctoral Research Associate, has worked on photoionization of atoms/ions and electron scattering. The project has been very productive since 25 publications have been generated with an additional 6 publications submitted for publication in refereed journals. Additionally, 31 papers have been presented at national and international conferences over the past three years. Three students, 2 M.S. and 1 undergraduate, in Physics have been supported and many have used the Workstation. An important accomplishment of this group has been its leadership in an international collaboration on small-angle electron scattering involving world-class experimenters from the United Kingdom, Canada, Germany, Yugoslavia, Poland, Brazil and the US. A paper was presented at the 1997 ICPEAC, Vienna, Austria, which is currently being expanded for publication in 1998. This paper uses our recent theoretical methods to guide measurements at and near zero scattering angles; it will be the standard work in this field where measurements are riddled with errors.

In January 1995, the Atomic and Molecular Theory Group collaborated with the CTSPS Wavelet-based Signal and Image Processing Group, a member of the Army Research Laboratory-Lockheed Martin Federated Consortium in Advanced Sensors, and sponsored through CTSPS the first workshop on Wavelet Theory and Quantum Mechanics at CAU. Leading researchers in the field of Wavelet Theory and Application, such as Dr. Alex Grossmann (Marseilles), Dr. Jean-Pierre Antoine (Belgium) and Dr. Marie Farge (France) participated. The workshop was very successful and it was suggested that another one be organized in the future. Subsequently, Professor X.-Q. Wang of CTSPS and collaborators incorporated Wavelet theory into their molecular dynamics code while Professors C. Handy and R. Murenzi have shown how to systematically implement continuous wavelet transform methods for one dimensional quantum mechanics problems. An important achievement by the group is that CTSPS and the Institute for Theoretical Atomic and Molecular Physics (ITAMP) at Harvard-Smithsonian Center for Astrophysics

have agreed to work closely together and will co-sponsor an International Workshop on Wavelet Theory and Quantum Mechanics at Harvard in 1998.

The Atomic and Molecular Group continues to develop novel approaches in small-angle electron scattering using Regge Pole theory. This approach will continue to revolutionize the field - an industry will be formed to produce reliable electron DCSs at and near zero scattering angles to guide measurements. Another important application will be in light scattering in the context of the various Light Sources being built throughout the world. As already indicated, Dr. Tayal has received funding from NASA and NSF to investigate effective collision strengths for use in modeling astrophysical plasmas.

## Research Results

The accomplishments of our research during the three-year project period are summarized below. The numbering are compatible with those under references.

### 1. Electron Collisions with Atoms and Molecules at Small Scattering Angles

Electron differential cross sections (DCS's) provide a stringent test of theory when theoretical results are compared with reliable experimental data. However, for optically allowed transitions the measured small angle DCS's are riddled with inaccuracies and uncertainties for two main reasons. (1) Generally, experiments measure relative DCSs and then obtain absolute values through various approaches, including the limiting behavior of the generalized oscillator strength (GOS) as the square of the momentum transfer,  $K^2 \rightarrow 0$ . (2) DCS's vary rapidly with decreasing scattering angle,  $\theta$  thus making measurements difficult. Consequently, accurate theoretical calculations are necessary to guide measurements. For finite impact energy,  $E$ ,  $K^2 = 0$  is non-physical; it corresponds to non-physical angles which are experimentally inaccessible. Until very recently [1] there was no rigorously derived expression to extrapolate the DCS through the non-physical region to the optical oscillator strength ( $K^2 = 0$ ). We have used the universal extrapolation function [1] to investigate several optically allowed transitions in atoms, ions and molecules at high to small impact energies to demonstrate the gravity of the problems referred to above and how they may be readily remedied. Also, we have attempted to delineate the importance of dynamic effects in various dipole-allowed transitions.

### 2. Dynamic Effects in Small-Angle Electron Differential Cross Sections for Excitation of H $2^2P$ , He $2^1P$ and Li $2^2P$ Levels

Experimental and theoretical small-angle electron DCS's for excitation of H  $2^2P$ , He  $2^1P$  and Li  $2^2P$  states from their respective ground states have been investigated [2] through the GOS and compared with GOS's from the universal function [1]. The objective was to delineate the behavior of dynamic effects as a function of impact energy,  $E$ . We found [2] the surprising result that for the Li  $2^2S \rightarrow 2^2P$  transition dynamic effects first decrease as  $E$  increases from 10eV to about 20eV where they reach a minimum. Thereafter, for a given  $K^2$ , away from the asymptotic region, their importance increases until the Born approximation regime is reached. In contrast, dynamic effects in H  $2^2P$  and He  $2^1P$  persist over a wide range of  $E$  values, all the way to the Born approximation limit where their significance diminish to zero.

### 3. Electron Excitation of Optically Allowed Transitions in Molecules: H<sub>2</sub>, CO<sub>2</sub>, CO, F<sub>2</sub>, SO<sub>2</sub>, and SF<sub>6</sub>

Integral cross sections for excitation from ground state to the dipole-allowed states  $B^1\Sigma_u^+$  and  $C^1\Pi_u^+$  in electron-H<sub>2</sub> scattering have been calculated [3] at 60eV using the universal formula for  $\theta < 10^\circ$  and experimental data for  $\theta \geq 10^\circ$ . The results for the  $C^1\Pi_u^+$  state show excellent agreement with the distorted-wave calculation. These results demonstrate the importance of reliable extrapolation of the experimental data using the universal formula. The unmeasured DCS's, mainly in the angular range  $0 \leq \theta \leq 2^\circ$  which is generally inaccessible experimentally, are found [4] to contribute significantly to the ICS's, varying from 40% at 300eV to 72% at 500eV for the fourth positive band of CO. Agreement is excellent between the universal function result and measurement for the inner-shell excitation of  $C_{1s}(2\sigma_g) \rightarrow 2\Pi_u$  in CO<sub>2</sub>. The universal formula is found to be applicable to molecular transitions at small scattering angles where it is inferred that dynamic effects are generally unimportant at small  $K^2$  values.

### 4. Study of Small-Angle DCS's for Optically-Allowed Transitions in H and K

The expansion of the universal extrapolation function in terms of  $K^2$  has been investigated. The merging of the Born approximation and the universal function GOS's in the region  $K^2 \rightarrow 0$  for the H 2p excitation demonstrates that the latter is suitable for extrapolating the GOS through the unphysical region to the optical oscillator strength (OOS). Small-angle experimental electron DCS's for the resonance transition in K have been contrasted [5] and compared with other theoretical calculations. For the excitation of the H 2p state, it is concluded that the R-matrix, the CC and DW methodologies do not calculate [6] the small-angle DCS's correctly at small and moderate impact energies. The fact that  $f^B = f^U \cong f^\circ [1 - 2.667 K^2]$  for H 2p as  $K^2 \rightarrow 0$  establishes the validity of the universal function for use in extrapolating the GOS to the OOS.

From the universal formula, a very useful formula has been derived [7] for calculating the excitation cross sections in the small-angular regime. It is given by

$$I = \frac{\pi f^\circ}{wE} \left[ \ln \frac{1+x^2-2xy_s}{1+x^2-2x} - 2 \ln \frac{1-xy_s}{1-x} \right] \quad (1)$$

where  $f^\circ$  is the OOS,  $w$  and  $E$  are respectively the excitation and impact energies,  $x^2 = 1 - w/E$  and  $y_s = \cos\theta_s$ .

Together with the universal formula, the above formula has been used to investigate both ICS's and DCS's for the resonance transition in K [5].

## 5. Differential Cross-Section Representations from First Principles Dispersion Relations: A Regge Pole Approach

A dispersion relation in the momentum transfer squared,  $K^2$  at *fixed energy* for electron scattering has been derived [8] from first principles. It is shown to describe the scattering by a *diffraction peak*. A global optimal parametrization of this diffraction peak which embeds the more reliable large scattering angle measurements permits an accurate extrapolation of the generalized oscillator strength down to  $K^2 = 0$  to obtain the optical oscillator strength. The Xe  $P_{3/2}$  and  $P_{1/2}$  data at 100 and 500eV have been used to illustrate the method. An experimental protocol is suggested for the use of our procedure. The new and unprecedented method exploits the reliable relatively large scattering angle measurements to obtain GOSs. It is also applicable to electron scattering from ions and molecules for both optically allowed and forbidden transitions.

The real part of the complex Regge exponent is responsible for the rapid drop of the GOS at small angles while the imaginary part is responsible for the oscillation in the GOS at larger  $K^2$  values. This provides a justification of the exponent in the universal formula [1] as used by Fomunung *et. al.* [4] and, recently by Chen and Msezane [14].

## 6. Collision Strengths for Dipole-Allowed and Intercombination Transitions in Fe XIII

The oscillator strengths in length and velocity formulations have been calculated [9] for all dipole-allowed and intercombination transitions between the levels of  $3s^23p^2$ ,  $3s3p^3$  and  $3s^23p3d$  configurations of Fe XIII using fairly extensive configuration-interaction wave functions. There is a good agreement between the length and velocity values, indicating the high accuracy of the wave functions used. These wave functions are also used to calculate collision strengths between fine-structure levels in an intermediate coupling scheme by the use of the R-matrix method. The 11 LS states:  $3s^23p^2$   $^3P$ ,  $^1D$ ,  $^1S$ ,  $3s3p^3$   $^3D^\circ$ ,  $^3P^\circ$ ,  $^1D^\circ$ ,  $^3S^\circ$ ,  $^1P^\circ$ ,  $3s^23p3d$   $^3P^\circ$ ,  $^3D^\circ$ ,  $^1D^\circ$  and 21 fine-structure levels of Fe XIII are included in the close-coupling expansion. Rydberg series of resonances converging to excitation thresholds are explicitly included in the calculation. The relativistic effects are included by means of the Breit-Pauli Hamiltonian. The calculated collision strengths are compared with the available distorted-wave results and some very significant differences are noted. The effective collision strengths are also calculated over a wide range of electron temperatures suitable for use in plasma modeling.

## 7. Generalized Oscillator Strengths at Zero Scattering Angles: A Stringent Test of Theory and Experiment

The recent theory of generalized oscillator strengths for forward electron scattering [10] provides a new and unique path,  $\Phi(x)$  to reach the optical oscillator strength without transversing the nonphysical region. The theory is applicable to optically allowed transitions over a wide range of impact energies. The resonance transitions in Li, Na and Cu, the Xe  $5p^6$   $^1S$ - $5p^5(^2P_{3/2})6s$  and the  $I$   $^1\Sigma_u^+$  ( $\nu = 0$ ) excitation in  $F_2$  are used as illustrative examples [11]. This provides one possible path to a long-standing problem of how to reach the limit of the GOS at  $K^2 = 0$  when Born Approximation is inapplicable. The  $\Phi(x)$  function can be viewed upon as the lower bound to the GOS, while the Born curve

represents the upper bound. As expected the two curves merge and converge to the OOS as  $K^2 \rightarrow 0$ .

The  $\Phi(x)$  curve provides a stringent test of both experiment and theory, as seen in the case of Na [12] while for Xe and  $F_2$  experiment is tested as  $K^2 \rightarrow 0$  since no data, within the experimental errors, should cross the  $\Phi(x)$  curve. The  $\Phi(x)$  curve has been used to demonstrate the unreliability of sophisticated methodologies [13] such as the 76 CCC of Fursa and Bray and the Distorted Wave of Madison *et. al.* to obtain accurate small-angle electron DCSs for optically allowed transitions.

## 8. Calculation of Excitation Cross Sections for the Lowest Five Dipole-Allowed Transitions in $e-N_2$

Two methods have been used [14] in the calculation of the integral excitation cross sections (ICSs) for the first time for the lowest five dipole-allowed transitions in  $e - N_2$  scattering in the energy range from 200 to 1000eV. The first method uses the universal extrapolation function together with the differential cross sections data, while the other uses Lassette's equation and the Bethe theory. Good agreement has been obtained between the two methods at 500eV. The calculation demonstrates that a significant contribution to the ICS comes from small scattering angles ( $0^\circ - 4.18^\circ$ ) where the experimental data are not available. Therefore a good extrapolation function is necessary in the calculation of the ICS from the DCS measurement in order to avoid the large uncertainties in the region of small scattering angles.

## 9. Generalized Oscillator Strengths for $SF_6$ in the S 2p Inner-Shell Region

An important accomplishment by this group has been the combined use of the momentum dispersion method [8], the universal formula [1] and the Lassette fitting formula to study small-angle electron excitations in molecules. In particular, Turci, *et. al.* have obtained OOS values for the  $T_{1u}(a_{1g})$ ,  $T_{1u}(t_{2g})$  and  $T_{1u}(e_g)$  states of  $SF_6$  at 1400eV that are compatible with published data when their GOSs were obtained from **total peak areas**, but with the Ying *et. al.* values when they employed **peak heights** for their GOSs.

The extrapolation to the optical oscillator strengths (OOSs) of the recently measured small-angle,  $\theta \leq 10^\circ$  generalized oscillator strengths (GOSs) for  $SF_6$  in the S 2p inner-shell region at 1400eV impact energy has been investigated [15] using various theoretical approaches. These methods include the recent momentum dispersion formula which has the more reliable larger scattering angle measurements embedded in it, the universal formula and the Lassette fitting formula. From the comparison between the measurements and the universal formula, it is concluded that dynamic effects are less significant for the  $T_{1u}(a_{1g})$  state for  $\theta \leq 8^\circ$ , but are important for the  $T_{1u}(t_{2g})$  and  $T_{1u}(e_g)$  states. We further conclude that the extrapolated OOSs depend sensitively upon the method of extrapolation. The momentum dispersion method produces extrapolated OOS values that are consistent with those of the experiment, thereby manifesting the importance of the accuracy of the larger scattering angle measurements in the extrapolation.

**10. Photoionization of K near the 3p Threshold:  
Coupling and Correlation Effects**

Channel-coupling, spin exchange interactions and CI effects in the initial and final states in the photoionization of the ground state of K have been investigated [16] using the R-matrix method. Two through five lowest extensive CI target states are coupled and results obtained in the length and velocity forms for photon energies from near the 3p inner-shell thresholds to about 70eV. We find that the inclusion of configurations  $3p^4 3d^2$  in the initial and final states improves the agreement between the length and velocity forms of the cross section. Channel-coupling, spin-exchange interactions and the addition of more states generally attenuate the individual and uncoupled cross sections near the 3p threshold. Results compare well with those of Be and Na where the triplet state cross section dominates and spin-exchange interactions and coupling enhance the cross section near the inner-shell thresholds.

**11. Resonant Excitation of Inelastic Transitions in Ar<sup>+</sup>**

Collision strengths for electron impact excitation of inelastic transitions in Ar<sup>+</sup> are calculated using the R-matrix method in two independent 9- and 19- state close-coupling approximations [17]. These Ar<sup>+</sup> states are represented by extensive configuration interaction wave functions which yield excitation energies and oscillator strengths that are in good agreement with experimental values and other calculations. The contribution of resonances has been fully and properly allowed for in the calculation. The effective collision strengths are also calculated over a wide range of temperatures.

**12. Energy Levels and Oscillator Strengths  
for Allowed Transitions in SIII**

Energy levels and oscillator strengths for dipole-allowed transitions between the terms belonging to the  $3s^2 3p^2$ ,  $3s 3p^3$ ,  $3s^2 3p 3d$ ,  $3s^2 3p 4s$ ,  $3s^2 3p 4p$  and  $3s^2 3p 4d$  configurations of SIII are calculated [18]. A large number of configurations is included in the configuration - interaction expansions to ensure convergence. Our calculation has resolved most of the existing discrepancies between the available calculations.

**13. Oscillator Strengths for Dipole-Allowed Transitions in Cd<sup>+</sup>**

Large scale configuration interaction calculation of oscillator strengths for electric-dipole allowed transitions among the Cd<sup>+</sup> ground  $4d^{10} 5s^2 S$  and excited  $4d^{10} 5p^2 P^0$ ,  $4d^{10} 6s^2 S$ , and  $4d^{10} 6p^2 P^0$  states is performed in the LS coupling scheme [19]. Twenty three orthogonal one-electron orbitals 1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, 4f, 5s, 5p, 5d, 5f, 5g, 6s, 6p, 6d, 7s, 7p, 8s and 8p are used to construct the configuration-interaction wave functions. A large number of configurations (up to about 10,000) are considered in the expansion of each state.

**14. Fe XII Emission Line Ratios**

A 29 level Fe XII model has been used in the statistical equilibrium plasma model calculation to obtain relative level populations and emission line strengths. Electron densities of the emitting plasma are deduced from the emission line ratios [20].

**15. Normalization of Relative Electron Differential Cross Sections for Optically Allowed Transitions**

The measured relative electron impact differential cross sections (DCSs) for optically allowed transitions in atoms and molecules can be brought to absolute values through the combined use of the recent forward scattering function and the momentum dispersion method [21]. The Ba  $6^1S - 6^1P^0$  and Cd  $5^1S - 5^1P^0$  transitions are used to demonstrate the procedure which is applicable for impact energies from near threshold to the Born Approximation limit.

**16. Electron Excitation of the  $^1\Pi$  and  $2^1\Sigma^+$  States of  $N_2O$**   
B. Marinkovic, Z. D. Pecc, R. Panajotovic, and D. M. Filipovic

A method for normalizing the differential cross sections (DCSs) employing the forward scattering function for generalized oscillator strengths (GOSs) has been applied to the electron excitation of the  $2^1\Sigma^+$  state of  $N_2O$  [22]. Measurements were made at electron impact energies of 15, 20, 30, 50 and 80eV, using the electron spectrometer briefly described here. For the transition from the ground state to the  $2^1\Sigma^+$  we determined the optical oscillator strengths (OOSs) to be 0.13 and 0.02, from the absolute values of the DCSs at 80eV and 30eV electron impact energy, respectively.

**17. Linear Variation of Small-Angle Electron Excitation Differential Cross Sections: Aid to Measurements**

The study of the electron differential cross section (DCS) representation through dispersion relations using a Regge Pole approach [8] has yielded the revealing forward scattering function,  $\Phi(K^2)$  [10] and consequently the present treatment. The function  $\Phi(K^2)$  provides a stringent test for both experimental and theoretical small-angle electron DCSs [12] through the generalized oscillator strength (GOS). Recently, it has also been used to predict and confirm anomalies in optically forbidden transitions in Mg and He.

In an appropriate representation the GOS varies linearly with the momentum transfer squared,  $K^2$  at small scattering angles and fixed impact energy, E for both optically allowed and forbidden atomic transitions [23]. This represents a breakthrough in small-angle electron DCS measurements, particularly for impact energies near threshold where the linear behavior is most dramatic; it can include angles as high as  $20^\circ$  or more. Thus the larger scattering angle measurements where the errors are relatively small can be employed to obtain reliable values at and near zero scattering angles. In turn, these data can be used to guide difficult measurements in this angular regime.

The representation of data on a log x log or log x linear graph will facilitate measurements and analyses of the angular regime near  $0^\circ$  which is difficult to access, particularly for complicated many-electron systems near threshold.

**18. Determination of Small-Angle Electron Differential Cross Sections from their Larger Angle Measurements**

It has been demonstrated [24] how small-angle electron differential cross sections (DCSs) for both optically allowed and forbidden transitions can be determined accurately

from their more reliably measured larger angle data [8]. The procedure is particularly effective for electron impact energy from near threshold to about ten times threshold. Examples are given for measured transitions in Li, Na, Mg, Xe, Hg, Ba, and N<sub>2</sub>O. Values of DCSs at an near zero scattering angles, a difficult angular regime to access experimentally were recommended.

**19. Electron Excitation of Optically Allowed Transitions at Small Scattering Angles**

The universal extrapolation (not interpolation) formula is justified through a complex angular momentum Regge pole representation of the electron differential cross sections. It is further demonstrated, using the recent forward electron scattering method for optically allowed transitions, that some of the sophisticated theoretical calculations are unreliable at and near zero scattering angles [25].

**20. Calculation of Energy Differences and Oscillator Strengths for the Electric-Dipole Transitions of Sulphur**

A large-scale configuration interaction (CI) calculation has been performed for the sulfur atom to obtain excitation energies and oscillator strengths of some electric-dipole transitions [27]. In the calculation, relativistic effects were included through the Breit-Pauli approximation. A fine-tuning technique was used for the adjustment of the diagonal matrix elements to achieve accurate transition energies and coefficients of the CI wavefunctions. The calculated excitation energies are mostly within 1% of the measurements. The agreement between the length and velocity forms of the oscillator strengths is also very good.

**21. Differential Cross Sections for H 2s-3s Excitation by Electron and Positron Impact**

Electron and positron impact differential cross sections for excitation of the 3s state of hydrogen atom from its metastable 2s state are calculated in a distorted wave approximation at 10 and 50eV [28]. The effects of both adiabatic and non-adiabatic distortion of the atomic charge cloud by the incoming electron or positron are included in the initial and final state wave functions. Contrary to an earlier prediction, no dramatic differences between the electron and positron results are found.

**22. Anomalous Behavior in Zero-Angle Electron Differential Cross Sections for Mg 3 <sup>1</sup>S → 3 <sup>1</sup>D and Cd 5 <sup>1</sup>S → 5 <sup>1</sup>D Excitations**

Anomalies in zero-angle electron differential cross sections for optically forbidden transitions can be predicted through a recent forward scattering function. Energy minima in Mg 3 <sup>1</sup>S → 3 <sup>1</sup>D and Cd 5 <sup>1</sup>S → 5 <sup>1</sup>D transitions are predicted for the first time and more precisely in He 1 <sup>1</sup>S → 2 <sup>3</sup>S [29].

23.

### Formula for the Calculation of Integral Cross Sections in a Fourier Expansion Method

A method has been developed to calculate the integral cross sections from the measured generalized oscillator strengths that are fitted by a Fourier expansion [30]. The method has been applied to the e-Xe and e-N<sub>2</sub> scattering problems. Excellent agreement has been obtained with existing measured values for the transitions to 5p<sup>5</sup>(<sup>2</sup>P<sub>3/2</sub>)6s and 5p<sup>5</sup>(<sup>2</sup>P<sub>1/2</sub>)6s of Xe at 100 and 500eV. For the vibrational states, v = 1 - 4 of the b<sup>1</sup>Π<sub>u</sub> electronic state of N<sub>2</sub> at 300eV good agreement with the data calculated by the Lassette expansion has also been achieved.

24.

### A New Method to Extract Optical Oscillator Strengths

A method, which filters the noise in measured generalized oscillator strengths (GOS's) by minimizing the  $\int_{x_0}^{x_n} f''(x)^2 dx + p(\sum_{i=0}^{i=n} (fx_i) - y_i^2 - s)$  with the cubic spline, has been developed and used to recover the smooth GOS function  $f_G$  [31]. The function  $f_G$  is then extrapolated to K<sup>2</sup> (momentum transfer squared) = 0 to obtain the optical oscillator strength (OOS). The method has been tested in the transition 1s - 2p in a simulated e - H scattering at 500eV. OOS's for some transitions in Ar, Kr, and the vibronic bands v = 1 - 4 of the b<sup>1</sup>Π<sub>u</sub> state of N<sub>2</sub> have been calculated and compared with those of other authors.

## References (Publications)

- [1] "Universal formula to extrapolate the generalized oscillator strength through the unphysical region to K<sup>2</sup> = 0", Alfred Z. Msezane and I. A. Sakmar, Phys. Rev. A**49**, 2405 (1994).
- [2] "Dynamic Effects in Small-Angle Electron Differential Cross Sections for Excitation of H 2 <sup>2</sup>P, He 2 <sup>1</sup>P and Li 2 <sup>2</sup>P Levels", A. Z. Msezane, P. Ozimba, Z. Felfli and Zhifan Chen, J. Phys. B**28**, 2509 (1995).
- [3] "Calculation of the Excitation Cross Sections for the B <sup>1</sup>Σ<sub>u</sub><sup>+</sup> and C <sup>1</sup>Π<sub>u</sub><sup>+</sup> States in e-H<sub>2</sub> Scattering at 60eV", Zhifan Chen and A. Z. Msezane, Phys. Rev. A**51**, 3745 (1995).
- [4] "Electron Excitation of Optically-Allowed Transitions in CO<sub>2</sub>, SF<sub>6</sub>, CO, F<sub>2</sub>, and SO<sub>2</sub>", I. W. Fomunung, Zhifan Chen and A. Z. Msezane, Phys. Rev. A**53**, 806 (1996).
- [5] "Small-Angle Electron Differential and Integral Cross Sections for the K 4s-4p Transition", P. Ozimba, Zhifan Chen and A. Z. Msezane, Can J. Phys., Submitted (1997).
- [6] "Small angle electron excitation of H 2p at 54.4eV", A. Z. Msezane and Zhifan Chen, J. Phys. B**28**, L64 (1995).
- [7] "Formula for the calculation of integral excitation cross sections at small scattering angles", Zhifan Chen and A. Z. Msezane, J. Chem. Phys. **102**, 3888 (1995).

- [8] "Differential Cross-Section Representation from Dispersion Relations: A Regge Pole Approach", A. Haffad, Z. Felfli, A. Z. Msezane and D. Bessis, *Phys. Rev. Lett.* **76**, 2456 (1996).
- [9] "Effective Collision Strengths for Electron Excitation of Fine-Structure Transitions in Fe III", S. S. Tayal, *Astrophys. J.* **446**, 895 (1995).
- [10] "Generalized Oscillator Strengths for Forward Electron Scattering", N. B. Avdonina, Z. Felfli and A. Z. Msezane, *J. Phys.* **B30**, 2591 (1997).
- [11] "Electron impact excitation of Optically Allowed Transitions at Small Angles", Z. Felfli, N. Avdonina, I. W. Fomunung and A. Z. Msezane, *NIMB* **119**, 337-344 (1996).
- [12] "Generalized oscillator strengths at zero scattering angles: A stringent test of theory and experiment" Zineb Felfli, Nina Avdonina, and Alfred Z. Msezane, *Phys. Rev. A* **55**, xxx (1997).
- [13] "Small-angle electron excitation of optically allowed transitions: reliability of theory", Alfred Z. Msezane, Zineb Felfli and Zhifan Chen, *J. Phys.* **B29**, L817-L824 (1996).
- [14] "Calculation of excitation cross sections for the lowest five dipole allowed transitions in e-N<sub>2</sub> scattering" Zhifan Chen and Alfred Z. Msezane, *J. Phys.* **B29**, 1525-1530 (1996).
- [15] "Generalized oscillator strengths for SF<sub>6</sub> in the S 2p inner-shell region", Z. Felfli, I. Fomunung, D. Bessis, A. Z. Msezane, *Chem. Phys.* **211**, 325-336 (1996).
- [16] "Photoionization of K near the 3p Threshold: Coupling and Correlation Effects", Z. Felfli and A. Z. Msezane, *Bull. Am. Phys. Soc.* **40**, 1551 (1995).
- [17] "Collision Strengths for Electron Impact Excitation of Inelastic Transitions in Ar II", S. S. Tayal and R. J. W. Henry, *J. Phys.* **B29**, 3443 (1996).
- [18] "Energy Levels and Oscillator Strengths for Allowed Transitions in S III", S. S. Tayal, *J. Phys.* **B28**, 5193 (1995).
- [19] "Oscillator Strengths for Dipole-Allowed Transitions in Cd<sup>++</sup>", S. S. Tayal, *Bull. Am. Phys. Soc.*, **41**, 1146 (1996).
- [20] "Fe XII Emission Lines in Spectra obtained with Solar EUV Rocket Telescope and Spectrograph (SERTS)", F. P. Keenan, R. J. Thomas, W. M. Neupert, V. J. Foster, P. J. F. Brown and S. S. Tayal, *Mon. Not. R. Astron. Soc.* **278**, 773 (1996).
- [21] "Normalization of Relative Electron Differential Cross Sections for Optically Allowed Transitions", Zineb Felfli and A. Z. Msezane, *J. Phys. B. Lett.*, Submitted (1997).
- [22] "Normalization of the Measured Relative Electron Differential Cross Sections for 2<sup>1</sup>Σ<sup>+</sup> and 1<sup>1</sup>Π States of N<sub>2</sub>O", B. Marinkovic, Z. D. Pejcev, R. Panajotovic, D. M. Filipovic, Z. Felfli and A. Z. Msezane, *J. Phys. B.*, Submitted (1997).

- [23] "Linear Variation of Small-Angle Electron Excitation Differential Cross Sections: Aid to Measurements", Z. Felfli and A. Z. Msezane, Proc. XX ICPEAC, Abstracts of Papers, Vienna, Austria, eds., F. Aumayr, G. Betz and H. P. Winder, Vol. II, P. MO 105 (1997).
- [24] "Determination of Small-Angle Electron Differential Cross Sections from their Larger Angle Measurements", Z. Felfli *et. al.*, Proc. XX ICPEAC, Abstracts of Papers, Vienna, Austria, eds., F. Aumayr, G. Betz and H. P. Winder, Vol. II, p. MO 107 (1997).
- [25] "Electron excitation of optically allowed transitions at small scattering angles", A. Z. Msezane and D. Bessis, J. Phys. B30, 445-450 (1997).
- [26] "Generalized Oscillator strengths for the vibronic excitation levels of the  $b\ ^1\Pi_u$  electronic state of  $N_2$ ", Z. Felfli, Zhifan Chen, D. Bessis and A. Z. Msezane, Chem. Phys. 222, 117 (1997).
- [27] "Calculation of Energy Differences and Oscillator Strengths for the Electric-Dipole Transitions of Sulphur", Zhifan Chen and A. Z. Msezane, J. Phys. B30, 3873 (1997).
- [28] "Differential Cross Sections for H 2s-3s Excitation by Electron and Positron Impact", N. C. Deb, A. Z. Msezane, K. Basu Choudhury and P. S. Mazumdar, J. Phys. B., Submitted (1997).
- [29] "Anomalous Behavior in Zero-Angle Electron Differential Cross Sections for Mg 3  $^1S$  - 3  $^1D$  and Cd 5  $^1S$  - 5  $^1D$  Excitations", Z. Felfli and A. Z. Msezane, J. Phys. B., Submitted (1997).
- [30] "Formula for the calculation of integral cross sections in a Fourier expansion method", Zhifan Chen and Alfred Z. Msezane, Phys. Rev. A 55, 812-814 (1997).
- [31] "A New Method to Extract Optical Oscillator Strengths", Zhifan Chen and A. Z. Msezane, J. Phys. B., To Appear (1997).

### **Presentations at National and International Conferences**

#### **DAMOP/DAMP '95 Meeting of the American Physical Society, Toronto, Canada, May 16-19, 1995:**

- [1] "Dynamic Effects in Small-Angle Electron Excitation of H  $2^2P$ , He  $2\ ^1P$ , and Li  $2\ ^2P$ ", A. Z. Msezane, P. Ozimba, Z. Felfli and Zhifan Chen, Bull. Am. Phys. Soc., 40, 1293 (1995).
- [2] "Electron Excitation of Fine-Structure Transitions in Fe XIII", S. S. Tayal, Bull. Am. Phys. Soc., 40, 1292 (1995).
- [3] "Small-Angle Electron Cross Sections for the Fourth Positive Band of CO and for  $CO_2\ 1s\ (2\sigma_g) \rightarrow 2\Pi_u$ ", I. Fomunung, Zhifan Chen and A. Z. Msezane, Bull. Am. Phys. Soc., 40, 1319 (1995).

**47th Annual Gaseous Electronics Conference, Gaithersburg, MD, October 18-21, 1994:**

- [4] "Small-Angle Differential and Integral Cross Sections for K 4s-4p", P. Ozimba, Zhifan Chen and A. Z. Msezane, *Bull. Am. Phys. Soc.* **39**, 1455 (1994).

**15th International Conference on Atomic Physics, Zeeman-Effect Centenary, University of Amsterdam, Amsterdam, August 5-9, 1996:**

- [5] "Generalized Oscillator Strength for Forward Electron Scattering: A Stringent Test of Theory and Experiment", Z. Felfli, I. W. Fomunung, N. Avdonina and A. Z. Msezane, *Proceedings of the Z ICAP, Amsterdam*, p. ThC6 (1996).
- [6] "Coupling Effects in Photoionization of Li near the 1s Inner-Shell Threshold: R-Matrix Calculation", Z. Felfli, A. Z. Msezane and K. A. Berrington, *Proceedings of Z ICAP, Amsterdam*, p. Tu15 (1996).

**1995 Annual Meeting of the South Eastern Section of the APS, Tallahassee, FL, November 9-11, 1995:**

- [7] "Generalized Oscillator Strengths for Vibronic Excitation Levels of the  $b^1\Pi_u$  Electronic State of  $N_2$ ", Z. Felfli, I. Fomunung, Z. Chen, D. Bessis and A. Z. Msezane, *Bull. Am. Phys. Soc.* **40**, 2084 (1995).

**1996 Division of Atomic, Molecular and Optical Physics Annual Meeting, Ann Arbor, MI, May 15-18, 1996:**

- [8] "Theory of Generalized Oscillator Strengths for Forward Electron Scattering", N. Avdonina, Z. Felfli and A. Z. Msezane, *Bull. Am. Phys. Soc.* **41**, 1109 (1996).
- [9] "A New Method to Calculate Optical Oscillator Strengths", Zhifan Chen and A. Z. Msezane, *Bull. Am. Phys. Soc.* **41**, 1145 (1996).
- [10] "Oscillator Strengths for Dipole-Allowed Transitions in  $Cd^+$ ", S. S. Tayal, *Bull. Am. Phys. Soc.* **41**, 1146 (1996).

**48th Annual Gaseous Electronic Conference, Berkeley, CA, October 9-13, 1995:**

- [11] "Photoionization of K Near the 3p Threshold: Coupling and Correlation Effects", Z. Felfli and A. Z. Msezane, *Bull. Am. Phys. Soc.* **40**, 1551 (1995).
- [12] "Universal Representation of Cross Sections from first Principles Dispersion Relations", D. Bessis, A. Haffad, Z. Felfli and A. Z. Msezane, *Bull. Am. Phys. Soc.* **40**, 1551 (1995).

**Seminar on Resolution Methods for Partial Differential Equations with Applications in Geometry and Physics, Porto-Novo, Benin, January 8-12, 1996:**

- [13] "Theory of Generalized Oscillator Strengths for Forward Electron Scattering", N. Avdonina, Z. Felfli and A. Z. Msezane, *Abstracts of Papers*, p. 18.

**XIX ICPEAC, Whistler, British Columbia, Canada, July 26-August 1, 1995:**

- [14] "Dynamic Effects in Small-Angle Electron Excitation of H 2 <sup>2</sup>P, He 2 <sup>1</sup>P and Li 2 <sup>2</sup>P Levels", A. Z. Msezane, P. Ozimba, Z. Felfli and Zhifan Chen, Abstracts of Papers, p. 492.
- [15] "Photoionization of the Ground State of Potassium: An R-matrix Calculation", Z. Felfli and A. Z. Msezane, Abstracts of Papers, p. 48.

**International Symposium on Electron- and Photon- Molecule Collisions and Swarms, Berkeley, CA, July 23-25, 1995:**

- [16] "Calculation of the Generalized Oscillator Strength for the Dipole-Allowed Transitions in e- N<sub>2</sub> Scattering", Zhifan Chen and A. Z. Msezane, Abstracts of Papers, p. H-26.

**Mini-Colloquium on Wavelets and Quantum Mechanics, CTSPS, Clark Atlanta University, Atlanta, GA, January 25-27, 1995:**

- [17] "Photoionization and Wave Function Calculations", Zineb Felfli.

**49th Annual Gaseous Electronics Conference, Argonne, IL, October 20-24, 1996:**

- [18] "Small-Angle Electron Impact Excitation of Optically Allowed Transitions: Reliability of Theory", Z. Felfli and A. Z. Msezane.
- [19] "Formula for the calculation of integral cross sections in a Fourier expansion method", Zhifan Chen and Alfred Z. Msezane.

**17th International Conference on X-ray and Inner-Shell Processes, Hamburg, Germany, September 9-13, 1996:**

- [20] "Coupling and Correlation Effects in the Photoionization of Potassium near the 3p Inner-Shell Threshold", Z. Felfli and A. Z. Msezane.
- [21] "Determination of Small-angle Electron Differential Cross Sections from Experimental Large-Angle Scattering", Z. Felfli, Nina Avdonina, D. Bessis and A. Z. Msezane.

**1997 Joint Meeting of the APS and AAPT with the Canadian Association of Physicists and the Sociedad Mexicana de Fisica, Washington, D.C., April 18-21, 1997:**

- [22] "Anomalous Behavior in Zero-Angle Electron Differential Cross-Sections for Mg 3 <sup>1</sup>S → 3 <sup>1</sup>D and Cd 5 <sup>1</sup>S → 5 <sup>1</sup>D Excitation", Z. Felfli and A. Z. Msezane, Bull. Am. Phys. Soc. **42**, 960 (1997).
- [23] "Accurate Determination of Small-Angle Electron Excitation Differential Cross Sections: Aid to Measurements", Z. Felfli and A. Z. Msezane, Bull. Am. Phys. Soc. **42**, 961 (1997).

- [24] "Calculation of energy levels and oscillator strengths for the electric-dipole transitions of sulfur", Zhifan Chen and Alfred Z. Msezane, *Bull. Am. Phys. Soc.* **42**, 1082 (1997).  
**XX International Conference on the Physics of Electronic and Atomic Collisions, Vienna, Austria, July 22-29, 1997:**
- [25] "Anomalies in Zero-Angle Electron Differential Cross Sections in He and Cd", Z. Felfli and A. Z. Msezane, *Proc. XX ICPEAC, Vol. II*, p. MO 106 (1997).
- [26] "Determination of Small-Angle Electron Differential Cross Sections from Their Larger Angle Measurements", Z. Felfli, *et. al.*, *Proc. XX ICPEAC, Vol. II*, p. MO 107 (1997).
- [27] "Linear Variation of Small-Angle Electron Excitation differential Cross Sections: Aid to Measurements", Z. Felfli and A. Z. Msezane, *Proc. XX ICPEAC, Vol. II*, p. MO 105 (1997).
- [28] "Calculation of Energy Differences and Oscillator Strengths for the Electric-Dipole Transitions of Sulfur", Zhifan Chen and A. Z. Msezane, *Proc. XX ICPEAC, Vol. II*, p. TU 198 (1997).  
**50th Annual Gaseous Electronics Conference, Madison, Wisconsin, October 6-9, 1997:**
- [29] "Normalization of Experimental Electron Cross Sections", N. Avdonina, Z. Felfli and A. Z. Msezane, *Bull. Am. Phys. Soc.* **42**, 1726 (1997).
- [30] "Photoionization of the Neon Isoelectronic Sequence Using RRPA", Nasreen Haque, A. Msezane, S. T. Manson and P. Deshmukh, *Bull. Am. Phys. Soc.* **42**, 1748 (1997).  
**Sixth Conference on Current Trends in Computational Chemistry, Vicksburg, Mississippi, November 7-8, 1997:**
- [31] "New Theoretical Advances in Small-Angle Electron Scattering", A. Z. Msezane and Z. Felfli, *Abstracts of Papers*, p. 33.

### Participants

- Dr. Alfred Z. Msezane, Professor of Physics and Director of CTSPS; Project Director
- Dr. Swaraj S. Tayal, Associate Professor of Physics (1994-1996)
- Dr. Zineb Felfli, Post-Doctoral Fellow (1994-1997)
- Mr. Ignatius Fomunung, completed M.S. Degree. Now at Georgia Tech. pursuing a Ph.D. degree in Transportation Modeling (partial support)
- Mr. Peter Ozimba, Ph. D. candidate (Physics) at Georgia State University (partial support)
- Mr. Albert Clark, undergraduate student

### Visitors

- Dr. Keith Berrington, Queen's University, Belfast, U.K., 1994 and 1995 (5 days each).
- Dr. Herb Jones, Professor of Physics, Florida A&M University, 1994 and 1995 (5 days each).

- Dr. Nina Avdonina, University of Pittsburgh, Summer 1995 (2 months), Summer 1996 (1 month), and Summer 1997 (1 month).