RCNP研究会「低エネルギー核物理と高エネルギー天文学で読み解く中性子星」 2022年8月4日(木) 14:00-14:30 (25+5min), 量子シミュレーション #2

Time-Dependent Density Functional Theory for the Inner Crust of Neutron Stars

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Hierarchy of Scales in the Universe

Smiling Face

10 Centimeter

Macroscopic world

Smiling Face

10 Centimeters

Microscopic world

Cosmic Eye - Universe Size Comparison: https://youtu.be/8Are9dDbW24

Hierarchy of Scales in the Universe

Neutron stars, NS merger, nucleosynthesis, GW, ...

lacroscopic

(Nuclear)Astrophysics

Nuclear structure, Equation of State (EoS) Superfluidity & Superconductivity Reaction rates, Fission fragments, ...

Microscopic

Neutron-star structure, Star quakes, GW Pulsar glitches, Cooling Stellar evolution, Nucleosynthesis, ...

Nuclear Many-Body Problem \leftarrow 10 fm Cosmic Eve - I

Cosmic Eye - Universe Size Comparison: https://youtu.be/8Are9dDbW24

Hierarchy of Scales in the Universe

Neutron stars, NS merger, nucleosynthesis, GW, ...

lacroscopic

vsics

lakes, GW

hesis, ...

Our Mission:

Nuclear structure.



To establish a concrete microscopic foundation of macroscopic models



Cosmic Eye - Universe Size Comparison: https://youtu.be/8Are9dDbW24

Today, I will talk about:

Dynamics of <u>quantum vortices</u> of superfluid neutrons

<u>Time-dependent band theory</u> for the inner crust of neutron stars









A theory which gives us access to the *exact* solution





The existence was proven, but its shape is unknown..

"Inverse Kohn-Sham"



Developing a better functional is an important subject in nuclear theory!





Great Success of the Density Functional Theory



Si crystal



0.0e+000 2.5e-002 5.0e-002 7.5e-002 1.0e-001

Y. Shinohara, K. Yabana, Y. Kawashita, J.-I. Iwata, T. Otobe, and G. F. Bertsch, Phys. Rev. B 82, 155110 (2010)

The seminal papers on DFT

C-Z. Gao et al.,

Fullerene: C₆₀

J. Phys. B: At. Mol. Opt. Phys. 48, 105102 (2015)

P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964) 19,015 citations!
 W. Kohn and L.J. Sham, Phys. Rev. 140, A1133 (1965) 24,384 citations!

All nuclei can be described with a single EDF



Neutron number

K. Sekizawa

All nuclei can be described with a single EDF



Neutron number

K. Sekizawa

Time-Dependent Density Functional Theory for the Inner Crust of Neutron Stars

TDDFT in Nuclear Physics

TDDFT is a versatile tool!!



Phys. Rev. C 84, 051309(R) (2011) I. Stetcu, A. Bulgac, P. Magierski, and K.J. Roche

Vortex-nucleus dynamics

Phys. Rev. Lett. **117**, 232701 (2016) G. Wlazłowski, K.S., P. Magierski, A. Bulgac, and M.M. Forbes

Induced fission of ²⁴⁰Pu



Phys. Rev. Lett. **116**, 122504 (2016) A. Bulgac, P. Magierski, K.J. Roche, and I. Stetcu

Low-energy heavy-ion reactions



Phys. Rev. Lett. **119**, 042501 (2017) P. Magierski, K.S., and G. Wlazłowski

Neutron-star "glitch"

Picture: https://astronomy.com/magazine/ask-astro/2017/12/stellar-magnets

What is the glitch?

Pulsar - a rotating neutron star

- ✓ First discovery in August 1967 → "Little Green Man" LGM-1 → PSR B1919+21
- ✓ Since then, more than 2650 pulsars have been observed
- ✓ It gradually <u>spins down</u> due to the EM radiation



Typical example: the Vela pulsar

Irregularity has been observed from continuous monitoring of the pulsation period



In daily life, a vortex is continuous..

In superfluid, vortices are quantized!!

W. Ketterle, MIT Physics Annual. 2001

The vortex mediated glitch: Naive picture



Rotation frequency

Time

To fully understand the glitches, we need to clarify:

Glitch dynamics

How do vortices move?

and, of course, details of NS matter..

Pinning mechanism

How are vortices pinned?

Trigger mechanism

How are vortices unpinned?

We attacked this problem using the state-of-the-art microscopic nuclear theory We attack this problem with HPC on GPU supercomputers with TDDFT for superfluid systems, TDSLDA!

TDSLDA (Time-Dependent Superfluid Local Density Approximation)

TDSLDA: TDDFT with local treatment of pairing

Kohn-Sham scheme is extended for non-interacting quasiparticles

TDSLDA equations (formally equivalent to TDHFB or TD-BdG equations)

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}u_{k,\uparrow}(\boldsymbol{r},t)\\u_{k,\downarrow}(\boldsymbol{r},t)\\v_{k,\uparrow}(\boldsymbol{r},t)\\v_{k,\downarrow}(\boldsymbol{r},t)\end{pmatrix} = \begin{pmatrix}h_{\uparrow\uparrow}(\boldsymbol{r},t) & h_{\uparrow\downarrow}(\boldsymbol{r},t) & 0 & \Delta(\boldsymbol{r},t)\\h_{\downarrow\uparrow}(\boldsymbol{r},t) & h_{\downarrow\downarrow}(\boldsymbol{r},t) & -\Delta(\boldsymbol{r},t) & 0\\0 & -\Delta^{*}(\boldsymbol{r},t) & -h_{\uparrow\uparrow}^{*}(\boldsymbol{r},t) & -h_{\uparrow\downarrow}^{*}(\boldsymbol{r},t)\\\Delta^{*}(\boldsymbol{r},t) & 0 & -h_{\downarrow\uparrow}^{*}(\boldsymbol{r},t) & -h_{\downarrow\downarrow}^{*}(\boldsymbol{r},t)\end{pmatrix} \begin{pmatrix}u_{k,\uparrow}(\boldsymbol{r},t)\\u_{k,\downarrow}(\boldsymbol{r},t)\\v_{k,\uparrow}(\boldsymbol{r},t)\\v_{k,\downarrow}(\boldsymbol{r},t)\end{pmatrix}$$

$$h_{\sigma} = \frac{\delta E}{\delta n_{\sigma}} \quad : \text{ s.p. Hamiltonian} \qquad \qquad n_{\sigma}(\boldsymbol{r}, t) = \sum_{E_k < E_c} |v_{k,\sigma}(\boldsymbol{r}, t)|^2 \quad : \text{ number density} \\ \Delta = -\frac{\delta E}{\delta \nu^*} \quad : \text{ pairing field} \qquad \qquad \nu(\boldsymbol{r}, t) = \sum_{E_k < E_c} u_{k,\uparrow}(\boldsymbol{r}, t) v_{k,\downarrow}^*(\boldsymbol{r}, t) \quad : \text{ anomalous density} \\ \boldsymbol{j}_{\sigma}(\boldsymbol{r}, t) = \hbar \sum_{E_k < E_c} \operatorname{Im}[v_{k,\sigma}^*(\boldsymbol{r}, t) \boldsymbol{\nabla} v_{k,\sigma}(\boldsymbol{r}, t)] \quad : \text{ current} \end{cases}$$

A large number (10⁴-10⁶) of 3D coupled non-linear PDEs have to be solved!! # of qp orbitals ~ # of grid points

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TDSLDA (Time-Dependent Superfluid Local Density Approximation)

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Vortex-nucleus dynamics within TDSLDA



G. Wlazłowski, <u>K. Sekizawa</u>, P. Magierski, A. Bulgac, and M.M. Forbes, Phys. Rev. Lett. **117**, 232701 (2016)

A key to understand the glitches is: <u>Vortex pinning mechanism in the inner crust of neutron stars</u>

Q. Is the vortex-nucleus interaction

Attractive?

or







"Nuclear pinning"

"Interstitial pinning"

Response of a spinning gyroscope when pushed



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Time-Dependent Density Functional Theory for the Inner Crust of Neutron Stars



Time-Dependent Density Functional Theory for the Inner Crust of Neutron Stars

1.4

1.6

0.7

0.8





TDSLDA equations (or TDHFB, TD-BdG)
$$\partial_{1} \left(a_{1} \left(n \right) \right)$$

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} h(\mathbf{r}) & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -h(\mathbf{r}) \end{pmatrix} \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix}$$

Computational details

75 fm × 75 fm × 60 fm $(50 \times 50 \times 40, \ \Delta x = 1.5 \text{ fm})$ $k_{\rm c} = \pi/\Delta x > k_{\rm F}$ $k_{\rm F} = (3\pi^2 \rho_n)^{1/3}$ Nuclear impurity: Z = 50 $\rho_n \simeq 0.014 \text{ fm}^{-3} (N \simeq 2,530)$ $\rho_n \simeq 0.031 \text{ fm}^{-3} (N \simeq 5,714)$ # of quasi-particle w.f. $\approx 100,000$

20 30 R=30fm 50 60 55 45 70 Z=50 $\rho(\mathbf{r})$ 50 40 30 20 10 $\rho_n \simeq 0.014 \, \mathrm{fm}^{-3}$

a vortex line exists here

TDSLDA equations (or TDHFB, TD-BdG)

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\begin{pmatrix}u_i(\mathbf{r})\\v_i(\mathbf{r})\end{pmatrix} = \begin{pmatrix}h(\mathbf{r}) & \Delta(\mathbf{r})\\\Delta^*(\mathbf{r}) & -h(\mathbf{r})\end{pmatrix}\begin{pmatrix}u_i(\mathbf{r})\\v_i(\mathbf{r})\end{pmatrix}$$

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MPI+GPU → 48h w/ 200GPUs for 10,000 fm/c



TITAN, Oak Ridge



NERSC Edison, Berkeley



HA-PACS, Tsukuba

Results of TDSLDA calculation: $\rho_n \simeq 0.014 \text{ fm}^{-3}$



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time= 8032 fm/c F_m (10.6)= 0.17 MeV/fm Q= 13 fm²



Results of TDSLDA calculation: $\rho_n \simeq 0.014 \text{ fm}^{-3}$



"Unpinned configuration"



"Pinned configuration"





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



The rest of the 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: <u>Anti-entrainment effects</u> in the slab phase

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(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.



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"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



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The "entrainment effect" is still a debatable problem

- The first consideration for 1D, square-well potential
- Band calculations for slab (1D) and rod (2D) phases

Entrainment effects are weak for the slab & rod phases:

K. Oyamatsu and Y. Yamada, NPA578(1994)184

B. Carter, N. Chamel, and P. Haensel, NPA748(2005)675

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

Band calculations for cubic-lattice (3D) phases

N. Chamel, NPA747(2005)109 (2005); NPA773(2006)263; PRC85(2012)035801; J. Low Temp. Phys. 189, 328 (2017)

<u>Significant</u> entrainment effects were found in a low-density region: $\frac{m^*}{m} \gtrsim 10$ or more! for the cubic lattice

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

"<u>*Reduction*</u>" of the effective mass was observed for the slab phase:

 $\left| { {m^\star \over m} \sim 0.65 \!-\! 0.75}
ight|$ for the slab phase

Yu Kashiwaba and T. Nakatsukasa, PRC100(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, PRC105(2022)045807

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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



Picture taken from AusPass by Australian National University

QPOs as "asteroseismology"

Monthly Notices of the ROYAL ASTRONOMICAL SOCIETY

MNRAS 489, 3022–3030 (2019) Advance Access publication 2019 August 29



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

Hajime Sotani⁰,¹* Kei Iida² and Kazuhiro Oyamatsu³

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

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

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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

Recently we have developed:

Time-Dependent Band Theory based on TDDFT



Structure and <u>dynamics</u> of infinite neutron-star matter can be described <u>microscopically</u> taking full account of <u>periodicity</u> of crystalline structure (*i.e.* band structure effects)

As the first step, it has been applied to the Slab phase!

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



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Results: Band structure $(Y_p = 0.1)$

K. Sekizawa, S. Kobayashi, and M. Matsuo, PRC105(2022)045807

Proton fraction: As $Y_{\rm p} = \frac{\bar{n}_{\rm p}}{\bar{n}_{\rm p} + \bar{n}_{\rm p}}$

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

Single-particle energy:

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

✓ <u>Dripped neutrons</u> show band structure (k_z dependence)



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



How to introduce spatially-uniform electric field

✓ TDKS equation in a "velocity gauge"

Spatially-uniform Vector potential

$$i\hbar \frac{\partial \widetilde{u}_{\alpha \mathbf{k}}^{(q)}(z,t)}{\partial t} = \left(\hat{h}^{(q)}(z,t) + \hat{h}_{\mathbf{k}(t)}^{(q)}(z,t)\right) \widetilde{u}_{\alpha \mathbf{k}}^{(q)}(z,t) \qquad \mathbf{k}(t) = \mathbf{k} + \frac{e}{\hbar c} \underbrace{A_z(t)}_{\mathbf{k}(t)} \hat{e}_z$$

Gauge transformation for the Bloch orbitals:Electric field:k-dependent term:Velocity operator: $\tilde{u}_{\alpha \mathbf{k}}^{(q)}(z,t) = \exp\left[-\frac{ie}{\hbar c}A_z(t)z\right]u_{\alpha \mathbf{k}}^{(q)}(z,t)$ $E_z(t) = -\frac{1}{c}\frac{dA_z}{dt}$ $\hat{h}_{\mathbf{k}}^{(q)}(z) = \frac{\hbar^2 \mathbf{k}^2}{2m_q^{\oplus}(z)} + \hbar \mathbf{k} \cdot \hat{v}^{(q)}(z)$ $\hat{v}^{(q)}(z) \equiv \frac{1}{i\hbar}[\mathbf{r}, \hat{h}^{(q)}(z)]$

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

Results: The collective mass



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Cause of the reduction of <u>the collective mass of protons</u>: the density-dependent "microscopic" effective mass



The continuity equation within Skyrme TDDFT reads:

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

where

$$p_{q}(\boldsymbol{r},t) = \boldsymbol{j}_{q}(\boldsymbol{r},t) + (\boldsymbol{q}) \frac{2m_{q}}{\hbar^{2}} \left(C_{0}^{\tau} - C_{1}^{\tau} \right) n_{n}(\boldsymbol{r},t) n_{p}(\boldsymbol{r},t) \left(\frac{\boldsymbol{j}_{p}(\boldsymbol{r},t)}{n_{p}(\boldsymbol{r},t)} - \frac{\boldsymbol{j}_{n}(\boldsymbol{r},t)}{n_{n}(\boldsymbol{r},t)} \right)$$

$$+1 \text{ for protons}$$

$$-1 \text{ for neutrons}$$
velocity difference

Then, what is the cause of the reduction of <u>the collective mass of the slab</u>?

 \rightarrow an "anti-entrainment" effect!



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

"Anti-entrainment" effect

Current density:

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

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



"Anti-entrainment" effect

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

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



"Anti-entrainment" effect

Current density:

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

Reduction of $M_{\rm slab}$

 \rightarrow enhancement of $n_{\rm c}$

 \rightarrow reduction of m^*

We interpret it as an "anti-entrainment" effect

$Y_{ m p}$	$n_{ m n}^{ m f}/ar{n}_{ m n}$	Static		Dynamic
		$n_{ m n}^{ m c}/ar{n}_{ m n}$	$m_{ m n}^{\star}/m_{ m n}$	$n_{ m n}^{ m c}/ar{n}_{ m n}$
0.3	$2.09 imes 10^{-4}$	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







Definitely, all are rooted with the wonder of nuclear physics which is basically a quantum many-body problem! ;)

Takeaway message







Microscopic, finite-

- Quantum many-body problem
- Nuclear force (\Leftrightarrow EoS, Structure & Reactions)
- Mass/binding energy (⇔ Crust compositions)
- Excitation properties (\Leftrightarrow GMR, GDR, EoS, ...)
- Nuclear reactions (\Leftrightarrow Stellar evolution, SNe, ...)

infinite- **Eq** • Outer crust

Micro-to-macro,

- Outer crus
- Inner crust
- Outer core
- Inner core



Density

Equation of State (EoS)

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See also:

