# Fermi Operator Expansion: Approach to Studying Neutron Star Inner Crust

Chengpeng Yu and Takashi Nakatsukasa

Center for Computational Sciences, University of Tsukuba
yu.chengpeng@nucl.ph.tsukuba.ac.jp, nakatsukasa@nucl.ph.tsukuba.ac.jp

## Introduction

**Background**

The pasta phases—the exotic inhomogeneous phases with nonspherical symmetry—in the inner crust of neutron stars are crucial for the phenomenology of the star. To fully understand the phases, one needs *3D coordinate-space* simulations.

**Technique to simulate the pasta phases**

One approach to the simulations is to use the energy density functional method of Hartree-Fock-Bogoliubov (HFB) theory.

The HFB theory involves the following mean-field Hamiltonian:

$$H = \sum_{ab}(h_{ab} - \mu)c_a^\dagger c_b + \frac{1}{2}\sum_{ab}(\Delta_{ab}c_a^\dagger c_b^\dagger + \Delta_{ab}^* c_b c_a). \tag{1}$$

Here, $c_a$ is the annihilation operator of particles, which are the free neutrons in the inner crust; The indices $a$, $b$ label the degrees of freedom of the particles, which are space coordinates $\boldsymbol{r}$ and spin $\sigma = \pm 1/2$ in this setup; $h_{ab}$ is the single particle Hamiltonian; $\Delta_{ab}$ is the pairing gap; $\mu$ is the chemical potential.

One can diagonalize the Hamiltonian by the Bogoliubov transformation, $c_a = \sum_\alpha (a_\alpha u_{\alpha a} + a_\alpha^\dagger v_{\alpha a}^*)$, where $a_\alpha$ represents a quasiparticle state, and show $u_{\alpha a}$ and $v_{\alpha a}$ obeys

$$\epsilon_\alpha \begin{pmatrix} u_{\alpha a} \\ v_{\alpha a} \end{pmatrix} = \sum_b (H_{\mathrm{HFB}})_{ab} \begin{pmatrix} u_{\alpha b} \\ v_{\alpha b} \end{pmatrix} = \sum_b \begin{pmatrix} h_{ab} - \mu & \Delta_{ab} \\ -\Delta_{ab}^* & -h_{ab}^* + \mu \end{pmatrix} \begin{pmatrix} u_{\alpha b} \\ v_{\alpha b} \end{pmatrix}. \tag{2}$$

where we refer to $H_{\mathrm{HFB}}$ as the HFB Hamiltonian.

The ground state of the system should be the vacuum state of the quasiparticles. At finite temperature, the ground-state normal and pair densities are

$$\rho_{ab} = \langle c_b^\dagger c_a \rangle = \sum_\alpha \left[ f(\epsilon_\alpha) u_{\alpha a} u_{\alpha b}^* + (1 - f(\epsilon_a))\, v_{\alpha a}^* v_{\alpha b} \right], \tag{3}$$

$$\kappa_{ab} = \langle c_b c_a \rangle = \sum_\alpha \left[ f(\epsilon_\alpha) u_{\alpha a} v_{\alpha b}^* + (1 - f(\epsilon_\alpha))\, v_{\alpha a}^* u_{\alpha b} \right], \tag{4}$$

where $f(\epsilon_\alpha) = 1/(1 + e^{E_\alpha/T})$ is Fermi-Dirac distribution of the quasiparticles.

To determine $h_{ab}$, $\Delta_{ab}$, $\rho_{ab}$, $\kappa_{ab}$, the energy density functional method of HFB theory introduces the energy of the system as a functional of the densities, $E[\rho, \kappa]$, and conducts the following steps:

1. Start from some initial guess of $h_{ab}$ and $\Delta_{ab}$
2. Use Eq. (2) to solve $u_{\alpha a}$ and $v_{\alpha a}$.
3. Use Eqs. (3), (4) to solve $\rho_{\alpha\beta}$ and $\kappa_{\alpha\beta}$.
4. Update $h_{ab}$ and $\Delta_{ab}$ using

$$h_{ab} = \frac{\delta E}{\delta \rho_{ba}},\ \Delta_{ab} = \frac{\delta E}{\delta \kappa_{ab}^*}. \tag{5}$$

5. Conduct step 2–4 iteratively until $\rho_{\alpha\beta}$ and $\kappa_{\alpha\beta}$ converge.

**Goal**

In the above recipe, step 2 is the most time-consuming. If one solves Eq. (2) by diagonalization, the time complexity is of $O(N^3)$ with $N$ being the number of space lattice sites, which is *formidably expensive* for 3D coordinate-space simulation. To reduce the time complexity, in this work, we, for the first time, study the *Fermi Operator Expansion (FOE) method of HFB theory with band structure*.

## Formulation

To study the pasta phase, we consider a system under a periodic potential, which is invariant under a translation vector $\boldsymbol{T}$. In this case, the index of the quasiparticles, $\alpha$, becomes the Bloch wave vector $\boldsymbol{k}$ and the band index $n$. The HFB equation becomes

$$\sum_{\sigma'} \int d\boldsymbol{r}'\, H_{\mathrm{HFB}}^{\boldsymbol{k}}(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma') \begin{pmatrix} \tilde{u}_n^{\boldsymbol{k}}(\boldsymbol{r}'\sigma') \\ \tilde{v}_n^{\boldsymbol{k}}(\boldsymbol{r}'\sigma') \end{pmatrix} = \epsilon_n^{\boldsymbol{k}} \begin{pmatrix} \tilde{u}_n^{\boldsymbol{k}}(\boldsymbol{r}\sigma) \\ \tilde{v}_n^{\boldsymbol{k}}(\boldsymbol{r}\sigma) \end{pmatrix}. \tag{6}$$

Here, as mentioned in the previous section, the indices $a$, $b$ are rewritten as $\boldsymbol{r}$, $\sigma$ and $\boldsymbol{r}'$, $\sigma'$, respectively; $H_{\mathrm{HFB}}^{\boldsymbol{k}} = e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} H_{\mathrm{HFB}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}}$.

We introduce the generalized density matrix defined as

$$R = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho^* \end{pmatrix}. \tag{7}$$

After a series of algebraic calculations, we prove

$$R = \frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} R^{\boldsymbol{k}} = \frac{1}{N_k} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}} f(\tilde{H}_{\mathrm{HFB}}^{\boldsymbol{k}}) e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}. \tag{8}$$

Here, $\tilde{H}_{\mathrm{HFB}}^{\boldsymbol{k}}$ is the projection of $H_{\mathrm{HFB}}^{\boldsymbol{k}}$ on the subspace spanned by periodic functions with respect to the translation $\boldsymbol{T}$; $f(\tilde{H}_{\mathrm{HFB}}^{\boldsymbol{k}})$ is a matrix function of $\tilde{H}_{\mathrm{HFB}}^{\boldsymbol{k}}$; $N_{\boldsymbol{k}}$ is the number of Bloch wave vectors in the numerical calculation.

Instead of solving $f(\tilde{H}_{\mathrm{HFB}}^{\boldsymbol{k}})$ by diagonalization, we expand it as a series of polynomials. We have

$$f(\tilde{H}_{\mathrm{HFB}}^{\boldsymbol{k}}) = \frac{a_0}{2} + \sum_{k=1}^{N_{\mathrm{cheb}}} a_k T_k(\tilde{H}_{\mathrm{HFB}}^{\boldsymbol{k}}/\epsilon_r), \tag{9}$$

Here, $T_k(x)$ are Chebyshev polynomials; $\epsilon_r$ is the estimated maximum quasiparticle energy; $a_0$, $a_k$ are the coefficients of Chebyshev expansion that can be computed in advance by considering the expansion of the scalar Fermi-Dirac distribution; $N_{\mathrm{cheb}}$ is a large number where we truncate the expansion.

Based on Eq. (9), we compute $R^{\boldsymbol{k}}$ using the recursive property of the Chebyshev polynomial:

$$R_{ij}^{\boldsymbol{k}} = \frac{a_0}{2}\delta_{ij} + \sum_{k=1}^{N_{\mathrm{cheb}}} a_k \langle i_0; \boldsymbol{k} | j_k; \boldsymbol{k} \rangle, \tag{10}$$

$$|j_0; \boldsymbol{k}\rangle = e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}|j\rangle,\ |j_1; \boldsymbol{k}\rangle = (\tilde{H}_{\mathrm{HFB}}^{\boldsymbol{k}}/\epsilon_r)|j_0; \boldsymbol{k}\rangle, \tag{11}$$

$$|j_k; \boldsymbol{k}\rangle = 2(\tilde{H}_{\mathrm{HFB}}^{\boldsymbol{k}}/\epsilon_r)|j_{k-1}; \boldsymbol{k}\rangle - |j_{k-2}; \boldsymbol{k}\rangle. \tag{12}$$

Here, $|j\rangle$ is the unit column vector with $\delta_{ij}$ as the $i$-th element in a given representation. The convergence speed of the Chebyshev polynomials does not depend on the number of lattice sites, so this algorithm is of $O(N^2)$ complexity. Furthermore, at finite temperature, the system is likely to be nearsighted, which means that there is a finite $r_N$, such that $R(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma') \simeq 0$ if $|\boldsymbol{r} - \boldsymbol{r}'| > r_N$. If this holds, the time complexity reduces to $O(N)$.

## Results

We verify the FOE method by considering a slab phase as shown in Fig. 1. We choose the temperature and chemical potential as $T = 0.1\,\mathrm{MeV}$, $\mu = 10\,\mathrm{MeV}$, which are typical values in the inner crust. We choose $h = K + U(z)$, where $K$ is the kinetic part and $U(z)$ is a periodic potential with $U(z) = -U_0/(1 + e^{(|z|-z_0)/a})$ at $-L/2 < z < L/2$. $U_0 = 50.00\,\mathrm{MeV}$, $z_0 = 10.00\,\mathrm{fm}$, $a = 2.00\,\mathrm{fm}$, $L = 48.00\,\mathrm{fm}$. We assume zero-region interaction of pairs, $\Delta(z) = g\kappa(z)$, and determine $\Delta(z)$ using the energy density functional method. We choose $g = 150$–$200\,\mathrm{MeV}\cdot(\mathrm{fm})^3$ such that the average pairing gap is $|\bar{\Delta}| \sim 1.00\,\mathrm{MeV}$.

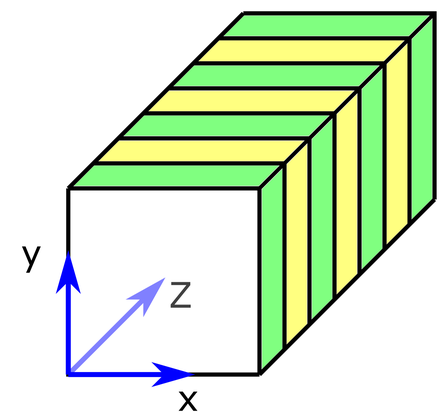


FIG.1: Schematic image of the slab phase.

We introduce local densities $\rho(z) = \sum_\sigma \rho(\boldsymbol{r}, \sigma, \boldsymbol{r}, \sigma)$ and $\kappa(z) = \rho(\boldsymbol{r}, +1/2, \boldsymbol{r}, -1/2)$. (The densities does not depends on $x$, $y$ and $x'$, $y'$ if $x = x'$ and $y = y'$.) We plot the $\rho(z)$, $\kappa(z)$ from the FOE method and the matrix diagonalization method of Eq. (2) on Fig. 2, 3. These figures show that with an increase of $N_{\mathrm{cheb}}$, both $\rho(z)$ and $\kappa(z)$ steadily approach the results of the diagonalization method. Furthermore, in these figures, the temperature is significantly low, but the densities still converge after a finite number of terms. This shows that although the FOE method is formulated for the finite temperature system, it applies to zero temperature systems as well.

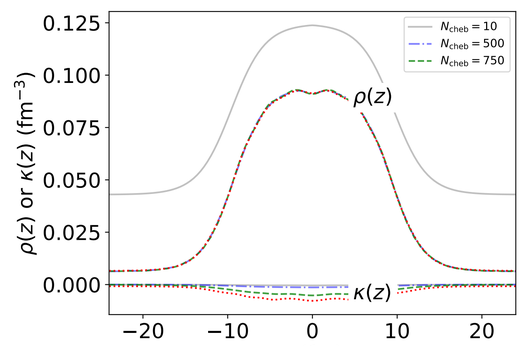


FIG. 2: The normal densities $\rho(z)$ and pair densities $\kappa(z)$ from the FOE method with fixed $N_{\mathrm{cheb}}$. The red dotted line is the result of the matrix diagonalization method. The average pairing gap is $|\bar{\Delta}| = 0.89\,\mathrm{MeV}$.

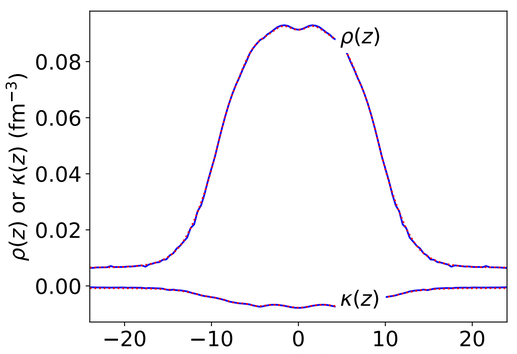


FIG. 3: The same as Fig. 2 but with $N_{\mathrm{cheb}}$ adaptively determined on each space lattice site. We have $N_{\mathrm{cheb}} \simeq 2500$ near $z = 0$.

## Conclusion

We introduce the FOE method of HFB band theory. The FOE method identifies the generalized density matrix with $f(\tilde{H}_{\mathrm{HFB}}^{\boldsymbol{k}})$, and computes $f(\tilde{H}_{\mathrm{HFB}}^{\boldsymbol{k}})$ by expanding it into Chebyshev series. It allows the calculation of normal and pair densities without diagonalizing the HFB Hamiltonian, and is a useful method for the HFB band theory calculation in the coordinate-space representation. It provides a promising tool for the simulation of the pasta phases in the inner crust of neutron stars.

Based on arXiv:2504.04735