

Time-Dependent Band Theory for the Inner Crust of Neutron Stars

Kazuyuki Sekizawa



Department of Physics, School of Science
Tokyo Institute of Technology



Today's talk is based on one of my most recent publications:

PHYSICAL REVIEW C **105**, 045807 (2022)

Time-dependent extension of the self-consistent band theory for neutron star matter: Anti-entrainment effects in the slab phase

Kazuyuki Sekizawa ^{1,2,*}, Sorataka Kobayashi,³ and Masayuki Matsuo ^{4,†}

¹Center for Transdisciplinary Research, Institute for Research Promotion, Niigata University, Niigata 950-2181, Japan

²Nuclear Physics Division, Center for Computational Sciences, University of Tsukuba, Ibaraki 305-8577, Japan

³Graduate School of Science and Technology, Niigata University, Niigata 950-2181, Japan

⁴Department of Physics, Faculty of Science, Niigata University, Niigata 950-2181, Japan



(Received 28 December 2021; accepted 4 April 2022; published 25 April 2022)

in collaboration with



Sorataka Kobayashi
(Finished MSc in Mar. 2019)



Masayuki Matsuo

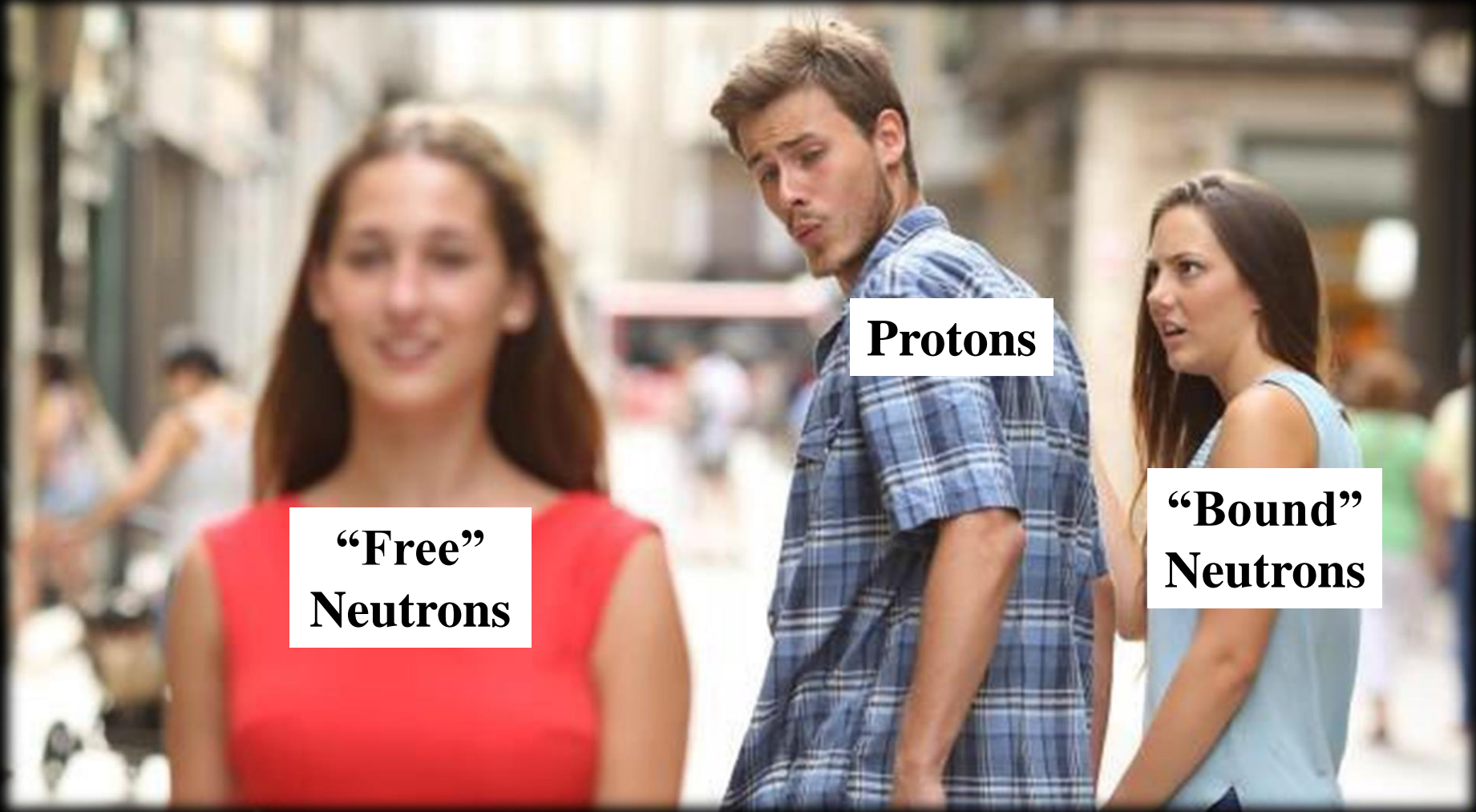


Kenta Yoshimura (M1)



What is the “entrainment” effect?

“Entrainment” is a phenomenon between two species (particles, gases, fluids, etc.), where a motion of one component attracts the other.



**“Free”
Neutrons**

Protons

**“Bound”
Neutrons**

“Entrainment” in the inner crust

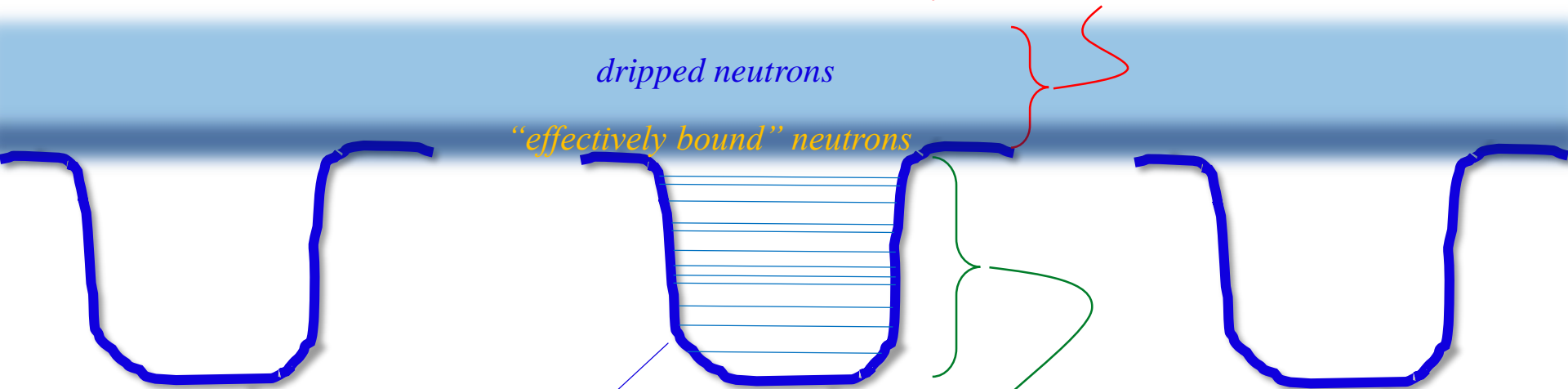
- Part of dripped neutrons are “effectively bound” (immobilized) by the periodic structure (due to Bragg scatterings), resulting in a larger effective mass

$$m_n n_n^f = m_n^* n_n^c$$

n_n^c : Conduction neutron number density
(neutrons that can actually flow)

m_n^* : (Macroscopic) Effective mass

Dripped neutrons extend spatially
→ Affected by the lattice, and a band structure is formed!



Entrainment leads:

- reduction of n_c
- enhancement of m^*

Potential for neutrons

Bound orbitals are well **localized**
→ Not affected by the lattice

The “entrainment effect” is still a debatable problem

- The first consideration for 1D, square-well potential

K. Oyamatsu and Y. Yamada, NPA**578**(1994)184

- Band calculations for slab (1D) and rod (2D) phases

B. Carter, N. Chamel, and P. Haensel, NPA**748**(2005)675

➡ Entrainment effects are **weak** for the slab & rod phases:

$$\frac{m^*}{m} \sim \begin{cases} 1.02 - 1.03 & \text{for the slab phase} \\ 1.11 - 1.40 & \text{for the rod phase} \end{cases}$$

- Band calculations for cubic-lattice (3D) phases

N. Chamel, NPA**747**(2005)109 (2005); NPA**773**(2006)263; PRC**85**(2012)035801; J. Low Temp. Phys. **189**, 328 (2017)

➡ **Significant** entrainment effects were found in a low-density region:

$$\frac{m^*}{m} \gtrsim 10 \text{ or more! for the cubic lattice}$$

- The first *self-consistent* band calculation for the slab (1D) phase (based on DFT with a BCPM EDF)

➡ “**Reduction**” of the effective mass was observed for the slab phase:

$$\frac{m^*}{m} \sim 0.65 - 0.75 \text{ for the slab phase}$$

Yu Kashiwaba and T. Nakatsukasa, PRC**100**(2019)035804

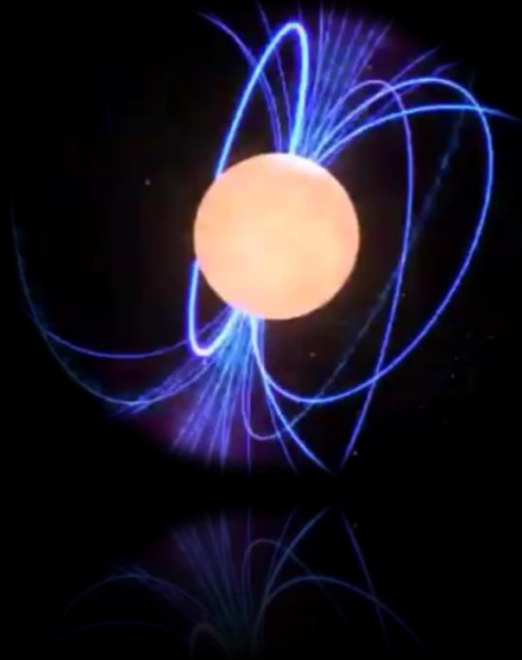
- **Time-dependent extension of the self-consistent band theory (based on TDDFT with a Skyrme EDF)**

➡ “**Reduction**” was observed, consistent with the Tsukuba group.

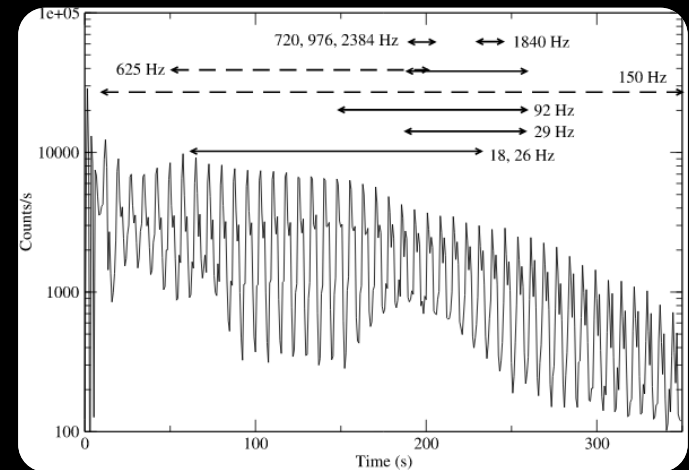
K. Sekizawa, S. Kobayashi, and M. Matsuo, PRC**105**(2022)045807

It may affect interpretation of various phenomena, e.g.:

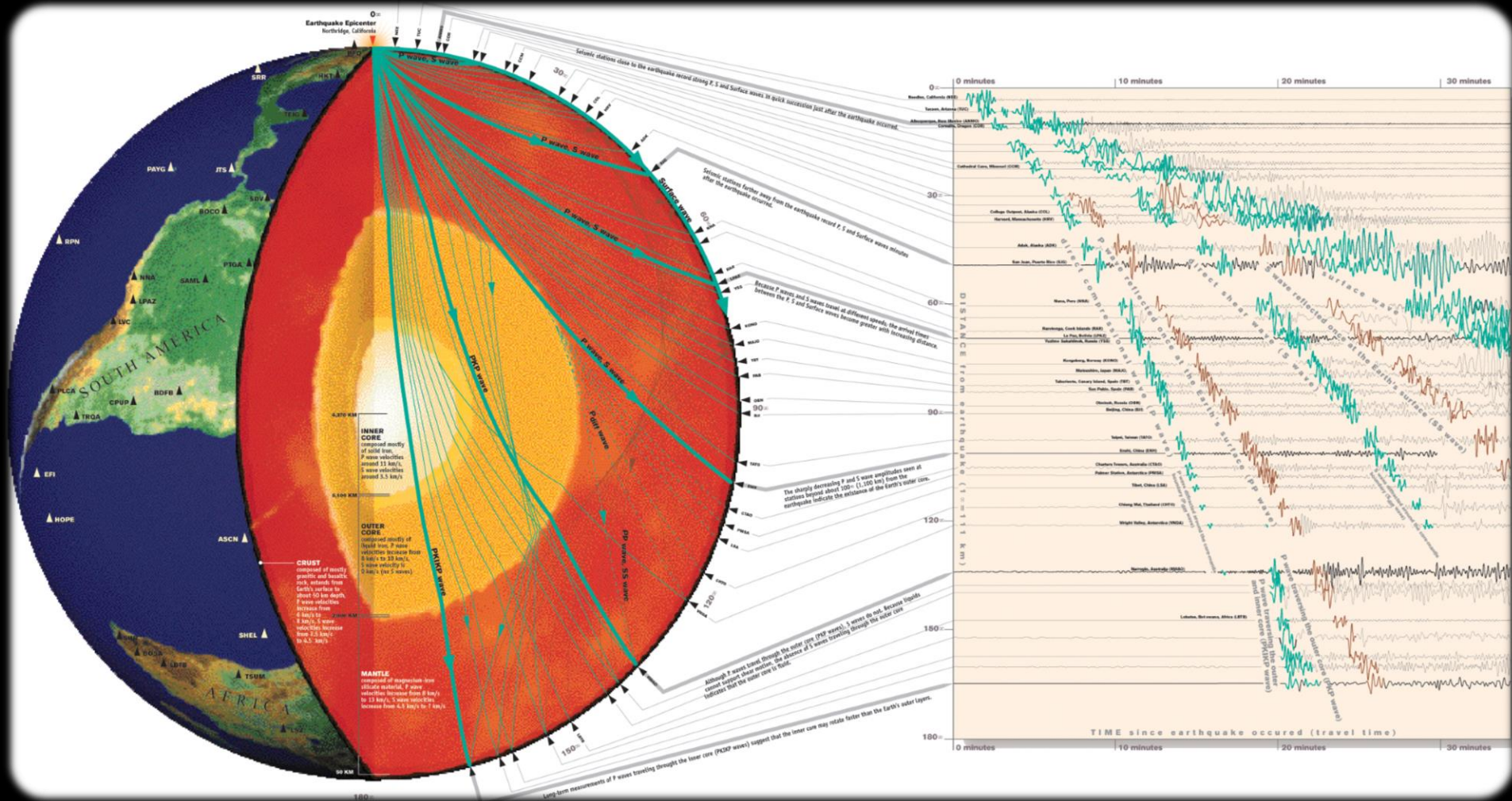
Neutron-star glitch



Quasi-periodic oscillation



Seismology (地震学): Studying inside of the Earth from earthquakes and their propagation





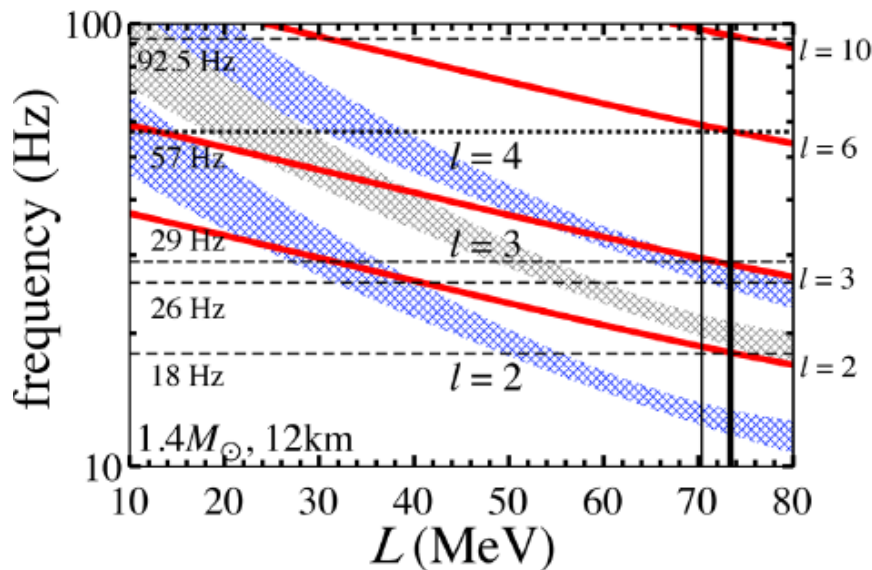
Astrophysical implications of double-layer torsional oscillations in a neutron star crust as a lasagna sandwich

Hajime Sotani¹,¹★ Kei Iida² and Kazuhiro Oyamatsu³

¹Division of Science, National Astronomical Observatory of Japan, 2-21-1 Osawa, Mitaka, Tokyo 181-8588, Japan

²Department of Mathematics and Physics, Kochi University, 2-5-1 Akebono-cho, Kochi 780-8520, Japan

³Department of Human Informatics, Aichi Shukutoku University, 2-9 Katahira, Nagakute, Aichi 480-1197, Japan



- Many (~30) observed QPO frequencies, and prediction by a Bayesian analysis, have been nicely explained by torsional oscillations of tube–bubble or sphere–cylinder layer

Astrophysical implications of double-layer torsional oscillations in a neutron star crust as a lasagna sandwich

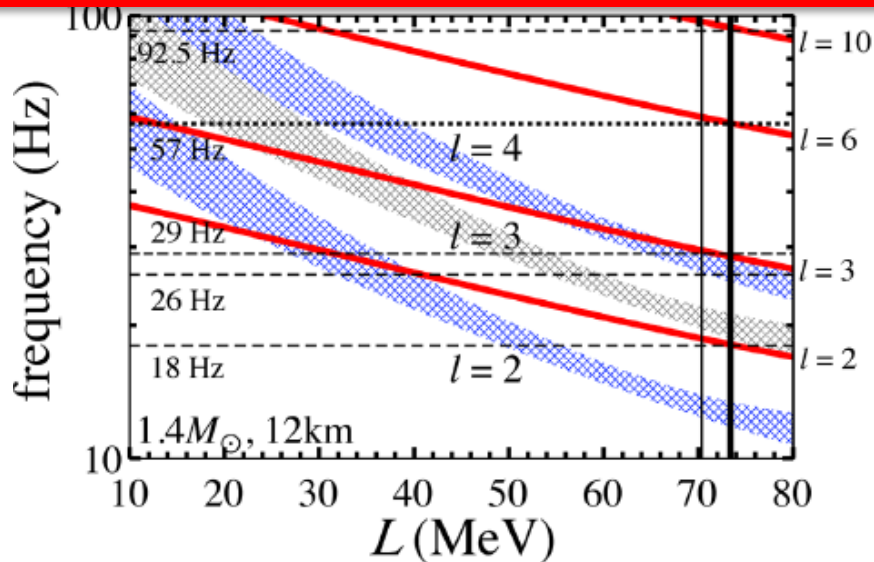
Hajime Sotani¹,¹★ Kei Iida² and Kazuhiro Oyamatsu³

¹Division of Science, National Astronomical Observatory of Japan, 2-21-1 Osawa, Mitaka, Tokyo 181-8588, Japan

²Department of Mathematics and Physics, Kochi University, 2-5-1 Akebono-cho, Kochi 780-8520, Japan

³Department of Human Informatics, Aichi Shukutoku University, 2-9 Katahira, Nagakute, Aichi 480-1197, Japan

The interpretation could be affected by the entrainment effects!



- Many (~30) observed QPO frequencies, and prediction by a Bayesian analysis, have been nicely explained by torsional oscillations of tube–bubble or sphere–cylinder layer

We employ the Skyrme-Kohn-Sham DFT with the Bloch boundary condition

✓ The Bloch boundary condition for single-particle orbitals

$$\psi_{\alpha\mathbf{k}}^{(q)}(\mathbf{r}) = \frac{1}{\sqrt{V}} u_{\alpha\mathbf{k}}^{(q)}(z) e^{i\mathbf{k}\cdot\mathbf{r}} \quad u_{\alpha\mathbf{k}}^{(q)}(z + na) = u_{\alpha\mathbf{k}}^{(q)}(z)$$

Periodicity of the slabs

α : Band index \mathbf{k} : Bloch wave vector q : Isospin (n or p) a : Period of the slabs

✓ Skyrme EDF

$$\frac{E}{A} = \frac{1}{N_b} \int_0^a \left(\frac{\hbar^2}{2m} \tau(z) + \sum_{t=0,1} \left[C_t^p [n] n_t^2(z) + C_t^{\Delta\rho} n_t(z) \partial_z^2 n_t(z) + C_t^{\tau} (n_t(z) \tau_t(z) - \mathbf{j}_t^2(z)) \right] + \mathcal{E}_{\text{Coul}}^{(p)}(z) \right) dz$$

Number density:

$$n_q(z) = 2 \sum_{\alpha,\mathbf{k}}^{\text{occ.}} |\psi_{\alpha\mathbf{k}}^{(q)}(\mathbf{r})|^2$$

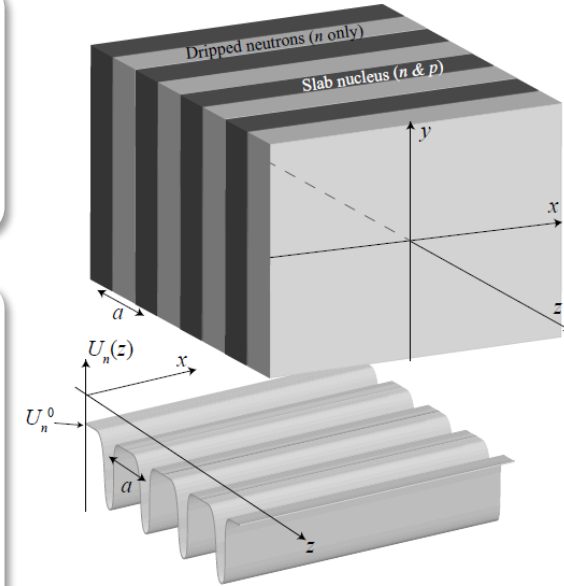
Kinetic density:

$$\tau_q(z) = 2 \sum_{\alpha,\mathbf{k}}^{\text{occ.}} |\nabla \psi_{\alpha\mathbf{k}}^{(q)}(\mathbf{r})|^2$$

Current (momentum) density:

$$\mathbf{j}_q(z) = 2 \sum_{\alpha,\mathbf{k}}^{\text{occ.}} \text{Im} [\psi_{\alpha\mathbf{k}}^{(q)*}(\mathbf{r}) \nabla \psi_{\alpha\mathbf{k}}^{(q)}(\mathbf{r})]$$

*Uniform background electrons are assumed for the charge neutrality condition: $n_e = \bar{n}_p$



Picture from PRC100(2019)035804

✓ Skyrme-Kohn-Sham equations

Note: While we deal with 3D slabs, the equations to be solved are 1D!

$$\hat{h}^{(q)}(z) \psi_{\alpha\mathbf{k}}^{(q)}(\mathbf{r}) = \varepsilon_{\alpha\mathbf{k}}^{(q)} \psi_{\alpha\mathbf{k}}^{(q)}(\mathbf{r}) \quad \rightarrow \quad \left(\hat{h}^{(q)}(z) + \hat{h}_{\mathbf{k}}^{(q)}(z) \right) u_{\alpha\mathbf{k}}^{(q)}(z) = \varepsilon_{\alpha\mathbf{k}}^{(q)} u_{\alpha\mathbf{k}}^{(q)}(z)$$

Ordinary single-particle Hamiltonian:

$$\hat{h}^{(q)}(z) = -\nabla \cdot \frac{\hbar^2}{2m_q^{\oplus}(z)} \nabla + U^{(q)}(z) + \frac{1}{2i} [\nabla \cdot \mathbf{I}^{(q)}(z) + \mathbf{I}^{(q)}(z) \cdot \nabla]$$

Additional (k -dependent) term:

$$\hat{h}_{\mathbf{k}}^{(q)}(z) = \frac{\hbar^2 \mathbf{k}^2}{2m_q^{\oplus}(z)} + \hbar \mathbf{k} \cdot \hat{\mathbf{v}}^{(q)}(z)$$

Velocity operator:

$$\hat{\mathbf{v}}^{(q)}(z) \equiv \frac{1}{i\hbar} [\mathbf{r}, \hat{h}^{(q)}(z)]$$

Results: Band structure ($Y_p = 0.4$)

Proton fraction:

$$Y_p = \frac{\bar{n}_p}{\bar{n}_n + \bar{n}_p}$$

Average nucleon density:

$$\bar{n}_q = \frac{1}{a} \int_0^a n_q(z) dz$$

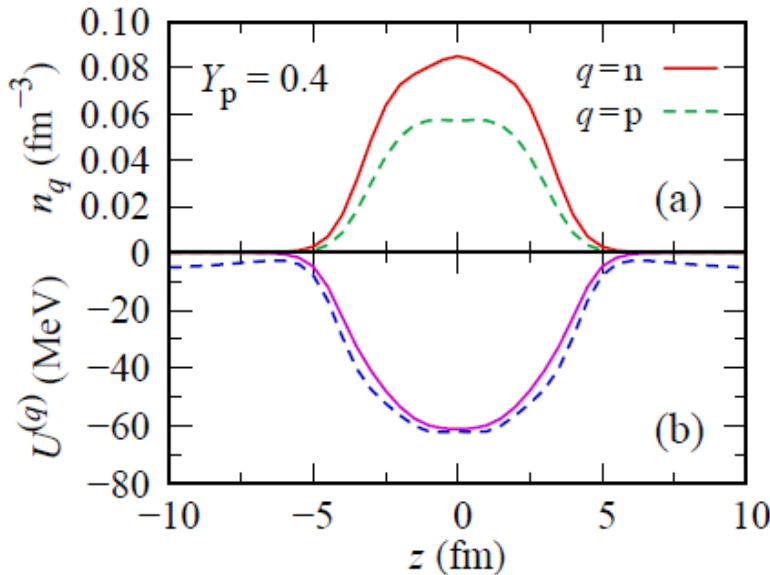
Single-particle energy:

$$\varepsilon_{\alpha\mathbf{k}}^{(q)} = \underbrace{e_{\alpha\mathbf{k}}^{(q)}}_{z\text{-component}} + \underbrace{\varepsilon_{\text{kin-xy},\alpha\mathbf{k}}^{(q)}}_{\approx \frac{\hbar^2 k_{\parallel}^2}{2m}} \quad k_{\parallel} = \sqrt{k_x^2 + k_y^2}$$

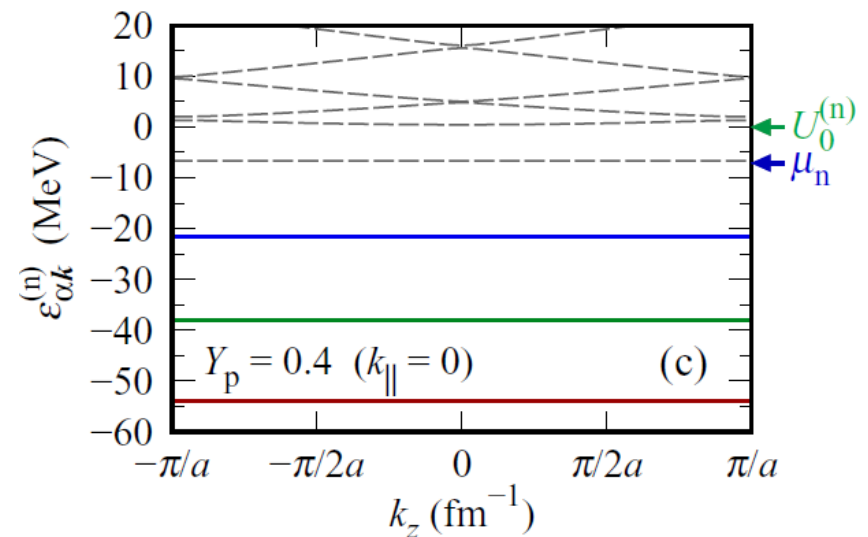
✓ Bound orbitals do not show band structure (k_z dependence)

$Y_p = 0.4, n_B = 0.4 \text{ fm}^{-3}$: Isolated slab (no neutron drip)

Density and potential



Neutron single-particle energies



Proton fraction:

$$Y_p = \frac{\bar{n}_p}{\bar{n}_n + \bar{n}_p}$$

Average nucleon density:

$$\bar{n}_q = \frac{1}{a} \int_0^a n_q(z) dz$$

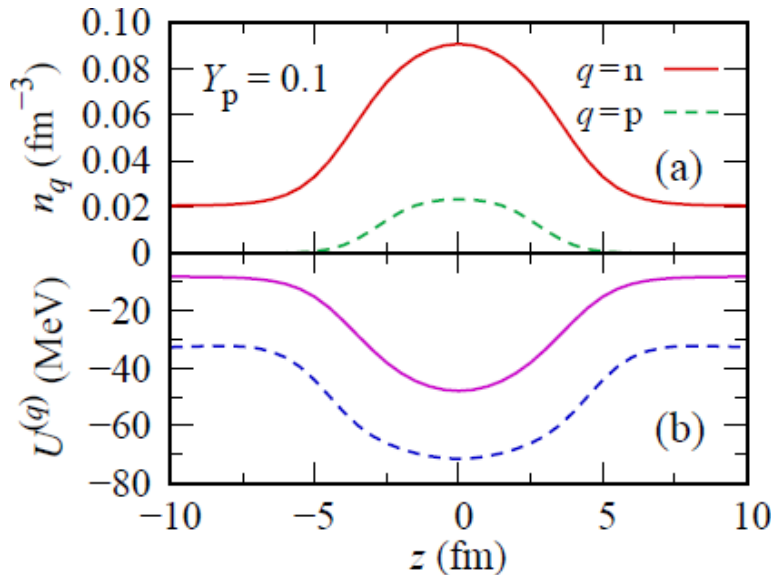
Single-particle energy:

$$\varepsilon_{\alpha\mathbf{k}}^{(q)} = \underbrace{e_{\alpha\mathbf{k}}^{(q)}}_{z\text{-component}} + \underbrace{\varepsilon_{\text{kin-xy},\alpha\mathbf{k}}^{(q)}}_{\approx \frac{\hbar^2 k_{\parallel}^2}{2m}} \quad k_{\parallel} = \sqrt{k_x^2 + k_y^2}$$

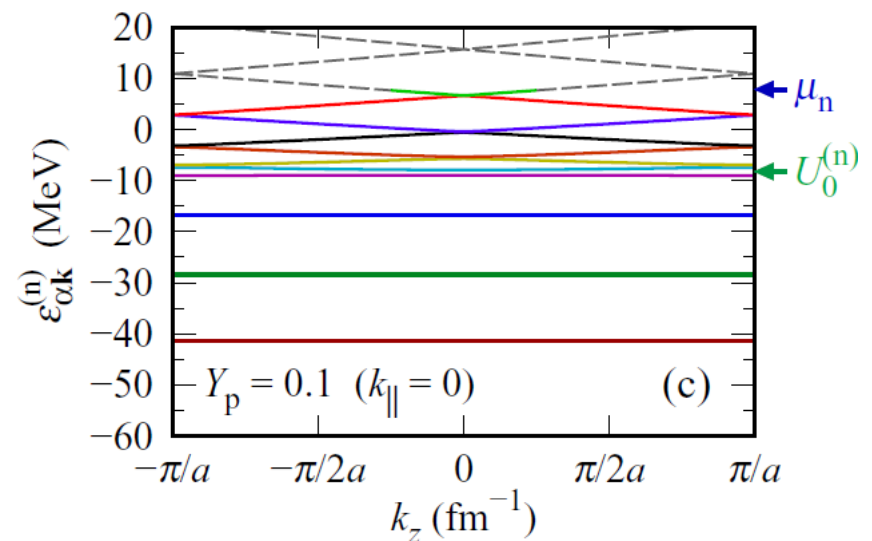
✓ Dripped neutrons show band structure (k_z dependence)

$Y_p = 0.1, n_B = 0.4 \text{ fm}^{-3}$: Neutron-dripped slab

Density and potential



Neutron single-particle energies



Proton fraction:

$$Y_p = \frac{\bar{n}_p}{\bar{n}_n + \bar{n}_p}$$

Average nucleon density:

$$\bar{n}_q = \frac{1}{a} \int_0^a n_q(z) dz$$

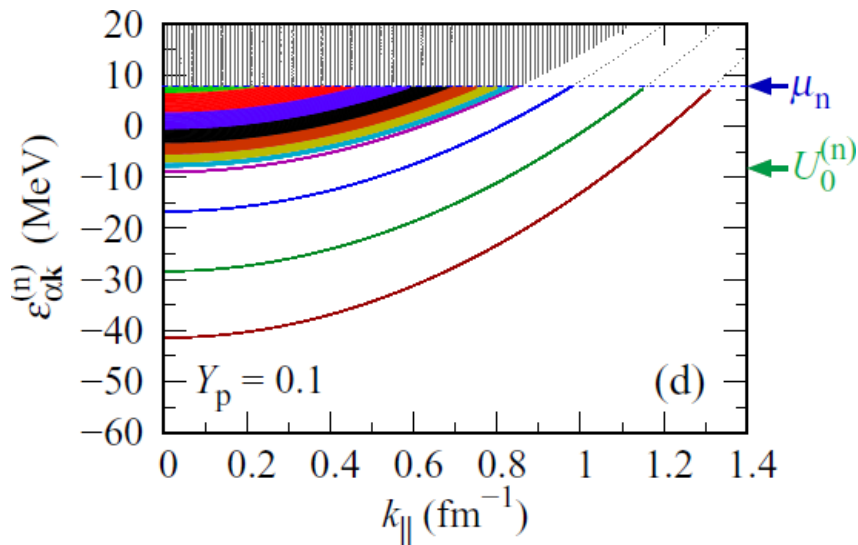
Single-particle energy:

$$\varepsilon_{\alpha\mathbf{k}}^{(q)} = \underbrace{e_{\alpha\mathbf{k}}^{(q)}}_{z\text{-component}} + \underbrace{\varepsilon_{\text{kin-xy},\alpha\mathbf{k}}^{(q)}}_{\approx \frac{\hbar^2 k_{\parallel}^2}{2m}} \quad k_{\parallel} = \sqrt{k_x^2 + k_y^2}$$

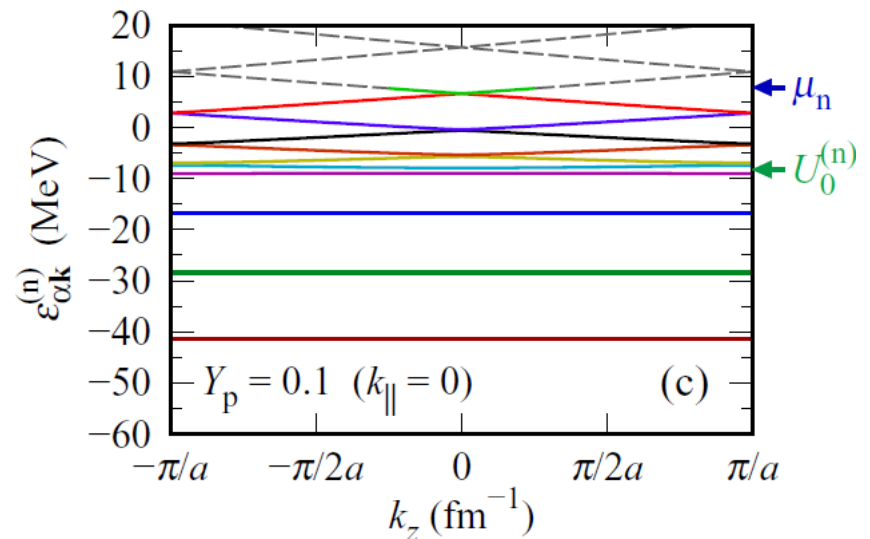
✓ Dripped neutrons show band structure (k_z dependence)

$Y_p = 0.1, n_B = 0.4 \text{ fm}^{-3}$: Neutron-dripped slab

k_{\parallel} dependence of s.p. energies:



Neutron single-particle energies



- ✓ In the static approach, **conduction neutrons** are analyzed

In the **static** approach, the *conduction neutron number density* is defined by

$$n_n^c \equiv m_{n,\text{bg}}^\oplus \mathcal{K}_{zz}^{(n)}$$

where $\mathcal{K}_{zz}^{(n)}$ is the so-called *mobility coefficient*:

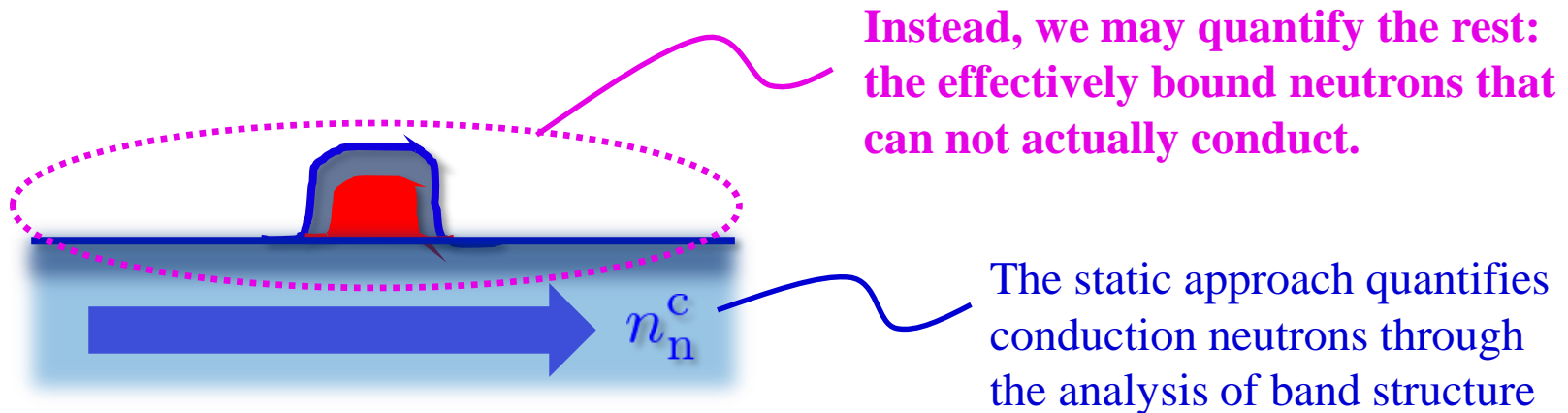
$$\mathcal{K}_{zz}^{(n)} = \frac{1}{\pi L} \sum_{\alpha, k_z} \int k_{\parallel} \left(m_{n,\alpha\mathbf{k}}^{\star-1} \right)_{zz} \theta(\mu_n - \varepsilon_{\alpha\mathbf{k}}^{(n)}) dk_{\parallel}$$

Inverse of the “macroscopic” effective mass tensor

$$\left(m_{n,\alpha\mathbf{k}}^{\star-1} \right)_{\mu\nu} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon_{\alpha\mathbf{k}}^{(n)}}{\partial k_{\mu} \partial k_{\nu}}$$

For bound orbitals, there is no k_z dependence $\Rightarrow 1/m \rightarrow 0$, i.e., $m \rightarrow \infty$ (can not conduct).
 \Rightarrow The mobility coefficient quantifies dripped neutrons that can actually conduct.

Let's look at the same phenomenon
from a different side



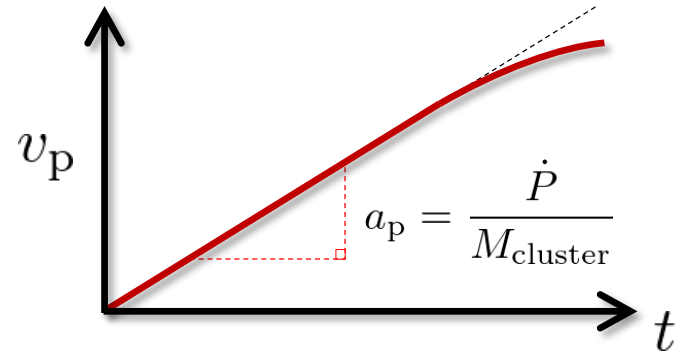
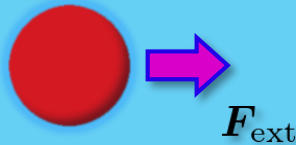




- ✓ The collective mass is extracted from **acceleration motion under constant force**

The real-time method: Idea

Dripped neutrons



How to introduce spatially-uniform electric field

- ✓ TDKS equation in a “velocity gauge”

$$i\hbar \frac{\partial \tilde{u}_{\alpha\mathbf{k}}^{(q)}(z, t)}{\partial t} = \left(\hat{h}^{(q)}(z, t) + \hat{h}_{\mathbf{k}(t)}^{(q)}(z, t) \right) \tilde{u}_{\alpha\mathbf{k}}^{(q)}(z, t)$$

Spatially-uniform
Vector potential

$$\mathbf{k}(t) = \mathbf{k} + \frac{e}{\hbar c} A_z(t) \hat{\mathbf{e}}_z$$

Gauge transformation for the Bloch orbitals:

$$\tilde{u}_{\alpha\mathbf{k}}^{(q)}(z, t) = \exp\left[-\frac{ie}{\hbar c} A_z(t) z\right] u_{\alpha\mathbf{k}}^{(q)}(z, t)$$

Electric field:

$$E_z(t) = -\frac{1}{c} \frac{dA_z}{dt}$$

k -dependent term:

$$\hat{h}_{\mathbf{k}}^{(q)}(z) = \frac{\hbar^2 \mathbf{k}^2}{2m_q^\oplus(z)} + \hbar \mathbf{k} \cdot \hat{\mathbf{v}}^{(q)}(z)$$

Velocity operator:

$$\hat{\mathbf{v}}^{(q)}(z) \equiv \frac{1}{i\hbar} [\mathbf{r}, \hat{h}^{(q)}(z)]$$

cf. K. Yabana and G.F. Bertsch, Phys. Rev. B **54**, 4484 (1996); G.F. Bertsch *et al.*, Phys. Rev. B **62**, 7998 (2000)

Results: The collective mass

Acceleration:

$$a_p = \frac{d^2 Z}{dt^2}$$

C.m. position of protons:

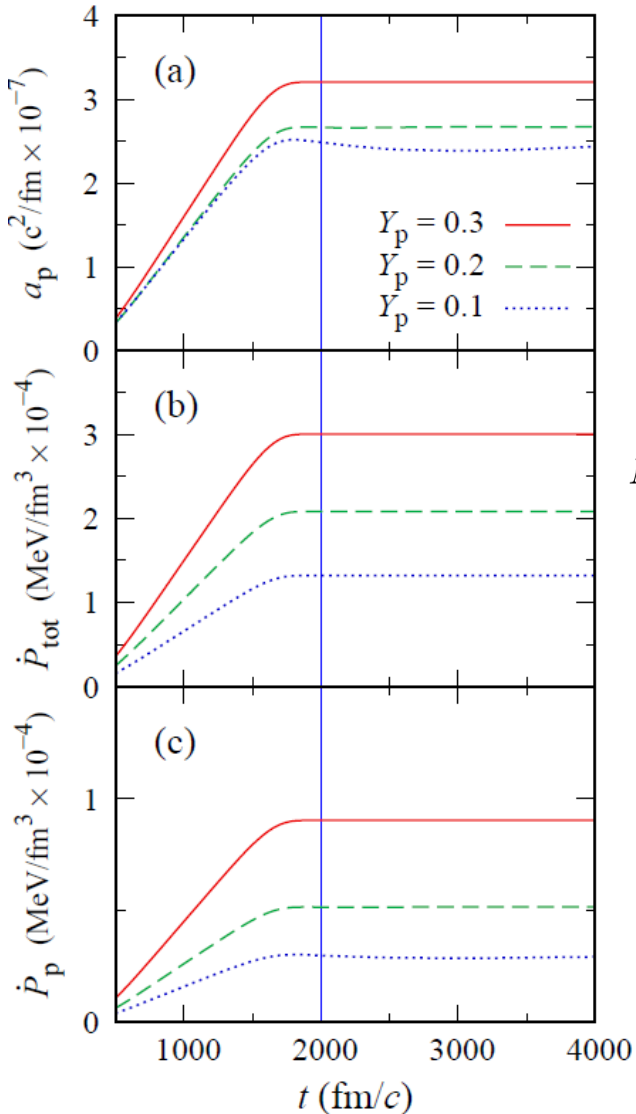
$$Z(t) = \frac{1}{a} \int_0^a z n_p(z, t) dz$$

Momentum of nucleons:

$$P_q(t) = \hbar \int_0^a j_q(z, t) dz$$

Total momentum:

$$P_{\text{tot}}(t) = P_n(t) + P_p(t)$$



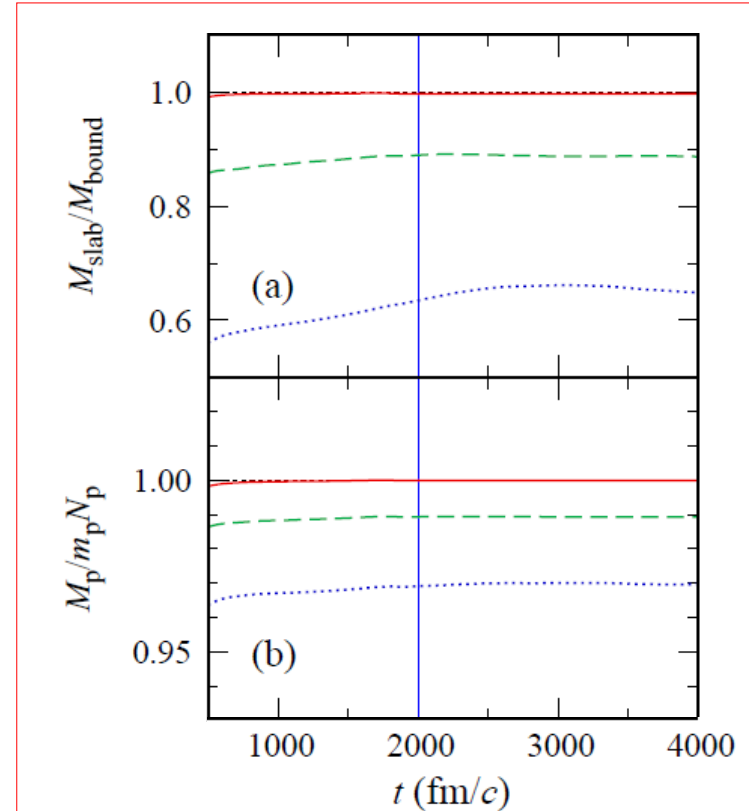
$$M_{\text{slab}} = \dot{P}_{\text{tot}}/a_p$$



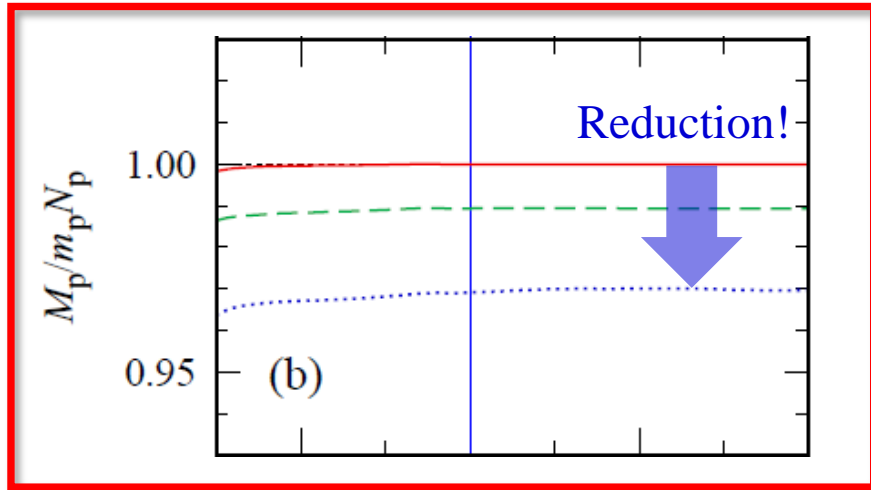
$$M_p = \dot{P}_p/a_p$$

✓ For neutron-dripped slabs, we find significant reduction of the collective mass!

➤ What is the origin of the reduction?



- ✓ Cause of the reduction of the collective mass of protons:
the density-dependent “microscopic” effective mass



Collective mass of protons

$$M_p \leq m_p N_p$$

$$\approx m_p^\oplus [n_n^{\text{b.g.}}] N_p$$

Protons and bound neutrons move together



There must be a velocity lag between protons and background neutrons!

The continuity equation within Skyrme TDDFT reads:

$$\frac{\partial \rho_q(\mathbf{r}, t)}{\partial t} + \hbar \nabla \cdot \mathbf{p}_q(\mathbf{r}, t) = 0$$

where

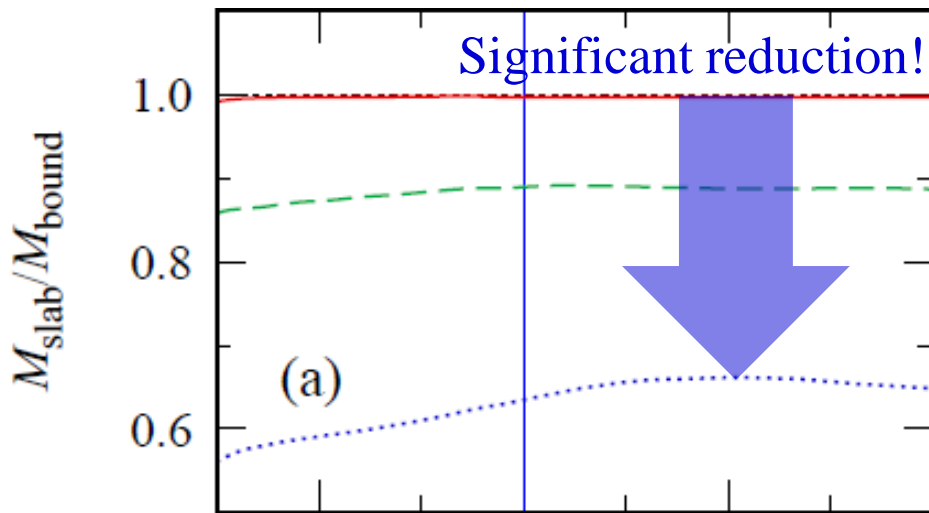
$$\mathbf{p}_q(\mathbf{r}, t) = \mathbf{j}_q(\mathbf{r}, t) + q \frac{2m_q}{\hbar^2} (C_0^\tau - C_1^\tau) n_n(\mathbf{r}, t) n_p(\mathbf{r}, t) \left(\frac{\mathbf{j}_p(\mathbf{r}, t)}{n_p(\mathbf{r}, t)} - \frac{\mathbf{j}_n(\mathbf{r}, t)}{n_n(\mathbf{r}, t)} \right)$$

+1 for protons
-1 for neutrons

velocity difference

Then, what is the cause of the reduction
of the collective mass of the slab?

→ an “anti-entrainment” effect!

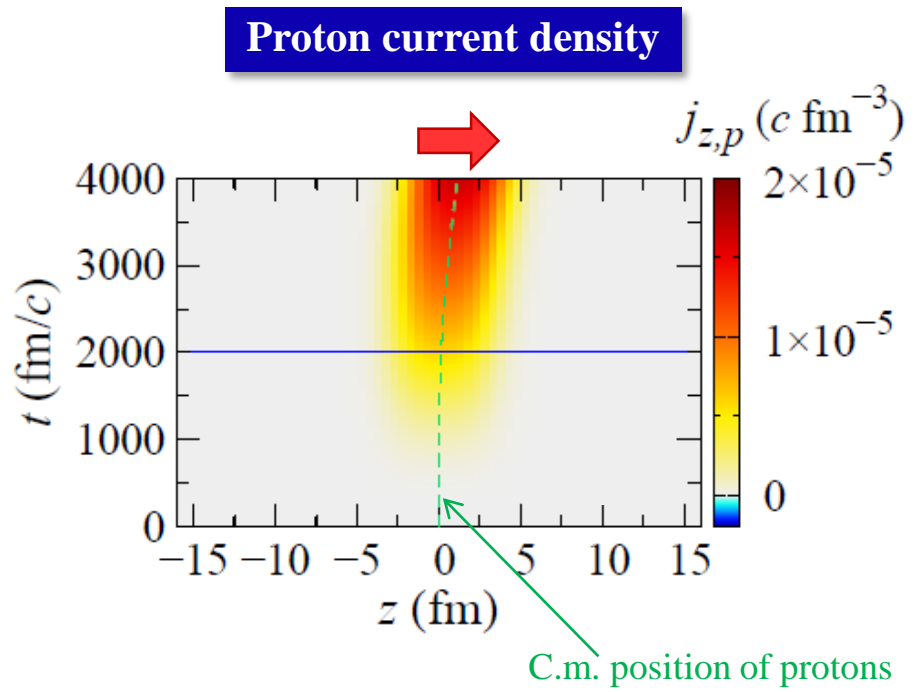


It can **not** be explained solely by
the microscopic effective mass.

Current density:

$$j_{z,q}(z,t) = \frac{\hbar}{m_q} \sum_{\alpha, \mathbf{k}}^{\text{occ.}} \text{Im}[\psi_{\alpha \mathbf{k}}^{(q)*}(\mathbf{r}, t) \nabla \psi_{\alpha \mathbf{k}}^{(q)}(\mathbf{r}, t)] = \frac{\hbar}{m_q} \frac{1}{aN_{k_z}} \sum_{\alpha, k_z} \int \frac{k_{\parallel}}{\pi} \text{Im}[u_{\alpha \mathbf{k}}^{(q)*}(z, t) (\partial_z + ik_z) u_{\alpha \mathbf{k}}^{(q)}(z, t)] \theta(\mu_q - \varepsilon_{\alpha \mathbf{k}}^{(q)}) dk_{\parallel}$$

✓ Protons inside the slab move toward the direction of the external force, as expected.



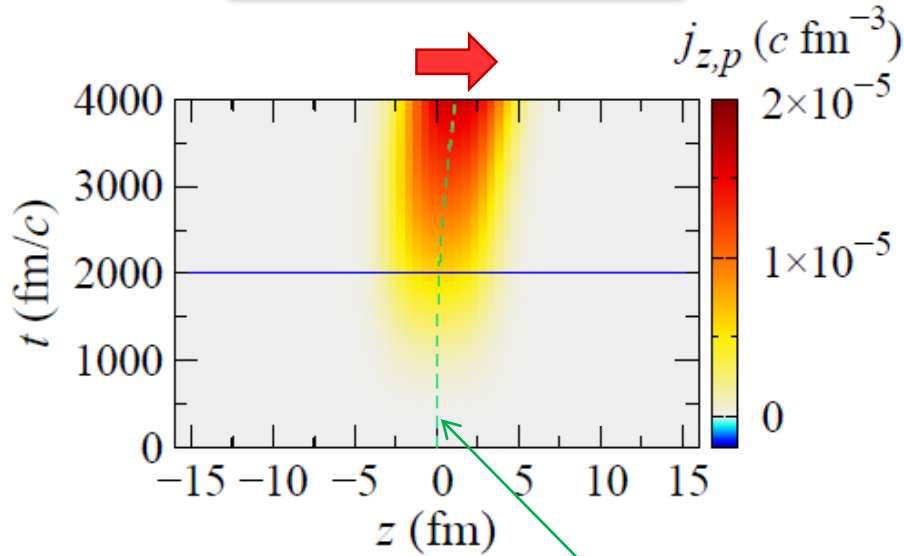
Current density:

$$j_{z,q}(z,t) = \frac{\hbar}{m_q} \sum_{\alpha,\mathbf{k}}^{\text{occ.}} \text{Im}[\psi_{\alpha\mathbf{k}}^{(q)*}(\mathbf{r},t) \nabla \psi_{\alpha\mathbf{k}}^{(q)}(\mathbf{r},t)] = \frac{\hbar}{m_q} \frac{1}{aN_{k_z}} \sum_{\alpha,k_z} \int \frac{k_{\parallel}}{\pi} \text{Im}[u_{\alpha\mathbf{k}}^{(q)*}(z,t) (\partial_z + ik_z) u_{\alpha\mathbf{k}}^{(q)}(z,t)] \theta(\mu_q - \varepsilon_{\alpha\mathbf{k}}^{(q)}) dk_{\parallel}$$

✓ Dripped neutrons outside the slab move toward the opposite direction!

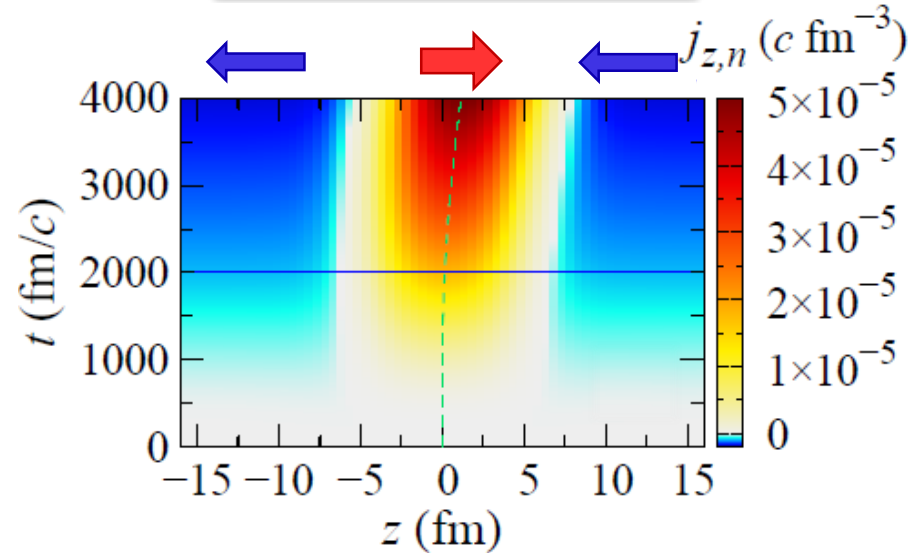
Since it reduces P_{tot} and \dot{P}_{tot} , $M_{\text{slab}} = \dot{P}_{\text{tot}}/a_p$ is reduced

Proton current density



C.m. position of protons

Neutron current density



$$(m_{n,\alpha\mathbf{k}}^{\star-1})_{\mu\nu} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon_{\alpha\mathbf{k}}^{(n)}}{\partial k_{\mu} \partial k_{\nu}}$$

Current density:

$$j_{z,q}(z,t) = \frac{\hbar}{m_q} \sum_{\alpha, \mathbf{k}}^{\text{occ.}} \text{Im}[\psi_{\alpha\mathbf{k}}^{(q)*}(\mathbf{r}, t) \nabla \psi_{\alpha\mathbf{k}}^{(q)}(\mathbf{r}, t)] = \frac{\hbar}{m_q} \frac{1}{aN_{k_z}} \sum_{\alpha, k_z} \int \frac{k_{\parallel}}{\pi} \text{Im}[u_{\alpha\mathbf{k}}^{(q)*}(z,t) (\partial_z + ik_z) u_{\alpha\mathbf{k}}^{(q)}(z,t)] \theta(\mu_q - \varepsilon_{\alpha\mathbf{k}}^{(q)}) dk_{\parallel}$$

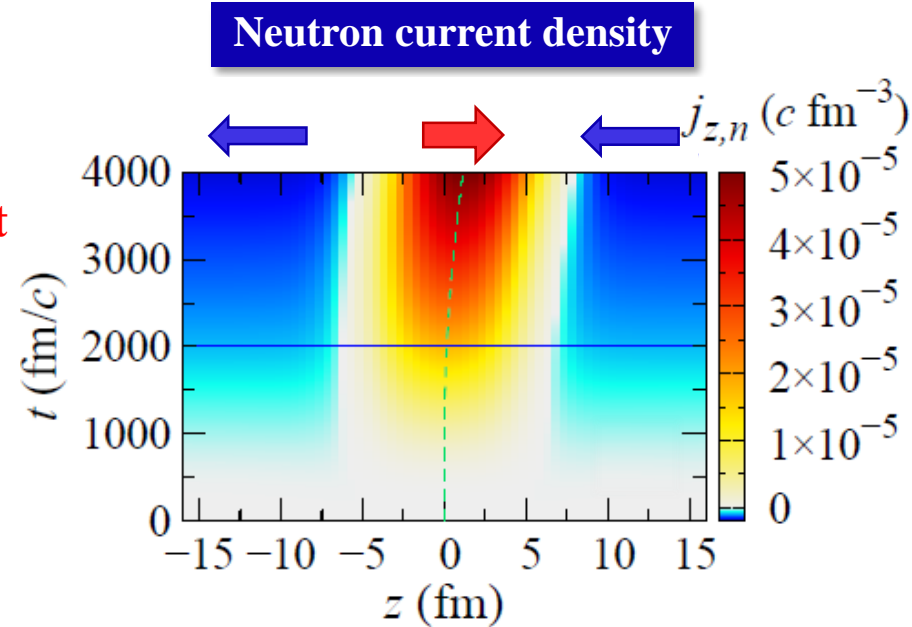
✓ Dripped neutrons outside the slab move toward the opposite direction!

Since it reduces P_{tot} and \dot{P}_{tot} , $M_{\text{slab}} = \dot{P}_{\text{tot}}/a_p$ is reduced

Reduction of M_{slab}
 → enhancement of n_c
 → reduction of m^*

We interpret it as an “anti-entrainment” effect

Y_p	n_n^f/\bar{n}_n	Static		Dynamic
		n_n^c/\bar{n}_n	m_n^*/m_n	n_n^c/\bar{n}_n
0.3	2.09×10^{-4}	0.005	0.040	0.005
0.2	0.127	0.256	0.496	0.229
0.1	0.362	0.630	0.574	0.586



$$(m_{n,\alpha\mathbf{k}}^{*-1})_{\mu\nu} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon_{\alpha\mathbf{k}}^{(n)}}{\partial k_{\mu} \partial k_{\nu}}$$



Summary

Takeaway messages

- ✓ A fully self-consistent **time-dependent band theory** based on TDDFT has been formulated with a Skyrme-type EDF and calculations were achieved, for the first time, for the slab phase of nuclear matter: [Phys. Rev. C **105**, 045807 \(2022\)](#).
- ✓ We have proposed **an intuitive, dynamic method to extract the collective masses** of a slab and protons from a dynamic response of a slab to an external force, which allows us to estimate the conduction neutron number density and, thus, the macroscopic effective mass.
- ✓ From the results, we have found a reduction of collective masses which is caused by: 1) the density-dependent *microscopic* effective mass and 2) **counterflow of dripped neutrons towards the direction opposite to the external force**. We interpret the latter as an “**anti-entrainment**” effect, which qualitatively agrees with the recent static band calculations by the Tsukuba group.
- We are now trying to extend it to include **pairing correlations** based on TDDFT for superfluid systems, time-dependent superfluid local density approximation (TDSLDA).

Kazuyuki Sekizawa

Associate Professor

Department of Physics, School of Science

Tokyo Institute of Technology

2-12-1 O-Okayama, Meguro, Tokyo 152-8551, Japan

sekizawa @ phys.titech.ac.jp

About me: <http://sekizawa.fizyka.pw.edu.pl/english/>

About us: <https://nuclphystitech.wordpress.com/>

See also:

