Superfluid band calculations for the neutron star inner crust

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INTRODUCTION

Nuclear Electron Correspondence

Density Functional Theory

Hohenberg-Kohn thm:

$$\delta E[\rho]/\delta\rho\big|_{\rho=\rho_0} = 0$$

Kohn-Sham Eq.

$$\hat{h}\phi_i(\boldsymbol{r}) = \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \hat{v}^{\mathrm{KS}}(\boldsymbol{r})\right]\phi_i(\boldsymbol{r}) = \varepsilon_i\phi_i(\boldsymbol{r})$$

Band theory:

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\tilde{\psi}_{n\boldsymbol{k}}(\boldsymbol{r})$$

$$\tilde{\psi}_{n\boldsymbol{k}}(\boldsymbol{r}+\boldsymbol{R}) = \tilde{\psi}_{n\boldsymbol{k}}(\boldsymbol{r})$$

Effective mass: $(m^\star)^{-1}_{\mu\nu} = \dfrac{\partial^2\varepsilon_{\boldsymbol{k}}}{\partial k_\mu \partial k_\nu}$

Nuclear systems

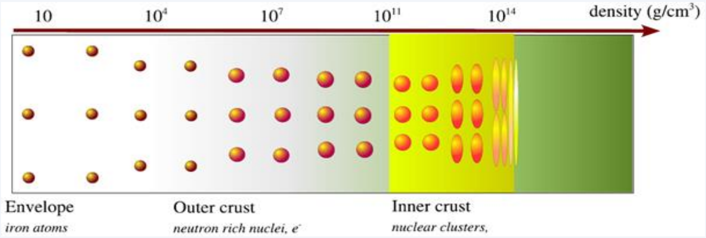
Hartree-Fock Eq.

$$\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \Gamma_H(\boldsymbol{r})\right]\phi_i(\boldsymbol{r}) + \int \mathrm{d}\boldsymbol{r}'\,\Gamma_F(\boldsymbol{r},\boldsymbol{r}')\phi_i(\boldsymbol{r}') = \varepsilon_i\phi_i(\boldsymbol{r})$$

Skyrme energy functional:

$$E = E_{\mathrm{Skyrme}}[\rho, \tau, \boldsymbol{j}, \ldots]$$

Nuclear ``matter”:



Our Interest?

- Application of the band theory to the nuclear DFT
- Thorough understandings of nuclear properties in the neutron star crust

History of Band calculation

N.Chamel, PRC85, 035801 (2012)

possible drastic change of effective mass (*entrainment*)

$\bar{n}$ (fm^{-3})	Z	A	n_n^f/n_n (%)	n_n^c/n_n^f (%)	$m_n^\star/m_n$
0.01	40	1215	88.9	15.5	6.45
0.02	40	1485	90.3	7.37	13.6
0.03	40	1590	91.4	7.33	13.6
0.04	40	1610	88.8	10.6	9.43
0.05	20	800	91.4	30.0	3.33

Self-consistency

Phys. Rev. C 100, 035804 (2019)

Phys. Rev. C 105, 045807 (2022)

- still w/o pairing
- only 1 dim. crystal
- effective mass *less* than bare mass

(anti-entrainment?)

Superfluidity

Phys. Rev. C 94, 065801 (2016)

Phys. Rev. Research 4, 033141 (2022)

- not self-consistent
- overestimation w/o self-consistency?

Our final goal :

1. develop ①self-consistent ②superfluid ③band theory
   for all crystalline structures realized in the neutron star inner crust
2. perform calculations and extract the *effective mass* of free neutrons
3. obtain the effective mass as a function of baryon densities,
   utilized for actual simulations for astronomical phenomena

THEORY

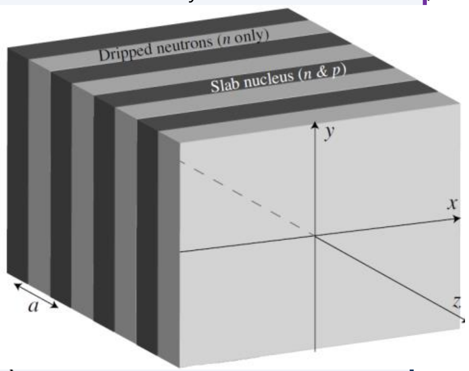
Band Theory

HFB theory

HFB equation: $$\begin{pmatrix} \hat{h}(\boldsymbol{r}) - \lambda & \Delta(\boldsymbol{r}) \\ \Delta^*(\boldsymbol{r}) & -\hat{h}^*(\boldsymbol{r}) + \lambda \end{pmatrix} \begin{pmatrix} u_\mu(\boldsymbol{r}) \\ v_\mu(\boldsymbol{r}) \end{pmatrix} = E_\mu \begin{pmatrix} u_\mu(\boldsymbol{r}) \\ v_\mu(\boldsymbol{r}) \end{pmatrix}$$

Densities: $$\rho(\boldsymbol{r}) = \sum_\mu |v_\mu(\boldsymbol{r})|^2 \quad \tau(\boldsymbol{r}) = \sum_\mu |\boldsymbol{\nabla} v_\mu(\boldsymbol{r})|^2 \quad \kappa(\boldsymbol{r}) = \sum_\mu v_\mu^*(\boldsymbol{r}) u_\mu(\boldsymbol{r})$$

Phys. Rev. C 100, 035804 (2019)



Superfluid Band Theory for one dimensional crystal

Bloch wave number: $$\boldsymbol{R} = T_x \hat{\boldsymbol{e}}_x + T_y \hat{\boldsymbol{e}}_y + n_z a \hat{\boldsymbol{e}}_z$$

Bloch transformation: $$u_{\mu\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \tilde{u}_{\mu\boldsymbol{k}}(\boldsymbol{r}) \quad v_{\mu\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \tilde{v}_{\mu\boldsymbol{k}}(\boldsymbol{r})$$

HFB Eq: $$\begin{pmatrix} \hat{h}(z) + \hat{h}_{\boldsymbol{k}}(z) - \lambda & \Delta(z) \\ \Delta^*(z) & -\hat{h}^*(z) - \hat{h}^*_{\boldsymbol{k}}(z) + \lambda \end{pmatrix} \begin{pmatrix} u_{\mu\boldsymbol{k}}(z) \\ v_{\mu\boldsymbol{k}}(z) \end{pmatrix} = E_{\mu\boldsymbol{k}} \begin{pmatrix} u_{\mu\boldsymbol{k}}(z) \\ v_{\mu\boldsymbol{k}}(z) \end{pmatrix}$$

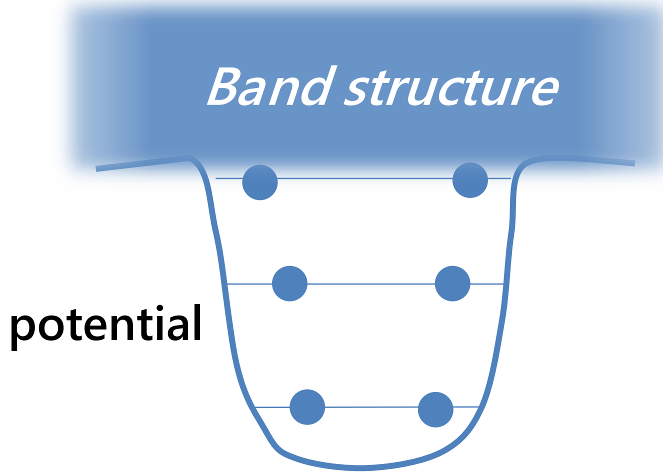
Points

- One-dimensional dependence
- Self-consistent equation
- Millions of orbitals (typically ~2400000)

⇒ Parallel computing with supercomputers

Effective Mass Calculation

Without band



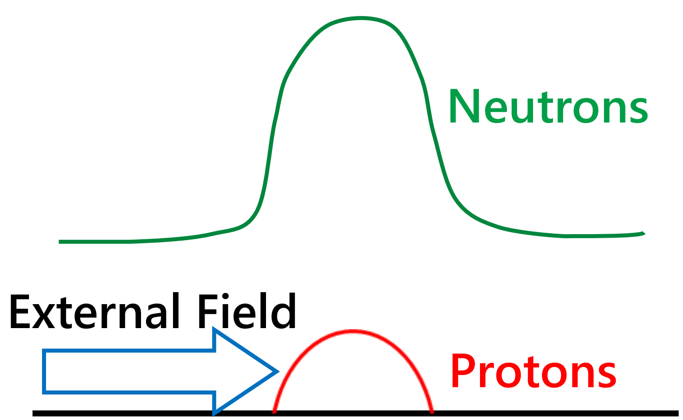
Free neutron density n_n^f

"bound" neutron

$$\sum_\mu \int \mathrm{d}z |v_\mu(z)|^2 \theta(e_\mu - U^{(0)})$$

Bound or free?

With band



TDDFT : $i\hbar \frac{\partial}{\partial t} \begin{pmatrix} u_{\mu \boldsymbol{k}\uparrow} \\ v_{\mu \boldsymbol{k}\downarrow} \end{pmatrix} = \hat{H} \begin{pmatrix} u_{\mu \boldsymbol{k}\uparrow} \\ v_{\mu \boldsymbol{k}\downarrow} \end{pmatrix}$

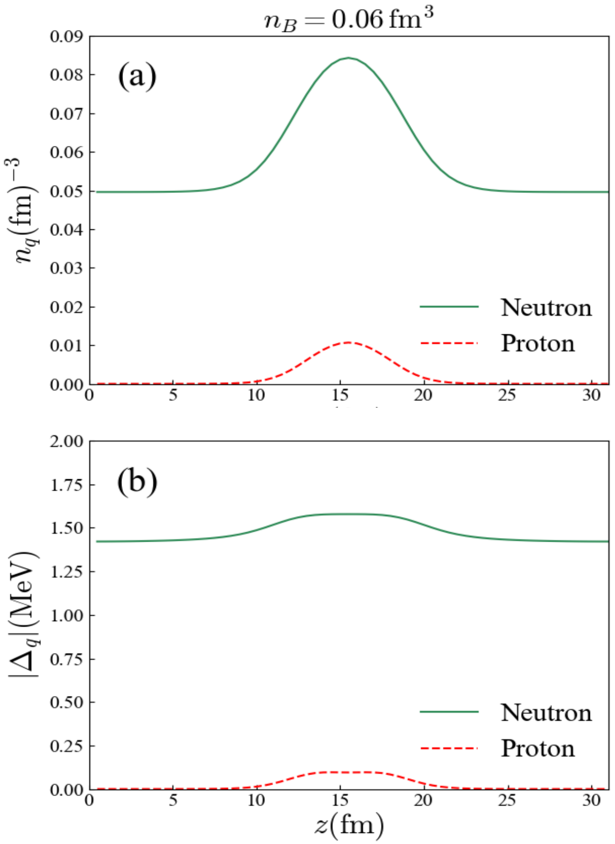
EoM : $F_{\mathrm{ext}} = M^{\mathrm{slab}} a$

Conduction number density n_n^c

Calc *effective mass* by $n_n^f m_n^{\mathrm{bare}} = n_n^c m_n^\star$

RESULT

Calc. Results and Effective Masses



Calculation Result : (nB = 0.05 fm^{-3}, β equilibrium)

(Upper : number density lower : pairing field)

- Highly n-rich (Yp ~ 0.03), centro-localized
- Both n & p have superfluidity (sup.conductivity)
- Most neutrons are dripped (about 70%)

Effective mass :

n_n^f … density of ***energetically*** free neutrons
n_n^c … neutrons ***effectively*** conducting freely

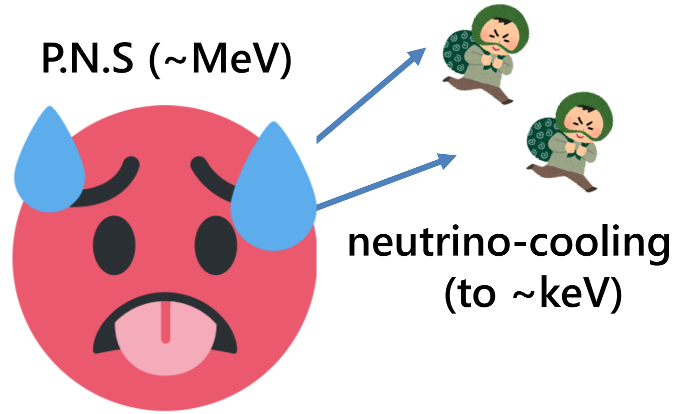
- Effective masses always less than baremass.
- Superfluidity slightly reduces eff. masses.

	Superfluid (TD)DFT			Normal (TD)DFT		
n_b	$n_n^f/\bar{n}_n$	$n_n^c/\bar{n}_n$	$m_n^\star/m_{n,bg}^\oplus$	$n_n^f/\bar{n}_n$	$n_n^c/\bar{n}_n$	$m_n^\star/m_{n,bg}^\oplus$
0.04	0.702	0.893	0.785	0.710	0.876	0.810
0.05	0.684	0.913	0.749	0.697	0.896	0.778
0.06	0.609	0.933	0.652	0.608	0.911	0.668
0.07	0.555	0.954	0.582	0.555	0.929	0.598

EXTENSION

Finite Temperature Extensions

F.T. Calculation is needed for ***Proto Neutron Star***



What we wanna know :

- How is the neutrino N.S. cooling?
- When nuclear pasta has been *cooked*?
- How many neutrons thermally superfluid?

F.T. Calculation

Density calculation : $\rho = \sum_{\mu \boldsymbol{k}} [f_D(E_{\mu \boldsymbol{k}})|u_{\mu \boldsymbol{k}}(\boldsymbol{r})|^2 + f_D(-E_{\mu \boldsymbol{k}})|v_{\mu \boldsymbol{k}}(\boldsymbol{r})|^2]$

Free Energy : $F(T) = E[\rho(T)] - S(T)T$

Specific Heat : $C_V(T) = \frac{\partial E(T)}{\partial T}$

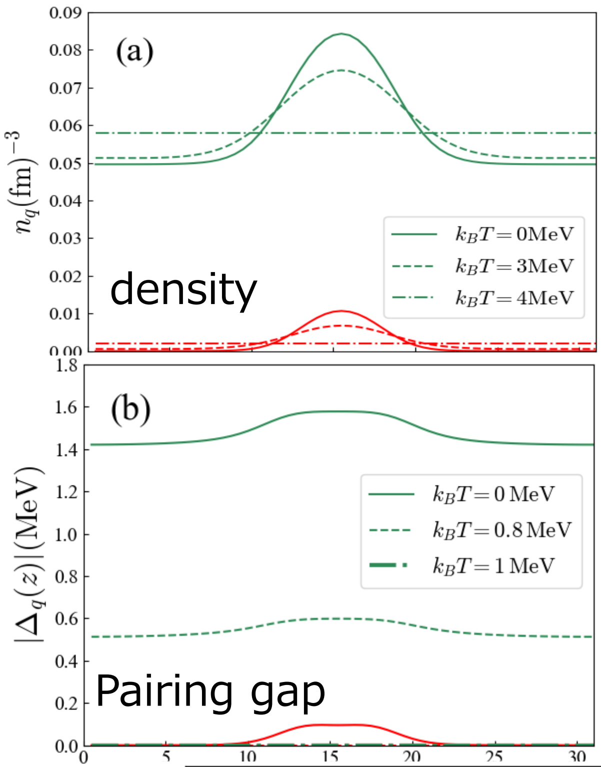
ν-pasta scattering

Neutrino *Opacity* : $\chi_T(E_\nu) = \frac{2G_F^2 E_\nu^2}{3\pi} n \left[c_V^2 \langle S_V(E_\nu)\rangle + 5c_A^2 \langle S_A(E_\nu)\rangle\right]$

Structure factors : $S^{(0)}_{\mathrm{el},q}(\boldsymbol{q}) = \frac{1}{N_q}\sum_{\mu \boldsymbol{k}}\left[f_D(E_{\mu \boldsymbol{k}})\, \langle v^{(q)}_{\mu \boldsymbol{k}}|e^{i\boldsymbol{q}\cdot\boldsymbol{r}}|v^{(q)}_{\mu \boldsymbol{k}}\rangle\, |\right]$ $S^{(0)}_{\mathrm{inel},q}(\boldsymbol{q}) = 1 - \frac{1}{N_q}\sum_{\alpha,\beta}\left[f_D(E_\alpha)f_D(E_\beta)\,\langle v^{(q)}_\alpha|e^{i\boldsymbol{q}\cdot\boldsymbol{r}}|v^{(q)}_\beta\rangle\right]$

$\langle S_V(E_\nu)\rangle = \frac{3}{4}\int_{-1}^{1} \mathrm{d}x (1-x^2)(S_{\mathrm{el}}(q) + S_{\mathrm{inel}}(q))$ $\langle S_A(E_\nu)\rangle = \frac{3}{20}\int_{-1}^{1} \mathrm{d}x (1-x)(3-x) S_{\mathrm{inel}}(q)$

Finite Temperature Extensions

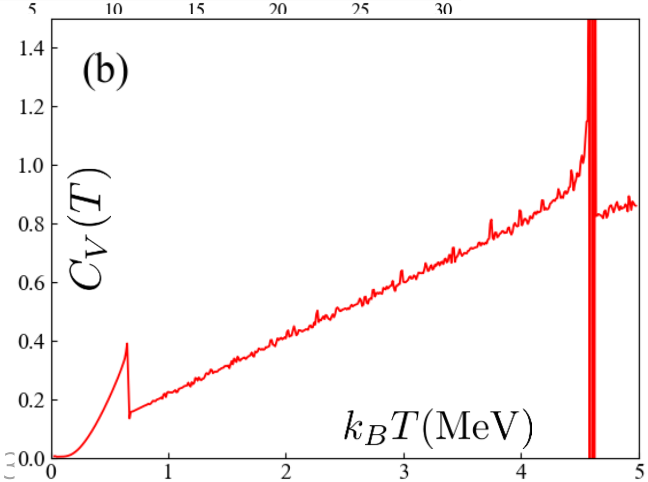


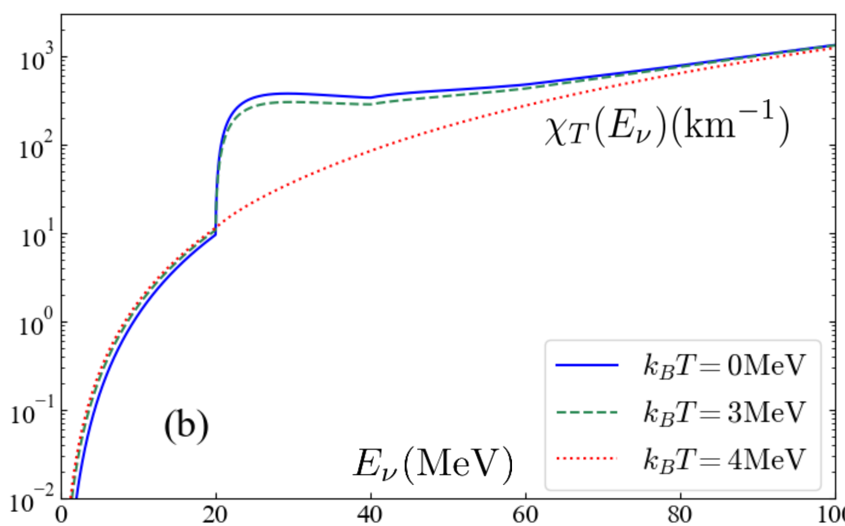
F.T. structure :

- Density change to uniform distribution
- Pairing goes to zero (normal fluid phase)
- Specific heat shows 2 phase transitions

Scattering calculation :

- Opacity shows peak structure at tens MeV
- Fluid phase doesn't change behaviour
- At 5MeV (uniform) there's no peak





Extension for mag-field systems

Why magnetic-field?

- Observational data supports the existence of ***magnetar***
- Theoretically predicted $B \sim 10^{18} G$ surface mag-field

How can we investigate?

- Electrons are ***Randau-Labi quantized***

$$e_\nu = \sqrt{c^2 p_z^2 + m_e^2 c^4 (1 + 2\nu B_\star)}$$

→Drastic change of nuclear composition?

- Recently effect on nucleus been investigated

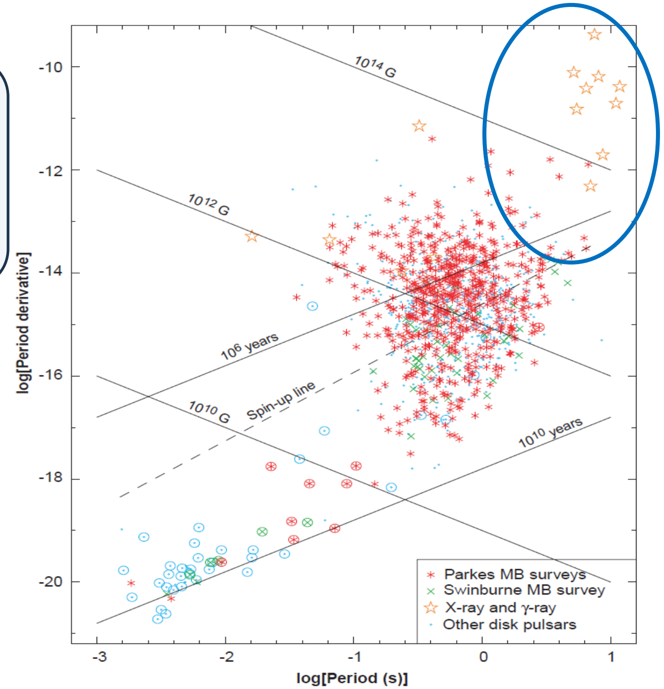
$$\hat{h}_q \rightarrow \hat{h}_q + \hat{h}_q^{(B)} \qquad \hat{h}_q^{(B)} = -\left(\boldsymbol{l}\delta_{q,p} + g_q \frac{\boldsymbol{\sigma}}{2} \right) \cdot \boldsymbol{B}_\star$$

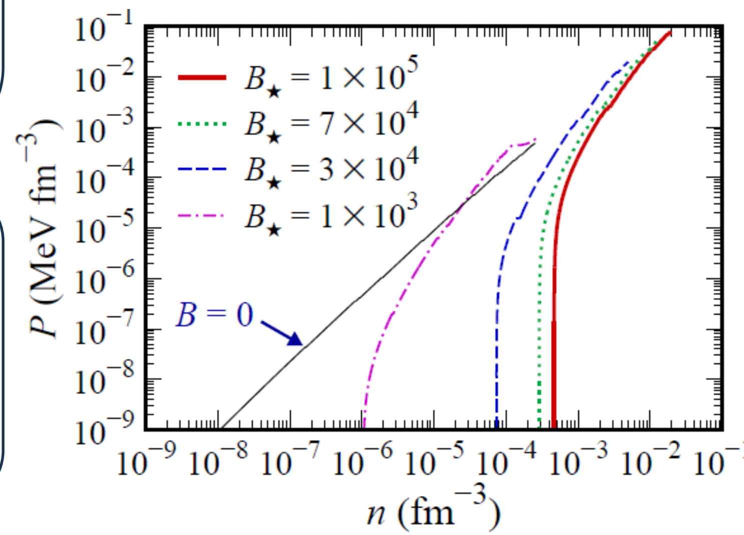
$$g_n = -3.826 \qquad g_p = 5.585$$

What we wanna know

- How structure changes?
- How affect on Equation of State?
- How pairing dynamics appear?

  (spin triplet superfluid, LOFF phase, etc...)





Extension for mag-field systems

Formulation

Additional magnetic-field term

$$\hat{h}_q \to \hat{h}_q + \hat{h}_q^{(B)} \qquad \hat{h}_q^{(B)} = -\left(\boldsymbol{l}\delta_{q,p} + g_q \frac{\boldsymbol{\sigma}}{2}\right) \cdot \boldsymbol{B}_\star$$

$$B^\star = B/B_c \qquad B_c = 2m_q c/e\hbar \sim 4.41 \times 10^{13} G$$

HFB equation with spin d.o.f. : $\hat{H}\begin{pmatrix} u_{\mu\boldsymbol{k}\uparrow}(\boldsymbol{r}) \\ u_{\mu\boldsymbol{k}\downarrow}(\boldsymbol{r}) \\ v_{\mu\boldsymbol{k}\uparrow}(\boldsymbol{r}) \\ v_{\mu\boldsymbol{k}\downarrow}(\boldsymbol{r}) \end{pmatrix} = E_{\mu\boldsymbol{k}} \begin{pmatrix} u_{\mu\boldsymbol{k}\uparrow}(\boldsymbol{r}) \\ u_{\mu\boldsymbol{k}\downarrow}(\boldsymbol{r}) \\ v_{\mu\boldsymbol{k}\uparrow}(\boldsymbol{r}) \\ v_{\mu\boldsymbol{k}\downarrow}(\boldsymbol{r}) \end{pmatrix}$

$$\hat{H} = \begin{pmatrix} \hat{h}_{\uparrow\uparrow} + \hat{h}_{\boldsymbol{k}} + \hat{h}^{(B)} - \lambda & 0 & 0 & \Delta \\ 0 & \hat{h}_{\downarrow\downarrow} + \hat{h}_{\boldsymbol{k}} - \hat{h}^{(B)} - \lambda & -\Delta & 0 \\ 0 & -\Delta^* & -\hat{h}^*_{\uparrow\uparrow} - \hat{h}^*_{-\boldsymbol{k}} - \hat{h}^{(B)} + \lambda & 0 \\ \Delta^* & 0 & 0 & -\hat{h}^*_{\downarrow\downarrow} - \hat{h}^*_{-\boldsymbol{k}} + \hat{h}^{(B)} + \lambda \end{pmatrix}$$

Electron energy calculation

Beta-equilibrium condition : $\mu_n = \mu_p + \mu_e$

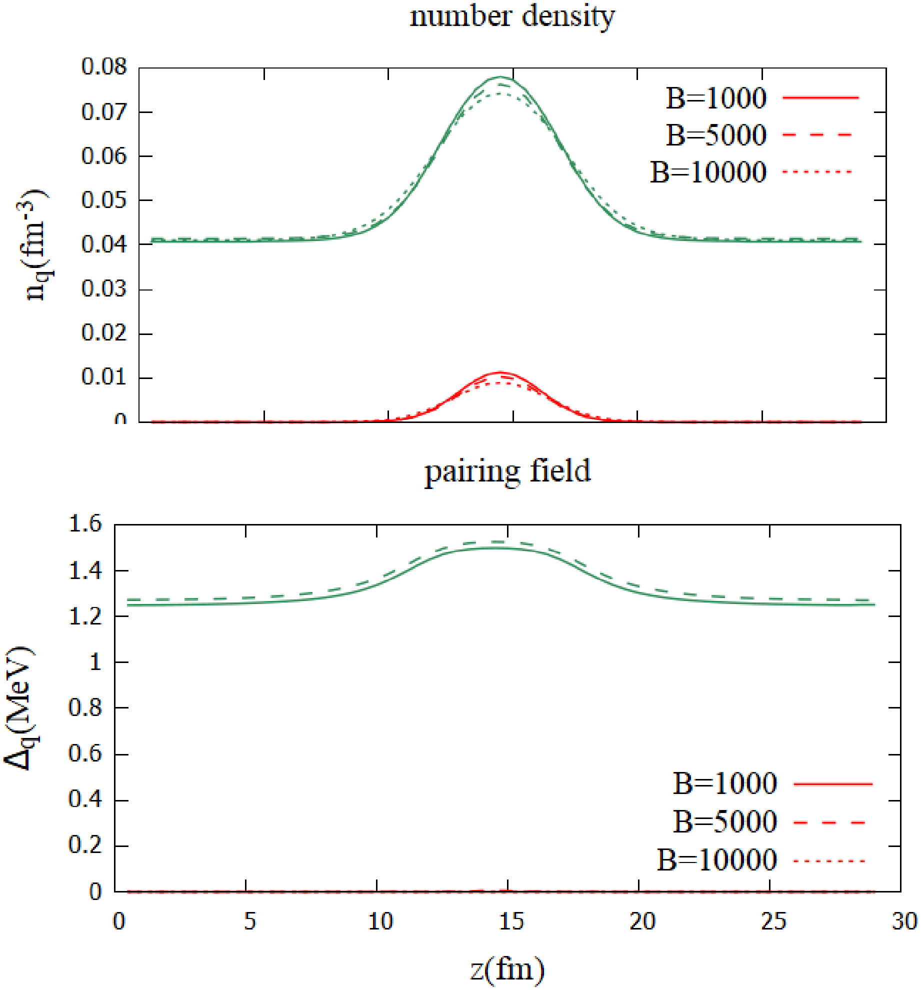
Charge neutrality : $\int (n_p - n_e) \mathrm{d}z = 0$

Electron energy level : $e_\nu = \sqrt{c^2 p_z^2 + m_e^2 c^4 (1 + 2\nu B_\star)}$

Electron density : $n_e = \dfrac{2B^\star}{(2\pi)^2 \lambda_e^3} \displaystyle\sum_{\nu=0}^{\nu_{\max}} g_\nu \sqrt{\gamma_e^2 - 1 - 2\nu B^\star}$

Calculation Result

<u>*Remark :*</u> 図中Bは全てB★ $B^\star = B/B_c$ $B_c = 2m_q c/e\hbar \sim 4.41 \times 10^{13} G$



数密度

- 磁場によって変化（一様に近づく？）
- でもあまり変わらないかも

ギャップ

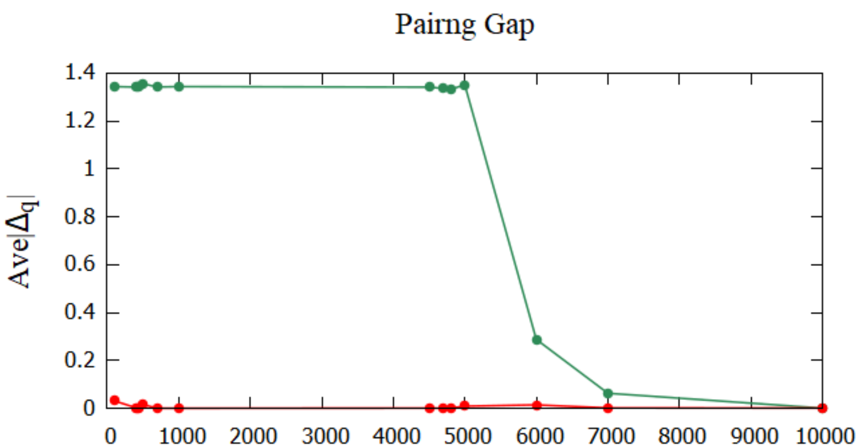
- 陽子は一瞬で壊れる（常伝導に）
- 中性子は割と耐える

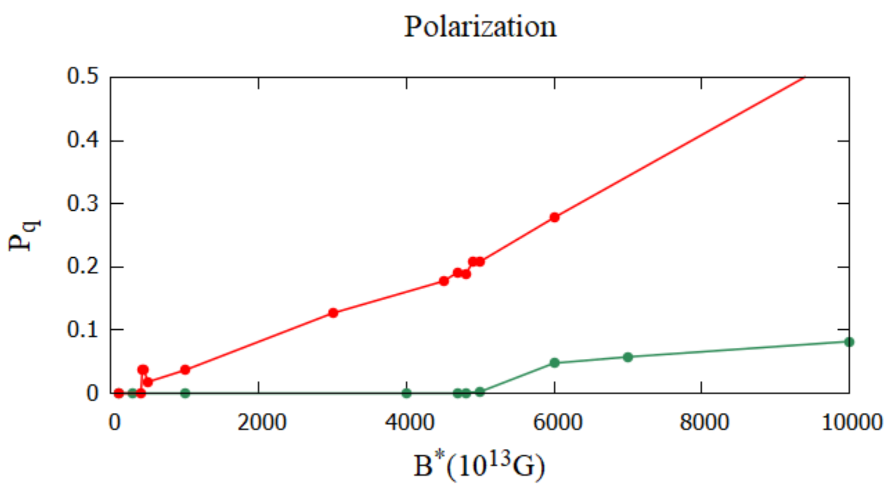
→強磁場では壊れる

Calculation Result

磁場を変数にPairing Gap、及び偏極度Pqを見る。

$$P = |N_\uparrow - N_\downarrow| / (N_\uparrow + N_\downarrow)$$





ギャップ

・陽子は一瞬で壊れる

→B*～6000前後で変化？（誤差かも）

・B*～6000で中性子は急激に変化

→すぐにゼロにはならない、
B*～7000くらいにかけてゼロに

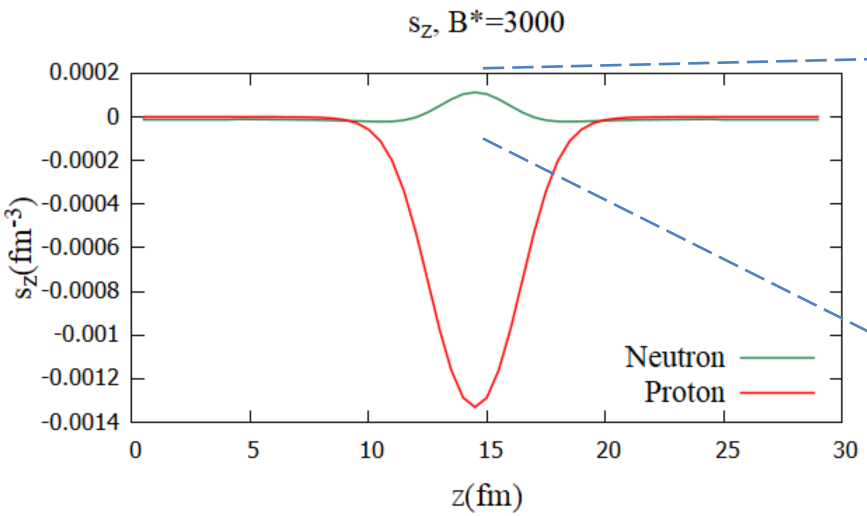
偏極度

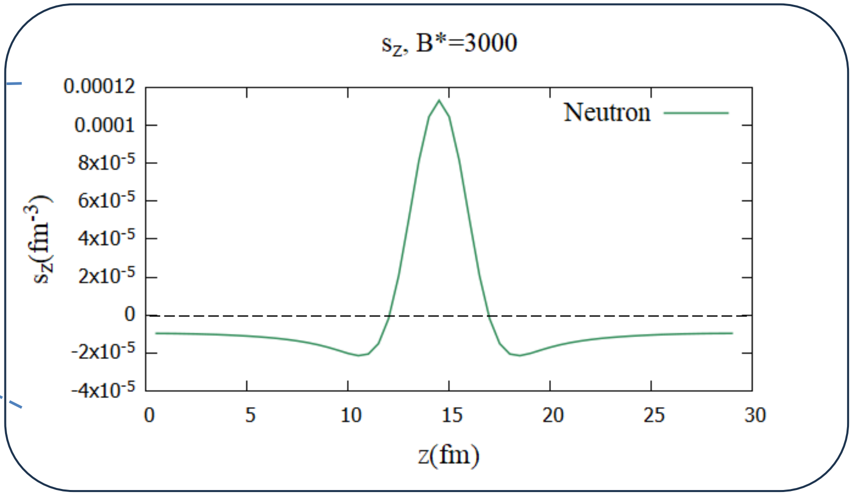
・陽子：B*～400くらいで偏極はじまる
→その後はほぼ線型に上がる

・中性子：B*～5000前後まではゼロ、
その直後一気に上がる
→その後は線型に上昇していく

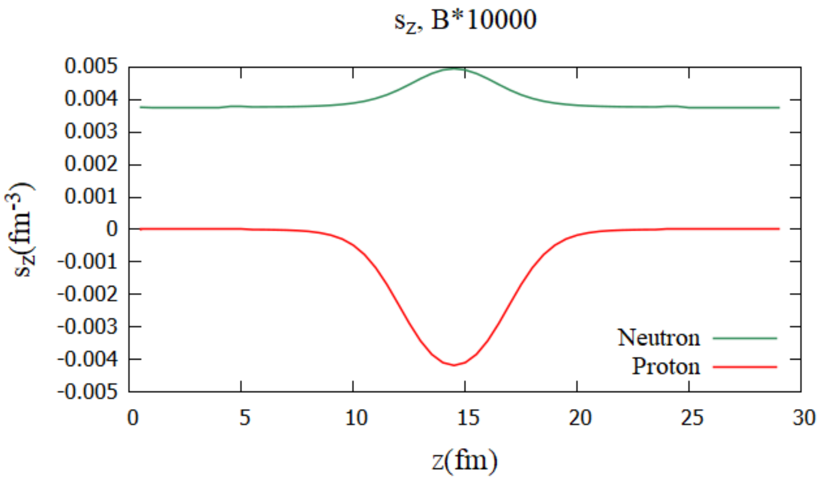
Calculation Result

B*=3000の偏極度分布





B*=10000の場合



- スラブ部分では陽子と逆方向に偏極
- 外側ではそれを打ち消すように偏極
- 全体とととして磁化0が保たれている
  （spin-spin interactionの影響？）

- 同じくらいの割合で偏極

Summary

What we've done

- developed the ①self-consistent ②superfluid ③band theory
  for nuclear pasta in the neutron star inner crust
- performed calculations and successfully extracted neutron ***effective mass***

Extensions

- For finite temperature systems,
  computing structure changes and ν-pasta scattering processes.
- For finite-magnetic-field systems,
  computing spin polarization and phase transitions

What we'll do

- Extensions for two- or three- dimensional crystalline phases,
  completing the "table" of effective mass as a function of density.

Thank you for your careful attention