Fermion Operator Expansion: Approach to Study Neutron Star Inner Crust

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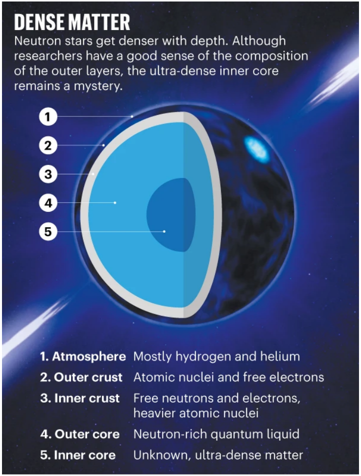
Background I

Neutron stars, highly compact celestial bodies composed of nuclear matter, exhibit layered structures.

In the crossover region of inner crust and core, nuclear matter forms exotic inhomogeneous phases (pasta phases).

The phases influence pulsar glitches, magnetic field decay, etc.



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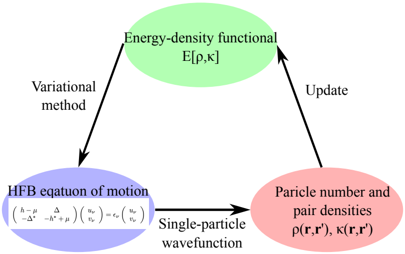
Background II

To study the pasta phases, one can perform coordinate-space energy density functional simulation.

This requires solving Hartree-Fock-Bogoliubov (HFB) equation in each iteration.

Complexity scales cubically with the measure (volume) of the system!

Difficult for 3D system!



Goal

Develop a method to perform the simulation without solving the HFB equation.

Idea:

$$\rho(\boldsymbol{x}\sigma, \boldsymbol{x}'\sigma'), \kappa(\boldsymbol{x}\sigma, \boldsymbol{x}'\sigma') \sim f(H). \tag{1}$$

H: Hamiltonian
$f(\cdot)$: the Fermi-Dirac distribution as a **matrix function**
$\rho(\boldsymbol{x}\sigma, \boldsymbol{x}'\sigma') = \langle \psi^\dagger(\boldsymbol{x}'\sigma')\psi(\boldsymbol{x}\sigma)\rangle$: density
$\kappa(\boldsymbol{x}\sigma, \boldsymbol{x}'\sigma') = \langle \psi^\dagger(\boldsymbol{x}'\sigma')\psi(\boldsymbol{x}\sigma)\rangle$: pair density

Key Question:

- $f(H)$ is $4N \times 4N$, ρ, κ is $2N \times 2N$.
- The band structure.

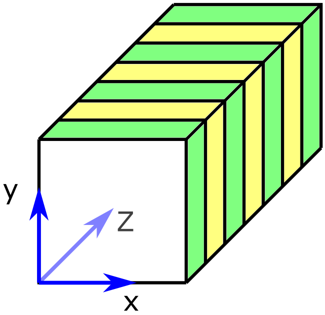
System configuration

Let us consider a slab phase.

$$H_{\text{HFB}}^{\boldsymbol{k}} = \begin{pmatrix} h^{\boldsymbol{k}} - \mu & \Delta(z) \\ -\Delta^*(z) & -h^{-\boldsymbol{k}*} + \mu \end{pmatrix}, \quad (2)$$

$$h^{\boldsymbol{k}} = -\frac{(\partial_z + ik_z)^2}{2m} + \frac{k_x^2 + k_y^2}{2m} + U(z). \quad (3)$$

$\boldsymbol{k} = (k_x, k_y, k_z)^T$, k_z is the Floquet wave vector. k_x, k_y are wave vectors of plane wave.



Theory I

We introduce the generalized density matrix:

$$R(\boldsymbol{x}\sigma, \boldsymbol{x}'\sigma') = \begin{pmatrix} \rho(\boldsymbol{x}\sigma, \boldsymbol{x}'\sigma') & \kappa(\boldsymbol{x}\sigma, \boldsymbol{x}'\sigma') \\ -\kappa^*(\boldsymbol{x}\sigma, \boldsymbol{x}'\sigma') & 1-\rho^*(\boldsymbol{x}\sigma, \boldsymbol{x}'\sigma') \end{pmatrix} \tag{4}$$

After some algebra, we show

$$\begin{aligned} R(\boldsymbol{x}\sigma, \boldsymbol{x}'\sigma') &= \frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} R^{\boldsymbol{k}}(\boldsymbol{x}\sigma, \boldsymbol{x}'\sigma') \\ &= \frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} \langle \boldsymbol{x}\sigma | e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{x}}} f(H_{HFB}^{\boldsymbol{k}}) e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{x}}} | \boldsymbol{x}'\sigma' \rangle, \end{aligned} \tag{5}$$

$\hat{\boldsymbol{x}}$ is the location operator.

Theory II

One can compute $f(H_{HFB}^{\boldsymbol{k}})$ by expansion.

Let $\bar{f}(x) = f(\epsilon_r x + \epsilon_c)$, $\epsilon_c = (\epsilon_{\mathrm{max}} + \epsilon_{\mathrm{min}})/2$, $\epsilon_r = (\epsilon_{\mathrm{max}} - \epsilon_{\mathrm{min}})/2$, $-1 < x < 1$.

Represent $\bar{f}(x)$ with Chebyshev series:

$$\bar{f}(x) = \frac{a_0}{2} + \sum_{k=1}^{N_{\mathrm{exp}}} a_k T_k(x), \tag{6}$$

$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$.

The required N_{exp} becomes small at finite temperature.

Theory III

For $f(H_{HFB}^{\mathbf{k}})$, let $\bar{H}_{HFB}^{\mathbf{k}} = (H_{HFB}^{\mathbf{k}} - \epsilon_c I)/\epsilon_r$,

$$f(H_{HFB}^{\mathbf{k}}) = \bar{f}(\bar{H}_{HFB}^{\mathbf{k}}) = \frac{a_0}{2} + \sum_{k=1}^{N_{\mathrm{exp}}} a_k T_k(\bar{H}_{HFB}^{\mathbf{k}}), \tag{7}$$

$$T_{n+1}(\bar{H}_{HFB}^{\mathbf{k}}) = 2\bar{H}_{HFB}^{\mathbf{k}} T_n(\bar{H}_{HFB}^{\mathbf{k}}) - T_{n-1}(\bar{H}_{HFB}^{\mathbf{k}}).$$

The convergence speed does not depend on the number of space lattice sites N.
The complexity is $O(N^2)$, smaller than the $O(N^3)$ of diagonalization.

Nearsightedness

At finite temperature, $R(\boldsymbol{x}, \boldsymbol{x}')$ is only nonzero when $|\boldsymbol{x} - \boldsymbol{x}'| < r_N$.

Baer and Head-Gordon shows:

$$r_N \sim r_{N0} = \sqrt{\frac{\hbar^2}{3m}(D-1)\beta}, \tag{8}$$

for reaching accuracy 10^{-D}.

When computing $T_{n+1}(\bar{H}^{\boldsymbol{k}}_{HFB}) = 2\bar{H}^{\boldsymbol{k}}_{HFB} T_n(\bar{H}^{\boldsymbol{k}}_{HFB}) - T_{n-1}(\bar{H}^{\boldsymbol{k}}_{HFB})$, we can discard the matrix elements (i, j) with $|\boldsymbol{x}_i - \boldsymbol{x}_j| > r_N$.

r_N does not depend on system size, so with fixed lattice spacing, the complexity reduces to $O(N)$.

Numerical setup

Potential:

$$U(z) = -\frac{U_0}{1 + e^{(z-z_0)/a}}, \quad -L/2 < z < L/2, \tag{9}$$

$U(z) = U(z + L)$.

Pair potential:

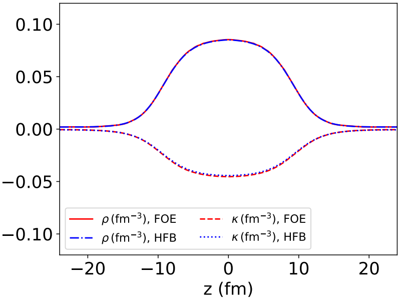
$$\Delta(z) = \int_{-L/2}^{L/2} g\kappa(z')\delta(z - z'), \tag{10}$$

$g = 1.00 \sim 1.50\,\mathrm{U_E} \cdot \mathrm{fm}^3$, $U_E = \hbar^2/(m^2\Delta z)^2 = 259.19\,\mathrm{MeV}$.

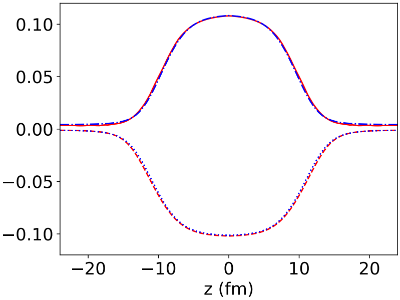
Solving $\rho(z) = \rho(z, z)$, $\kappa(z) = \kappa(z, z')$ iteratively until $\kappa(z)$ converges.

Results I

Comparing different methods



$g = 1.00\,\mathrm{U_E} \cdot \mathrm{fm}^3,\ T = 0.50\,\mathrm{MeV},\ \mu = 4.50\,\mathrm{MeV}$



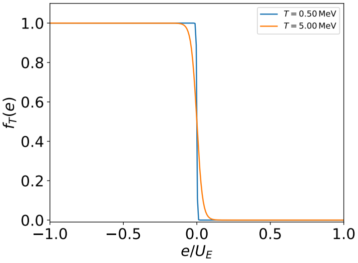
$g = 1.50\,\mathrm{U_E} \cdot \mathrm{fm}^3,\ T = 5.00\,\mathrm{MeV},\ \mu = 4.50\,\mathrm{MeV}$

FOE = "Fermion Operator Expansion"; HFB = "Solving HFB equation by Diagonalization"

Results II

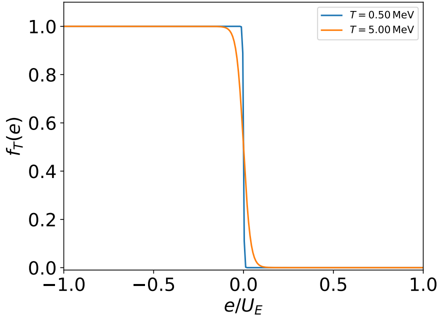
We determine the number of Chebyshev terms self-consistently.
Left: $N_{\text{expansion}}|_{z=0} = 1700$;
Right: $N_{\text{expansion}}|_{z=0} = 300$.

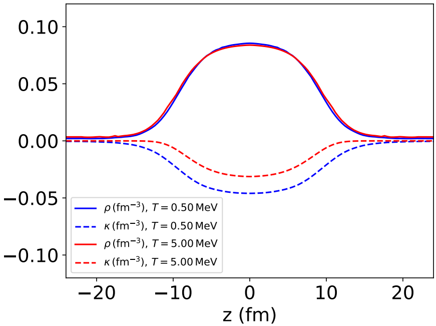
This method works out nicely for even low-temperature cases.



Results III

Speed of convergence: temperature

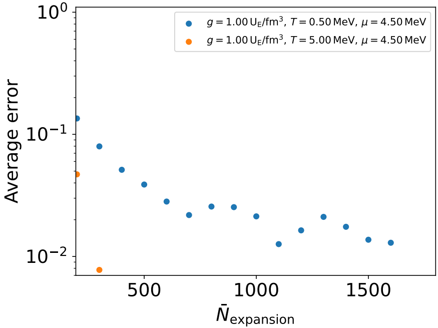


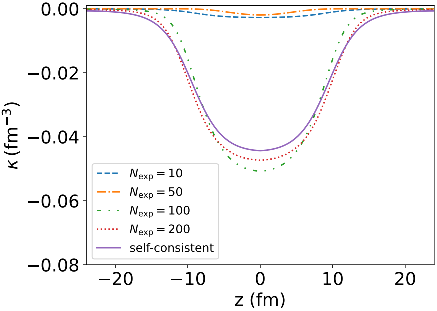


$g = 1.00\,\mathrm{U_E}\cdot\mathrm{fm}^3$, $\mu = 4.50\,\mathrm{MeV}$

$U_E = \hbar^2/(m^2\Delta z)^2 = 259.19\,\mathrm{MeV}$ is the energy scale determined by the lattice spacing.

Results IV



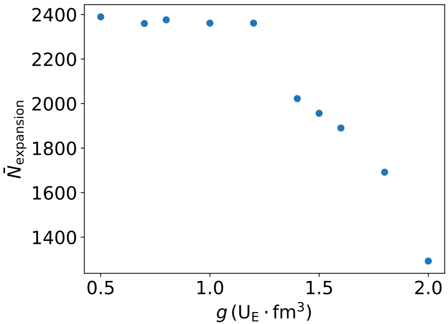


$g = 1.00\,\mathrm{U_E} \cdot \mathrm{fm}^3,\ T = 0.50\,\mathrm{MeV},\ \mu = 4.50\,\mathrm{MeV}$

The finite-temperature results converge much faster.

Results V

Speed of convergence: pairing strength

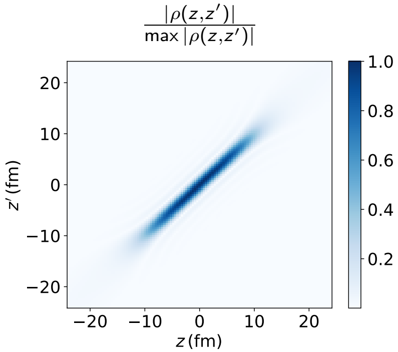


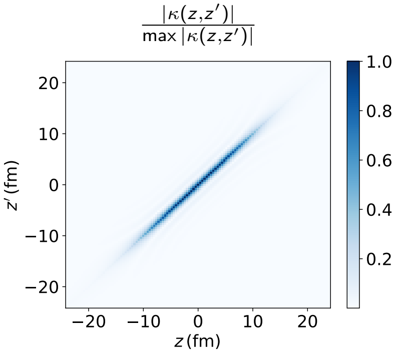
$T = 0.50\,\mathrm{MeV}$, $\mu = 4.50\,\mathrm{MeV}$

The increase of g and paring gap leads to faster convergence.

Results VI

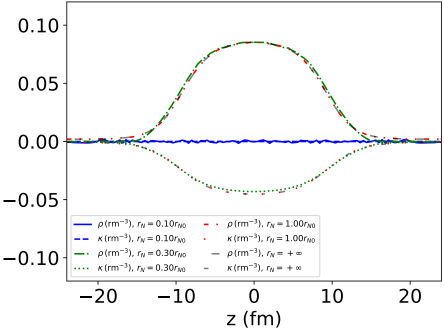
Nearsightedness





$g = 1.50\,\mathrm{U_E}\cdot\mathrm{fm}^3,\ T = 0.50\,\mathrm{MeV},\ \mu = 4.50\,\mathrm{MeV}$

Results VII



$g = 1.00\,\mathrm{U_E}\cdot\mathrm{fm}^3,\ T = 0.50\,\mathrm{MeV},\ \mu = 0.45\,\mathrm{MeV}$

$r_{N0} \approx 7.44\,\mathrm{fm}$ is a reasonable estimation.

Results VIII

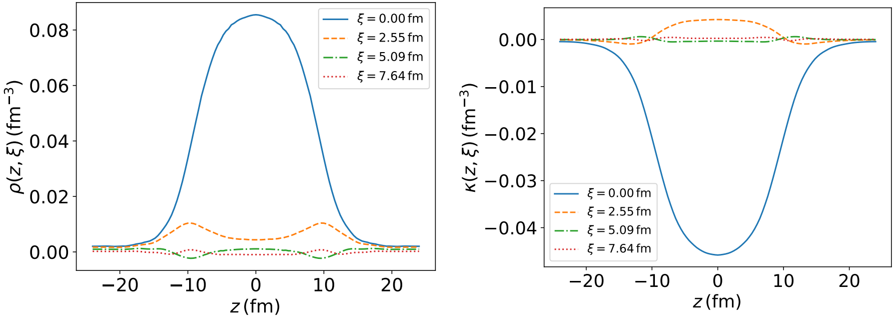
Transverse dependence

With a little algebra, we show

$$R^{\boldsymbol{k}}(\boldsymbol{x}\sigma, \boldsymbol{x}'\sigma') \propto J_0(k_\xi \xi), \tag{11}$$

$\xi = \sqrt{x^2 + y^2}$, $k_\xi = \sqrt{k_x^2 + k_y^2}$

Results IX



$g = 1.00\,\mathrm{U_E} \cdot \mathrm{fm}^3,\ T = 0.50\,\mathrm{MeV},\ \mu = 0.45\,\mathrm{MeV}$

Nearsightedness also emerges in the transverse direction.

Summary

We have developed the Fermion Operator Expansion method for coordinate-space DFT simulation based on HFB theory with band structure.

The core idea is to compute $\langle \boldsymbol{x} | f(H) | \boldsymbol{x}' \rangle$ instead of solving HFB equation.

When the nearsightedness approximation applies, the time complexity of the method only scales linearly with the measure of system. It is ideal for performing finite-temperate 3D simulation.

It is promising for studying the pasta phases in the bottom of neutron crust.