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and Their Effect on Stellar Models

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NEW ASTROPHYSICAL OPACITIES AND THEIR EFFECT ON STELLAR MODELS

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Recent advances in astrophysical opacity calculations are discussed. A description and comparison of results from two new independent efforts is given. The large increases in the calculated opacity in the few hundred-thousand degree range have led to improved agreement with a wide range of observations. Some directions for future work are suggested.

I. INTRODUCTION

The rapid increase in the breadth and quality of stellar observations in recent years has presented a challenge to stellar models. The most widely known example has been attempts to explain the solar neutrino production rate. This, plus a number of other observed properties of stars that could not be adequately explained by theoretical models were known to be sensitive to the opacity. It was noticed that arbitrarily increasing the opacity in the few hundred-thousand degree temperature range by factors of 2-3 would improve some properties of variable stars (Fricke, Stobie, and Strittmatter 1971; Peterson 1974; Stellingswerf 1978; Simon 1982), increasing the opacity by about 40% at slightly higher temperatures would improve the calculated Li abundance in the Hyades cluster (Swenson, Stringfellow, and Faulkner 1990), and increasing the opacity by 10-20% in the few million degree range would improve the predicted solar p-mode frequencies (Christensen-Dalsgaard, et al. 1985; Korzenik and Ulrich 1989; Cox et al. 1989).

The primary source of opacity data from the early 1960's until recently has been the Los Alamos National Laboratory (Cox and Stewart 1962; Cox and Tabor 1976; Huebner et al. 1977). St Andrews University has also provided opacity data (Carson, Mayers, and Stibbs 1968; Caron 1976). In response to a plea by Simon (1982) to reinvestigate the opacity, Magee et al. (1984) concluded that errors in the existing Los Alamos data were around 20% and rejected the possibility of large increases in the theoretical opacity.

Due to the importance of radiation transport in opacity for a wide range of stellar properties, the Los Alamos study notwithstanding, two groups undertook completely new, independent efforts to calculate astrophysical opacities. One of these, known as the Opacity Project (OP), is an international collaboration concerned with stellar envelopes. The other, known as OPAL and located at Lawrence Livermore National Laboratory, is concerned with the full range of interior opacities needed in stellar modeling. Contrary to the conclusions of Magee et al. (1984) preliminary OPAL results showed substantial increases in opacity (Iglesias, Rogers, and Wilson 1987) and up to factors of four have been reported in more complete calculations (Iglesias and Rogers 1991; Rogers and Iglesias 1992; Seaton et al. 1994). These increases are largely due to the rich spectrum of transitions originating in M-shell iron with an important contribution from the intra-M-shell transitions neglected by Los Alamos.

The format of the paper is as follows. Section II gives a brief description of the OP and OPAL efforts and Section III discusses the equation of state approaches that underlie the opacity calculations. New calculations of astrophysical opacities that include very heavy
elements are presented in Section IV and Section V suggests some future directions for opacity work.

II. OPACITY

The radiation transfer equation describes the transport of energy by photons and is equivalent to the Boltzmann equation in the kinetic theory of particle transport (Mihalas 1978). For steady-state conditions it is given by

$$\frac{dI_V(s,n)}{ds} = -\kappa_V I_V(s,n) + j_V$$

(1)

where \(I_V(s,n)\) is the intensity of radiation of frequency \(v\) in the direction \(n\) as a function of distance \(s\), \(j_V\) is the emissivity, and \(i\) is the elemental type. The monochromatic opacity, \(\kappa_V\), is given by

$$\kappa_V = \sum_i \chi_i \left( \kappa_{ib}^i + \kappa_{bf}^i + \kappa_{ff}^i \right)(1-e^{-hv/kT}) + \kappa_s,$$

(2)

where \(\chi_i\) is the number fraction, \(\kappa_{ib}^i\), \(\kappa_{bf}^i\), and \(\kappa_{ff}^i\) are the bound-bound, bound-free, and free-free absorption cross-sections, respectively, \(\kappa_s\) is the scattering cross-section and the factor \((1-\exp^{-hv/kT})\) is the correction factor for stimulated emission.

Conditions inside a star are close to local thermodynamic equilibrium so that according to Kirchhoff's law,

$$j_V = \kappa_V B_v(T),$$

(3)

where,

$$B_v = \frac{(2hv^3 / c^2)(e^{hv/kT} - 1)^{-1}}$$

(4)

is the Planck function. In addition, conditions change slowly over many photon mean-free paths and the radiation transfer equation greatly simplifies. In this limit, known as the diffusion approximation, \(\kappa_V\) can be replaced with a flux weighted harmonic mean according to

$$\frac{1}{\kappa_R} = \int_0^\infty d\nu \frac{1}{\kappa_V} \int_0^\infty dT \frac{dB_v}{dT}.$$  (5)

In Eq. (5) \(\kappa_R\) is the Rosseland mean opacity or simply the opacity. A large value of the opacity indicates strong absorption from a beam of photons, whereas a small value indicates that the beam loses very little energy as it passes through the medium.

It was apparent from the beginning that the most intensive part of the opacity calculations would be the vast amount of atomic data needed to calculate bound-bound and bound-free absorption cross-sections. Several possible levels of detail for including atomic data are possible. For example, consider transitions that connect two electrons in an sp configuration to a p\(^2\) configuration through a one electron jump. In the simplest approximation the transitions are degenerate. Opacity calculations that carry out a sum over a large number of configurations in this approximation are referred to as detailed
configuration accounting (DCA) methods. However, the DCA approach neglects non-spherical interactions that remove the degeneracy and lead to configuration term structure. In light elements the dominant non-spherical term is the Coulomb interaction between the electrons, which leads to pure LS coupling. In LS coupling the single spectral line of the DCA method is split into three distinct lines corresponding to a triplet and two singlet terms. With heavier elements, such as those in the iron group, the interaction between the electron spin and the magnetic field resulting from the electron orbital motion is no longer negligible and requires intermediate coupling (Cowan 1981). In intermediate coupling the three lines of the LS coupling scheme in our example split into eight lines having no net total spin change, \( \Delta S=0 \), and 6 intercombination lines having \( \Delta S=\pm 1 \). In more complicated configurations the increase in the number of spectral lines can be more dramatic.

To calculate the required atomic data the OPAL group developed a parametric potential method that is fast enough to allow on-line calculations, while achieving accuracy comparable to single configuration Dirac-Fock results (Rogers, Iglesias, and Wilson 1988). This on-line capability also provides flexibility to study easily the effects of atomic physics approximations such as various angular momentum couplings or data averaging methods. By contrast, the OP group uses first principle methods to construct detailed atomic databases that can be used in other types of investigations (Seaton 1987; Seaton \textit{et al.} 1994). The large increase in the iron opacity obtained with the LS coupling scheme compared to calculations that neglect term splitting were an indication that fine structure should also be included (Rogers and Iglesias 1992). The OPAL group responded with calculations that include the spin-orbit effects in full intermediate coupling (Iglesias, Rogers, and Wilson 1992), while the OP group uses an approximate method that does not include spin changing transitions (Seaton \textit{et al.} 1994). The OPAL calculation assumes single configurations, while OP includes configuration-interaction effects in both the bound-bound and bound-free calculations. Configuration-interaction is most important for neutral and near neutral transitions. The available Los Alamos opacity data is mostly in the DCA approximation, but more detailed calculations are in progress (Magee 1992).

The OPAL calculations include degeneracy and plasma collective effects in the free-free absorption using a screened form of the parametric potentials, whereas, these effects are not included in OP. In both OPAL and OP collective effects on the Thomson scattering are obtained from the method of Boercker (1987). In OPAL spectral line broadening for one, two, and three electrons ions are obtained from a suite of codes provided by R.W. Lee (1988) that include linear Stark theory. For all other transitions the OPAL calculations use Voigt profiles where the Gaussian width is due to Doppler broadening and the Lorentz width is due to natural plus electron impact collision broadening (Dimitrievic and Konjevic 1980). The OP line broadening follows similar lines, except broadening by ions is included only for hydrogenic systems and HeI (Seaton 1990).

The source of the largest opacity increases obtained by the OPAL and OP groups has been improved atomic physics, but equation of state and line-broadening improvements have also been important.

**III. EQUATION OF STATE**

The equation of state plays an important role in opacity calculations by providing the occupation numbers needed to evaluate Eq. (5). The OP and OPAL equation of state approaches are quite different, but for typical stellar conditions give very similar thermodynamic results (Däppen 1992). However, the predicted occupation numbers are
different for highly excited states that can affect the opacity at high density; the OPAL values being somewhat larger. The OP calculation is based on a free energy minimization, or chemical picture method, whereas the OPAL calculation is based on activity expansions of the grand canonical ensemble, or physical picture method.

A major difficulty that arises in existing free energy minimization methods is obtaining a convergent partition function. To treat this problem the OP work uses an occupation probability formalism that is thermodynamically consistent and produces continuous free energies (Däppen, Anderson, and Mihalas 1987; Hummer and Mihalas; Mihalas, Däppen, and Hummer 1988). It is commonly referred to as the MHD equation of state. Based on experimental measurements of level shifts (Goldsmith, Griem and Cohen 1984), they assume that the bound states of atoms and ions are unshifted by the plasma environment.

The MHD approach is based on the observation that if a configurational free energy, \( f(V,T,\{n_i\}) \), that depends explicitly on the occupation numbers of the individual states is added to the ideal free energy terms, then the ratio of the occupation of a state \( i \) of a given ion to the total occupation is given by

\[
n_i / n = \exp[-\beta(E_i + \partial f / \partial n_i)] / \tilde{Z}_{\text{int}} \tag{6}
\]

where

\[
\tilde{Z}_{\text{int}} = \Sigma_i \exp[-\beta(E_i + \partial f / \partial n_i)] \tag{7}
\]

plays the role of the internal partition function,

\[
\omega_i = \exp[-\beta \partial f / \partial n_i] \tag{8}
\]

is the occupation probability, \( n_i \) is the occupation number for state \( i \) and \( n \) is the total occupation for a given species. The occupation probability is a measure of the number of bound states of type \( i \) that are available to be occupied. The quantity \( 1 - \omega_i \) is, thus, a measure of the fraction of total states that have been severely affected by plasma perturbations and no longer act like localized states. In order to make progress it is necessary to have either a good estimate for \( f \) or a good estimate for \( \omega_i \), whichever is easier.

The MHD approach mixes the two possibilities. In the case of neutral particle interactions the free energy of a parameterized hard sphere gas is used to determine the occupation probability. For ion-ion interactions the occupation probabilities are determined from the electric microfield (Stark-ionization theory). For ion-neutral interactions a product of the two forms is used. The method is thus phenomenological, but uses experimental data to fit free parameters in the occupation probability function. The MHD method has been used in numerous stellar modeling sensitivity studies (Christensen-Dalsgaard and Däppen 1993; Dziembowski, Pamyatnykh, and Sienkiewicz 1992). A method similar to MHD has also been developed by Sevastyanenko (1985).

The OPAL approach treats the system in terms of its fundamental constituents, so that bound complexes arise naturally from the theory. The procedure is to expand the pressure as a sum of two body, three body terms etc., i.e., a cluster expansion. The long range of the Coulomb potential introduces substantial complications. In addition, the quantum nature of
electrons introduces degeneracy and exchange corrections. The attractive electron-ion interaction leads to short distance divergences in classical cluster coefficients, so that the use of quantum mechanical methods is essential. The activity expansion method uses graphical resummation procedures to remove the long-range divergences occurring in all cluster coefficients of plasmas. Composite particles, i.e., ions, atoms, and molecules, arise naturally in the physical picture, such that plasma screening effects on the bound states are determined from theory (Rogers 1994; 1989; 1986). This is a definite advantage over the chemical picture methods in current use which must introduce intuitive models to obtain these effects. A detailed description of the procedure is given elsewhere (Ebeling et al. 1976; Kraeft et al. 1986; Rogers 1981).

The simple case of a hydrogen plasma can be used to illustrate results from the physical picture (Rogers 1994; 1989; 1986). To relate the results to the chemical picture we display the low density free energy obtained in the physical picture, as described in Rogers (1994),

\[ \frac{F}{kT} = -N_e \ln \left( \frac{e^g_e}{\rho_e \lambda_e^3} \right) - N_p \ln \left( \frac{e^g_p}{\rho_p \lambda_p^3} \right) - N_H \ln \left( \frac{e^g_H}{\rho_H \lambda_H^3} \right) - \frac{F_{DH}}{kT} \]  

where

\[ Z_{int}^l = \sum_{n} (2 \ell + 1)(e^{-\beta E_{nl}} - 1 + \beta E_{nl}) \]  

is the so called Planck-Larkin partition function and

\[ \frac{F_{DH}}{kT} = -\frac{V}{12\pi} \left( \frac{kT}{4\pi e^2 \sum_{i} Z_i^2 \rho_i} \right)^{3/2} \]

is the Debye-Hückel free energy, and \( \rho_i \) is the number density of ions of type \( i \) including electrons. The sum in \( Z_{int}^l \) ranges over the allowed states in a screened potential that approaches the Debye-Hückel potential at very low density. However as described in Rogers (1986; 1981) the energy levels appearing in \( Z_{int}^l \) are unscreened except for high lying states near the plasma continuum. The states that are screened change with plasma conditions. As a result \( Z_{int}^l \) is both finite and a continuous function of temperature and density; although the density dependence is very slight for normal stellar conditions. The MHD equation of state displays a similar property through the use of the occupation probability formalism. The OPAL approach obtains systematic higher order Coulomb corrections not considered in the OP work and is expected to produce more realistic results at higher density.

IV. NEW RESULTS

Accurate models of stellar structure require detailed computer calculations. However, in regions where radiation pressure dominates, the ratio of the matter pressure to the radiation pressure is approximately constant (Bohm-Vitense 1992). Using the non-relativistic ideal gas pressure in combination with the Stefan-Boltzmann law, one obtains
with the above assumption a constant value for density/(temperature)$^3$. Thus, it is convenient to tabulate the Rosseland mean opacity at constant values of $R$ against temperature where $R=\rho/T_6^3$, $\rho$ is the material density in g/cm$^3$, and $T_6$ is the temperature in units of 10$^6$ Kelvin.

In order to calculate the opacity it is necessary to specify the chemical composition. Estimated elemental abundances have changed appreciably over the years and have been a major source of opacity uncertainties. For example, improvements in measuring techniques have brought the solar photospheric abundances into close agreement with the meteoritic abundances. Of particular importance to the opacity calculations is the recent 30% reduction in the photospheric iron abundance (Biemont et al. 1991). Although, abundance estimates are available for all naturally occurring elements, those above zinc have not been included in any of the existing astrophysical opacity calculations. The abundance of a number of elements of odd atomic number and a few of even atomic number below zinc are also very low. It has been computationally expedient to eliminate these elements from the calculations by combining their abundance with their neighbors. The most recent changes in solar abundances have been small (Grevesse and Noels 1993).

Figure 1 displays the opacity as a function of temperature for log $R$=3 for the abundances used by Cox-Tabor (1976). The mixture in this example assumes a hydrogen mass fraction $X=0.7$. OPAL results are displayed for a mixture having no metals and for a mixture that is composed of 2% metals by mass. In the astrophysical literature metals refers to all elements heavier than helium and their total fractional mass is indicated by the symbol Z. The helium mass contents of the two mixtures are, thus, $Y=0.3$ and 0.28, respectively. The results for a commonly used set of Los Alamos opacities (Cox and Tabor 1976) with $Z=0.02$ are also plotted. The curves show a series of bumps in log $\kappa_R$ that are due to strong absorption features in the spectrum of the indicated species. The H, He and He$^+$ bumps long have been associated with pulsational driving in variable stars (Bohm-Vitense 1992). However, the substantial bump in the new opacities around log $T_6$=5.4 is missing in the old results. This new Z bump has been shown to resolve several long-standing pulsation problems. The bump near log $T_6$=6.3 is important to helioseismology as well as Li depletion. A major reason that large deficiencies in the astrophysical opacities persisted over such a long time was due to the lack of laboratory experiments. A few experiments that measure opacity for conditions relevant to stellar envelopes have recently appeared (DaSilva et al. 1992; Springer et al. 1992).

The OPAL calculations were carried out with a 14 element mixture; reduced first from the Anders-Grevesse (1989) abundances and later the Grevesse (1991) abundances. As a consequence of the large increase in opacity resulting from a careful treatment of transitions originating from the M-shell, even lowly abundant elements from the iron group make contributions to the total opacity (Rogers and Iglesias 1992). More recent OP data has been calculated including Cr, Mn, and Ni (Seaton et al. 1994). OPAL calculations that include these elements in the opacity tables are underway. In Fig. 2 we compare OP and OPAL opacities for the same reduced 14 element Grevesse 1991 mixture having $X=0.7$ and $Z=0.02$. The overall agreement is good. The largest differences (30-40%) occur for log $R$ $\geq-2$ and log $T_6 \geq 5.8$ and for log $R < -3$ and log $T_6 = 5.2$. In both cases the OP opacity is lower than OPAL. A comparison of the same OPAL data with the 17 element OP data reduced from Noels and Grevesse (1992) that includes Cr, Mn, Ni is given in Fig. 18 of Seaton et al. (1994). This brings the OP results closer to OPAL, which are in this situation slightly lower than OP in some places. Similar increases in the OPAL data can be expected.
when the same 17 element mixture is used.

A large number of calculations have been reported that use the new opacities; e.g., Rogers and Iglesias (1994). For example: pulsational instability for β-Cephei stars, as actually observed, is now predicted (Cox et al. 1992; Kiriakidis, El Eid, and Glatzel 1992; Moskalik and Dziembowski 1992) and calculated period ratios for double mode classical Cepheids and RR-Lyrae stars agree closely with observation at evolutionary masses (Kovacs, Buchler and Marom 199; Cox 1991; Moskalik, Buchler and Marom 1992). In addition the location of stellar models in the observational planes relating mass, luminosity, effective temperature, and radius is substantially improved for main-sequence stars (Stothers and Chin 1991); the observed lithium abundance of stars in the Hyades cluster can now be modeled without invoking exotic theories (Swenson et al. 1994); the solar seismic frequencies as well as the calculated radius of the inner boundary of the solar convection zone are in close agreement with observations (Dziembowski, Pamyatnykh, and Sienkiewicz 1992; Guenther et al. 1992; Bahcall and Pinsonneault 1992; Cox and Guzik 1993); and the calculated light curves for the decay phase of classical novae agree better with observation (Kato 1994).

V. EFFECTS OF VERY HEAVY ELEMENTS ON OPACITY

The iron number fraction in the sun is down by almost 5 orders of magnitude compared to hydrogen and represents only about 2% of the number fraction of elements heavier than helium. Even so the major reason for the large increase in opacity in the few hundred-
FIG. 2. Comparison of OPAL and OP for the reduced G91 abundances. The calculations assume X=0.7 and Z=0.02. The OPAL results are represented by solid lines, OP results by dashed lines. Plots are shown for five values of log R.

thousand degree temperature range with OPAL and OP is due to a better treatment of the atomic physics of iron. The combined number abundance of Cr and Ni is more than an order of magnitude less than iron, but still can increase the total opacity by as much as 20%. Consequently, even though the abundance of still heavier elements is down another couple orders of magnitude, the aggregate effect of these elements needs to be examined. Especially since they will display N shell (and higher) spectra that have still greater photoabsorption than the M-shell spectra.

Preliminary calculations that approximately include the effects of heavy elements up to neodymium have recently been carried out by Iglesias et al. (1994). The procedure was to augment the 14 element OPAL calculations for the Grevesse-Noels (1993) mixture with the calculations of very heavy elements from the Super Transition Array (STA) code (Bar-Shalom et al. 1994). The STA code uses statistical methods to treat the very large number of lines in heavy elements, where detailed accounting of individual lines becomes intractable. It includes in an approximate way all possible transitions between electronic states of the various ions in the plasma. The STA code uses parametric potentials, similar to OPAL, to obtain reasonably accurate atomic data (Klapisch 1971; Klapisch et al. 1977) and includes configuration interactions between neighboring j-j configurations. The statistical approach makes it possible to address cases where the number of relevant configurations is immense.
A comparison between OPAL and STA shown in Fig. 3 helps clarify the STA method. The calculations are for Ga at a temperature and density near the peak of the absorption bump due to transitions originating in the M-shell. The STA accurately reproduces the envelope of the OPAL results, but since it is a statistical approach it does not resolve the details of the spectrum. Consequently the STA method tends to overestimate the Rosseland mean opacity (Iglesias, Rogers, and Wilson 1990). The advantage is that the STA approach is computationally fast and can be applied to the heavier elements where the detailed line accounting methods are not practical.

The Iglesias et al. (1994) calculations treated the heavy elements in groups of five, placing the total abundance with the central element of the group. They found that for solar element abundances that the effect is insignificant for $T_6 > 1$. An example is given in Fig. 4 for conditions near the bottom of the solar convection zone ($T_6 = 3$). The individual element absorption is greater for the heavy elements at these high temperatures, but that increase is not enough to overcome the greatly decreased abundances. However, for stars with peculiar element abundances, such as those of type $A_m$ and $A_p$, that have significant increases in some heavy elements, there may be important contributions to the opacity. For normal solar composition the heavy elements make the largest contribution in the $0.1 < T_6 < 1$ temperature region similar to the iron group elements.

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**FIG. 3.** Monochromatic opacity vs. $u=\text{photon energy}/kT$ for gallium. The STA results have been multiplied by 0.01.
VI. NEW DIRECTIONS

The applications of the new opacities have so far concentrated on main sequence and near main sequence stars. It remains to be seen what the effects of the new opacity will be on more evolved stars that have exhausted most of their core hydrogen and perhaps even their helium. Depending on their initial mass and metallicity, these stars can display a wide range of phenomena ending up as exploding supernova in one extreme or as cooling white dwarfs in the other.

The current OPAL opacity tables only extend far enough to model white dwarf stars whose surface temperatures are greater than about 15000 K (even higher with OP). However, the coolest white dwarfs (Teff = 4000 K) are remnants of the first generation of stars in the local disk of the Galaxy. Opacities that allow for the study of these white dwarfs would provide an independent estimate of the age of the local disk and could shed some light on the formation of spiral galaxies in general. This will require extending the equation of state and opacity calculations several orders of magnitude in density, presenting new challenges to the calculations.

There has been speculation that observed stellar abundance anomalies in the envelopes of some A and B stars may be produced by radiative levitation of highly absorptive heavy elements and diffusion (Richer, Michaud, and Proffitt 1992; Proffitt 1994). The radiation force acting on different species in a stellar mixture is given by a formula very similar to Eq. 1 (Michaud 1976) and can be calculated using slight modifications to the OP and OPAL codes.
There are a number of recent neutron star flux detections with the Hubble telescope UV and especially the ROSAT soft X-ray satellites. These stars have dense iron atmospheres and calculations of the emergent spectrum are sensitive to the opacity (Romani 1987). Modeling of the atmospheres of neutron stars is also sensitive to non-ideal Coulomb corrections in the thermodynamic properties. In addition the presence of large magnetic fields in some neutron stars may affect the opacity and thermodynamic properties (Van Riper 1988).

Cool stars with surface temperatures below 5000 K can form a wide variety of molecules in their atmospheres. Molecular opacities in these stars affect the surface temperature and are important for determining their masses. A substantial part of the mass in the galaxy may be locked-up in low mass, cool stars and reliable opacities are needed to answer this question. Several groups are in the process of improving molecular opacities and new results are becoming available (Alexander and Ferguson 1994; Allard et al. 1994; Sharp 1993).

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