Energy density functional approaches to inhomogeneous superfluid neutron-star matter

Nakatsukasa, Takashi

University of Tsukuba

Supported by

QNP2024 @Barcelona, Spain, 2024.7.8-12
Contents

• Fermi Operator Expansion (FOE) method

• Self-consistent description of the inner crust
  • Band calculation for 1D slab (lasagna) phase
  • Effect of superfluidity

• Finite-temperature HFB in the 3D coordinate-space representation
  • Toward 2D, 3D phases
Crust of neutron stars

Chamel and Haensel, Living Rev. Relativity 11, 10 (2008)
Nuclei beyond the neutron drip line
+ low-density neutrons gas
+ electrons gas

(\rho_0 = 3 \times 10^{14} \text{ g cm}^{-3})

William G. Newton (2013)
Phenomena associated with crust

• Crustal oscillation
  Low frequency oscillation

• Cooling process
  Direct URCA process

• Pulsar glitch
  Entrainment for conduction neutrons

Static crust structure
Dynamic transport properties
Energy density functional method

• Energy density functional $E[\rho, \kappa]$
  • $\rho$: One-body density
  • $\kappa$: Pair density (abnormal density)

• Potentials
  • $V = \delta E / \delta \rho$: One-body (Kohn-Sham) potential
  • $\Delta = \delta E / \delta \kappa^*$: One-body (Kohn-Sham)

• Kohn-Sham-Bogoliubov equation
  • $\begin{pmatrix} h - \mu & \Delta \\ -\Delta^* & -(h - \mu)^* \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}$

• Diagonalization produces $\rho = V^*V^T, \kappa = V^*U^T$

• **Diagonalization** requires cost of computation $\propto N^3$
EDITORS' SUGGESTION

Fermi operator expansion method for nuclei and inhomogeneous matter with a nuclear energy density functional

Calculations for nuclear structure at high excitation energy or of nuclear matter in explosive stellar phenomena and neutron stars require intensive computations. The author tests the performance of a numerical method based on Fermi operator expansion that requires neither diagonalization nor Gram-Schmidt orthonormalization. The approach is suitable for massively parallel computing with distributed memory, and the calculations promise to scale well for large space sizes. Applied to finite nuclei and inhomogeneous nuclear matter, the method is efficient at high temperature, and the calculations clearly show the liquid-gas phase transition.

Takashi Nakatsukasa
Phys. Rev. C 107, 015802 (2023)
Density operator at finite $T$

- Fermi-Dirac distribution function
  \[ f_T(E) = \left( 1 + e^{\beta(E-\mu)} \right)^{-1} \]

- Fermi-Dirac distribution operator
  \[ f_T(\hat{H}) = \left( 1 + e^{\beta(\hat{H}-\mu)} \right)^{-1} \]

- One-body density
  \[ \rho_T = \sum_n |n\rangle f_T(E_n) \langle n| = f_T(\hat{H}) \approx \sum_{k=0}^{M} a_k T_k(\hat{H}) \]
  \[ H |n\rangle = E_n |n\rangle \]
Chebyshev expansion of $f_T(E)$

\[ f_T(E) = \frac{1}{1 + e^{\beta(E - \mu)}} \approx \sum_{k=0}^{M} a_k T_k(E) \]

$\mu = -14 \text{ MeV}$

$T = 5 \text{ MeV}, \quad M = 200$
Code

• Test Fortran code with MPI+OpenMP
• Energy density functional *w/o* pairing
  • Rectangular box with periodic boundary condition
  • FFT to construct the Coulomb potential
  • Kinetic energy computed with the finite difference
  • 3D square lattice

\[ \rho_T | \vec{r} \rangle = \sum_{k=0}^{M} a_k T_k (H) | \vec{r} \rangle \]

(25 fm)³ = 25³
Shape phase transition: $^{24}\text{Mg}$
Inhomogeneous symmetric nuclear matter

Box: $(23 \text{ fm})^3$
$n_b = 2.63 \times 10^{-3} \text{ fm}^{-3}$

From Bcc to simple cubic

$T = 5 \text{ MeV}$

$T = 2 \text{ MeV}$
Order-\(N\)

- Iterative computation of \(T_k(H)|i\rangle\)

\[ H |\vec{r}\rangle = \sum_{\vec{d}} c_{\vec{d}} |\vec{r} + \vec{d}\rangle \]

- Calculation of \(\rho_T(\vec{r}, \vec{r}')\) requires only a region around \(\vec{r}'\)

- Truncation for \(H^n |\vec{r}\rangle\), setting \(c_{\vec{d}} = 0\) for \(|\vec{d}| > d_0\)

\[ H^n |\vec{r}\rangle = \sum_{\vec{d}} c_{\vec{d}} |\vec{r} + \vec{d}\rangle \]

Off-diagonal elements of $\rho(0, \vec{r})$

$\rho_B = 0.03 \text{ fm}^{-3}$

$T = 5 \text{ [ MeV ]}$

$\rho(0, r) \text{ [ fm}^{-3}]$

$T = 10 \text{ [ MeV ]}$

$T = 50 \text{ [ MeV ]}$
Off-diagonal elements of $\rho(0, \vec{r})$

$log|\rho(0, r)|$

$\rho_B = 0.03 \text{ fm}^{-3}$
Pulsar glitch
Most promising glitch mechanisms

- Glitch origin: Inner crust
Moment of inertia ratio \((I_n: \text{Neutron Mol}, I: \text{Total Mol})\)

\[
I_n/I \approx 2\tau_c \mathcal{A}, \quad \text{where} \quad \mathcal{A} = \frac{1}{t_{\text{obs}}} \left( \sum_{i} \Delta \Omega^i_p / \Omega_p \right).
\]

<table>
<thead>
<tr>
<th>PSR</th>
<th>(\tau_c) (kyr)</th>
<th>(\mathcal{A}) (\times 10^{-9}/d)</th>
<th>(I_n/I) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>J0537-6910</td>
<td>4.93</td>
<td>2.40</td>
<td>0.9</td>
</tr>
<tr>
<td>B0833-45 (Vela)</td>
<td>11.3</td>
<td>1.91</td>
<td>1.6</td>
</tr>
<tr>
<td>J0631+1036</td>
<td>43.6</td>
<td>0.48</td>
<td>1.5</td>
</tr>
<tr>
<td>B1338-62</td>
<td>12.1</td>
<td>1.31</td>
<td>1.2</td>
</tr>
<tr>
<td>B1737-30</td>
<td>20.6</td>
<td>0.79</td>
<td>1.2</td>
</tr>
<tr>
<td>B1757-24</td>
<td>15.5</td>
<td>1.35</td>
<td>1.5</td>
</tr>
<tr>
<td>B1758-23</td>
<td>58.4</td>
<td>0.24</td>
<td>1.0</td>
</tr>
<tr>
<td>B1800-21</td>
<td>15.8</td>
<td>1.57</td>
<td>1.8</td>
</tr>
<tr>
<td>B1823-13</td>
<td>21.5</td>
<td>0.78</td>
<td>1.2</td>
</tr>
<tr>
<td>B1930+22</td>
<td>38.8</td>
<td>0.95</td>
<td>2.7</td>
</tr>
<tr>
<td>J2229+6114</td>
<td>10.5</td>
<td>0.63</td>
<td>0.5</td>
</tr>
</tbody>
</table>
Observation constraint

Andersson et al., PRL 109, 241103 (2012)

Moment of inertia ratio \( (I_n: \text{Neutron Mol}, I: \text{Total Mol}) \)

\[
I_n/I \approx 2\tau_c \mathcal{A}, \quad \text{where } \mathcal{A} = \frac{1}{t_{\text{obs}}} \left( \sum_i \frac{\Delta \Omega^i_p}{\Omega_p} \right).
\]

The characteristic age of pulsar

\[
\tau_c = -\frac{\Omega_p}{2\dot{\Omega}_p}.
\]

<table>
<thead>
<tr>
<th>PSR</th>
<th>( \tau_c ) (kyr)</th>
<th>( \mathcal{A} ) ( \times 10^{-9} / d )</th>
<th>( I_n/I ) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>J0537-6910</td>
<td>4.93</td>
<td>2.40</td>
<td>0.9</td>
</tr>
<tr>
<td>B0833-45 (Vela)</td>
<td>11.3</td>
<td>1.91</td>
<td>1.6</td>
</tr>
<tr>
<td>J0631+1036</td>
<td>43.6</td>
<td>0.48</td>
<td>1.5</td>
</tr>
<tr>
<td>B1338-62</td>
<td>12.1</td>
<td>1.31</td>
<td>1.2</td>
</tr>
<tr>
<td>B1737-30</td>
<td>20.6</td>
<td>0.79</td>
<td>1.2</td>
</tr>
<tr>
<td>B1757-24</td>
<td>15.5</td>
<td>1.35</td>
<td>1.5</td>
</tr>
<tr>
<td>B1758-23</td>
<td>58.4</td>
<td>0.24</td>
<td>1.0</td>
</tr>
<tr>
<td>B1800-21</td>
<td>15.8</td>
<td>1.57</td>
<td>1.8</td>
</tr>
<tr>
<td>B1823-13</td>
<td>21.5</td>
<td>0.78</td>
<td>1.2</td>
</tr>
<tr>
<td>B1930+22</td>
<td></td>
<td></td>
<td>2.7</td>
</tr>
<tr>
<td>J2229+6114</td>
<td></td>
<td></td>
<td>0.5</td>
</tr>
</tbody>
</table>

These ratios are consistent with the superfluid neutrons in the inner crust.
Entrainment effect

Nuclear lattice

N. Chamel, PRC 85, 035801 (2012)

Neutron gas is not “free”. Neutron mobility is significantly reduced.

$m_n^* / m_n \geq 10$
Observation constraint (mod.)

Moments of inertia ratio with entrainment

\[ \frac{I_n}{I} \approx 2\tau_c \mathcal{A} \frac{\langle m_n^* \rangle}{m_n} \text{ where } \mathcal{A} = \frac{1}{t_{\text{obs}}} \left( \sum_i \frac{\Delta \Omega_i}{\Omega_p} \right). \]

Need more superfluid neutrons in the crust

Contradiction with standard nuclear matter EOS
Effective masses

• (Microscopic) effective mass due to velocity-dependent potential

\[ \frac{m^*}{m} \sim 0.7 - 0.8 \Rightarrow \frac{m^*}{m} = 1 \]

• (Macroscopic) effective mass due to Bragg scattering of periodic potential

\[ \frac{m^*}{m} \text{ can be very large/small or even negative} \]
Energy functional

Barcelona-Catania-Paris-Madrid (BCPM) density functional


• **Volume term**: local density approximations
  based on ab initio nuclear and neutron matter EOS
  \[
  (m^*/m = 1, \ L=52.96 \text{ MeV, } K_0=212.4 \text{ MeV})
  \]
  \[
  E_{vol} = \int dr \left[ (1 - \beta^2(r)) \sum_{n=1}^{5} a_n \rho^n(r) + \beta^2(r) \sum_{n=1}^{5} b_n \rho^n(r) \right] \rho(r)
  \]

• **Surface term**: Gaussian folding
  fixing binding energy of finite 579 even-even nuclei
  \[
  E_{suf} = \sum_{q,q'=p,n} V_{qq'} \left[ \int dr dr' \rho_q(r) \rho_{q'}(r') e^{-(r-r')^2/r_0^2} - \int dr e^{-r^2/r_0^2} \int dr' \rho_q(r') \rho_{q'}(r') \right]
  \]
Band calculation of inner crust

• Treatment of dripped neutrons
• Self-consistent band calculation
  • Large space = Many Bloch $k$
  • Structure optimization “without external potentials”

![Diagram of fcc and bcc structures](image)

Localized protons

Delocalized neutrons
Band calculation

• Single-particle states in a periodic potential
  • Bulk matter \(\rightarrow\) Unit cell with many Bloch wave numbers \(k\)

• Effect of Bragg scattering (entrainment)
  • \(k\)-dependence of bands

• Former calculations (Chamel et al.)
  • Thomas-Fermi approx. to fix the potential

• **Present work**: Self-consistent band cal.
  • 1D slab phase, near the crust bottom
Dripped neutrons (n only)

Slab nucleus (n & p)
Density distributions in the slab phase

\[ \rho = 0.06 \text{ fm}^{-3} \]

Beta equilibrium

\[ \mu_n = \mu_p + \mu_e \]

\[ n \rightleftharpoons p + e + \nu \]

\[ Y_p = 0.02 - 0.04 \]

Protons are also dripped near the transition to uniform matter
Neutron bands

\[ n_B = 0.07 \text{ fm}^{-1} \]

\[ \mu_n = 11.9 \text{ MeV} \]

Confined neutrons

Free neutrons

\[ -\pi/a \quad 0 \quad \pi/a \]

\[ k_z \text{ [ fm}^{-1} \text{]} \]
Effective mass

- Effective mass due to Bragg scattering
  \[ \frac{m_n^*}{m_n} = \frac{n^f}{n^c} \]

- Conduction neutron density: \[ n^c = m_n K^{zz} \]
  \[ K^{zz} \equiv \frac{m_n}{\pi a N_k} \sum_{\alpha, k_z}^{\text{occ}} d^2 e_{\alpha, k_z}^{(n)} \frac{d k_z^2}{d k_z^2} (\mu_n - e_{\alpha, k_z}^{(n)}) \]

- Free neutron density: \[ n^f \]

- Group velocity of neutrons
  \[ \nu_{\alpha, k} = \nabla_k \epsilon_{\alpha, k} \]

- Neutrons in “flat” bands are defined “Confined”.
Effective mass


The Bragg scattering enhances the neutron mobility!

Anti-entrainment effect

Similar results with TDDFT calculation:
Sekizawa, Kobayashi, Matsuo, PRC 105, 045807 (2022)
Superfluidity (inclusion of pairing)

FOE method for HFB can be achieved by

\[ f_T(H) \text{ with } H \text{ as HFB Hamiltonian} \]
Effect of superfluidity

• Superfluid neutrons may reduce the effective mass (Watanabe, Pethick, PRL 119, 062701, 2017)

• TDHFB cal. with accelerated protons [1D] (Yoshimura, Sekizawa, PRC 109, 065804 (2024)) ⇒ Small effect

• Moving frame [1D] (Almirante, Urban, PRC 109, 045805 (2024)) ⇒ Small effect
Superfluid current

• Introducing quasi-momentum $Q$

\[ \Delta(r) \rightarrow \Delta(r)e^{2iQ \cdot r} \]

• Supercurrent density: $j(r)$

\[ \frac{1}{V} \int_V j(r) dr = \frac{n}{m^*} Q = \frac{n_s}{m} Q \]

$n_s$: Superfluid neutron density
$n$: Neutron density
$m^*$: Neutron effective mass
Superfluid neutron density

• Adopting the potential at $n_B = 0.07 \text{ fm}^{-3}$

\[ n_s/n \]

\[ \Delta n [\text{ MeV}] \]

\[ \mu_n = 11 \text{ MeV} \]
Superfluid neutron density

- Adopting the potential at $n_B = 0.07 \text{ fm}^{-3}$
Effective mass for superfluid neutrons

N. Chamel, PRC 85, 035801 (2012)

<table>
<thead>
<tr>
<th>( \bar{n} ) (fm(^{-3} ))</th>
<th>Z</th>
<th>A</th>
<th>( n_n^f/n_n ) (%)</th>
<th>( n_n^c/n_n^f ) (%)</th>
<th>( m_n^*/m_n )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0003</td>
<td>50</td>
<td>200</td>
<td>20.0</td>
<td>82.6</td>
<td>1.21</td>
</tr>
<tr>
<td>0.001</td>
<td>50</td>
<td>460</td>
<td>68.6</td>
<td>27.3</td>
<td>3.66</td>
</tr>
<tr>
<td>0.005</td>
<td>50</td>
<td>1140</td>
<td>86.4</td>
<td>17.5</td>
<td>5.71</td>
</tr>
<tr>
<td>0.01</td>
<td>40</td>
<td>1215</td>
<td>88.9</td>
<td>15.5</td>
<td>6.45</td>
</tr>
<tr>
<td>0.02</td>
<td>40</td>
<td>1485</td>
<td>90.3</td>
<td>7.37</td>
<td>13.6</td>
</tr>
<tr>
<td>0.03</td>
<td>40</td>
<td>1590</td>
<td>91.4</td>
<td>7.33</td>
<td>13.6</td>
</tr>
<tr>
<td>0.04</td>
<td>40</td>
<td>1610</td>
<td>88.8</td>
<td>10.6</td>
<td>9.43</td>
</tr>
<tr>
<td>0.05</td>
<td>20</td>
<td>800</td>
<td>91.4</td>
<td>30.0</td>
<td>3.33</td>
</tr>
<tr>
<td>0.06</td>
<td>20</td>
<td>780</td>
<td>91.5</td>
<td>45.9</td>
<td>2.18</td>
</tr>
<tr>
<td>0.07</td>
<td>20</td>
<td>714</td>
<td>92.0</td>
<td>64.6</td>
<td>1.55</td>
</tr>
<tr>
<td>0.08</td>
<td>20</td>
<td>665</td>
<td>104</td>
<td>64.8</td>
<td>1.54</td>
</tr>
</tbody>
</table>

Superfluid effect: Reduction in effective mass (1/4 at low density)
Consistency with inner-crust origin of pulsar glitch phenomena
Full 3D calculation

- Various configurations (fcc, bcc, rod, slab, anti-rod, anti-fcc/bcc, etc.)
- Large 3D box
- Nuclear superfluidity
- Finite temperature
3D finite-temperature HFB calculation

- KSBdG (HFB) eq.
  \[
  \begin{pmatrix}
  h - \mu & \Delta \\
  -\Delta^* & -(h - \mu)^*
  \end{pmatrix}
  \begin{pmatrix}
  U_k \\
  V_k
  \end{pmatrix}
  = E_k
  \begin{pmatrix}
  U_k \\
  V_k
  \end{pmatrix}
  \]

- Densities
  \[
  \rho = UFV^+ + V^*(1 - f)V^T
  \]
  \[
  \kappa = UFV^+ + V^*(1 - f)U^T
  \]
  \[
  f_{kk'} = \delta_{kk'}/(1 + e^{\beta E_k})
  \]

- Self-consistent iteration

- Diagonalization of the matrix
  - High computational cost
  - Low parallel efficiency
Green’s function

- HFB Green’s function

\[ G(z; \xi, \xi') = \begin{pmatrix} G_{uu}(z; \xi, \xi') & G_{uv}(z; \xi, \xi') \\ G_{vu}(z; \xi, \xi') & G_{vv}(z; \xi, \xi') \end{pmatrix} \]

\[ G_{\phi\psi}(z; \xi, \xi') = \sum_{k>0} \left[ \frac{\phi(\xi)\psi^*(\xi')}{z - E_k} + \frac{\psi(\xi)\phi^*(\xi')}{z - E_k} \right] \]

- Identity

\[ (zI - H_{HFB})G(z) = I \]
\[ R_T = \begin{pmatrix} \rho_T & \kappa_T \\ -\kappa_T^* & 1 - \rho_T^* \end{pmatrix} = \frac{1}{2\pi i} \oint_C f_T(z) G(z) dz + T \sum_{|\omega_n| < h} G(i\omega_n) \]

\[ f_T(z) = \left(1 + e^{\beta z}\right)^{-1} \]

Matsubara frequencies: \( \omega_n = (2n + 1)\pi T \)
Pairing & shape transitions

Thermal pairing & shape transitions in $^{146}$Ba

- On average, $C_V \propto T$
- Kinks in $C_V$ at the pairing & quadrupole-shape phase transition points
- Disappearance of octupole shape has a minor effect on $C_V$

Benchmark calculation (fcc)

Beta equilibrium state with fcc in a cell of $(45 \text{ fm})^3$

Av. density: $n_B = 0.045 \text{ fm}^{-3}$
Proton/Neutron #: $Z = 136, \; N = 3936$

Emergence of deformed Se nuclei “beyond drip line”
Higher density

Beta equilibrium state starting from fcc in a cell of $\text{(45 fm)}^3$

Neutron chemical potential:

$\mu_n = 10 \text{ MeV}$

$\mu_n = 14 \text{ MeV}$

Emergence of sliced swiss cheese
Summary

• Self-consistent band calculation for the slab phase of inner crust in neutron stars
  [Kashiwaba, TN, PRC 100, 035804 (2019)]

• Enhanced mobility by the entrainment effect
  \( m^*/m \approx 0.7 \) at \( n_B = 0.07 - 0.08 \text{ fm}^{-3} \)

• Effect of superfluid neutrons
  Minor effect for slab phase: \( n_B = 0.07 - 0.08 \text{ fm}^{-3} \)
  \( m^*/m \approx 1/4 \) at \( n_B = 0.02 - 0.03 \text{ fm}^{-3} \)
  Possible revival of pulsar glitch model

• FT-HFB calculation in the 3D coordinate space representation
  • Green’s function method [Kashiwaba, TN, PRC 101, 045804 (2020)]
  • Fermion operator expansion method [TN, PRC 107, 015802 (2023)]
Collaborators

• Chengpeng Yu (Postdoc at Univ. Tsukuba)
• Yu Kashiwaba (former PhD student)
• Mao Tsuchida (former Msc student)
# Oakforest-PACS System

<table>
<thead>
<tr>
<th>Specification</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total peak performance</td>
<td>25 PFLOPS</td>
</tr>
<tr>
<td>Total number of compute nodes</td>
<td>8,208</td>
</tr>
<tr>
<td>Compute node</td>
<td>Fujitsu PRIMERGY CX600 M1 (2U) + CX1640 M1 x 8 node</td>
</tr>
<tr>
<td>Processor</td>
<td>Intel® Xeon Phi™ 7250 (Code name: Knights Landing), 68 cores, 1.4 GHz</td>
</tr>
<tr>
<td>Memory High BW</td>
<td>16 GB, 490 GB/sec (MCDRAM, effective rate)</td>
</tr>
<tr>
<td>Memory Low BW</td>
<td>96 GB, 115.2 GB/sec (peak rate)</td>
</tr>
<tr>
<td>Interconnect</td>
<td>Intel® Omni-Path Architecture</td>
</tr>
<tr>
<td>Link speed</td>
<td>100 Gbps</td>
</tr>
<tr>
<td>Topology</td>
<td>Fat-tree with (completely) full-bisection bandwidth</td>
</tr>
<tr>
<td>Parallel File System</td>
<td>Lustre File System</td>
</tr>
<tr>
<td>Total Capacity</td>
<td>26.2 PB</td>
</tr>
<tr>
<td>Product</td>
<td>DataDirect Networks SFA14KE</td>
</tr>
<tr>
<td>Aggregate BW</td>
<td>500 GB/sec</td>
</tr>
<tr>
<td>File Cache System</td>
<td>Burst Buffer, Infinite Memory Engine (by DDN)</td>
</tr>
<tr>
<td>Total capacity</td>
<td>940 TB (NVMe SSD, including parity data by erasure coding)</td>
</tr>
<tr>
<td>Product</td>
<td>DataDirect Networks IME14K</td>
</tr>
<tr>
<td>Aggregate BW</td>
<td>1,560 GB/sec</td>
</tr>
<tr>
<td>Power consumption</td>
<td>4.2 MW (including cooling)</td>
</tr>
<tr>
<td># of racks</td>
<td>102</td>
</tr>
</tbody>
</table>

*Oakforest-PACS is operated by JCAHPC: Joint Center for Advanced High Performance Computing*