Thermodynamics and radiation transport in dense plasmas

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1 Introduction

The development of theoretical models to simulate the Equation Of State (EOS) for dense plasmas had been mostly finished in 40s-50s. In principle, the material presented in [1] is sufficient to solve numerically the thermodynamic parameters and radiation transport in high-temperature plasmas, if: (1) the researcher is perfectly familiar with atomic physics, quantum mechanics and quantum electrodynamics and (2) he/she has an unlimited access to databases for atomic and ion "parameters" such as all ionization potentials, an excitation energy for all levels, as well as the degeneracy for both ground and energy levels). Even in this hypothetic case the researcher may be tempted to solve the coupled system of *the Saha equations*, which relate the populations of ions with different cherge numbers. The latter approach appears to be inoptimal, if plausible at all.

Of course, there are tabulated EOS as well as the opacity tables. However, it is intereting to summarize here the methods which allows researchers to compute both the EOS functions and opacities for the radiation transport, at least under some simplifying assumptions.

Particularly, here we employ the assumption of a Local Thermodynamic Equilibrium. This means that we assume the popolation of all atomic and ionic states to be excatly the same as those calculated using the methods of statistical physics [2].

The paper is split to two parts, the first of them being entirely devoted to the thermodynamic analisys applied to LTE dense plasmas. It is more focused on the EOS function calculation, however, the obtained populations and partition function are also used in the second part, to find opacities. This makes the overall aproach to the radiation hydrodynamics to be consistent.

The second part describes the way to apply the results of the first part to a problem of the radiation transport in plasmas. This transport is treated in the framework of Multi-Group Diffusion (MGD). The assumtions of LTE and MGD are key points of the presented paper.

2 Effect of the Fermi statistics on Thermal Ionization

While simulating the ionization equilibrium in partially ionized electron-ion plasmas using Saha equations, the electrons are usually assumed to be an ideal Boltzmann gas. However, the electron is a Fermion with spin of 1/2. In practical calculations the conditions for applicability of the Boltzmann gas model for electrons are often not satisfied, resulting in very low accuracy. Therefore, it is worth while checking whether or not one needs to assume Boltzmann statistics for the electrons when solving the ionization equlibrium.

It appears that for realistic quantitative simulations this assumption is completly unnecessary, as solving the ionization equilibrium under the incorrect assumption of Boltzmann statistics is not any easier than that with the correct Fermi statistics for electrons.

In a partially ionized plasma the free electron density, corrected by the effects of the Fermi statistics ('the exchange interaction'), should be used in solving the Equation-Of-State (EOS), which is also directly affected by the exchange interactions. There is no need to remind that *at the given electron density* the exchange interaction increases the electron pressure and the internal energy density (see [2]). On the other hand, in partially ionized plasmas this effect may be partially or even fully balanced by the electron density decrease due to the exchange interaction effect on the ionization equilibrium.

Helmholtz free energy. Consider an ionized monatomic gas with positive non-complex ions. The Helmholtz free energy, $F = F_{ion} + F_e$, is assumed to be the total of contributions from each of the ion charge states, $i = 0$ to $i_{\max}$ (we apply Eq.(42.3) from [2] to account for these contributions), as well as the contribution from electrons:

$$F = -T \sum_{i=0}^{i_{max}} N_i \log \left[g_i \frac{eV}{N_i} \left(\frac{MT}{2\pi\hbar^2} \right)^{3/2} \exp\left(-\sum_{j=0}^{i-1} \frac{I_j}{T} \right) \right] + F_e, \qquad (1)$$

where $N_i = n_i V$ is the total number of ions in the charge state i in the volume V and I_j $(j = 0, 1, 2, \ldots)$ is the energy needed to ionize an atom or ion from the charge state j to the charge state $j + 1$ (the ionization potential), and g_i is a statistical weight of an ion (atom) in a given charge state (see Section IV for more detail).

Ionization equilibrium: formulation of the problem. Now we formulate the requirement for the ionization equilibrium with respect to the reaction $(i) \leftrightarrow (i+1)+e$ for each ion charge state, i. The Helmholtz free energy is a minimum at the equilibrium set of N_i and N_e. Therefore, the total derivative of F with respect to N_e should be zero:

$$\frac{\partial F}{\partial N_e} + \frac{dN_i}{dN_e}\frac{\partial F}{\partial N_i} + \frac{dN_{i+1}}{dN_e}\frac{\partial F}{\partial N_{i+1}} = 0. \tag{2}$$

For the reaction under consideration, the increments in the particle numbers should be related as follows: $dN_i = -dN_{i+1} = -dN_e$. Therefore the requirement, $dF/dN_i - dF/dN_{i+1} - dF/dN_e = 0$, gives:

$$-T\log\left[\frac{g_i}{N_i}e^{-\sum_{j=0}^{i-1} I_j/T}\right] + T\log\left[\frac{g_{i+1}}{N_{i+1}}e^{-\sum_{j=0}^{i} I_j/T}\right] - \mu_e = 0, \tag{3}$$

where we applied the definition of the chemical potential, $\mu = (\partial F/\partial N)_{T,V}$, to the electron gas. The solution of the ionization equilibrium, therefore, reads:

$$N_{i+1}/g_{i+1} = (N_i/g_i)e^{(-\mu_e - I_i)/T}, \tag{4}$$

or, applying this recursively:

$$N_i/g_i = (N_0/g_0)e^{(-i\mu_e - \sum_{j=0}^{i-1} I_j)/T} = (N_0/g_0)(g_e)^i e^{-\sum_{j=0}^{i-1} I_j/T}, \quad g_e = e^{-\mu_e/T}, \tag{5}$$

where g_e is the effective statistical weight of a free electron. Indeed, the effective statistical weight of i electrons combined with an ion in the charge state, i, is the product of statistical weights for each of the particles under consideration, $(g_e)^i g_i$, in accordance with Eq.(5).

In the limiting case of $g_e \gg 1$ (a Boltzmann gas of electrons with large negative value of μ_e), g_e might be interpreted as the large number of elementary quantum states the detached electron can occupy, which facilitates the ionization by resulting in a higher total probability for the ionized state. In the opposite limiting case of a degenerate Fermi gas of electrons, the positive chemical potential, $\mu_e > 0$, tends to the Fermi energy E_F, which in this limiting case is much greater than the temperature. Accordingly, the exponentially low value of $g_e = e^{-E_F/T}$ in this case means the low probability for an electron to jump from a bound state with negative energy to a free state above the threshold of the positive Fermi energy.

Partition function and electron density. We now introduce the ion partition function, $p_i = N_i/N_a$, N_a, being the total number of atoms. Since the partition function is normalized by unity, we have:

$$p_i = \frac{g_i (g_e)^i e^{-E_i/T}}{S}, \tag{6}$$

where we introduced the statistical sum:

$$S = \sum_{i=0}^{i_{max}} \left[g_i (g_e)^i e^{-E_i/T} \right], \tag{7}$$

as well as the total ionization energy spent to ionize the atom to the state i:

$$E_i = \sum_{j=0}^{i-1} I_j. \tag{8}$$

Introducing the averaging operator acting on an arbitrary function of the ion charge number, $\langle f_i \rangle = \sum p_i f_i$, and assuming quasi-neutrality, $N_e = \sum i N_i$, we obtain the expression for the electron density:

$$Z = N_e/N_a = \langle i \rangle. \tag{9}$$

On the other hand, for given T and $n_a = N_a/V$ the electron concentration may be found as a function of $g_e (= e^{-\mu_e/T})$. Now we assume electrons form an ideal Fermi gas. This assumption immediately gives us another relationship between the electron density and g_e (see Eq.(56.5) from [2]):

$$Z = g_{e1} \mathrm{Fe}_{1/2}(g_e). \tag{10}$$

The coupled equations (9) and (10) are used below to solve Z and g_e. Here

$$g_{e1}(T, N_a/V) = \frac{2V}{N_a} \left(\frac{m_e T}{2\pi \hbar^2} \right)^{3/2} \tag{11}$$

is a value such that in the *Boltzmann* electron gas $g_e = g_{e1}/Z$ would hold. $\mathrm{Fe}_\nu(g_e)$ is the Fermi function:

$$\mathrm{Fe}_\nu(g_e) = \frac{1}{\Gamma(\nu+1)} \int \frac{x^\nu dx}{g_e e^x + 1}, \tag{12}$$

where Γ-function is introduced as usually: $\Gamma(\nu+1) = \nu\Gamma(\nu)$, $\Gamma(1/2) = \pi^{1/2}$. Below we use the following auxiliary functions:

$$R^-(g_e) = \frac{\mathrm{Fe}_{-1/2}(g_e)}{\mathrm{Fe}_{1/2}(g_e)}, \qquad R^+(g_e) = \frac{\mathrm{Fe}_{3/2}(g_e)}{\mathrm{Fe}_{1/2}(g_e)}. \tag{13}$$

Detailed discussion on the Fermi functions is delegated to Appendix A.

Derivatives along the ionization curve. Taking differential of the equation of ionization equilibrium, $G = 0$, one gets an equation relating the differentials of different variables along the curve of ionization equilibrium:

$$\frac{dg_e}{g_e}\left(\langle i^2\rangle - Z^2 + ZR^-(g_e)\right) + \frac{dT}{T^2}\left(\langle iE_i\rangle - \langle E_i\rangle Z\right)) = \left(\frac{3}{2}\frac{dT}{T} + \frac{dV}{V}\right)Z, \tag{14}$$

here we substitute wherever possible Z for $\langle i\rangle$ and $g_{e1}\mathrm{Fe}_{1/2}(g_e)$. Accordingly, the differential of Z is:

$$dZ = \left(\frac{3}{2}\frac{dT}{T} + \frac{dV}{V} - \frac{R^-(g_e)dg_e}{g_e}\right)Z. \tag{15}$$

To solve the ionization equilibrium for the given T and $n_a = N_a/V$, one needs to solve g_e from equation $G(g_e) = 0$, $G(g_e) = \langle i\rangle - g_{e1}\mathrm{Fe}_{1/2}(g_e)$, which is obtained by means of excluding Z from Eqs.(9,10). It may be solved using the Newton-Rapson iterations with any trial value, $\log(g_e)_{old}$, the improved value, $\log(g_e)_{new}$, is obtained from the equation as follows:

$$\log(g_e)_{new} = \log(g_e)_{old} - \frac{\langle i\rangle - g_{e1}\mathrm{Fe}_{1/2}((g_e)_{old})}{\langle i^2\rangle - \langle i\rangle^2 + ZR^-((g_e)_{old})}, \tag{16}$$

where the derivative $g_e G'$, which should stand in the denominator of Eq.(16), is derived using the easy-to-check equations as follows:

$$g_e\frac{d\mathrm{Fe}_\nu(g_e)}{dg_e} = -\mathrm{Fe}_{\nu-1}(g_e), \tag{17}$$

and for any set of values in the charge states, f_i:

$$g_e\frac{\partial\langle f_i\rangle}{\partial g_e} = \langle if_i\rangle - \langle f_i\rangle\langle i\rangle, \tag{18}$$

which is a particular case of Eq.(131).

We see that to solve iterations in Eq.(16) for Fermi gas of electrons is not a more computationally intense problem compared to the same problem assuming electrons to be a Boltzmann gas. In the latter case, $g_e \to +\infty$, we have $\mathrm{Fe}_\nu(g_e) \approx 1/g_e$ (see Eq.(29) below) and $g_e \approx g_{e1}/Z$, which allows us to iterate Eq.(16) as a somewhat simpler equation for Z: $\log(Z_{new}) = \log(Z_{old}) + (\langle i \rangle - Z_{old})/(Z_{old} + \langle i^2 \rangle - \langle i \rangle^2)$. However in any case, the most cumbersome computations while solving Eq.(16) for a Fermi gas, or the equation for Z for a Boltzmann gas, is in explicitly calculating the numerous partition functions for many charge states and excitation levels. Compared with these bulk computations, the presence of the Fermi functions in Eq.(16), which may be tabulated for all interesting cases of $\nu = -1/2, 1/2, 3/2$, does not matter at all.

Therefore, we do not see any reason for applying the assumption of a Boltzmann electron gas in modelling the ionization equilibrium in real dense plasmas.

Plasma thermodynamics and Equation-Of-State. Now we substitute the ion partition function into Eq.(1). After some algebra we obtain:

$$F = -TN_a \log\left[\frac{eV}{N_a}\left(\frac{MT}{2\pi\hbar^2}\right)^{3/2}\right] - TN_a \log S + \Omega_e, \tag{19}$$

the thermodynamic potential $\Omega_e = F_e - \mu_e Z N_a$ for Fermi gas of electrons is given by Eq.(56.6) from [2]:

$$\Omega_e = -[g_{e1}N_a]T\mathrm{Fe}_{3/2}(g_e), \tag{20}$$

the product in the square brackets, being independent of N_a because $g_{e1} \sim N_a^{-1}$. Eq.(19) provides the free energy in the case of local thermodynamic equilibrium with the first term being the contribution from the ion translational energy. This term may be written as the function of the ion temperature, in the case the latter differs from the electron temperature. Unless the ion-ion interaction is taken into account, this first term gives the contributions of $n_a T_i$ and $3n_a T_i/2$ to the total plasma pressure and total energy density correspondingly. The second term is the Boltzmann distribution of ions over the ionization and excitation states, expressed in terms of the statistical sum. Finally, the electron gas with the variable particle number gives the contribution of Ω_e instead of F_e.

While differentiating Eq.(19) with respect to T and V, it is important that the derivatives by g_e from the second and third terms cancel each other:

$g_e(\partial \log S/\partial g_e) = \langle i \rangle = Z$ and $-g_e g_{e1} \mathrm{Fe}'_{3/2}(g_e) = g_{e1}\mathrm{Fe}_{1/2} = Z$. That is why for the internal energy density, $\mathcal{E}$, and for the pressure we find:

$$\mathcal{E} = -\frac{T^2}{V}\left(\frac{\partial}{\partial T}\left(\frac{F}{T}\right)\right) = \mathcal{E}_i + \mathcal{E}_e, \qquad \mathcal{E}_i = \frac{3}{2}Tn_a, \qquad \mathcal{E}_e = n_a\left[\frac{3}{2}TZR^+(g_e) + \langle E_i \rangle\right], \tag{21}$$

$$P = -\frac{\partial F}{\partial V} = P_i + P_e, \qquad P_i = n_a T, \qquad P_e = n_a TZR^+(g_e). \tag{22}$$

However, while calculating the second order thermodynamic derivatives, like the specific heat, the derivatives of g_e essentially sophisticate the calculations. The result may be expressed in terms of covariances: $\langle \delta^2 i \rangle = \langle (i-Z)^2 \rangle$, $\langle \delta^2 E_i \rangle = \langle (E_i - \langle E_i \rangle)^2 \rangle$ and $\langle \delta i \delta E_i \rangle = \langle (E_i - \langle E_i \rangle)(i - Z) \rangle$. In a similar way one can find the specific heat in an isochoric process, per the unit of volume:

$$C_{Ve} = \frac{\partial \mathcal{E}_e}{\partial T} = n_a\left[\frac{\langle \delta^2 E_i \rangle}{T^2} + \frac{15}{4}ZR^+ - \frac{\left(\frac{3}{2}Z - \frac{\langle \delta E_i \delta i \rangle}{T}\right)^2}{\langle \delta^2 i \rangle + ZR^-}\right], \tag{23}$$

the temperature derivative of pressure:

$$\frac{\partial P_e}{\partial T} = n_a Z\left[\frac{5}{2}R^+ - \frac{\frac{3}{2}Z - \frac{\langle \delta E_i \delta i \rangle}{T}}{\langle \delta^2 i \rangle + ZR^-}\right], \tag{24}$$

as well as the isothermal compressibility:

$$V\frac{\partial P_e}{\partial V} = -\frac{Z^2 n_a T_e}{\langle \delta^2 i \rangle + ZR^-}. \tag{25}$$

For simplicity in the above equations, the contributions due to ion translational motions,

$$C_{Vi} = \frac{3}{2}n_a, \qquad \frac{\partial P_i}{\partial T} = n_a, \qquad V\frac{\partial P_i}{\partial V} = -n_a T, \tag{26}$$

are omitted.

The speed of sound, C_s, is defined in terms of the adiabatic comressibility (at constant entropy), $C_s^2 = \left(\frac{\partial P}{\partial \rho}\right)_{\mathrm{ad}}$, which may be parametrized in terms of effective adiabatic index, γ, such that $\gamma\frac{P}{\rho} = \left(\frac{\partial P}{\partial \rho}\right)_{\mathrm{ad}}$, herewith ρ is the mass density. To calculate this, one can take Eq.(3.72) from [7],

$$\left(\frac{\partial P}{\partial \rho}\right)_{\mathrm{ad}} = \left(\frac{\partial P}{\partial \rho}\right)_T - \frac{\rho}{C_V}\left[\left(\frac{\partial(\mathcal{E}/\rho)}{\partial \rho}\right)_T - \frac{P}{\rho^2}\right]\left(\frac{\partial P}{\partial \rho}\right)_T.$$

Note that in [7] both the internal energy and the specific heat are related per a unit of mass, while we relate them to the unit of volume. Now we apply the thermodynamic identity as follows:

$$\left(\frac{\partial(\mathcal{E}/\rho)}{\partial\rho}\right)_T - \frac{P}{\rho^2} = -\frac{T}{\rho^2}\left(\frac{\partial P}{\partial T}\right)_\rho, \tag{27}$$

which gives:

$$\gamma = \frac{\rho}{P}\left(\frac{\partial P}{\partial\rho}\right)_T + \left(\frac{\partial P}{\partial T}\right)_\rho^2 \frac{T}{C_V P}. \tag{28}$$

Note that in the last three equations we denote the derivative at constant V as that at constant ρ and used the derivatives over ρ instead of those over V: $V\frac{\partial}{\partial V} = -\rho\frac{\partial}{\partial\rho}$.

Discussion: Estimating the effect of the Fermi statistics on the ionization degree. Eqs.(14,15) allow us to evaluate the effect of electron Fermi statistics on ionization. From Eq.(29) one can see that for large g_e (Boltzmann gas) the equation, $G(g_e) = 0$, reduces to $\langle i\rangle - g_{e1}/g_e = \delta_{\rm Fe}$, where $\delta_{\rm Fe}$ is a small negative correction to the Fermi function at $g_e \to \infty$:

$$\mathrm{Fe}_\nu(g_e) = \frac{1}{\Gamma(\nu+1)}\int\frac{x^\nu dx}{g_e e^x + 1} = \frac{1}{\Gamma(\nu+1)}\int\frac{x^\nu dx}{g_e e^x} + \delta_{\rm Fe} = \frac{1}{g_e} + \delta_{\rm Fe}. \tag{29}$$

Assuming $\delta_{\rm Fe}$ to be a small increment in the right hand side of Eqs.(14,15), and by finding $dg_e/\delta_{\rm Fe}$ from Eq.(14) at $dV = dT = 0$ and then finding $dZ/\delta_{\rm Fe}$ from Eq.(15) gives:

$$\delta Z = Z\delta_{\rm Fe}\frac{\langle i^2\rangle - Z^2}{\langle i^2\rangle - Z^2 + Z}. \tag{30}$$

The correction is negative as long as $\delta_{\rm Fe}$ is negative. Thus, due to the Fermi gas effects for detached electrons, the ionization degree is always lower than that predicted by the Saha equilibrium equations under the assumption of a Boltzmann electron gas.

This effect should be accounted for while treating the effect of the Fermi statistics for electrons in the equation of state. Specifically, *at constant electron density* the exchange interactions between the electrons increases the electron pressure, but in the partially ionized plasma the magnitude (if not the sign!) of this effect can be compromised by the pressure reduction due to the decrease in electron density.

3 Madelung approximation of electrostatic energy

Coulomb interactions may be accounted for within the Madelung approximation. According to this model, we assume that the net charge of an ion and all of the electrons bound to it is concentrated in one point. For an ion in the charge state i, i free electrons are considered to be coupled with it, being uniformly distributed over its *ion sphere,* which is a sphere of volume $1/n_a$, with the ion at its center. While calculating the electrostatic energy we neglect the Coulomb interactions between charges related to different ion spheres. As a result, we only need to calculate the electrostatic energy of an ion with free electrons coupled to it, which is equal to the energy of electron-electron interactions and the energy required to put the ion at the center of the ion sphere:

$$E_E = \frac{1}{2}\int_{r=0}^{r_{iono}} q_e n_e \varphi_e(r) dV - q_e i \varphi_e(0) = \frac{3}{5}\frac{q_e^2 i^2}{r_{iono}} - \frac{3}{2}\frac{q_e^2 i^2}{r_{iono}} = -\frac{9}{10}\frac{q_e^2 i^2}{r_{iono}}, \quad (31)$$

where r_{iono} stands for the radius of the ion sphere, and the potential of the electrostatic field of electrons is as follows:

$$\varphi_e(r) = ei\left(-\frac{3}{2}\frac{1}{r_{iono}} + \frac{1}{2}\frac{r^2}{r_{iono}^3}\right). \quad (32)$$

Helmholtz free energy. The extra term in the free energy, which accounts for the electrostatic energy, is as follows (see also Eq.(3.50) in [7]):

$$F_M = -E_M \sum_{i=0}^{i_{max}} i^2 N_i, \qquad E_M = \frac{9}{10}\frac{q_e^2}{r_{iono}}, \qquad r_{iono} = \left(\frac{4\pi}{3} n_a\right)^{-\frac{1}{3}}. \quad (33)$$

Here the Madelung energy,

$$E_M = \frac{9}{10}\frac{q_e^2}{r_{iono}} = \frac{1.8 Ry}{(r_{iono}/a)}, \quad (34)$$

characterizes the electrostatic energy related per atomic cell. It is conveniently expressed in terms of the Rydberg constant, $Ry = \frac{q_e^2}{2a} \approx 13.60$ eV, as long as the ion sphere radius, r_{iono}, is related to the Bohr radius, $a = \hbar^2/m_e q_e^2 \approx 0.5 \cdot 10^{-10}$ m.

Ionization equilibrium. Accordingly, in the requirement for ionization equilibrium, $\partial F/\partial N_i - \partial F/\partial N_{i+1} - \partial F/\partial N_e = 0$ (with respect to the reaction $(i) \leftrightarrow (i+1)+e$), the term $\partial F_M/\partial N_i - \partial F_M/\partial N_{i+1}$ will give the contribution of $(2i+1)E_M$ to the left side:

$$-T\log\left[\frac{g_i}{N_i}e^{\sum_{j=0}^{i-1} I_j/T}\right] - i^2 E_M + T\log\left[\frac{g_{i+1}}{N_{i+1}}e^{\sum_{j=0}^{i} I_j/T}\right] + (i+1)^2 E_M - \mu_e = 0. \tag{35}$$

The solution of the ionization equilibrium, hence, reads:

$$\frac{N_{i+1}}{g_{i+1}} = \frac{N_i}{g_i}\exp\left(-\frac{1}{T}\left(I_i - (2i+1)E_M + \mu_e\right)\right), \tag{36}$$

or, applying recursively and reducing the sum $\sum_{j=0}^{i-1}(2j+1) = i^2$,

$$\frac{N_i}{g_i} = \frac{N_0}{g_0}(g_e)^i \exp\left(i^2\frac{E_M}{T} - \frac{\sum_{j=0}^{i-1} I_j}{T}\right). \tag{37}$$

This may be interpreted as the ionization potential lowering caused by the Coulomb interaction. Each of the potentials, I_i, is reduced by $(2i+1)E_M$. Energy of the ion of the charge state i is:

$$E_i^* = \sum_{j=0}^{i-1} I_j - i^2 E_M. \tag{38}$$

This effect shifts the ionization equilibrium towards higher ionization degrees for a given temperature and atomic density.

Partition function. The common multiplier, $\frac{N_0}{g_0}$, in each of Eqs.(37) may be also represented as $\frac{N_a}{S}$. From the normalization condition, $\sum N_i = N_a$, we find that S is a statistical sum:

$$S = \sum_{i=0}^{i_{max}} g_i (g_e)^i \exp\left(-\frac{E_i^*}{T}\right), \tag{39}$$

so that:

$$p_i = \frac{N_i}{N_a} = \frac{1}{S} g_i (g_e)^i \exp\left(-\frac{E_i^*}{T}\right). \tag{40}$$

Differentials along the curve of ionization equilibrium obey the following equations:

$$A_{g_e}\frac{dg_e}{g_e} = A_V\frac{dV}{V} + A_T\frac{dT}{T}, \tag{41}$$

$$A_{g_e} = \langle \delta^2 i\rangle + ZR^-(g_e), \qquad A_T = \frac{3}{2}Z - \frac{\langle \delta i \delta E_i^*\rangle}{T}, \qquad A_V = Z + L\langle \delta(i^2)\delta i\rangle, \tag{42}$$

where

$$L = \frac{E_M}{3T} = \frac{3}{5}\frac{Ry[eV]}{T[eV]r_{iono}[a]}. \tag{43}$$

Again, we express the result in terms of covariances, $\langle \delta a \delta b\rangle = \langle (a - \langle a\rangle)(b - \langle b\rangle)\rangle$, and mean values, which are now being calculated using the modified partition functions. Differentiation of mean values, which is necessary for derivation of the above equation on differentials, is not a complicated problem with the following formula:

$$d\langle f_i\rangle = \left\langle \delta f_i \delta\left(\frac{dp_i}{p_i}\right)\right\rangle, \tag{44}$$

where f_i is a function of the only argument i, for example, iE_i or $i^2 + i$.

The ionization equilibrium can be solved using the old technique, i.e. the Newton-Rapson iterations, defined in Eq.(16).

The full Helmholtz free energy now includes the contribution of the electrostatic field energy as in Eq.(33):

$$F = -T\sum_{i=0}^{i_{max}} N_i \log\left[g_i \frac{eV}{N_i}\left(\frac{MT}{2\pi\hbar^2}\right)^{3/2} \exp\left(-\sum_{j=0}^{i-1}\frac{I_j}{T}\right)\right] + F_e - \sum_{i=0}^{i_{max}} N_i i^2 E_M. \tag{45}$$

With the ion partition functions in Eq.(40) one can rewrite Eq.(45) in the following form:

$$F = -TN_a \log\left[\frac{eV}{N_a}\left(\frac{MT}{2\pi\hbar^2}\right)^{3/2}\right] - TN_a \log S + \Omega_e, \tag{46}$$

where, again, $\Omega_e = F_e - \mu_e N_a \sum i p_i = F_e - \mu_e N_a \langle i\rangle$.

Plasma thermodynamics and Equation-Of-State. While differentiating Eq.(46) with respect to T and V, again we see that the derivatives by g_e from the second and third terms cancel each other: $g_e(\partial \log S/\partial g_e) = \langle i\rangle = Z$, which is evident from $d\log S = \langle d(\log p_i)\rangle$, and $-g_e g_{e1}\mathrm{Fe}'_{3/2}(g_e) = g_{e1}\mathrm{Fe}_{1/2} = Z$. Accordingly, for the internal energy density, $\mathcal{E}$, and for the pressure, P, we find the following general expressions:

$$\mathcal{E} = -\frac{T^2}{V}\left(\frac{\partial}{\partial T}\left(\frac{F}{T}\right)\right) = \mathcal{E}_i + \mathcal{E}_e, \qquad \mathcal{E}_i = \frac{3}{2}Tn_a, \qquad \mathcal{E}_e = n_a\left[\frac{3}{2}TZR^+ + \langle E_i^*\rangle\right], \tag{47}$$

$$P=-\frac{\partial F}{\partial V}=P_i+P_e,\quad P_i=n_aT,\quad P_e=n_a\left[TZR^+-V\langle\frac{\partial E_i^*}{\partial V}\rangle\right], \tag{48}$$

where we assume a general dependence $E_i^*=E_i^*(V)$, such as that in Eq.(38).

In the above equations we add the Madelung corrections to the energy of the electron gas, $\mathcal{E}_e$, and to the electron pressure, P_e, because those corrections are controlled by the electron temperature.

The thermodynamic derivatives can also be expressed in a general form for $E_i^*=E_i^*(V)$ in such a way that one can find the specific heat in an isochoric process, per the unit volume:

$$C_{Ve}=\frac{\partial\mathcal{E}_e}{\partial T}=n_a\left[\frac{\langle\delta^2E_i^*\rangle}{T^2}+\frac{15}{4}ZR^+-\frac{\left(\frac{3}{2}Z-\frac{\langle\delta E_i^*\delta i\rangle}{T}\right)^2}{\langle\delta^2 i\rangle+ZR^-}\right], \tag{49}$$

the temperature derivative of pressure:

$$\frac{\partial P_e}{\partial T}=n_a\left[\frac{5}{2}ZR^+-\left(Z+\frac{V}{T}\langle\delta\frac{\partial E_i^*}{\partial V}\delta i\rangle\right)\frac{\frac{3}{2}Z-\frac{\langle\delta E_i^*\delta i\rangle}{T}}{\langle\delta^2 i\rangle+ZR^-}-\frac{V}{T^2}\langle\delta\frac{\partial E_i^*}{\partial V}\delta E_i^*\rangle\right], \tag{50}$$

as well as the isothermal compressibility:

$$V\frac{\partial P_e}{\partial V}=n_aT\left[-\frac{\left(Z+\frac{V}{T}\langle\delta i\delta\frac{\partial E_i^*}{\partial V}\rangle\right)^2}{\langle\delta^2 i\rangle+ZR^-}+\frac{V^2}{T^2}\langle\delta^2\frac{\partial E_i^*}{\partial V}\rangle-\frac{V^2}{T}\langle\frac{\partial^2E_i^*}{\partial V^2}\rangle\right]. \tag{51}$$

Again, for simplicity in the above equations the contributions due to ion translational motions,

$$C_{Vi}=\frac{3}{2}n_a,\qquad\frac{\partial P_i}{\partial T}=n_a,\qquad V\frac{\partial P_i}{\partial V}=-n_aT, \tag{52}$$

are omitted.

To apply the Madelung theory we calculate the first and the second partial derivatives of the energy levels over volume using Eq.(38):

$$\frac{V}{T}\frac{\partial E_i^*}{\partial V}=Li^2,\qquad\frac{V^2}{T}\frac{\partial^2E_i^*}{\partial V^2}=-\frac{4}{3}Li^2. \tag{53}$$

Eqs.(38,53) allow for specification of all averages and covariances in the expressions for thermodynamic variables and derivatives.

Simulation results. The following table shows the values of Z calculated for Xenon at various electron temperatures (given in electron-volts – the value of $k_B T_e$, where k_B is in eV/K) and heavy particle concentrations, given in number of particles per cm^3. The ”no” columns contain the same values calculated without Coulomb interation taken into account.

Na[1/cm^3]	10^{18}		10^{19}		10^{20}		10^{21}		10^{22}		10^{23}	
Te[eV]	no	Mad	no	Mad	no	Mad	no	Mad	no	Mad	no	Mad
5.	3.4	3.4	2.8	3.0	2.2	2.5	1.3	1.9	0.6	1.4	0.2	2.9
10.	6.3	6.4	5.2	5.4	4.1	4.6	3.0	3.7	1.7	3.2	0.7	3.9
15.	7.3	7.3	6.9	6.9	5.9	6.3	4.4	5.4	2.7	4.6	1.1	4.8
20.	9.2	9.3	7.7	7.9	6.9	7.1	5.6	6.5	3.6	5.7	1.6	5.6
25.	11.8	12.0	9.4	9.7	7.6	8.0	6.5	7.1	4.5	6.5	2.1	6.2
30.	13.8	14.0	11.5	11.9	8.9	9.5	7.1	7.8	5.4	7.0	2.6	6.7
35.	15.7	15.9	13.3	13.7	10.4	11.3	7.8	8.9	6.0	7.6	3.1	7.2
40.	17.2	17.4	14.9	15.3	12.1	12.9	8.7	10.2	6.6	8.3	3.6	7.8
45.	18.1	18.2	16.4	16.7	13.4	14.2	9.9	11.6	7.1	9.2	4.1	8.5
50.	19.0	19.2	17.4	17.7	14.7	15.5	11.1	12.9	7.6	10.3	4.6	9.3
55.	20.5	20.7	18.1	18.4	15.9	16.7	12.3	14.0	8.2	11.4	5.0	10.1
60.	22.0	22.2	19.0	19.3	16.9	17.5	13.3	15.1	8.8	12.4	5.5	11.0
65.	23.3	23.5	20.1	20.6	17.6	18.1	14.3	16.0	9.6	13.4	5.9	11.9
70.	24.4	24.6	21.4	21.9	18.2	18.8	15.2	16.8	10.4	14.3	6.2	12.7
75.	25.3	25.4	22.6	23.0	19.0	19.7	16.1	17.5	11.2	15.1	6.6	13.5
80.	25.7	25.7	23.6	24.0	19.8	20.7	16.8	18.0	12.0	15.8	6.9	14.2
85.	25.9	25.9	24.5	24.8	20.8	21.8	17.4	18.6	12.7	16.5	7.3	14.9
90.	25.9	25.9	25.1	25.3	21.9	22.7	17.9	19.2	13.5	17.0	7.7	15.5
95.	26.0	26.0	25.5	25.6	22.8	23.6	18.5	20.0	14.2	17.5	8.0	16.0
100.	26.1	26.1	25.7	25.8	23.6	24.3	19.1	20.8	14.8	18.0	8.4	16.5
105.	26.2	26.2	25.9	25.9	24.3	24.9	19.7	21.6	15.4	18.4	8.9	16.9
110.	26.4	26.5	25.9	26.0	24.8	25.3	20.5	22.4	16.0	18.9	9.3	17.3
115.	26.9	27.0	26.0	26.0	25.2	25.5	21.3	23.1	16.5	19.5	9.8	17.7
120.	27.5	27.6	26.1	26.1	25.5	25.7	22.0	23.7	17.0	20.1	10.2	18.1
125.	28.3	28.4	26.2	26.3	25.7	25.8	22.7	24.3	17.5	20.7	10.7	18.4

4 Excited states of atoms and ions

To account for excitation of atoms and ions we need not only to involve the distribution over the ionization states, i, but also to quantify the ion distribution over the ground and excited levels.

For simplicity, multiple excitation and autoionization are neglected. We count as the separate excited levels only those for which the principal quantum number, n, of the outermost electron, exceeds that for the atom or ion in its ground state, n_{gr}, by at least one. The excited states, therefore, can be enumerated using two indexes, namely, the ion charge, $i = 0, 1, 2...$, and the principal quantum number $n(i) = n_{gr}(i), n_{gr}(i) + 1, ...$

The partition function, p_i, describing the ion distribution over charge state i (recall that $\sum_i p_i = 1$), is now split into smaller populations, $p_{i,n}$, with each relating to a particular excitation level, n. Note that:

$$\sum_n p_{i,n} = p_i, \qquad \sum \frac{p_{i,n}}{p_i} = 1. \tag{54}$$

Which is why the statistical weights, $w_{i,n}$, and, hence, the statistical sum and the partition functions become more complex:

$$w_{i,n} = g_{i,n} \cdot g_e^i \exp\left(-\frac{E^*_{i,n}}{T}\right), \qquad S = \sum_{i=0}^{i_{max}} \sum_{n=n_{gr}}^{\infty} w_{i,n}, \qquad p_{i,n} = \frac{w_{i,n}}{S}, \tag{55}$$

where $g_{i,n}$ stands for the excited level degeneracy, and the energy of the excited state,

$$E^*_{i,n} = E^*_i + E^{exc}_{i,n}, \tag{56}$$

now includes the contribution from the ionization energy, the excitation energy and, generally speaking, the contribution from the electrostatic energy.

We take the values of the excitation energy, $E^{exc}_{i,n}$, from several sources: [27], [26], [28], [29]. When some values are missing in those sources, we calculate them using the following formula:

$$E^{exc}_{i,n} = I_i - Ry\frac{(i+1)^2}{n^2}. \tag{57}$$

For the degeneracies of excited levels we assume $g_{i,n} = 2n^2$. To calculate the ground level degeneracy we use the electron configurations from [30]. Some of the values of degeneracies have been modified to match the data from [8].

Up to this point mean values and covariances were being calculated over $i_{max}+1$ possible values of i, but now i is not the only variable that the energy levels depend on. Accounting for excitation levels in the way described above leads to energy levels being a function of i and n. This only increases the number of terms in the statistical sum, but does not change anything in principle. To obtain the thermodynamic variables and the thermodynamic functions we can just replace the mean values over i with mean values over i and n in the Eqs.(47), (48), (49), (50), (51) and substitute the new expression, as in Eq.(57), for energy levels.

To calculate the covariances over i and n we use Eq.(133).

The following table is intended to compare the reference data with the values of excitation energies obtained using Eq.(57). Here for each charge state of nitrogen ion, i, and principal quantum number of the excited electron, n, we have the value given by the formula, which does not depend on the orbital momentum of the excited electron, l, or the reference data (Table is removed to because its style is outdated).

5 Pressure ionization

We account for pressure ionization via energy levels correction as follows:

$$\Delta E_{i,n,l} = f(i,n,l)(r_{iono}[a])^{-3\theta}, \qquad E_{i,n,l} = E_i^* + E_x, \qquad E_x = E_{i,n}^{exc} + \Delta E_{i,n,l}, \tag{58}$$

where the function f and the constant value θ must be adjusted according to the particular model being used. Now we distingish quantum states also by the azimuthal quantum number, l, because the effect of pressure ionization depends on the orbital type.

Besides the continuum lowering due to Coulomb interactions, the effect of pressure ionization raises the excitation levels. When the excitation energy exceeds the energy at continuum, the corresponding excitation level vanishes. Application of the Madelung theory results in the condition for energy level elimination as follows:

$$E_{i,n}^{exc} + \Delta E_{i,n,l} > I_i - (2i+1)E_M. \tag{59}$$

We can still use the Eqs.(47), (48), (49), (50), (51), where mean values and covariance should now be calculated over all possible triplets (i,n,l).

Substitution of the partial derivatives of E with respect to V as follows:

$$-V\frac{\partial(\Delta E_{i,n,l})}{\partial V} = \theta \cdot f(i,n,l)(r_{iono}[a])^{-3\theta} = \theta \cdot \Delta E_{i,n,l}, \tag{60}$$

$$V^2\frac{\partial^2(\Delta E)}{\partial V^2} = \theta(\theta+1) \cdot f(i,n,l)(r_{iono}[a])^{-3\theta} = \theta(\theta+1) \cdot \Delta E_{i,n,l}, \tag{61}$$

gives us the following formulas for thermodynamic derivatives:

$$P = n_a\left[T(1+ZR^+ - L\langle i^2\rangle) + \theta\langle\Delta E\rangle\right], \tag{62}$$

$$\mathcal{E} = n_a\left[\frac{3}{2}T(1+ZR^+) + \langle E\rangle\right], \tag{63}$$

$$C_V = n_a\left[\frac{3}{2} + \frac{\langle\delta^2 E\rangle}{T^2} + \frac{15}{4}ZR^+ - \frac{(\frac{3}{2}Z - \frac{\langle\delta i\delta E\rangle}{T})^2}{\langle\delta^2 i\rangle + ZR^-}\right], \tag{64}$$

$$\begin{aligned}\frac{\partial P}{\partial T} &= n_a\Bigg[1 + \frac{5}{2}ZR^+ - \left(Z + L\langle\delta i\delta(i^2)\rangle - \theta\frac{1}{T}\langle\delta i\delta\Delta E\rangle\right)\frac{\frac{3}{2}Z - \frac{\langle\delta i\delta E\rangle}{T}}{\langle\delta^2 i\rangle + ZR^-} - \\ &- L\frac{\langle\delta E\delta(i^2)\rangle}{T} + \theta\frac{\langle\delta E\delta\Delta E\rangle}{T^2}\Bigg],\end{aligned} \tag{65}$$

$$\begin{aligned}V\frac{\partial P}{\partial V} &= n_a T\Bigg[-1 - \frac{(Z + \langle Li^2 - \theta\frac{\Delta E}{T}\rangle)^2}{\langle\delta^2 i\rangle + ZR^-} + \frac{4}{3}L\langle i^2\rangle - \theta(\theta+1)\frac{\langle\Delta E\rangle}{T} + \\ &+ \left\langle\delta^2\left(Li^2 - \theta\frac{\Delta E}{T}\right)\right\rangle\Bigg].\end{aligned} \tag{66}$$

To calculate the covariances over i, n and l we use Eq.(133), giving:

$$\langle\delta^2 E\rangle = \langle\langle\delta^2 E_x\rangle_{n,l}\rangle_i + \langle\delta^2\langle E\rangle_{n,l}\rangle_i, \tag{67}$$

$$\langle\delta E\delta i\rangle = \langle i\langle E\rangle_{n,l}\rangle_i - \langle i\rangle_i\langle E\rangle, \tag{68}$$

$$\frac{V}{T}\langle\delta i\delta\frac{\partial E}{\partial V}\rangle = \frac{V}{T}\langle\delta i\delta\frac{\partial E_i^*}{\partial V}\rangle_i + \langle\delta i\delta(\frac{V}{T}\langle\frac{\partial E_x}{\partial V}\rangle_{n,l})\rangle_i, \tag{69}$$

$$\frac{V^2}{T^2}\langle\delta^2\frac{\partial E}{\partial V}\rangle = \langle\frac{1}{T^2}V^2\langle\delta^2\frac{\partial E_x}{\partial V}\rangle_{n,l}\rangle_i + \langle\delta^2(\frac{V}{T}\frac{\partial E_i^*}{\partial V} + \frac{V}{T}\langle\frac{\partial E_x}{\partial V}\rangle_{n,l})\rangle_i, \tag{70}$$

$$-\frac{V}{T^2}\langle\delta\frac{\partial E}{\partial V}\delta E\rangle = -\frac{V}{T^2}\langle\delta\frac{\partial E_i^*}{\partial V}\delta\langle E\rangle_{n,l}\rangle_i - \frac{V}{T^2}\langle\langle\delta E_x\delta\frac{\partial E_x}{\partial V}\rangle_{n,l}\rangle_i - \frac{V}{T^2}\langle\delta\langle\frac{\partial E_x}{\partial V}\rangle_{n,l}\delta\langle E\rangle_{n,l}\rangle_i. \tag{71}$$

PART 2. RADIATION TARNSPORT IN DENSE PLASMAS

6 Multi-group diffusion: governing equations and general ralationships

Governing equation to describe the radiation transport in the multigrop diffusion approximation may be written as the partial differential equation for the spectral energy density, E_ε, which is related to the unit ov volume and the unit interval of the photon energy, ε. The energy is assumed to be integrated over the solid angle of directions of the photon propagation. Once the spectral energy is integrated density over photon energies, the total radiation energy density is obtained:

$$E = \int_0^\infty E_\varepsilon d\varepsilon. \tag{72}$$

The governing equation for the spectral energy density is as follows:

$$\frac{\partial E_\varepsilon}{\partial t} + \nabla\cdot(\mathbf{u}E_\varepsilon) - (\gamma_R - 1)(\nabla\cdot\mathbf{u})\varepsilon\frac{\partial E_\varepsilon}{\partial \varepsilon} = \text{diffusion} + \text{emission} - \text{absorption}. \tag{73}$$

The second and third terms in the left hand side of Eq.(73) express the time evolution of the spectral energy density resulting from: (1) the radiation advection and comression with the background, which moves with the velocity, $\mathbf{u}$; as well as (2) the photon systematic blue (red) shift in the convergent (divergent) motions, which is analogous to the first order Fermi acceleration of chanrged particles in a moving plasma with the frozen in magnetic field. Herwith $\gamma_R = 4/3$ is the adiabat index of a relativistic (photon) gas. The processes described by the symbolic terms in the right hand side of Eq.(73) are described below.

A set of multi-group equations may be indroduced when we choose a set of frequency groups. Here we enumerate groups with the index, $g = 1, G$. The interval of the photon energies, relating to the gth group is denoted as $[\varepsilon_{g-1/2}, \varepsilon_{g+1/2}]$. The discrete set of unknowns, E_g, is introduced in terms of the integrals of the spectral energy density of the frequency group interval:

$$E_g = \int_{\varepsilon_{g-1/2}}^{\varepsilon_{g+1/2}} E_\varepsilon d\varepsilon. \tag{74}$$

Note that according to Eqs.(72,74)

$$E = \sum_g E_g. \tag{75}$$

Although some of the formulae below are not sensitive to the choice of the group set, here we specify the boundaries of the frequency groups to be such that *the frequency logarithm* is equally spaced (rather than the frequency itself):

$$\log(\varepsilon_{g+1/2}) - \log(\varepsilon_{g-1/2}) = \Delta(\log\varepsilon) = const. \tag{76}$$

Note that as long as the number of groups, G, tends to infinity, the ratio $E_g/\Delta(\log\varepsilon)$ tends to the local value of $\varepsilon E_\varepsilon$, rather than to E_ε. Therefore, the grequency integrals on the equally spaced logarithmic frequency grid allow us to approximate not a spectral energy density, but its product by the photon energy:

$$\frac{E_g}{\Delta(\log\varepsilon)} \approx \varepsilon E_\varepsilon. \tag{77}$$

Now we can integrate Eq.(73) to arrive at the desired set of the multigroup equations:

$$\begin{aligned}\frac{\partial E_q}{\partial t} &+ \nabla\cdot(\mathbf{u}E_g) + (\gamma_R - 1)(\nabla\cdot\mathbf{u})E_g + \\ &+ [-(\gamma_R - 1)(\nabla\cdot\mathbf{u})]\left[\varepsilon_{g+1/2}E_\varepsilon(\varepsilon_{g+1/2}) - \varepsilon_{g-1/2}E_\varepsilon(\varepsilon_{g-1/2})\right] = \\ &= \int_{\varepsilon_{g-1/2}}^{\varepsilon_{g+1/2}} (\text{diffusion} + \text{emission} - \text{absorption})d\varepsilon. \end{aligned} \tag{78}$$

If the number of frequency groups, G is sufficiently large, we employ the approximation as in Eq.(77), which allows us to close Eq.(78) in the following form:

$$\frac{\partial E_q}{\partial t} \; + \; \nabla\cdot(\mathbf{u}E_g)+(\gamma_R-1)(\nabla\cdot\mathbf{u})E_g+\frac{-(\gamma_R-1)(\nabla\cdot\mathbf{u})}{\Delta(\log\varepsilon)}\left[E_{g+1/2}-E_{g-1/2})\right]=$$
$$= \int_{\varepsilon_{g-1/2}}^{\varepsilon_{g+1/2}}(\text{diffusion}+\text{emission}-\text{absorption})d\varepsilon. \qquad (79)$$

where the values $E_{g\pm1/2}$ should be interpolated from the mesh-centered values E_g towards the frequency values corresponding to the inter-group boundary.

Note that we arrived to difference-differential equation, with the left-hand side including: (1) the conservative advection of the radiation energy density with the velocity $\mathbf{u}$; the work done by the radiation pressure $P_g=(\gamma_R-1)E_g$; (3) and, as a new element, a linear conservative advection with respect to the log-frequency coordinate. The flux-to-control-volume ratio for the latter effect equals

$$F_{g-1/2}=-(\gamma_R-1)(\nabla\cdot\mathbf{u})E_{g-1/2}/\Delta(\log\varepsilon).$$

Eq.(79) provides us a ready numerical scheme to solve this advection numerically. The recipi to construct a numerical flux for a linear advection equation are well-known. Specifically, we apply a limited reconstruction procedure, with the 'superbee' limiter function,

$$L(a,b)=\frac{1}{2}[\mathrm{sign}(a)+\mathrm{sign}(b)]\min(\max(|a|,|b|),2|a|,2|b|),$$

to obtain left and right interpolated values,

$$E^{(L)}_{g-1/2}=E_{g-1}+\frac{1}{2}L(E_g-E_{g-1},E_{g-1}-E_{g-2}),$$

$$E^{(R)}_{g-1/2} = E_g - \frac{1}{2}L(E_{g+1} - E_g, E_g - E_{g-1})$$

. With these interpolated values the upwinded numerical flux is constructed as follows:

$$\begin{aligned} F_{g-1/2} &= -(\gamma_R - 1)(\nabla \cdot \mathbf{u})E^{(R)}_{g-1/2}/\Delta(\log\varepsilon), \qquad (\nabla \cdot \mathbf{u}) \geq 0, \\ F_{g-1/2} &= -(\gamma_R - 1)(\nabla \cdot \mathbf{u})E^{(L)}_{g-1/2}/\Delta(\log\varepsilon), \qquad (\nabla \cdot \mathbf{u}) \leq 0 \end{aligned} \tag{80}$$

Eqs.(79) with the numerical fluxes as in Eq.(80) may be further discretized using the control volume methods and solved numerically, assuming the right hand side to be zero, as the coupled element of the system of hydrodynamic (or magneto-hydro-dynamic) equations involving the ratiation pressure contributions. Note, that suming up Eqs.(79) we obtain the equation of the gray radiation diffusion:

$$\frac{\partial E}{\partial t} + \nabla\cdot(\mathbf{u}E) + (\gamma_R - 1)(\nabla\cdot\mathbf{u})E = \int_0^\infty (\text{diffusion} + \text{emission} - \text{absorption})d\varepsilon. \tag{81}$$

If, again, we assume the right hand side of Eq.(81) to be zero, then only Eq.(81) is two-way coupled to the system of equation of the plasma motion, since in these equations the radiation effects the plasma motion only via the total radiation pressure:

$$P = (\gamma_R - 1)E. \tag{82}$$

On advancing the solution of this coupled system through the time step, the numerical solution of each of Eqs.(79) may be also advanced through the time step, Δt, as long as $\mathbf{u}$ is known. Depending on the value of $\Delta(\log\varepsilon)$ one may prefer to treat the advection over frequency as: (1) an extra flux (the control volume in this case is treated as the four-dimentional rectangular box $\Delta x * \Delta y * \Delta z * \Delta(\log\varepsilon)$); or (2) an extra advance operator, which can be split out and hanled separately. In the second case the second order of accuracy, $o((\Delta t)^2)$, may be achieved with the choice of the numerical flux as follows:

$$\begin{aligned}
\Delta t F_{g-1/2} &= -\mathrm{CFL}\left[E_g - \frac{1-\mathrm{CFL}}{2} L(E_{g+1}-E_g, E_g - E_{g-1})\right], \qquad (\nabla\cdot\mathbf{u}) \geq 0,\\
\Delta t F_{g-1/2} &= \mathrm{CFL}\left[E_{g-1} + \frac{1-\mathrm{CFL}}{2} L(E_g - E_{g-1}, E_{g-1} - E_{g-2})\right], \qquad (\nabla\cdot\mathbf{u}) \leq 0, \qquad (83)
\end{aligned}$$

where

$$\mathrm{CFL} = \frac{(\gamma_R - 1)\Delta t}{\Delta(\log\varepsilon)} |\nabla\cdot\mathbf{u}| \geq 0 \tag{84}$$

is the Courant-Friedrichs-Levi number.

7 Absroption, emission and stimulated emission

An account of the stimuated emission is not less important in the context of the multi-group radiation diffusion than the use of the locat termodynamic equailibrium assumption. As long as the stimulated emission is not often discussed in books regarding the diffisive radiation transport, the code developer may meet a problem while bridging from the absorption coefficient, a_ε, which is calculated from single-photon diagrams of Quantum ElectroDynamics (QED), describing an absorption of a single photon, to the absorption coefficient which is to be used in the radiation trasport simulations. Below we follow [1], in which this subject is presented quite transparently.

Consider a part of the radiation spectrum, of a small width of $\Delta\varepsilon$, about the photon energy, ε, which is resonant with some bound-bound transition, that is

$$\varepsilon = \mathcal{E}_E - \mathcal{E}_A, \tag{85}$$

where $\mathcal{E}_A$ and $\mathcal{E}_E$ are some energy states of an atom (or ion, below we refer the system in these states to as an Emitter or an Absorber). For the sake of simplicity, assume for a while that the degeneracy (multiplicity) is equal to one for both upper and lower level:

$$g_E = 1, \qquad g_A = 1,$$

the use of the same denotation for the degeneracy as for the group index should not confuse the reader.

Assume there is no photon in the initial state. The only radiation process which can occur in this case is the spontaneous emission. Introduce the probability, $dw_p/d\mathbf{o}$, for the spontaneous emission from a single emitter, into the element of a solid andgle, with a given polarization of the photon, p, per a unit of time. The total spontaneous emission from the unit of volume is, hence,

$$N_E \frac{dw_p}{d\mathbf{o}} d\mathbf{o},$$

where $N_{E,A}$ are the abundancies of the emitters and the absorbers correspondingly. The contribution from the spontaneous emission to Eq.(74) should have an extra factor of 4π (due to the integration over the photon directions) times 2 (summation by polarizations) times ε (an emitted energy per a photon) divided by $\Delta\varepsilon$.

Now assume that there are N_p photons in the considered unit volume of plasma, which are in the same as the emitted photon. The rules to express the probability of stimulated emission and absorption may be found in any textbook on QED, particularly, we follow [3]. The probability of a total emission (spontaneous plus stimilated) equals

$$(1 + N_p) \frac{dw_p}{d\mathbf{o}}$$

while the number of the absorbed photons from the same photon state, per an absorber, equals

$$(1 + N_p)\frac{dw_p}{d\mathbf{o}}$$

On integrating the total absorbtion and emission by $d\mathbf{o}$ and suming the result up by polarizations, we arrive at the following expression for the emission and absoption terms in Eq.(74):

$$\text{emission} - \text{absortion} = \frac{8\pi\varepsilon}{\Delta\varepsilon}\frac{dw_p}{d\mathbf{o}}(N_E(1 + N_p) - N_A N_p)$$

Now we may abandon the assumption about non-degeneracy of the emeitter and absorber states. The extra freedom of the ssytem in its *final* state to occupy any of g_f final states simply multiplies the transition probability by a factor of g_f. Properly applying the factors $g_f = g_E$ and $g_f = g_A$, we find:

$$\text{emission} - \text{absortion} = \frac{8\pi\varepsilon}{\Delta\varepsilon}\frac{dw_p}{d\mathbf{o}}(N_E g_A(1 + N_p) - N_A g_E N_p).$$

The population of the photon state, N_p, may be related to the spectral energy density. A radiation energy in the unit volume within the interval of the photon energies, $d\varepsilon$, may be written as $E_\varepsilon d\varepsilon$. The same energy may be obtained if we multiply $2N_p\varepsilon$ (the factor of two accounts for two polarizations of the photon) by the number of photon states within $d\varepsilon$. In the unit volume the number of photon states per the pase volume of $dk_x dk_y dk_z$ equals $dk_x dk_y dk_z/(2\pi)^3$, with k_x, k_y, k_z being the three components of the wave vector. The number of photon states per the interval of dk is, hence, $4\pi k^2 dk/(2\pi)^3 = 4\pi\varepsilon^2 d\varepsilon/(hc)^3$. We find:

$$E_\varepsilon = \frac{8\pi N_p \varepsilon^3}{h^3 c^3},$$

and

$$\text{emission} - \text{absorption} = ca_\varepsilon \left[\frac{N_E g_A}{N_A g_E} \left(\frac{8\pi\varepsilon^3}{h^3c^3} + E_\varepsilon \right) - E_\varepsilon \right]. \quad (86)$$

where the absorption coefficient is introduced (the radiation energy dissipation per a unit of length), which is related to the emission probability as follows:

$$a_\varepsilon = \frac{h^3c^2 N_A g_E}{8\pi\varepsilon^2} \frac{dw_p}{d\mathbf{o}\Delta\varepsilon}. \quad (87)$$

Under the condition of a local thermodynamic equilibrium, the partition function of atoms and ions in different charge and energy states is governed by the Boltzmann statistics, so that the abundance of each excited level is proportianal to its mutiplicity and to the Boltzbann factor, $\exp(-E/(k_BT))$. Therefore, under these circumstances, using Eq.(85), we find

$$N_{E,A} \propto g_{E,A} \exp[-E_{E,A}/(k_BT)], \qquad \frac{N_E g_A}{N_A g_E} = \exp\left[\frac{E_A - E_E}{k_BT}\right] = \exp[-\varepsilon/(k_BT)] \quad (88)$$

and

$$\text{emission} - \text{absorption} = ca'_\varepsilon \left(\frac{8\pi}{h^3c^3} \frac{\varepsilon^3}{\exp[\varepsilon/(k_BT)] - 1} - E_\varepsilon \right). \quad (89)$$

where the effective absorption coefficient, a'_ε, is indroduced, which is corrected to account for stimulated emission:

$$a'_\varepsilon = a_\varepsilon \left(1 - \exp\left[-\frac{\varepsilon}{k_BT} \right] \right) \quad (90)$$

Following [1] we can make now two important conclusions. First, the assoption coefficient to be used in simulationg the radiation transport should be corrected for the stimulated emission, by means of applying a simple correction factor. Second, the spontaneous emission from a plasma with the equilibrium distribution over the energy states is related to the corrected absorption coefficient in sunch a way that their ratio,

$$E_\varepsilon^{(Pl)}(T,\varepsilon) = \frac{8\pi}{h^3c^3}\frac{\varepsilon^3}{\exp[\varepsilon/(k_BT)]-1}, \tag{91}$$

is the spectral energy density distribution of the black body radiation (the Planckian). We will also apply it in a normalized form as follows:

$$E_\varepsilon^{(Pl)}(T,\varepsilon) = \alpha T^4\frac{15}{\pi^4}\frac{x^3}{\exp(x)-1}\frac{1}{k_BT}, \qquad \alpha=\frac{8\pi^5k_B^4}{15h^3c^3}, \qquad x=\frac{\varepsilon}{k_BT}. \tag{92}$$

The spectral function in (91) is normalized by a unity:

$$\int_0^\infty \frac{15}{\pi^4}\frac{x^3}{\exp(x)-1}\frac{d\varepsilon}{k_BT} = \frac{15}{\pi^4}\int_0^\infty\frac{x^3dx}{\exp(x)-1}=1,$$

about the intregrals like this see §58 in [2]. Therefore the total energy density in the Planck spectrum equals αT^4, as it should.

8 Bound-bound absroption

TBC

9 Photoionization and photorecombination: effect of the Fermi statistics.

The formula for the photoionization cross-section from atom (ion) in the charge state, ζ, and with the electron configuration, i, reads:

$$\sigma^{ion}_{\zeta,i\to\zeta+1,j}=\sigma_0\frac{w_\eta n_\eta}{(\zeta+1)^2}\left(\frac{E_{ij}}{h\nu}\right)^3. \tag{93}$$

Here

$$\sigma_0=\frac{64\pi}{3\sqrt{3}}\alpha a_0^2\approx 7.9\cdot 10^{-22}[\mathrm{m}^2], \tag{94}$$

is the near-threshold ($E_{ij}=h\nu$) semi-classical cross-section of the photoionization of the hydrogen atom from the ground state ($\zeta=0$, $w_\eta=1$, $n_\eta=1$), which may be found in [1]

$$\alpha=\frac{e^2}{\hbar c}\approx 1/137.04 \tag{95}$$

is a fine structure constant, and

$$a_0=\frac{\hbar^2}{m_e e^2}\approx 0.5\cdot 10^{-10}[\mathrm{m}] \tag{96}$$

is the Bohr radius. Eqs.(95,96) are only valid in CGSE system of units, however, with the known numerical values for them all the other formulae become insensitive to the choice of units. $h\nu$ is the energy of the photon, which is absorbed in the course of the photoionization. It should exceed the transition energy,

$$h\nu\geq E_{ij}. \tag{97}$$

The transition energy equals:

$$E_{ij}=I_\zeta-E_{\zeta,i}+E_{\zeta+1,j}, \tag{98}$$

where the excitation energy, $E_{\zeta,i}\geq 0$ is introduced, which is the non-negative difference between the energy of the given electron configuration with respect to the ground state energy for the atom (ion) with the charge number equal to ζ.

We consider only the transition to states j, such that the electron confiruration in these states are obtained from the initial configuration, i, by removing a single electron from ηth electron orbit. w_η and n_η in Eq.(93) mean the number of electron on this orbit and its principal quantum number correspondingly.

However, if the photoionization occurs in a plasma and the effects of the Fermi- statistics in this plasma are not negligible, Eq.(93) should be revisited. Recall, that the probabilities of the photon absorption processes in Quantum ElectroDynamics (QED) are calculated as follows (see [3]): (1) first, the matrix element of perturbation is calculated using the wave functions of bound and free electrons in initial and final states; (2) and then the matrix element should be integrated over all possible value of the free electron momentum, $\mathbf{p}$, as long as there is a free electron in the final state. In this integration the number of free electron states per the unit of space volume is introduced as follows:

$$N_{\mathbf{p}} = 2\frac{dV d^3\mathbf{p}}{(2\pi\hbar)^3}. \tag{99}$$

To account for the Fermi statistics effect on the electron gas we should note that: (1) the calculation of the matrix element does not change, because in any case the wave function for a free electron is a plane wave; (2) however, the way to calculate the number of states of free electrons change specifically. Specifically, we find that among the states as in Eq.(99) some places are already occupied, with the occupation numbers equal to $1/(\exp[(\varepsilon_e - \mu)/(k_B T)] + 1)$ (see [2]). Here μ is a chemical potential of a free electron gas and $\varepsilon(\mathbf{p})$ is its non-relativistic kinetic energy of the electron. With this account, the actual number of free electron states is

$$N^{corr}_{\mathbf{p}} = 2\frac{dV d^3\mathbf{p}_e}{(2\pi\hbar)^3}\left(1 - \frac{1}{\exp[\frac{\varepsilon_e-\mu}{k_BT}]+1}\right) = N_{\mathbf{p}}\frac{\exp[\frac{\varepsilon_e-\mu}{k_BT}]}{\exp[\frac{\varepsilon_e-\mu}{k_BT}]+1}. \tag{100}$$

Therefore, the corrected cross-section becomes:

$$\sigma^{corr,ion}_{\zeta,i\to\zeta+1,j} = \sigma^{ion}_{\zeta,i\to\zeta+1,j}\frac{\exp[\frac{\varepsilon_e-\mu}{k_BT}]}{\exp[\frac{\varepsilon_e-\mu}{k_BT}]+1}. \tag{101}$$

The electron energy here is related to the photon energy, $h\nu$, via the conservation law:

$$\varepsilon_e = h\nu - E_{ij} \tag{102}$$

The contribution from the bound-free transition to the absorption coefficient (not yet corrected for the stimulated emission) may be now written in terms of the corrected cross-section:

$$\kappa^{bf}_{\nu} = \sigma_0 \sum_{\zeta,i,j} N_{\zeta,i}\frac{w_\eta n_\eta}{(\zeta+1)^2}\left(\frac{E_{ij}}{h\nu}\right)^3 \frac{\exp[\frac{h\nu-E_{ij}-\mu}{k_BT}]}{\exp[\frac{h\nu-E_{ij}-\mu}{k_BT}]+1}, \tag{103}$$

where $N_{\zeta,i}$ is the concentration of ions with the given electron configuration.

Now, the cross-section of a photorecombination of an electron on a collision with the ion in the state, $\zeta+1, j$ is related to the cross-section as in Eq.(93) in the following way:

$$\sigma^{rec}_{\zeta+1,j\to\zeta,i} = \frac{g_{\zeta,i}}{g_{\zeta+1.j}}\frac{(h\nu)^2}{2m_ec^2}\frac{1}{\varepsilon_e}\sigma^{ion}_{\zeta,i\to\zeta+1,j} = \frac{g_{\zeta,i}p_p^2}{g_{\zeta+1.j}p_e^2}\sigma^{ion}_{\zeta,i\to\zeta+1,j}, \tag{104}$$

where $p_p = \varepsilon_p/c$ and $\varepsilon_p = h\nu$ are the momentum and the energy of a photon correspondingly.

The rule as in Eq.(104) expresses the so-called *cross-invariance* property of all QED processes, which claims the possibility to relate the probability of the direct and inverse processes if we accordingly account for the weights of the initial and final states. This property comes from the point that the matrix elements for the direct and reverse processes are exactly the same, the difference in the cross-sesctions occurs when the matrix element is integrated over the final states, which are different, because the final and initial states in the cross-invariant processes are changed by places. We emphasize, that the relationship as in Eq.(104) holds with the *uncorrected* cross-section $\sigma^{ion}_{\zeta,i\to\zeta+1,j}$, because it is based on the *uncorrected* statistical weight of free electron as in Eq.(99), which results in the multiplier, p_e^2, in the denominator of (104). If we account the correcting factors both in $\sigma^{ion}_{\zeta,i\to\zeta+1,j}$ and in (99) these factors cancel each other and the expression for $\sigma^{rec}_{\zeta+1,j\to\zeta,i}$ keeps unchanged.

Integrate $(p_e/m_e)\sigma^{rec}_{\zeta+1,j\to\zeta,i}$ with the distribution function, $f_{\mathbf{p}}$, of an ideal Fermi gas of electrons,

$$f_{\mathbf{p}} d^3\mathbf{p}_e = \frac{2}{\exp[\frac{\varepsilon_e-\mu}{k_BT}]+1}\frac{d^3\mathbf{p}_e}{(2\pi\hbar)^3}, \tag{105}$$

and represent the result of integration by the electron momentum directions in the following form.

$$\int \frac{8\pi}{c^2h^3}\sigma_0\frac{g_{\zeta,i}}{g_{\zeta+1.j}}\frac{w_\eta n_\eta}{(\zeta+1)^2}\frac{1}{h\nu}\frac{E_{ij}^3 d\varepsilon_e}{\exp[\frac{\varepsilon_e-\mu}{k_BT}]+1}. \tag{106}$$

Now discuss the physical meaning of the integrand as in (106). In accordance with Eq.(102), $d\varepsilon_e = d\varepsilon_p = d(h\nu)$. Hence the integrand in (106) may be interpreted as the probability of emission, per a unit time interval, from an ion in the given state, with the emitted photon being within the energy interval $d(h\nu) = d(E_{ij}+\varepsilon_e)$. Once been multiplied by $(h\nu)$, this becomes the emitted energy and once multipled by the emitters density, $N_{\zeta+1,j}$, it becomes the volumetric emissivity due to recombination, per a unity interval of the photon energies, $\mathcal{E}_\varepsilon$:

$$\mathcal{E}^{bf}_\varepsilon = \frac{8\pi}{c^2h^3}\sigma_0 \sum_{\zeta,i,j} N_{\zeta+1,j}\frac{g_{\zeta,i}}{g_{\zeta+1.j}}\frac{w_\eta n_\eta}{(\zeta+1)^2}\frac{E^3_{ij}}{\exp[\frac{h\nu-E_{ij}-\mu}{k_BT}]+1}. \quad (107)$$

Discuss briefly the interaction of plasma with the euqilibrium black-body radiation. The absroption of the black-body radiation (again, our Eq.(103) is not yet corrected for a stimulated emission) balances the emissivity, if the following condition is satisfied:

$$\mathcal{E}^{bf}_\varepsilon = \frac{8\pi(h\nu)^3\exp[-(h\nu)/(k_BT)]}{c^2h^3}\kappa^{bf}. \quad (108)$$

Comparing this with Eqs.(103,107), we find that the condition is satisfied, if:

$$\frac{g_{\zeta,i}N_{\zeta+1,j}}{g_{\zeta+1.j}N_{\zeta.i}} = \exp[\frac{-E_{ij}-\mu}{k_BT}] = \exp[\frac{-I_\zeta+E_{\zeta,i}-E_{\zeta+1,j}-\mu}{k_BT}]. \quad (109)$$

This is exactly the expression relating the populations of the electron states in ions, which are in a thermodynamic equilibrium with a Fermi gas of electrons (see Part 1).

10 Free-Free opacity

The analisys of free-free absorption is mostly based on the same considerations as that for bound-free absorption. The distinction is in the use of the Fermi-Dirac distribution function not only for a free electron in the final state (what we did in the previous section) but also for the electron in the initial state.

The emission from an electron having the velocity, v_E (again the subscript E means "emitter", subscript A means "absorber"), is given by Eq.(5.11) from [**?**]:

$$\frac{dE_\varepsilon}{dt} = \frac{32\pi^2 e^6}{3\sqrt{3}c^3 h m_e^2 v_E} N_e \sum_\zeta N_\zeta \zeta^2 G_f f \tag{110}$$

11 Spectral temperature and group spectral temperatures

In [2] it was mentioned that for any known spectral energy distribution , E_ε at any value of ε, the local spectral temperature, $T^{Spectral}(E_\varepsilon(\varepsilon), \varepsilon)$ may be introduced, such that the spectral energy density $E_\varepsilon(\varepsilon)$ is locally equal to the Planckian spectral energy density at the temperature $T^{Spectral}$:

$$E_\varepsilon(\varepsilon) = E_\varepsilon^{(Pl)}(T^{Spectral}, \varepsilon). \tag{111}$$

Of course, if the radiation spectrum differs from that for equilibrium black-body radiation, the values of $T^{Spectral}$ are different at different energies, generally speaking.

In other words, for non-equilibrium spectrum, the distribution of spectral temperature may be used instead of the spectral energy density, as the spctrum characteristics. The relationship between the spectral temperature and spectrum energy density is one-to-one mapping. For a given spectral temperature, the spectral energy density is given by Eq.(91). For a given spectral energy density the spectral temperature amy be found using Eq.(63.26) from [2] which in our denotations may be written as follows:

$$T^{Spectral} = \frac{\varepsilon/k_B}{\log\left(1 + \frac{8\pi}{h^3c^3}\frac{\varepsilon^3}{E_\varepsilon}\right)} \tag{112}$$

Now we introduce the discrete analog of a spectral temperature. Specifically, we introduce *a group temperature*, T_g, such that the spectral energy of a black-body radiation, once integrated over the photon energy within a given group, would equal the given value of E_g:

$$E_g(T_g) = \int_{\varepsilon_{g-1/2}}^{\varepsilon_{g+1/2}} E_\varepsilon^{(Pl)}(T_g,\varepsilon)d\varepsilon = \alpha T_g^4 \frac{15}{\pi^4}\int_{\varepsilon_{g-1/2}/(k_BT_g)}^{\varepsilon_{g+1/2}/(k_BT_g)} \frac{x^3dx}{\exp(x)-1}. \tag{113}$$

We will also need an expression for the group specific heat of the radiation, per a unit of volume:

$$C_g = \frac{dE_g}{dT_g} = 4\alpha T_g^3 \frac{15}{4\pi^4}\int_{\varepsilon_{g-1/2}/(k_BT_g)}^{\varepsilon_{g+1/2}/(k_BT_g)} \frac{x^3\exp(x)dx}{[\exp(x)-1]^2}. \tag{114}$$

The procedure which allows us to obtain the radiation energy density per group and radiation specific heat per group from the given group temperature is straightforward. However, the inverse procedure is not that simple, because Eq.(112) now only holds as an approximate one:

$$T^g \approx \frac{\sqrt{\varepsilon_{g-1/2}\varepsilon_{g+1/2}}/k_B}{\log\left(1+\frac{\alpha\varepsilon^2_{g-1/2}\varepsilon^2_{g+1/2}}{k_B^4}\frac{15}{\pi^4}\frac{\Delta(\log\varepsilon)}{E_g}\right)} \tag{115}$$

To satisfy Eq.(113), one needs to improve the accuracy using Newton-Rapson procedure:

$$T_g^{n+1} = T_g^n + (E_g - E_g(T_g^n))/C_g(T_g^n). \tag{116}$$

TBC

12 Averaging opacities

TBC

13 Reduction of the multi-group diffusion equations to symmetric system of N temperature diffusion equations

TBC

14 Appendix A: The Fermi function calculation approach

For $g_e \geq 1$, $\nu > -1$ the Fermi function may be developed into convergent power series (see Eq.(5) from [5]):

$$\mathrm{Fe}_\nu(g_e) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^{\nu+1}(g_e)^n}. \tag{117}$$

The Taylor series in powers of $-\log(g_e)$ (see Eq.(6) from [5]):

$$\mathrm{Fe}_\nu(g_e) = \sum_{i=0}^{\infty} \frac{(1 - 2^{i-\nu})\zeta(\nu + 1 - i)}{i!}(-\log(g_e))^i. \tag{118}$$

is only used for $g_e \in [e^{-3}; 1)$, because it converges when $|\log(g_e)| < \pi$.

For $0 < g_e < e^{-3}$ we use the following asymptotic series (see Eq.(8) from [5]):

$$\mathrm{Fe}_\nu(g_e) \sim \frac{(-\log(g_e))^{\nu+1}}{\Gamma(k+2)} \left(1 + \sum_{i=1}^{\infty} a_{2i}(\log(g_e))^{-2i}\right). \tag{119}$$

where

$$a_{2i} = \frac{(1 - 2^{1-2i})(k+1)!(2\pi)^{2i}}{(k+1-2i)!} \frac{|B_{2i}|}{(2i)!}. \tag{120}$$

where B_j denotes a standard Bernoulli number. The last formula can be simplified using the following expression for the Bernoulli numbers (see Eq.(9.616) from [4]):

$$B_{2i} = \frac{(-1)^{i-1}(2i)!}{2^{2i-1}\pi^{2i}}\zeta(2i). \tag{121}$$

so that

$$a_{2i} = \frac{2(1 - 2^{1-2i})(k+1)!}{(k+1-2i)!}|\zeta(2i)|. \tag{122}$$

We only calculate the first three sum terms of the asymptotic series to get the best approximation of $\mathrm{Fe}_\nu(g_e)$ for g_e around e^{-3}:

$$\mathrm{Fe}_\nu(g_e) \approx \frac{(-\log(g_e))^{\nu+1}}{\Gamma(k+2)} \left(1 + \frac{a_2}{(\log(g_e))^2} + \frac{a_4}{(\log(g_e))^4}\right). \quad (123)$$

An asymptotic series does not guarantee an improvement in accuracy while increasing the number of the sum terms involved. In our particular case the use of either more than or less than three sum terms noticeably lowers the accuracy of $\mathrm{Fe}_\nu(g_e)$ for $g_e \in [e^{-5}, e^{-3}]$.

In both series $\zeta(x)$ denotes the Riemann zeta-function. At $x > 0$ it can be calculated as a convergent series (see Eq.(9.522.2) from [4]):

$$\zeta(x) = \frac{1}{1-2^{1-x}} \sum_{n=1}^{\infty} (-1)^{n+1} \frac{1}{n^x}. \quad (124)$$

At $x < 0$ we use the following reflection formula (see Eq.(7) from [5]):

$$\zeta(x) = 2^x \pi^{x-1} \sin(\frac{\pi x}{2}) \Gamma(1-x) \zeta(1-x). \quad (125)$$

15 Appendix B: Partition function and excitation

Common properties of mean values and covariances. Recall the definition of mean value (also referred to as "expected value"):

$$\langle f_i \rangle = \sum_i p_i f_i. \quad (126)$$

Where p_i acts as the probability of occurence of state i. Covariance is constructed using the definition of mean value described

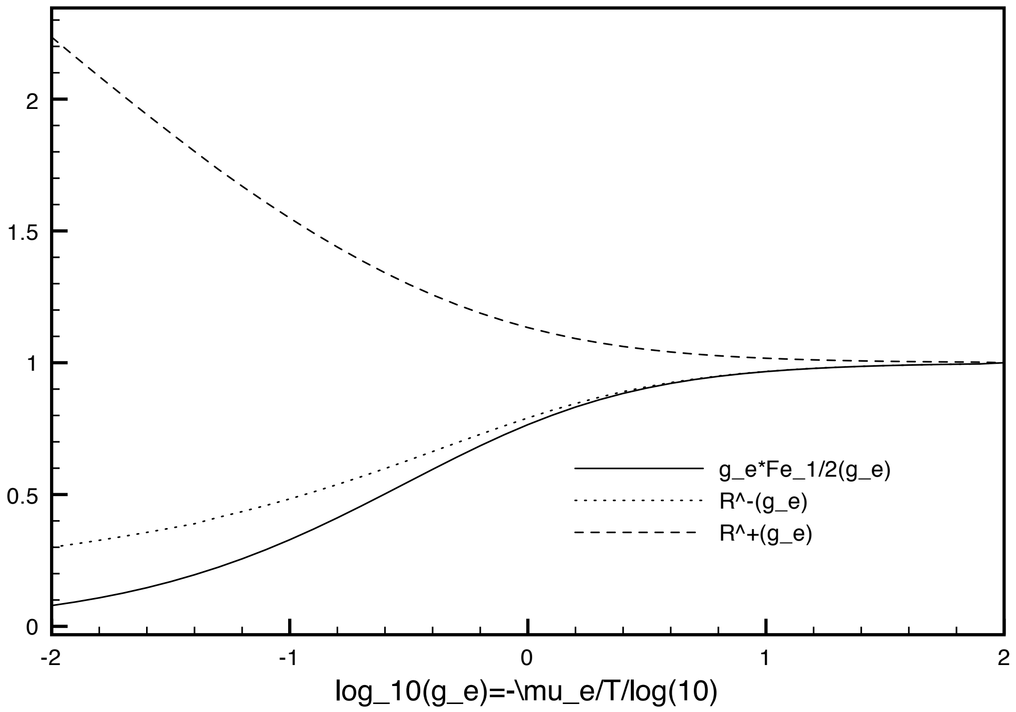

Figure 1: The Fermi function of index 1/2 multiplied by g_e (solid) and the ratio functions (dashed) calculated using the described algorithm.

above:

$$Cov(a,b) = \langle \delta a \delta b \rangle = \langle (a - \langle a \rangle)(b - \langle b \rangle) \rangle, \qquad (127)$$

where $\delta a = a - \langle a \rangle$. One of the useful properties of covariance is as follows:

$$\langle \delta a \delta b \rangle = \langle ab \rangle - \langle a \rangle \langle b \rangle, \qquad (128)$$

$$proof : \langle (a - \langle a \rangle)(b - \langle b \rangle) \rangle = \langle ab - a\langle b \rangle - b\langle a \rangle + \langle a \rangle \langle b \rangle \rangle =$$
$$\langle ab \rangle - 2\langle a \rangle \langle b \rangle + \langle a \rangle \langle b \rangle = \langle ab \rangle - \langle a \rangle \langle b \rangle.$$

Another property we actually use in the code to optimize the calculation of covariances is as follows:

$$\langle \delta a \delta b \rangle = \langle (a - \langle a \rangle) b \rangle, \tag{129}$$

$$proof : \langle \delta a \delta b \rangle = \langle ab \rangle - \langle a \rangle \langle b \rangle = \langle ab \rangle - \langle \langle a \rangle b \rangle = \langle (a - \langle a \rangle) b \rangle. \tag{130}$$

Even having no idea about particular properties of either p_i and f_i, one can derive the formula for $d\langle f_i \rangle$ as follows:

$$d\langle f_i \rangle = \langle \delta f_i \delta \left(\frac{dp_i}{p_i} \right) \rangle + \langle df_i \rangle, \tag{131}$$

which is useful to calculate partial derivatives of $\langle f_i \rangle$, for example, $\frac{\partial \langle f_i \rangle}{\partial g_e}$.

Proof:

$$\begin{aligned} d\langle f_i \rangle &= d \left(\frac{\sum w_i f_i}{\sum w_i} \right) = \frac{d(\sum w_i f_i)}{\sum w_i} - \frac{d(\sum w_i) \sum w_i f_i}{\sum w_i} = \\ &= \frac{\sum (w_i df_i + f_i dw_i)}{\sum w_i} - \frac{\sum dw_i}{\sum w_i} \langle f_i \rangle = \\ &= \langle df_i \rangle + \langle f_i \frac{dw_i}{w_i} \rangle - \langle \frac{dw_i}{w_i} \rangle \langle f_i \rangle = \langle \delta f_i \delta \left(\frac{dw_i}{w_i} \right) \rangle + \langle df_i \rangle, \end{aligned} \tag{132}$$

where $w_i = p_i S$ are non-normalized partition functions.

To calculate covariances over several indices one can separate the indices using this formula:

$$\langle \delta f_{i,n} \delta g_{i,n} \rangle_{i,n} = \left\langle \langle \delta f_{i,n} \delta g_{i,n} \rangle_n \right\rangle_i + \left\langle \delta \left\langle f_{i,n} \right\rangle_n \delta \left\langle g_{i,n} \right\rangle_n \right\rangle_i . \tag{133}$$

16 Appendix C: Debye-Huekel approximation of electrostatic energy

The Debye-Huekel approximation may also be used to account for Coulomb interactions. This model considers the coupled free electrons to be distributed according to the Boltzmann distribution with respect to the electrostatic field of the corresponding ion.

Helmholtz free energy. The extra term in the free energy, which accounts for the potential of the Coulomb field created in the location of a given particle by all other particles, is as follows (see Eq.(78.11) in [2]):

$$F_{DH} = -\frac{VT}{12\pi R_D^3}, \quad \frac{1}{R_D^2} = \frac{4\pi q_e^2 (N_e + \sum_i i^2 N_i)}{VT}. \tag{134}$$

Accordingly, in Eq.(3) the term $\partial F_{DH}/\partial N_i - \partial F_{DH}/\partial N_{i+1} - \partial F_{DH}/\partial N_e$ will contribute $(i+1)q_e^2/(TR_D)$ to the left hand side. The partition function with the Coulomb interaction, thus becomes:

$$\frac{N_i}{g_i} = \frac{N_0}{g_0}(g_e)^i e^{\frac{(i^2+i)}{2R_D T} - \frac{\sum_{j=0}^{i-1} I_j}{T}}. \tag{135}$$

This may be interpreted as the ionization potential lowering, which results from the Coulomb interaction: each of the potentials, I_i, is reduced by $(i+1)q_e^2/R_D$. The total reduction in the energy of the ion of charge state i is, therefore, $(i^2+i)q_e^2/2R_D$, where the terms proportional to i^2 and i stand for ion and electrons electrostatic energy correspondingly. This effect shifts the ionization equilibrium towards higher ionization degrees, for a given temperature and atomic density.

The partition function can be derived the same way it was in the Madelung approximation of electrostatic energy (see Eqs.(39) and (40)), where E_i^* should be modified according to the Debye-Huekel theory:

$$E_i^* = \sum_{j=0}^{i-1} I_j - \frac{i^2+i}{2R_D}. \tag{136}$$

Taking exact partition functions leads us to the following equations for differentials of g_e, T, V and $1/R_D$:

$$\frac{dg_e}{g_e}\left[\langle\delta^2 i\rangle + ZR^-\right] + dT\left[\frac{\langle\delta E_i^*\delta i\rangle}{T^2} - \frac{3}{2}\frac{Z}{T}\right] + \tag{137}$$
$$+d\left(\frac{1}{R_D}\right)3LR_D\langle\delta(i^2+i)\delta i\rangle = \frac{Z}{V}dV.$$

Here we should substitute $d(1/R_D)$ obtained by differentiation of Eq.(142):

$$d\left(\frac{1}{R_D}\right) = \frac{1}{2R_D}\frac{-\frac{dV}{V} + \frac{dg_e}{g_e}\frac{\langle\delta(i^2+i)\delta i\rangle}{\langle i^2+i\rangle} + \frac{dT}{T}\left(\frac{\langle\delta(i^2+i)\delta E_i^*\rangle}{T\langle i^2+i\rangle} - 1\right)}{1 - \frac{3}{2}L\frac{\langle\delta^2(i^2+i)\rangle}{\langle i^2+i\rangle}}, \tag{138}$$

so that the coefficients in Eq.(41) become:

$$A_{g_e} = \langle\delta^2 i\rangle + ZR^- + \frac{\langle\delta(i^2+i)\delta i\rangle^2}{\frac{2}{3L}\langle i^2+i\rangle - \langle\delta^2(i^2+i)\rangle}, \qquad A_V = Z + \frac{\langle\delta(i^2+i)\delta i\rangle}{\frac{2}{3L} - \frac{\langle\delta^2(i^2+i)\rangle}{\langle i^2+i\rangle}}, \tag{139}$$

$$A_T = \frac{3}{2}Z - \frac{\langle\delta E_i^*\delta i\rangle}{T} + \frac{\langle\delta(i^2+i)\delta i\rangle\left(\langle i^2+i\rangle - \frac{\langle\delta(i^2+i)\delta E_i^*\rangle}{T}\right)}{\frac{2}{3L}\langle i^2+i\rangle - \langle\delta^2(i^2+i)\rangle}. \tag{140}$$

Helmholtz free energy. Using the new ion partition functions with the correction as in Eq.(134) added, one can rewrite Eq.(19) in the following form:

$$F = -TN_a\log\left[\frac{eV}{N_a}\left(\frac{MT}{2\pi\hbar^2}\right)^{3/2}\right] - TN_a\log S + \Omega_e + \frac{VT}{24\pi R_D^3}, \tag{141}$$

where

$$\frac{1}{R_D^2} = \frac{4\pi q_e^2 N_a\langle i+i^2\rangle}{VT}, \tag{142}$$

and the equation for the electron statistical weight now reads:

$$Z = \langle i \rangle = g_{e1} \mathrm{Fe}_{1/2}(g_e). \tag{143}$$

Both the averages and the statistical sum should be calculated with the partition functions as in Eq.(135), which depend not only on T and g_e, but also on R_D. Again, it is easy to check the partial derivatives of Eq.(141) over g_e and over $1/R_D$ to confirm that both vanish. To simplify further formula derivations and to make them independent of system of units, we introduce a dimensionless variable L:

$$L_{CGS} = \frac{q_e^2}{6R_D T}, \qquad L = \frac{Ry[eV]}{3T[eV]R_D[a]}, \tag{144}$$

where $R_D[a]$ stands for the Debye radius expressed in the units of Bohr radius, so that we obtain a simpler formula for R_D:

$$\frac{1}{R_D^3} = 24\pi n_a \langle i^2 + i \rangle L. \tag{145}$$

Thermodynamic functions. By differentiating the free energy over temperature we find the internal energy and by differentiating over the volume we find the pressure:

$$\mathcal{E} = \mathcal{E}_i + \mathcal{E}_e, \qquad \mathcal{E}_i = \frac{3}{2} T n_a, \qquad \mathcal{E}_e = n_a \left[\frac{3}{2} T Z R^+ + \langle E_i^* \rangle \right], \tag{146}$$

$$P = P_i + P_e, \qquad P_i = n_a T, \qquad P_e = n_a T (1 + Z R^+ - L\langle i^2 + i \rangle), \tag{147}$$

Results. Below we add the calculation of the Debye-Huekel correlation energy as well as the Madelung energy.

Na[1/cm^3]	10^{18}	10^{19}	10^{20}	10^{21}
Te[eV]	$DH\vert Mad$	$DH\vert Mad$	$DH\vert Mad$	$DH\vert Mad$
5.	1.7 — 2.4	3.3 — 3.7	5.0 — 4.9	4.6 — 4.7
10.	7.8 — 8.4	14.1 — 12.4	22.9 — 17.2	27.5 — 19.5
15.	9.7 — 11.1	25.6 — 21.2	52.8 — 34.4	70.2 — 41.6
20.	17.0 — 17.8	31.5 — 26.8	71.4 — 46.3	128.2 — 68.4
25.	31.9 — 29.2	51.9 — 40.3	86.8 — 56.8	175.1 — 90.6
30.	46.8 — 40.0	87.1 — 60.5	125.5 — 77.2	206.0 — 107.4
35.	63.4 — 51.5	123.2 — 80.2	190.7 — 107.3	253.0 — 129.6
40.	78.6 — 62.2	160.5 — 100.0	274.0 — 142.9	333.3 — 162.8
45.	85.3 — 68.3	201.1 — 120.9	354.6 — 176.5	453.0 — 207.8
50.	94.6 — 75.8	230.1 — 137.0	439.2 — 210.8	608.5 — 262.0
55.	113.1 — 88.1	247.1 — 148.3	529.5 — 246.6	777.2 — 318.5
60.	134.6 — 101.8	270.8 — 162.3	607.2 — 278.1	946.8 — 373.9
65.	153.4 — 114.1	311.5 — 183.0	660.8 — 302.2	1122.0 — 430.1
70.	169.6 — 125.1	361.9 — 207.3	706.1 — 323.7	1304.8 — 487.5
75.	180.8 — 133.6	410.9 — 230.9	765.4 — 349.5	1482.7 — 543.2
80.	183.7 — 137.9	453.9 — 252.1	851.4 — 383.4	1636.8 — 592.8
85.	181.8 — 139.8	490.2 — 270.8	959.0 — 423.6	1762.8 — 635.6
90.	178.2 — 140.6	514.5 — 285.0	1072.9 — 465.2	1875.2 — 675.0
95.	174.6 — 141.2	523.8 — 293.7	1180.9 — 505.0	1995.4 — 716.4
100.	171.5 — 141.9	523.0 — 298.5	1277.6 — 541.4	2141.5 — 763.9
105.	169.7 — 143.2	517.2 — 301.1	1358.8 — 573.3	2322.5 — 819.6
110.	170.5 — 145.9	509.8 — 302.9	1418.2 — 599.1	2534.8 — 882.4
115.	175.4 — 150.9	502.6 — 304.5	1453.0 — 618.0	2765.7 — 949.1
120.	184.8 — 158.5	496.8 — 306.5	1466.8 — 630.8	2999.9 — 1016.3
125.	196.7 — 167.5	494.3 — 309.7	1466.3 — 639.2	3223.7 — 1080.8

17 Appendix D: How to solve coupled system of N temperature equations.

The numerical solution of the non-linear heat conduction problem in the coupled system of the energy equations (say, for internal energy of radiation, electrons and/or ions) is reduced to a numerical solution of the system of linear equations with a sparse matrix, which is symmetric, definite positive and diagonal-dominant.

17.1 Governing equations and their symmetry

Consider the coupled system of the energy equations as follows:

$$\frac{\partial \mathcal{E}_\alpha}{\partial t} = \nabla \cdot (\kappa_\alpha \nabla T_\alpha) + \sum_{\beta \neq \alpha} R_{\alpha\beta}(T_\beta - T_\alpha), \tag{148}$$

where $\mathcal{E}$ is the internal energy density, index $\alpha = 1, ..., N$ enumerates N different components involved into a consideration, such as plasma as a single component or electrons and ions as two separate components and/or radiation; T_α being the temperature of the component (for radiation $aT_r^4 = \mathcal{E}_r$, hence, $T_r = (\mathcal{E}_r/a)^{1/4}$); the heat fluxes are assumed to have a form of $-\kappa_\alpha \nabla T_\alpha$; and $R_{\alpha\beta}$ characterizes the rate of energy exchange between different components. For gray radiation absorbtion the latter coefficient is:

$$R_{re} = \frac{ck_p(aT_e^4 - E_r)}{T_e - T_r} = ck_p a(T_e + T_r)(T_e^2 + T_r^2), \tag{149}$$

where k_p is the Planck opacity. Note also that in analogous manner the diffusive flux of the gray radiation energy, which is usually expressed in terms of the radiation energy density gradient, $\nabla \mathcal{E}_r$, may be reduced to the form as in Eq.(148), because $\nabla \mathcal{E}_r = 4aT_r^3 \nabla T_r$. All the variables and parameters may be dependent on temperatures as well as on the other plasma parameters (density, ionization degree etc)

17.2 Symmetry and positivity

In accordance with the second law of thermodynamics, the heat always transferred from the body with higher temperature to that with lower one, so that:

$$\kappa_\alpha \geq 0, \quad R_{\alpha\beta} \geq 0. \tag{150}$$

Another property of the governing equations comes from the detailed equilibrium principle which relates the energetic rates for direct and reverse processes and requires, that:

$$R_{\alpha\beta} = R_{\beta\alpha}. \tag{151}$$

In particular, Eq.(151) ensures the total energy conservation: $\frac{d}{dt}\sum_\alpha \int \mathcal{E} dV = 0$, because on the right hand side of Eq.(148) the divergence of the heat flux vanishes in integrating over a volume, while the energy exchange rates cancel each other locally on suming by α.

17.3 Discretization

Consider the semi-discrete set of equations, obtained by applying the finite volume formulation to Eq.(148) and employing the set of control volumes, V_i, enumerated by a single index, $i = 1, ..., I$:

$$V_i \frac{d\mathbf{E}_i}{dt} + \sum \mathbf{F}_{ij} + V_i \mathbf{R}_i \cdot \mathbf{T}_i = 0, \tag{152}$$

Here the elements $E_{\alpha i}$ of the state vector in the ith volume are the averaged value of the energy density, $\mathcal{E}_\alpha$. The fluxes, $F_{\alpha ij}$

may be obtained by approximating the temperature gradient: $F_{\alpha ij} = \kappa_{\alpha ij} S_{ij} (T_{\alpha i} - T_{\alpha j})/\|x_i - x_j\|$. The index j enumerates the control volumes which have the common face with the ith control volume, the face area being S_{ik} and the distance between the cell centers being $\|x_i - x_j\|$. The elementss of $N * N$ matrix, $\mathbf{R}_i$, are: $-R_{\alpha\beta i}$, for off-diagonal elements ($\alpha \neq \beta$), and $\sum_{\beta \neq \alpha} R_{\alpha\beta i}$, for the αth diagonal element.

All the coefficients and variables in Eq.(152), again, may be highly non-linear functions of temperature. However, now we employ the *principle of frozen coefficients*. Specifically, in advancing the solution through a time step, $\Delta t = t^{n+1} - t^n$, we assume all the coefficients, $\kappa_{\alpha ij}$ and $\mathbf{R}_i$ to be constant in time and keep their values as in the time instant, t^n. Moreover, we also approximate the time derivative of $\mathcal{E}_\alpha$ in terms of that of temperature, $\partial \mathcal{E}_\alpha / \partial t = C_\alpha \partial T_\alpha / \partial t$, where $C_\alpha = \partial \mathcal{E}_\alpha / \partial T_\alpha$ is the specific heat. Thus, Eq.(152) becomes:

$$V_i \mathbf{diag}\{C_\alpha\}_i \cdot \frac{d\mathbf{T}_i}{dt} + \sum_j \frac{S_{ij} \mathbf{diag}\{\kappa_{\alpha ij}\} \cdot (\mathbf{T}_i - \mathbf{T}_j)}{\|x_i - x_j\|} + V_i \mathbf{R}_i \cdot \mathbf{T}_i = 0, \tag{153}$$

where $\mathbf{diag}\{C_\alpha\}$ denotes $N * N$ matrix with the diagonal $\alpha\alpha$ element being C_α. Now we advance the solution of Eq.(153) through the time step using fully implicit scheme. To achieve this, one needs to solve a linear system as follows:

$$\frac{V_i \mathbf{diag}\{C_\alpha\}_i \cdot \mathbf{T}_i^{n+1}}{\Delta t} + \sum_j \frac{S_{ij} \mathbf{diag}\{\kappa_{\alpha ij}\} \cdot \left(\mathbf{T}_i^{n+1} - \mathbf{T}_j^{n+1}\right)}{\|x_i - x_j\|} + \\ + V_i \mathbf{R}_i \cdot \mathbf{T}_i^{n+1} = \frac{V_i \mathbf{diag}\{C_\alpha\}_i \cdot \mathbf{T}_i^n}{\Delta t} \tag{154}$$

The left hand side of this equation is the product, $\mathbf{A} \cdot \mathbf{T}^{n+1}$, of the $I * I$ block matrix, $\mathbf{A}_{ij}$, the elements of the block matrix being

$N * N$ matrices, with the block I-vector, $\mathbf{T}_i^{n+1}$, the elements of the block vector being N-vectors. In the matrix $\mathbf{A}$ all off-diagonal blocks are diagonal $N * N$ matrices:

$$\mathbf{A}_{ij} = \mathbf{A}_{ji} = -\frac{S_{ij}\mathbf{diag}\{\kappa_{\alpha ij}\}}{\|x_i - x_j\|},\ i \neq j. \tag{155}$$

We see that the off-diagonal block part of the matrix $\mathbf{A}$ is symmetric and all numbers in this part are non-positive, according to Eq.(150). The diagonal blocks are:

$$\mathbf{A}_{ii} = \frac{V_i\mathbf{diag}\{C_\alpha\}_i}{\Delta t} - \sum_{j\neq i}\mathbf{A}_{ij} + V_i\mathbf{R}_i. \tag{156}$$

The off-diagonal elements in the matrix $\mathbf{R}_i$ are again symmetric and non-positive, due to Eqs.(150,151). Hence, the matrix $\mathbf{A}$ is symmetric. It is also diagonal-dominant: taking the difference between the diagonal element and the sum of absolute values of all off-diagonal elements in the same line, one can see, that:

$$A_{\alpha\alpha ii} - \sum_{\beta\neq\alpha}|A_{\alpha\beta ii}| - \sum_{i\neq j}|A_{\alpha\alpha ij}| = \frac{V_i C_{\alpha i}}{\Delta t} > 0. \tag{157}$$

Thus, we proved that the matrix $\mathbf{A}$ is symmetric and diagonal-dominant. As a consequence, it is positive definite, but the diaginal domination is more strong and usefull property. There is a variety of tools allowing to solve efficiently the system of equations with such kind of matrices, for example, preconditioned conjugated gradients.

Finally, we show how to employ $\mathbf{T}^{n+1}$ found from non-conservative Eq.(153) to advance the solution of original Eq.(152), which conserves the energy. To do this, one needs to express the fluxes and energy in Eq.(152) in terms of $\mathbf{T}^{n+1}$, still keeping the coefficients frozen. After a simple algebra we obtain:

$$\mathcal{E}_{\alpha i}^{n+1} = \mathcal{E}_{\alpha i}^{n} + C_{\alpha i}(T_{\alpha i}^{n+1} - T_{\alpha i}^{n}). \tag{158}$$

The corrected temperature at the time instant t^{n+1} then should be recovered from $\mathcal{E}$ using the equation of state, and, for plasma with the temperature-dependent specific heat. it may differ from T^{n+1}. Note also that at this final stage, theoretically, the choice of too large time step may result in negative temperature. Indeed, although $\mathbf{T}^{n+1}$ are all positive, it is not guaranteed that at $T^{n+1} \ll T^n$ the energy $\mathcal{E}^{n+1}$ found from Eq.(158) exceeds the value corresponding to zero temperature. The advance through the timestep in this case may be done in two stages, getting the temperature drop limited.

17.4 Generalizations: $N+M$ temperatures, and temperature powered n.

Note some more or less trivial generalizations of the developed approach.

Non-linear temperature. So far we considered only the temperaature values for different components of the physical system, as the unknowns to be solved numerically. However, in many problems of the thermodynamics the term “temperature” implies “...or any monotonous function on it”. Particularly any monotonous function of temperature, $T_{\rm new}(T)$ can be introduced instead of the the temperature, into the governing equations or into the finite volume formulation. In the latter case while setting the frozen coefficients the *Lipshitz derivative* should be used, which is the symmetric positive function, $T'_{\rm new}(T_1, T_2)$, of two input parameters, T_1 and T_2, such that for any T_1 and T_2,

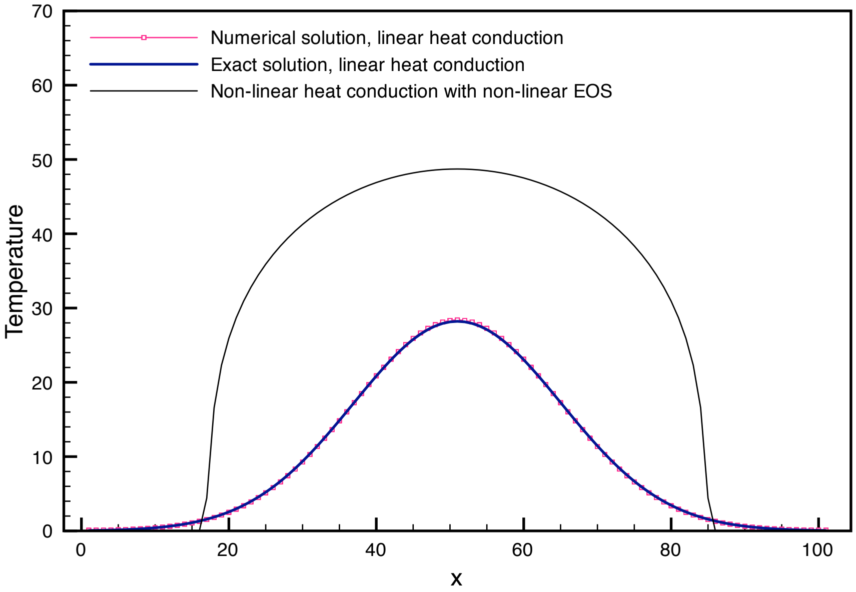

Figure 2: The test result for N-temperature model using conjugeted gradients method with Jacobi block preconditioner ($\mathbf{A}_{ii}$ matrix is exactly inverted): (1) linear heat conduction equation compared with the anylitical solution (to test the CG routine) and the numerical solution of the non-linear heat conduction equation is compared to that of the coupled system of heat conduction with very high energy exchange rate (1000 per time step) and the same total conduction and heat capacity as for a single equation. Not surprisingly, the solution of the strongly coupled system is not different from that for a single equation, but remarkable is the fact that such the high energy exchange rate does not affect the iteration convergence rate.

by definition,

$$T'_{\rm new}(T_1,T_2)=\frac{T_{\rm new}(T_1)-T_{\rm new}(T_2)}{T_1-T_2}. \qquad (159)$$

Particularly, for the power law $T_{\rm new}(T)=aT^L$ with the integer index, L, the Lipshitz derivative is $T'_{\rm new}(T_1,T_2)=a\sum_{l=0}^{L-1}T_1^{L-1-l}T_2^l$. The system of linear equations, (154), as formulated in terms of $T^{n+1}_{\alpha i}$, has the same form as before, bur the frozen coefficients in it are frozen in a different way:

$$C_{\alpha i}\to\frac{C_{\alpha i}}{T'_{\rm new}(T^n_{\alpha i},T^n_{\alpha i})},\qquad R_{\alpha\beta i}\to\frac{R_{\alpha\beta i}}{T'_{\rm new}(T^n_{\alpha i},T^n_{\beta i})}, \qquad (160)$$

$$\kappa_{\alpha ij}\to\frac{\kappa_{\alpha ij}}{T'_{\rm new}(T^n_{\alpha i},T^n_{\alpha j)}}, \qquad (161)$$

Positivity, symmetry and the diagonal domination are proved in the same way as above, using the positivity ond symmetry of the Lipshitz derivative. Since the Lipshitz derivatives are taken as the frozen coefficients, the non-linear temperature approach implies another choice of the linerization procedure in the governing equations.

Partial inversion of the advancing operator may or may not make sense, if the heat transfer for one or some of the physical components is negligible (for, example the ion heat conduction usually, but not always, is small as compared with the electron one). In this case one can re-write Eq.(154) in the following manner, which lists only N equations including heat conduction, with extra term describing the energy exchange with M non-heat-conducting components, for which the temperature is denoted as Θ_{Mi} and the enumerating index for these components is denoted with upper case M :

$$\frac{V_i\mathbf{diag}\{C_\alpha\}_i\cdot\mathbf{T}_i^{n+1}}{\Delta t}+\sum_j\frac{S_{ij}\mathbf{diag}\{\kappa_{\alpha ij}\}\cdot\left(\mathbf{T}_i^{n+1}-\mathbf{T}_j^{n+1}\right)}{\|x_i-x_j\|}+$$
$$+V_i\mathbf{R}_i\cdot\mathbf{T}_i^{n+1}-V_i\|R_{\alpha M}\|_i\cdot\mathbf{\Theta}_i^{n+1}=\frac{V_i\mathbf{diag}\{C_\alpha\}_i\cdot\mathbf{T}_i^n}{\Delta t}.\tag{162}$$

Note that the diagonal elements of the $\mathbf{R}$ matrix includes a contribution from the energy exchange between heat-conducting and non-heat-conducting components. Analogously, $M*M$ $\mathbf{r}_i$ matrix for the energy exchange between non-heat-conducting components also includes the diagonal elements accounting for the contributions from heat-conducting components. The equation for non-heat-conducting components reads:

$$\frac{\mathbf{diag}\{C_M\}_i\cdot\mathbf{\Theta}_i^{n+1}}{\Delta t}+\mathbf{r}_i\cdot\mathbf{\Theta}_i^{n+1}-\|R_{M\alpha}\|_i\cdot\mathbf{T}_i^{n+1}=\frac{\mathbf{diag}\{C_M\}_i\cdot\mathbf{\Theta}_i^n}{\Delta t}.\tag{163}$$

All this derivations make sense as long as the matrix of the advancing operator in Eq.(163) may be inverted, to find:

$$\mathbf{B}_i^{-1}=\left(\frac{\mathbf{diag}\{C_M\}_i}{\Delta t}+\mathbf{r}_i\right)^{-1}.\tag{164}$$

Using the inverted matrix, one can exclude $\mathbf{\Theta}_i^{n+1}$ from (162) using the following equation:

$$\mathbf{\Theta}_i^{n+1}=\mathbf{B}_i^{-1}\cdot\left(\frac{\mathbf{diag}\{C_M\}_i\cdot\mathbf{\Theta}_i^n}{\Delta t}+\|R_{M\alpha}\|_i\cdot\mathbf{T}_i^{n+1}\right).\tag{165}$$

On excluding $\mathbf{\Theta}_i^{n+1}$ Eq.(162) again takes the form of Eq.(154) with the following modifications:

$$\mathbf{R}_i\to\mathbf{R}_i-\|R_{\alpha M}\|_i\cdot\mathbf{B}_i^{-1}\cdot\|R_{\alpha M}\|_i,$$
$$\mathbf{diag}\{C_\alpha\}_i\cdot\mathbf{T}_i^n\to\mathbf{diag}\{C_\alpha\}_i\cdot\mathbf{T}_i^n+\|R_{\alpha M}\|_i\cdot\mathbf{B}_i^{-1}\cdot\mathbf{diag}\{C_M\}_i\cdot\mathbf{\Theta}_i^n\tag{166}$$

So, the detailed algorithm in this case may be as follows: (1) in each point, i, find the inverted matrix $\mathbf{B}_i^{-1}$; (2) modify the matrix of the equation for heat-condicting components using (166); (3) solve Eq.(154), with the modified relaxation matrices and changed right hand side, througout the whole computational domain; (4) at each point solve temperatures for non-heat-condicting components, using (165). The symmetry of the modified matrix $\mathbf{R}$ is evident, less evident is its diagonal domination. The latter is a consequence of the above mentioned contributions from the cross interactions, into the diagonal elements of $\mathbf{R}$ and $\mathbf{r}$ matrices.

17.5 Summary

Thus, to update the conservative system of non-linear heat conduction equations one needs: (1) to calculate coeffecients in the matrix $\mathbf{A}$, (2) solve the predicted values of temperature from the system of linear equations with symmetric, positive definite and diagonal-dominant matrix, (3) update the energy using Eq.(158)

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