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The DAVROS opacity code: Detailed term accounting calculations for LTE plasmas☆

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ABSTRACT

The radiative opacity of a plasma is a key parameter in understanding a diverse range of high energy density systems including inertial confinement fusion and astrophysics. The accurate calculation of opacity is hampered by the potentially enormous number of ionic configurations, the detailed internal structure of each giving rise to the term structure, and the line broadening models which must typically be applicable across densities from 10^{-6} g/cc to several times solid.

The DAVROS opacity code (**D**etailed **A**ccounting of **V**arious configurations for **R**adiative **O**pacity **S**pectra) has been developed at AWE over recent years, and by making use of the large scale High Performance Computing (HPC) systems, implements a number of models and algorithms aimed at a more direct calculation of opacities than has traditionally been feasible. The results are both more physically based and spectrally accurate than codes based upon statistical accounting approximations. In particular, the bound–bound line spectrum can be explicitly calculated using the Detailed Term Accounting (DTA) method, which, although computationally expensive, is necessary to understand the true frequency dependent structure of the opacity spectrum. Additionally, M. Baranger (1958) [1] quantum mechanical formulism of pressure (or electron impact) broadening is implemented, thereby representing a significant improvement upon alternative approximations.

We present a summary of some of the key issues, models and algorithms in the code, and show some representative results, including comparisons with opacity measurements made at AWE.

1. Overview

The interaction of radiation with a plasma is central to understanding high energy density physics (HEDP) systems. A key parameter for practicable radiation transport calculations is the Rosseland mean opacity

$$\frac{1}{\kappa_R} = \frac{15}{4\pi^4}\int_0^\infty \frac{u^4 e^u}{\kappa(uT)(e^u-1)^2}\,\mathrm{d}u \qquad (1)$$

where $\kappa(\nu)$ is the monochromatic opacity computed at a photon energy ν and $u=\nu/kT$. Unfortunately, κ_R can be sensitive to the detailed structure of the spectrum. An example of this is shown in Table 1 for Ni calculated using the DAVROS code at a temperature of 30 eV and a density of 0.003 g/cc. In this example, the density is sufficiently low that line broadening is weak and the individual spectral lines resulting from a detailed term accounting (DTA) treatment remain separated. On the other ahnd, using the unresolved transition array (UTA) approximation, this gives a rather poor estimate of $\kappa_{R,UTA} = 7283.6$ cm^2/g as compared to the DTA value of $\kappa_{R,DTA} = 4850.4$ cm^2/g.

One of the more established AWE codes used to calculate the radiative opacity of materials is the CASSANDRA code [2] which uses statistical techniques based upon an average-atom model and it is fundamentally a UTA code. In recent years, with the availability of large scale high-performance computer (HPC) systems, the DAVROS opacity code has been developed to perform more direct calculations based upon the relatively straight-forward, but computationally expensive, methods of detailed configuration accounting (DCA) and detailed term accounting (DTA). At the DCA

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Table 1
Example for spectator configuration accounting in Fe. As an increasing number of spectator electrons are added (first column) the number of possible configurations grows rapidly in a combinatorial manner. However the contribution to the total partition function decreases rapidly and thus the contribution to the low energy photon region of the opacity spectrum can be well represented by a much smaller number of configurations. The recursive algorithm used to estimate spectator configuration energies (and hence related properties) encapsulated by eq. (11) is key to iterating this vast number of configurations efficiently.

	# Configs total	# Configs spectrum	P.F. Total	P.F. Spect.
1	375,063	375,063	5.4749	5.4749
2	7,501,260	7,434,269	2.5178	2.5174
3	102,440,284	4,791,785	0.7771	0.3517
4	1,073,430,306	0	0.1810	0.0000
5	9,197,217,950	0	0.0391	0.0000
6	67,064,034,096	0	0.0053	0.0000
Tot	77,444,998,959	12,601,117	8.9901	8.3441

level, one typically calculates the properties of specific real configurations which are expected to be representative of the plasma, but retains the approximation that the spectral lines are approximated by the UTA model. Extending the computation to explicitly include the detailed line structure due to each configuration gives rise to the DTA method (sometimes referred to as detailed level accounting (DLA)).

It should be appreciated that the number of distinct ion configurations within a plasma may be extremely large. It is only with the recent development of large scale HPC systems that direct atomic physics calculations of realistic numbers of configurations that are representative of systems of interest have become feasible. The DAVROS code has been developed from scratch to make use of these new resources efficiently. Having the advantage of being an entirely new code, it has enabled us to use a number of novel techniques to directly compute the opacity spectrum in more detail than has traditionally been practicable. This paper gives a brief summary of some of the key principles and methods used in DAVROS. A small number of representative results are also illustrated.

2. Code Description

2.1. Configuration accounting

2.1.1. Core configurations

We begin with an average atom calculation which is used to identify which electronic shells are either closed (fully occupied) or open. We then initially estimate the energies of all possible (nl) configurations with occupied orbitals having a maximum value of n such that we exclude all shells that do not have any nl sub-shells with an occupancy probability $p_i = q_i/g_i < 0.01$ – with q_i and g_i being the electron occupancy and statistical weight of the i^{th} sub-shell. For example if the $n=2$ shell is opened, we may also see that the average atom predicts appreciable fractions of electrons in the $n=3$ and $n=4$ shells, but negligible occupancies in higher sub-shells (The inclusion of these in an approximate manner is discussed later). An estimate of the energies of these configurations is given by a Taylor series expansion from the average atom [3].

$$E = E^{\text{ref}} + \sum_j \left(q_j - q_j^{\text{ref}}\right)\frac{\partial E^{\text{ref}}}{\partial q_j} + \frac{1}{2}\sum_j\sum_k \left(q_j - q_j^{\text{ref}}\right) \times \left(q_k - q_k^{\text{ref}}\right)\frac{\partial^2 E^{\text{ref}}}{\partial q_j \partial q_k} \quad (2)$$

where E^{ref} is the energy of the reference configuration – here the average atom – and the summations run over the occupied sub-shells j,k with occupancies of $q_{j,k}$ electrons. The partial derivatives are determined from the average atom by straight forward numerical differentiation.

The probability of the i^{th} configuration is then estimated via the Saha–Boltzmann equations

$$p_i = w_i/\Pi_0 \quad (3)$$

$$\Pi_0 = \sum_i w_i \quad (4)$$

$$w_i = g_i \exp\left(\frac{E_i + \mu\left(Z - z_i^b\right)}{kT}\right) \quad (5)$$

where μ is the plasma chemical potential and z_i^b is the number of bound electrons in the configuration.

The resulting list of configurations is then sorted by descending order of probability and from hereafter only the top $\mathscr{N}$ configurations are retained such that the majority of the partition function, Π_0, is represented to within some tolerance τ

$$\left(\Pi_0 - \sum_{\widehat{i}}^{\mathscr{N}} w_{\widehat{i}}\right) \Big/ \Pi_0 = \tau \quad \tau \sim 0 \quad (6)$$

where $\widehat{i}$ represents the $\widehat{i}^{\text{th}}$ most probable in the sorted list. These remaining configurations will be referred to as *core* configurations.

Each core configuration is then split into all possible underlying relativistic (nlj) configurations. This enables the code to subsequently calculate spectra in either the *JJ* or intermediate coupling representations depending upon the atomic number/degree of ionisation. Each of these core (nlj) configurations then has an individual atomic structure calculation performed in a unique self-consistent-field (SCF) using a Dirac-Hartree-Slater (DHS) type of potential. The potential in each case includes a contribution from the Thomas-Fermi distribution of free electrons from the bulk plasma as estimated from the average atom calculation. In this way the effect of the plasma, e.g. wavefunction distortion and continuum lowering, is explicitly included in the subsequent determination of the atomic properties.

The quality of the atomic structure, (e.g. as measured by transition energies), can be significantly improved by using an individual potential for each sub-shell j such that self-interaction arising from other electrons in the j^{th} sub-shell is explicitly excluded [4]. DAVROS thus uses the DHS potential

$$V_j(r) = V_{\text{nuc}}(r) + \frac{1}{2}\int \frac{\rho_j(r)}{\max(r, r_2)} dr_2 + V_{\text{xc}}(r) \quad (7)$$

with

$$\rho_j(r) = \rho_{\text{free}}(r) + \sum_k \left(q_k - \delta_{j,k}\right)\left(P_k^2(r) + Q_k^2(r)\right) \quad (8)$$

where P and Q are the large and small components of the Dirac wave functions and V_{xc} is the exchange and correlation potential [5]. The use of a different potential for each occupied sub-shell results in non-orthogonal wave functions. The effect is generally small but is easily corrected with an inexpensive Gram-Schmidt orthogonalisation within the SCF loop.

The major computational expense involved in the SCF calculations is due to the evaluation of the Coulomb potential in eq. (8) The