RADIATIVE OPACITIES

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ABSTRACT A review is given of opacity calculations made during the past decade.

SOME DEFINITIONS

The net outward radiative flux inside a star is

$$F = -\frac{1}{\kappa_B} \frac{4\pi}{3} \frac{dB}{dT} \frac{dT}{dr} \tag{1}$$

where r is radius, T is temperature,

$$B = \frac{2\pi^4}{15c^2h^3}(kT)^4\tag{2}$$

is the integrated Planck function and κ_R is the Rosseland mean opacity, defined as a harmonic mean weighted by the temperature derivative of the monochromatic Planck function. The working formula is

$$\frac{1}{\kappa_R} = \int \frac{f(u)}{\kappa(u)} \ du \tag{3}$$

where $u = h\nu/kT$, $\kappa(u)$ is the monochromatic opacity and

$$f(u) = (15/4\pi^4)u^4 \exp(-u)/[1 - \exp(-u)]^2.$$
 (4)

This function is normalised to

$$\int f(u) \ du = 1, \tag{5}$$

is proportional to u^2 for u small, has a maximum value at u = 3.830..., and decreases exponentially for u large.

The monochromatic opacity is obtained on summing over all processes leading to extinction of radiation,

$$\kappa(u) = \sum_{i} N_{i} \sigma_{i}(u) \times E_{i}$$
 (6)

where N_i is the number-density of particles of type i, $\sigma_i(u)$ is a cross section and E_i a correction-factor for stimulated emission: $E_i = [1 - \exp(-u)]$ for absorption processes, $E_i = 1$ for scattering.

Use of equations such as (6) gives opacities per-unit-length. Those are the quantities which enter directly into the equation of radiative transfer and they are also the most convenient for general presentation of the theory. Numerical results, however, are usually given as opacities per-unit-mass (in units of cm² g⁻¹). The relation is $\kappa(\text{per-unit-length}) = \rho \times \kappa(\text{per-unit-mass})$, where ρ is the mass-density. In attempting to calculate opacities we face two main problems.

- Determine the populations, N_i . That is the problem of the equation of state (EOS).
- Determine the cross sections, σ_i . That is a problem of atomic physics.

One must consider very large numbers of atomic processes: bound-bound (spectrum lines); bound-free (photoionisation); free-free; and scattering (mainly by free electrons). For the line contributions one requires, in addition to line-frequencies and f-values, information about the line profiles determined by radiation damping, thermal motions and pressure-broadening.

We may distinguish between two regions "inside the stars", envelopes and interiors. So far as opacity work is concerned, I define envelopes to be those regions in which there are no major plasma perturbations of the systems i giving dominant contributions to opacities; and interiors those in which such perturbations are important. For the calculation of envelope opacities one requires an acceptable EOS and large amounts of accurate atomic data. For interiors one has the additional, and difficult, problem of calculating the cross-sections $\sigma_i(u)$ allowing for plasma perturbations.

BACKGROUND TO RECENT WORK.

I will not attempt to review the earlier literature: see Cox(1965) and Carson (1973). For more than two decades extensive use has been made of opacities calculated at the Los Alamos National Laboratory in the USA (see Cox and Stewart, 1965 and 1970; Cox and Tabor, 1976; Hübner et al. 1977; Hübner, 1985; and Weiss et al. 1990). I shall refer to that work as LAOL (Los Alamos Opacity Library). Substantial use has also been made of the St. Andrews opacities (Carson et al., 1968). The reasons for some discrepancies between the LAOL and the St. Andrews work have been explained (Carson et al., 1984).

In his now-famous paper of 1982, Simon made a plea for the re-examination of the heavy-element contributions to opacities. He showed that an increase in the contributions from elements heavier than helium, by factors of two or three in envelope regions, would resolve a number of outstanding problems in the theory of pulsating stars. Although Magee et al. (1984) argued that such a large increase would be incompatible with atomic physics, two groups responded to Simon's plea. The first was at the Lawrence Livermore National Laboratory (F.J. Rogers, C.A. Iglesias and B.G. Wilson) and I will refer to it as OPAL, the name of their computer code. The second is a project with which I have been associated and which has involved quite a large team of workers from a number

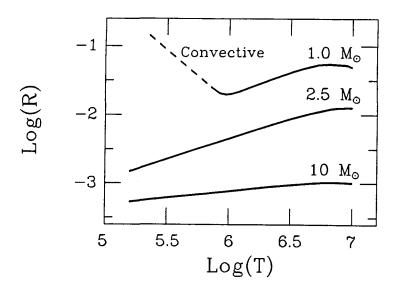


FIGURE I Values of $\log(R)$ against $\log(T)$ for three initial main sequence models, from Schwarzschild (1958). $R=\rho/T_6^3$ with ρ in g cm⁻³ and $T_6=10^{-6}\times T$ with T in K

of countries (France, Germany, the UK, the USA and Venezuela). We refer to it as *The Opacity Project* and I will refer to it here as OP. The remainder of the present review will be mainly concerned with the presentation of OPAL and OP results, and comparisons with those from LAOL.

The Rosseland mean, κ_R , depends on temperature T, density ρ and chemical composition. For any stellar model higher temperatures correspond to higher densities. The OPAL team use the variable $R = \rho/T_6^3$ with ρ in g cm⁻³ and $T_6 = 10^{-6} \times T$ with T in K. For a given stellar model, R is approximately constant — at least, to within a factor of 10 or so: Figure I shows $\log(R)$ against $\log(T)$ for 3 early stellar models (Schwarzschild, 1958). Thus a plot of κ_R against T for fixed R gives an impression of the variation of κ_R with depth inside a star. I will make use of such plots in the present review.

THE OPAL AND OP APPROACHES

The OPAL approach.

The EOS work, of both OPAL and OP, is discussed further by W. Däppen at this meeting and therefore need not be discussed in detail here. The OPAL work is based on a sophisticated approach to the plasma EOS problem developed over many years (see Rogers 1986, 1991 and references therein). The method is firmly the "physical picture" in which one starts by considering an assembly of electrons and nuclei. As the plasma conditions permit, the electrons can become bound to the nuclei to form states of atomic ions. In general such states

are perturbed by the plasma environment and their wave-functions must be calculated with inclusion of plasma potentials. The simplest example of such a potential is the static screened Coulomb potential $\exp(-r/r_D)/r$ replacing the Coulomb potential 1/r, r_D being the Debye radius. The use of such potentials has, however, been criticised by Hummer and Mihalas (1988).

For lower densities, and states which are not highly excited, the plasma perturbations become small and can be neglected. For unperturbed atomic states Rogers (1981) and Rogers et al. (1988) use parametric potentials of the type

 $V(r) = -\frac{2}{r} \left[z + \sum_{i} C_{i} \exp(-\alpha_{i} r)\right]$ (7)

where z is the residual charge on the ion and C_i the number of electrons in shell i. With such potentials they use a spin-averaged Dirac equation to calculate atomic radial functions. For states with principal quantum numbers $n \leq 4$ they take full account of LS angular-momentum coupling and adjust the parameters α_i in (7) so as to obtain good agreement with experimental ionisation energies. For $n \geq 5$ they use a simple central-field model. In later work (Iglesias et al, 1992) they consider the use of intermediate coupling.

The OPAL atomic calculations are made on-line, that is to say the atomic data are not stored but are calculated as they are required. There is doubtless some cost in computer time but the approach does give the advantage of great flexibility and of allowing for the possibility to include plasma potentials as and when required. The OPAL EOS calculations are made on solving coupled equations for full mixtures at each density and temperature point. Their results for opacities are tabulated as functions of $\log(R)$ and T_6 .

The OP approach

For a plasma, define a mean inter-particle separation r_0 by $(4\pi/3)r_0^3N=1$ and let r_i be the mean radius for absorber i (for hydrogenic systems with principal quantum number n, $r_n=(5n^2+1)/(4z)$ atomic units). For envelopes it is assumed that $r_i\gg r_0$ for all absorbers contributing significantly to the opacity. Hummer and Mihalas (1988) tentatively adopy $\rho=10^{-2}$ g cm⁻² for the lower boundary of envelopes. That corresponds to $r_0\simeq 5.5$ atomic units.

The OP work is concerned with the determination of envelope opacities using results from extensive ab initio calculations of atomic data. The main atomic calculations are made R-matrix methods (see Berrington et al., 1987) and are described in a series of papers "Atomic Data for Opacity Calculations" in the Journal of Physics B (to date, 17 papers published or submitted). For systems containing up to 12 electrons the OP atomic data can be considered to be "near definitive": with the exception only of a fairly small number of cases for which highly optimised calculations have been made, they are more accurate than other data available, and much more extensive. For systems with more than 12 electrons, particularly those involving configurations $3s^x 3p^y 3d^z$, supplementary calculations are made using the code SUPERSTRUCTURE (Eissner and Nussbaumer, 1969; Nussbaumer and Storey, 1988).

The OP EOS work is described in four papers "The Equation of State for Stellar Envelopes" (Hummer and Mihalas, 1988; Mihalas et al., 1988; Däppen et al., 1988; and Mihalas et al., 1990). The approach is firmly the "chemical

picture" in which atomic particles are assumed to exist. In order to avoid divergences of partition functions (essentially, the exclusion of states with r_i not $\gg r_0$) it is necessary to introduce occupation probabilities, W_i . Equations for the determination of ionisation equilibria are obtained from minimisation of the free energy. It is found that, to a very good approximation, the equilibria depend only on temperature T and electron density N_e . Opacities are calculated separately for each chemical element as functions of T and N_e and are archived. Results for any mixture can then be calculated rapidly. The OP opacity tables give ρ and κ_R as functions of T and N_e and interpolation routines provide values of κ_R for any required value of T and ρ within the range of the tables.

Comparisons of the two approaches

Envelopes and interiors

The main thrust of the OP work is in the calculation of opacities for envelopes, say $\rho \le 10^{-2} \text{ g cm}^{-2}$. For deeper interiors the OPAL results are to be preferred.

Equations of State

Comparisons between OPAL and OP EOS results have been made by Däppen, Lebreton and Rogers (1990). For envelope regions they find good agreement for basic thermodynamic quantities. Further comparisons of ionisation equilibria have also been made by members of the two teams and, again for envelopes, the agreement is quite good. Larger differences can be expected — and exist — if the OP EOS calculations are extended to interiors.

Atomic data

The OP R-matrix data are obtained with allowance for configuration interaction (CI), which is neglected in the OPAL work. For unperturbed atomic systems the OP atomic data should therefore be the more accurate.

When CI is neglected one can obtain bound states above the ionisation limit. Inclusion of CI leads to coupling between those states and continuum states and hence to auto-ionisation features. Many of the OP photo-ionisation cross sections contain very complicated auto-ionisation structures. An example is shown in Figure II. These features are included by OPAL as ordinary lines (transition to the "bound states" above the ionisation limits) but the auto-ionisation broadening is neglected. The figure also shows results from central-field calculations which are probably in close agreement with results used by OPAL.

Line profiles

The treatment of line profiles should be basically similar. A distinction is made between hydrogenic systems (nl states degenerate with respect to l) for which Stark effects are important (a detailed account is given by Seaton, 1990) and non-hydrogenic systems for which "isolated-line" approximations are used. For the isolated lines, both teams use methods related to those introduced by Griem (1968) which employ an extension to line-broadening theory of the \overline{g} -approximation of atomic collision theory. This gives expressions for line-widths in terms of oscillator strengths and some empirical factors. OPAL uses factors

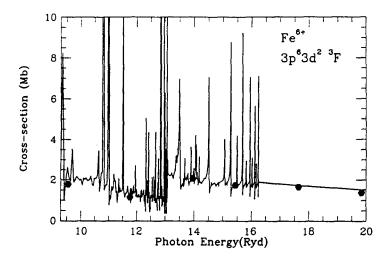


FIGURE II Cross section for photo-ionisation of the Fe⁶⁺ ground state, from Saraph *et al.* (1992). The solid hexagons are from central-field calculations by Reilman and Manson (1979).

determined by Dimitrijevič and Konijevič (1980) from fitting to experimental data while OP uses data fitted to results from R-matrix calculations. Table 12 of Seaton (1988) shows that the two approaches give close agreement. It may be desirable to consider further the use of the sharp distinction between the hydrogenic and non-hydrogenic cases.

For the widths of the auto-ionisation features, neither approach may be be entirely satisfactory. For those features, OP allows for auto-ionisation broadening but neglects other broadening mechanisms (Doppler and pressure), whereas OPAL includes those other mechanisms but neglects auto-ionisation.

Mesh points

There are two OP codes, one developed by Yu Yan and D. Mihalas in Illinois and the other by myself in London. The Illinois code uses a constant interval in $\log(u)$ and 10^5 mesh points, sufficient to resolve all Doppler profiles. I use a constant interval in u, $0 \le u \le 20$. If one reduces the number of frequency-mesh points some narrow lines may be missed altogether but, with trapezoidal-rule integrations, one will obtain over-estimates of contributions due to lines with centre-frequencies close to mesh points. These effects tend to cancel. I find that use of 10^4 frequency points, compared with 10^5 , gives errors no larger than 1 % or so. These errors are not important in themselves but can produce a slight lack of smoothness which may be just discernable in some of the plots which I shall show later.

OP uses intervals of 0.25 in $\log(N_e)$ and 0.025 in $\log(T)$. OPAL uses 5×10^3 frequency points and intervals in $\log(\rho)$ and $\log(T)$ somewhat larger than those used by OP.

RESULTS FOR OPACITIES

OPAL results.

Results for a Cepheid model

The first published OPAL results (Iglesias et al., 1987) were for $\rho=10^{-5}$ g cm⁻² and kT=20 and 60 eV (T=2.32 and 6.97×10^5 K) and showed that an improved treament of the atomic physics could lead to significant opacity enhancements. That these could be at least as large as those postulated by Simon (1982) was first shown by Iglesias et al. (1990), who gave results for a model of a Cepheid envelope previously considered by Rozsnayi (1989). The top part of Figure III shows $\log(R)$ against $\log(T)$ for the model (the highest density is $\rho=0.0136$) and the lower part compares OPAL opacities with those from LAOL as used by Simon. The largest ratio, $\kappa_R(\text{OPAL})/\kappa_R(\text{LAOL})$, is 3.34.

In discussing Rosseland opacities one must consider the nature of the harmonic mean defined by (3) (failure to do so was the main source of error in the paper by Magee et al., 1984). Any extended region in which $\kappa(u)$ is small will give a large contribution to the integrand in (3) and hence leads to a small value of κ_R (the radiation escapes in regions of high transparency). Iglesias et al. identify two effects in the LAOL work which lead to localised under-estimates of $\kappa(u)$. The first is neglect of $\Delta n=0$ transitions, a consequence of the use of hydrogenic f-values. The second is the almost-complete neglect of term-splitting. Without such splitting transitions between two configurations are represented by a single line. When one allows for LS quantum numbers of initial and final states, and for all possible internal couplings of angular momenta, that single line is replaced by many lines with a significant spread in frequency. The most striking effects are for transitions involving configurations $3s^x 3p^y 3d^z$ in iron ions, which can give rise to very large numbers of lines.

The solar radiative interior

In constructing stellar models the net outward energy flux is generally a known quantity, determined by the rate of energy production in the deep interior. When conduction and convection can be neglected, the total flux is equal to the radiative flux and the temperature gradient, dT/dr, is then given by equation (1) and is proportional to the Rosseland mean opacity. Throughout much of the solar interior convection is important and in those regions knowledge of the Rosseland mean is not of such great significance. It is, however, again of importance in the solar radiative interior, the region below the convection zone. Accurate opacity determinations for that region are required in connection with studies of the solar neutrino problem and in considering sound-speeds determined by helio-seismology.

Iglesias and Rogers (1991) give a very careful and detailed discussion of opacities in the solar interior. They present OPAL results for $T \geq 10^6$ K, 3 values of $\log(R)$ and a number of different chemical mixtures. The differences between LAOL and OPAL for the solar interior are much smaller than those for the Cepheid envelope — for $T \geq 2 \times 10^6$ K the differences are no larger than 11 %. The revisions suggested by the OPAL work are, nevertheless, of considerable importance for problems in solar physics.

At the solar centre the opacity is mainly determined by free-free transitions

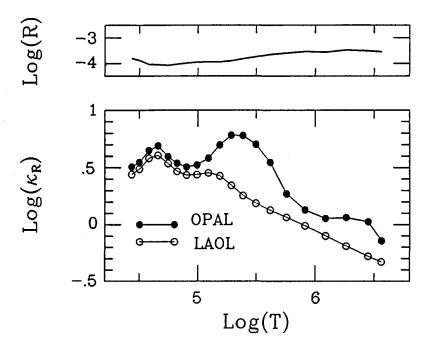


FIGURE III Opacities for a Cepheid model. OPAL results from Iglesias et al. (1990), LAOL results as used by Simon (1982). The top figure shows $\log(R)$ for the model.

and by electron scattering. In OPAL, free-free is calculated using parametric potentials screened for plasma correlations. The theory of Boercker (1987) is used for electron scattering. The OPAL/LAOL differences in the centre region are no more than 1 to 3 %.

The biggest OPAL/LAOL differences occur in the region just below the convection zone, with the OPAL results being the larger. Iglesias et al. conclude that these differences are mainly due to different treatments of the EOS problems. Different assumed chemical compositions can also lead to opacity differences of up to 5 % or so.

Comprehensive OPAL opacity tables

In a paper of major importance, Rogers and Iglesias (1992) give comprehensive tables of OPAL opacities. I have already given an outline description of the methods which they use. I will defer discussion of their results in order to compare them with those from OP.

OP opacities

First results for opacities from the OP work were presented at a Workshop on Astrophysical Opacities in Caracas, July 1991 (Yu Yan, 1992). Unfortunately those results were not entirely correct. I take full responsibility for the error, in one line of my code. Corrected results will be published in a post-script to the Workshop proceedings, added some months after the end of the meeting (Seaton, 1992). Further OP calculations have now been completed. Results can be provided, on request, for any required mixture together with the interpolation routine which give κ_R for all values of ρ and T covered by the tables.

Comparison and discussion of results

Mixtures are defined by X, Y and Z, fractions by weight of hydrogen, helium and all heavier elements. In the results presented here I will use the relative abundances of the heavier elements as given by Anders and Grevesse (1989).

Hydrogen and helium

Figure IV gives results for X = 0.7, Y = 0.3, Z = 0.0 and $\log(R) = -4$, -3 and -2. The OPAL and OP results are seen to be in close agreement. For OP I use a dashed line in regions with $\log(\rho) > -2$.

At the lower temperatures there are important contributions from H⁻ bound-free and free. From Figure IV it is seen that there are 3 maxima sometimes known, from left to right, as X-, Y- and Z-bumps. The first, at $\log(T) \simeq 4.1$, is due to absorption by H⁰, and to a lesser extent He⁰, in excited states. At these low temperatures the threshold for absorption by ground states comes at too high a frequency to make a significant contribution to the Rosseland mean. The next bump, at $\log(T) \simeq 4.7$, is due to absorption by the H⁰ ground state with some contributions from the He⁰ ground state and He⁺ excited states. The third bump (more like a shoulder for He and He alone), at $\log(T) \simeq 5.2$, is due to absorption by the He⁺ ground state.

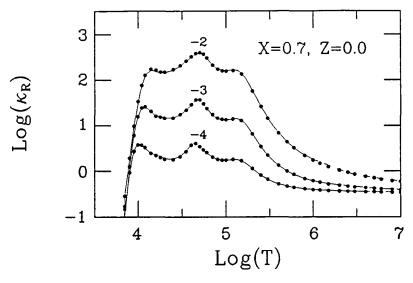


FIGURE IV Opacities for a mixture of hydrogen and helium. Full lines, OP; filled circles, OPAL. The curves are labelled with values of log(R)

The RR Lyrae case

Figure V shows, for the case of $\log(R) = -3$, the effect of adding 0.1% of heavy elements. There are two curves, one for Z = 0.000 and the other for Z = 0.001. There is, again, quite close agreement between the two calculations. Even for this low value of Z there is a substantial opacity enhancement for $5.0 \ge \log(T) \ge 6.5$, much larger than the enhancement given by LAOL. These results present some problems in studies of RR Lyrae stars.

Solar abundances

Figure VI shows results for X=0.7, Z=0.02 and $\log(R)=-4$, -3 and -2. Comparisons with LAOL for a similar composition have already been given in Figure III, and the effects producing an enhancement in metal contributions have been discussed in section 4.1.1. The agreement between OPAL and OP is fairly good although there are some differences with a tendency for the OP results to be the smaller. The reason for these differences should be studied further.

Figure VI shows that there is another bump in the opacities, which I will refer to it as the A-bump, at $\log(T) \simeq 6.3$.

Contributions from the different elements

Figure VII shows some OP results all made for the same mixture, X = 0.7, Z = 0.02, and $\log(R) = -3$. In order to show the contributions of different groups of elements, their opacities have been successively "switched on". There are 4 curves: (a) H and He; (b) as (a) plus C, N, O and Ne; (c) as (b) plus Na, Mg, Al, Si, S, Ar and Ca; (d) as (b) plus Fe. The A-bump is mainly due to absorption

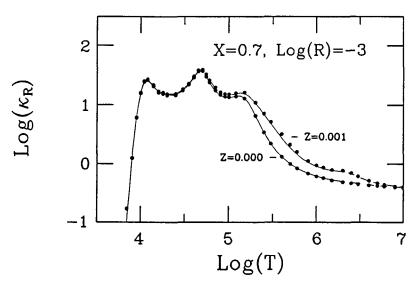


FIGURE V Opacities for X = 0.7, $\log(R) = -3$ and Z = 0.000 and 0.001. Curves as in Figure IV.

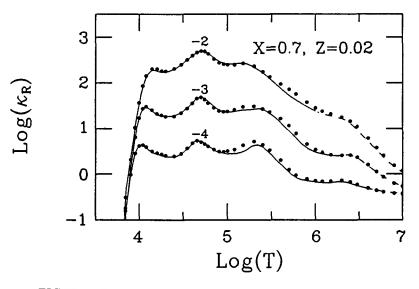


FIGURE VI Opacities for a solar mix, $X=0.7,\ Z=0.02.$ Curves as in Figure IV.

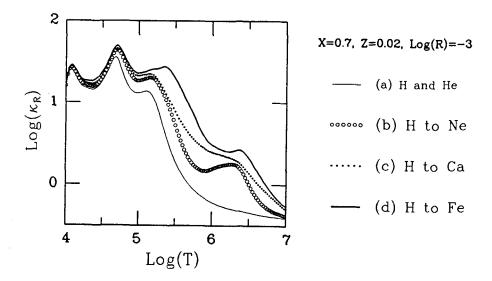


FIGURE VII Contributions to opacities from different groups of elements. OP calculations

from ground states in hydrogen-like and helium-like C, N and O. The elements from Na to Ca make important contributions in the vicinity of $\log(T) = 5.8$. The contribution of iron is important for all $\log(T) \geq 5$ but particularly in the vicinity of the Z-bump at $\log(T) \simeq 5.5$.

Inclusion of fine-structure

It has been seen that allowance for term-splitting (LS quantum numbers) produces major changes in results for opacities. It is therefore natural to ask whether allowance for fine-structure (introduction of J quantum numbers) will lead to further enhancements. This question has been considered recently by both the OPAL team (Iglesias et al., 1992) and the OP team, with findings in good agreement. At high densities the line-widths are comparable to the LS-coupling line-separations, the lines form a quasi-continuum and allowance for fine structure hardly makes any change. At low densities the lines are much narrower and inclusion of fine structure does lead to opacity enhancements. Thus at $\log(R) = -5$, inclusion of fine-structure leads to an enhancement by nearly 50 % at the peak of the Z-bump; while at $\log(R) = -2$ inclusion of fine-structure produces negligible change.

SUMMARY

Work which has been done during the past decade, and which is now nearing completion, has led to major revisions in envelope opacities, by factors as large as 3 or 4. There are also some revisions in results for deeper layers, which are important but not so pronounced. Use of the new opacities will require a

re-examination of a wide range of problems in stellar astrophysics.

It is very fortunate that two groups, OPAL and OP, took up the challenge. Their results do not agree exactly but there is generally close agreement, leaving no doubt about the magnitude of the changes in opacities compared with the earlier work.

ACKNOWLEDGMENTS

I thank Forrest Rogers and Carlos Iglesias for many helpful discussions, and all members of the OP team for their cheerful collaboration.

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