NSE EOS Notes

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1 Introduction

Here we describe the components of an equation of state (EOS) that goes beyond the single nucleus approximation and naturally transitions to nuclear statistical equilibrium (NSE). It is assumed that the bulk free energy is known, so our model is a generic, phenomenological description of the non-uniform phase during the nuclear liquid-gas phase transition. In different limits, it reduces to the excluded volume model of Hempel, the single nucleus approximation of Lattimer, or to a simple two charge Gibbs phase construction.

2 The free energy

Basically, our model assumes a multi-phase medium where each phase bubble – aside from the exterior bulk – is constrained to have a fixed neutron and proton number. This is a straight forward generalization of LS. Clearly, a phase bubble can alternatively thought of as a nucleus. In the spirit of LS, our model Helmholtz free energy for nuclear matter is

$$F = \sum_{i}^{\text{nuclei}} F_i(v_i, n_i, T) + V_o f_B(n_{p,o}, n_{n,o}, T). \tag{1}$$

Here f_B is the free energy of homogeneous nuclear matter, n_x is the number density of species x, v_i is the volume of nucleus (or phase) i, the subscript o denotes nucleons outside of nuclei and corresponds to the low density phase (at densities below pasta formation). The total free energy of phase i is modeled as

$$F_i = \mathcal{N}_i \left[v_i f_B(\frac{Z_i}{v_i}, \frac{N_i}{v_i}, T) + F_{FS}(v_i, Z_i, N_i, n_{p,o}, n_{n,o}, n_e, T) + T \ln\left(\frac{n_i}{n_Q A_i^{3/2}}\right) - T + E_{0,i} \right], \tag{2}$$

where $\mathcal{N}_i = V n_i$, $n_Q = (m_n T/2\pi)^{3/2}$, n_e is the number density of uniform electrons, and F_{FS} is the free energy contribution from finite size effects such as surface tension and Coulomb corrections. Shell and pairing effects can be included through $E_{0,i}$. If we assumed there were a single nucleus (i.e. only one N_i and Z_i) and allowed these neutron and proton number of the nucleus to vary, we arrive at the model free energy used in LS.

2.1 Minimization of the Free Energy

To find the thermodynamic state of the system, we must minimize our free energy with respect to the free parameters in our model subject to the constraints of total neutron number, proton number, and volume conservation. These constraints are written as

$$\begin{aligned}\sum \mathcal{N}_i Z_i + Z_o &= Z \\ \sum \mathcal{N}_i N_i + N_o &= N \\ \sum \mathcal{N}_i v_i + V_o &= V,\end{aligned}$$

where $Z_o = n_{p,o} V_o$ and $N_o = n_{n,o} V_o$. Choosing $\mathcal{N}_i$ and v_i as our independent variables gives the relations

$$\begin{aligned} Z_i + \frac{\partial Z_o}{\partial \mathcal{N}_i} = 0, \quad N_i + \frac{\partial N_o}{\partial \mathcal{N}_i} = 0 \\ v_i + \frac{\partial V_o}{\partial \mathcal{N}_i} = 0, \quad \mathcal{N}_i + \frac{\partial V_o}{\partial v_i} = 0 \end{aligned}$$

and results in the system of equations

$$\frac{\partial F}{\partial \mathcal{N}_i} = v_i f_{B,i} + F_{FS,i} + \mu_{K,i} + E_{0,i} - Z_i \mu_{p,o} - N_i \mu_{n,o} + v_i P_o = 0 \tag{3}$$

$$\frac{\partial F}{\partial v_i} = \mathcal{N}_i \left(-P_{B,i} - P_{FS,i} + P_{B,o} \right) = 0 \tag{4}$$

$$\sum Z_i n_i + \left(1 - \sum v_i n_i\right) n_{p,o} = n_p = n_e \tag{5}$$

$$\sum N_i n_i + \left(1 - \sum v_i n_i\right) n_{n,o} = n_n, \tag{6}$$

where we have defined $\mu_{K,i} = T \ln(A_i^{-3/2} n_i / n_Q)$.

2.2 Connection to NSE

When the outside densities are low, P_o is negligible and the second constraint equation results in

$$P_{B,i} + P_{FS,i} = 0.$$

As long as the finite size term is not strongly affected by the exterior medium (which is expected at low densities), this equation only depends on v_i. Therefore, it just determines the volume of nucleus i in vacuum, and thereby its total energy and entropy. The first constraint equation then results in

$$n_i = A_i^{3/2} n_Q \exp(Z_i \mu_{p,o} + N_i \mu_{n,o} - v_i P_o - B_i),$$

where $B_i = -v_i f_{B,i} - F_{FS,i} - E_{0,i}$. This is almost the same form as we would recover for standard NSE with excluded volume corrections, but at first glance there appears to be no contribution from the internal partition function. This is of course not the case, since B_i is temperature dependent and contains information about the internal excitation as well as the ground state energy. Combined with the proton and neutron density constraint equations, this results in the standard NSE system that is used by Hempel, for instance.

■ **[TODO: Work out what the internal partition function is in more detail]** ■

2.3 Reduction to Gibbs Phase Equilibrium

The Gibbs phase construction assumes there are no surface effects and that the phase bubbles are stationary. Employing these two approximations forces us to set $E_{FS,i}$ and $\mu_{K,i}$ to zero (or assume they are negligible). Our constraint equations are then

$$\begin{aligned} n_i P_{B,i} &= n_i P_o \\ v_i f_{B,i} + E_{0,i} &= Z_i \mu_{p,o} + N_i \mu_{n,o} - v_i P_o. \end{aligned}$$

The relation $P_B = n_p \mu_p + n_n \mu_n - f_B$ can then be employed to recast the constraints as

$$\begin{aligned} n_i P_{B,i} &= n_i P_o \\ Z_i \left(\mu_{p,i} - \mu_{p,o}\right) + N_i \left(\mu_{n,i} - \mu_{n,o}\right) &= 0 \end{aligned}$$

These equations are either satisfied by nucleus i when it's density is zero or when it satisfies the Gibbs phase equilibrium conditions. Since there is no difference between different nuclei with the same Y_p because there is are no finite size effects, this will just look like a two phase construction.

3 Thermodynamic Quantities

The pressure is given by

$$P = P_o + \sum n_i \left[T + \frac{\partial F_{FS,i}}{\partial \ln n_e} + u_o \frac{\partial F_{FS,i}}{\partial \ln n_{p,o}} + u_o \frac{\partial F_{FS,i}}{\partial \ln n_{n,o}} \right] \tag{7}$$

and the entropy is given by

$$s = u_o s_{B,o} + \sum n_i \left(S_{B,i} + \frac{5}{2} - \frac{\mu_{K,i}}{T} - \frac{\partial F_{FS,i}}{\partial T} \right). \tag{8}$$

The chemical potentials are

$$\mu_p = \mu_{p,o} + \sum_i \frac{n_i}{u_0} \frac{\partial F_{FS,i}}{\partial n_{p,o}}, \tag{9}$$

$$\mu_n = \mu_{n,o} + \sum_i \frac{n_i}{u_0} \frac{\partial F_{FS,i}}{\partial n_{n,o}}. \tag{10}$$

I think the finite size correction should be there, but this bears double checking. The LS model would predict them to be zero, since their F_{FS} is independent of the external densities. In any case, these corrections should always be quite small for nuclei. They can potentially be large for voids.

4 Model for Finite Size Effects

4.1 Coulomb Corrections

We currently employ the Wigner-Seitz approximation to Coulomb corrections. In principle more complicated models could easily be used. The volume of a charge neutral spherical cell containing a nucleus of charge Z_i is

$$v_{WS,i} = \frac{Z_i - v_i n_{p,o}}{n_e - n_{p,o}}$$

and the fraction of this volume filled by the nucleus is

$$u_i = v_i / v_{WS,i} = \frac{n_e - n_{p,o}}{n_{p,i} - n_{p,o}}.$$

The total Coulomb contribution to the free energy for a single nucleus is then given by

$$F_{C,i} = \frac{3\alpha}{5 r_i} \left(Z_i - v_i n_{p,o}\right)^2 \mathcal{D}(u_i), \tag{11}$$

where $\mathcal{D}(u) = 1 - 3/2 u^{1/3} + u/2$. This expression is valid wether the exterior phase is low or high density and is applicable when calculating voids. Derivatives of this are also required

$$\begin{aligned}
\frac{\partial F_{WS,i}}{\partial \ln n_e} &= F_{WS,i} \frac{\mathcal{D}'}{\mathcal{D}} \frac{\partial u_i}{\partial \ln n_e} \\
\frac{\partial F_{WS,i}}{\partial \ln n_{p,o}} &= F_{WS,i} \frac{\mathcal{D}'}{\mathcal{D}} \frac{\partial u_i}{\partial \ln n_{p,o}} - v_i \frac{F_{WS,i}}{Z_i - v_i n_{p,o}} \\
\frac{\partial F_{WS,i}}{\partial v_i} &= \frac{F_{WS,i}}{v_i} \left[\frac{\mathcal{D}'}{\mathcal{D}} \frac{\partial u_i}{\partial \ln v_i} - \frac{2 n_{p,o}}{n_{p,i} - n_{p,o}} - \frac{1}{3} \right].
\end{aligned}$$

4.2 Surface Tension

■ **[TODO: Come up with a decent surface tension prescription]** ■

5 Dealing with nuclear inversion

■ **[TODO: Not sure how to deal with it smoothly]** ■

6 Numerics

■ **[TODO: Write up what you are doing]** ■

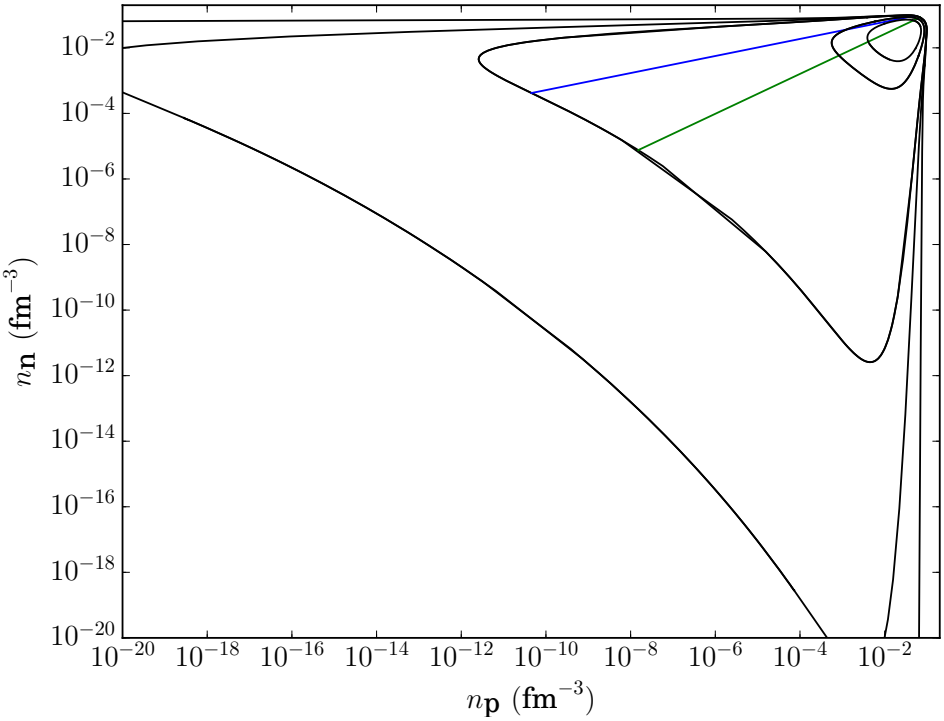

Figure 1: Phase boundaries for a variety of temperatures with LS Skyrme.

6.1 Gibbs Phase Equilibrium Solver

6.2 NSE Solver