ASTROPHYSICAL OPACITIES AT LLNL

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ABSTRACT. In an effort to reduce uncertainties in the theoretical radiative opacities a new code has been developed at LLNL which removes several of the approximation present in past calculations. Results from the new code with comparisons to other available opacity calculations are presented as well as experiments.

1. INTRODUCTION

The calculation of plasma radiative properties involves detailed knowledge of both atomic and plasma physics. As a result, the problem is complex and has been fully addressed by only a few groups. However, due to the complexity, approximations have been made in the past which may limit the accuracy of the results. Unfortunately, direct experimental measurements of the opacity are essentially nonexistent so that the success or failure of theoretical results must be determined indirectly. For example, the calculation of period ratios in Cephieds based on stellar models does not agree with experimental observations. It has been suggested by Simon[1] and later by Andreasen[2] that an arbitrary increase in the Rosseland mean opacity of the metals without increasing their abundance can explain the discrepancy. Comparison of observed and predicted p-mode oscillations in the sun can be improved by increasing the opacity[3]. The solar neutrino rate is sensitive to the opacity as well. There are other outstanding problems which could be solved by changes in the input opacity calculations. Probably the discrepancies will not all disappear with improved opacities, however, it will be easier to find the explanations if uncertainties in the opacities were reduced.

At present there are about ten theoretical efforts throughout the world developing radiative opacity codes. Although there is some overlap, the groups vary somewhat in approach and tend to emphasize different matter conditions. There are also some experimental efforts trying to measure directly the photon absorption[4]. These are difficult experiments and definite results are not presently available. Perhaps all this activity coupled to the astrophysical and astronomical community, which at present offer the best laboratories (stellar matter), will result in opacity calculations being better understood and uncertainties reduced.

Several reviews have appear in the literature[5] which discuss opacities and is not the purpose here to go over this ground, but rather to describe a new opacity effort at LLNL: the OPAL code. We shall consider temperatures sufficiently high (a few eV) that molecular absorption is negligible and photon energies low enough (less than about 10keV) that relativistic effects are

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small. These conditions cover the relevant plasma temperature and photon energy ranges for computing opacities inside the sun. Under these circumstances the dominant absorption processes are electronic transitions in the field of ions; that is, line transitions (bound-bound), photoionization (bound-free), and inverse bremsstrahlung (free-free). At high temperatures nuclei are completely striped of any bound electrons and photon scattering from free electrons becomes important.

For conditions of interest here, collisions between the plasma constituents are sufficiently frequent that the plasma can be assumed to be in local thermodynamic equilibrium (LTE). Since the mean free path of an average photon is small compared to the scale of the matter temperature gradients inside a star, the photons are in equilibrium with the matter and have a black body spectrum at the material temperature. The transport of photons will then be well desscribed by the diffusion approximation with the diffusion constant given by the Rosseland mean opacity, K_R,

$$\frac{1}{K_R} = \int_0^\infty du \, \frac{1}{\tilde{K}(u)} \, \frac{\partial B(u,T)}{\partial T} \tag{1}$$

where the weighting function

$$\frac{\partial B(u,T)}{\partial T} = \frac{15}{4\pi^4} \, \frac{u^4 e^u}{(1-e^u)^2} \tag{2}$$

peaks at u (=photon energy/T) = 4 with T the matter temperature in units of energy. The extinction coefficient is defined by

$$\tilde{K}(u) = K_{abs}(u)(1-e^{-u}) + K_{sc}(u) \tag{3}$$

where K_{abs} is the absorption coefficient and K_{sc} is the scattering cross section,

$$K_{abs}(u) = \sum_{ijk} N_{ijk} \, \sigma_{ijk}(u)$$

$$K_{sc}(u) = N_e \, \sigma_{sc}(u). \tag{4}$$

Here, N_{ijk} is the number of ions of charge j in electronic level k of element species i, $\sigma_{ijk}(u)$ is the absorption cross section for photons with energy u by those levels, and N_e the free electron number density with $\sigma_{sc}(u)$ the photon scattering cross section.

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2. THEORY

2.1 Equation of State (EOS)

Every opacity calculation begins with the EOS to obtain the occupation numbers, N_{ijk}. Our EOS was developed by Rogers[6] and is based on an activity expansion for the grand canonical partition function. The approach relies on quantum statistical mechanics and does not require any *ad hoc* cutoffs so familiar in free energy minimization techniques. The well known problem in the latter is related to the internal partition function,

$$\sum_{j=0}^{N} g_j \exp\left(-\frac{E_j}{T}\right) \propto N^3 \tag{5}$$

where the sum is over bound levels, g_j is the level degeneracy, and E_j the level energy. The divergence requires a phenomenological argument for truncating the series.

A proper solution to the problem recognizes that the partition function for the plasma involves a trace over all states. The many-body activity expansion developed by Rogers[6] and Ebeling et al.[7] not only avoids the *ad hoc* cutoffs but shows how the divergences are removed by including the scattering states. It starts from a description of the system in terms of electrons and nuclei interacting through the Coulomb potential and makes no assumptions about the internal states of composites (ions and atoms). This fundamental particle activity expansion is then renormalized to account for the composites. Ebeling will describe the EOS in another chapter of the present volume so that only brief remarks concerning the method will be given here.

For simplicity assume a plasma in LTE made up of protons and electrons interacting through the Coulomb potential. Following quantum statistical mechanics, one can write the pressure, P, in terms of an activity expansion and cluster coefficients,

$$\frac{P}{T} = \sum_{\alpha} z_\alpha + \sum_{\alpha}\sum_{\alpha'} z_\alpha z_{\alpha'} b_{2,\alpha\alpha'} + \cdots \tag{6}$$

where z_α is the activity for species α, b_n's are the n-body cluster coefficients, and α is an electron or proton. As an example consider the electron-proton cluster coefficientt[8]

$$b_{2,ep} \propto Tr_{ep}\left\{\exp\left(-\frac{H_{ep}}{T}\right) - \exp\left(-\frac{H^0_{ep}}{T}\right)\right\} \tag{7}$$

where Tr_{ep} is a trace over a complete set of electron-proton states, with H_{ep} and H^0_{ep} the electron-proton Hamiltonian with and without the Coulomb interaction, respectively. The cluster b_2 has a simple interpretation: It contains two-body interaction corrections to the pressure, the H_{ep} term, but one must be careful to subtract the non-interacting two body contributions already included in the ideal gas term, subtracted H^0_{ep} term. In this form it is easy to see that b_2 is not the two body partition function and to interpret it as such may lead to confusion.

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Since the Coulomb interaction depends only on relative coordinates, the center of mass motion separates from the relative motion and we find after some manipulations[8]

$$b_{2,ep} \propto \sum_{j(bound)} g_j \exp\left(-\frac{E_j}{T}\right) + \frac{1}{\pi}\sum_l (2l+1)\int_0^\infty dp\, \frac{d\delta_l(p)}{dp} \exp\left(-\frac{p^2}{2\mu T}\right) \quad (8)$$

where E_j are the bound state eigenvalues of H_{ep}, $\delta_l(p)$ are the scattering state phase shifts with momentum p, and μ is the reduced mass. At this point it appears that $b_{2,ep}$ also diverges due to the bound state contributions. However, an integration by parts leads to

$$b_{2,ep} \propto \sum_{j(bound)} g_j\left[\exp\left(-\frac{E_j}{T}\right)-1\right] + \frac{2}{\pi\mu T}\sum_l (2l+1)\int_0^\infty dp\, p \exp\left(-\frac{p^2}{2\mu T}\right)\delta_l(p) \quad (9)$$

where use has been made of Levinson's theorem[8]

$$\delta_l(p) = \pi(\text{number of bound states of quantum number } l) \quad (10)$$

We can see in Eq. (9) that the contribution from the scattering states compensates for the leading divergence in the bound state contribution. Higher order Levinsons theorems have been proven for the Coulomb potential[9] and a second integration by parts yields

$$b_{2,ep} \propto \sum_{j(bound)} g_j\left[\exp\left(-\frac{E_j}{T}\right)-1+\frac{E_j}{T}\right] + \frac{2}{\pi\mu^2T^2}\sum_l (2l+1)\int_o^\infty dp \exp\left(-\frac{p^2}{2\mu T}\right)\left[\int dp\, p^2\, \delta_l(p)\right] \quad (11)$$

and the bound state divergences are now fully compensated by the scattering states. This manipulations have redefined the continuum such that weakly bound states are treated with the scattering states in many-body perturbation. The sum over bound states in Eq. (11) is the so-called Plank-Larkin partition function which, of course, is <u>not</u> a partition function, but rather the bound state contribution from two-body bound states to the pressure.

There are other divergences in the activity expansion of the pressure which do not compensate. These are present even in classical Coulomb systems without bound states and are associated with the long-ranged Coulomb interaction. Their removal is well understood and involves summing certain classes of terms appearing in the expansion. The above procedures and their extensions to higher order cluster coefficients has been discussed extensively by Refs. 6 and 7

Even though the activity expansion provides a formalism for the EOS, it does not automatically yield occupation numbers for the plasma radiative properties. A final step described by Rogers[6] is necessary where a formal comparison of pressure expressions from the activity expansion and the free energy minimization was done. The results show that strongly bound state

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occupation numbers are described by Boltzman factors while weakly bound states require many-body corrections.

2.2. Absorption Cross Sections

The approach followed for computing the opacity is the so-called detailed configuration method in which every electronic configuration and corresponding term structure is considered explicitly. Such an approach requires vast amounts of atomic data. One possibility is to create a large data base with energy levels and cross sections. The data base, however, will not contain any density effects which may be important for high density plasma in stellar interiors. A second possibility, and the one chosen here, is to compute the atomic data "on-line". In the past, on-line calculations were too slow or not sufficiently accurate. Fortunately, we have developed a parametric potential method which is both fast and accurate[10]. The parametrization procedure required reproduction of experimental energy level data. Solving the Dirac equation with these parametric potentials provides wavefunctions and energies which in turn are used to compute the photon absorption cross sections. The parametric potentials have been developed for valence and inner shell electrons as well as multiply excited configurations. The accuracy of this method is comparable to single configuration, self-consistent-field calculations with relativistic corrections. The method affords the possibility of including density effects by suitable modifications of the Coulomb tail by plasma screening. It also allows for testing of various atomic physics issues by changing the atomic package in the code. Something not easily done with data bases. Finally, it is important to note that data bases are not "complete" and that on-line atomic calculations, much simplified over those in the data base,would still be necessary to supplement the data base approach. It is possible that a hybrid approach would be best where a very accurate, relatively small data base is supplemented with fast and reasonably accurate on-line method such as ours.

Previous opacity calculations have not included this level of accuracy in their atomic data, partly due to the limited computer facilities available at the time. Consequently, they have in some plasma conditions important for Cephied variables underestimated the opacity of the metals by large factors[11].

Below follows a brief description of how the three dominant absorption processes are computed in OPAL. It is important to realize that as in most calculations, it is assumed that many-body physics can be well described by an appropriate single particle representation.

2.2.1. *Bound-Bound Transitions.* The accuracy obtained in calculating bound-bound transitions depends on the line location and associated oscillator strength. Using the parametric potential we can obtain 1% or better accuracy for the configuration averaged energies when compared to experiment for ions relevant to the solar interior. In order to match real experiments, it necessary to include the configuration term splitting. The angular momentum coupling is done using standard perturbation theory methods and includes either Russell-Saunders or intermediate coupling depending on the levels and nuclear charge. The term splitting results are not as accurate as the configuration averages but are better than 10% when compared to experiment. The strong oscillator strengths are also in the order of 10% accuracy, but very little experimental data are available. Of course, the comparisons are done for isolated ions and it must be emphasize that little is known of how ions behave under the extreme conditions of stellar interiors. Not all transitions are computed with term splitting. Transition from lower bound levels with quantum number greater than 5 are considered in the configuration average only. If in the future this "switch" is

insufficient (perhaps in the much colder regions in the photosphere) it is easily change in the code to some higher value.

In nature spectral lines experience broadening, for example, Doppler effects, collisions, and natural lifetimes. In OPAL lines from single electron ions are treated with standard linear Stark theory[12]. These line shapes are in good agreement with experiment. In the near future we will include similar calculations for Helium-like and Lithium-like ions which have also compared well with experiments. For all other transitions we use Voigt profiles where the Gaussian width is due to doppler broadening and the lorentz width is due to estimated natural plus electron impact collisions.[12] The latter is computed using second order dipole approximation. These are not scaled hydrogenic results but use the same wavefunctions as in the atomic data calculations.

2.2.2. *Bound-Free Cross Sections.* These cross sections are computed explicitly for all levels with angular momentum quantum number less than 5. For levels with principal quantum number greater than 5, the configuration term structure is neglected. The resulting bound-free cross sections have compared well with experiments even for neutral atoms[6] except when configuration interaction effects are important. Such effects, however, are expected to be very small for solar interior calculations. For the remaining levels we use scaled hydrogenic cross sections.

2.2.3. *Free-Free Absorption.* Since the parametric potential model provides good results for bound-free cross sections where both bound and scattering states are required, we assume that the parametric potential method will also be valid for free-free calculations where only scattering states are necessary. We compute explicitly the dipole matrix elements except in some limiting regions where simpler approximations are valid. For example, for small photon energies elastic scattering cross sections are useful and easy to compute. Plasma screening effects are introduced into the electron-ion interaction. These effects are described by Rogers[6] and reduce to the Debye-Huckel[13] result for weakly coupled plasmas. This approach provides two improvements over calculations using Coulomb Gaunt factors. The first is corrections due to the plasma screening at small photon energies. The second is corrections at large photon energies where the scattering electron can penetrate the bound electron orbits and see a higher effective charge.

2.3 Scattering

The treatment of photon scattering from free electrons follows Boercker[14]. There, the transport cross section is computed including the many electron effects; that is,

$$\sigma_{sc}(k) = \sigma_t \int_{-1}^{1} d(\cos\theta)\,[1+\cos^2\theta][1-\cos\theta]\,S(k) \tag{12}$$

where

$$k = \frac{4\pi}{\lambda}\sin\left(\frac{\theta}{2}\right) \tag{13}$$

$$S(k) = 1 + h_{RPA}(k) + h_x(k) \tag{14}$$

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where θ is the photon scattering angle, λ the photon wavelength, with h_{RPA} and h_x are the electron-electron correlation functions in the Random Phase Approximation and first order exchange, respectively.

3. Experiments

As mentioned earlier, absorption experiments are difficult. Firstly, they require LTE conditions which are difficult to obtain in laboratory plasmas. Independent measurements of the plasma density and temperature are necessary and care is require in order to avoid circular arguments. For comparison with theoretical calculations error bars would be quite useful in helping to discriminate between various models. Finally, the experiments will be restricted to low densities.

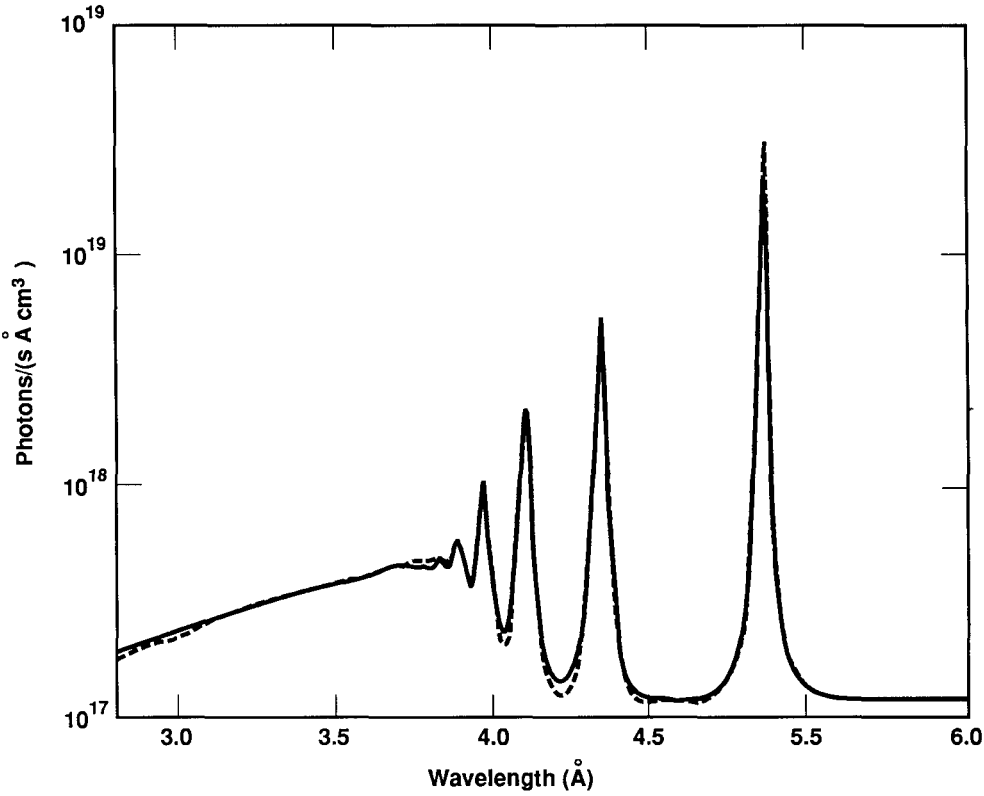

Fig. 1. Emissivities at N_e=1.8x10^{17}electrons/cm^3 and T=1.0x10^{4}K.
Dashed line: Wiese et al.[15]. Solid line: OPAL

In spite of all the difficulties there are some experiments with hydrogen. In Figures 1 and 2 we compare our results for the emissivity with experimental data by Wiese et al.[15]. In looking at

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the comparison one should note that the experiments were not in strict LTE and that the chosen plasma conditions were obtained by the experimentalist assuming LTE conditions. Similar experiments and comparisons have been done by other researchers[16,17].

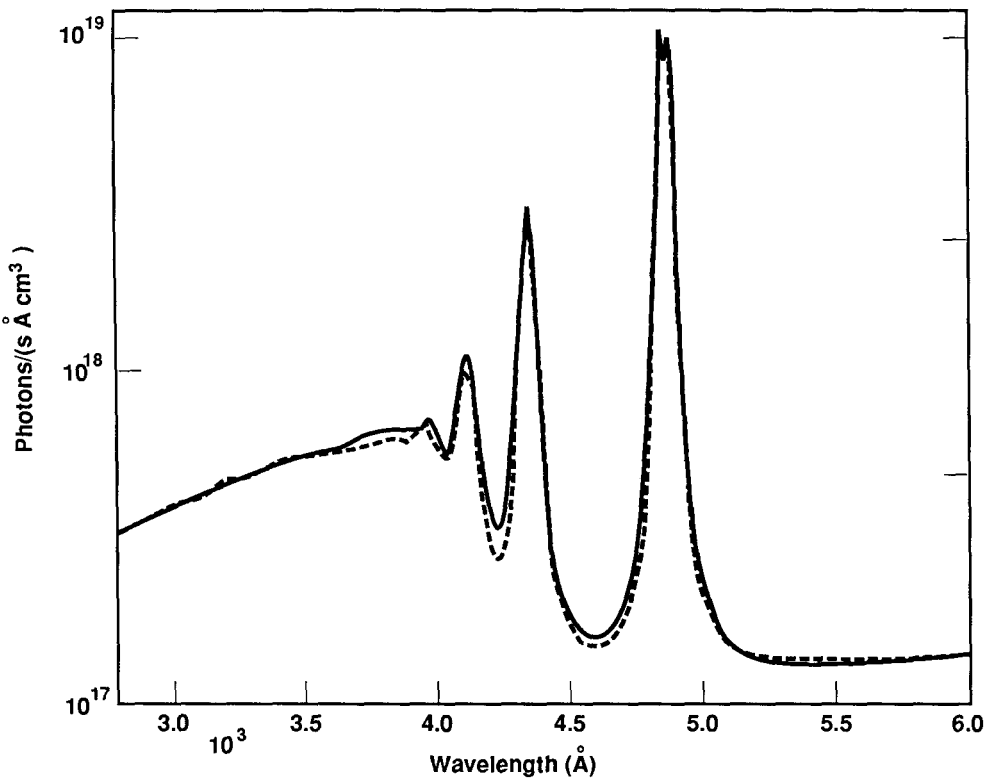

Fig. 2. Same as Fig. 1 with $N_e = 9.3 \times 10^{17}$ electrons/cm^3 and $T = 1.33 \times 10^4$.

Unfortunately, the Wiese et al.[15] experiment is not a sensitive test for EOS or occupation numbers, but rather it is an excellent test for Stark broadening of Hydrogen spectral lines as originally intended by the authors. The reason is that Saha-type EOS formulations with principal quantum number cutoff above the Inglis-Teller[18] limit will reproduce reasonably well the experimental data[16]. The difficulty is in reproducing the line spectra near threshold where a careful theory, which is not presently available, would need to Stark mix many states with different quantum numbers plus the continuum. What has been done with some success in the past are phenomenological methods[16,17] that mimic the line broadening of overlapping lines. These methods are in effect "smoothing" procedures which conserve the oscillator strengths. Just as important, they restrict the line radiation to the region near threshold while standard line broadening theories have unphysical broadening to regions far from line center leaving a spectral window.

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4. Opacity Results for the Sun

The Rosseland mean opacities are compared with the results from the Los Alamos Astrophysical Library published in Bahcall et al.[19]. The comparisons are presented in Table 1. The assumed solar mixture (labelled Ross-Aller'76) was obtained from Table IV of Ref. 19 and the Los Alamos Rosseland means from Table VI. We see no significant differences until the matter temperature drops below $7x10^6$ K. As the temperature continues to drop, the opacity difference increases to approximately 18% at $1x10^6$ K. Such increases are significant to Helioseismological data.

The opacity is also sensitive to uncertainties in the element mixture. For comparison, we did our calculations assuming the same temperatures and densities but assumed a more recent Aller[20] element abundance (labelled Aller'86). This mixture is richer in both Fe and Ne. In Table 1 one can see that near the solar center where Fe is important to the opacity there is a few percent increase in the Rosseland mean due to changes in the mixture when using the OPAL code. Similarly, near $3x10^6$ K Ne is important and there is an 8% increase.

TABLE 1. Comparison of OPAL and Los Alamos[19] Rosselasnd mean opacities (cm^2/g) where X=0.35 and Z=0.0179.

T ($x10^6$K)	ρ (g/cm^3)	Ross-Aller'76		Aller'86
		Ref.19	OPAL	OPAL
15.7	135.0	1.18	1.17	1.21
12.8	73.4	1.34	1.33	1.37
11.3	50.5	1.45	1.44	1.47
10.0	35.0	1.61	1.58	1.60
7.0	12.0	2.54	2.53	2.55
4.5	3.19	5.85	6.23	6.39
3.0	0.945	13.6	14.6	15.8
1.8	0.204	31.0	35.4	36.5
1.0	0.035	49.9	59.3	57.3

The differences between the results of the two codes are mostly due to the improved atomic physics package in OPAL. We have done some comparisons of the occupation numbers, N_{ijk}, but found small differences on the most relevant levels. There are also differences in the treatment of line broadening since the lorentz widths are not the same in the two codes. The subject of line broadening, in particular line wings, remains an open question in opacity calculations. The problem of line broadening of spectral lines in multi-electron ions has just begun to be explored.

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5. Conclusions

The differences in the numerical results between the two codes may be interpreted as a measure of the uncertainties in opacity calculations for solar interior. However, a word of caution is necessary. Even though the codes were independently developed and several of the approximations in the previous calculations were removed, there are no experiments to guide the theory for such extreme temperature and density conditions. In the past, single particle representations of many-body problems have been successful, but usually experiments were necessary in order to pinpoint the important physics of the particular problem. Perhaps with very accurate astronomical experiments, such as the p-mode oscillation measurements, it will be possible to improve our understanding of EOS and absorption properties of very hot, dense matter.

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