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EXCITATION AND IONIZATION OF HIGHLY CHARGED IONS
BY ELECTRON IMPACT

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ABSTRACT

Two approaches for very rapid calculation of atomic data for high temperature plasma modeling have been developed. The first uses hydrogenic basis states and has been developed and applied in many papers discussed in previous progress reports. Hence, it is only briefly discussed here. The second is a very rapid, yet accurate, fully relativistic approach that has been developed over the past two or three years. It is described in more detail. Recently it has been applied to large scale production of atomic data. Specifically, it has been used to calculate relativistic distorted wave collision strengths and oscillator strengths for the following: (1) all transitions from the ground level to the $n = 3$ and 4 excited levels in the 71 Neon-like ions with nuclear charge number Z in the range $22 \leq Z \leq 92$; (2) all transitions among the $2s_{1/2}$, $2p_{1/2}$ and $2p_{3/2}$ levels and from them to all nlj levels with $n = 3, 4$ and 5 in the 85 Li-like ions with $8 \leq Z \leq 92$; (3) all transitions among the $3s_{1/2}$, $3p_{1/2}$, $3p_{3/2}$, $3d_{3/2}$ and $3d_{5/2}$ levels and from them to all nlj levels with $n = 4$ and 5 in the 71 Na-like ions with $22 \leq Z \leq 92$; and (4) all transitions among $4s_{1/2}$, $4p_{1/2}$, $4p_{3/2}$, $4d_{3/2}$, $4d_{5/2}$, $4f_{5/2}$ and $4f_{7/2}$ levels and from them to all nlj levels with $n = 5$ in the 33 Cu-like ions with $60 \leq Z \leq 92$. Also the program has been extended to give cross-sections for excitation to specific magnetic sublevels of the target ion by an electron beam and very recently it has been extended to give relativistic distorted wave cross sections for ionization of highly charged ions by electron impact.

I.Introduction

This is the final report on the work done under Grant DE-FG02-85ER53208. The work on this Grant done prior to April 30, 1987, has been covered rather completely in previous progress reports. Hence, the main emphasis here will be on the more recent work done during the period May 1, 1987 until October 31, 1989, the final day of the present Grant period.

We note that work in the area of this Grant has been supported by the Division of Applied Plasma Physics, Office of Fusion Energy, Department of Energy, since April 1, 1976, initially under contract DE-AC02-76-ET53056 and then under the present Grant DE-FG02-85ER53208. Since February 7, 1985 the work in this area has been jointly supported by the Lawrence Livermore National Laboratory under subcontract 6181405. Also since September 15, 1988 this work has been partially supported by the Ultrashort Wavelength Laser Program, Innovative Science and Technology Office, Strategic Defense Initiative Organization under contract No. 00014-88-K-2021.

The purpose of the work reported here is to calculate the atomic data needed for application to the study and understanding of very high temperature plasmas such as occur in fusion energy research, astrophysical research and research to develop X-ray lasers. In particular, we have been calculating the atomic data needed to model and diagnose such plasmas. For fusion energy research this includes the data needed to determine energy losses due to impurity ions. Most of our emphasis has been on calculating collision strengths or cross sections for excitation and ionization of highly charged ions by electron impact, but radiative line strengths or oscillator strengths and, in some cases, autoionization rates are also calculated.

An immense amount of atomic data is needed for plasma applications. Hence, we have emphasized the development and application of very rapid approaches for calculating these atomic data. During the period of support by DOE we have developed two such approaches. One of these was developed and used during most of the period of DOE support. Since it has been covered quite thoroughly in previous progress reports it is only briefly discussed in the next section. The other more accurate approach is a very rapid

fully relativistic approach that has been developed in the past two or three years. The remaining sections cover it and its applications in more detail.

II. Calculations using Hydrogenic Basis States

During most of the period of support by DOE we developed and applied in a large number of papers (Ref. 1 - 45) a very rapid approach in which the complete electron-electron interaction and all relativistic interactions were treated as a perturbation. Hence, the approach used hydrogenic basis states. Comparisons with other more elaborate calculations and experiment, when available, have indicated that this approach is generally quite accurate (within about 15 or 20%) for electron impact excitation when the condition:

$$2.5N \text{ or } 3N \leq Z \leq 50 \text{ or } 60 \quad (1)$$

is satisfied, where N is the number of bound electrons per ion and Z is the nuclear charge number. The range of Z given by Eq.(1) is approximately the range at which both the electron-electron interaction and the relativistic interactions are quite small. For lower values of Z the electron-electron interaction becomes too large to be treated as a perturbation and for higher Z the relativistic interactions become too large to be treated perturbatively. For ionization the range of validity of the approach is somewhat greater, presumably because ionization is like excitation summed over many final states for the active electron and errors tend to cancel in the summation.

This approach and practically all of the work done with it are covered rather completely in our previous progress reports^{46,47}. Thus, we only mention a few points for completeness here. First we note that the two papers on innershell ionization of Na-like and Li-like ions as a mechanism for populating excited levels of Ne-like and He-like ions, which were discussed in Ref.47, have been published^{41,42}. Also, a similar paper on inner-shell ionization of Cu-like ions as a mechanism for populating excited levels of Ni-like ions has been published⁴³. In all three cases it appears that this mechanism is an important one for producing excited levels of the next higher stage of ionization, especially if there are a few nonthermal high energy electrons present. Also it appears that the formula for $n - n'$ transitions and ionization for hydrogenic ions given in Ref.44 are quite accurate. This has

recently been confirmed by unitarized distorted wave calculations of R.E.H.Clark⁴⁸ at Los Alamos. It should be mentioned that according to his test calculations the modification given by Eq.(14) of Ref.44, which we proposed to approximately take account of the effects of strong coupling between initial and final levels for $n - n + 1$ transitions, should not be made. Then the formula appears to be accurate to within about 25% even for $Z = 3$ and the accuracy increases quite rapidly with increase in Z . With the use of effective Z values, these formulae should be very useful for treating the less important transitions involving high n values in complex ions, while using a more detailed treatment of the lower more important levels. In fact it is my understanding that this is now the standard practice of the plasma modelers at the Lawrence Livermore National Laboratory (LLNL). We also note that the papers on collision strengths and oscillator strengths for excitation of Neon-like ions to the $n = 3$ and 4 levels and innershell excitation of Na-like ions, which were discussed in our last progress report⁴⁷, have been published in Ref.40 and 45.

III.Fully Relativistic Distorted Wave Calculations.

After some preliminary work in Ref.49 and 50 on quasirelativistic line strengths for hydrogenic ions, we have recently succeeded in developing a very rapid fully relativistic approach and associated computer programs (with still faster quasirelativistic (QR) options) for treating ions satisfying the condition:

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

A detailed description of the approach together with illustrative numerical results and comparison with results of other more elaborate relativistic approaches have been published in Ref.51 and 52. It should be noted that, although the lower limit of Z in Eq.(2) is not much lower than in Eq.(1) the comparisons made in Ref.51 and 52 and in the more recent work of Ref.53-56 indicate that the accuracy of the new relativistic approach within the range of Z given by Eq.(2) is considerably higher than that of our earlier approach within the range of Z given by Eq.(1). In fact within most of the range of Z given by Eq.(2), the results by our new relativistic approach appear to be essentially as accurate as those by the most elaborate relativistic distorted wave programs now available.

Before we proceed to an outline of the principal features of this new relativistic approach we summarize the accomplishments made thus far with it.

(a) Summary of Accomplishments with Our Relativistic Approach

First we note that our new relativistic approach has been applied to large scale production of atomic data for several classes of transitions of interest for high temperature plasma applications in Ref.53-56. It is of interest that during the course of that work the programs have been further optimized so they are now over a factor of 3 times faster than they were at the time the calculations in Ref.53 and 54 were made. In fact, at present the CPU time required on Cray-XMP at the NMFEC at Livermore, CA, per collision strength data point averages only about 0.1 sec for the cases considered in Ref.53-56.

In the work of those references it was demonstrated that when the collision strengths are expressed in the factorized form of Bar-Shalom et al⁵⁷ they can be accurately obtained for a large portion of an isoelectronic sequence with the use of fits to power series in Z , the nuclear charge number, after detailed calculations have been made for only a few values of Z . For example, in Ref.53 relativistic collision strengths were obtained for the 88 transitions from the ground level to the excited levels with $n = 3$ and 4 in the 71 Ne-like ions with $22 \leq Z \leq 92$ after making detailed calculations for only the 6 values, $Z = 22, 30, 42, 56, 74$ and 92. Similarly in Ref.54 collision strengths were obtained for the 3 transitions among the $2s_{1/2}$, $2p_{1/2}$ and $2p_{3/2}$ levels and the 63 transitions from them to the nlj levels with $n = 3, 4$ and 5 in the 85 Li-like ions with $8 \leq Z \leq 92$ after detailed calculations were made for only the 8 Z values $Z = 8, 14, 22, 30, 42, 56, 74$ and 92. In Ref.55, similar calculations were made for Na-like ions. Specifically the relativistic collision strengths were obtained for the 10 transitions among the $3s_{1/2}$, $3p_{1/2}$, $3p_{3/2}$, $3d_{3/2}$, $3d_{5/2}$ levels and the 80 transitions from these levels to the nlj levels with $n = 4$ and 5 in the 71 Na-like ions with $22 \leq Z \leq 92$, where, as for neon-like ions, the detailed calculations were made for the 6 values $Z = 22, 30, 42, 56, 74$ and 92. In Ref.56 the relativistic collision strengths were obtained for the 21 transitions among the $4s_{1/2}$, $4p_{1/2}$, $4p_{3/2}$, $4d_{3/2}$, $4d_{5/2}$, $4f_{5/2}$ and $4f_{7/2}$ levels and the 63 transitions from them to the nlj levels with $n = 5$ in the 33 Cu-like ions with $60 \leq Z \leq 92$ after detailed calculations were made for the 4 values

$Z = 60, 70, 80$ and 92 . In making all of these calculations, when considering a particular class of transitions, the results are obtained for the same set of six scattered or final electron energies E' given in units of Z_{eff}^2 Rydbergs, where Z_{eff} is given approximately by:

$$Z_{eff} = Z - 0.833(N - 1) \quad (3)$$

In addition, our new relativistic programs have been expanded to give a program for calculating relativistic distorted wave collision strengths for excitation of highly charged ions to specific magnetic sublevels M_f by an electron beam. This work was complicated by the fact that these cross sections, or collision strengths, depend on the so called Coulomb phase factor of the scattered electron, but modified to account for the fact that the potential is actually not that of a pure Coulomb field. The work was written up in Ref.58. It was done at the request of LLNL for use in comparing with and interpreting their electron beam ion trap (EBIT) experiments⁵⁹.

Also, we have recently expanded our collision program to obtain a fully relativistic distorted wave electron impact ionization program, with a faster quasirelativistic option. This program needs to be further tested and optimized and a paper on it has not yet been written. However, we expect to write one very soon containing some illustrative numerical results and we expect to apply the program to several cases of interest for high temperature plasma research in the coming year.

(b) Outline of Our Relativistic Approach

In our relativistic approach, when treating a given class of transitions, all orbitals, bound and free, are solutions of the Dirac equation with the same relativistic Hartree-Fock-Slater, or Dirac-Fock-Slater central potential. Hence, all orbitals are automatically orthogonal and exchange can be handled in a simple, consistent manner. This potential is given in Rydbergs by:

$$V(r) = -\frac{2Z}{r} + V_c(r) - \left(\frac{24}{\pi}\rho\right)^{\frac{1}{3}} \quad (4)$$

where

$$V_c(r) = \sum_{n'\kappa'} \omega_{n'\kappa'} \int_0^\infty \frac{2}{r_2} [P_{n'\kappa'}^2(r_2) + Q_{n'\kappa'}^2(r_2)] dr_2 \quad (5)$$

and

$$\rho(r) = \frac{1}{4\pi r^2} \sum_{n'\kappa'} \omega_{n'\kappa'} [P_{n'\kappa'}^2(r_2) + Q_{n'\kappa'}^2(r_2)] \quad (6)$$

Here $\omega_{n'\kappa'}$ is the occupation number of subshell $n'\kappa' = n'l'j'$, the summation is over all occupied subshells, $r_>$ is the greater of r and r_2 , and $P_{n'\kappa'}$ and $Q_{n'\kappa'}$ the so called large and small components of the radial function of an electron in the $n'\kappa'$ subshell.

In considering a given class of transitions a single mean configuration with fractional occupation numbers for some subshells is used in determining the potential with Eqs.(4)-(6). For example in the application to excitation to the $n = 3$ and $n = 4$ levels in neon-like ions considered in Ref.53 we used the mean configuration:

$$\begin{aligned} &1s_{1/2}^2 \ 2s_{1/2}^{1.9} \ 2p_{1/2}^{1.9} \ 2p_{3/2}^{3.7} \ 3s_{1/2}^{0.04} \ 3p_{1/2}^{0.04} \ 3p_{3/2}^{0.04} \ 3d_{3/2}^{0.04} \ 3d_{5/2}^{0.04} \\ &\times 4s_{1/2}^{0.04} \ 4p_{1/2}^{0.04} \ 4p_{3/2}^{0.04} \ 4d_{3/2}^{0.04} \ 4d_{5/2}^{0.04} \ 4f_{5/2}^{0.05} \ 4f_{7/2}^{0.05} \end{aligned} \quad (7)$$

which corresponds to a total hole of 0.5 electrons in the $n = 2$ subshells and an occupation of 0.5 electrons in the $n = 3$ and 4 subshells. This can be regarded as equal splitting of the active electron between initial and final subshells which is the prescription we usually use. Actually test cases^{51,52} have indicated that slight changes in occupation numbers within a shell have little effect on results.

It should be noted that the mean configuration is used solely in determining the potential with Eqs.(4)-(6) and the calculations are generally multiconfiguration calculations, except in simple cases such as transitions involving only a single valence electron. Generally we include at least all the mixing among the states in a complex, i.e. having the same set of n values, parity and J value. In fact, in Ref.53, where we found that some of the $n = 4$ levels overlapped some of the $n=3$ levels for low and high Z values, we included mixing among all the $n = 3$ and $n = 4$ levels with the same parities and J values.

For most cases the length of the calculations of collision strengths is determined principally by the number of radial wave functions and radial scattering matrix elements or integrals. Hence, it is important to keep this number to a minimum. In addition to the other convenient aspects of using the same potential in determining the orbitals of all the electrons, as we have described, this helps to minimize the number of radial integrals in

treating complex ions. This occurs because, in contrast to some multiconfiguration treatments the bound electron contribution to the radial scattering integrals is then the same for all transitions in which the same orbital transition $n_a l_a j_a - n'_a l'_a j'_a$ enters, which can be very large for complex ions. Of course, the free-electron contribution to these radial integrals differs for each different initial and final free-electron energy. In order to minimize this effect we use the following procedure: In considering a given class of transitions, such as all the $n = 2$ to $n = 3$ and 4 transitions in neon-like ions considered in Ref.53, we calculate results for a fixed set of scattered electron energies (usually six) beginning near zero and spanning the range needed to obtain accurate collision rates. For each of these we calculate results for three impact-electron energies spanning the range of transition energies for the class of transitions considered. Then we interpolate on these three sets of results for the radial scattering integrals to get the values for the correct transition energy for each particular transition in the complex ion. When the factorized form for the collision strength is used, as we do in large scale production runs, the interpolation is done on the Q^λ , see Eq.(8) below. Since the radial integrals and the Q^λ vary smoothly and quite slowly with energy, this procedure works very well and leads to a large reduction in the number of radial integrals occurring in the treatment of complex ions.

In order to obtain results for a given class of transitions for a large portion of an isoelectronic sequence, as done in Ref.53-56, it is convenient to use the factorized form of Bar-Shalom et al⁵⁷ for the collision strength. In the factorized form the collision strength can be written:

$$\Omega = 8 \sum_{\substack{j_a j'_a \\ j_{a_1} j'_{a_1}}} \sum_{\lambda} B^\lambda(j_a j'_a, j_{a_1} j'_{a_1}) Q^\lambda(j_a j'_a, j_{a_1} j'_{a_1}) \quad (8)$$

where the abbreviations $j_a = n_a l_a j_a$, $j'_a = n'_a l'_a j'_a$ etc. have been used. Here j_a and j_{a_1} represent orbitals of active electrons in the initial target ion wave function, while j'_a and j'_{a_1} represent corresponding quantities in the final target ion wave function. A very convenient feature of Eq.(8) is that B^λ is a function only of the target ion quantum numbers and the 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 summation over the free electron momenta performed within it. The B^λ can vary rapidly with Z , but they can be regarded

as essentially part of the atomic structure portion of the calculations and require little time to compute. In fact, for the relatively simple cases considered in Ref.54-56, they are unity, but for the cases considered in Ref.53, they are products of mixing coefficients, e.g. Eq.(18) of Ref.52. In general, most of the computing time goes into calculating the Q^λ . However, $Z^2 Q^\lambda$ varies slowly and smoothly with N and Z . In fact in our earlier rapid method based on hydrogenic basis functions, which was used in Ref.1-45, the $Z^2 Q^\lambda$ would be independent of Z and N . Thus one should expect to be able to make accurate fits of the Q^λ to N and Z , and it is fits of Q^λ not Ω to power series in Z that have been used in Ref.53-56. For example in Ref.53 we fit Q^λ to the form:

$$Z^2 Q^\lambda = a_1 Z^3 + a_2 Z^2 + a_3 Z + a_4 + a_5 Z^{-1} + a_6 Z^{-2} \quad (9)$$

while in Ref.54 we used:

$$Q^\lambda = [a_1 Z^4 + a_2 Z^3 + a_3 Z^2 + a_4 Z + a_5 + a_6 Z^{-1} + a_7 Z^{-2} + a_8 Z^{-3}]^{-2} \quad (10)$$

However, in simple cases such as those considered in Ref.54-56 involving no mixing, fits of Ω instead of Q^λ to power series in Z are only slightly less accurate. Extensive test calculations have indicated that in practically all cases the fit procedures used in Ref.53-56 give numerical accuracy to better than 1% , usually much better. In fact the maximum error found was 1.4%.

IV.Tentative Future Plans

Although it appears that the Division of Applied Plasma Physics, Office of Fusion Energy of DOE will no longer be supporting our future work in this area, we think the work will be of general interest and value for high temperature plasma applications, including those in fusion energy research. Hence, we give here a summary of our tentative future plans.

Now that our relativistic distorted wave collision strength program has been optimized considerably over the past few months, we expect to apply it in the coming year to some of the more complex and lengthy cases of interest for modeling high temperature plasmas,

such as excitation of fluorine-like ions, Ni-like and possibly cobalt like ions. Also during the coming year we expect to have built up a sufficient data base of the Q^λ that we can use to demonstrate that accurate fits of the Q^λ to N as well as Z can be made. In more distant future work it is anticipated that a sufficiently complete file of Q^λ 's will have been obtained for each class of orbital transitions, such as the 15 $n = 2$ to $n = 3$ orbital transitions, to allow one to obtain collision strengths for any N and Z of interest very rapidly. To be specific, this file might consist of the Q^λ for 6Z values and 4N values. In a particular plasma modeling application one would calculate the structure data for all the N values of interest for the particular value of Z of interest and form the B^λ . Then one would read in the Q^λ files for the orbital transitions of interest and make fits to Z for each of the 4 values of N to obtain values for the Q^λ for the particular Z of interest. Then one would make fits to N for that Z value to obtain the Q^λ values for every N of interest. Finally after interpolations to obtain the Q^λ for each precise transition energy, as discussed in the previous section, one would apply the Q^λ and B^λ to Eq.(8) and obtain the collision strengths for each transition needed for modeling the plasma under consideration. With this procedure, once the Q^λ files have been made the calculations of collision strengths for highly charged ions will take almost a trivial amount of computing time.

With regard to ionization we first note that, although we eventually expect to develop a general state to state ionization program, the present relativistic program calculates results only for ionization cross sections having the form of those for hydrogenic ions. However, it can use radial functions computed with any potential. In particular, we use the same relativistic Hartree-Fock-Slater, or so called Dirac-Fock-Slater, potential determined with the use of a mean configuration as described in Section III (b) for all electrons bound and free so all the orbitals are automatically orthogonal. Of course, this program applies directly for ionization of the valence electron in ions with a single valence electron such as Li-like, Na-like and Cu-like ions. In addition, as follows from the Appendix of Ref.41, the program can be used in obtaining relativistic cross sections for innershell ionization of these ions or any other case in which there is no mixing either among the initial states or the final states of the target ion. Thus, for example, it can also be used in obtaining ionization cross sections for fluorine like and cobalt like ions as well as He-like, Ne-like, and

Ni-like ions in their ground levels. Hence, it can be used for most cases of major interest for high temperature plasma applications. During the coming year while optimizing the program, we will also apply it to some of these cases of interest. In doing this, we expect to be able to demonstrate that for a given value of N the results for ionization from a relativistic subshell nlj can be accurately fit to Z after making detailed calculations for only a few Z values, analogous to the case for excitation discussed previously. Eventually, we expect to be able to show that accurate fits to N can be made as well.

Also in the future we expect to generalize our relativistic distorted wave ionization program into a general state to state ionization program that can be applied to any complex ion. We also expect to include the generalized Breit interaction in both our relativistic structure program and in the collisional excitation program. In addition it is planned to expand the programs to include photoionization and autoionization. As is well known the latter can then be applied to many indirect processes such as the resonance contribution to excitation cross sections, the branching ratios needed for the contribution of innershell excitation to ionization cross sections and dielectronic recombination.

REFERENCES

1. D. H. Sampson, "Electron Impact Excitation Cross Sections for Complex Ions I. Theory for Ions with One and Two Valence Electrons", *Astrophys. J. Suppl.* 28, 309-321 (1974).
2. D. H. Sampson and A. D. Parks, "Electron Impact Excitation Cross Sections for Complex Ions II. Applications to the Isoelectronic Series of Helium and Other Light Elements", *Astrophys. J. Suppl.* 28, 323-334 (1974).
3. A. D. Parks and D. H. Sampson, "Inner Shell Excitation of Lithium-Like Ions by Electron Impact", *J. Phys. B: Atom. Molec. Phys.* 8, 774-777 (1975).
4. A. D. Parks and D. H. Sampson, "Electron Impact Excitation Cross Sections for Complex Ions. III. Highly Charged Ions with Three Valence Electrons", *Astrophys. J.* 209, 312-318 (1976).
5. A. D. Parks and D. H. Sampson, "Electron Impact Excitation of Highly Charged Beryllium-Like Ions with Inclusion of Configuration Mixing", *Phys. Rev. A* 15, 1382-1392 (1977).
6. D. H. Sampson, A. D. Parks and R. E. H. Clark, "Effects of Configuration Mixing and Parentage Mixing on Inner Shell Excitation of Highly Charged Lithium-Like Ions", *Phys. Rev. A* 15, 1393-1406 (1977).
7. L. B. Golden and D. H. Sampson, "Ionization of Highly Charged Ions by Electron Impact", *J. Phys. B: Atom. Molec. Phys.* 10, 2229-2237 (1977).
8. D. H. Sampson and L. B. Golden, "Electron Impact Ionization Results by the $Z = \infty$ Method", *J. Phys. B: Atom. Molec. Phys.* 11, 541-549 (1978).
9. D. H. Sampson, A. D. Parks and R. E. H. Clark, "Intermediate Coupling Collision Strengths for Fine Structure Transitions between S and P Levels and S and D Levels in Highly Charged He-Like Ions", *Phys. Rev. A* 17, 1619-1633 (1978).
10. R. E. H. Clark, "Intermediate Coupling Collision Strengths from LS Coupled R-Matrix Elements", *Comput. Phys. Commun.* 16, 119-127 (1978).
11. L. B. Golden and D. H. Sampson "Scaled Coulomb-Born-Oppenheimer Collision Strengths for Electron Impact Excitation to Levels with $n \leq 5$ in Hydrogenic Ions with $Z = \infty$ ", *Astrophys. J. Suppl.* 38, 19-28 (1978).
12. L. B. Golden, D. H. Sampson and K. Omidvar, "Ionization from the 3s Sublevel of Highly Charged Ions", *J. Phys. B: Atom. Molec. Phys.* 11, 3235-3243 (1978).
13. R. E. H. Clark and D. H. Sampson, "Intermediate-Coupling Collision Strengths for P-P and P-D Transitions Produced by Electron Impact on Highly Charged He-Like Ions", *At. Data Nucl. Data Tables* 22, 527-546 (1978).
14. D. H. Sampson, R. E. H. Clark and A. D. Parks, "Intermediate-Coupling Collision Strengths for Inner Shell Excitation of Highly Charged Li-Like Ions", *J. Phys. B: Atom. Molec. Phys.* 12, 3257-3272 (1979).

15. D. H. Sampson and L. B. Golden, "Ionization Cross Sections for Li-Like Ions Including Excitation-Autoionization Contributions", J. Phys. B: Atom. Molec. Phys. 12, L785-L791 (1979).
16. D. L. Moores, L. B. Golden, D. H. Sampson, "Ionization from the 3p and 3d Sublevels of Highly Charged Ions", J. Phys. B: Atom. Molec. Phys. 13, 385-395 (1980).
17. L. B. Golden and D. H. Sampson, "Ionization from the 4s, 4p, 4d and 4f Sublevels of Highly Charged Ions", J. Phys. B: Atom. Molec. Phys. 13, 2645-2652 (1980).
18. D. H. Sampson and R. E. H. Clark, "Intermediate Coupling Collision Strengths for $\Delta n = 0$ Transitions Produced by Electron Impact on Highly Charged Ions I. Theoretical Development and Application to $n = 2$ Levels in He-Like Ions", Astrophys. J. Suppl. 44, 169-191 (1980).
19. D. H. Sampson, R. E. H. Clark and L. B. Golden, "Intermediate Coupling Collision Strengths for $\Delta n = 0$ Transitions Produced by Electron Impact on Highly Charged Ions II. Transitions between States of the $1s^2 2s^2$ and $1s^2 2p^2$ Configurations and Those of the $1s^2 2s 2p$ Configurations in Be-like Ions", Astrophys. J. Suppl. 44, 193-213 (1980).
20. R. E. H. Clark, D. H. Sampson and A. D. Parks, "Intermediate Coupling Collision Strengths for $\Delta n = 0$ Transitions Produced by Electron Impact on Highly Charged Ions III. Transitions within the $1s^2 2s 2p$ and $1s^2 2p^2$ Configurations and between the $1s^2 2s^2$ and $1s^2 2p^2$ Configurations in Be-like Ions", Astrophys. J. Suppl. 44, 215-222 (1980).
21. S. J. Goett, R. E. H. Clark and D. H. Sampson "Intermediate Coupling Collision Strengths for $\Delta n = 0$ Transitions Produced by Electron Impact on Highly Charged He- and Be-Like Ions", At. Data Nucl. Data Tables 25, 185-217 (1980).
22. D. H. Sampson and L. B. Golden, "Ionization Cross Sections with Inclusion of Excitation-Autoionization Contributions for Ions with Five or Fewer Bound Electrons", J. Phys. B: Atom. Molec. Phys. 14, 903-913 (1981).
23. L. B. Golden, R. E. H. Clark, S. J. Goett and D. H. Sampson, "Scaled Collision Strengths for Hydrogenic Ions", Astrophys. J. Suppl. 45, 603-612 (1981).
24. D. H. Sampson, R. E. H. Clark and S. J. Goett, "Intermediate-Coupling Collision Strengths and Line Strengths for Certain Transitions to $n = 3$ Levels in Highly Charged Be-Like Ions", Phys. Rev. A 24, 2979-2994 (1981).
25. R. E. H. Clark, D. H. Sampson and S. J. Goett, "Scaled Collision Strengths for $\Delta n \geq 1$ Transitions Involving $n \leq 5$ in Hydrogenic Ions", Astrophys. J. Suppl. 49, 545-554 (1982).
26. D. H. Sampson, "Ionization of Na-Like Ions Including Excitation-Autoionization", J. Phys. B: Atom. Molec. Phys. 15, 2087-2099 (1982).
27. S. J. Goett, D. H. Sampson and R. E. H. Clark, "Intermediate-Coupling Collision Strengths for Transitions between Doubly Excited Levels Produced by Electron Impact on Highly Charged He-Like Ions", At Data Nucl. Data Tables 28, 279-297 (1983).

28. D. H. Sampson, S. J. Goett and R. E. H. Clark, "Electron-Impact Collision Strengths for Inner-Shell Excitation of Doubly Excited Levels from Singly Excited Levels in He-Like Ions", At. Data Nucl. Data Tables 28, 299-331 (1983).
29. D. H. Sampson, S. J. Goett and R. E. H. Clark, "Electron-Impact Collision Strengths for Excitation of He-Like Ions from the Levels with $n = 1$ and 2 to All Singly Excited Levels with Higher $n \leq 5$ ", At. Data Nucl. Data Tables 29, 467-534 (1983).
30. S. J. Goett, D. H. Sampson, "Collision Strengths for Innershell Excitation of Li-Like Ions from Levels of the $1s^2 2s$ and $1s^2 2p$ Configurations to Levels of the $1s 2l 2l'$ Configurations", At. Data Nucl. Data Tables 29, 535-572 (1983).
31. S. J. Goett, D. H. Sampson and R. E. H. Clark, "Innershell Excitation of Li-Like Ions", Astrophys. J. Suppl. 54, 115-125 (1984).
32. D. H. Sampson, S. J. Goett and R. E. H. Clark, "Collision Strengths and Line Strengths for Fine-Structure Transitions between the $2l_a 2l_b$ Configurations and the $2l'_a 3l'_b$ Configurations in Be-Like Ions", At. Data Nucl. Data Tables 30, 125-260 (1984).
33. R. E. H. Clark and D. H. Sampson, "Ionization from the Sublevels $n l$ with $n = 5$ and 6 in Highly Charged Ions", J. Phys. B: Atom. Molec. Phys. 17, 3311 (1984).
34. D. H. Sampson, S. J. Goett, G. V. Petrou, H. Zhang and R. E. H. Clark, "Collision Strengths for Innershell Excitation of Li-Like Ions from the $1s^2 2s$ and $1s^2 2p$ Levels to the $1s 2l 3l'$ Levels", At. Data Nucl. Data Tables 32, 343 (1985).
35. D. H. Sampson, G. V. Petrou, S. J. Goett and R. E. H. Clark, "Collision Strengths for Innershell Excitation of Li-Like Ions from the $1s^2 3l$ Levels to the $1s 2l' 3l''$ Levels", At. Data Nucl. Data Tables 32, 403 (1985).
36. 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 in Boron-Like Ions", At. Data Nucl. Data Tables 35, 223 (1986).
37. H. Zhang, D. H. Sampson and R. E. H. Clark, "Collision Strengths and Line Strengths for all Transitions among the levels of the $1s 2l 2l'$ Configurations in Li-Like Ions", At. Data Nucl. Data Tables 35, 267 (1986).
38. D. H. Sampson, "Branching Ratios for Excitation to Highly Excited Levels or Ionization of Complex Ions", Phys. Rev. A. 34, 986 (1986).
39. H. Zhang and D. H. Sampson, "Collision Rates for Excitation of He-Like Ions with Inclusion of Resonance Effects", Astrophys. J. Suppl. 63, 487 (1987).
40. H. Zhang, D. H. Sampson, R. E. H. Clark and J. B. Mann, "Collision Strengths and Oscillator Strengths for Excitation to the $n=3$ and 4 Levels of Neon-Like Ions", Atom. Data Nucl. Data Tables 37, 17 (1987).
41. 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 (1987).

42. 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 (1988).
43. 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 (1988).
44. D. H. Sampson and H. L. Zhang, "Semiempirical Formulas for Electron Impact Excitation and Ionization of Hydrogenic Ions," *Astrophys. J.* 335, 516 (1988).
45. 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," *At. Data Nucl. Data Tables* 41, 1 (1989).
46. D. H. Sampson, "Excitation and Ionization of Highly Charged Ions by Electron Impact," Progress Report for Sept. 1, 1985-April 30, 1986, DOE/ER/53208-1.
47. D. H. Sampson, "Excitation and Ionization of Highly Charged Ions by Electron Impact," Progress Report for May 1, 1986-April 30, 1987, DOE/ER/53208-2.
48. R. E. H. Clark, "Distorted Wave Collision Strengths for n - n' Transitions in Hydrogenic Ions," scheduled for Nov. 1989 issue of *Astrophys. J.*
49. A. K. Mohanty and D. H. Sampson, "A Comparison of Relativistic and Quasirelativistic Line Strengths," *Physica Scripta* 35, 645 (1987).
50. A. K. Mohanty and D. H. Sampson, "Reply to 'Comment on 'A Comparison of Relativistic and Quasirelativistic Line Strengths,'" *Physica Scripta* 38, 557 (1988).
51. 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 (1989).
52. 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 (1989).
53. 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 $22 \leq Z \leq 92$," *At. Data Nucl. Data Tables* 43, 1 (1989).
54. H. L. Zhang, D. H. Sampson and C. J. Fontes "Relativistic Distorted Wave Collision Strengths and Oscillator Strengths for the 85 Li-Like Ions with $8 \leq Z \leq 92$," accepted by *At. Data Nucl. Data Tables*.
55. 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 $22 \leq Z \leq 92$," submitted to *At. Data Nucl. Data Tables*.

56. 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 $60 < Z < 92$," submitted to At. Data Nucl. Data Tables.
57. A. Bar-Shalom, M. Klapisch and J. Oreg. Phys. Rev. A 38, 1773 (1988).
58. 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," accepted by Phys. Rev. A.
59. R. E. Marrs, M. A. Levine, D. A. Knapp and J. R. Henderson, Phys. Rev. Lett. 60, 1715 (1988).

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