Heavy Nuclei in Neutron Star Crust

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Neutron Star Structure

- At the meeting of the American Physical Society in December 1933 (the proceedings were published in January 1934), Walter Baade and Fritz Zwicky proposed the existence of neutron stars, less than two years after the discovery of the neutron by Sir James Chadwick. (Wikipedia)
- Neutron stars was born from core-collapsing supernova explosion

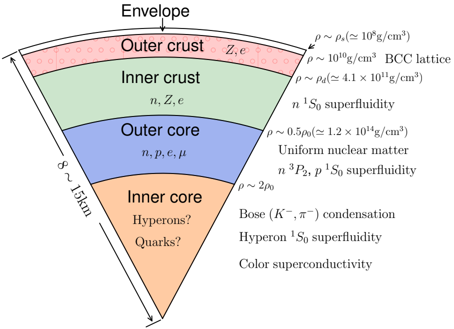


Figure : Schematic picture of neutron star structure

- Neutron stars consist of inner core, outer core, inner crust, and outer crust
- Superfluidity and Superconductivity
- Unknown properties for inner core
- Uniform nuclear matter in the outer core
- inhomogeneous nuclear matter in the inner crust
- ionized nuclei in the outer crust

- Neutron Star Mass and Radius : TOV equations

$$\frac{dp}{dr} = -e^{2\lambda}(\epsilon + p)\left(\frac{m}{r^2} + 4\pi r p\right),$$
$$\frac{dm}{dr} = 4\pi r^2 \epsilon.$$

- $\epsilon, p \rightarrow$ Nuclear equation of state
- Energy density functional

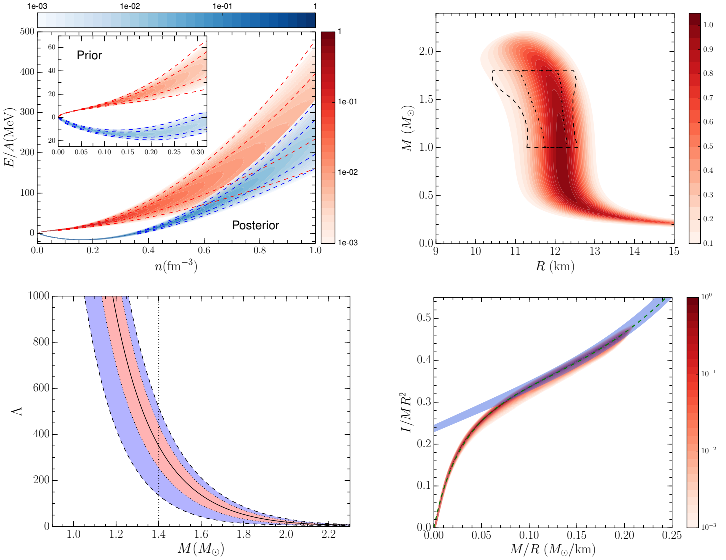
$$\mathcal{E}(n,x) = \frac{1}{2m}\tau_n + \frac{1}{2m}\tau_p + (1-2x)^2 f_n(n) + \left[1-(1-2x)^2\right] f_s(n)\,, \qquad (1)$$

  where n is the nucleon number density, τ_n and τ_p are the neutron and proton kinetic energy densities, x is the proton fraction,

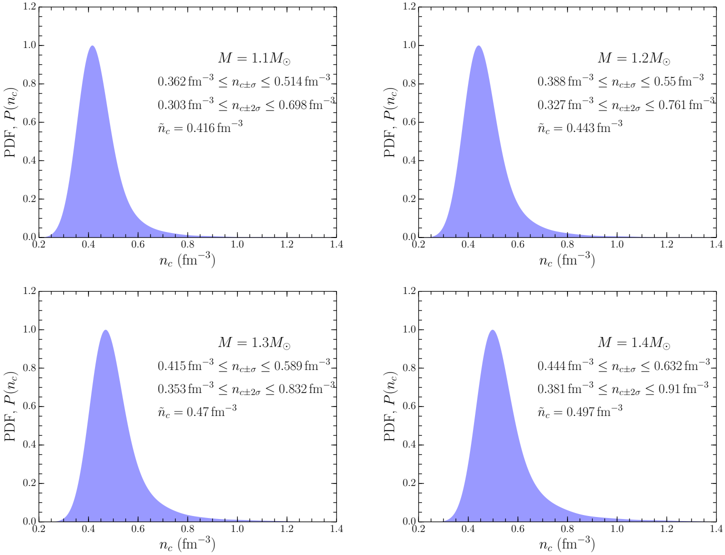
$$f_s(n) = \sum_{i=0}^{3} a_i n^{(2+i/3)}\,, \quad f_n(n) = \sum_{i=0}^{3} b_i n^{(2+i/3)} \qquad (2)$$

- Neutron & Symmteric matter from EFT (N2LO450, N2LO500, N3LO414, N3LO450, N3LO500)
- Symmetric matter from Finite nuclei properties (205 Skyrme force models)
- Neutron matter from FLT
- Or Bayesian (EFT$\rightarrow$ prior, Skyrme, FLT $\rightarrow$ Likelihood)

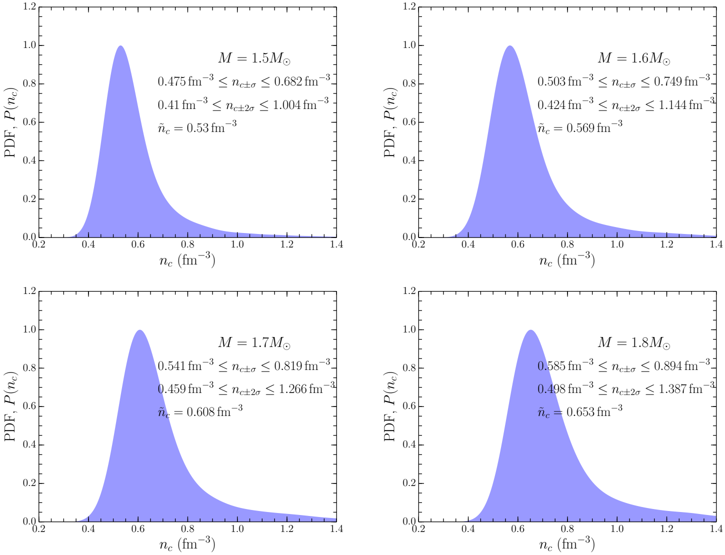
Neutron Star Phenomenology



Probability distribution of central density I



Probability distribution of central density II



Topology in neutron star crust

- Outer crust : isolated nuclei with unbound electrons
- Inner crust : Inhomogeneous nuclear matter
- Core-Crust boundary : Nuclear pasta phase

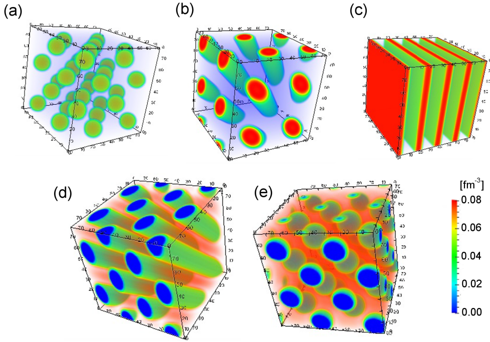


Figure : Pasta phase Okamoto et al. Phys.Rev. C88 (2013)

Numerical Method

- How can we calculate density profile of inhomogeneous nuclear matter?
- Liquid drop model
- Thomas Fermi Approximation
- Hartree-Fock method

Liquid Drop Model

- Well known method to calculate nuclear mass - Bulk, Surface, Coulomb, Pairing, Shell
- Density discontinuity at the surface
- Easy to manipulate
- Fast and accurate

$$F = un_i f_i + \frac{\sigma(x_i) u d}{r_N} + 2\pi(n_i x_i e r_N)^2 u f_d(u) + (1-u) n_{no} f_o \,, \tag{3}$$

where u is the filling factor for heavy nuclei to Winger-Seitz cell, n_i is the nuclear density of heavy nuclei, x_i is the proton fraction, f_i is the energy per baryon in heavy nuclei, $\sigma(x_i)$ is the surface tension as a function of proton fraction,

$$\sigma(x) = \sigma_0 \frac{2^{\alpha+1} + q}{(1-x)^{-\alpha} + q + x^{-\alpha}} . \tag{4}$$

$$\mu_{ni} - \frac{x_i \sigma'(x_i) d}{r_N n_i} = \mu_{no}\,, \tag{5a}$$

$$P_i - 2\pi (n_i x_i e r_N)^2 \frac{\partial (u f_d)}{\partial u} = P_{no}\,, \tag{5b}$$

$$n - u n_i - (1-u) n_{no} = 0\,, \tag{5c}$$

$$n Y_p - u n_i x_i = 0\,. \tag{5d}$$

The nuclear virial theorem tells $E_S = 2E_C$, where we can obtained from $\partial f / \partial r_N = 0$. This gives $E_S + E_C = \beta \mathcal{D}$,where $\beta = \left(\frac{243\pi}{2}\right)^{1/3} (n_i x_i e \sigma)^{2/3}$ and $\mathcal{D}(u) = u \left[\frac{d^2 f_d}{9}\right]^{1/3}$. If we allow d is continuous, we can find the shape function $\mathcal{D}$, which represents all pasta phase within single formula. We adopt the $\mathcal{D}$ used in Lattimer-Swesty EOS,

$$\mathcal{D}(u) = u(1-u) \frac{(1-u) f_3^{1/3} + u f_3^{1/3} (1-u)}{u^2 + (1-u)^2 + 0.6 u^2 (1-u)^2}\,. \tag{6}$$

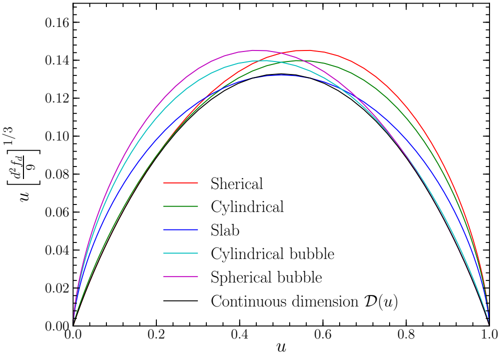


Figure : (Color online) Shape function, $\mathcal{D}(u)$ for specific dimension and continuous dimension. The continuous dimension is always minimum among other functions. Y. Lim and J.W. Holt, Phys. Rev. C 95, 065805 (2017)

Thomas Fermi Approximation

- Realistic density profile

$$n_t(r) = \begin{cases} (n_{ti} - n_{to}) \left[1 - \left(\frac{r}{R_t}\right)^{\alpha_t}\right]^3 + n_{to} & \text{if} \quad r < R_t\,, \\ n_{to} & \text{if} \quad r \geq R_t\,. \end{cases} \tag{7}$$

- Find Q for surface energy

When $\mu_n > 0$, $n_{no} \neq 0$, thus n_{no} represents the density of free gas of neutrons. Depending on the density, all parameters $(n_{ti}, n_{to}, r_t, R_t, \alpha_t)$ are to be obtained numerically from free energy minimization. The total energy minimized is given as

$$E = \int \Big[\mathcal{H}(n_n, n_p, \nabla n_n, \nabla n_p) + m_n n_n + m_p n_p + \mathcal{E}_{el}(n_e) + \mathcal{E}_{Coul}(n_p, n_e) + \mathcal{E}_{ex}(n_p, n_e)\Big]\, d\mathbf{r}\,, \tag{8}$$

where the Hamiltonian $\mathcal{H}$ is given as

$$\mathcal{H}(n_n, n_p, \nabla n_n, \nabla n_p) = \frac{\hbar^2}{2m_n}\tau_n + \frac{\hbar^2}{2m_p}\tau_p + V_{NN}(n_n, n_p) + \frac{1}{2}Q_{nn}(\nabla n_n^2 + \nabla n_p^2) + Q_{np}\nabla n_n \nabla n_p\,. \tag{9}$$

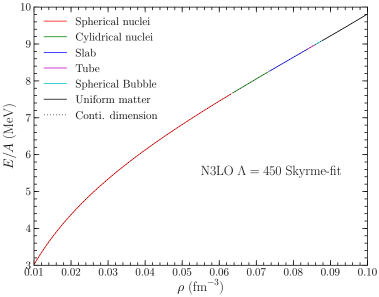


Figure : Energy per baryon of inhomogeneous nuclear matter. Left (LDM), Right (TF), Y. Lim and J.W. Holt, Phys. Rev. C 95, 065805 (2017)

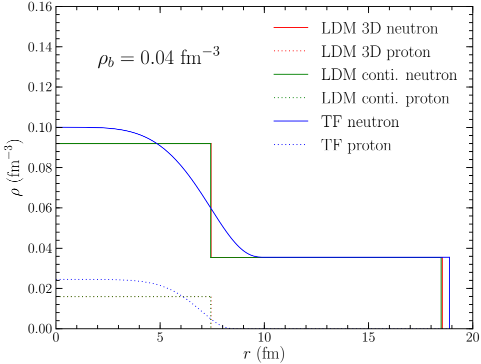


Figure : Neutron and proton density profile using three different numerical methods with $\Lambda = 450$. The neutron density of free gas are similar for each method. Y. Lim and J.W. Holt, Phys. Rev. C 95, 065805 (2017)

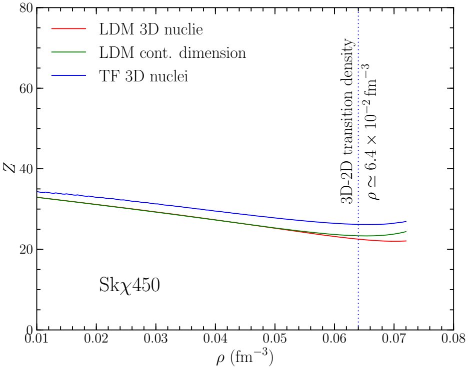


Figure : Atomic number for a given baryon number density. Y. Lim and J.W. Holt, Phys. Rev. C 95, 065805 (2017)

Hot dense matter : LDM

Hot dense matter EOS can be simply obtained by solving Fermi-Dirac statistics

$$\rho_t = \frac{1}{4\pi^2\hbar^3}\int_0^\infty f_t d^3p\,, \quad \tau_t = \frac{1}{4\pi^2\hbar^5}\int_0^\infty f_t p^2 d^3p \tag{10}$$

where t is the type of nucleon and f_t is the Fermi occupation fuction,

$$f_t = \frac{1}{1+\exp\left(\frac{\varepsilon_t-\mu}{k_B T}\right)}\,. \tag{11}$$

At $T = 0$ MeV, this equation simply gives $\tau_t = \frac{3}{5}(3\pi^2)^{2/3}\rho_t^{5/3}$.

And alpha particle

$$\begin{aligned} F =& u n_i f_i + \frac{\sigma(x_i)ud}{r_N} + 2\pi(n_i x_i e r_N)^2 u f_d(u) + (1-u)n_{no}f_o\,, \\ \rightarrow& \\ F =& u n_i f_i + \frac{\sigma(x_i)ud}{r_N} + 2\pi(n_i x_i e r_N)^2 u f_d(u) + (1-u)(1-n_\alpha v_\alpha)n_o f_o + (1-u)n_\alpha f_\alpha \end{aligned} \tag{12}$$

Hot dense matter : TF

α particle density

$$n_\alpha(r) = \begin{cases} n^o_\alpha - n^o_\alpha \left[1 - \left(\frac{r}{R_p}\right)^{\tau_p}\right]^3 & \text{if} \quad r < R_p \\ n^o_\alpha & \text{otherwise}\,. \end{cases} \tag{13}$$

Free energy density

$$F = \frac{1}{V}\int_0^{R_{WS}} [1 - n_\alpha(r) v_\alpha] F_N(n_n, n_p)\, d^3r + \frac{1}{V}\int_0^{R_{WS}} F_\alpha(n_\alpha)\, d^3r + \frac{1}{V}\int_0^{R_{WS}} F_C d^3r + \frac{1}{V}\int_0^{R_{WS}} F_\nabla d^3r\,. \tag{14}$$

Need to minimize the free energy w.r.t. $n_{n_i}, n_{p_i}, n_{n_o}, n_{p_0}, R_n, R_p, t_n, t_p, n^0_\alpha$

Hot dense matter phase boundaries : preliminary

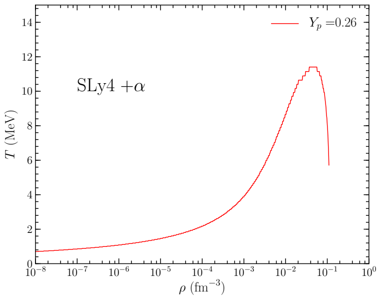


Figure : Phase boundaries of hot dense matter. Left (LDM), Right (TF), Y. Lim and J.W. Holt, in preparation

Hartree Fock Approximation

- Schrodinger or Dirac equation
- Microscopic approach
- Takes too long
- Shell energy effect : Spin-orbit coupling

$$
\begin{aligned}
v_{i,j}(\mathbf{k},\mathbf{k}') &= t_0(1+x_0P_\sigma)\delta(\mathbf{r}_i-\mathbf{r}_j) \\
&+ \frac{t_1}{2}(1+x_1P_\sigma)\left[\delta(\mathbf{r}_i-\mathbf{r}_j)\mathbf{k}^2+\mathbf{k}'^2\delta(\mathbf{r}_i-\mathbf{r}_j)\right] \\
&+ t_2(1+x_2P_\sigma)\mathbf{k}'\cdot\delta(\mathbf{r}_i-\mathbf{r}_j)\mathbf{k} \\
&+ \frac{1}{6}t_3(1+x_3P_\sigma)\rho^\alpha\delta(\mathbf{r}_i-\mathbf{r}_j) \\
&+ iW_0\mathbf{k}'\delta(\mathbf{r}_i-\mathbf{r}_j)\times\mathbf{k}\cdot(\boldsymbol{\sigma}_i+\boldsymbol{\sigma}_j)\,,
\end{aligned}
\tag{15}
$$

where P_σ is the spin exchange operator, $\mathbf{k}=\frac{1}{2i}(\nabla_i-\nabla_j)$, and $\mathbf{k}'=-\frac{1}{2i}(\nabla_i'-\nabla_j')$.

$$\left[-\frac{d}{dr}\mathcal{M}\frac{d}{dr} + \mathcal{U} + \mathcal{M}\frac{l(l+1)}{r^2} + \mathcal{M}'\frac{1}{r} + \mathcal{U}_{s.o.}\right] u = Eu\,, \tag{16}$$

where

$$\mathcal{M}_q = \frac{\hbar^2}{2m_q^*(n_q, n_{q'})} \tag{17}$$

By introducing new variables $u = \varphi/\sqrt{\mathcal{M}}$, we have

$$\left[-\mathcal{M}\frac{d^2}{dr^2} + V\right] \varphi = E\varphi\,, \tag{18}$$

where

$$V = \mathcal{U} + \mathcal{M}\frac{l(l+1)}{r^2} + \mathcal{M}'\frac{1}{r} + \mathcal{U}_{s.o.} + \frac{1}{2}\mathcal{M}'' - \frac{1}{4}\frac{\mathcal{M}'^2}{\mathcal{M}}\,, \tag{19}$$

where $\mathcal{M}' = \frac{d\mathcal{M}}{dr}$ and $\mathcal{M}' = \frac{d^2\mathcal{M}}{dr^2}$.

- Negele and Vautherin Nuclear Physics A 207, 298 (1973)
  - use DME
  - Boundary condition

$$\begin{cases} \left.\dfrac{d\psi}{dr}\right|_{r=R_c} = 0 & \text{if } l \text{ is even} \\ \psi(R_c) = 0 & \text{if } l \text{ is odd} \end{cases} \tag{20}$$

  - Spin-orbit interaction only for proton
  - Uniform electron density
  - No exchange Coulomb potential
  - Flattening of density at the surface

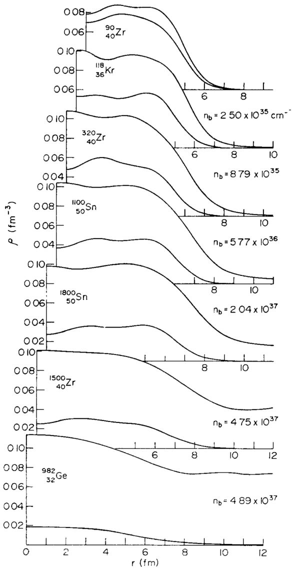
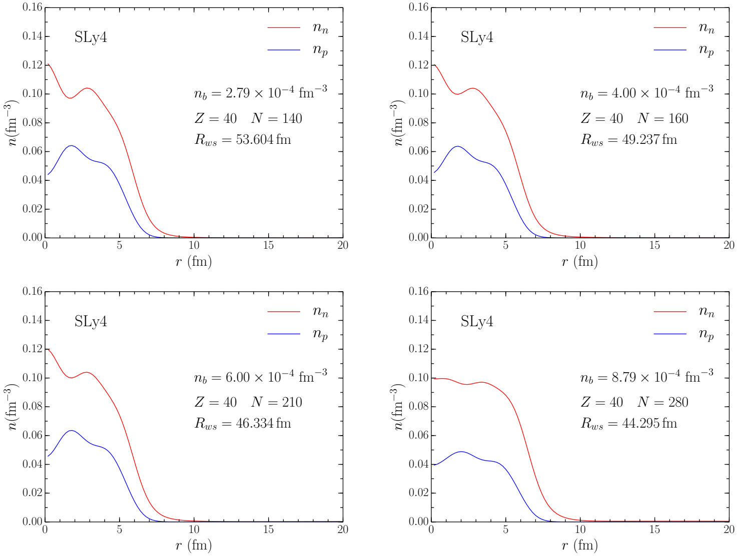
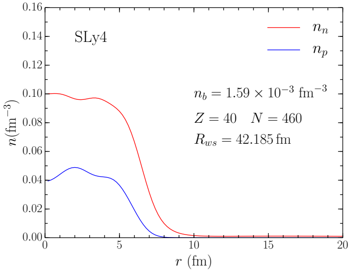


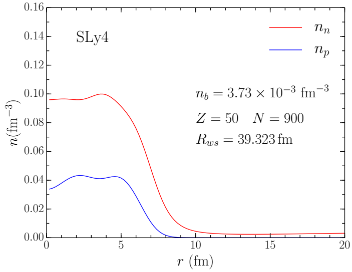
Figure : Nuclear density profile of heavy nuclei in the inner crust of neutron stars

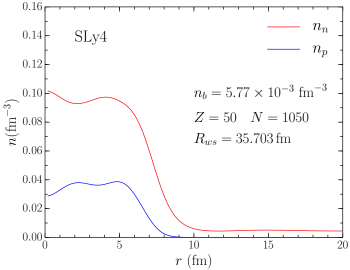
Preliminary I., Y.Lim & J.W. Holt, in preparation

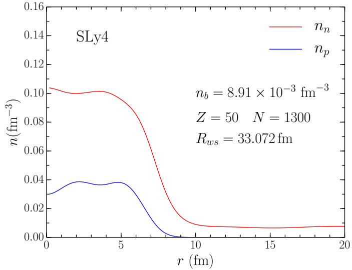


Preliminary II

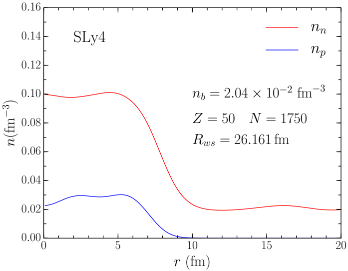


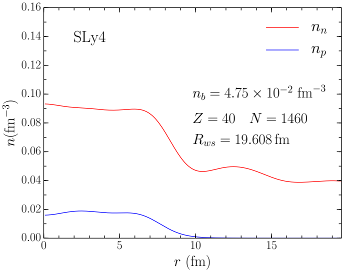


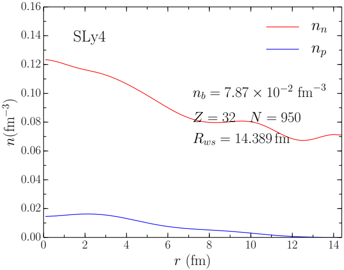




Preliminary III

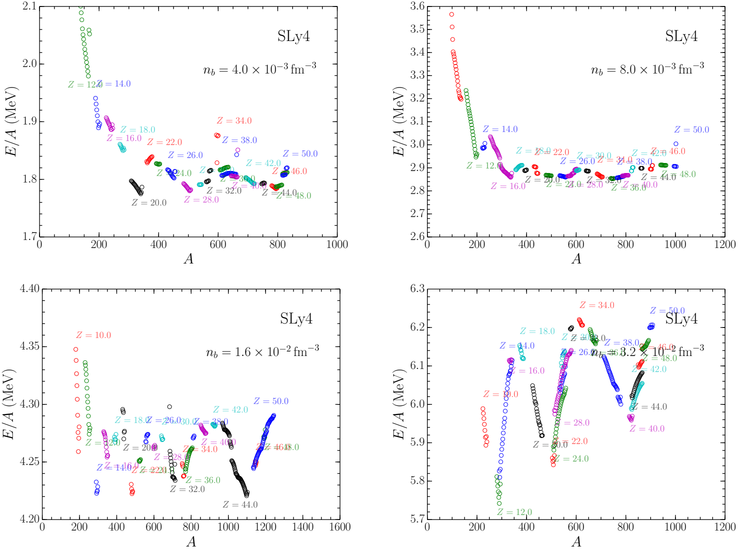




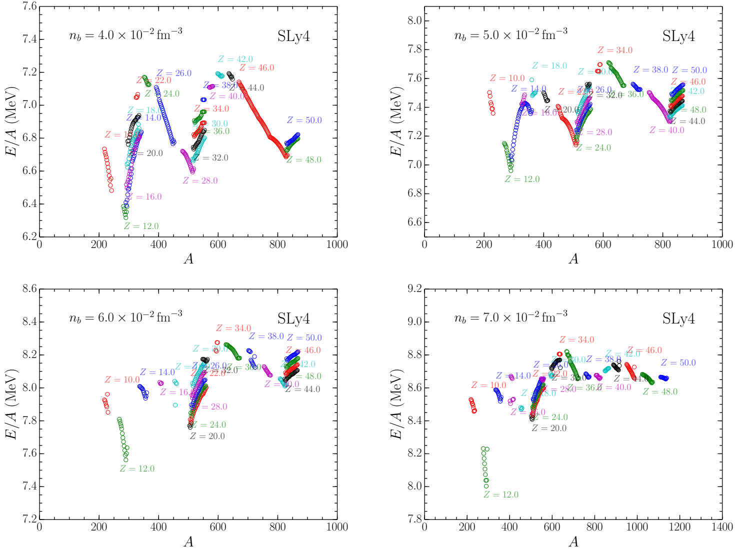


- The ground state for a given baryon number density
  - Have to search all possible configuration
  - Most time consuming
- Does not agree with the previous study by NV
  - Spin-orbit interaction is not strong
  - Might check the interaction

Preliminary IV



Preliminary V



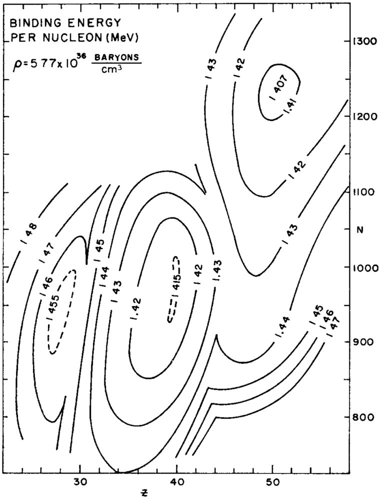


Figure : Contour plot of Z and A in NV, Nuclear Physics A 207, 298 (1973)

- NV calculation gives ground state $Z \geq 32$
- SLy4 $Z \geq 12$ is the ground state
- Energy from Spin-orbit small
- Domain for searching ground state is different
- Way to deal the density at the cell boundary is different
- Need to consider if we need to search ground state from $Z \geq 20$.
- Need to compare with LDM, and TF results

Wisdom from condensed matter physics

- Periodic boundary conditions

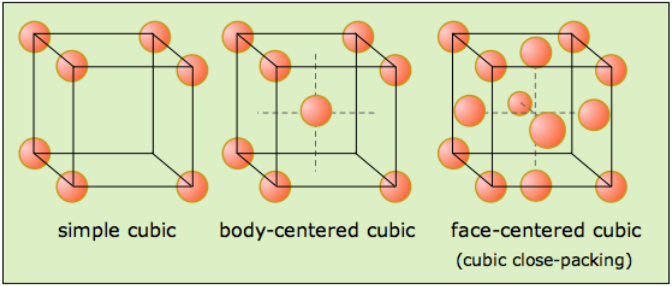


Figure : Simple lattice structure in sold

- Outer crust : Heavy nuclei in lattice site and unbound electrons (non-conductor)
- Inner crust : Valence neutrons floating around lattice sites (conductor)

Periodic condition

Few points about the periodic solid:

- Any translation of a Bravais lattice can be written as an integral multiple of primitive vectors
$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3\,. \tag{21}$$
Here $\mathbf{a}_i$ are primitive translations
- The reciprocal lattice vectors $\mathbf{K} = n_a\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3$ also form a Bravais lattice and the reciprocal primitive vectors are $\mathbf{b}_1 = 2\pi\frac{\mathbf{a}_2\times\mathbf{a}_3}{\mathbf{a}_1\cdot(\mathbf{a}_2\times\mathbf{a}_3)}$ and permutations.

- Any periodic function in a crystal satisfying $f(\mathbf{r}+\mathbf{R}) = f(\mathbf{r})$, has nonzero Fourier components only for reciprocal lattice vectors $\mathbf{K}$
  Example: Nuclear position, electron density,..
- The wave function in a solid satisfies the Bloch theorem

$$\boxed{\Psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})} \tag{22}$$

  where $u_{\mathbf{k}}(\mathbf{r})$ is periodic function $u(\mathbf{r}+\mathbf{R}) = u(\mathbf{r})$. Momentum $\mathbf{k}$ is a good quantum number. (Translation comutes with Hamiltonian).
- Any momentum can be written as a sum of a vector from a first Brillouin zone $\mathbf{k} = \frac{n_1}{N_1}\mathbf{b}_1 + \frac{n_2}{N_2}\mathbf{b}_2 + \frac{n_3}{N_3}\mathbf{b}_3$ and reciprocal lattice vector $\mathbf{K}$, i.e. $\mathbf{q} = \mathbf{k} + \mathbf{K}$. Here Ni is number of all lattice points in i-th direction and n_i is integer between 0 and $N_i - 1$. Obviously, number of $\mathbf{k}$ -points is the same as number of lattice points.

Augmented Plane Wave Method (APW)
The solution for wave functions in crystal is constructed as a linear combination of the APW basis functions

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{K}} A_{\mathbf{K}}(\mathbf{k}) \chi^{APW}_{\mathbf{k}+\mathbf{K}}(\mathbf{r}) \tag{23}$$

where

$$\chi^{APW}_{\mathbf{k}+\mathbf{K}}(\mathbf{r}) = \begin{cases} e^{i(\mathbf{k}+\mathbf{K})\cdot\mathbf{r}} & \text{if} \quad r > S; \\ \sum_L C_L(\mathbf{k}+\mathbf{K})\psi_L(\varepsilon, \mathbf{r}) & \text{if} \quad r < S \end{cases} \tag{24}$$

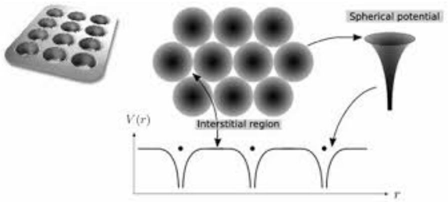


Figure : Schematic picture of lattice calculation

For sphere, $\psi_L(\varepsilon, \mathbf{r}) = i^l Y_L(\hat{\mathbf{r}})\psi_l(\varepsilon, r)$,

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + V(r) - \varepsilon\right] r\psi_l = 0\,. \tag{25}$$

Plane wave expansion in spherical coordinates,

$$e^{i\mathbf{qr}} = 4\pi \sum_L i^l j_l(qr) Y_L^*(\hat{\mathbf{q}}) Y_L(\hat{\mathbf{r}}) \tag{26}$$

where j_l are spherical Bessel functions. Matching in values at $r = S$,

$$C_L(\mathbf{q}) = 4\pi j_l(qr)\frac{Y_L^*(\mathbf{q})}{\psi_l(\varepsilon, S)}\,. \tag{27}$$

The secular equation in APW base takes the form

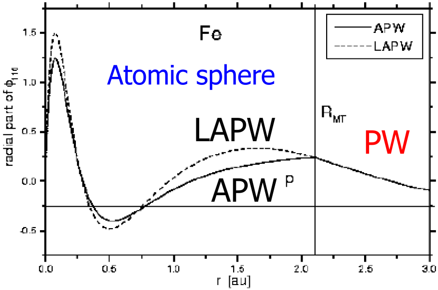
$$\sum_{\mathbf{K}} \langle \chi_{k+\mathbf{K}'}^{APW} | H - \varepsilon_{\mathbf{k}} | \chi_{k+\mathbf{K}'}^{APW} \rangle A_{\mathbf{K}}(\mathbf{k}) = 0\,. \tag{28}$$

Linear Augmented Plane Wave Method (LAPW)

The basic idea of any method starting with L (LAPW or LMTO) is to solve the Schroedinger equation for fixed energy E_ν rather than for the eigen-energy $\varepsilon_{\mathbf{k}} = \varepsilon$ (which would need to be determined self-consistently). To keep the good precision of the solution, one expands the solution of the Schroedinger equation in Taylor series (usually only to the linear order), i.e.,

$$\psi_l(\varepsilon, r) = \psi_l(E_\nu) + (\varepsilon - E_\nu)\frac{\partial}{\partial \varepsilon}\psi_l(E_\nu, r) \equiv \psi_l(E_\nu) + (\varepsilon - E_\nu)\dot{\psi}_l(E_\nu, r) \quad (29)$$

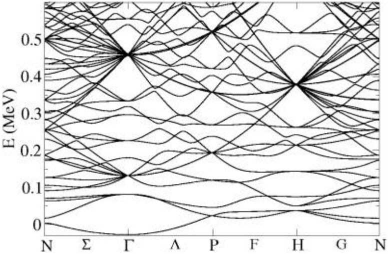
$$\chi^{LAPW}_{\mathbf{k}+\mathbf{K}}(\mathbf{r}) = \begin{cases} e^{i(\mathbf{k}+\mathbf{K})\cdot\mathbf{r}} & \text{if} \quad r > S; \\ \sum_L A_L(\mathbf{k}+\mathbf{K})\psi_L(\varepsilon, \mathbf{r}) + B_L(\mathbf{k}+\mathbf{K})\dot{\psi}_L(\varepsilon, \mathbf{r}) & \text{if} \quad r < S \end{cases} \quad (30)$$

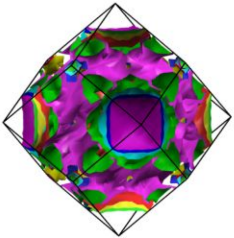


Figure

Nuclear Band Theory

The band theory is particularly well suited for studying the dynamics of the neutron superfluid, especially the reduction of the neutron superfluid density due Bragg scattering.





N. Chamel, Nucl. Phys. A747(2005), 109.

Preliminary VI, Y.Lim & J.W. Holt, in preparation

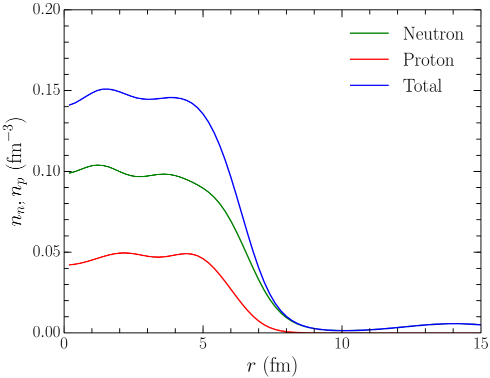


Figure : Density profile of finite nuclei ($Z = 40$, $A = 180$) using LAPW, Y.Lim & J.W. Holt, in preparation

Summary

- Neutron Star crust can be studied by
  - LDM, TF, HF (HFB), and LAPW
- Finite Temperature
  - Easily extended (LDM, TF)
  - Supernovae EOS
- Skyrme Hartree Fock 1D calculation for inhomogeneous matter
  - Might or might not work
  - Deformation
  - Thermodynamic consistency (p,ε, μ_n, μ_p,...)
- LAPW needs to be considered as a new method for physics in the crust
  - Huge matrix algebra