Time-Dependent Band Theory for the Inner Crust of Neutron Stars: Extension to Include Superfluidity

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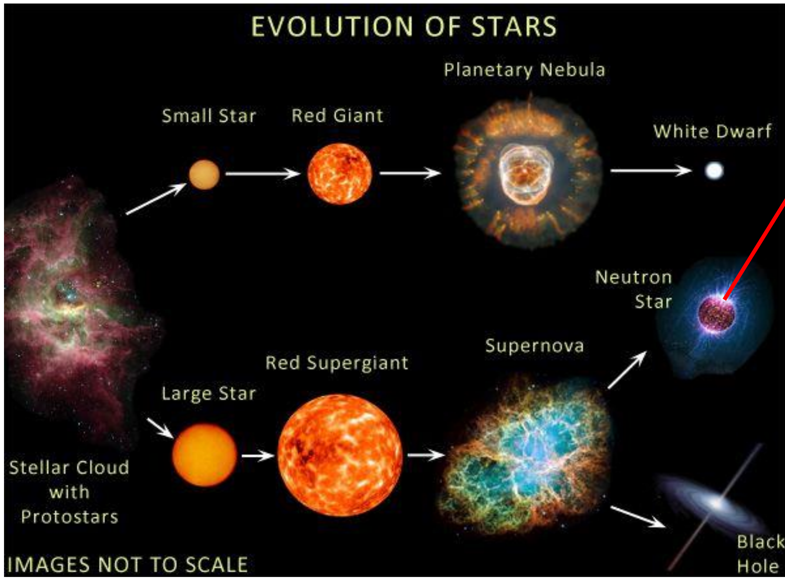
Contents

- Motivation
  - What is Neutron Star?
  - Entrainment Effect
- Theoretical Framework
  - Formulation
  - Derivation of Effective Mass
- Calculation Result
  - Distributions
  - Effective Mass
- Extensions
  - Beta-Equilibrium
  - Finite Temperature Systems
- Summary

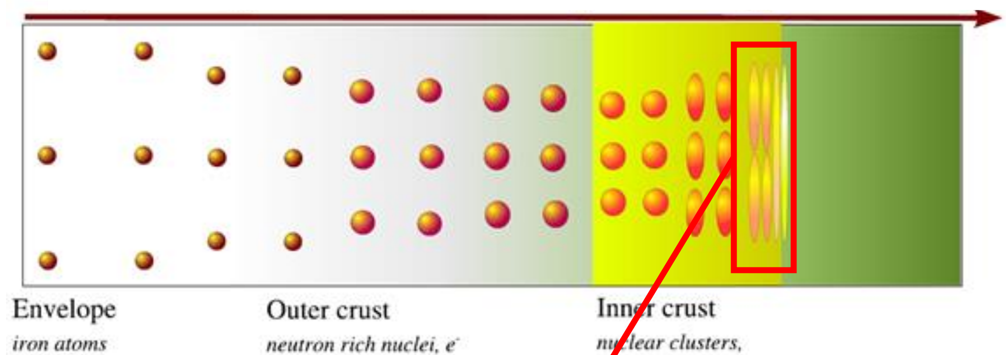
What is Neutron Star?

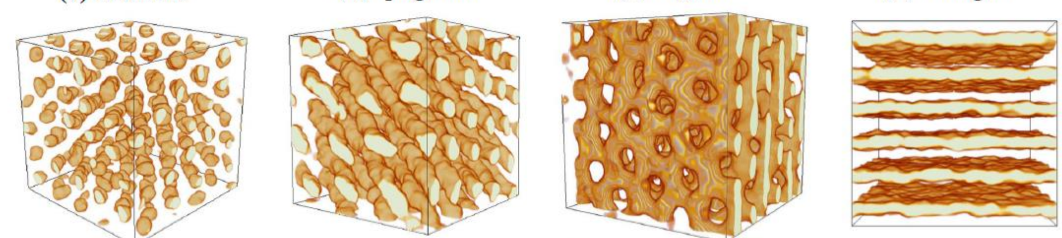
https://blackholecam.org/a-massive-star-collapsing-in-upon-itself-forms-a-black-hole/



Mass: $1.4M_{\odot}$, Radius: 12km

N. Chamel and P. Haensel, Living Rev. Relativity 11, 10 (2008)





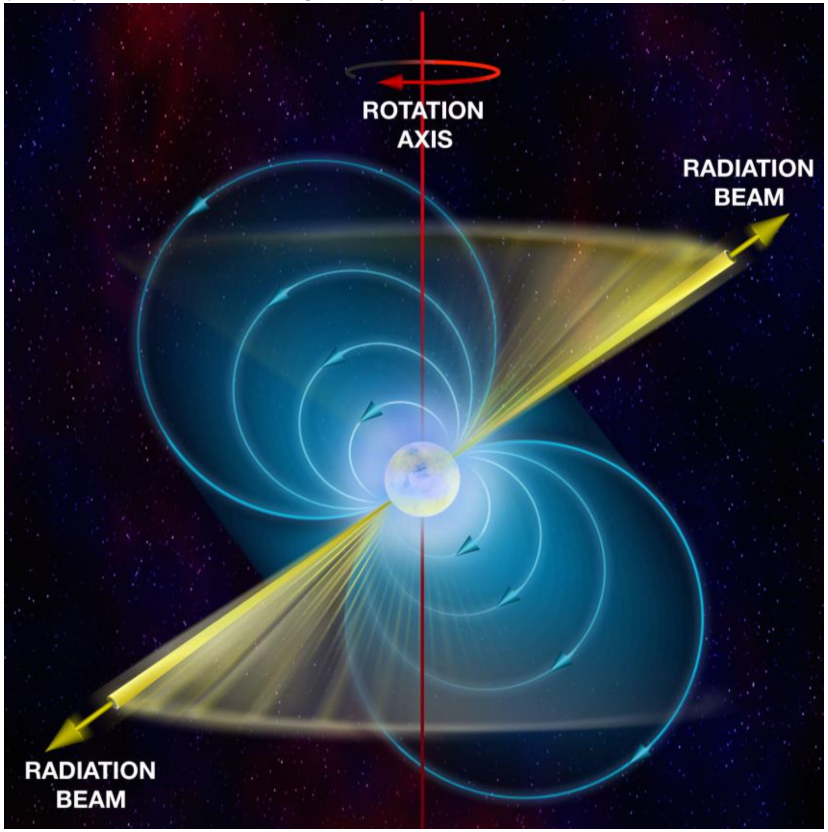
H. Heiselberg, arXiv: astro-ph/0201465.

The “Pasta Structure” is realized at the bottom layer of “inner crust”

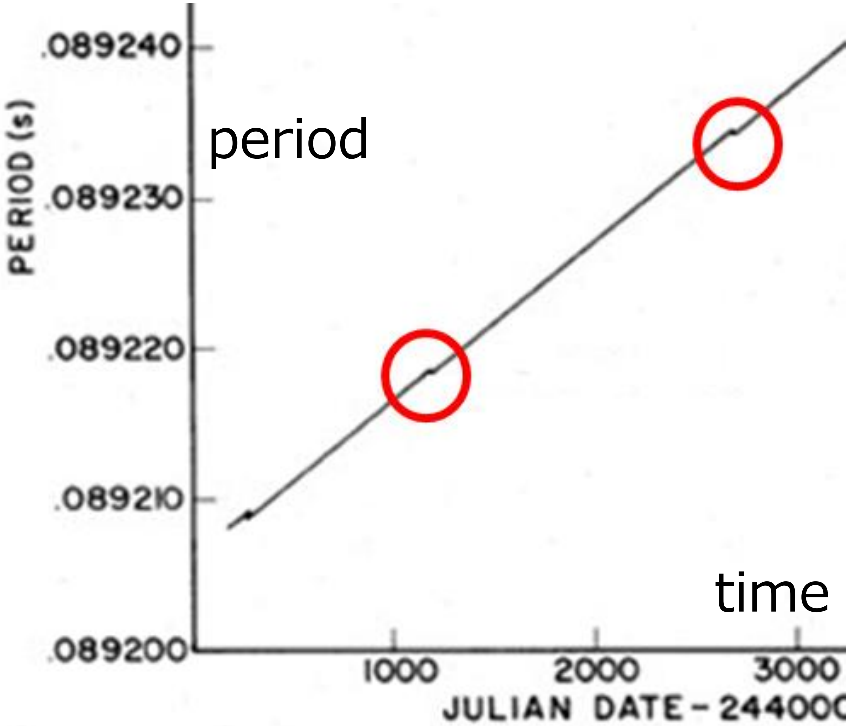
We’re now investigating the states and structures of these Pasta phases by using DFT combined with HFB theory and Band theory.

What is Neutron Star?

https://public.nrao.edu/gallery/parts-of-a-pulsar/



Neutron stars are called "**pulsar**", because of their periodic pulses which are radiated by the magnetic pole.

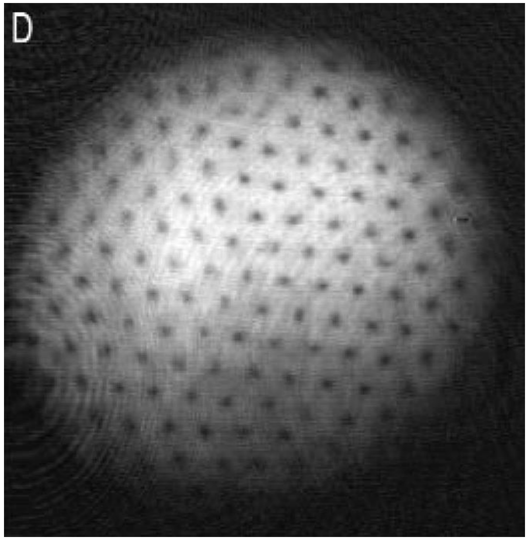


https://www2.kek.jp/imss/cmrc/other/workshop20190114/14-5 iida.pdf

The time series of period shows gradual increase due to the magnetic radiation, and irregular recovery which is called "**glitch**" phenomenon.

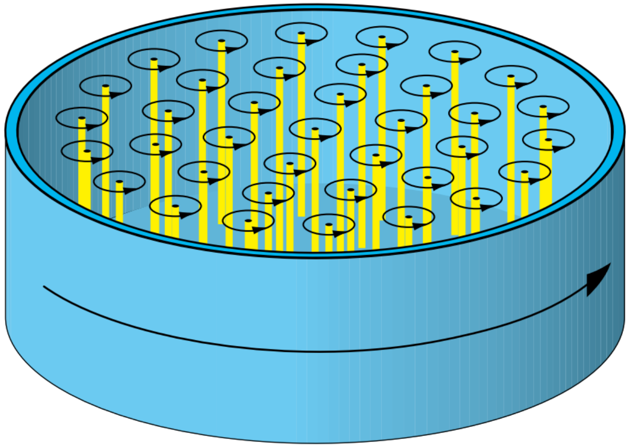
Glitch and Quantum Vortices

In recent researches, it has been advocated the superfluidity of neutrons in inner crust is influential in the interpretation of glitch phenomena.



"Topological" defect of superfluid yields **quantum "vortices"** which store angular momentum.

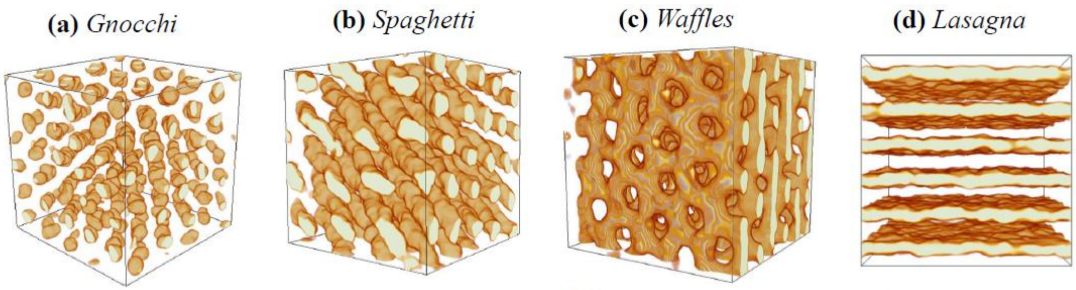
Dissolution of a mass of vortices contributes to the recover of rotational speed···?



Computational Simulation!

Entrainment Effect

H. Heiselberg, arXiv: astro-ph/0201465.



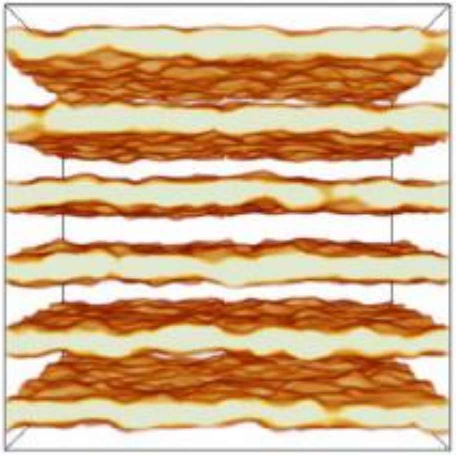
- N.Chamel, PRC85, 035801 (2012)
  The first research in which they simulated the states of pasta structure using "**Density Functional Theory**" combined with "**Band theory**".

$\bar{n}$ (fm^{-3})	Z	A	n_n^f/n_n (%)	n_n^c/n_n^f (%)	$m_n^\star/m_n$
0.0003	50	200	20.0	82.6	1.21
0.001	50	460	68.6	27.3	3.66
0.005	50	1140	86.4	17.5	5.71
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
0.06	20	780	91.5	45.9	2.18

Captured by periodical structure, the **conduction** of dripped neutrons are strikingly disturbed, moreover there are density areas where the "**effective mass**" reaches ten times of bare mass!!

Precedent Research

However, in the following studies…



- Y.Kashiwaba and T.Nakatsukasa, PRC100, 035804 (2019)
  The first self-Consistent band calculations for slab phases of inner crust.

- K.Sekizawa, S.Kobayashi, and M.Matsuo, PRC105, 045807 (2022)
  A new approach using TDDFT and derive effective mass dynamically by analyzing the response to fixed external fields.

⇩

Both calculations give effective masses less than bare mass!
(anti-entrainment?)

For more comprehensive understanding of entrainment, we have to take into account superfluidity.(We're now trying to!)

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  - Derivation of Effective Mass
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Formulation

Kohn-Sham theory

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + v_{\mathrm{KS}}[\rho]\right]|\psi_n\rangle = \varepsilon_n |\psi_n\rangle$$

with densities,

$\rho[\psi(\boldsymbol{r})]$, $\tau[\psi(\boldsymbol{r})]$, $\boldsymbol{j}[\psi(\boldsymbol{r})]$, etc⋯

HFB theory

$$\begin{pmatrix} \hat{h}-\lambda & \Delta_{\uparrow\downarrow} \\ \Delta^{\star}_{\uparrow\downarrow} & -\hat{h}^{\star}+\lambda \end{pmatrix}\begin{pmatrix} u_{k\uparrow} \\ v_{k\downarrow} \end{pmatrix} = E_k \begin{pmatrix} u_{k\uparrow} \\ v_{k\downarrow} \end{pmatrix}$$

$\Delta_{\uparrow\downarrow}$ ⋯pairing field

λ ⋯chemical potential

$$u_{\alpha\boldsymbol{k}}(z) = \tilde{u}_{\alpha\boldsymbol{k}}(z)e^{i\boldsymbol{k}\boldsymbol{r}}$$

$$v_{\alpha\boldsymbol{k}}(z) = \tilde{v}_{\alpha\boldsymbol{k}}(z)e^{i\boldsymbol{k}\boldsymbol{r}}$$

Band theory

$$\psi_{\alpha\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{\Omega}}\tilde{\psi}_{\alpha\boldsymbol{k}}(\boldsymbol{r})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{r}}$$

$$\tilde{\psi}_{\alpha\boldsymbol{k}}(\boldsymbol{r}+\boldsymbol{T}) = \tilde{\psi}_{\alpha\boldsymbol{k}}(\boldsymbol{r})$$

In 1D periodical system⋯

$$\psi_{\alpha\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{\Omega}}\tilde{\psi}_{\alpha\boldsymbol{k}}(z)\mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{r}}$$

The we can finally get

$$\begin{pmatrix} \hat{h}^{(q)}+\hat{h}^{(q)}_{\boldsymbol{k}}-\lambda & \Delta_{\uparrow\downarrow} \\ \Delta^{*}_{\uparrow\downarrow} & -\hat{h}^{(q)*}-\hat{h}^{(q)*}_{\boldsymbol{k}}+\lambda \end{pmatrix}\begin{pmatrix} u^{(q)}_{\alpha\boldsymbol{k}.\uparrow} \\ v^{(q)}_{\alpha\boldsymbol{k}.\downarrow} \end{pmatrix} = E_{\alpha\boldsymbol{k}}\begin{pmatrix} u^{(q)}_{\alpha\boldsymbol{k}.\uparrow} \\ v^{(q)}_{\alpha\boldsymbol{k}.\downarrow} \end{pmatrix}$$

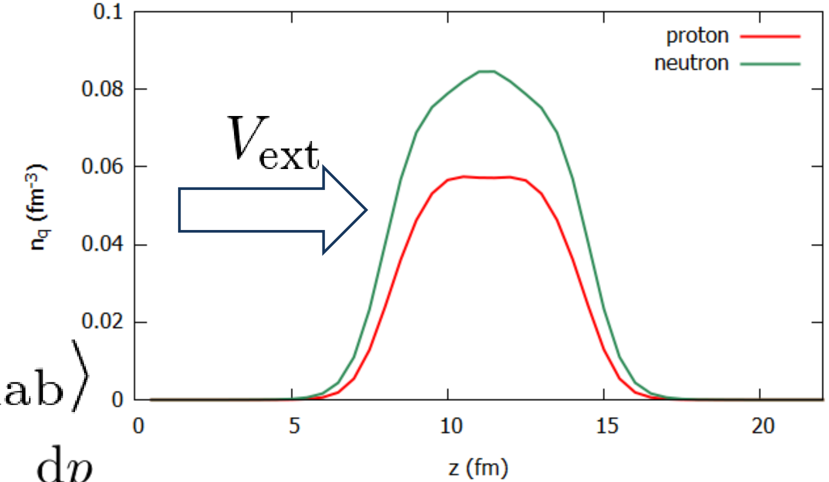
Formulation

We can extend this calculation into time-dependent form as

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_k(z,t) \\ v_k(z,t) \end{pmatrix} = \begin{pmatrix} \hat{h}(z,t) & \Delta(z,t) \\ \Delta^*(z,t) & -\hat{h}^*(z,t) \end{pmatrix}\begin{pmatrix} u_k(z,t) \\ v_k(z,t) \end{pmatrix}$$

We set the external field coupling to only protons as

$$\hat{h}(\boldsymbol{r},t) = \hat{h}(\boldsymbol{r}) + V_{\mathrm{ext}}(t)\delta_{qp}$$



Tracing the response to the external force,

we can get the acceleration a_{slab}

and

the momenta of protons and slab $\langle P_p\rangle\langle P_{\mathrm{slab}}\rangle$

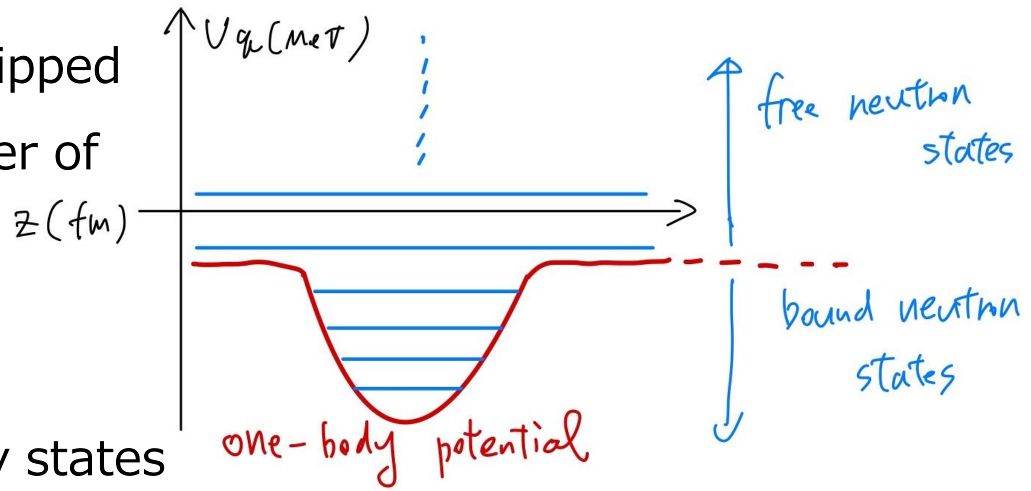
From the classical relation $ma = \frac{\mathrm{d}(mv)}{\mathrm{d}t} = \frac{\mathrm{d}p}{\mathrm{d}t}$ we can get

$$M_{\mathrm{slab}} = \frac{\langle P_{\mathrm{slab}}\rangle}{a_{\mathrm{slab}}} \qquad M_{\mathrm{p}} = \frac{\langle P_{\mathrm{p}}\rangle}{a_{\mathrm{slab}}}$$

Then we can calculate mass of neutrons belonging to slab $M_{n.\mathrm{effbound}}$

Derivation of effective mass

To evaluate the effective mass of dripped neutrons, we have to get the number of neutrons not bound in nuclei.



To get it, we have to separate energy states into ones whose one-particle energies are below the potential and not.

We define "free neutron density" as $n_n^f = \frac{N_{\mathrm{local}}}{a} - n_n$

where $N_{\mathrm{local}} = \frac{1}{N_{kz}} \sum_{\alpha, k_z} \int \frac{k_\parallel}{\pi} \left[\frac{1}{a} \int_0^a |v_{\alpha \boldsymbol{k}}^{(q)}(z)|^2 dz \right] \theta(U_0^{(q)} - e_{\alpha \boldsymbol{k}}^{(q)})$

This is the free neutron number without the effect of periodical system.

Derivation of effective mass

Next we will the number of neutrons which “effectively” contribute to the conduction of the dripped neutrons.

Using $M_{n.\mathrm{effbound}}$ gotten in TD-calculation, we can get

$$N_{n.\mathrm{effbound}} = \frac{M_{n.\mathrm{effbound}}}{m^{\oplus}_{\mathrm{drip}}}$$

Then we define the “conduction number density” as

$$n_n^c = \frac{N_n - N_{n.\mathrm{effbound}}}{a}$$

Now we can represent the extent of the effect of periodical structure by

$$\frac{m_n^\star}{m_n} = \frac{n_n^f}{n_n^c}$$

which we call “collective effective mass”.

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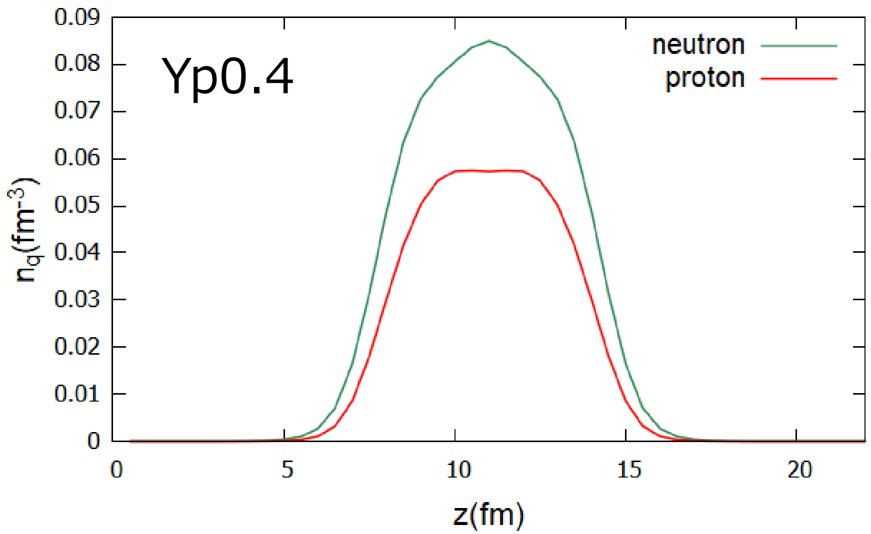
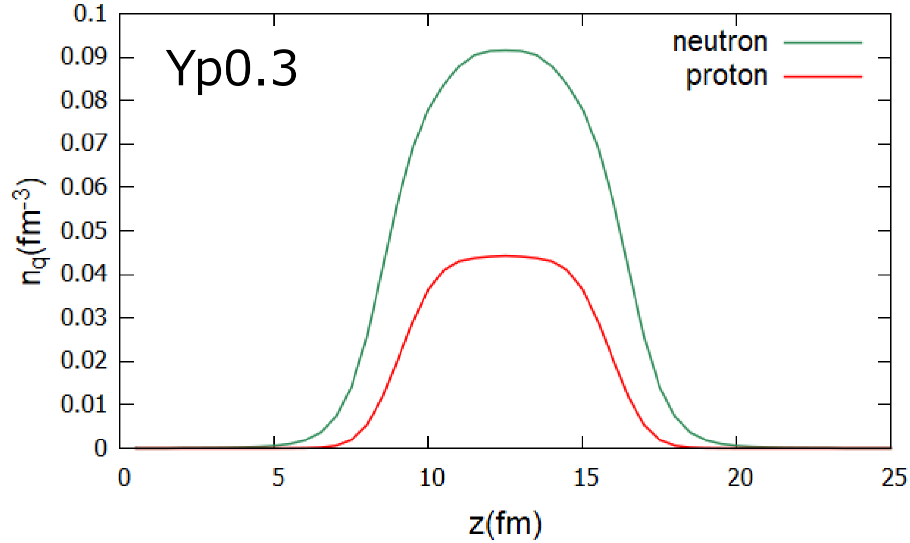
Computational Settings

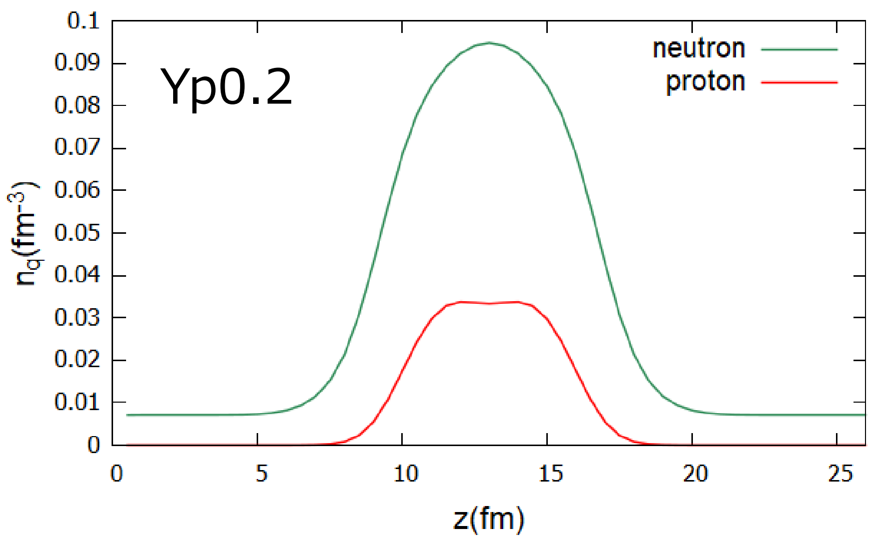
- We normally fix baryon density $n_B = 0.04$ and proton proportion $Y_p = 0.1, 0.2, \ldots, 0.5$, and adjusted λ such as particle numbers conserve.
- For EDF, we used as a parameter set "Sly4"
- For the coordinates we set $\mathrm{d}z = 0.5\,\mathrm{fm}$ and period length a such as the total energy of the system gives the minimum (later)
- We recognize the period direction as z axis and discretize wavenumber k_z into N_{k_z} points within 1st Brillouin zone $-\pi/a \leq k_z \leq \pi/a$

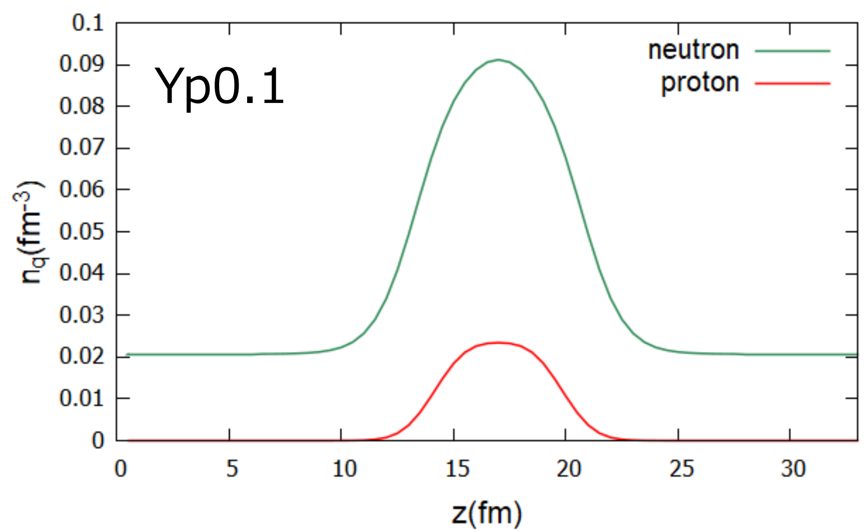
  The other parts k_x k_y are reduced into $k_{||} = \sqrt{k_x^2 + k_y^2}$ and discretized as $\mathrm{d}k_{||} = 0.1$, $0 \leq k_{||} \leq 1.5$
- For the TD-calculation we set $\mathrm{d}t = 0.1\,\mathrm{fm/c}$ and time developed until $t = 3000\,\mathrm{fm/c}$ or $t = 4000\,\mathrm{fm/c}$
- All the calculations are parallelized by MPI and executed in Yukawa-21

Density Distribution



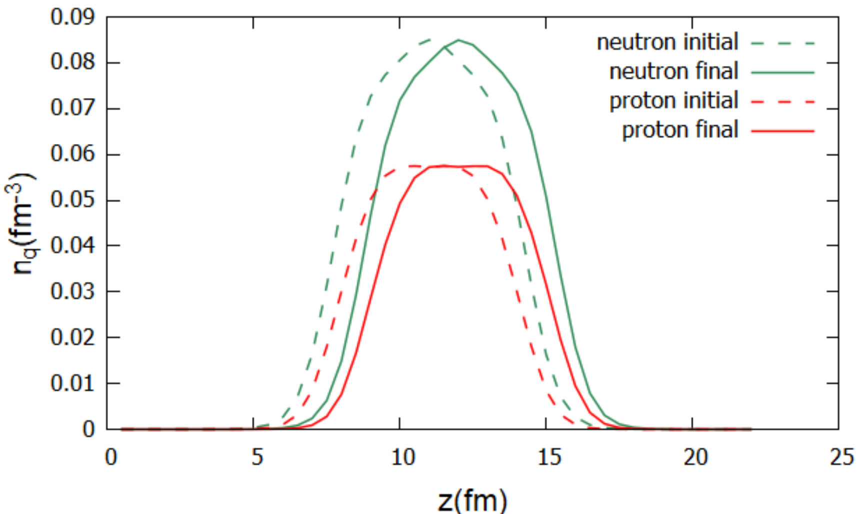


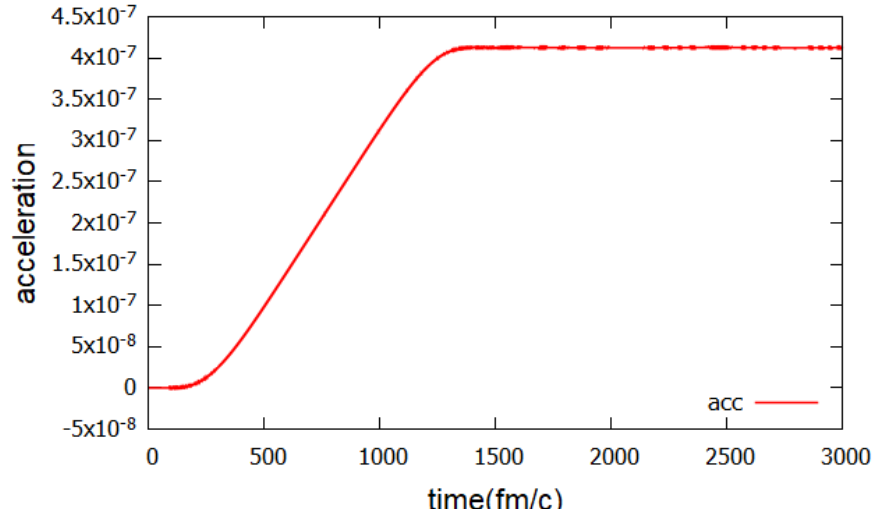




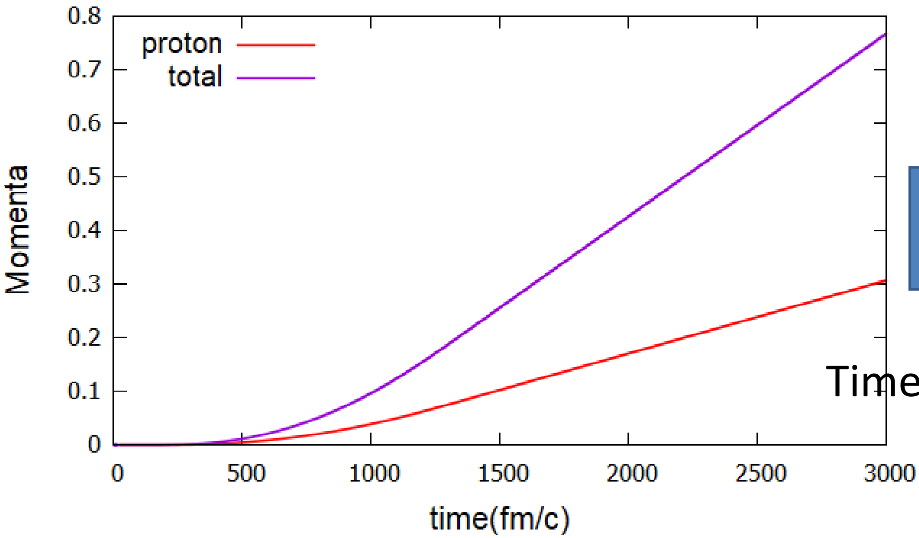
TD-Calculation Result

In the Yp0.4 setting, the change of densities and acceleration are like

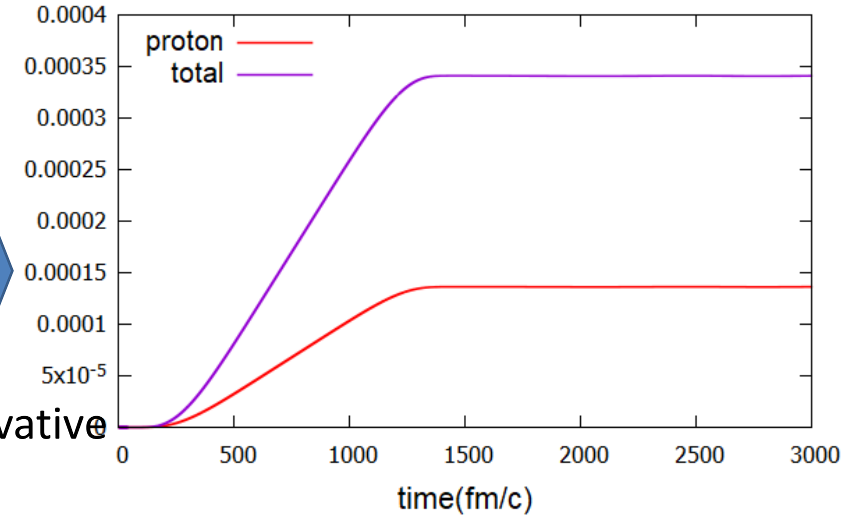




The change of momenta is



Time derivative



Effective Mass

We can get free neutron densities from static calculations, and conduction number densities from TD calculation.

The very preliminary results are

Yp	n_f	n_c	m*/m	precedent
0.1	0.382	0.632	0.605	0.617
0.2	0.138	0.243	0.568	0.555
0.3	9.37E-03	3.23E-03	2.90	0.043
0.4	5.68E-03	9.78E-05	0	0

? ? ? ?

There is a bit of difference against the precedent research, but we can get generally consistent results.

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  - Effective Mass
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  - **Finite Temperature Systems**
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Beta Equilibrium

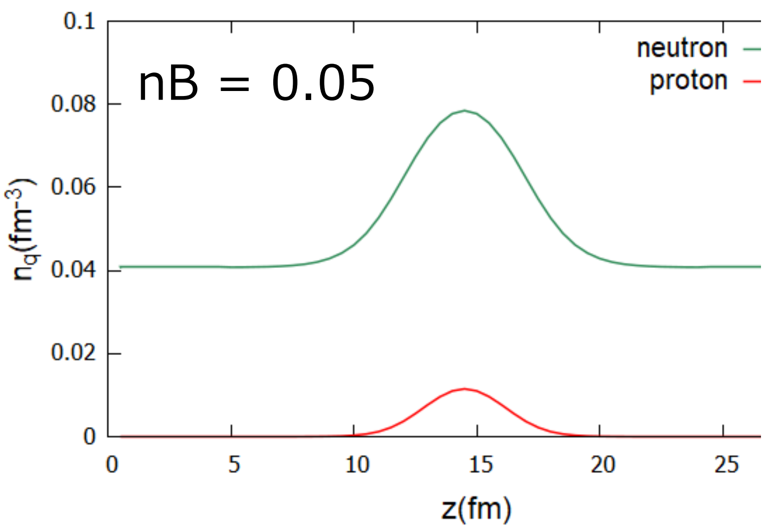
Instead fixing Y_p , we set β-equilibrium condition

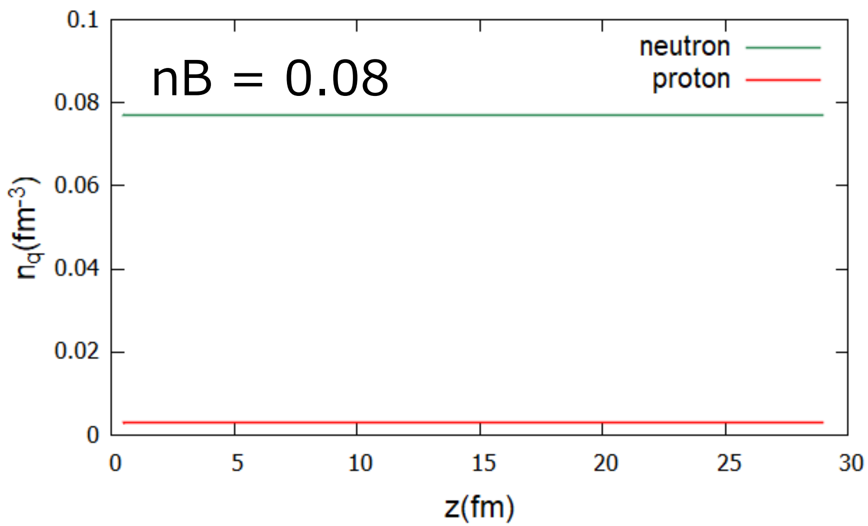
$$\mu_n = \mu_p + \mu_e$$

We investigate how Y_p changes with respect to baryon density n_B

nB	0.04	0.05	0.06	0.07
Yp	0.031	0.030	0.037	0.035
a	38	29	29	25

n_B gets more than 0.08, nuclei melt and distribute uniformly :

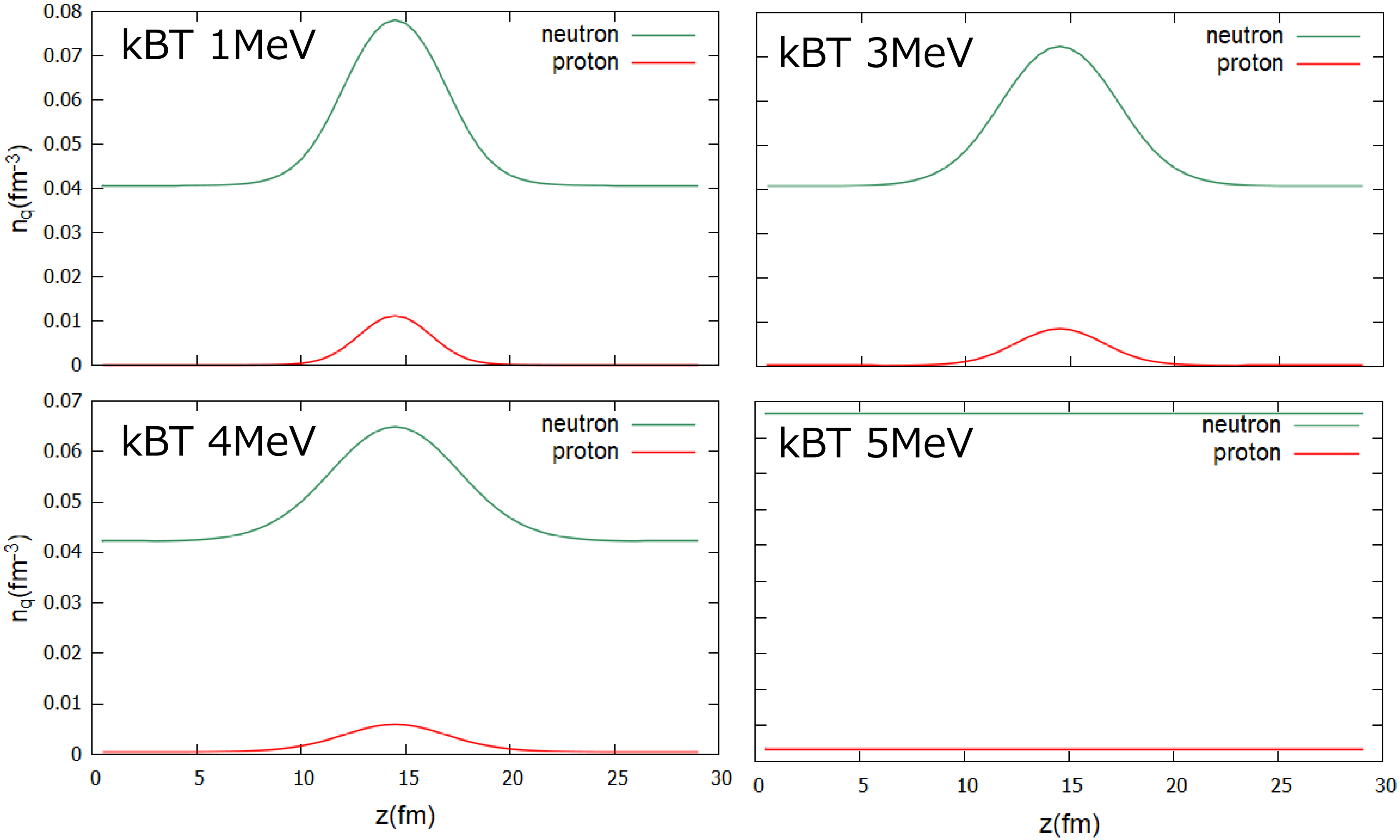




Finite Temperature Extension

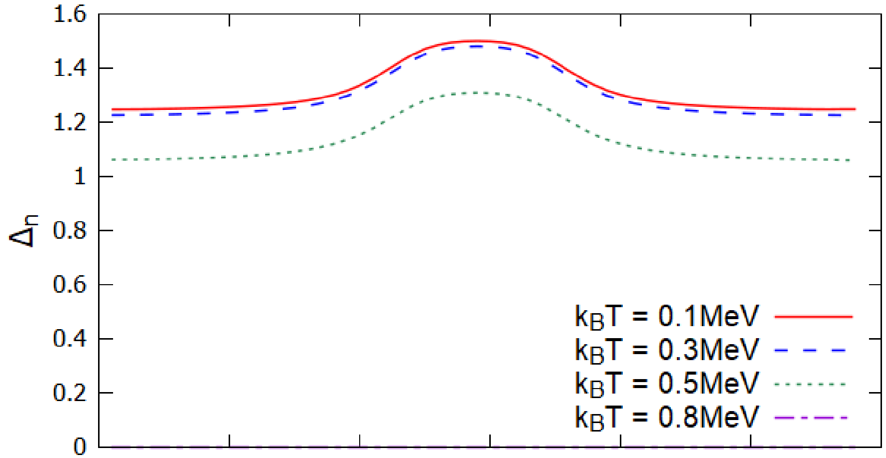
We can easily extend these calculations into finite temp. systems.

in nB = 0.05 settings, nuclei are changed with respect to kBT as



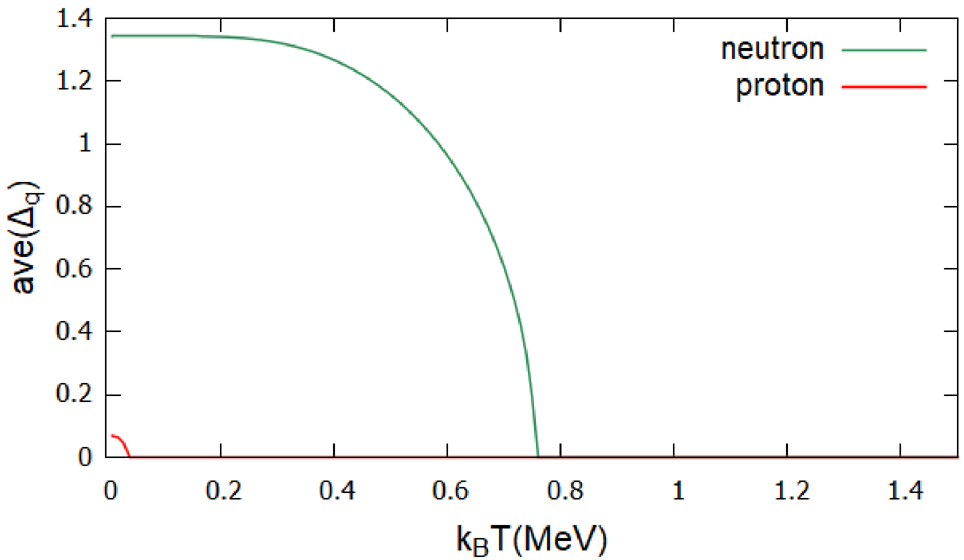
Finite Temperature Extension

Pairing field $\Delta_{\uparrow\downarrow}$ is of course affected by the change of temperature.



We can see that as kBT increases, $\Delta_{\uparrow\downarrow}$ get less values and suddenly fall into zero.

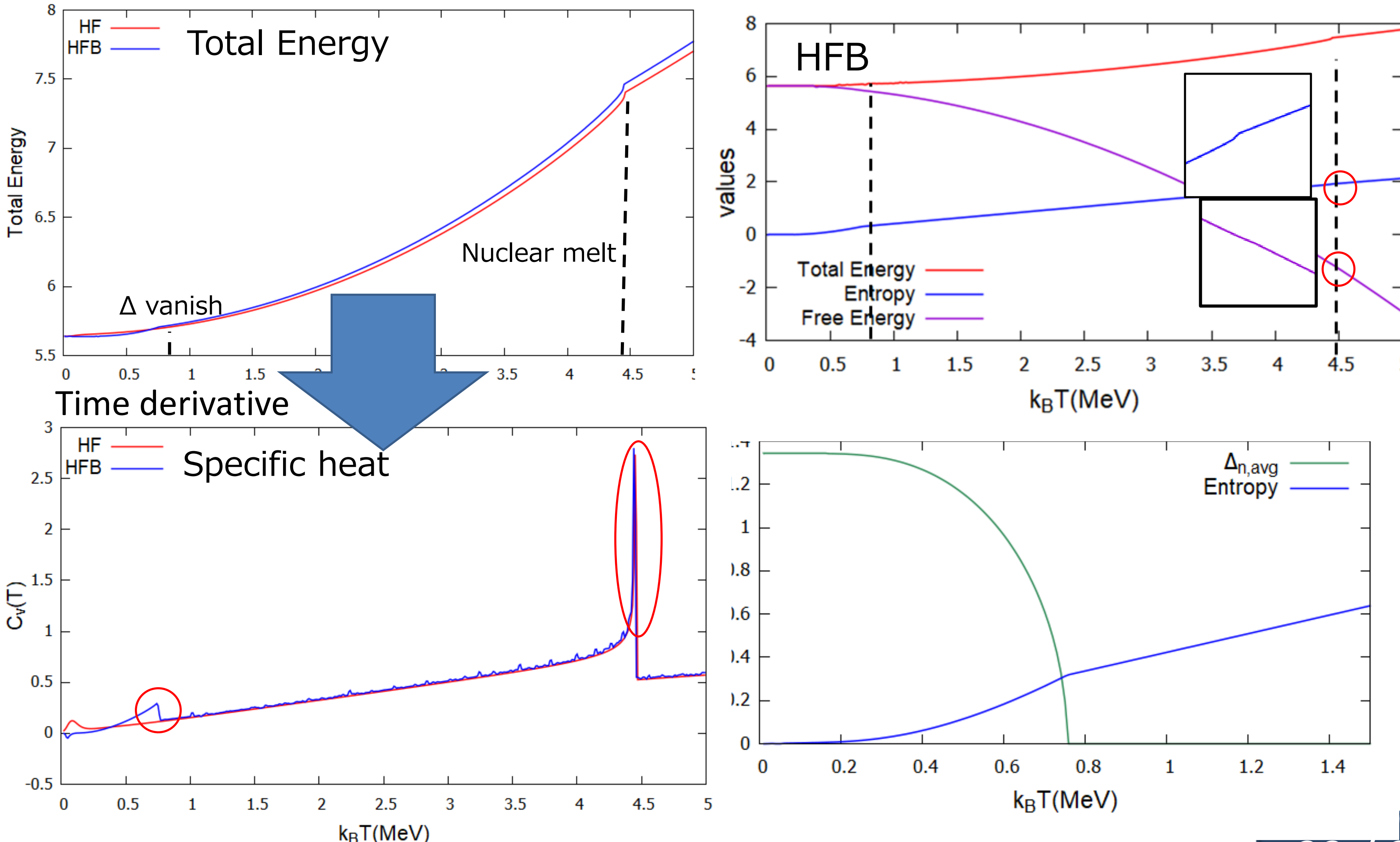
When we take average value, its change w.r.t temperature is like



We can see that under about 0.8 kBT pairing field totally disappears.

Finite Temperature Extension

We trace change of total energy, entropy and free energy w.r.t. temperature :



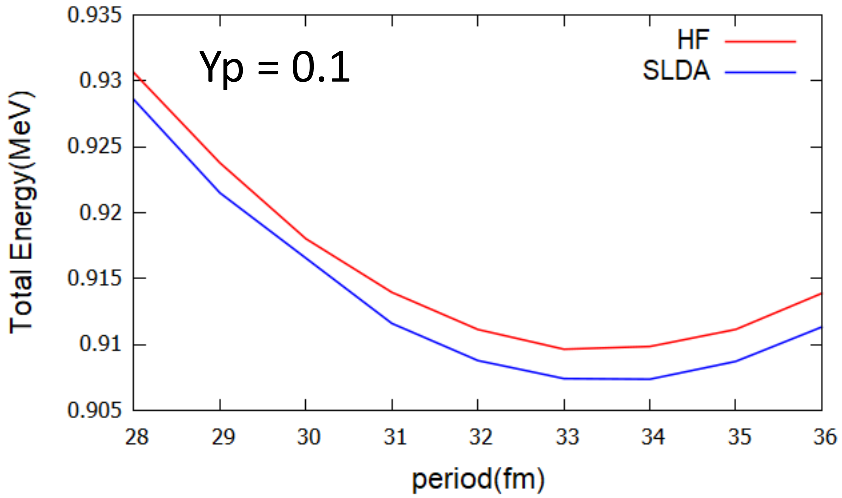
Summary

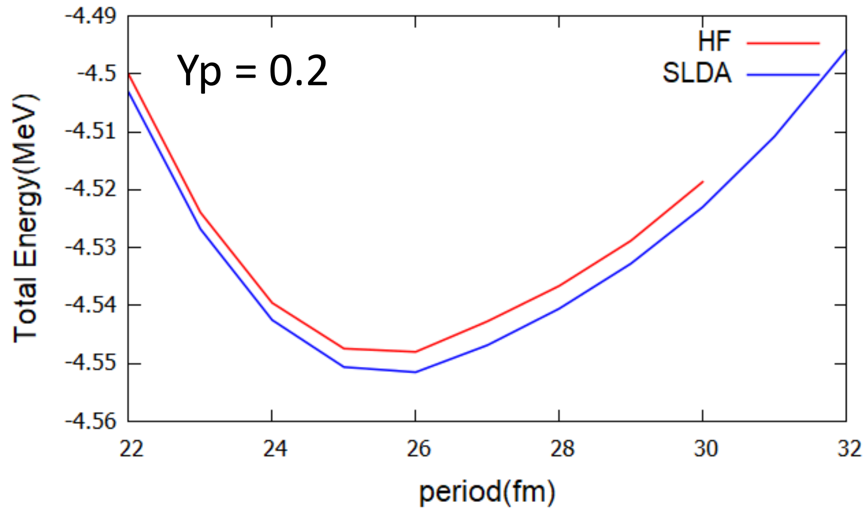
・Based on Kohn-Sham theory, HFB theory, and Band theory, we can simulate systems of neutron-rich nuclei bound in 1-dimensional periodical potential with pairing correlation self-consistently.

・After getting convergence solution statically, we time developed the system and investigate conduction of dripped neutrons dynamically, which leads to derivation of collective effective mass.

・HFB is quite general framework to descript states of nuclei and it is expected that we can extend these calculations into systems under various situation and settings.

System's Energies w.r.t. Periods



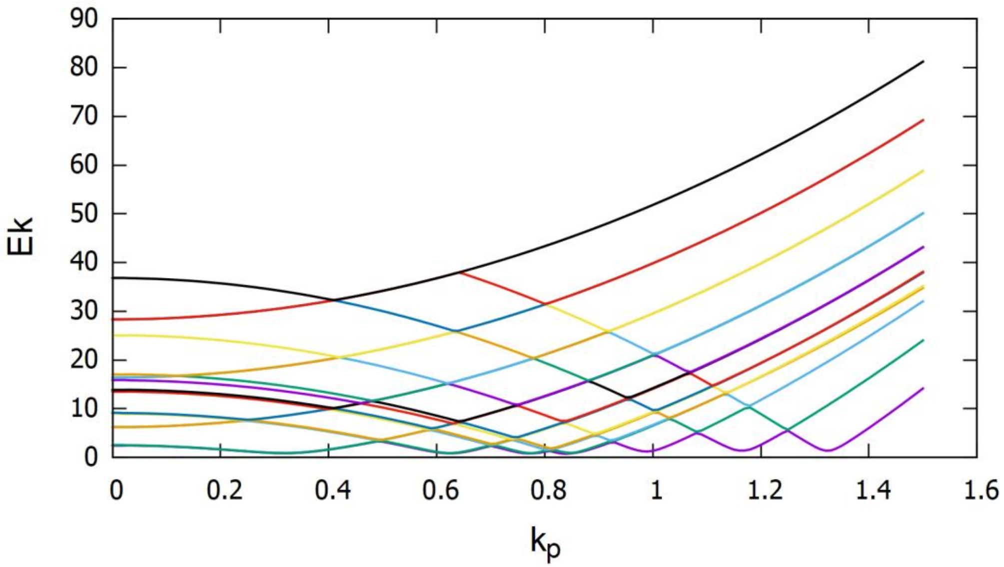


Total energies become lower than HF under any period and Yp, and optimal periods are almost the same between two methods.

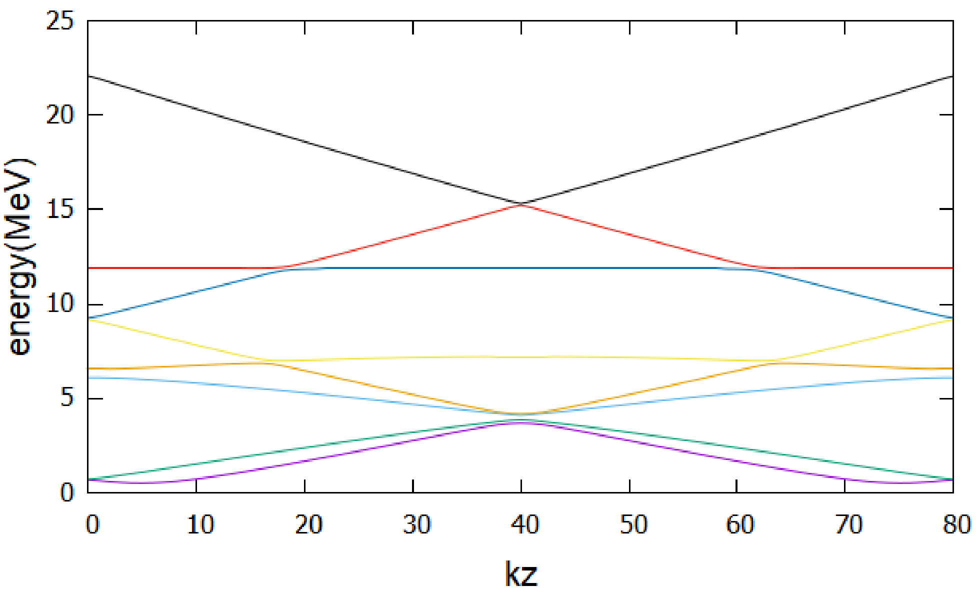
Looking at each part of a certain total energy, we can see slight increase of kinetic energy and interaction terms' compensation and overtake.

	Yp = 0.2	a = a_HF	
	HF	SLDA_old	SLDA_new
Kin_n	15.662	15.984	15.73
Kin_p	2.319	2.4	2.32
Pair_n	0	-0.028	-0.029
Pair_p	0	-0.004	-0.004
Coul	0.392	0.3914	0.392
Skyrme	-22.92	-22.8	-22.96
Total	-4.549	-4.055	-4.552

Energy States



vs $k_{||}$



vs k_z

Pairing field