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OPACITY CALCULATIONS
FOR LOW-SPACE AND HIGH-Z MATERIAL

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A short note on opacity calculations for low- and high-Z materialsS.J. Rose

The purpose of this short note is to look in quite general terms at the calculation of the opacity of both low- and high-Z materials and to point out areas in which new initiatives may be made. The comments made here are simply meant to stimulate discussion.

Introduction.

The calculation of the radiative opacity of a plasma requires in principle, the same information for both low- and high-Z materials. Assuming that the temperature is sufficiently high that the contribution from molecules can be ignored, an accurate knowledge of the energies and absorption strengths of each bound-bound, bound-free and free-free transition is required for each ion in the plasma. If the opacity model is not to be based exclusively on experimental data, this requires a model of the ionic electronic structure. Many different models of varying accuracy have been used in opacity calculations. Coupled with this atomic physics information, the probability that a particular ion is found in the plasma is required. For L.T.E. systems this involves solving the Saha and Boltzmann equations (or some approximation to them). A line (or edge) shape is then required for each absorption feature. The physical basis of the broadening will depend on the temperature and density of the plasma and the approximations used for the line shape have varied in their sophistication. The remarks on the atomic and statistical physics have been made under the assumption that the plasma is at a low density. The effects of finite plasma density need to be taken into account in all opacity calculations, but the effects are believed to become particularly marked for densities approaching solid, which makes the effect of density relevant to both

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laboratory and astrophysical plasmas.

Present opacity calculations.

Several excellent reviews of opacity calculations have appeared in the literature^{1,2,3,4,5}, and it is not the purpose of this note to go over that ground in such detail, but rather to summarize some of the approximations in the physical theory which are used in present opacity calculations.

Atomic physics

In discussing atomic physics models used to date, it is desirable to consider separately the detail and the accuracy of the calculations.

Considering firstly the detail, opacity codes at both L.L.N.L. and L.A.S.L. consider the splitting of each one-electron transition into the different transitions from one configuration to another. However, in no code known to the author has the term-splitting been included explicitly (by which is meant that the position and strength of each transition in the array is calculated separately), although in the L.L.N.L. code Moszkowski's⁶ method of describing the splitting as a continuous distribution has been included. It could well be the case that because the number of configurations which occur in high-Z systems is generally very high, such a statistical description is adequate. In low-Z opacity calculations the number of configurations has always made consideration of transitions between one configuration and another necessary and feasible. Because in general the configurations involve orbitals of lower angular momentum than in the high-Z case, explicit consideration of term-splitting is also included in some calculations⁷. Although LS-coupling appears to be adequate for systems of very low-Z and/or low ionization, it has recently been shown that for highly ionized systems intermediate coupling may be needed (see Appendix). Many of the calculations of the opacity of low-Z material which are in use, however, do not include term-splitting.⁸ A study of the plasma conditions under which the inclusion of term-splitting

is important for opacity calculations has never appeared, to the author's knowledge, in the literature.

Considering secondly the accuracy of the atomic physics models in opacity calculations, we need to distinguish between average-atom models, which are used in many low-Z and all high-Z calculations, and models which use experimental data or accurate calculated values, which have been used in some low-Z calculations^{5,6}. Average-atom models calculate the atomic physics from a single set of one-electron orbitals for particular plasma conditions. Although it has been recognised for some time that this can produce line and edge positions which are very inaccurate¹⁰ (especially for low degrees of ionization), it has only recently been appreciated that similar errors can be produced in high-Z calculations (again especially for low degrees of ionization). These errors arise from the neglect of orbital relaxation and the effect is particularly important in certain low-temperature laser-produced plasmas.

Statistical Mechanics.

Although the Saha and Boltzmann equations are usually used to calculate the probability that a particular ion is found in the plasma for low-Z material (but see 3), for the high-Z case an approximation based on individual orbital occupancies, which is much easier to compute, is often used. The error involved is usually referred to as the neglect of statistical correlation. In general it appears that this approximation becomes worse as the temperature decreases¹¹.

Density Effects.

This is an area of physical theory which is not well understood. Originally continuum lowering and shifts in the positions of lines and edges due to the plasma were included either, for average-atom calculations, through the average-atom potential due to the plasma, or for isolated-ion calculations, using perturbation theory with a plasma potential (such as Debye-Huckel or the uniform free-electron model). There

are good theoretical reasons to doubt these formulations although there is little experimental data against which to test theories. Recently a much more complete theoretical description has been produced¹² and an assessment of its impact on opacity values awaits its inclusion in an opacity code.

Future Opacity Calculations.

It is obviously desirable to include all improvements which are believed to be important in any new opacity calculation. For low-Z material it appears feasible to include term-splitting explicitly, to provide accurate absorption strengths beyond the average-atom approximation, to use accurate statistical mechanics and to account for plasma density effects with the most accurate and complete theoretical formulation available. Also for low-Z material, it may be possible to use many-electron line-shape calculations. A large effort is required to write a code to calculate opacities at this level of complexity and this is being provided by the low-Z opacity group at L.L.N.L. The results of their detailed calculations will be of particular interest to the astrophysical community who work in the field of stellar structure and evolution.

For calculations of the opacity of high-Z materials the situation is different in that it does not appear possible to include term-splitting explicitly. The only feasible methods appear to be those used by Moszkowski⁶, the more modern variant of Bauche-Arnoult¹³ or possibly the methods of Bloom and Goldberg¹⁴. Because of this, the calculation of individual line-broadening is far less critical than in low-Z calculations. Current average-atom high-Z calculations produce inaccurate values of line and edge positions for low states of ionization because of their neglect of orbital relaxation. In high-Z opacity calculations it would therefore be desirable to include this effect. Liberman¹⁵ has recently demonstrated a fast, accurate method for the calculation of transition energies between one configuration and another which includes orbital relaxation and Albritton¹⁵ has written a fast method of solving the statistical mechanical

equations. It therefore appears that it would be possible to write a high-Z opacity code based on these two pieces of work coupled with one of the descriptions of term broadening discussed above, which would go beyond the present calculations based on the average-atom. This would plainly be of great use for comparison with present opacity calculations and experimental data.

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RELATIVISTIC AND NON-RELATIVISTIC CALCULATIONS OF TRANSITION ARRAYS

S. J. Rose

The purpose of this short note is to discuss the limitations of LS-coupling in the description of term-splitting in low-Z opacity calculations. We have calculated absorption spectra of the lines resulting from a transition between one configuration and another in two different approximations. The first uses a relativistic multiconfiguration Dirac-Fock calculation¹ to predict, within the single-manifold approximation,* the line positions and strengths. The second approximation is exactly equivalent to the first except that the value of the speed of light in the calculation has been increased by a factor of 10^4 , which makes the calculation effectively non-relativistic.

Calculations for several different cases have been performed in this way. The materials Al, Cl and Fe have been chosen to cover a range of atomic number of interest for which a difference between the two calculations may be expected. In each case $gf\phi(\nu)$ is plotted against photon energy where g is the degeneracy of the ground state of the transition, f is the oscillator strength and $\phi(\nu)$ is the normalized Doppler profile at the

*This approximation includes all the jj-states which reduce to a single non-relativistic configuration in the formal limit $c \rightarrow \infty$.

temperature shown (chosen so as to be approximate in each case for the degree of ionization involved). For Al and Cl results of the calculations are shown for the transitions

$$1s^2 2s^2 2p^3 \rightarrow 1s 2s^2 2p^4$$

whereas for Fe results are shown for

$$1s^2 2s^2 2p^2 \rightarrow 1s 2s^2 2p^3 \text{ and } 1s^2 2s^2 2p^3 \rightarrow 1s 2s^2 2p^4 .$$

In each case, the lines calculated in the non-relativistic approximation lie to lower energy than in the relativistic calculation. The largest change is, however, a small percentage of the transition energy and this effect would not be in itself a major error in an opacity calculation. However, in the relativistic calculation there are more lines. This is due to both the fine-structure splitting and the breakdown in the $\Delta S=0$ selection rule. Although for Al and Cl the effect is relatively small, in Fe the absorption profile is completely different in the relativistic calculation. Examination of the eigenvectors shows that although the non-relativistic calculation is in exact LS-coupling, for the case of Fe in the relativistic calculations the eigenvectors are in intermediate coupling.

In conclusion, it appears that although the shift in transition energy due to the effect of relativity is unimportant for the calculation of opacity, the inclusion of intermediate coupling is necessary for the description of the distribution of lines in transition arrays. This latter effect is particularly necessary for elements of atomic number as high as Fe.

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Al $1s^2 2s^2 2p^3 \rightarrow 1s 2s^2 2p^4$ (100eV)

non-relativistic

photon energy (keV)

AL $1s^2 2s^2 2p^3 \rightarrow 1s 2s^2 2p^4$ (100 eV)
relativistic

gfa

Cl $1s^2 2s^2 2p^3 \rightarrow 1s 2s^2 2p^4$ (300 eV)
non-relativistic

Cl $1s^2 2s^2 2p^3 \rightarrow 1s 2s^2 2p^4$ (300 eV)

relative

gfd

Fe $1s^2 2s^2 2p^2 \rightarrow 1s 2s^2 2p^3$ (1000eV)