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Analytical Expressions for Radiative Opacities of Low Z Plasmas

J G Rubiano^{1,2,3,} P Martel^{1,2}, JM Gil^{1,2}, R. Rodriguez^{1,2}, R. Florido^{1,2}, M A Mendoza¹ and E Minguez²

¹Departamento de Física, Universidad de Las Palmas de GC, Las Palmas de GC, Spain ²Instituto de Fusión Nuclear (DENIM), Universidad Politécnica de Madrid, Madrid, Spain

E-mail: jgarcia@dfis.ulpgc.es

Abstract. In this work we obtain analytical expressions for the radiative opacity of several low Z plasmas (He, Li, Be, and B) in a wide range of temperatures and densities. These formulas are obtained by fitting the proposed expression to mean opacities data calculated by using the code ABAKO/ RAPCAL. This code computes the radiative properties of plasmas, both in LTE and NLTE conditions, under the detailed-level-accounting approach. It has been successfully validated in the range of interest in previous works.

1. Introduction

The accurate determination of the radiative properties of hot dense matter is needed in several research fields such as ICF target physics analysis, magnetic fusion or astrophysics, and the radiative opacity is a key factor to be determined. Thus, ICF target simulation involves the use of hydrodynamic radiation codes that require the input of thousands of spectrally resolved opacity data for each point of a fine mesh of temperatures and densities and determining them takes a large computation time. A usual approach consists of weighting these opacities in a small number of multigroups opacities or even only one group using then the Rosseland and Planck mean opacities. Even in this case, the accurate computation of these quantities is too huge to be used in-line with a hydrodynamic code.

For these reasons, analytical formulas giving mean radiatives properties versus temperature and density of the plasma are a useful tool. In this work, our main goal is to obtain analytical expressions for the Rosseland and Planck mean radiative opacities of several low Z plasmas in a wide range of temperature and densities. These formulas are obtained by fitting the free parameters of the proposed expression to data calculated by the code ABAKO/ RAPCAL [1]. This code computes the radiative properties of plasmas such as the spectrally resolved opacity or the Rosseland and Planck mean opacities, both in LTE and NLTE conditions, under the detailed-level-accounting approach. The code has been successfully tested by comparing its results with reference codes in the fourth and fifth Kinetic Code Comparison Workshops [2, 3]. It also has demonstrated to be useful for diagnostic of experiments [4].

³ To whom any correspondence should be addressed.

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2. Opacity calculation

We have carried on a detailed analysis of the mean opacity for helium, lithium, beryllium and boron plasma, using high quality atomic data obtained using the FAC code [5]. This code provides atomic magnitudes calculated into the DLA approach, using appropriate coupling schemes and including configuration interaction. The calculation of ionic charge state distributions and level populations is performed by solving a collisional-radiative steady-state model (CRSS). The level populations are computed with a reasonable accuracy for plasmas of any element in a wide range of conditions embracing Coronal Equilibrium (CE), non-LTE and LTE situations. The spectrally resolved opacity is obtained as a sum of the bound-bound, bound free, free-free and scattering contributions

$$\kappa(\nu) = \frac{1}{\rho} \Big(\mu_{bb}(\nu) + \mu_{bf}(\nu) + \mu_{ff}(\nu) + \mu_{scatt}(\nu) \Big)$$
(1)

The bound-bound spectrum includes all the allowed transitions in the dipole approximation along with all the detailed atomic levels considered. Line profiles incorporate Doppler, natural and electron-impact widths. The bound-free and free-free processes are calculated using the Kramer's semiclassical expressions. The Rosseland and Planck mean opacities are then computed by:

$$\frac{1}{\kappa_{Rosseland}} = \int_{0}^{\infty} d\nu B'(\nu, T) / \kappa(\nu) \qquad \qquad \kappa_{Planck} = \int_{0}^{\infty} d\nu B(\nu, T) [\kappa(\nu) - \kappa_{scatt}(\nu)] \qquad (2)$$

where κ_{scatt} is the absorption coefficient contribution by scattering (Thomson cross section), and B(v,T) and B'(v,T) are the Planck weighting function and its derivative.

3. Results and discussion

Analytical expressions can be found in the literature [6–8] for the opacity of low-Z plasmas in a wide range of temperatures and densities. The expression most commonly used to model Rosseland and Planck mean opacities is a power law depending on temperature and density,

$$k_{R,P} = e^a \rho^b T^c \tag{3}$$

where T is the temperature (eV) and ρ is the mass density (g·cm⁻³). The definition of the parameter a can change depending on the author. These formulas are usually fit to match LTE data but there are no values for a wide range of density and temperature conditions where NLTE assumptions are important. In a logarithmic representation, equation (3) is a plane surface over the entire range of temperatures and densities. This geometrical form can give a good fit for highly ionized plasmas, but it fails at low temperatures where the atomic structure leads to local modulations of the mean opacity.

In order to extend its range of application, we have modified this formula including a multiplicative term depending on the temperature and the electron density, thus,

$$\mu_{R,P}(cm^{-1}) = \rho \kappa_{R,P} = e^{a_0} T^{a_1} \rho^{a_2} f(x, y)$$
(4)

with

$$f(x, y) = \left[\exp a_3 xy + a_4 x^2 + a_5 y^2 \right]$$
(5)

where $x = \log(T)$ and $y = \log(\rho)$. We have fit the mass absorption coefficient μ instead of the radiative opacity because it has a smoother behavior. This new expression is a quadratic fit to surface which gives more flexibility in relation to a linear one.

In figure 1, it is shown the average ionization for a beryllium plasma in the range $1-10^3$ eV for several densities from 10^{-9} to 10^{-1} g·cm⁻³. At low temperatures the behaviour of the mean ionization depends strongly on the plasma density, thus under 10 eV we found huge variations in the average ionization. In the range 15 - 100 eV the low density curves trend to mach and for temperatures above 300 eV the fully striped ion dominates for all the cases studied. This complexity found in the ionization at low temperature has its counterpart in the mean opacity, and it is necessary to perform different fits for each range of temperatures.

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In figure 2 we plot the behavior of the Planck mean absorption coefficient (a) and its fit (b) for boron plasmas in the temperature range between 1 and 10^3 eV and density from 10^{-10} to 10^{-1} g cm⁻². Figures 3(a) and 3(b) show the Rosseland mean for beryllium plasmas under the same conditions. The fit has been performed using a quadratic response surface model and since it is not possible fit the whole surface in the entire range of temperature, a piecewise fit has been done. One can appreciate that performing a linear fit over the entire range of temperatures and densities will yield a poor representation of the data, whereas equation 4 provides a better representation of the behavior of the Planck and Rosseland means at low temperatures.



Figure 1. Average ionization computed by ABAKO vs. temperature at several densities for a Beryllium plasma



Figure 2. (a) Planck absorption coefficient (cm^{-1}) for a boron plasma (b) fit using equations (4)-(5).

Figure 3. (a) Rosseland absorption coefficient (cm^{-1}) for a beryllium plasma (b) fit using equations (4)-(5).

Values of the parameters obtained for several low Z elements are given in Table 1. These results should be used with caution because the accuracy of the fit increases with the temperature, thus for the range $10^2 - 10^3$ eV we find local deviations around 10-20 % in the opacities but in the range 1 -10 eV they can deviate by factor 5 from the calculated values. Nevertheless this fit could be a useful tool in the study of phenomena in hydrodynamics involving radiative transport, when these local deviations can be assumed.

		Planck Rosseland								
Z=2										
	2≤T≤5 eV	5 <t≤ 10="" ev<="" th=""><th>10<t≤10<sup>3 eV</t≤10<sup></th><th>2≤T≤10 eV</th><th>10<t≤ 10<sup="">2 eV</t≤></th><th>$10^2 < T \le 10^3 \text{ eV}$</th></t≤>	10 <t≤10<sup>3 eV</t≤10<sup>	2≤T≤10 eV	10 <t≤ 10<sup="">2 eV</t≤>	$10^2 < T \le 10^3 \text{ eV}$				
\mathbf{a}_0	1.5483E+01	-6.5726E+00	2.7636E+01	1.5179E+01	2.9428E+01	1.3474E+00				
\mathbf{a}_1	-5.8973E+00	2.1957E+01	-4.5688E+00	2.8546E+00	-5.8835E+00	-4.5316E-01				
\mathbf{a}_2	1.3979E+00	1.2924E+00	2.2334E+00	2.2316E+00	2.9015E+00	1.1514E+00				
a ₃	2.2544E-02	1.8327E-01	1.6779E-02	-6.2619E-02	-2.6930E-01	-2.3174E-02				
\mathbf{a}_4	3.1109E+00	-5.5971E+00	5.1518E-02	-1.2338E+00	-7.2351E-03	0.0000E+00				
a ₅	1.1628E-02	2.0203E-02	3.9707E-02	1.4569E-02	2.3920E-02	0.0000E+00				
Z=3										
	1≤T≤10 eV	$10 < T \le 10^2 \text{ eV}$	$10^2 < T \le 10^3 \text{ eV}$	1≤T≤10 eV	$10 < T \le 10^2 \text{ eV}$	$10^2 < T \le 10^3 \text{ eV}$				
\mathbf{a}_0	2.1195E+01	9.3986E+00	2.7807E+01	1.9424E+01	1.5594E+01	2.4996E+01				
\mathbf{a}_1	-9.5624E+00	4.2568E+00	-5.1315E+00	-7.7632E+00	1.5201E+00	-7.6016E+00				
\mathbf{a}_2	2.1810E+00	1.5861E+00	1.7701E+00	2.2338E+00	2.8647E+00	1.4683E+00				
a ₃	-3.8400E-01	2.8961E-02	-3.7040E-03	-1.0297E-01	-2.4069E-01	-4.3706E-02				
\mathbf{a}_4	2.4094E+00	-1.0845E+00	1.0344E-01	2.0365E+00	-8.6555E-01	5.5563E-01				
a ₅	1.2152E-02	2.3232E-02	2.5038E-02	1.7773E-02	2.5594E-02	7.0353E-03				
			Z=4							
	1 ≤T≤ 10 eV	$10 < T \le 10^2 eV$	$10^2 < T \le 10^3 \text{ eV}$	1 ≤T≤ 10 eV	$10 < T \le 10^2 \text{ eV}$	$10^2 < T \le 10^3 \text{ eV}$				
\mathbf{a}_0	2.5021E+01	-1.3335E+01	3.1069E+01	2.1479E+01	1.0988E+01	4.2232E+01				
\mathbf{a}_1	-1.1426E+01	1.5940E+01	-6.1691E+00	-5.2281E+00	1.8834E+00	-1.2768E+01				
\mathbf{a}_2	1.9024E+00	1.4265E+00	1.4141E+00	2.0529E+00	2.6111E+00	1.5055E+00				
a ₃	-8.7274E-02	-2.4457E-02	-4.7942E-03	-1.9886E-01	-1.3254E-01	-4.8302E-02				
\mathbf{a}_4	2.6164E+00	-2.5665E+00	1.8157E-01	-1.5990E-01	-5.5587E-01	9.4243E-01				
a ₅	1.5436E-02	1.1775E-02	1.4057E-02	4.6793E-03	3.0221E-02	7.5590E-03				
Z=5										
	1 ≤T≤ 20 eV	20 <t≤2×10<sup>2eV</t≤2×10<sup>	$2 \times 10^{2} < T \le 10^{3} eV$	1 ≤T≤ 10 eV	20 <t≤2×10<sup>2eV</t≤2×10<sup>	$2 \times 10^2 < T \le 10^3 eV$				
\mathbf{a}_0	1.6109E+01	-2.0046E+01	3.0288E+01	1.7740E+01	8.6753E+00	5.2951E+01				
\mathbf{a}_1	-8.8648E-01	1.6572E+01	-5.6685E+00	-5.7576E-01	2.1382E+00	-1.5937E+01				
\mathbf{a}_2	1.4934E+00	1.2575E+00	1.1586E+00	1.9185E+00	2.5659E+00	1.1639E+00				
a ₃	4.5994E-02	-2.7165E-02	-2.0608E-03	-1.2073E-01	-1.3522E-01	-1.2894E-02				
\mathbf{a}_4	-2.8942E-01	-2.3022E+00	1.2952E-01	-9.2101E-01	-5.0343E-01	1.1695E+00				
a ₅	1.5892E-02	5.6522E-03	6.2114E-03	3.6289E-03	2.8486E-02	3.1661E-03				

Table 1. Fit coefficients for He, Li, B and Be Plasma.

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