Opacity calculation based on average atom model*

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Abstract The relativistic self-consistent average atom model is employed to calculate the radiative opacities for high Z plasma. One-electron transitions are considered for bound-bound process. The line distribution from ionic configurations are calculated ion by ion. The Rosseland mean opacities and the Planck mean ones for europium with D=0.1 g/cm^3, kT=60~10^4 eV are given and compared with data given by SESAME data base.
Keywords Radiative opacity, Plasma, Ionic configuration, Average atom model

1 Introduction

In radiative transfer work, two frequency-averaged radiative opacities play an important role. For optically-thick plasmas, the Rosseland mean opacity is important, whereas the Planck mean opacity is of interest in optically-thin plasmas. Their usual definitions are

$$\frac{1}{K_{\rm R}({\rm cm^2/g})}=\frac{15}{4\pi^4}\int_0^{\infty}\frac{u^4\exp(-u){\rm d}u}{K_{\rm t}(u)[1-\exp(-u)]^2} \tag{1}$$

$$K_{\rm P}({\rm cm^2/g})=\frac{15}{\pi^4}\int_0^{\infty}\left[K_{\rm bf}(u)+K_{\rm ff}(u)+K_{\rm bb}(u)\right]u^3\exp(-u){\rm d}u \tag{2}$$

where

$$K_{\rm t}(u)=\left[K_{\rm bf}(u)+K_{\rm ff}(u)+K_{\rm bb}(u)\right]\left[1-\exp(-u)\right]+K_{\rm s} \tag{3}$$

$u=h\nu/kT$. $K_{\rm bf}(u)$, $K_{\rm ff}(u)$, $K_{\rm bb}(u)$ and $K_{\rm s}$ are the frequency-dependent opacity from photoionization (b-f), inverse bremsstrahlung (f-f), photoexcitation (b-b) and scattering, respectively. Each of them equals their respective cross section multiplied by corresponding particle number per unit mass. In present work, for inverse bremsstrahlung cross section, the Kramer's classical formula $\sigma_{\rm ff}^{\rm K}(u)$ is used,[1] and for scattering process, the Thomson cross-section $\sigma_{\rm T}$= 6.653×10^{-25} cm^2 is used.

2 Atomic model

In order to give the $\sigma_{\rm bf}(u)$, $\sigma_{\rm bb}(u)$ and population (or particle number), the one-component Dirac equation (in a.u.) for the average atom (AA) as the following

$$\frac{{\rm d}^2G_i(r)}{{\rm d}r^2}-\frac{\alpha^2/2}{1+\alpha^2(E_i+V)/2}\frac{{\rm d}V(r)}{{\rm d}r}\frac{{\rm d}G_i(r)}{{\rm d}r}$$

$$+\left[2(E_i+V)-\frac{K_i(K_i+1)}{r^2}+\alpha^2(E_i+V)^2-\frac{\alpha^2/2}{1+\alpha^2(E_i+V)/2}\frac{{\rm d}V(r)}{{\rm d}r}\frac{K_i}{r}\right]G_i(r)=0 \tag{4}$$

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was solved by Hartree-Fock-Slater (HFS) self-consistent potential method,[2,3] where α is the fine-structure constant, $V(r)$ is the self-consistent potential, K_i is the relativistic quantum number, E_i and $G_i(r)$ are the single particle level and the wave function for the i-th state, respectively. The boundary conditions of Eq.(4) for AA are

$$V(R_0) = 0, \qquad \frac{\mathrm{d}V(r)}{\mathrm{d}r}\Big|_{r=R_0} = 0,$$
$$\lim_{r\to 0} rV(r) = Z \tag{5}$$

where Z is the nuclear charge and $R_0 = (3\Omega_0/4\pi)^{1/3}$ the WS radius, Ω_0 the atomic volume determined by the plasma density. The AA model assumes that the electronic levels are populated according to the Fermi-Dirac statistics:

$$\overline{N_i} = \frac{2\,|\,K_i\,|}{\exp\left[(E_i - \mu)/kT\right] + 1} \tag{6}$$

where T is the temperature of plasma, μ the chemical potential determined by requiring charge neutrality in the ion-sphere. The level E_i, the mean population $\overline{N_i}$, the chemical potential μ, the wave function $G_i(r)$ and the self-consistent potential $V(r)$ can be obtained by the self-consistent solution. Based on $V(r)$, the continuum wave functions of free electrons and the photoionization cross section can be calculated.[4] So can the photoionization opacities $K_{\mathrm{bf}}(u)$ be given easily.

3 Photoexcitation

The calculation of photoexcitation opacities $K_{\mathrm{bb}}(u)$ are most complicated. It is the key to the opacity calculations. The average atom has only a statistically mean sense. Actually, in a hot plasma, there are statistical fluctuations of electronic occupation about the mean value $\overline{N_i}$ for each level. The fluctuations of electronic occupation cause the differing amounts of screening and, in an ensemble of radiating atoms (ions), split each generically one-electron transition into many lines. This splitting is called configuration splitting. The spectrum corresponding to one-electron transition from the initial level (nlj) to the final one $(n'l'j')$ is called a transition cluster.

From the Dirac Eq.(4) the shift $\Delta E_i^{(c)}$ of the i-th level, due to population changes from $\overline{N_j}$ to $N_j^{(c)}$ for all of other levels j, is given by

$$\Delta E_i^{(c)} = -\Sigma_{j\neq i}(\overline{N_j} - N_j^{(c)})E_{ij} \tag{7}$$

where $N_j^{(c)}$ is a set of integers for a configuration (c).

$$E_{ij} = \int_0^{R_0} G_i^2\Big\{\big[1 + \alpha^2(E_i + V) + \frac{\alpha^4}{8}[1 + \alpha^2(E_i + V)/2]^{-2}\frac{\mathrm{d}V}{\mathrm{d}r}\Big(\frac{K_i}{r} + \frac{1}{G_i}\frac{\mathrm{d}G_i}{\mathrm{d}r}\Big)\big]V_{ij}^{(1)}(r)$$
$$+\frac{\alpha^2}{4}[1 + \alpha^2(E_i + V)/2]^{-1}\Big(\frac{K_i}{r} + \frac{1}{G_i}\frac{\mathrm{d}G_i}{\mathrm{d}r}\Big)V_{ij}^{(2)}(r)\Big\}\mathrm{d}r \tag{8}$$

$$V_{ij}^{(1)}(r) = \Big[\frac{1}{r}\int_0^r G_j^2(r')\mathrm{d}r' + \int_r^{R_0}\frac{1}{r'}G_j^2(r')\mathrm{d}r'\Big] - \frac{G_j(r)}{G_i(r)}\delta(m_i^{\mathrm{s}}, m_j^{\mathrm{s}})$$
$$\times\Big[\frac{1}{r}\int_0^r G_j(r')G_i(r')\mathrm{d}r' + \int_r^{R_0}\frac{1}{r'}G_j(r')G_i(r')\mathrm{d}r'\Big] \tag{9}$$

$$V_{ij}^{(2)}(r) = \frac{1}{r^2}\int_0^r G_j^2(r')\mathrm{d}r' - \frac{G_j(r)}{G_i(r)}\delta(m_i^{\mathrm{s}}, m_j^{\mathrm{s}})\frac{1}{r^2}\int_0^{R_0} G_j(r')G_i(r')\mathrm{d}r' \tag{10}$$

where $\delta(x)$ is the Dirac' δ function; m_i^{s}, m_j^{s} the spin quantum number of the i-th state and the j-th state, respectively. Likewise, there are the similar expressions for the level f but only changing i into f in Eqs.(7~10). The energy shift $\Delta(h\nu_{if})^{(c)}$ of the transition line i to f (i-f:J) is expressed as

$$\Delta(h\nu_{if})^{(c)} = \Delta E_i^{(c)} - \Delta E_f^{(c)} \tag{11}$$

The place of the line J for a configuration (c) is

$$(h\nu_{if})^{(c)} = h\nu_{if} + \Delta(h\nu_{if})^{(c)} \quad (12)$$

The exiting probability $P^{(c)}$ for a configuration (c) is

$$P^{(c)} = \Pi_j \frac{g_j!}{(g_j - N_j^{(c)})!N_j^{(c)}!}\exp[-\frac{\mu N^{(c)} - E^{(c)}}{kT}] \quad (13)$$

where g_j is the statistical weight of the j-th state,

$$N^{(c)} = \Sigma_j N_j^{(c)}, \qquad E^{(c)} = \Sigma_j N_j^{(c)} E_j^{(c)},$$

$$E_j^{(c)} = E_j + \Delta E_j^{(c)} \quad (14)$$

$N_j^{(c)}$ is selected in the limits:

$$\overline{N_j} - \Delta N_j \leq N_j^{(c)} \leq \overline{N}_j + \Delta N_j \quad (15)$$

$$\Delta N_j = \overline{N}_j \sqrt{\overline{N}^{-1} - g_j^{-1}} \quad (16)$$

The probable configurations are those with integer occupation numbers $N_j^{(c)}$ close to the mean values $\overline{N}_j$. In our work only those configurations with probability larger than $10^{-3} \times P_{\rm M}^{(c)}$ are kept, where $P_{\rm M}^{(c)}$ stands for the probability of the most probable configuration. This configuration is obtained by truncating the AA level populations to the nearest integer value. Using the above two limits, several thousand configurations are considered usually for high Z plasmas.

Finally the frequency dependent photoexcitation opacities $K_{\rm bb}(h\nu)$ is written as

$$K_{\rm bb}(h\nu) = \frac{N_0}{A}\Sigma_J \Sigma_{(c)}\sigma_J^{(c)}(h\nu) = \frac{8\pi^3 e^2 a_0^2}{3ch}\frac{N_0}{A}\Sigma_J B(lj, l'j')[\int_0^{R_0} G_{nlj} \cdot r \cdot G_{n'l'j'}{\rm d}r]^2$$
$$\times \Sigma_{(c)} P^{(c)} \cdot h\nu_{if}^{(c)} \cdot I_{\rm V}^{(c)}(h\nu, \Gamma) N_i^{(c)}(1 - N_f^{(c)}/g_f) \quad (17)$$

where N_0 is Avogadro's number; A the atomic weight of plasma;

$$B(lj, l'j') = (2l+1)(2j'+1)\begin{pmatrix} l & l' & 1 \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{Bmatrix} l & 1 & l' \\ j & 1/2 & j' \end{Bmatrix}^2 \quad (18)$$

where l and j (l' and j') are the quantum numbers of the orbital and total angular momenta of electron in the initial state (final state), respectively, $\begin{pmatrix} l & l' & 1 \\ 0 & 0 & 0 \end{pmatrix}$ and $\begin{Bmatrix} l & 1 & l' \\ j & 1/2 & j' \end{Bmatrix}$ are the 3-j symbol and the 6-j symbol;

$I_{\rm V}^{(c)}(h\nu, \Gamma)$ is the Voigt profile of the line transition, and can be expressed as[5]

$$I_V^{(c)}(h\nu, \Gamma) = \frac{\ln 2}{\pi^{3/2}} \cdot \frac{\Gamma_t}{\Gamma_{\rm D}^2} \cdot \int_{-\infty}^{\infty} \frac{\exp(-y)^2{\rm d}y}{(b-y)^2 + a^2} \quad (19)$$

where

$$y = \sqrt{\ln 2}[E' - (h\nu_{if})^{(c)}]/\Gamma_{\rm D}, \quad a = \Gamma_t\sqrt{\ln 2}/\Gamma_{\rm D}, \quad b = [h\nu - (h\nu_{if})^{(c)}]\sqrt{\ln 2}/\Gamma_{\rm D} \quad (20)$$

here E' is the dumb variable in the convolution, $\Gamma_{\rm D}$ stands for the half-width of the Doppler line shape at half maximum, Γ_t for the sum of the electron collision half-width Γ_c and the Stark half-width Γ_S (the natural half-width was ignored),

$$\Gamma_{\rm D}[(h\nu_{if})^{(c)}] = [2kT\ln 2/Mc^2]^{1/2}(h\nu_{if})^{(c)} \quad (21)$$

$$\Gamma_c = \frac{8\pi^2}{9}(\frac{2}{3\pi})^{1/2}\frac{\hbar^3}{m^{3/2}}\frac{N_0 n_f D}{A}(kT)^{-1/2}\Sigma_{l'j'}B(lj, l'j')[\int_0^{R_0} G_{nlj} \cdot r \cdot G_{n'l'j'}{\rm d}r]^2 \quad (22)$$

$$\Gamma_s = \frac{5}{2}\frac{n_f a_0 e^2}{R_0^2}[\int_0^{R_0} G_i^2 \cdot r \cdot \mathrm{d}r + \int_0^{R_0} G_f^2 \cdot r \cdot \mathrm{d}r] \tag{23}$$

in which, $n_f = Z - \Sigma_j \overline{N}_j$ is the mean ionization degree of the AA, M the atom mass, D the density of plasma.

4 Results of calculation

The calculating program (OPINCH) for the above model was written on the computer Galaxy II made in China. Up to now the radiative opacities for a number of elements have been calculated with this program. Here the partial results on europium are given as an example. Fig.1 and Fig.2 show the Rosseland mean opacities and the Planck mean opacities for Eu at D=0.1 g/cm^3 and $kT = 60 \sim 10^4$ eV, respectively, where the SESAME values[6](dots) are also shown. A agreement is found for the Rosseland mean, but for the Planck mean there is an evident deviation in the range of kT >2 keV. We have nothing to say for this deviation because no detailed informations have been published on how the SESAME tables were generated.

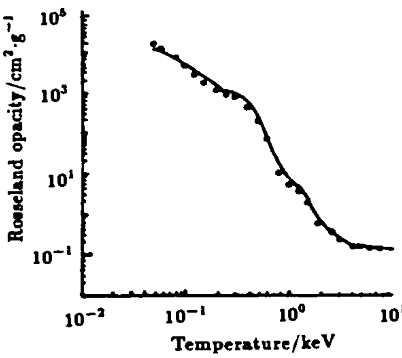

Fig.1 Rosseland mean opacities vs temperature for Eu at $D = 0.1$ g/cm^3

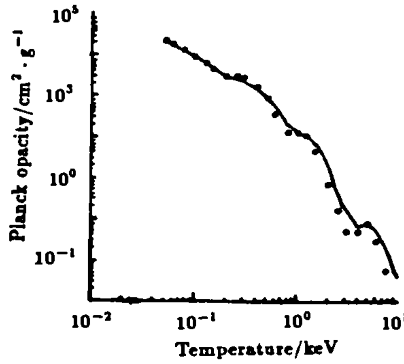

Fig.2 Planck mean opacities vs temperature for Eu at D=0.1 g/cm^3

The solid line represents the results of present work, the dots are from the SESAME opacity library

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