Default NSE Corrections in NucNet Tools

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This document presents some notes on the default Coulomb corrections used in NucNet Tools. We use the expression for the Helmholtz free energy in the one-component plasma (OCP) given in [3]:

$$\frac{F(\Gamma)}{NkT} = g_1(\Gamma) = a\Gamma + 4b\Gamma^{1/4} - 4c\Gamma^{-1/4} + d\ln(\Gamma) - [a + 4(b-c)] + \frac{F(1)}{kT} \quad (1)$$

where k is Boltzmann's constant and T is the temperature. Here, the Coulomb coupling parameter Γ is given by

$$\Gamma = Z^{5/3}\Gamma_e \quad (2)$$

where Z is the ion charge and Γ_e is given by

$$\Gamma_e = \left(\frac{e^2}{a_e kT}\right) \quad (3)$$

with the electron cloud radius a_e given in terms of the electron number density n_e as

$$a_e = \left(\frac{3}{4\pi n_e}\right)^{1/3} \quad (4)$$

As suggested by [1], when $\Gamma < 1$ we take

$$\frac{F(\Gamma)}{NkT} = g_2(\Gamma) = -\frac{1}{\sqrt{3}}\Gamma^{3/2} + \frac{\beta}{\gamma}\Gamma^{\gamma} \quad (5)$$

The constants β and γ are determined by matching the expressions in Eqs (1) and (5) and their first derivatives at $\Gamma = 1$.

It is possible to compute thermodynamic quantities from Eq. (1) or Eq. (5). The chemical potential μ is given by

$$\mu = \left(\frac{\partial F}{\partial N}\right)_{T,V} \quad (6)$$

If we do not change n_e in the variation, then we simply find

$$\frac{\mu}{kT} = g(\Gamma) \quad (7)$$

where we choose $g = g_1$ for $\Gamma > 1$ and $g = g_2$ for $\Gamma < 1$.

The entropy S is given by

$$S = -\left(\frac{\partial F}{\partial T}\right)_{V,N} \tag{8}$$

We first note that

$$\left(\frac{\partial \Gamma}{\partial T}\right)_{V,N} = -\frac{\Gamma}{T} \tag{9}$$

With this result, we note that

$$\frac{S}{Nk} = -g + \Gamma\frac{\partial g}{\partial \Gamma} \tag{10}$$

where g is either g_1 or g_2. For $\Gamma > 1$, $g = g_1$, so

$$\Gamma\frac{\partial g}{\partial \Gamma} = a\Gamma + b\Gamma^{1/4} + c\Gamma^{-1/4} + d \tag{11}$$

From this, we find

$$\frac{S}{Nk} = -3b\Gamma^{1/4} + 5c\Gamma^{-1/4} + d - d\ln(\Gamma) + o \tag{12}$$

where

$$o = a + 4(b - c) - \frac{F(1)}{kT} \tag{13}$$

For $\Gamma < 1$, $g = g_2$, so

$$\Gamma\frac{\partial g}{\partial \Gamma} = -\frac{\sqrt{3}}{2}\Gamma^{3/2} + \beta\Gamma^{\gamma} \tag{14}$$

In this case, the entropy for $\Gamma < 1$ is

$$\frac{S}{Nk} = -\frac{1}{2\sqrt{3}}\Gamma^{3/2} + \beta\left(1 - \frac{1}{\gamma}\right)\Gamma^{\gamma} \tag{15}$$

The energy U is given by

$$\frac{U}{NkT} = \frac{F + TS}{NkT} = \frac{F}{NkT} + \frac{S}{Nk} = \Gamma\frac{\partial g}{\partial \Gamma} \tag{16}$$

For $\Gamma > 1$, we find from Eq. (11)

$$\frac{U}{NkT} = a\Gamma + b\Gamma^{1/4} + c\Gamma^{-1/4} + d \tag{17}$$

For $\Gamma < 1$, we find from Eq. (14)

$$\frac{U}{NkT} = -\frac{\sqrt{3}}{2}\Gamma^{3/2} + \beta\Gamma^{\gamma} \tag{18}$$

The pressure P is given by

$$P = -\left(\frac{\partial F}{\partial V}\right)_{T,N} \tag{19}$$

From the expression for Γ, we find

$$\left(\frac{\partial \Gamma}{\partial V}\right)_{T,N} = -\frac{\Gamma}{3V} \tag{20}$$

With this,

$$P = \frac{NkT}{3V}\Gamma\frac{\partial g}{\partial \Gamma} = \frac{1}{3}\frac{U}{V} \tag{21}$$

For the default NSE correction treatment in NucNet Tools, the constants a, b, c, and d are taken from [2]. The value of $F(1)/NkT = -0.420$, as suggested by [3].

When more than one ion species is present (a multi-component plasma), we use the usual "additive approximation" in which each species is computed as if it were a OCP and then the contributions of each ion are weighted by the ion's abundance. In this case, we consider the abundance per nucleon of species i as $Y_i = N_i/N$, where N is the total number of nucleons in the system. The Coulomb entropy per nucleon (in units of k) for species i is then

$$s_i = Y_i\left(-g + \Gamma\frac{\partial g}{\partial \Gamma}\right) \tag{22}$$

Similarly, the energy per nucleon for species i is

$$\frac{u_i}{kT} = Y_i\Gamma\frac{\partial g}{\partial \Gamma} \tag{23}$$

The partial pressure for species i is

$$P_i = \frac{1}{3}nu_i \tag{24}$$

where n is the number density of total nucleons.

References

[1] E. Bravo and D. García-Senz. Coulomb corrections to the equation of state of nuclear statistical equilibrium matter: implications for SNIa nucleosynthesis and the accretion-induced collapse of white dwarfs. *Mon. Not. Royal. Astron. Soc.*, 307:984–992, August 1999.

[2] S. Ogata and S. Ichimaru. Critical examination of N dependence in the Monte Carlo calculations for a classical one-component plasma. *Phys. Rev. A*, 36:5451–5454, December 1987.

[3] W. L. Slattery, G. D. Doolen, and H. E. Dewitt. Improved equation of state for the classical one-component plasma. *Phys. Rev. A*, 21:2087–2095, June 1980.