

Statistical Methods in Nuclear Physics

: Practical Approach

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Write down the total binding energy as a function density and think the way to solve it !

$$E = -BA + E_S A^{2/3} + E_C \frac{Z^2}{A^{1/3}}; \quad \text{In compressible model} \quad (1)$$

$$\begin{aligned} -B &\rightarrow -B + S_v(1 - 2x)^2 + \frac{K}{18} \left(1 - \frac{n}{n_0}\right)^2 \\ A &\rightarrow \frac{4\pi}{3} R^3 n, \quad E_S \rightarrow \sigma(x); \quad x \rightarrow \text{proton fraction} \end{aligned}$$

※ $\sigma(x)$ is the surface tension which can be obtained semi-infinite nuclear matter density profile. This is an quantities related to two phase(dense matter, dilute matter) equilibrium. Thus it is a thermodynamic quantity.

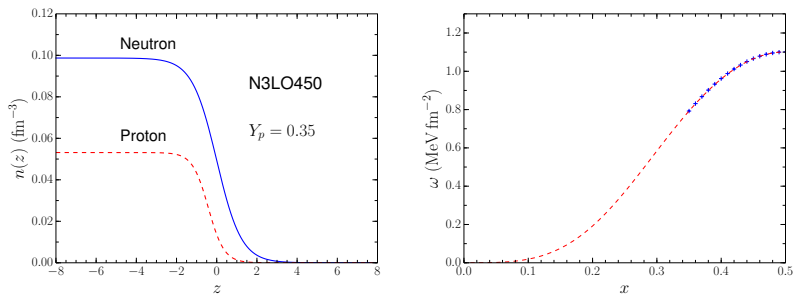


Figure: surface density profile (left) and surface tension (right)

$$\sigma(x) \simeq \sigma(x = 0.5) - \sigma_\delta(1 - 2x)^2 \quad (2)$$

$$f(n, x) = \left[-B + S_v(1 - 2x)^2 + \frac{K}{18} \left(1 - \frac{n}{n_0} \right)^2 \right] A \quad (3)$$
$$+ 4\pi R^2 \sigma(x) + \frac{3}{5} \frac{Z^2 e^2}{R}; \quad \text{Compressible model}$$

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No we forgot the constraints

$$A = \frac{4\pi}{3} R^3 n, \quad x = \frac{Z}{A} \quad (5)$$

Lagrange Multiplier Method

- How can we minimize some quantities with certain constraints?

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$$2x + \lambda = 0, \quad 2y + \lambda = 0, \quad x + y - 1 = 0 \quad (9)$$

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$$\mu_n = \frac{\partial F_N}{\partial n_n}, \quad \mu_p = \frac{\partial F_N}{\partial n_p}, \quad \mu_e = \frac{\partial F_e}{\partial n_e}, \quad \mu_\mu = \frac{\partial F_\mu}{\partial n_\mu}, \quad (12)$$

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$$\mu_n = \mu_p + \mu_e, \quad \mu_e = \mu_\mu, \quad (13)$$

- Apply Lagrange Multiplier method to the compressible liquid drop model

$$\begin{aligned}
 g(n, x) = & \left[-B + S_v(1 - 2x)^2 + \frac{K}{18} \left(1 - \frac{n}{n_0} \right)^2 \right] A \\
 & + 4\pi R^2 [\sigma_0 - (1 - 2x)^2 \sigma_\delta] + \frac{3}{5} \frac{Z^2 e^2}{R} \\
 & + \lambda_1 \left(A - \frac{4\pi R^3}{3} n \right) + \lambda_2 \left(\frac{Z}{A} - x \right)
 \end{aligned} \tag{14}$$

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- What are unknowns ? $n, x, R, \lambda_1, \lambda_2$

Using the notation $f_B(n, x) = -B + S_v(1 - 2x)^2 + \frac{K}{18} \left(1 - \frac{n}{n_0}\right)^2$

$$\frac{\partial g}{\partial n} = 0; \quad \frac{\partial f_B}{\partial n} A - \frac{4\pi R^3}{3} \lambda_1 = 0, \quad (15)$$

$$\frac{\partial g}{\partial x} = 0; \quad \frac{\partial f_B}{\partial x} A - 16\pi R^2 \delta^2 \sigma_\delta - \lambda_2 = 0, \quad (16)$$

$$\frac{\partial g}{\partial R} = 0; \quad 8\pi R[\sigma_0 - \delta^2 \sigma_\delta] + \frac{\partial E_C}{\partial R} - \lambda_1 4\pi R^2 n = 0, \quad (17)$$

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Next job is to reduce the equations as many as possible!

- λ_1 and λ_2 are related to chemical potential of neutrons and protons

$$\lambda_1 = n \frac{\partial f_B}{\partial n}, \quad \lambda_2 = \frac{\partial f_B}{\partial n} A - 16\pi R^2 \delta\sigma_\delta, \quad x = \frac{Z}{A} \quad (20)$$

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- The remaining two unknowns are n and x which can be obtained from two equations.

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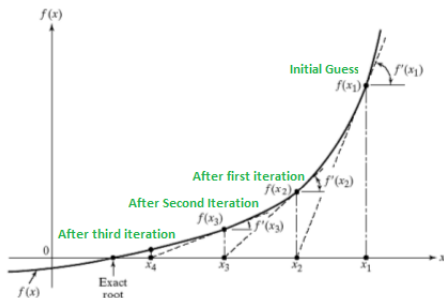
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Non-linear equations !

It's time to learn how to solve non-linear solutions.

Newton Raphson

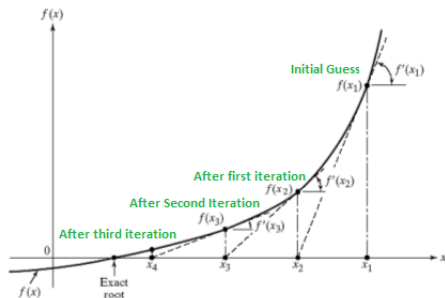
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$$x_{n+1} = x_n - f(x_n)/f'(x_n) \quad (22)$$

- Numerical derivative

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Depending on the relative size of x_j , λ_j (scale factor) is introduced,
 $\Delta x_j = -\lambda_j D_{ij}^{-1} f_i$

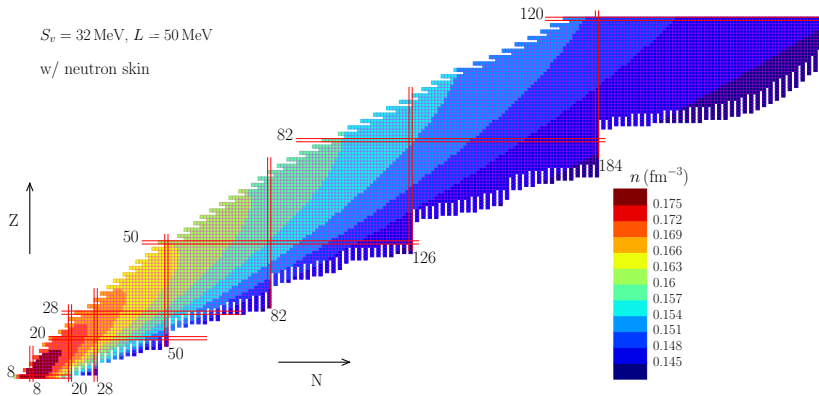


Figure: Bound nuclei with compressible model

Take home problem III

- If you can write a code (python, fortran, c, c++,...), Try to solve Eq.(21) for ^{56}Fe .
- You may use $B = -16 \text{ MeV}$, $S_v = 32 \text{ MeV}$, $K = 235 \text{ MeV}$, $\sigma_0 = 1.12 \text{ MeV fm}^{-2}$, $\sigma_\delta = 2.0 \text{ MeV fm}^{-2}$.
- You can try with initial guess $n = 0.16 \text{ fm}^{-3}$, $R = 1.12A^{1/3} \text{ fm}$.
- If you can solve for a given value of B , S_v , K , σ_0 , σ_δ , you can also find the optimized σ_0 and σ_δ .
- In the same manner, you can also find the pairing gap Δ and Shell corrections in the compressible model.
- See how the energy difference changes for N , Z , especially magic number.

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Tips

As you may know, if you meet some numerical problems, it always works if you can simplify the problems. In this case, you may start $f_B = -B$ or $\sigma_\delta = 0$ and increase the complexities to check your code.

Take Home Problem IV

- Energy density functional is a simple analytic function to describe energy density as a function of baryon number density and proton fraction (n, x).

$$\mathcal{E}(n, x) = \frac{\hbar^2}{2m} \tau_n + \frac{\hbar^2}{2m} \tau_p + (1 - 2x)^2 f_n(n) + [1 - (1 - 2x)^2] f_s(n),$$

- We can get the coefficients for Energy Density Functional utilizing the results from state of the art calculation for pure neutron matter EOS and symmetric nuclear matter properties.

First, the kinetic energy densities (τ_n, τ_p) (in the uniform) are given as

$$\tau_n = \frac{3}{5} (3\pi^2)^{2/3} (n(1-x))^{5/3}, \quad \tau_p = \frac{3}{5} (3\pi^2)^{2/3} (nx)^{5/3}$$

The potential energy parts are assumed to be

$$f_s(n) = \sum_{i=0}^3 a_i n^{(2+i/3)}, \quad f_n(n) = \sum_{i=0}^3 b_i n^{(2+i/3)}$$

- The definition of symmetric nuclear matter properties are

$$-B = \frac{\mathcal{E}}{n}, P = n^2 \frac{\partial}{\partial n} \left(\frac{\mathcal{E}}{n} \right), K = 9n^2 \frac{\partial^2}{\partial n^2} \left(\frac{\mathcal{E}}{n} \right), Q = 27n^3 \frac{\partial^3}{\partial n^3} \left(\frac{\mathcal{E}}{n} \right).$$

where every quantity is evaluated at $n = n_0$, $x = 1/2$.

From the properties finite nuclei, we have $B = 16\text{MeV}$,
 $P = 0$ ($n_0 = 0.16 \text{ fm}^{-3}$), $K = 235\text{MeV}$, $Q = -300\text{MeV}$

- Find the coefficient a_i from the symmetric nuclear matter properties !
- Find the coefficient b_j from the neutron matter EOS !

Fitting

This problem is related with the last lecture and a problem in there.

This is the data file for pure neutron matter from Many body perturbation calculation using chiral potential and three body forces.

k_F (fm ⁻¹)	n (fm ⁻³)	E/A (MeV)	k_F (fm ⁻¹)	n (fm ⁻³)	E/A (MeV)
0.66651	0.01	2.87933	1.48231	0.11	11.73104
0.83975	0.02	4.27096	1.52593	0.12	12.56379
0.96127	0.03	5.33345	1.56719	0.13	13.42159
1.05802	0.04	6.23757	1.60639	0.14	14.29794
1.13972	0.05	7.05834	1.64376	0.15	15.19301
1.21113	0.06	7.83732	1.6795	0.16	16.10768
1.27499	0.07	8.59843	1.71379	0.17	17.03337
1.33302	0.08	9.35958	1.74675	0.18	17.97216
1.3864	0.09	10.13324	1.77852	0.19	18.91497
1.43595	0.1	10.92077	1.80919	0.20	19.86317

LDM for the neutron star crust

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- First of all, we have to think the presence of electrons
- As density increases, neutrons drips out of neutron rich heavy nuclei
Unbound neutron exists
- Write energy contribution and apply Lagrange Multiplier Method with constraints !

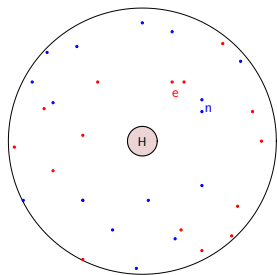
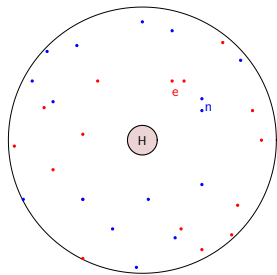
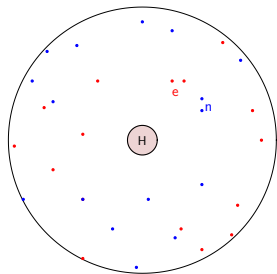


Figure: Wigner Seitz cell



F_i : Energy density of a heavy nucleus

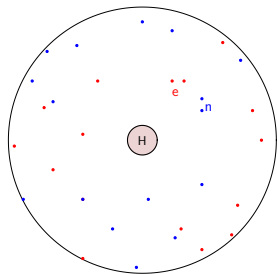
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F_i : Energy density of a heavy nucleus

F_s : Surface energy density

Figure: Wigner Seitz cell

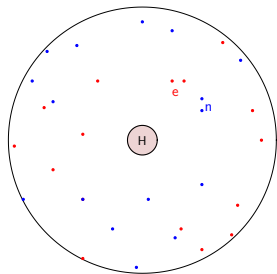


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F_s : Surface energy density

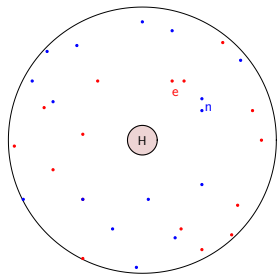
F_c : Coulomb energy density

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- F_i : Energy density of a heavy nucleus
- F_s : Surface energy density
- F_c : Coulomb energy density
- F_o : Energy density of outside nucleons

Figure: Wigner Seitz cell



- F_i : Energy density of a heavy nucleus
- F_s : Surface energy density
- F_c : Coulomb energy density
- F_o : Energy density of outside nucleons
- F_e : Electron energy density

Figure: Wigner Seitz cell

Nuclear pasta phase

- The ground state of nuclear shape is determined by the competition between Coulomb interaction and surface tension.

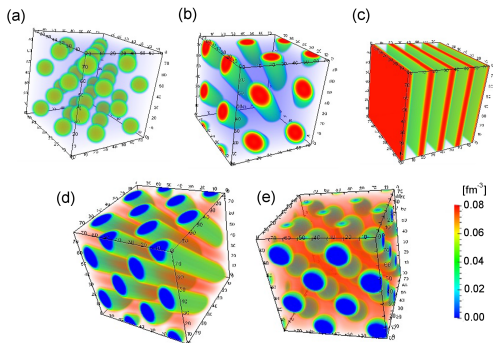


Figure: Numerical calculation of nuclear pasta phase. Figure from the work of Okamoto et al., Phys. Rev. C 88, 025801 (2013).

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 & + (1 - u)n_{no} f_o + f_e,
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with constraints

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 nY_p - un_i x_i &= 0, \\
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- $\partial F / \partial r_N \rightarrow F_S = 2F_C$ (the nuclear virial theorem)
- $\partial G / \partial n_e = 0$, the beta equilibrium is made.
- Finally, the unknowns will be (n_i, x_i, u, n_{no}) for a given (n, Y_p) .

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- Thermodynamic quantities from free energy density and during the process of looking for solutions

Take Home Problem V

- In this example, you may obtain the neutron star outer crust EOS using LDM.
- Since the outer crust does not have any unbound neutrons, Eq. (26) is simplified a lot.
- The valid dimension is $d = 3$. That is, spherically symmetric nuclei would be the ground state.
- The surface tension and discrete dimensional Coulomb f_d are given by

$$\begin{aligned}\sigma(x) &= \sigma_0 \frac{2^{\alpha+1} + q}{(1-x)^{-\alpha} + q + x^{-\alpha}}, \\ f_d(u) &= \frac{1}{d+2} \left[\frac{2}{d-2} \left(1 - \frac{1}{2} du^{1-2/d} \right) + u \right],\end{aligned}\tag{28}$$

where $\sigma_0 = 1.12 \text{MeV fm}^{-2}$, $q = 45$, and $\alpha = 3$.

- First, assume the electron energy but maintain f_d . Try to get Equations to solve in the outer crust, using the constraints for a given (n, Y_p)
- What happens if you add the electrons and minimize the energy density w.r.t. Y_p
- Estimate when $\mu_n > 0$ so that the neutron drip density is determined.