UCRL CR 105110
S/C - 6181405

Final Progress Report for
Lawrence Livermore National Laboratory Subcontract 6181405

Title
Electron Impact Collision Strengths for
Excitation of Highly Charged Ions

UCRL-CR--105110

DE91 002666

by
Douglas H. Sampson
Department of Astronomy and Astrophysics
The Pennsylvania State University
University Park, PA 16802
(814) 865 - 0261

Period Covered
February, 1985 - August 15, 1990

Date Prepared: August 20, 1990

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

NOV 15 1990

MASTER *db*

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

DISCLAIMER

Work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial products, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

The principal task given us by the Lawrence Livermore National Laboratory (LLNL) to perform under Subcontract 6181405 was to develop a method and corresponding computer programs to make very rapid, yet accurate, fully relativistic and quasirelativistic calculations of cross sections or collision strengths for electron impact excitation of highly charged ions with any value for the nuclear charge number Z . Also while this major code development was being done we were asked to calculate cross sections of interest using our previous rapid, more approximate codes, which used hydrogenic basis functions and screening constants with both the electron-electron Coulomb interaction and relativistic interactions included by perturbation theory. This was done in references 1-5 for the cases indicated by the titles of those papers. We were also asked to determine the branching ratio for ionization to various final states in complex cases, where two or more states corresponding to the final configuration of the ion were possible. This was done in Ref. 6.

It was also suggested by LLNL scientists (e.g. Ref. 7) that innershell ionization of Na-like ions might be a significant mechanism for populating excited states of neon-like ions and it was suggested that we obtain cross sections and rates for this process. This was done in Ref. 8. Also similar results for populating excited levels of He-like and Ni-like ions by innershell ionization of Li-like and Cu-like ions were obtained in Ref. 9 and 10.

Another project suggested by LLNL scientists was for us to obtain improved collision rates for excitation to highly excited levels with principal quantum number $n \geq 5$, for transitions among these levels and for ionization from these levels, which in most of the plasma modeling programs are labeled by n value alone. This was done in Ref. 11. At that time it was thought that the rates were accurate (to 20% or 25%) except possibly for the $n \rightarrow n+1$ transitions, where initial and final states are strongly coupled for low Z . At our request Dr. R.E.H. Clark at Los Alamos made unitarized distorted wave calculations of the cross sections for $n \rightarrow n+1$ and $n \rightarrow n+2$ transitions for $Z = 3, 10$ and 26 in Ref. 12 and found that our formula, without the modification for strong coupling given by Eq (14) of Ref. 11 for $n \rightarrow n+1$ transitions, was accurate to within 20% to 30% even near threshold for $Z = 3$ and was considerably better for higher Z and energies.

Returning to the discussion of our principal task of developing a rapid set of fully relativistic and quasirelativistic codes, we first made some tests of possible quasirelativistic approaches by comparing line strengths in Ref. 13 and 14. By the summer of 1987 we had preliminary versions of both the atomic structure and collision programs operating and reported this in Ref. 15. Further refinements and improvements were made and the detailed description of our fully relativistic (FR) approach, a faster quasirelativistic (QR) approach, and the corresponding computer programs were given in Ref. 16 and 17. Large scale calculations of collision strengths and oscillator strengths using the fully relativistic option in these programs have been made for various cases of interest in Ref. 18 - 22. In addition, similar calculations for Ni-like ions are nearly completed.²³

Some of the principal features of these programs are the following: The same relativistic Hartree-Fock-Slater, or Dirac-Fock-Slater, potential evaluated using a mean configuration is used in calculating all orbitals, bound and free, in considering a given class of transitions, such as the $n = 2 - n = 3$ transitions in fluorine-like ions. Hence, all orbitals are automatically orthogonal. In order to further reduce the number of radial functions and radial scattering integrals we calculate them for a fixed set of final, or scattered electron energies (usually six) starting near zero and going out to sufficiently high values to allow accurate determination of collision rates. For each of these we compute the radial integrals for three impact electron energies spanning the range of transition energies for the class of transitions being considered. Then we interpolate on these results to obtain values for the exact transition energy in each case. It should be mentioned that, although we usually calculate collision strengths for a fixed set of final electron energies in our large scale calculations, our computer programs have the option to calculate collision strengths for a set of impact electron energies, which are sometimes preferred by the LLNL scientists. If the factorization method of Bar-Shalom et al²⁴ is used, the interpolation is done on the Q^λ . In general we do use the factorization method²⁴ whenever we do large scale calculations for a big portion of an isoelectronic sequence, as in Ref. 18-23. Then the collision strength Ω has the form

$$\Omega = 8 \sum_{\substack{j_a, j'_a \\ j_{a1}, j'_{a1}}} \sum_{\lambda} B^\lambda(j_a j'_a, j_{a1} j'_{a1}) Q^\lambda(j_a j'_a, j_{a1} j'_{a1}), \quad (1)$$

Here j_{a1} and j_a represent orbitals in the initial target ion wave function, and j'_{a1} and j'_a represent orbitals in the final target ion wave function. A convenient feature of Eq (1) is that B^λ is a function

only of target ion quantum numbers and mixing coefficients plus λ , while the Q^λ contains the radial contribution and depends only on λ and the bound and free orbitals with the summations over the free-electron momenta performed within it. Since the Q^λ vary smoothly with Z , in treating a given class of transitions for a large portion of an isoelectronic sequence, one needs to make detailed calculations of the Q^λ for only a few values of Z (typically one in ten) and then these can be fitted to a power series in Z that generally gives accurate results to within a percent for the complete range of Z being considered. Since usually the Q^λ calculation is the lengthy part, this typically leads to a factor of 10 reduction in computing time. The present factorization version of our collision program is not totally general, but a totally general factorization version will be available within the coming year, if our funding continues.

The quasirelativistic option of our programs corresponds to dropping the small component of the radial functions and normalizing the large component as though it were the complete radial function. In addition, for the free electrons one uses the average (over j) value $\kappa = -1$ in the effective potential determining the free radial functions. They then become independent of j . This is a good approximation because one sums over j values for the free electrons in calculating the collision strength. Although as discussed in Ref. 17 the quasirelativistic results are quite accurate for most Z values, it only saves about a factor of 2.5 in computing time and it was not used in the large scale calculations of Ref. 18 - 23.

Recently a new option to include the generalized Breit interaction and the vacuum polarization and self energy QED corrections perturbatively has been added to our relativistic atomic structure program. These were included in the calculations done in Ref. 22 and 23. They affect the mixing coefficients significantly in a few cases for large groups of mixed states for high Z and they also improve the energies significantly for high Z , but they (in particular the Breit interaction) do greatly increase the length of the calculations. For example, in the work on F-like ions, use of this option increased the length of computing time for the atomic structure part of the calculations, which is otherwise essentially negligible relative to the time for the collision part, so that the total time for the calculations was approximately doubled. In order to give an indication of the current speed of the programs, we note that the total average CPU time on the Cray XMP at the LLNL Open Computing Facility (OCF) was a little less than 0.01 sec per collision strength data point for F-like ions when the option to include the generalized Breit interaction and the other QED corrections in the structure part of the calculations was omitted and this time was slightly more than doubled when this option was used. However, we expect to reduce the time required by this option in future work (assuming we get funding) so that even with its inclusion, the atomic structure part again requires almost negligible time in large scale calculations of collision strengths. One way this can probably be done is by fitting the radial parts of the Breit matrix elements to a power series in Z after detailed evaluations for a few Z values. It should also be noted that without this option the transition energies for $\Delta n \geq 1$ transitions appear generally to be accurate to within better than 1% and the effect on mixing coefficients is usually small so that omitting this option will give sufficient accuracy for many purposes. We should also mention that at least for excitation from the 1s subshell when $Z \geq 40$ or 50, the generalized Breit interaction probably makes a significant contribution to the scattering matrix elements and we will investigate this if funding for that purpose is obtained.

A version of our relativistic collision program that gives cross sections for excitation to specific magnetic sublevels of the target ion by directive electrons has also been obtained.²⁵ This was done at the request of LLNL scientists for use in comparing with and interpreting the electron beam ion trap (EBIT) experiments. For this purpose we have used this program to calculate results for several cases of interest as requested by LLNL scientists. If our funding is continued, this program could be expanded to include an option to calculate differential cross sections.

The collision program has also recently been expanded to give a rapid program for relativistic distorted wave electron impact ionization cross sections (see Ref. 26, copy attached). This gives very good agreement with other recent relativistic ionization work done in Ref. 27-30. It presently gives cross sections with the form of hydrogenic cross sections except that the orbitals are calculated using the Hartree-Fock-Slater potential for the target ion. Hence, the present ionization program can obviously be applied to ionization of the valence electron in Li-like, Na-like and Cu-like ions. However, as shown in the Appendix of Ref. 8, a program such as the present one has much wider applications. In particular it applies whenever both the initial and final states are pure states, such as is the case for ionization of He-like, Ne-like and Ni-like ions in their ground levels, and it also

applies if only either the initial or final level is a pure state. Hence, it is applicable for ionization of F-like and Co-like ions as well as innershell ionization of Li-like, Na-like and Cu-like ions. In order to make application to these more complex cases one must multiply by the initial occupation number $w_{n\kappa}$ of the active subshell $n\kappa = nlj$ and, if more than one state for the final ion is possible, one must multiply by a branching ratio factor R considered, for example, in Ref. 6. Also if mixing occurs in the initial or final level, one must multiply by the square of the mixing coefficient and sum over the mixed states. It is also convenient to express results in terms of a reduced cross section Q_R by factoring out a $\pi a_0^2/I(Ryd)^2$ factor, where I is the ionization energy. Then, if both initial and final states are pure ones, the cross section for ionization from subshell $n\kappa$ is given by

$$Q = \frac{\pi a_0^2}{I(Ryd)^2} w_{n\kappa} R Q_R, \quad (2)$$

while, if either the initial or final state is a mixed one, Eq (2) should be multiplied by the square of the mixing coefficient and summed over the mixed states, as mentioned previously.

It is interesting that the relativistic distorted wave values for the Q_R are close to the non-relativistic Coulomb-Born-Exchange values of Ref. 31 for hydrogenic ions Q_R^H except for high Z and/or energies. Since the Q_R^H have been fitted to simple functions of the electron energy in threshold units that are readily integrated over a Maxwellian electron distribution function to obtain ionization rates, one would expect that accurate fits of the relativistic results for the reduced cross section could be made, as well, probably using the same functional form given by Eq (6) of Ref. 31, but allowing the coefficients to be slowly varying functions of an effective Z or of Z and N , where N is the number of bound electrons per ion. This would be very convenient for applications to plasma modeling. If our funding continues we would expect to do this in the coming year. Also we would expect to consider ionization from higher subshells and we would expect to extend our rapid approach to autoionization so that we could treat the excitation-autoionization contribution, which sometimes considerably exceeds the direct contribution to ionization even for high Z as shown in Ref. 32. Of course, once our programs have been expanded to treat autoionization we could use them to rapidly calculate other indirect or resonance processes such as dielectronic recombination and the resonance contributions to excitation rates. In addition, if our funding continues, we expect to expand the present ionization program to give a general state to state relativistic distorted wave ionization program to handle those cases not involving initial and/or final pure states, where the present program does not apply.

Some LLNL scientists have also expressed strong interest in a relativistic program that would compute cross sections for ionization to specific sublevels of the final ion for applications to some EBIT experiments. A version of our programs that would do this could also be developed, if our funding continues.

It is probably of interest to note that our ionization program also includes a quasi-relativistic option like that discussed previously with regard to our excitation program. However, contrary to our expectations, this only saves about a factor of 1.6 in computing time. The reason for this is that so called triangular conditions limit the number of relativistic ionization scattering matrix elements so they are not much greater than in non-relativistic calculations.

Very analogous to our relativistic ionization program, a very rapid version of our relativistic excitation program calculates cross sections $Q_H^p(nlj - n'l'j')$ of the same form as relativistic hydrogenic ones except that the potential used in calculating the orbitals is the Dirac-Fock-Slater potential evaluated using a mean configuration. These programs are of direct use for the mean relativistic configuration model being used in some plasma modeling work at LLNL. Of course, to be applicable to this model the cross sections must be multiplied by the occupation w_{nlj} of the initial subshell of the active electron and by the fraction of final states available, that is by the total factor $w_{nlj}[2j' + 1 - w_{n'l'j'}]/(2j' + 1)$, where $w_{n'l'j'}$ is the initial occupation number of the final subshell. We have found that the $Q_H^p(nlj - n'l'j')$ for a given transition and fixed N can be fitted accurately (to within 1 or 2%) to a power series in Z for a fixed N . Also fits to a power series in N can be made. Hence, one need calculate them for only a fraction of Z and N values. Also we suspect that similar to the ionization cross sections the $Q_H^p(nlj - n'l'j')$ can be fitted to quite simple functions of the excitation energy in the threshold units with coefficients that are functions of an effective Z or Z and N . If our funding continues, this could be investigated in future work.

Finally we note that, as discussed in Ref. 16 - 23, comparisons of collision strengths with results by other more elaborate relativistic programs such as that of Hagelstein and Jung³³ and the very elaborate program of Kim³⁴ and Kim and Desclaux³⁵, and comparison of oscillator strengths with those by the multiconfiguration Dirac-Fock program of Grant et al³⁶⁻³⁸ indicate that the results by the present rapid programs are essentially as accurate as those by the most elaborate relativistic programs available when

$$Z \geq 2N \text{ or } 2.5N. \quad (3)$$

References

1. D.H. Sampson, G.M. Weaver, S.J. Goett, H.L. Zhang and R.E.H. Clark, "Collision Strengths and Line Strengths for all Transitions Among the Levels of the $1s^2 2s^2 2p$, $1s^2 2s 2p^2$ and $1s^2 2p^3$ Configurations of Boron-Like Ions", *Atom. Data Nucl. Data Tables* **35**, 223-266 (1986).
2. H.L. Zhang, D.H. Sampson and R.E.H. Clark, "Collision Strengths for all Transitions Among the Levels of the $1s 2l 2l'$ Configurations of Li-Like Ions", *Atom. Data Nucl. Data Tables* **35**, 267-318 (1986).
3. H.L. Zhang and D.H. Sampson, "Collision Rates for Excitation of Helium-Like Ions with Inclusion of Resonance Effects", *Astrophys. J. Suppl.* **63**, 487-514 (1987).
4. H.L. Zhang, D.H. Sampson, R.E.H. Clark and J.B. Mann, "Collision Strengths and Oscillator Strengths for Excitation to the $n = 3$ and $n = 4$ Levels in Neon-Like ions", *Atom. Data Nucl. Data Tables* **37**, 17-51 (1987).
5. H.L. Zhang, D.H. Sampson, R.E.H. Clark and J.B. Mann, "Collision Strengths and Oscillator Strengths for Innershell Excitation of Na-Like Ions", *Atom. Data Nucl. Data Tables*, **41**, 1-58 (1989).
6. D.H. Sampson, "Branching Ratios for Excitation to Highly Excited Levels or Ionization of Highly Charged Ions", *Phys. Rev. A* **34**, 986-1006 (1986).
7. B.L. Whitten and A.U. Hazi, in *Laser Interaction and Related Plasma Phenomena*, edited by H. Hora and G.H. Miley (Plenum, New York, 1986), Vol 7, p. 53.
8. D.H. Sampson and H. L. Zhang, "Rate Coefficients for Populating Excited Levels of Neon-Like Ions by Innershell Ionization of Na-like Ions", *Phys. Rev. A* **36**, 3590-3606 (1987).
9. D.H. Sampson and H. L. Zhang, "Rate Coefficients for Populating Excited Levels of He-Like Ions by Innershell Ionization of Li-like Ions", *Phys. Rev. A* **37**, 3765-3776 (1988).
10. D.H. Sampson, H. L. Zhang and A.K. Mohanty, "Rate Coefficients for Populating Excited Levels of Ni-Like Ions by Innershell Ionization of Cu-like Ions", *Phys. Rev. A* **38**, 4569-4573 (1988).
11. D.H. Sampson and H.L. Zhang, "Semi-Empirical Formulae for Electron Impact Excitation and Ionization of Hydrogenic Ions", *Astrophys. J.* **335**, 516-524 (1988).
12. R.E.H. Clark, *Astrophys. J.* **354**, 382 (1990).
13. A.K. Mohanty and D.H. Sampson, "A Comparison of Relativistic and Quasirelativistic Line Strengths", *Physica Scripta* **35**, 645-649 (1987).
14. A.K. Mohanty and D.H. Sampson, "Reply to 'Comment on 'A Comparison of Relativistic and Quasirelativistic Line Strengths''", *Physica Scripta* **38**, 557-559 (1988).
15. H.L. Zhang, D.H. Sampson and A.K. Mohanty, in Abstracts from the Sixth Topical Conference of the American Physical Society on Atomic Processes in High Temperature Plasmas, Santa Fe, NM, 1987, Los Alamos National Laboratory Publication No. LALP-87-30.
16. D.H. Sampson, H.L. Zhang, A.K. Mohanty and R.E.H. Clark, "A Dirac-Fock-Slater Approach to Atomic Structure for Highly Charged Ions", *Phys. Rev. A* **40**, 604-615 (1989).
17. H.L. Zhang, D.H. Sampson and A.K. Mohanty, "Fully Relativistic and Quasirelativistic Distorted Wave Methods for Calculating Collision Strengths for Highly Charged Ions", *Phys. Rev. A* **40**, 616-632 (1989).
18. H.L. Zhang and D.H. Sampson, "Relativistic Distorted Wave Collision Strengths for Excitation to the $88\ n = 3$ and $n = 4$ Levels in all 71 Neon-Like Ions with $22 \leq Z \leq 92$ ", *Atom. Data Nucl. Data Tables*. **43**, 1-69 (1989).

19. H.L. Zhang, D.H. Sampson and C.J. Fontes, "Relativistic Distorted Wave Collision Strengths and Oscillator Strengths for the 88 Li-Like Ions with $8 \leq Z \leq 92$ ", *Atom. Data Nucl. Data Tables*, 44, 31-77 (1990).
20. D.H. Sampson, H.L. Zhang and C.J. Fontes, "Relativistic Distorted Wave Collision Strengths and Oscillator Strengths for the 71 Na-Like Ions with $22 \leq Z \leq 92$ ", *Atom. Data Nucl. Data Tables*, 44, 209-271 (1990).
21. H.L. Zhang, D.H. Sampson and C.J. Fontes, "Relativistic Distorted Wave Collision Strengths and Oscillator Strengths for the 33 Cu-Like Ions with $60 \leq Z \leq 92$ ", *Atom. Data Nucl. Data Tables*, 44, 273-304 (1990).
22. D.H. Sampson, H.L. Zhang and C.J. Fontes, "Relativistic Distorted Wave Collision Strengths and Oscillator Strengths for the 71 F-Like Ions with $22 \leq Z \leq 92$ ", being submitted to *Atom. Data Nucl. Data Tables*.
23. H.L. Zhang, D.H. Sampson and C.J. Fontes, "Relativistic Distorted Wave Collision Strengths for Excitation to the 249 $n=4$ and $n=5$ Levels in the 33 Ni-like Ions with $60 \leq Z \leq 92$ ", being prepared for submission to *Atom. Data Nucl. Data Tables*.
24. A. Bar-Shalom, M. Klapisch and J. Oreg, *Phys. Rev. A* 38, 1773 (1988).
25. H.L. Zhang, D.H. Sampson and R.E.H. Clark, "Relativistic Cross Sections for Excitation of Highly Charged Ions to Specific Magnetic Sublevels by an Electron Beam", *Phys. Rev. A*, 41, 198-206 (1990).
26. H.L. Zhang and D.H. Sampson, "A Rapid Relativistic Distorted Wave Approach for Calculating Cross Sections for Ionization of Highly Charged Ions", accepted by *Phys. Rev. A*.
27. M. S. Pindzola and M. J. Buie, *Phys. Rev. A* 37, 3232 (1988).
28. M. S. Pindzola and M. J. Buie, *Phys. Rev. A* 39, 1029 (1989).
29. M. S. Pindzola, D. L. Moores and D. C. Griffin, *Phys. Rev. A* 40, 4941 (1989).
30. D. L. Moores and M. S. Pindzola, *Phys. Rev. A* (in press).
31. D.L. Moores, L.B. Golden and D.H. Sampson, *J. Phys. B* 13, 385 (1980).
32. K.J. Reed, M.H. Chen and D.L. Moores, *Phys. Rev. A* 41, 550 (1990).
33. P.L. Hagelstein and R.K. Jung, *Atom. Data Nucl. Data Tables* 37, 121 (1987).
34. Y.-K. Kim, private communication (1988) and Hazi Atomic Physics Workshop, LLNL, June 20-22 (1988).
35. Y.-K. Kim and J.P. Desclaux, *Physica Scripta* 36, 796 (1987).
36. I.P. Grant, B.J. McKenzie, P.H. Norrington, D.F. Mayers and N.C. Pyper, *Compt. Phys. Commun.* 21, 207 (1980).
37. B.J. McKenzie, I.P. Grant and P.H. Norrington, *Compt. Phys. Commun.* 21, 233 (1980).
38. K.G. Dyall, I.P. Grant, C.T. Johnson, F.A. Parpia and E.P. Plummer, *Compt. Phys. Commun.* 55, 425 (1989).

END

DATE FILMED

12 / 03 / 90