COO-4264-5

Oscillator Strengths for Highly Ionized Atomic Systems

Progress Report
for period May 1, 1978-April 30, 1979

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January, 1979

Prepared for

The U.S. Department of Energy under contract
No. EG-77-S-02-4264

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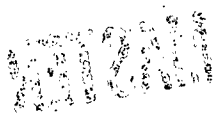

NOTICE

CONTENTS

I. ABSTRACT

Evidence has been found recently that the cascade process may be more important in the analysis of beam-foil decay curves than anticipated. In order to assist the analysis of such data the multiconfiguration Hartree-Fock program (MCHF77) has been applied to the theoretical study of several transitions which are part of a cascade process for a resonance transition.

i) $\{3p^2, 3s\ 3d\}^1D - \{3p\ 3d, 3s\ 4f\}^1F$ and $\{3s\ 3d\}^3D - \{3p\ 3d, 3s\ 4f\}^3F$ transitions in the Mg sequence.

For higher members of the sequence, MCHF77 was modified to include the relativistic effects which shift the energy of a configuration as a whole, and intermediate coupling calculations were performed.

ii) $4s\ 4p\ ^1P - \{4p^2, 4s\ 4d\}^1D$ transitions in the Zn I sequence.

A strong interaction exists between $4p^2$ and $4s\ 4d\ ^1D$ and it has been shown that much of the earlier experimental material concerning the ^1D terms are in error. Comparison with a few recent experimental investigations shows good agreement.

Relatively few levels have been identified in Fe XIV. Because of the importance of the iron ions both in astrophysics and tokamak plasma research, a line list has been produced for levels with three electrons in the M shell. gf-values for allowed transitions and intercombination lines are tabulated.

II. RESEARCH PROGRESS

Research has proceeded in three different but related areas.

i) Software for Atomic Structure Calculations

The multiconfiguration Hartree-Fock program[1] MCHF77 has been published and made available for distribution. The program also has been modified to include certain relativistic corrections which shift the energy of one configuration relative to another, namely the mass-velocity correction, the Darwin term, and part of the spin-spin contact term. (Expressions for these corrections are given by Hartmann and Clementi[2]). These MCHF results may then be used in intermediate coupling calculations which include spin-orbit interactions as well as the "relativistic shift" effects mentioned above. The relativistic Dirac Hartree-Fock (DHF) calculations are much lengthier than non-relativistic equations; thus it is important that the numerical methods used are as efficient as possible. Some studies were performed to adapt direct procedures found to be effective for HF equations[1] to the DHF equations. The method of solution is iterative and the rate of convergence for the Dirac equation was compared with the method used by Desclaux et al[3]. A comparison of the accuracy and rate of convergence is given in Table 1.

Table 1. Comparison of the rate of convergence for direct methods with the in-out integration used by Desclaux et al[3] applied to the Dirac equation for hydrogen.

Electron	Direct Method		In-Out	
	Error	# of Iterations	Error	# of Iterations
$2p_{1/2}$	4.42×10^{-7}	4	7.0×10^{-9}	12
$3d_{3/2}$	3.54×10^{-7}	5	1.5×10^{-9}	9
$4f_{5/2}$	2.83×10^{-7}	5	4.7×10^{-9}	8
$3s_{1/2}$	6.19×10^{-7}	5	1.7×10^{-9}	15
$4p_{3/2}$	9.49×10^{-7}	5	2.8×10^{-9}	9
$5d_{5/2}$	8.67×10^{-7}	4	3.6×10^{-9}	9

The two test calculations are not entirely comparable since the stopping criterion for the in-out method is smaller. But even taking this factor into account it appears that direct methods are appreciably faster and further studies would be worthwhile.

ii) F-value Trends

The simulation of the beam-foil decay curve for the resonance transition of Kr VIII performed by Younger and Wiese[4] showed the importance of the cascade process in the analysis of beam-foil data. Since a system of levels is decaying simultaneously, it appears that the lifetime of a given level cannot always be deduced reliably from one beam-foil decay curve. The decay of at least some of the levels entering into the cascade process should be considered also. Younger and Wiese's[4] study showed that yrast cascade effects were most important.

In the Mg sequence, the resonance transition is $3s^2\ ^1S - 3s\ 3p\ ^1P$ and the yrast chain includes $4f \rightarrow 3d \rightarrow 3p$ transitions. Some f-values are available for $3d \rightarrow 3p$ transitions but little was known about $3d - 4f$ transitions. Calculations have been performed for a variety of D - F transitions in Mg sequence[5]. Experimental f-values for $3s\ 3d\ ^1D - 3s\ 4f\ ^1F$ are available only for neutral Mg. For the triplet series, good agreement was observed between theoretical f-values and those obtained from experiment for $3s\ 3d\ ^3D - 3p\ 3d\ ^3F$ even for Ar VI, but for $3s\ 3d\ ^3D - 3s\ 4f\ ^3F$ the agreement deteriorated with increasing degree of ionization. The results for Ar VI are given below:

	theory	experiment
$\lambda(\mathring{A})$	299.8	297.6
f	0.85	0.38

In the Zn isoelectronic sequence, the important cascade contribution arises from the $4s\ 4p\ ^1P - 4s\ 4d\ ^1D$ transition. However, the interaction of the latter with $4p^2\ ^1D$ is exceptionally strong and the crossing of the two levels has been observed only recently. A theoretical study was

performed for the ^1D sequence[6] and it was found that some of the levels in Ge III and As IV had been identified incorrectly. Better agreement was found with more recent experiments. For higher degrees of ionization the state which is predominantly a 4s 4d ^1D configuration state, is the upper ^1D. For this state the interaction with $4p^2\ ^1D$ leads to constructive interference or enhancement in the calculation of the f-value. In the region Kr VIII - Sn XXI the approximate relativistic f-value for a transition to the upper state is about six times larger than a transition to the lower state. Thus the cascade correction to the 4s 4p ^1P beam-foil decay curve may be large which could account for the discrepancy between theory and experiment observed in the earlier study of the $4s^2\ ^1S$ - 4s 4p ^1P sequence[7].

	theory	experiment
f for Kr VII	1.61	0.81, 0.94

iii) Analysis of Spectra

Iron at all stages of ionization has been of interest in astrophysics for some time. Of all the ionization stages in which the ground state has electrons in the M shell, Fe XIV has the fewest identified lines. Our earlier study found that precisely in Fe XIV the $3p\ 3d^2$ energy levels were crossing those for $3s^2\ 4p$ with $3p\ 3d^2(^1S, ^1D)\ ^2P$ below $3s^2\ 4p$ and $3p\ 3d^2(^3P)\ ^2P$ above $3s^2\ 4p$, and this may account for the paucity of identified levels.

Recently Poppe[8] has shown how theoretical gf-values can be used to aid the identification of observed energy levels. To assist such an analysis, theoretical energy levels were computed for all states of Fe XIV

with three electrons in the M shell. A line list for all allowed transitions and inter-combination lines has been tabulated[9], according to increasing wavelength (Å)

i) with gf for the line greater than 0.4

ii) with gf for the line greater than 0.01 and the lower state being a low lying state, most of which have been identified.

iv) Correlation Effects on Energy Levels

Correlation effects for the $3d^n$ group have been shown to be important[10] even when the 3d group is part of the core, and particularly when relative energies of configurations with differing number of 3d electrons are required. Examples are the $3d^4\ 4s\ 4p\ ^7P$ and $3d^5\ 4p\ ^7P$ states of Cr I. When correlation within $3d^n$ is ignored, theoretical calculations predict the two levels in the wrong order. A partially extended MCHF model produces results in far better agreement with observation[10].

In multi-photon laser spectroscopy many high-lying Rydberg states are being investigated[11]. These have been analyzed[12] using quantum defect theory for continuim process and extrapolating the theory to levels below the ionization limit. Another, possibly more reliable, approach would be to perform calculations for the low lying states, where energy level data is available for comparison to determine the important correlation effects, and then proceeding to the higher excited states. Work is now in progress to determine correlation effects in Ca for $4s\ ns\ ^1S$ and $4s\ nd\ ^1D$ states, n = 4 to 7.

v) Bibliographic References

1. C. Froese Fischer, "A general multi-configuration Hartree-Fock program," Comput. Phys. Commun. 14 (1978) 145.

2. H. Hartmann and E. Clementi, "Relativistic correction for analytic Hartree-Fock wavefunctions," Phys. Rev. 133 (1964) A1295.

3. J. P. Desclaux, D. F. Mayers and F. O'Brien, "Relativistic atomic wave functions," J. Phys. B 4 (1971) 631.

4. S. M. Younger and W. L. Wiese, "Theoretical simulation of beam-foil decay curves for resonance transitions of heavy ions," Phys. Rev. A17 (1978) 1944.

5. C. Froese Fischer, "Oscillator strengths for some D - F transitions in the Mg Sequence," JOSA (accepted).

6. C. Froese Fischer and J. E. Hansen, "4s 4d ^{1}D - 4p^2 ^{1}D interactions in the Zn I isoelectronic sequence," (submitted to Phys. Rev.).

7. _____, "Theoretical oscillator strengths for the resonance transitions in the Zn I isoelectronic sequence," Phys. Rev. A 17 (1978) 1956.

8. R. Poppe, "Extended analysis of Ni IV," Physica, 81 C (1976) 351.

9. C. Froese Fischer, "Energy levels and oscillator strengths for Fe XIV," Technical Report COO-4264-4.

10. C. Froese Fischer, "The multiconfiguration Hartree-Fock method for atomic energy levels and transition probabilities," Invited talk presented at the Sixth International Conference on Atomic Physics, Conference Paper COO-4264-3.

11. P. Esherick, J. A. Armstrong, R. W. Dreyfus, and J. J. Wynne, "Multiphoton ionization spectroscopy of high-lying even parity states in calcium," Phys. Rev. Lett. 36 (1976) 1296.

12. J. A. Armstrong, P. Esherick, and J. J. Wynne, "Bound even-parity J = 0 and 2 spectra of Ca: A multichannel quantum defect theory analysis," Phys. Rev. A 15 (1977) 180.

III. PRINCIPAL INVESTIGATOR'S CONTRIBUTION

The principal investigator collaborated with a full-time Research Associate (first J. E. Hansen, then R. Glass) and directed a half-time graduate student for six months. A total of at least three months were devoted by the principal investigator to this contract with the time distributed as indicated below.

May,	1978	20%
June,	1978	80%
July,	1978	20%
August,	1978	60%
September,	1978	15%
October,	1978	15%
November,	1978	15%
December,	1978	15%
January,	1979	15%
February,	1979	15%
March,	1979	15%
April,	1979	15%

An invited talk was presented by the principal investigator at the Sixth International Conference on Atomic Physics in Riga, August 1978 and will appear in the conference proceeding. Two papers submitted during the period of this contract as well as a technical report were entirely the work of the principal investigator.

A complete list of publications for the contract period is given in Section IV.

IV. RESEARCH PUBLICATIONS (Copies Attached)

1. "Levels of $2p^5\ 3p^5$ in Ar^{2+}," (with D. Ridder) J. Phys. B. 11 (1978) 2267-2272.

2. "A General Multi-Configuration Hartree-Fock Program," Comput. Phys. Commun. 14 (1978) 145-153.

3. "Theoretical Oscillator Strengths for the Resonance Transitions in the Zn I Isoelectronic Sequence," (with J. E. Hansen) Phys. Rev. A 17 (1978) 1956-1965.

4. "The $4s\ ^2S - 4p\ ^2P$ Transitions in the Al Sequence," Can. J. Phys. 56 (1978) 983.

5. "The Multiconfiguration Hartree-Fock Method for Atomic Energy Levels and Transition Probabilities," Invited talk presented at the Sixth International Conference on Atomic Physics, Riga, 1978 (to appear in Conference Proceedings) Conference paper No. COO-4264-3.

6. "Oscillator Strengths for Some D - F Transitions in the Mg Sequence," J.O.S.A. (accepted-preprint attached).

7. "$4s\ 4d\ ^1D - 4p^2\ ^1D$ Interaction in the Zn I Isoelectronic Sequence" (with J. E. Hansen) (submitted to Phys. Rev.-preprint attached).

8. "Energy Levels and Oscillator Strengths for Fe XIV," Technical Report COO-4264-4.

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A strong interaction exists between $4p^2$ and $4s\ 4d\ ^1D$ and it has been shown that much of the earlier experimental material concerning the ^1D terms are in error. Comparison with a few recent experimental investigations shows good agreement.

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