NSE EOS Notes

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Contents

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

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

where f_B is the free energy of homogeneous nuclear matter per volume, 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). Here, $V_o = V - \sum v_i \mathcal{N}_i$ is the volume not taken up by nuclei. 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

$$\sum \mathcal{N}_i Z_i + Z_o = Z \tag{3}$$
$$\sum \mathcal{N}_i N_i + N_o = N \tag{4}$$
$$\sum \mathcal{N}_i v_i + V_o = V, \tag{5}$$

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

$$Z_i + \frac{\partial Z_o}{\partial \mathcal{N}_i} = 0, \quad N_i + \frac{\partial N_o}{\partial \mathcal{N}_i} = 0 \tag{6}$$
$$v_i + \frac{\partial V_o}{\partial \mathcal{N}_i} = 0, \quad \mathcal{N}_i + \frac{\partial V_o}{\partial v_i} = 0 \tag{7}$$

and results in the system of equations

$$\frac{\partial F}{\partial \mathcal{N}_i} = v_i f_{B,i} + F_{FS,i} + \mu_{K,i} + E_{0,i} - Z_i \mu_{p,o} - N_i \mu_{n,o} + v_i P_o = 0 \tag{8}$$
$$\frac{\partial F}{\partial v_i} = \mathcal{N}_i \left(-P_{B,i} - P_{FS,i} + P_o\right) = 0 \tag{9}$$
$$\sum Z_i n_i + \left(1 - \sum v_i n_i\right) n_{p,o} = n_p = n_e \tag{10}$$
$$\sum N_i n_i + \left(1 - \sum v_i n_i\right) n_{n,o} = n_n, \tag{11}$$

where we have defined $\mu_{K,i} = T \ln(A_i^{-3/2} n_i / n_Q)$, $P_{B,i} = -\partial(v_i f_{B,i})/\partial v_i$, and $P_{FS,i} = -\partial(F_{S,i})/\partial v_i$.

2.2 Connection to NSE

Here we discuss the physics of NSE for an ensemble of non-interacting nuclei and show how a similar formulation results from our multi-nucleus Gibbs construction.

2.2.1 Basic NSE

For a reaction $i \leftrightarrow j + k$, it is easy to show that the principle of detailed balance implies that

$$\mu_i = \mu_j + \mu_k \tag{12}$$

holds when the forward rate balances the backward rate. When all strong interactions are in equilibrium with their inverses, invoking detailed balance for all of the reactions implies that

$$\mu_i = N_i \mu_n + Z_i \mu_p. \tag{13}$$

where N_i is the number of neutrons and Z_i is the number of protons in a nucleus of species i. This of course implies that if the neutron and proton number densities are known, the number densities of all other species in the medium are known. Assuming that the heavy nuclei obey Boltzmann statistics (i.e. $\mu_i = m_i + T \ln [n_i/(G_i n_Q)]$ gives

$$n_i = A_i^{3/2} G_i(T) n_Q \exp\left(\left[Z_i \mu_p + N_i \mu_n - m_i\right]/T\right), \tag{14}$$

where G_i is the temperature dependent internal partition function of species i. When neutrons and protons also obey Boltzmann statistics, the number density can be expressed as

$$n_i = \frac{A_i^{3/2} G_i(T)}{2^{A_i} n_Q^{A_i-1}} n_n^{N_i} n_p^{Z_i} \exp(BE_i/T), \tag{15}$$

where BE_i is the binding energy and G_i is the internal partition function of species i.

Rather than being given the free proton and neutron densities, we often only know the total neutron and proton densities. In that case the equations of neutron and proton number conservation must be solved as functions of the free proton and neutron number densities

$$n_{n,o} + \sum_i^{\text{nuclei}} N_i n_i(n_{n,o}, n_{p,o}) = n_n, \tag{16}$$

$$n_{p,o} + \sum_i^{\text{nuclei}} Z_i n_i(n_{n,o}, n_{p,o}) = n_p. \tag{17}$$

The equations of NSE can also be derived by writing minimizing the free energy of a multi-component gas subject to the constraints of neutron and proton number conservation. The free energy is just

$$F_{NSE} = V f_B(n_{p,o}, n_{n,o}, T) + \sum_i^{\text{nuclei}} \mathcal{N}_i \mathrm{f}_i(\mathcal{N}_i/V, T), \tag{18}$$

where V is the total volume of the system, $\mathcal{N}_i$ is the total number of particles of species i, and

$$\mathrm{f}_i = m_i + T \ln\left[\frac{\mathcal{N}_i}{V G_i(T)} \left(\frac{2\pi\hbar^2}{m_i T}\right)^{3/2}\right] - T \tag{19}$$

is the specific free energy of species i. ■ **[WARNING: We need to be careful about including the rest mass in the free energy, the Skyrme output does not include it so the nucleon binding energies should come in. This needs to be cleaned up both in the notes and in the code (although the code is currently consistent)]** ■ The NSE equations (equations 14, 16, and 17) result if this free energy is minimized with respect to the $\mathcal{N}_i$ while maintaining fixed total neutron number, proton number, and volume (similar to the procedure in section 2.1).

2.2.2 NSE with Excluded Volume Correction

A slightly more complicated for nuclei in a medium takes into account that the nuclei take up volume. The nuclei can exist in the whole volume, but neutrons and protons can only exist in the volume not taken up by nuclei. The free energy for this system can be written as

$$F_{EV} = \sum_i^{\text{nuclei}} V f_i(\mathcal{N}_i/V, T) + \left(1 - \sum_i^{\text{nuclei}} \mathcal{N}_i v_i\right) V \left[f_n + f_p\right]. \tag{20}$$

Minimizing this free energy results in a very similar set of equations to the NSE equations, but with a correction term to the number density of species i because of the energetic cost of excluding nucleons from its volume

$$n_{i,EV} = A_i^{3/2} G_i(T) n_Q \exp\left(\left[Z_i \mu_p + N_i \mu_n - m_i - v_i(P_n + P_p)\right]/T\right). \tag{21}$$

2.2.3 Relation of Multi-nucleus Gibbs to NSE

The constraint equations for our model free energy bear a strong resemblance to the excluded volume NSE equations (by construction). This can be seen by recasting equation 8 to

$$n_i = A_i^{3/2} n_Q \exp(Z_i(\mu_{p,o} - m_p) + N_i(\mu_{n,o} - m_n) + \tilde{B}_i - v_i P_o), \tag{22}$$

where

$$\tilde{B}_i(v_i, n_{p,o}, n_{n,o}, T) = Z_i m_p + N_i m_n - v_i f_{B,i} - F_{FS,i} - E_{0,i}. \tag{23}$$

We can also see that equation 9 is independent of $\mathcal{N}_i$ when n_i is non-zero. This allows us to express the nuclear volume as a function of only the properties of the external medium, $v_i = v_i(n_{p,o}, n_{n,o}, T)$, so that $\tilde{B}_i = \tilde{B}_i(n_{p,o}, n_{n,o}, T)$ is just an external density dependent binding energy for species i. For some choices of the properties of the external medium, the pressure equilibrium conditions cannot be met for any volume. This just implies that n_i must be zero, which also provides a solution to equation 9. When solutions are admitted, the expression for the number density of species i can be further massaged to look like standard NSE by expressing the thermal average of the excitation energy above the ground state as

$$\langle E^* \rangle = T \frac{d \ln G}{d \ln T}, \tag{24}$$

where $G(T)$ is the internal partition function of the gas and E^* is the excitation energy above the zero temperature ground state. To get the internal partition function outside the exponential as would be the case in NSE, we must make the identification $G_i = \exp(d \ln G / d \ln T)$. ■ **[TODO: This probably should reduce to something like a fermi gas model for the level density. Check if this is in fact the case.]** ■

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

$$P_{B,i} + P_{FS,i} = 0. \tag{25}$$

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. Combined with the proton and neutron density constraint equations, this results in the excluded volume NSE equations employed by Hempel, for instance. Further assuming that $\sum v_i n_i$ and $v_i P_o$ are negligible, which is a very good approximation at low density, results in the standard equations for low density NSE.

2.3 Connection 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

$$n_i P_{B,i} = n_i P_o \tag{26}$$
$$v_i f_{B,i} + E_{0,i} = Z_i \mu_{p,o} + N_i \mu_{n,o} - v_i P_o. \tag{27}$$

The relation $P_B = n_p \mu_p + n_n \mu_n - f_B$ (which holds for homogeneous matter) can then be employed to recast the constraints as

$$n_i P_{B,i} = n_i P_o \tag{28}$$
$$Z_i \left(\mu_{p,i} - \mu_{p,o}\right) + N_i \left(\mu_{n,i} - \mu_{n,o}\right) = 0 \tag{29}$$
$$\tag{30}$$

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.

2.4 Connection to the Single Nucleus Approximation

■ **[TODO: Write down constraint equations with single nuclear species with N and Z allowed to vary.]** ■

3 Thermodynamic Quantities

Remember the total energy is :

$F_{EV} = \sum_i N_i(F_i + F_{FS,i}) + (V - \sum_i N_i v_i)F_o = \sum_i N_i(F_i + F_{FS,i}) + V_o f_o$.

Here, $F_i = F_{bulk,i} + F_{CM,i}$.

And, the dependence on the volume of the individual nucleus has been used as a constraint:

$$\frac{\partial F_{EV}}{\partial v_i} = \frac{\partial F_i}{\partial v_i} + \frac{\partial F_{FS,i}}{\partial v_i} + \frac{\partial F_o}{\partial v_i} = 0 \tag{31}$$

Then, pressure is given by

$$\begin{aligned}
P = & -\frac{\partial F_{EV}}{\partial V} = -\frac{\partial V_o}{\partial V}\frac{\partial F_{EV}}{\partial V_o} \\
= & -\sum_i \mathcal{N}_i\left(\frac{\partial F_i}{\partial V_o} + \frac{\partial F_{FS,i}}{\partial V_o}\right) - \frac{\partial F_o}{\partial V_o} \\
= & P_o + \sum_i n_i T - \sum_i n_i V \left[\frac{\partial F_{FS,i}}{\partial n_{p,o}}\frac{\partial n_{p,o}}{\partial V_o} + \frac{\partial F_{FS,i}}{\partial n_{n,o}}\frac{\partial n_{n,o}}{\partial V_o} + \frac{\partial F_{FS,i}}{\partial n_e}\frac{\partial n_e}{\partial V}\right] \\
= & P_o + \sum_i n_i T - \sum_i n_i V \left[\frac{\partial F_{FS,i}}{\partial n_{p,o}}\left(-\frac{n_{p,o}}{V_o}\right) + \frac{\partial F_{FS,i}}{\partial n_{n,o}}\left(-\frac{n_{n,o}}{V_o}\right) + \frac{\partial F_{FS,i}}{\partial n_e}\left(-\frac{n_e}{V}\right)\right] \\
= & P_o + \sum_i n_i \left[T + \frac{1}{u_o}\frac{\partial F_{FS,i}}{\partial \ln n_{p,o}} + \frac{1}{u_o}\frac{\partial F_{FS,i}}{\partial \ln n_{n,o}} + \frac{\partial F_{FS,i}}{\partial \ln n_e}\right]
\end{aligned} \tag{32}$$

where $\frac{\partial \square}{\partial \ln n_q} \equiv n_q \frac{\partial \square}{\partial n_q}$.

?

$$P = P_o + \sum n_i \left[T + \frac{\partial F_{FS,i}}{\partial \ln n_e} + u_o \frac{\partial F_{FS,i}}{\partial \ln n_{p,o}} + u_o \frac{\partial F_{FS,i}}{\partial \ln n_{n,o}} \right] \tag{33}$$

The entropy is given by

$$s = u_o s_{B,o} + \sum n_i \left(S_{B,i} + \frac{5}{2} - \frac{\mu_{K,i}}{T} - \frac{\partial F_{FS,i}}{\partial T} \right). \tag{34}$$

The chemical potentials are

$$\mu_p = \mu_{p,o} + \sum_i \frac{n_i}{u_0} \frac{\partial F_{FS,i}}{\partial n_{p,o}}, \tag{35}$$

$$\mu_n = \mu_{n,o} + \sum_i \frac{n_i}{u_0} \frac{\partial F_{FS,i}}{\partial n_{n,o}}. \tag{36}$$

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 expressions for F_{FS} are 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

$$v_{WS,i} = \frac{Z_i - v_i n_{p,o}}{n_e - n_{p,o}} \tag{37}$$

and the fraction of this volume filled by the nucleus is

$$u_i = v_i / v_{WS,i} = \frac{n_e - n_{p,o}}{n_{p,i} - n_{p,o}}. \tag{38}$$

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

$$F_{C,i}(v_i, n_{p,o}, n_e) = \frac{3\alpha}{5 r_i} \left(Z_i - v_i n_{p,o} \right)^2 \mathcal{D}(u_i), \tag{39}$$

where $\mathcal{D}(u) = 1 - 3/2u^{1/3} + u/2$. 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

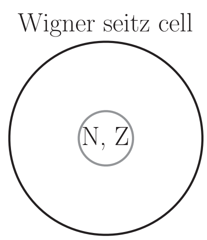
$$\frac{\partial F_{WS,i}}{\partial \ln n_e} = F_{WS,i}\frac{\mathcal{D}'}{\mathcal{D}}\frac{\partial u_i}{\partial \ln n_e} \tag{40}$$

$$\frac{\partial F_{WS,i}}{\partial \ln n_{p,o}} = F_{WS,i}\frac{\mathcal{D}'}{\mathcal{D}}\frac{\partial u_i}{\partial \ln n_{p,o}} - v_i\frac{F_{WS,i}}{Z_i - v_i n_{p,o}} \tag{41}$$

$$-P_{C,i} \quad = \quad \frac{\partial F_{WS,i}}{\partial v_i} = \frac{F_{WS,i}}{v_i}\left[\frac{\mathcal{D}'}{\mathcal{D}}\frac{\partial u_i}{\partial \ln v_i} - \frac{2n_{p,o}}{n_{p,i} - n_{p,o}} - \frac{1}{3}\right]. \tag{42}$$

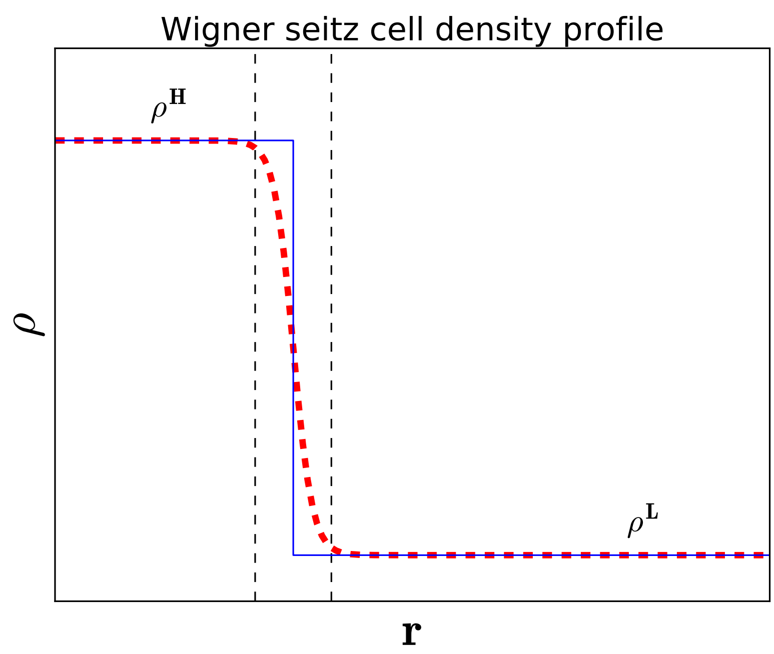
4.2 Surface Tension

Our description of the Wigner seitz cell:



Woods-Saxon model:

The desnity profile of the Wigner seitz cell is decomposed in terms of the Woods - Saxon function for the high density region (nucleus) and the low denisty region (nuclear medium outside):



$$
\begin{aligned}
n(r) =&n_{Nuc}(r) + n_{gas}(r) \\
=&\frac{n^H}{1+\exp[(r-R^{WS})/a_{WS}]} + \frac{n^L}{1+\exp[-(r-R^{WS})/a_{WS}]}
\end{aligned} \tag{43}
$$

where,

$$
\begin{aligned}
a_{WS} =&\alpha + \beta(\delta^H_{np})^2,\ \alpha \approx 0.53 \text{ fm}, \beta_n \approx 1.14 \text{ fm},\ \beta_p \approx 0.35 \text{ fm} \\
R^{WS} =&R_i[1 - \frac{\pi^2}{3}(\frac{a}{R_i})^2] \\
R_i =&(\frac{3V_i}{4\pi})^{1/3} \\
=&(\frac{3A_i}{4\pi n^H})^{1/3}
\end{aligned} \tag{44}
$$

Assuming $a \ll R_i \to R^{WS} \approx R_i$.

In our model, we assume two homogeneous phases of matter at different densities with a sharp transition from one to the other. This is represented by the step function in the figure. In order to make the 2 descriptions match, our description needs to include a surface contribution:

$$
E^H(R^{WS}-4a, R) + E^L(R, R^{WS}+4a) + E^S = E^{WS}(R^{WS}-4a, R^{WS}+4a),\ E^S = 4\pi(R^{WS})^2\sigma \tag{45}
$$

where, $E^H,\ E^L$ are the energies of homogeneous matter at $\rho^H,\ \rho^L$ respectively. E^{WS} is the energy of non-constant matter.

The skyrme energy density:

$$
\begin{aligned}
E/V =& \sum_{t=n,p}\frac{\hbar^2}{2M_q}\tau_q + \frac{1}{4}t_0\Big[(2+x_0)n^2 - (1+2x_0)\sum_{q=n,p}n_q^2\Big] \\
&+ \frac{1}{8}\Big[a(n\tau + \frac{3}{4}(\nabla n)^2) + 2b\sum_{q=n,p}(n_q\tau_q + \frac{3}{4}(\nabla n_q)^2)\Big] \\
&+ \frac{1}{24}t_3 n^\alpha\Big[(2+x_3)n^2 - (1+2x_3)\sum_{q=n,p}n_q^2\Big] \\
&= (E/V)_{\text{homogeneous}} + \frac{3}{32}\Big[a(\nabla n)^2 + 2b\sum_{q=n,p}(\nabla n_q)^2)\Big]
\end{aligned} \tag{46}
$$

Again assuming $a \ll R^{WS}$:

$$
\begin{aligned}
4\pi(R^{WS})^2\,\sigma \approx&[4\pi(R^{WS})^2 \times 8a_{WS}] \times \frac{3}{32}\Big[a(\nabla n)^2 + 2b\sum_{q=n,p}(\nabla n_q)^2)\Big] \leftrightarrow \\
\sigma =&\frac{3a_{WS}}{4}\Big[a(\frac{dn}{dr})^2 + 2b\big((\frac{dn_n}{dr})^2 + (\frac{dn_p}{dr})^2\big)\Big]\Big|_{R^{WS}}
\end{aligned} \tag{47}
$$

Given the functional form of the density profile: $(\frac{dn}{dr})^2\Big|_{r=R^{WS}} = \frac{(n_H-n_L)^2}{16\ {a_{WS}}^2}$. And, $a_{WS} = a_B \approx a_n$:

$$
\sigma =\frac{3}{64}\frac{(n_H-n_L)^2}{a_{WS}}\big[a\ + 2b(1+\frac{a^2_{WS}}{a^2_p})\big] \leftrightarrow \tag{48}
$$

$$
\boxed{\begin{aligned}
\sigma(n_H - n_L, \delta_{np}^H) =& \frac{3}{64}\frac{(n_H - n_L)^2}{\alpha + \beta_n\, {\delta_{np}^H}^2}\left[a \;+ 2b(1 + \frac{(\alpha + \beta_n\, {\delta_{np}^H}^2)^2}{(\alpha + \beta_p\, {\delta_{np}^H}^2)^2})\right] \\
a_{WS} =& \alpha + \beta(\delta_{np}^H)^2,\ \alpha \approx 0.53 \text{ fm}, \beta_n \approx 1.14 \text{ fm},\ \beta_p \approx 0.35 \text{ fm}
\end{aligned}}
$$

For ordinary nuclei (no surrounding nuclear medium) the diffuseness parameter is $a_{WS} = 0.55 \pm 0.05$ fm.

Thus, we can improve our model by accounting for medium effects in the surface tension.

$$
\begin{aligned}
E_i^S =& (36\pi)^{1/3} v_i^{2/3} \sigma(n_H - n_L, \delta_{np}^H) \\
P_i^S =& -\frac{2}{3}(36\pi)^{1/3} v_i^{-1/3} \sigma(n_H - n_L, \delta_{np}^H) + (36\pi)^{1/3} v_i^{2/3} \frac{\partial \sigma}{\partial v_i} \\
=& -\left[\frac{2E_i^S}{3v_i} + \frac{2E_i^S n_H}{v_i(n_H - n_L)}\right] \\
=& -\frac{2E_i^S}{3v_i}\left(1 + \frac{3n_H}{n_H - n_L}\right)
\end{aligned} \tag{49}
$$

If the diffunesess of ordinary nuclei is used, the assymetry dependence can be negleted:

$$
\sigma(n_H - n_L) = \frac{3}{64}\frac{(n_H - n_L)^2}{a_{WS}}(a + 4b),\ a_{WS} \approx 0.55 \text{ fm} \tag{50}
$$

Since the surface tension is a function of density, it will contribute to the chemical potentials of the mixed phase:

$$
\begin{aligned}
&\frac{\partial F_{S,i}}{\partial \ln n_e} = 0 \\
&\frac{\partial F_{S,i}}{\partial \ln n_{p,0}} = -2n_{p,0}\frac{E_{S,i}}{(n_H - n_L)} \\
&\frac{\partial F_{S,i}}{\partial \ln n_{n,0}} = -2n_{n,0}\frac{E_{S,i}}{(n_H - n_L)} \\
&\frac{\partial F_{S,i}}{\partial \ln n_{p,i}} = 2n_{p,i}\frac{E_{S,i}}{(n_H - n_L)} \\
&\frac{\partial F_{S,i}}{\partial \ln n_{n,i}} = 2n_{n,i}\frac{E_{S,i}}{(n_H - n_L)}
\end{aligned} \tag{51}
$$

5 Dealing with nuclear inversion

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

6 Numerics

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

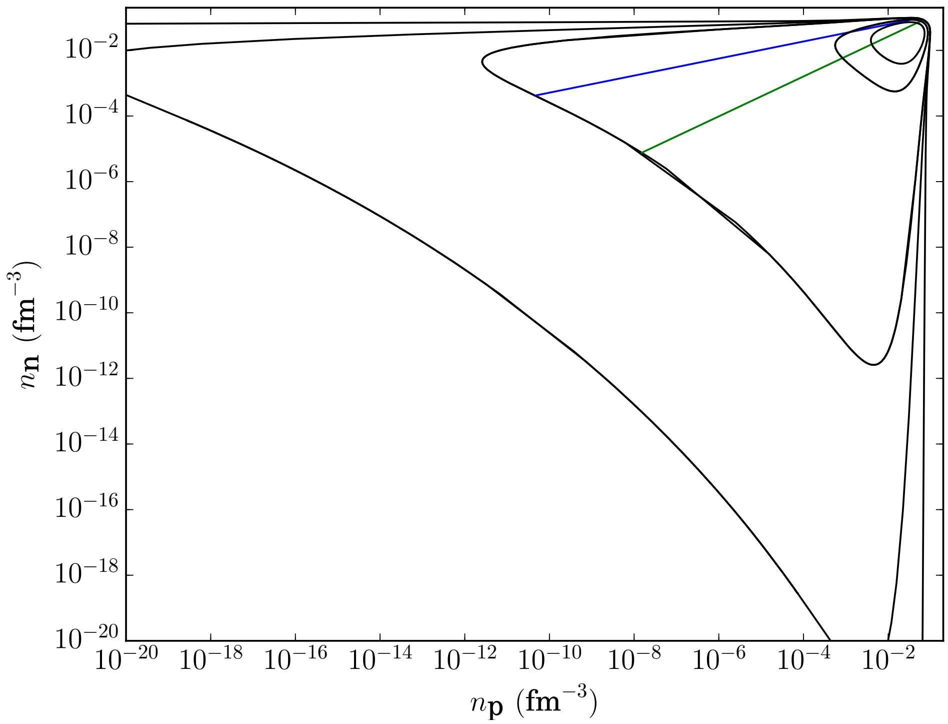


Figure 1: Phase boundaries for a variety of temperatures with LS Skyrme.

6.1 Gibbs Phase Equilibrium Solver

6.2 NSE Solver

The NSE solver and equation of state are found in the file `src/EquationsOfState/EOSNSE.hpp`. As was shown above, standard NSE, excluded volume NSE, and our model free energy share a very similar form. Therefore, a generic NSE solver with excluded volume corrections has been implemented. It takes a vector of nuclear species that all inherit from the class `NucleusBase`. For a given exterior state, these nuclei can return their binding energy, their internal partition function ■ **[TODO: implement the partition function for generality]** ■, and their volume. This implies that the NSE solver should be agnostic about what type of nuclei are being passed to it. Often, it is hard to find a solution to the NSE equations when the composition is dominated by nuclei. To increase the range over which the solver converges, we use a trick where we turn on the binding energies and volumes of the nuclei as if they were a perturbation. The number densities then are given by

$$n_i = A_i^{3/2} G_i(T) n_Q \exp\left(\left[Z_i(\mu_p - m_p) + N_i(\mu_n - m_n) - \lambda_B B_i - \lambda_v v_i P_o\right]/T\right). \tag{52}$$

A solution can easily be found when the λs are zero, and then they can be slowly increased to find a solution to our actual system of equations. There also seem to be problems when the neutrons and protons are assumed to be an interacting gas. This results in the chemical potentials decreasing with increasing density and prevents a solution from being found. Currently, it is unclear to me why this is the case. ■ **[TODO: Understand why this is the case.]** ■

7 Uniform Matter Thermodynamics

This section deals with the various relationships between the thermodynamic potentials and their derivatives in the framework of uniform matter. The set of independent parameters is given by (V, N, Y_i, T). In homogeneous matter, $\mathcal{E} = T\mathcal{S} - P + \mu_i n_i$, $\mathcal{F} = \mathcal{E} - T\mathcal{S} = -P + \mu_i n_i$. For constant volume calculations, the indpendent set of parameters becomes (n, Y_i, T) and the first law of thermodynamics can be written as follows,

$$d\mathcal{E} = Td\mathcal{S} + \mu_i dn_i, \;\; d\mathcal{F} = -\mathcal{S}dT + \mu_i dn_i, \; dP = SdT + n_i d\mu_i \tag{53}$$

where, $\mathcal{S} = S/V$, $n_i = N_i/V$, $n = \sum_i n_i, s = S/N = \mathcal{S}/n$, $f = F/N = \mathcal{F}/n$ and when taking partial derivatives, all other independent parameters are kept constant. Then, $\mu_i = \partial_{n_i}\mathcal{F}$, $\mathcal{S} = -\partial_T \mathcal{F} = \partial_T P$, $\mu_i = \partial \mu_i P$. In practice it is more convenient to work with the following set of parameters, $\mu = \mu_n - \mu_p$, $Y = Y_n - Y_p$ where,$1 = Y_n + Y_p$:

$$\begin{aligned} &d\mathcal{E} = Td\mathcal{S} + \mu dn, \;\; d\mathcal{F} = -\mathcal{S}dT + \mu dn, \; dP = SdT + nd\mu \\ &\mu = \partial_n \mathcal{E} = \partial_n \mathcal{F}, \; \mathcal{S} = -\partial_T \mathcal{F} = \partial_T P, \; n = \partial \mu P \end{aligned} \tag{54}$$

The 1^{st} order partial derivatives of f with respect to (n, Y, T) can be found:

$$\begin{aligned} &\partial_n f = -\mathcal{F}/n^2 + \partial_n \mathcal{F}/n = (-\mathcal{F} + \mu n)/n^2 = P/n^2 \\ &\partial_Y f = \frac{\partial \mathcal{F}}{n \partial Y} = \partial_n \mathcal{F} = \mu \\ &\partial_T f = \partial_T \mathcal{F}/n = -s \end{aligned} \tag{55}$$

So,

$$\boxed{\partial_n f = P/n^2, \; \partial_Y f = \mu, \; \partial_T f = -s} \tag{56}$$

And the 1^{st} law of thermodynamics for the pressure, $dP = SdT + nd\mu$, with (n, T, Y) as independent parameters:

$$\begin{aligned} \partial_n P =& n\partial_n \mu \\ \partial_T P =& S = ns + \partial_T \mu \\ \partial_Y P =& n\partial_Y \mu \end{aligned} \tag{57}$$

The 2^{nd} order mixed partial derivatives give thermodynamic relations among (P, μ, s):

$$\begin{aligned} \partial_{Tn} f = \partial_{nT} f \rightarrow -\partial_n s =& \partial_T P/n^2 \\ \partial_{TY} f = \partial_{YT} f \rightarrow \partial_T \mu =& -\partial_Y s \\ \partial_{Yn} f = \partial_{nY} f \rightarrow \partial_n \mu =& \partial_Y P/n^2 \end{aligned} \tag{58}$$

Combining the 2 set of identities above:

$$\begin{aligned} -\partial_n s = \partial_T P/n^2 = (ns + \partial_T \mu)/n^2 =& s/n \partial_T \mu/n^2 = s/n - \partial_Y s/n^2 \leftrightarrow \\ s =& \partial_Y s/n - n\partial_n s \end{aligned} \tag{59}$$

Also,

$$\begin{aligned}\partial_T P =& ns + \partial_T \mu \leftrightarrow \\ \partial_{YT} f =& n^2 \partial_{nT} f + n \partial_T f\end{aligned} \tag{60}$$

The remaining 2^{nd} order partial derivatives:

$$\begin{aligned}\partial_{nn} f =& \partial_n (P/n^2) = \partial_n P/n^2 - 2P/n^3 \\ =& \partial_{\{nY\}} f/n - 2\partial_n f/n \\ \partial_{YY} f =& \partial_Y \mu \\ =& \partial_Y P/n \\ =& n\partial_{nY} f \\ \partial_{TT} f =& -\partial_T s\end{aligned} \tag{61}$$

Since all mixed partial derivatives should be equal under permutations of the order of taking the derivatives, for higher order derivatives all possible permutations will be denoted by $\{\}$. For instance, all mixed derivatives from T, n, Y will be denoted by $\partial_{\{YTn\}} f$.

Thus, at 2^{dn} order, there are only 3 independent partial derivatives and the rest can be calculated from them:

$$\boxed{\begin{aligned}\partial_{YY} f =& n\partial_{\{nY\}} f = n^2 \partial_{nn} f + 2n\partial_n f \\ \partial_{\{YT\}} f =& n^2 \partial_{\{nT\}} f + n\partial_T f\end{aligned}} \tag{62}$$

$$\boxed{\begin{aligned}&\partial_{\{nY\}} f = \partial_n P/n = \partial_n \mu = \partial_Y P/n^2 = \partial_Y \mu/n \\ &\partial_{\{nT\}} f = s/n + \partial_T \mu/n^2 = s/n - \partial_Y s/n^2 = \partial_T P/n^2 = -\partial_n s \\ &\partial_{TT} f = -\partial_T s\end{aligned}} \tag{63}$$

All 3^{rd} order derivatives based on $\partial_{TT} f$:

$$\begin{aligned}\partial_{TTT} f =& -\partial_{TT} s \\ \partial_{\{TTn\}} f =& \partial_{\{TTY\}} f/n^2 - \partial_{TT} f/n \\ =& -\partial_{\{Tn\}} s = \partial_T s/n + \partial_{TT}\mu/n^2 = \partial_T s/n - \partial_{YT} s/n^2 = \partial_{TT} P/n^2\end{aligned} \tag{64}$$

All remaining 3^{rd} order derivatives based on $\partial_{nT} f$:

$$\begin{aligned}\partial_{\{nnT\}} f =& \partial_n \left[\partial_{\{YT\}} f/n^2 - \partial_T f/n\right] \\ =& \partial_{\{nTY\}} f/n^2 - 2\partial_{\{YT\}} f/n^3 - \partial_{\{nT\}} f/n + \partial_T f/n^2 \\ =& \partial_{\{nTY\}} f/n^2 - 3\partial_{\{nT\}} f/n + 2\partial_T f/n^2 \\ =& \partial_{\{Tn\}} P/n^2 - 2\partial_T P/n^3 = -\partial_{nn} s \\ =& \partial_n s/n - s/n^2 + \partial_{Tn}\mu/n^2 - 2\partial_T \mu/n^3 = \partial_n s/n - s/n^2 - \partial_{\{Yn\}} s/n^2 + 2\partial_Y s/n^3 \\ =& 3\partial_Y s/n^3 - 2s/n^2 - \partial_{\{Yn\}} s/n^2\end{aligned} \tag{65}$$

All remaining 3^{rd} order derivatives based on $\partial_{nY} f$:

$$\begin{aligned}\partial_{\{YYn\}} f =& \partial_{YYY} f/n = n\partial_{\{nnY\}} f + \partial_{\{nY\}} f = n^2 \partial_{nnn} f + 4n\partial_{nn} f + 2\partial_n f \\ \partial_{\{nnY\}} f =& \partial_{nY} P/n = \partial_{YY} P/n^2 = \partial_{nY}\mu = \partial_{YY}\mu/n\end{aligned} \tag{66}$$

Thus, at $3^r d$ order there are 4 independent partial derivatives:

$$\boxed{\begin{aligned}&\partial_{\{TTn\}} f = \partial_{\{TTY\}} f/n^2 - \partial_{TT} f/n \\ &\partial_{\{nnT\}} f = \partial_{\{nTY\}} f/n^2 - 3\partial_{\{nT\}} f/n + 2\partial_T f/n^2 \\ &\partial_{\{YYn\}} f = \partial_{YYY} f/n = n\partial_{\{nnY\}} f + \partial_{\{nY\}} f = n^2\partial_{nnn} f + 4n\partial_{nn} f + 2\partial_n f\end{aligned}} \tag{67}$$

$$\boxed{\begin{aligned}\partial_{TTT} f =& -\partial_{TT} s \\ \partial_{\{TTn\}} f =& -\partial_{\{Tn\}} s = \partial_T s/n + \partial_{TT}\mu/n^2 = \partial_T s/n - \partial_{YT} s/n^2 = \partial_{TT} P/n^2 \\ \partial_{\{nnT\}} f =& \partial_{\{Tn\}} P/n^2 - 2\partial_T P/n^3 = -\partial_{nn} s \\ =& \partial_n s/n - s/n^2 + \partial_{Tn}\mu/n^2 - 2\partial_T \mu/n^3 = 3\partial_Y s/n^3 - 2s/n^2 - \partial_{\{Yn\}} s/n^2 \\ \partial_{\{nnY\}} f =& \partial_{\{nY\}} P/n = \partial_{YY} P/n^2 = \partial_{\{nY\}}\mu = \partial_{YY}\mu/n\end{aligned}} \tag{68}$$

All 4^{th} order derivatives based on $\partial_{TTT} f$:

$$\begin{aligned}\partial_{TTTT} f =& -\partial_{TTT} s \\ \partial_{\{TTTn\}} f =& \partial_{\{TTTY\}} f/n^2 - \partial_{TTT} f/n \\ =& -\partial_{\{TTn\}} s = \partial_{\{TT\}} s/n + \partial_{TTT}\mu/n^2 = \partial_{\{TT\}} s/n - \partial_{\{YTT\}} s/n^2 = \partial_{TTT} P/n^2\end{aligned} \tag{69}$$

All remaining 4^{th} order derivatives based on $\partial_{TTn} f$:

$$\begin{aligned}\partial_{\{TTnn\}} f =& \partial_{\{TTYn\}} f/n^2 - 2\partial_{\{TTY\}} f/n^3 + \partial_{\{TT\}} f/n^2 - \partial_{\{nTT\}} f/n \\ =& \partial_{\{TTYn\}} f/n^2 - 3\partial_{\{TTY\}} f/n^3 + 2\partial_{TT} f/n^2 \\ =& -\partial_{\{nnT\}} s = \partial_{\{Tn\}} s/n - \partial_T s/n^2 + \partial_{\{nTT\}}\mu/n^2 - 2\partial_{TT}\mu/n^3 \\ =& \partial_{\{Tn\}} s/n - \partial_T s/n^2 - \partial_{\{YTn\}} s/n^2 + 2\partial_{\{YT\}} s/n^3 \\ =& 3\partial_{\{YT\}} s/n^3 - 2\partial_T s/n^2 - \partial_{\{YTn\}} s/n^2 \\ =& \partial_{\{TTn\}} P/n^2 - 2\partial_{TT} P/n^3 \\ \partial_{\{TTnY\}} f =& \partial_{\{TTYY\}} f/n^2 - \partial_{\{TTY\}} f/n\end{aligned} \tag{70}$$

All remaining 4^{th} order derivatives based on $\partial_{nnT} f$:

$$\begin{aligned}
\partial_{\{nnnT\}} f =& \partial_n \left[\partial_{\{nTY\}} f/n^2 - 3\partial_{\{nT\}} f/n + 2\partial_T f/n^2 \right] \\
=& \partial_{\{nnTY\}} f/n^2 - 2\partial_{\{nTY\}} f/n^3 - 3\partial_{\{nnT\}} f/n + 5\partial_{\{nT\}} f/n^2 - 2\partial_T f/n^3 \\
=& \partial_{\{nnYT\}} f/n^2 - 5\partial_{\{TYn\}} f/n^3 + 14\partial_{\{nT\}} f/n^2 - 8\partial_T f/n^3 \\
=& \partial_{\{nnT\}} P/n^2 - 4\partial_{\{nT\}} P/n^3 + 6\partial_T P/n^4 = -\partial_{nnn} s \\
=& \partial_{nn} s/n - 2\partial_n s/n^2 + 2s/n^3 + \partial_{\{Tnn\}} \mu/n^2 - 4\partial_{\{Tn\}} \mu/n^3 + 6\partial_T \mu/n^4 \\
=& 5\partial_{\{nY\}} s/n^3 - 9\partial_Y s/n^4 - 2\partial_n s/n^2 + 4s/n^3 - \partial_{\{nnY\}} s/n^2 \\
\partial_{\{nnTY\}} f =& \partial_{\{YYnT\}} f/n^2 - 3\partial_{\{nTY\}} f/n + 2\partial_{\{TY\}} f/n^2
\end{aligned} \tag{71}$$

And, from $\partial_{YYn} f$:

$$\partial_{\{YYnT\}} = f\partial_{\{YYYT\}} f/n = n\partial_{\{nnYT\}} f + \partial_{\{nYT\}} f \ = n^2 \partial_{\{nnnT\}} f + 4n\partial_{\{nnT\}} f + 2\partial_{\{nT\}} f \tag{72}$$

All remaining 4^{th} order derivatives based on $\partial_{YYn} f$:

$$\begin{aligned}
\partial_{\{YYnn\}} f =& \partial_{\{YYYn\}} f/n - \partial_{YYY} f/n^2 = n\partial_{\{nnnY\}} f + 2\partial_{\{nnY\}} f = n^2 \partial_{nnnn} f + 6n\partial_{nnn} f + 6\partial_{nn} f \\
\partial_{\{nnnY\}} f =& \partial_{\{nnY\}} P/n - \partial_{\{nY\}} P/n^2 = \partial_{\{YYn\}} P/n^2 - 2\partial_{YY} P/n^3 = \partial_{\{nnY\}} \mu = \partial_{\{YYn\}} \mu/n - \partial_{YY} \mu/n^2
\end{aligned} \tag{73}$$

Thus, at $4^t h$ order there are 5 independent partial derivatives:

$$\boxed{\begin{aligned}
\partial_{\{TTTn\}} f =& \partial_{\{TTTY\}} f/n^2 - \partial_{\{TTT\}} f/n \\
\partial_{\{TTnn\}} f =& \partial_{\{TTYn\}} f/n^2 - 3\partial_{\{TTY\}} f/n^3 + 2\partial_{TT} f/n^2 \\
=& \partial_{\{TTYY\}} f/n^4 - 4\partial_{\{TTY\}} f/n^3 + 2\partial_{TT} f/n^2 \\
\partial_{\{nnYT\}} f =& \partial_{\{YYnT\}} f/n^2 - 3\partial_{\{nTY\}} f/n + 2\partial_{\{TY\}} f/n^2 \\
=& n^2 \partial_{\{nnnT\}} f + 5\partial_{\{nTY\}} f/n - 14\partial_{\{nT\}} f + 8\partial_T f/n \\
\partial_{\{YYnn\}} f =& \partial_{\{YYYn\}} f/n - \partial_{YYY} f/n^2 = n\partial_{\{nnnY\}} f + 2\partial_{\{nnY\}} f \\
=& n^2 \partial_{nnnn} f + 6n\partial_{nnn} f + 6\partial_{nn} f
\end{aligned}} \tag{74}$$

$$
\boxed{\begin{aligned}
\partial_{TTTT}f =& -\partial_{TTT}s\\
\partial_{\{TTTn\}}f =& -\partial_{\{TTn\}}s = \partial_{\{TT\}}s/n + \partial_{TTT}\mu/n^2 = \partial_{\{TT\}}s/n - \partial_{\{YTT\}}s/n^2 = \partial_{TTT}P/n^2\\
\partial_{\{TTnn\}}f =& -\partial_{\{nnT\}}s = \partial_{\{Tn\}}s/n - \partial_T s/n^2 + \partial_{\{nTT\}}\mu/n^2 - 2\partial_{TT}\mu/n^3\\
=&\partial_{\{Tn\}}s/n - \partial_T s/n^2 - \partial_{\{YTn\}}s/n^2 + 2\partial_{\{YT\}}s/n^3\\
=&3\partial_{\{YT\}}s/n^3 - 2\partial_T s/n^2 - \partial_{\{YTn\}}s/n^2\\
=&\partial_{\{TTn\}}P/n^2 - 2\partial_{TT}P/n^3\\
\partial_{\{nnnT\}}f =&\partial_{\{nnT\}}P/n^2 - 4\partial_{\{nT\}}P/n^3 + 6\partial_T P/n^4 = -\partial_{nnn}s\\
=&\partial_{nn}s/n - 2\partial_n s/n^2 + 2s/n^3 + \partial_{\{Tnn\}}\mu/n^2 - 4\partial_{\{Tn\}}\mu/n^3 + 6\partial_T\mu/n^4\\
=&5\partial_{\{nY\}}s/n^3 - 9\partial_Y s/n^4 - 2\partial_n s/n^2 + 4s/n^3 - \partial_{\{nnY\}}s/n^2\\
\partial_{\{nnnY\}}f =&\partial_{\{nnY\}}P/n - \partial_{\{nY\}}P/n^2 = \partial_{\{YYn\}}P/n^2 - 2\partial_{YY}P/n^3\\
=&\partial_{\{nnY\}}\mu = \partial_{\{YYn\}}\mu/n - \partial_{YY}\mu/n^2
\end{aligned}} \tag{75}
$$

5^{th} order partial derivatives based on $\partial_{TTTT}f$:

$$
\begin{aligned}
&\partial_{TTTTT}f = -\partial_{TTTT}s\\
&\partial_{\{TTTTY\}}f = n^2\partial_{TTTTn}f + n\partial_{TTTT}f\\
&\partial_{\{TTTTn\}}f = -\partial_{\{TTTn\}}s = \partial_{\{TTT\}}s/n + \partial_{TTTT}\mu/n^2 = \partial_{\{TTT\}}s/n - \partial_{\{TTTY\}}s/n^2 = \partial_{TTTT}P/n^2
\end{aligned} \tag{76}
$$

5^{th} order partial derivatives based on $\partial_{TTnn} f$:

$$
\begin{aligned}
\partial_{TTnnY} f =& \partial_{\{TTYYn\}} f/n^2 - 3\partial_{\{TTYY\}} f/n^3 + 2\partial_{\{TTY\}} f/n^2 \\
=& \partial_{\{TTYYY\}} f/n^4 - 4\partial_{\{TTYY\}} f/n^3 + 2\partial_{\{TTY\}} f/n^2 \\
=& -\partial_{\{nnTY\}} s = \partial_{\{TnY\}} s/n - \partial_{\{TY\}} s/n^2 + \partial_{\{nYTT\}} \mu/n^2 - 2\partial_{\{TTY\}} \mu/n^3 \\
=& \partial_{\{YTn\}} s/n - \partial_{\{YT\}} s/n^2 - \partial_{\{YYTn\}} s/n^2 + 2\partial_{\{YYT\}} s/n^3 \\
=& 3\partial_{\{YYT\}} s/n^3 - 2\partial_{\{TY\}} s/n^2 - \partial_{\{YYTn\}} s/n^2 \\
=& \partial_{\{TTnY\}} P/n^2 - 2\partial_{\{TTY\}} P/n^3 \\
\partial_{TTTnn} f =& \partial_{\{TTTYn\}} f/n^2 - 3\partial_{\{TTTY\}} f/n^3 + 2\partial_{TTT} f/n^2 \\
=& \partial_{\{TTTYY\}} f/n^4 - 4\partial_{\{TTTY\}} f/n^3 + 2\partial_{TTT} f/n^2 \\
=& -\partial_{\{nnTT\}} s = \partial_{\{TTn\}} s/n - \partial_{TT} s/n^2 + \partial_{\{TTTn\}} \mu/n^2 - 2\partial_{TTT} \mu/n^3 \\
=& \partial_{\{TTn\}} s/n - \partial_{TT} s/n^2 - \partial_{\{TTYn\}} s/n^2 + 2\partial_{\{TTY\}} s/n^3 \\
=& 3\partial_{\{TTY\}} s/n^3 - 2\partial_{TT} s/n^2 - \partial_{\{TTYn\}} s/n^2 \\
=& \partial_{\{TTTn\}} P/n^2 - 2\partial_{TTT} P/n^3 \\
\partial_{TTnnn} f =& \partial_n \left[\partial_{\{TTYn\}} f/n^2 - 3\partial_{\{TTY\}} f/n^3 + 2\partial_{TT} f/n^2\right] \\
=& \partial_n \left[\partial_{\{TTYY\}} f/n^4 - 4\partial_{\{TTY\}} f/n^3 + 2\partial_{TT} f/n^2\right] \\
=& \partial_{\{TTnnY\}} f/n^2 - 5\partial_{\{TTYn\}} f/n^3 - 9\partial_{\{TTY\}} f/n^4 + 2\partial_{\{TTn\}} f/n^2 - 4\partial_{TT} f/n^3 \\
=& \partial_{\{TTnnY\}} f/n^2 - 5\partial_{\{TTYn\}} f/n^3 - 7\partial_{\{TTY\}} f/n^4 - 6\partial_{TT} f/n^3 \\
=& \partial_{\{TTYYn\}} f/n^4 - 4\partial_{\{TTYY\}} f/n^5 - 4\partial_{\{TTYn\}} f/n^3 + 12\partial_{\{TTY\}} f/n^4 + 2\partial_{\{TTn\}} f/n^2 - 4\partial_{TT} f/n^3 \\
=& \partial_{\{TTYYn\}} f/n^4 - 4\partial_{\{TTYY\}} f/n^5 - 4\partial_{\{TTYn\}} f/n^3 + 14\partial_{\{TTY\}} f/n^4 - 6\partial_{TT} f/n^3 \\
=& \partial_{\{TTYYn\}} f/n^4 - 8\partial_{\{TTYY\}} f/n^5 + 16\partial_{\{TTY\}} f/n^4 - 6\partial_{TT} f/n^3
\end{aligned}
\tag{77}
$$