YITP Workshop on "*Fundamentals in density functional theory* (DFT2022)"
December 8, 2022 @ Y306, Yukawa Hall, YITP, Kyoto University

Nuclear TDDFT: Past, Present, and Future

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"End Credits" from "E.T. the Extra-Terrestrial": https://youtu.be/YuhZ80YHFns

Outline

1. An informal introduction to nuclear DFT
2. Some remarks on fundamentals of TDDFT
3. Selected topics: from nuclear reactions to neutron stars
4. Summary and perspective

Outline

1. **An informal introduction to nuclear DFT**

2. **Some remarks on fundamentals of TDDFT**

3. **Selected topics: from nuclear reactions to neutron stars**

4. **Summary and perspective**

✓ Nucleons inside a nucleus are not really relativistic.

Note: Throughout the lectures we will restrict ourselves to ***non-relativistic*** treatments.

Only from the saturation density, you can already infer, as follows:

✓ **Nuclear saturation density:**

$$n_0 = 0.16\ [\mathrm{fm}^{-3}] \qquad \left(n_0/2 = 0.08\ [\mathrm{fm}^{-3}] \ \text{for } n \text{ or } p \right)$$

➢ **Fermi wave number:**

$$k_\mathrm{F} = (3\pi^2 n_0/2)^{1/3} \approx 1.33\ [\mathrm{fm}^{-1}]$$

➢ Fermi momentum:

$$p_\mathrm{F} \approx 262 \left[\frac{\mathrm{MeV}}{c}\right]$$

➢ Fermi energy:

$$\varepsilon_\mathrm{F} = \frac{\hbar^2 k_\mathrm{F}^2}{2m} \approx 36.5\ [\mathrm{MeV}]$$

➢ **Fermi velocity:**

$$\frac{v_\mathrm{F}}{c} = \frac{\hbar c\, k_\mathrm{F}}{mc^2} \approx \frac{197\ [\mathrm{MeV\ fm}] \times 1.33\ [\mathrm{fm}^{-1}]}{940\ [\mathrm{MeV}]} \approx 0.28$$

Lorentz factor: *Quite small!*

$$\boxed{\gamma = \frac{1}{\sqrt{1-(v/c)^2}} \approx 1.04}$$

*Note that there are relativistic approaches, such as relativistic mean-field (RMF) theory or covariant DFT, which are rooted with the meson-exchange picture, explains the origin of spin-orbit and time-odd interactions, ...

$\hbar c \approx 197.3269631\ [\mathrm{MeV\ fm}]$	$m_n > m_p$	$mc^2 \gg \varepsilon_\mathrm{F}$
$m_n c^2 = 939.56542052\ [\mathrm{MeV}]$	$\tau_n \approx 877.74\ [\mathrm{s}]$	(about 15 min)
$m_p c^2 = 938.27208816\ [\mathrm{MeV}]$	$\tau_p > 10^{34}\ [\mathrm{y}]$	(cf. Super-Kamiokande experiment)

If you agree with the use of non-relativistic treatments

Our ultimate goal would be **to solve the many-body Schrödinger equation:**

$$\hat{H}\,\Psi(\boldsymbol{r}_1\sigma_1 q_1,\ldots,\boldsymbol{r}_A\sigma_A q_A) = E\,\Psi(\boldsymbol{r}_1\sigma_1 q_1,\ldots,\boldsymbol{r}_A\sigma_A q_A)$$

That's it!

However, it's **practically impossible**.. Why?

E. Schrödinger (1887-1961)

Portrait: https://en.wikipedia.org/wiki/Erwin_Schr%C3%B6dinger

We want to solve this, but can't in practice. Why?

$$\hat{H}\,\Psi(\boldsymbol{r}_1\sigma_1 q_1,\ldots,\boldsymbol{r}_A\sigma_A q_A) \;=\; E\,\Psi(\boldsymbol{r}_1\sigma_1 q_1,\ldots,\boldsymbol{r}_A\sigma_A q_A)$$

The problem is two-fold:

1. It's computationally too demanding.

- ❑ The number of degrees of freedom of Ψ is: $(\underbrace{3}_{x,y,z} \times \underbrace{2}_{\uparrow,\downarrow} \times \underbrace{2}_{\mathrm{n,p}})^A$ ➡ 6×10^{10} for A=10, 8×10^{107} for A=100
- ❑ To store Ψ on a HDD, one needs: $\underbrace{16}_{\text{double precision complex (byte)}} \times (\underbrace{N_{xyz}}_{N_x\times N_y\times N_z} \times \underbrace{2}_{\uparrow,\downarrow} \times \underbrace{2}_{\mathrm{n,p}})^A$ ➡ 2×10^{25} TB for 10^3, A=10, 3×10^{636} TB for 100^3, A=100

In other words, "**Ψ contains enormous amount of information!**" (*may be too much!*)

2. We don't really know actual form of nuclear interactions.

- ❑ Lattice QCD calculations are under way, but still have not provided the actual force.
- ❑ One may parametrize the "bare" NN interaction, and fit to reproduce NN scattering data. (It is called "realistic nuclear force." It shows a repulsive core which requires a caution.)

What is DFT?

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

Equivalent!
(for a special EDF)

$$\hat{H}\Psi(\boldsymbol{r}_1,\dots,\boldsymbol{r}_N) = E\Psi(\boldsymbol{r}_1,\dots,\boldsymbol{r}_N)$$

Kohn-Sham equation

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

EDF

This is the key!

$$v_{\mathrm{KS}}[\rho(\boldsymbol{r})] = \frac{\delta\mathcal{E}[\rho]}{\delta\rho} \qquad \rho(\boldsymbol{r}) = \sum_{i=1}^{N}|\phi_i(\boldsymbol{r})|^2$$

Energy can also be written as a functional of density

$$E[\rho] = \langle \underline{\Psi[\rho]} | \hat{H} | \underline{\Psi[\rho]} \rangle$$

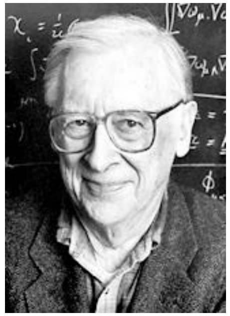
w.f. is a functional of density

P. Hohenberg and W. Kohn, Phys. Rev. B **136**, 864 (1964)

Great Success of the Density Functional Theory

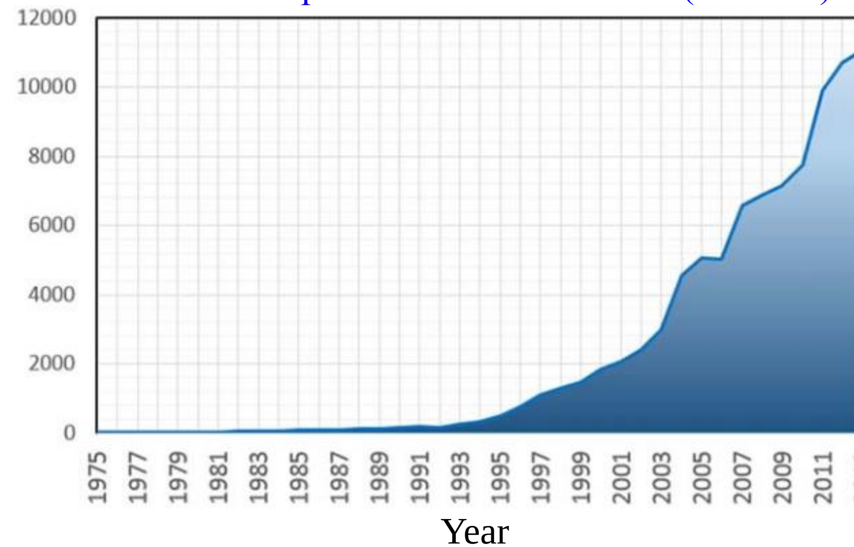
The Nobel Prize in Chemistry 1998

Walter Kohn



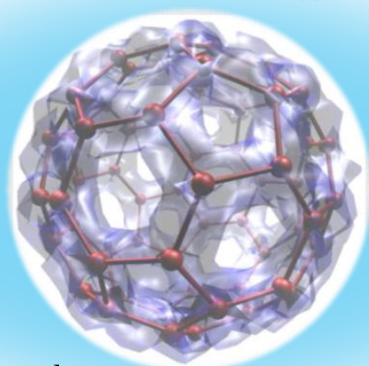
John Pople

Number of publications with “DFT” (till 2013)



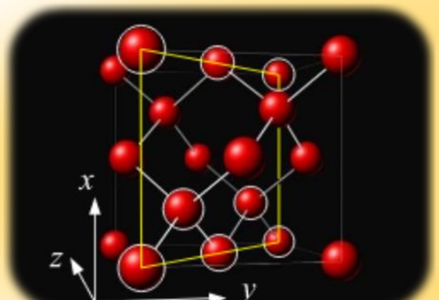
A. Galano and J.R. Alvarez-Idadoy, J. Compt. Chem. **35**, 2019 (2014)

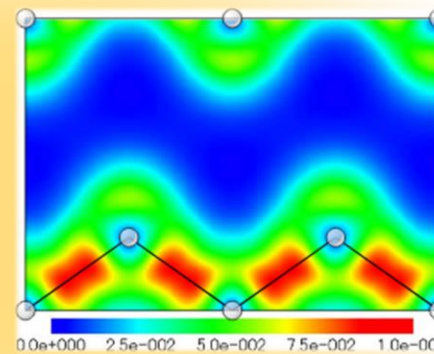
Fullerene: C_{60}



C-Z. Gao et al.,
J. Phys. B: At. Mol. Opt. Phys. **48**, 105102 (2015)

Si crystal





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

- P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964) ➡ **38,725 citations!**
- W. Kohn and L.J. Sham, Phys. Rev. **140**, A1133 (1965) ➡ **46,208 citations!**

CAUTION!

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

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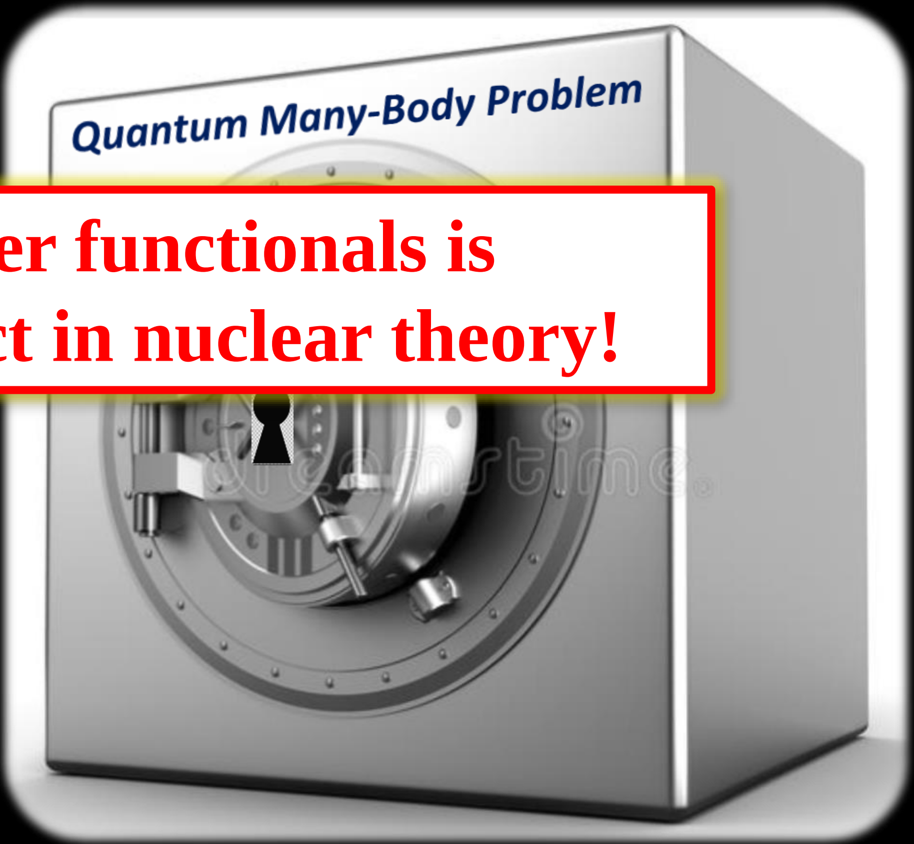
"Inverse Kohn-Sham"

CAUTION!

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

“Inverse Kohn-Sham”



Developing better functionals is an important subject in nuclear theory!

May the DFT be with you..

The Jedi of DFT

In principle,

it is an ***exact*** *approach..*

(if we find the universal EDF)

Anakin Skywalker: https://starwars.fandom.com/wiki/Anakin_Skywalker

May the DFT be with you..

The Jedi of DFT

In principle,

*it is an **exact** approach..*

(if we find the universal EDF)

The Darkside of DFT

In practice,

*it would **never** be **exact**!!*

(since we don't know the universal EDF)

Anakin Skywalker: https://starwars.fandom.com/wiki/Anakin_Skywalker Darth Vader: https://www.eiganohimitsu.com/1810.html

In electronic systems:

$$\hat{H} = \text{Kinetic} + \underset{\text{btw electrons}}{\text{Coulomb}} + \underset{\text{from ions}}{\text{Coulomb}}$$

The interaction is <u>exactly known</u> :)

In nuclear systems:

"Something complicated"

$$\hat{H} = \text{Kinetic} + \underset{\text{btw protons}}{\text{Coulomb}} +$$

NN interaction
3-body interaction
LS, tensor, ...
repulsive core ...

The interaction is <u>not completely known</u> :(

➢ In practice, a ***zero-range* effective NN interaction** has been applied

Skyme (zero-range, contact-type, density-dependent) effective interaction

$$\hat{v}_{ij} = \hat{v}(\boldsymbol{r}_i\sigma_i, \boldsymbol{r}_j\sigma_j) = t_0(1+x_0\hat{P}_\sigma)\delta(\boldsymbol{r}_i-\boldsymbol{r}_j) + \frac{1}{6}t_3\,\rho^\alpha\Big(\frac{\boldsymbol{r}_i+\boldsymbol{r}_j}{2}\Big)(1+x_3\hat{P}_\sigma)\delta(\boldsymbol{r}_i-\boldsymbol{r}_j)$$
$$+\frac{1}{2}t_1(1+x_1\hat{P}_\sigma)\Big\{\delta(\boldsymbol{r}_i-\boldsymbol{r}_j)\hat{\boldsymbol{k}}^2+\hat{\boldsymbol{k}}'^2\delta(\boldsymbol{r}_i-\boldsymbol{r}_j)\Big\}$$
$$+t_2(1+x_2\hat{P}_\sigma)\hat{\boldsymbol{k}}'\cdot\delta(\boldsymbol{r}_i-\boldsymbol{r}_j)\hat{\boldsymbol{k}}+\mathrm{i}W_0\,(\hat{\boldsymbol{\sigma}}_i+\hat{\boldsymbol{\sigma}}_j)\cdot\{\hat{\boldsymbol{k}}'\times\delta(\boldsymbol{r}_i-\boldsymbol{r}_j)\hat{\boldsymbol{k}}\}$$

Spin exchange operator:

$$\hat{P}_\sigma = \frac{1}{2}(1+\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)$$

Relative-wave-vector operator:

$$\hat{\boldsymbol{k}} = \frac{\boldsymbol{\nabla}_i-\boldsymbol{\nabla}_j}{2i}$$

($\hat{\boldsymbol{k}}'$ is a C.C. of $\hat{\boldsymbol{k}}$ acting to the left)

$t_{0\text{-}3}$, $x_{0\text{-}3}$, α, and W_0 are parameters, which are adjusted to reproduce known nuclear properties.

Then, the resulting HF energy becomes **a functional of various *local* densities**:

$$E_{\mathrm{SHF}} = \langle\Phi|\hat{H}_{\mathrm{Skyrme}}|\Phi\rangle = E[\rho,\tau,\nabla\rho,\nabla^2\rho,J\ldots]$$

*It looks as if there are only local (direct) terms, but it contains the exchange terms.

Skyrme Hartree-Fock vs. DFT

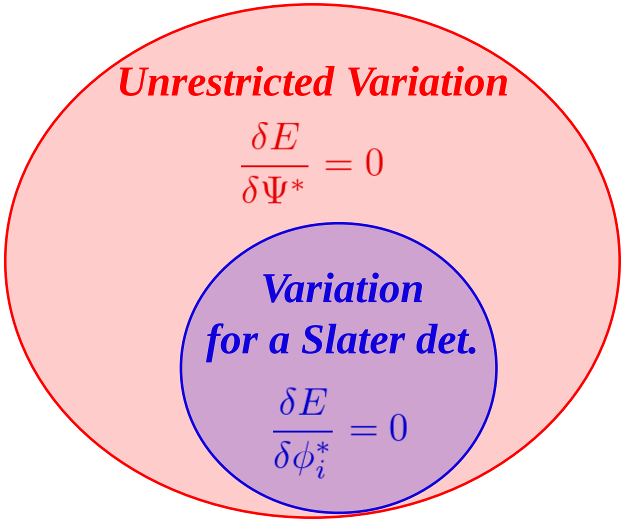
Regarding E_{Skyrme} as an EDF, Skyrme-HF eq. may be regarded as KS eq. in DFT

Unrestricted variation

Schrödinger eq:

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

so, of course, HF ≠ DFT



Variation for a Slater determinant

Hartree-Fock eq: **Integro-differential eq.*

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \Gamma_{\mathrm{H}}(\boldsymbol{r})\right)\phi_i(\boldsymbol{r}) + \int \Gamma_{\mathrm{F}}(\boldsymbol{r},\boldsymbol{r}')\phi_i(\boldsymbol{r}')d\boldsymbol{r}' = \varepsilon_i\phi_i(\boldsymbol{r})$$

Slater determinant:

$$\Phi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N) = \frac{1}{\sqrt{N!}}\det\{\phi_i(\boldsymbol{r}_j)\}$$

Orthonormal condition:

$$\langle\phi_i|\phi_j\rangle = \delta_{ij}$$

Hartree potential (direct term):

$$\Gamma_{\mathrm{H}}(\boldsymbol{r}) = \int v(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}'$$

Fock potential (exchange term):

$$\Gamma_{\mathrm{F}}(\boldsymbol{r},\boldsymbol{r}') = v(\boldsymbol{r},\boldsymbol{r}')\sum_i \phi_i(\boldsymbol{r})\phi_i^*(\boldsymbol{r}')$$

$$E = \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

$$\hat{H} = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i<j} v(\boldsymbol{r}_i,\boldsymbol{r}_j)$$

Regarding E_{Skyrme} as an EDF, Skyrme-HF eq. may be regarded as KS eq. in DFT

- One may also regard Skyrme-TDHF as TDKS in TDDFT

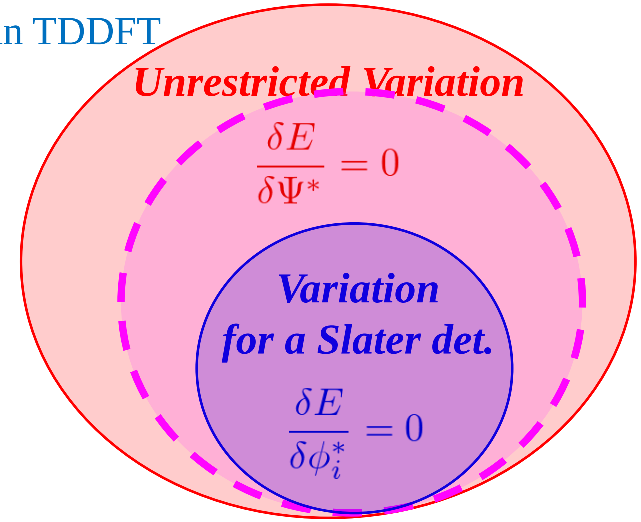
Unrestricted variation

Schrödinger eq:

$$\hat{H}\big|\Psi\big\rangle = E\big|\Psi\big\rangle$$

Kohn-Sham equation:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + v_{\text{KS}}[\rho(\boldsymbol{r})]\right]\phi_i(\boldsymbol{r}) = \varepsilon_i\,\phi_i(\boldsymbol{r})$$



Variation for a Slater determinant

Hartree-Fock eq: **Integro-differential eq.*

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \Gamma_{\text{H}}(\boldsymbol{r})\right)\phi_i(\boldsymbol{r}) + \int \Gamma_{\text{F}}(\boldsymbol{r},\boldsymbol{r}')\phi_i(\boldsymbol{r}')d\boldsymbol{r}' = \varepsilon_i\phi_i(\boldsymbol{r})$$

Skyrme "effective interaction" *$t_{0\text{-}3}$, $x_{0\text{-}3}$, W_0, and α are the parameters

T.H.R. Skyrme, Philos. Mag. **1**, 1043 (1956)

$$\hat{v}_{ij} = t_0(1+x_0\hat{P}_\sigma)\delta(\boldsymbol{r}) + \frac{1}{6}t_3\rho^\alpha(\boldsymbol{R})(1+x_3\hat{P}_\sigma)\delta(\boldsymbol{r})$$
$$+\frac{1}{2}t_1(1+x_1\hat{P}_\sigma)\left[\delta(\boldsymbol{r})\hat{\boldsymbol{k}}^2 + \hat{\boldsymbol{k}}'^2\delta(\boldsymbol{r})\right] + t_2(1+x_2\hat{P}_\sigma)\hat{\boldsymbol{k}}'\cdot\delta(\boldsymbol{r})\hat{\boldsymbol{k}}$$
$$+iW_0(\hat{\boldsymbol{\sigma}}_i + \hat{\boldsymbol{\sigma}}_j)\cdot\left[\hat{\boldsymbol{k}}'\times\delta(\boldsymbol{r})\hat{\boldsymbol{k}}\right]$$

$\boldsymbol{r} = \boldsymbol{r}_i - \boldsymbol{r}_j$: Relative coordinate

$\boldsymbol{R} = (\boldsymbol{r}_i + \boldsymbol{r}_j)/2$: C.M. coordinate

$\hat{\boldsymbol{k}} = (\nabla_i - \nabla_j)/2i$: Relative momentum op.

$\hat{P}_\sigma$: Spin exchange op.

Skyrme-Hartree-Fock eq:

$$-\frac{\hbar^2}{2m}\nabla^2\phi_i(\boldsymbol{r},\sigma) + \sum_{\sigma\sigma'}\Gamma^{\text{HF}}_{\sigma\sigma'}(\boldsymbol{r})\phi_i(\boldsymbol{r},\sigma') = \varepsilon_i\phi_i(\boldsymbol{r},\sigma)$$

$$E_{\text{Skyrme}} = \big\langle\Phi\big|\hat{H}_{\text{Skyrme}}\big|\Phi\big\rangle = E[\rho,\tau,\boldsymbol{j},\boldsymbol{s},\boldsymbol{T},J_{\mu\nu}]$$

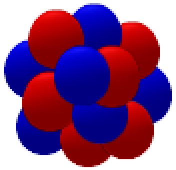
$$\sum_\alpha \frac{\delta E}{\delta\xi_\alpha}\frac{\delta\xi_\alpha}{\delta\phi_i^*(\boldsymbol{r},\sigma)}$$

*E is a functional of various densities

*ξ_α stands here for various densities

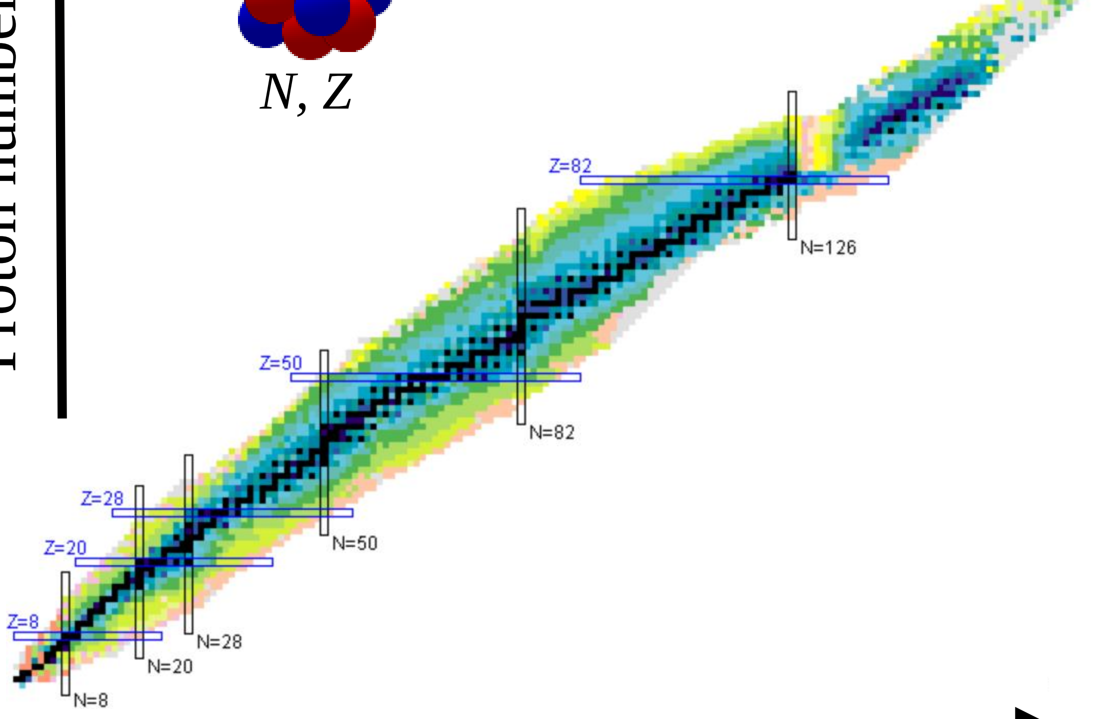
Then, how does it work?

All nuclei can be described with a *single* EDF



N, Z

Proton number

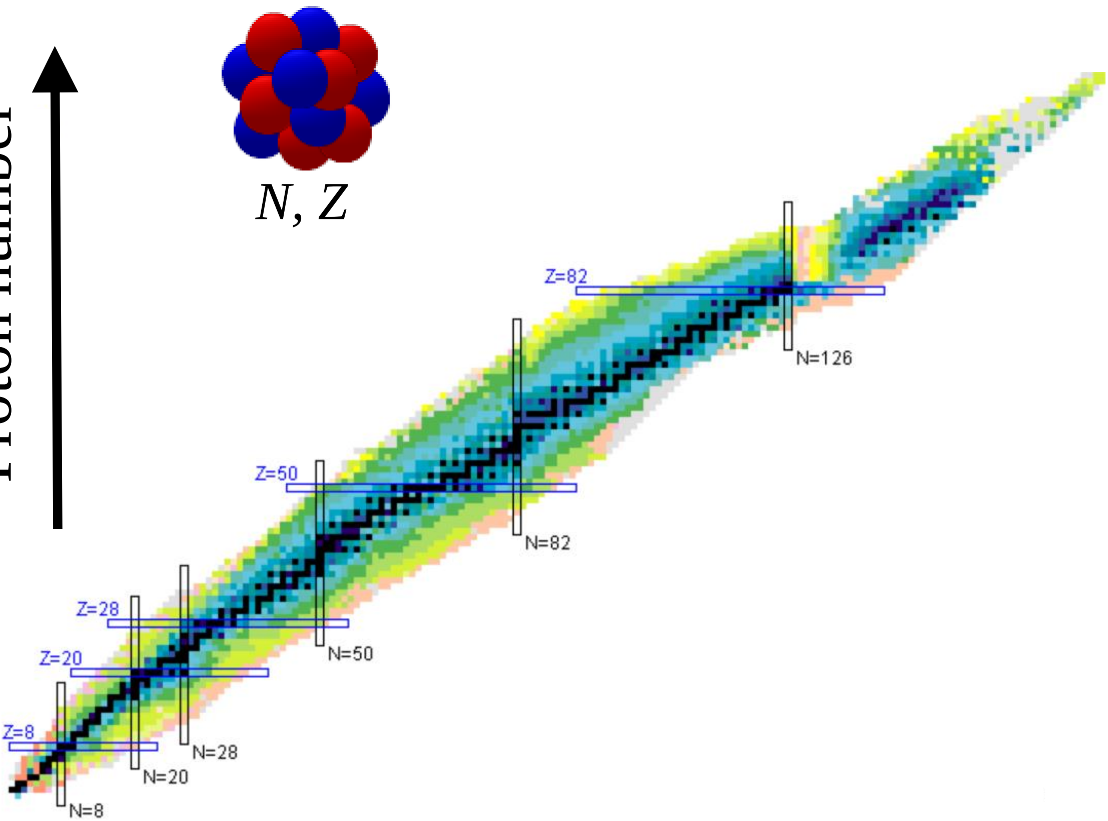


Neutron number

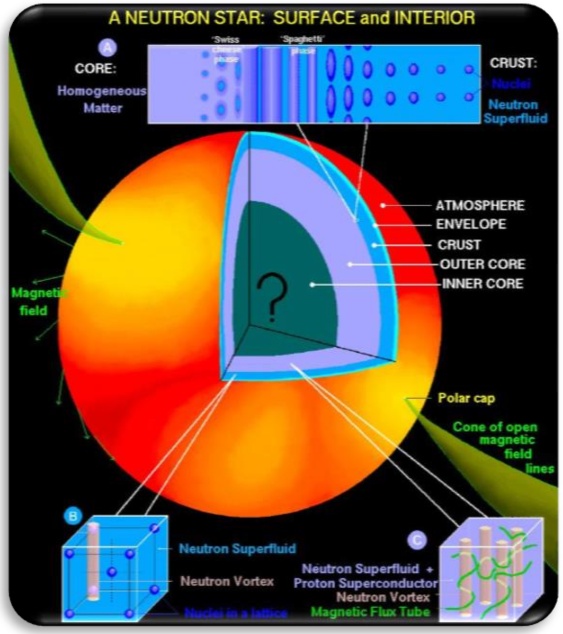
All nuclei can be described with a *single* EDF

N, Z

Proton number



Neutron star



Neutron number

Let us switch from DFT to TDDFT

Brief (over)look at a chronology: from past to present

DFT for ***superconductor***
Oliveira, Gross, and Kohn, PRL**60**(1988)2430

TDDFT for ***superconductor***
Wacker, Kümmel, and Gross, PRL**73**(1994)2915

LDA for *superfluid Fermi gas* (***SLDA***)
Kurth, Marques, Lüders, and Gross, Phys. Rev. Lett. **83**, 2628 (1999)
Bulgac and Yu, PRL**88**(2002)042504; Bulgac, PRC**65**(2002)051305(R)

TD-LDA for *superfluid Fermi gas* (***TDSLDA***)
Bulgac and Yoon, PRL**102**(2009)085302; Bulgac *et al.*, Science**332**(2011)1288

Other Sides (Cond. Mat. or DFT)

Real-space TDDFT for molecules
K. Yabana and G.F. Bertsch, Phys. Rev. B **54**, 4484 (1996)

Real-space TDDFT for solids
Bertsch, Iwata, Rubio, and Yabana, Phys. Rev. B **62**, 7998 (2000)

"Birth of DFT" *"Birth of TDDFT"* ***SLDA*** ***TDSLDA***

1956,59 1964,65 1970 1976 1984 1996 1998 2000 2010 2022

Skyrme's interaction

Skyrme "HF", "TDHF"

"Birth of KS" **(1988)**

"Nuclear DFT or EDF" was spread over the field..

Linear-response, RPA
FAM: PRC76(2007)024318
Density-Constrained TDHF
QRPA, TDHFB, ...

(TD)DFT for solid crusts of neutron stars 2019 (2022)~

Nuclear Side

Real-space "TDHF" for nuclear collisions
1D: P. Bonche, S. Koonin, and J.W. Negele, Phys. Rev. C **13**, 1226 (1976)
3D: R.Y. Cusson, R.K. Smith, and J.A. Maruhn, Phys. Rev. Lett. **36**, 1166 (1976)

Real-space "Skryme HF" for atomic nuclei
D. Vautherin and D.M. Brink, Phys. Lett. **32B**, 149 (1970); Phys. Rev. C **5**, 626 (1972); *ibid.* **7**, 296 (1973)

Skryme's "effective interaction"
T.H.R. Skyrme, Phil. Mag. **1**, 1043 (1956); Nucl. Phys. **9**, 615-640 (1959)

➢ **TDDFT is a time-dependent extension of DFT, but derivations are different**

	DFT	**TDDFT**
❑ **For what?**	**Ground state**	**Excited states, dynamics**
❑ **Relies on:**	**Hohenberg-Kohn theorem**	**Runge-Gross theorem**
	$n(\boldsymbol{r}) \overset{\text{H.K.}}{\Leftrightarrow} V_{\text{ext}}(\boldsymbol{r}) \Leftrightarrow \hat{H} \overset{\text{S.E.}}{\Leftrightarrow} \Psi$	$n(\boldsymbol{r},t) \overset{\text{R.G.}}{\Leftrightarrow} V_{\text{ext}}(\boldsymbol{r},t) \Leftrightarrow \hat{H}(t) \overset{\text{TDSE}}{\Leftrightarrow} \Psi(t)$
	$\Psi(\boldsymbol{r}_1,\dots,\boldsymbol{r}_N) = \Psi[n(\boldsymbol{r})]$	$\Psi(\boldsymbol{r}_1,\dots,\boldsymbol{r}_N,t) = \Psi[n(\boldsymbol{r},t)]$
❑ **Based on:**	**Variational principle**	**Taylor expansions**
	$E_{\text{g.s.}} = \min_n \left[\min_{\Psi\to n} \langle \Psi[n] \vert \hat{H} \vert \Psi[n] \rangle \right] = E[n_{\text{g.s.}}]$	$f(\boldsymbol{r},t) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\partial^n f(\boldsymbol{r},t)}{\partial t^n}\Big\vert_{t=t'} (t-t')^n$
❑ **Magic of:**	**Kohn-Sham Scheme → KS eq.**	**van Leeuwen's theorem → TDKS eq.**

TDDFT in a tiny nutshell - the Runge-Gross theorem

E. Runge and E.K.U. Gross, Phys. Rev. Lett. **52**, 997 (1984)

One-body density:

$$\rho(\boldsymbol{r},t) = N\int d\boldsymbol{r}_2\cdots\int d\boldsymbol{r}_N |\Psi(t)|^2$$

One-body current density:

$$\boldsymbol{j}(\boldsymbol{r},t) = \frac{\hbar N}{2im}\int d\boldsymbol{r}_2\cdots\int d\boldsymbol{r}_N \big[\Psi^*(t)\nabla\Psi(t) - \Psi(t)\nabla\Psi^*(t)\big]$$

TDSEs:

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi \qquad i\hbar\frac{\partial\Psi'}{\partial t} = \hat{H}'\Psi'$$

$$\Psi = \Psi(\boldsymbol{r}_1,\dots,\boldsymbol{r}_N,t) \qquad \hat{H} = \hat{T} + \hat{V} + \hat{V}_{\rm ext}$$

$$\hat{H}' = \hat{T} + \hat{V} + \hat{V}'_{\rm ext}$$

The rate of change of the current density reads:

$$\frac{\partial\boldsymbol{j}}{\partial t} = \frac{N}{2m}\int d\boldsymbol{r}_2\cdots\int d\boldsymbol{r}_N \Big[(H\,\Psi)^*\nabla\Psi - \Psi^*\,\nabla(H\,\Psi) + (H\,\Psi)\nabla\Psi^* - \Psi\,\nabla(H\,\Psi)^*\Big] \quad \cdots \text{(a)}$$

$$\frac{\partial\boldsymbol{j}'}{\partial t} = \frac{N}{2m}\int d\boldsymbol{r}_2\cdots\int d\boldsymbol{r}_N \Big[(H'\Psi')^*\nabla\Psi' - \Psi'^*\nabla(H'\Psi') + (H'\Psi')\Psi'^* - \Psi'\nabla(H'\Psi')^*\Big] \quad \cdots \text{(b)}$$

(a) − (b)

$$\boxed{\frac{\partial}{\partial t}\big[\boldsymbol{j}(\boldsymbol{r},t) - \boldsymbol{j}'(\boldsymbol{r},t)\big] = -\frac{1}{m}\rho(\boldsymbol{r},t)\nabla\underbrace{\big[v_{\rm ext}(\boldsymbol{r},t) - v'_{\rm ext}(\boldsymbol{r},t)\big]}_{\neq c(t)}} \quad \cdots (\bigstar)$$

*One can obtain equations for higher-order derivatives in the same manner

As in the case of static DFT, we have a TDKS scheme according to the following one-to-one correspondences:

$$\hat{H}(t) \overset{\text{TDSE}}{\Leftrightarrow} \Psi(t) \overset{\text{RG}}{\Leftrightarrow} \boldsymbol{j}(\boldsymbol{r},t)\ \&\ \rho(\boldsymbol{r},t)$$

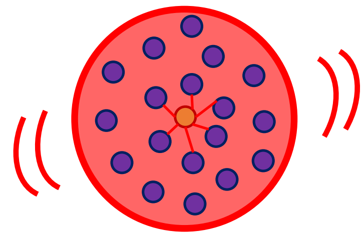
*Taking divergence of Eq.(★) and using the continuity equation, one can obtain equations for the density.

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\boldsymbol{j} = 0$$

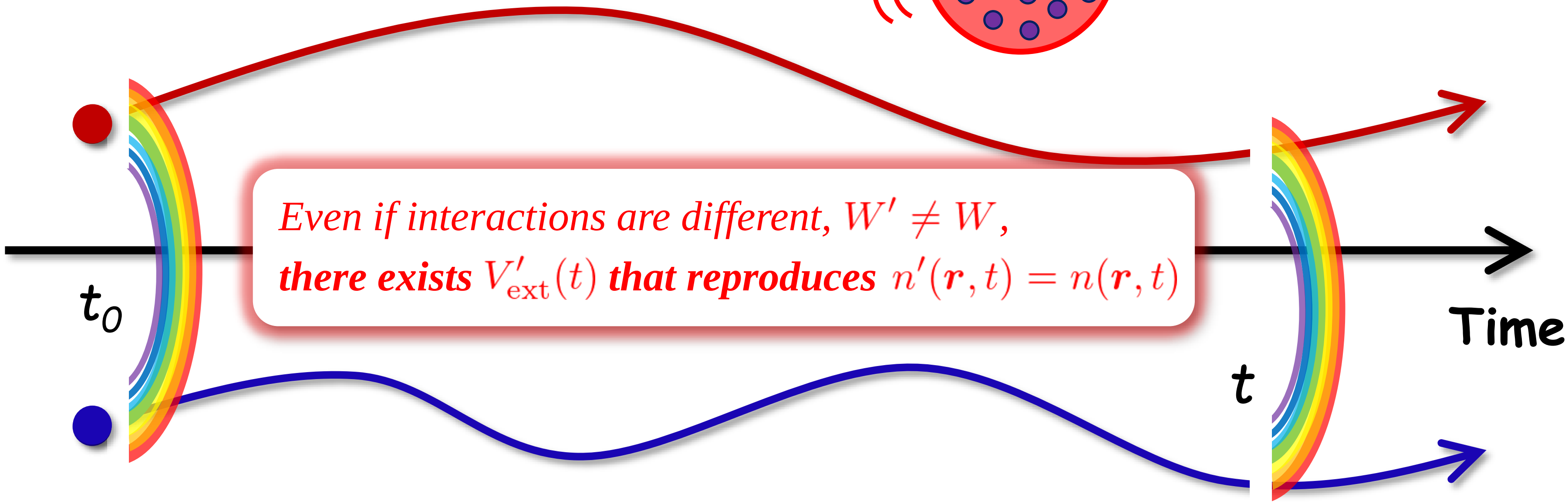
TDDFT is a time-dependent extension of DFT

TDSE for an *N*-body system

$$i\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r}_1,\dots,\boldsymbol{r}_N,t) = \hat{H}\Psi(\boldsymbol{r}_1,\dots,\boldsymbol{r}_N,t)$$



$$\hat{H}(t) = \hat{T} + \hat{W} + \hat{V}_{\text{ext}}(t)$$



Even if interactions are different, $W' \neq W$,
there exists $V'_{\text{ext}}(t)$ ***that reproduces*** $n'(\boldsymbol{r},t) = n(\boldsymbol{r},t)$

TDSE for another *N*-body system (*with a different interaction* W')

$$i\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r}_1,\dots,\boldsymbol{r}_N,t) = \hat{H}'\Psi(\boldsymbol{r}_1,\dots,\boldsymbol{r}_N,t)$$

$$\hat{H}'(t) = \hat{T} + \hat{W}' + \hat{V}'_{\text{ext}}(t)$$

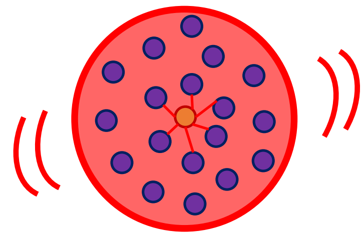
R. van Leeuwen, Phys. Rev. Lett. **82**, 3863 (1999)

What is the van Leeuwen's theorem? $W' = W \Rightarrow$ RG $W' = 0 \Rightarrow$ TDKS

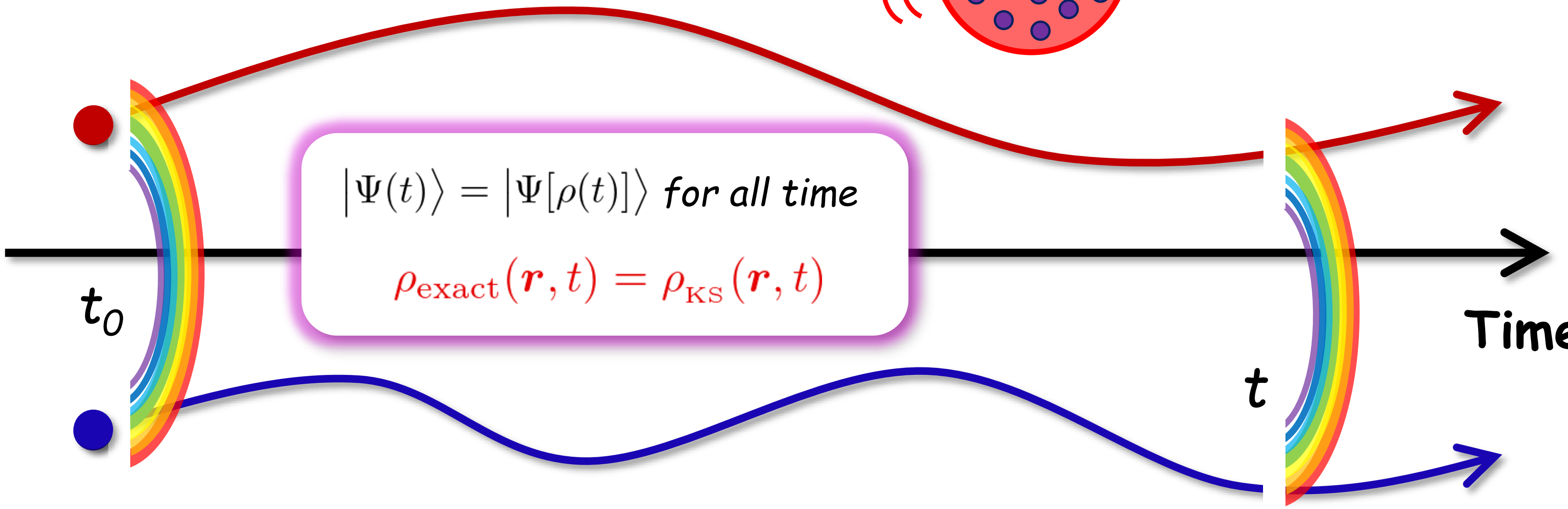
TDDFT is a time-dependent extension of DFT

TDSE for an *N*-body system

$$i\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r}_1,\dots,\boldsymbol{r}_N,t) = \hat{H}\Psi(\boldsymbol{r}_1,\dots,\boldsymbol{r}_N,t)$$

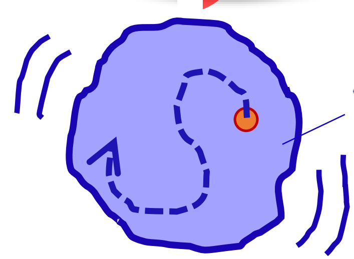


$$\hat{H}(t) = \hat{T} + \hat{W} + \hat{V}_{\rm ext}(t)$$



TDKS eq. in TDDFT ($W' = 0$, *i.e., a non-interacting system*)

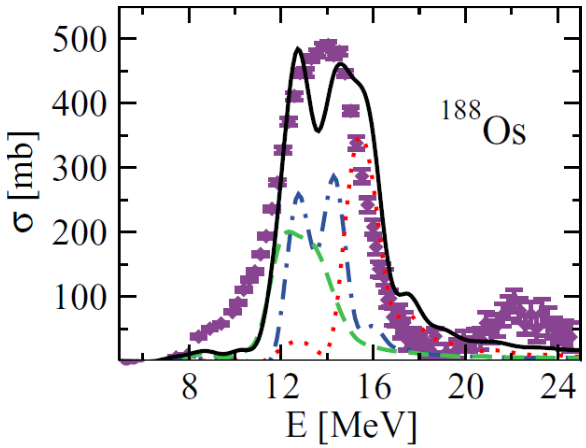
$$i\hbar\frac{\partial\phi_i(\boldsymbol{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + v_{\rm KS}[\rho(\boldsymbol{r},t)]\right]\phi_i(\boldsymbol{r},t)$$



R. van Leeuwen, Phys. Rev. Lett. **82**, 3863 (1999)

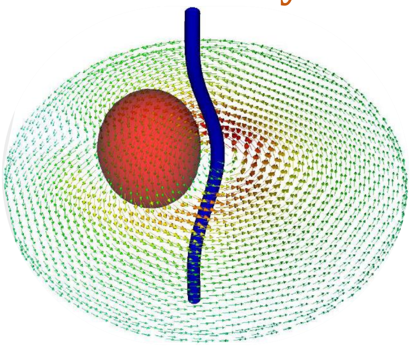
TDDFT is a versatile tool!!

IVGDR



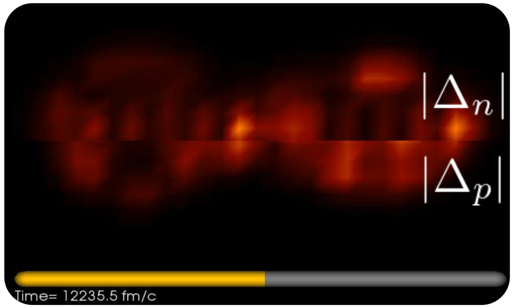
Phys. Rev. C **84**, 051309(R) (2011)
I. Stetcu, A. Bulgac, P. Magierski, and K.J. Roche

Vortex-nucleus dynamics



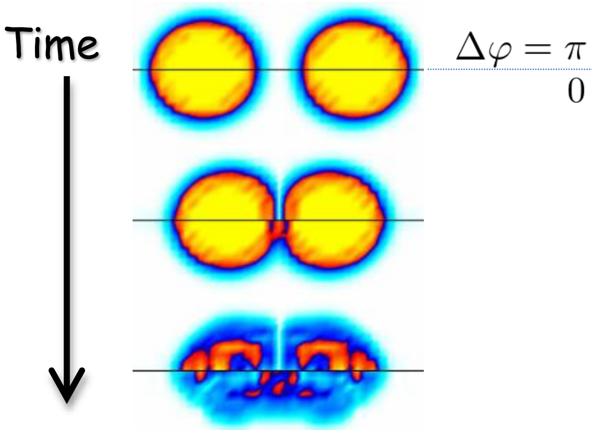
Phys. Rev. Lett. **117**, 232701 (2016)
G. Wlazłowski, K.S., P. Magierski, A. Bulgac, and M.M. Forbes

Induced fission of ^{240}Pu



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

Low-energy heavy-ion reactions

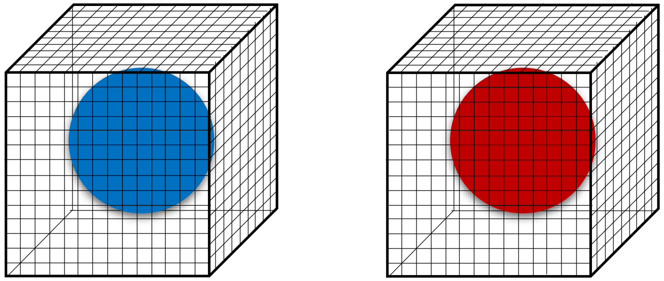


Phys. Rev. Lett. **119**, 042501 (2017)
P. Magierski, K.S., and G. Wlazłowski

Low-energy heavy-ion reactions

Once an EDF is given, there are no empirical parameters

1. Prepare ground states of projectile and target nuclei

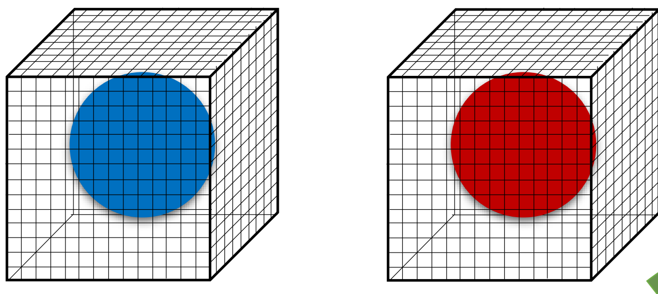


KS (or HF) equations

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

Once an EDF is given, there are no empirical parameters

1. Prepare ground states of projectile and target nuclei



KS (or HF) equations

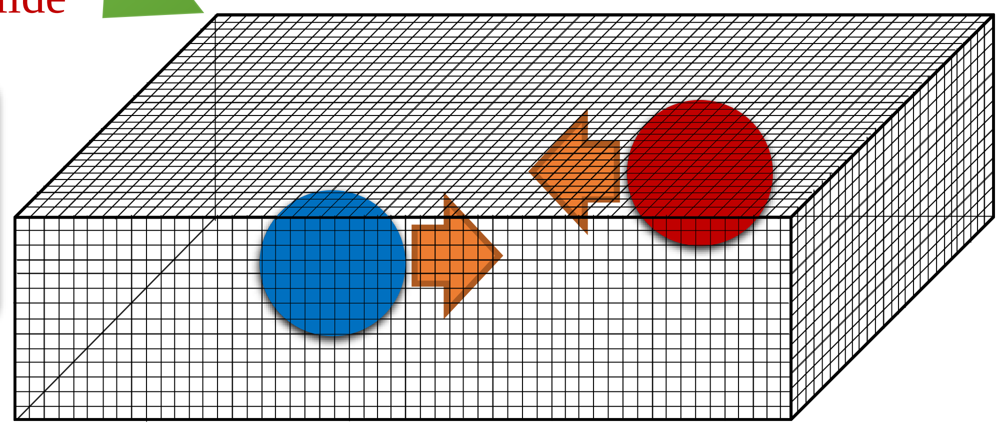
$$\left[-\frac{\hbar^2}{2m}\nabla^2 + v_{\text{KS}}[\rho(\boldsymbol{r})]\right]\phi_i(\boldsymbol{r}) = \varepsilon_i\,\phi_i(\boldsymbol{r})$$

2. Put them into a larger box

3. Give relative momentum, and let them collide

TDKS (or TDHF) equations

$$i\hbar\frac{\partial\phi_i(\boldsymbol{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + v_{\text{KS}}[\rho(\boldsymbol{r},t)]\right]\phi_i(\boldsymbol{r},t)$$

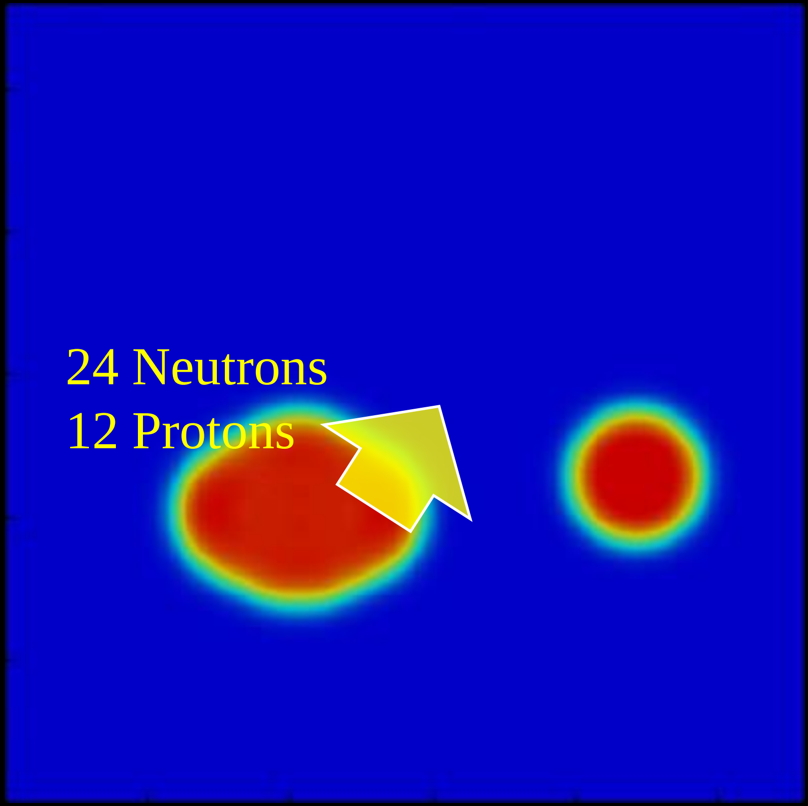


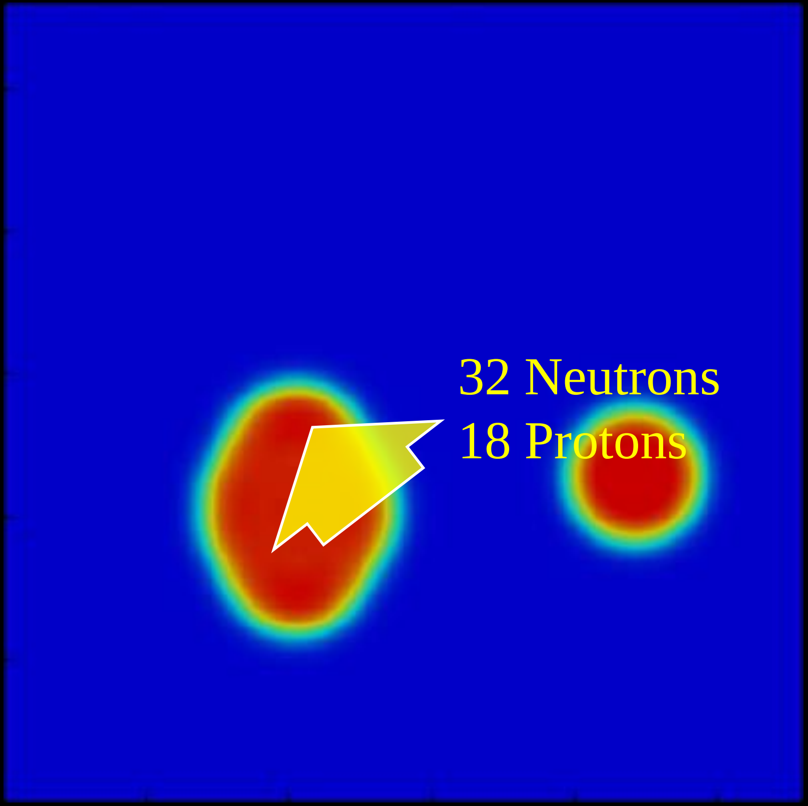
^{64}Ni+^{238}U at E_{lab}=390 MeV

K.S. and K. Yabana, PRC**93**(2016)054616

Quasifission dynamics in TDDFT

Tip collision	Side collision
Shell effects of ^{208}Pb	More mass-symmetric



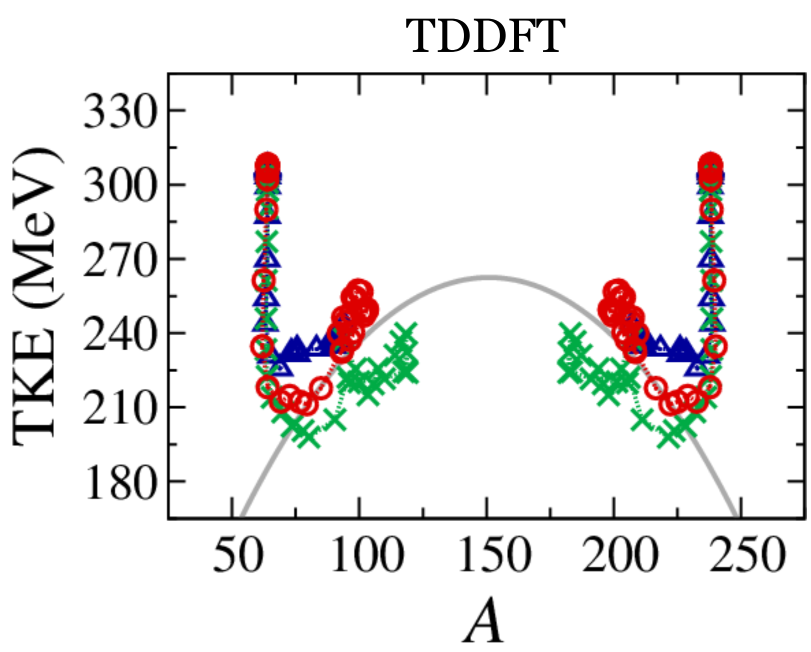


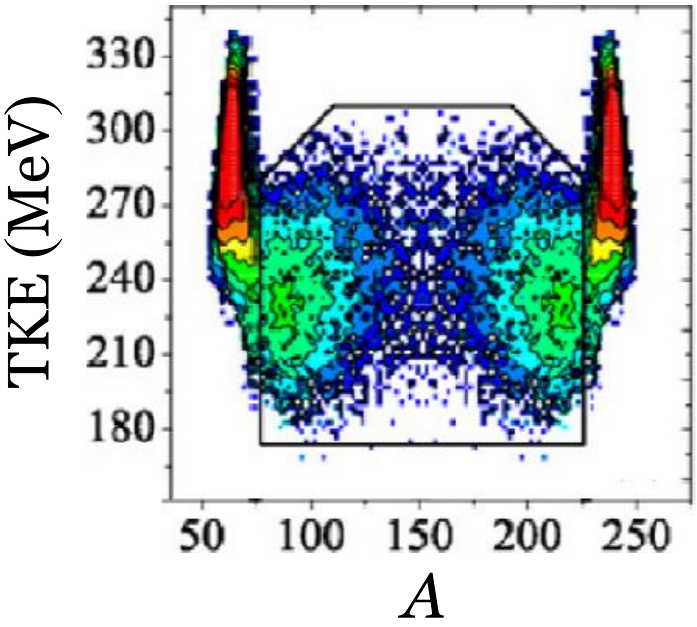
$^{64}Ni+^{238}U$ at E_{lab}=390 MeV

K.S. and K. Yabana, PRC**93**(2016)054616

TDDFT provides quantitative description of quasifission dynamics

TKE-*A* distribution: Comparison with experimental data



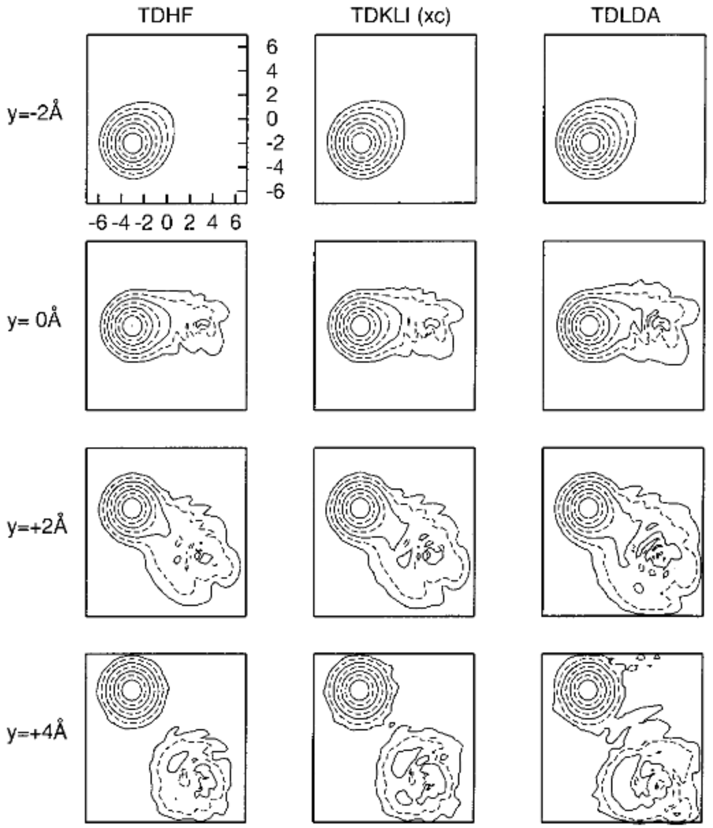


Expt.: E.M. Kozulin *et al.*, PLB**686**(2010)227

One may extract transfer probabilities, though $\Phi_{\mathrm{KS}}[n(\boldsymbol{r},t)] \neq \Psi_{\mathrm{exact}}[n(\boldsymbol{r},t)]$

H.J. Lüdde and R.M. Dreizler, J. Phys. B: Atom. Mol. Phys. **16**, 3973 (1983)
R. Nagano, K. Yabana, T. Tazawa, and Y. Abe, PRA**62**(2000)062721

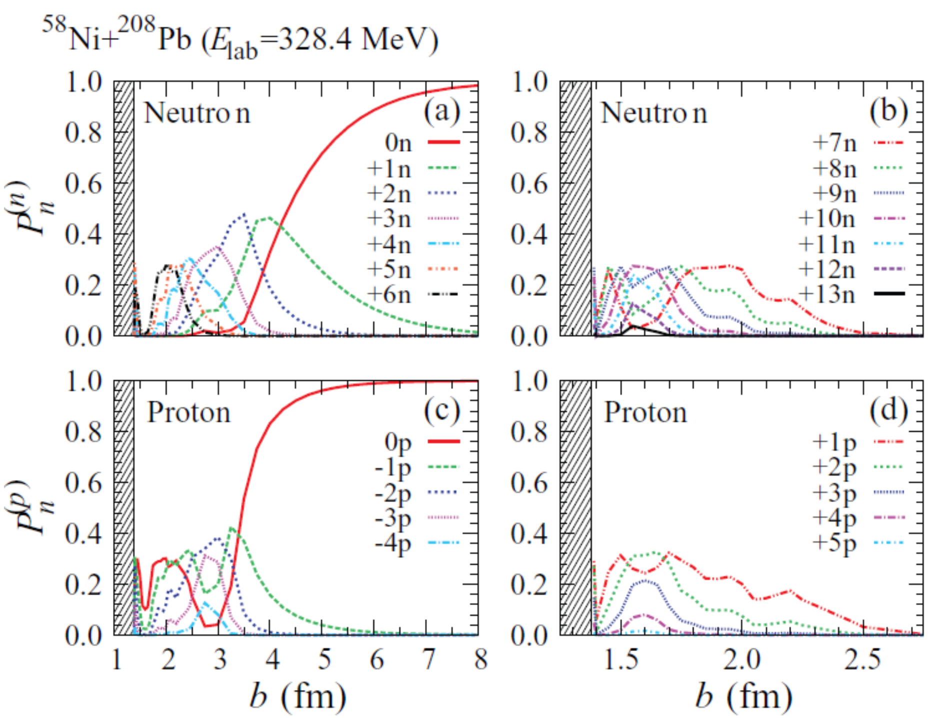
Electron transfer in collisions of Ar^{8+} and Ar



S.E. Koonin, K.T.R. Davies, V. Maruhn-Rezwani, H. Feldmeier, S. J. Krieger, and J. W. Negele, PRC**15**(1977)1359

Particle-number projection for TDHF:
C. Simenel, PRL**105**(2010)192701
K. Sekizawa and K. Yabana, PRC**88**(2013)014614

Nucleon transfer in collisions of ^{58}Ni and ^{208}Pb



From nuclei to **neutron stars**

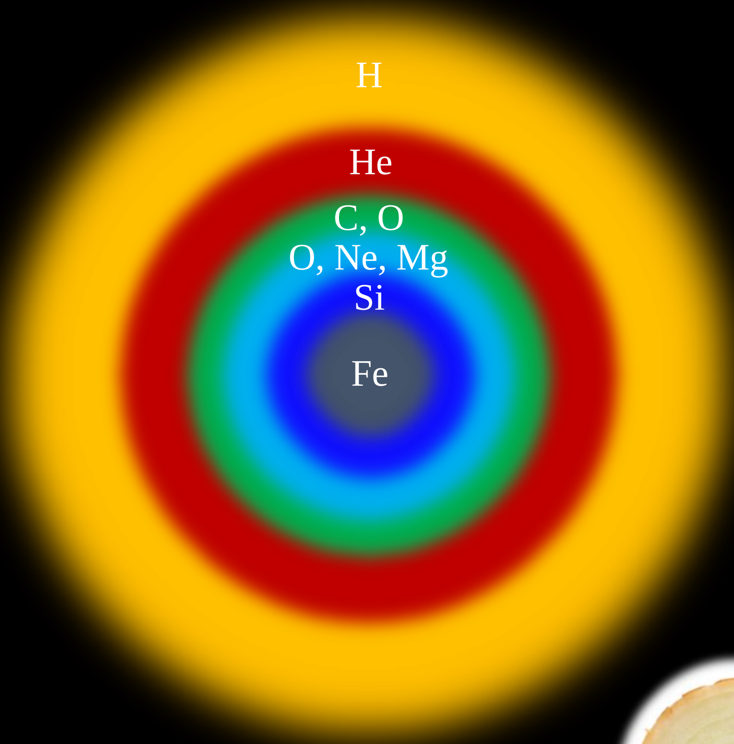
“3d hyperspace background with warp tunnel effect Free Photo” @freepik

The fate of a massive star

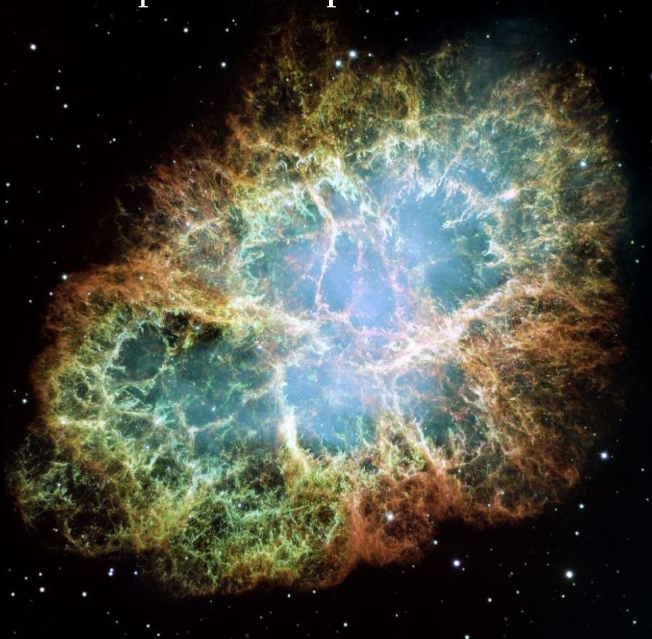
Nuclear reactions:

$^{1}\mathrm{H} \rightarrow {}^{4}\mathrm{He} \rightarrow {}^{12}\mathrm{C} \rightarrow {}^{16}\mathrm{O} \rightarrow {}^{20}\mathrm{Ne} \rightarrow {}^{24}\mathrm{Mg} \rightarrow {}^{28}\mathrm{Si} \rightarrow \ldots \rightarrow {}^{56}\mathrm{Fe}$

"Onion structure"



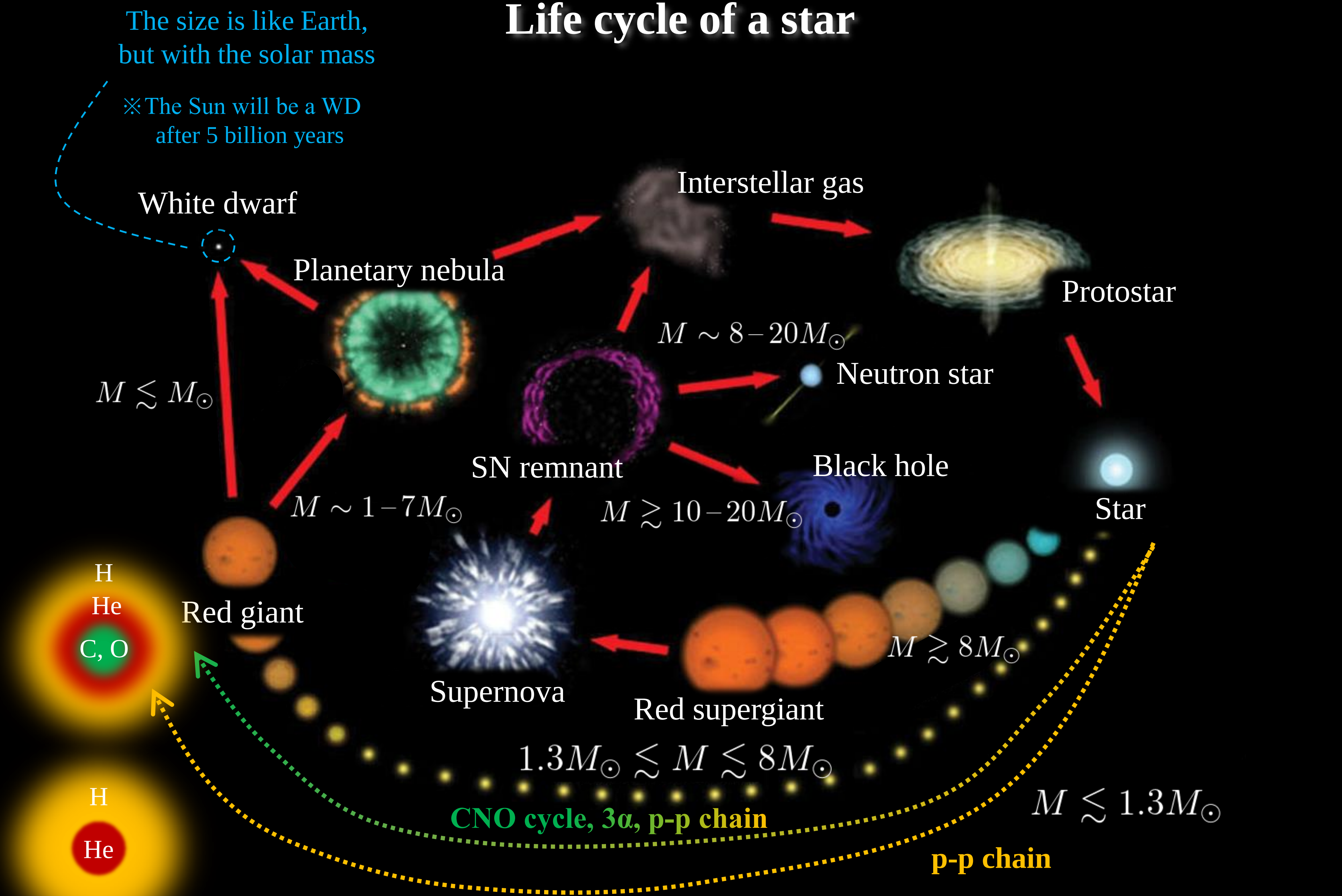
After forming the iron core…
→ no more fuel
→ gravitational collapse
→ supernova explosion



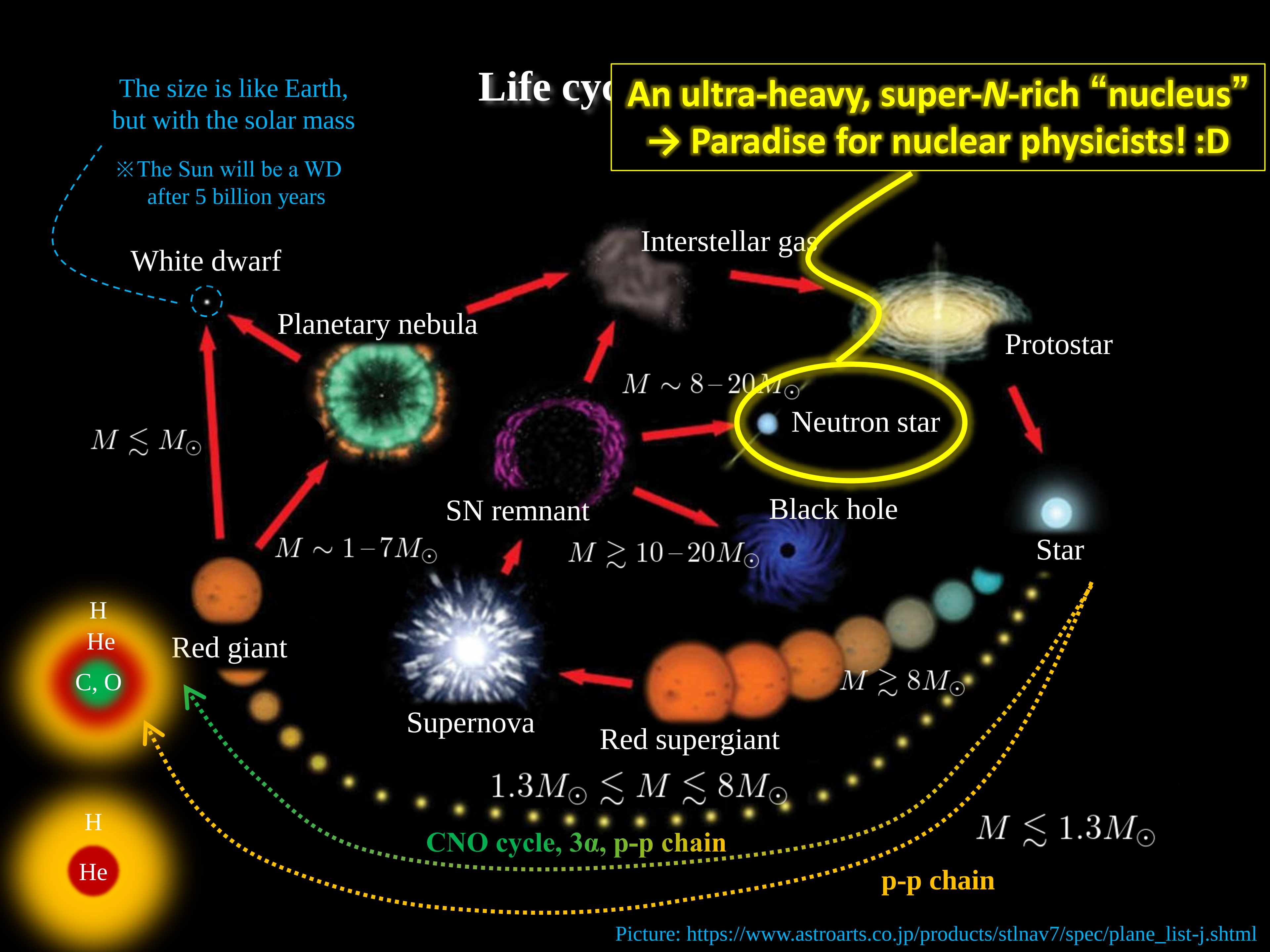
The Crab Nebula
Remnant of the SN in 1054

Picture: https://en.wikipedia.org/wiki/Crab_Nebula

Life cycle of a star



Picture: https://www.astroarts.co.jp/products/stlnav7/spec/plane_list-j.shtml



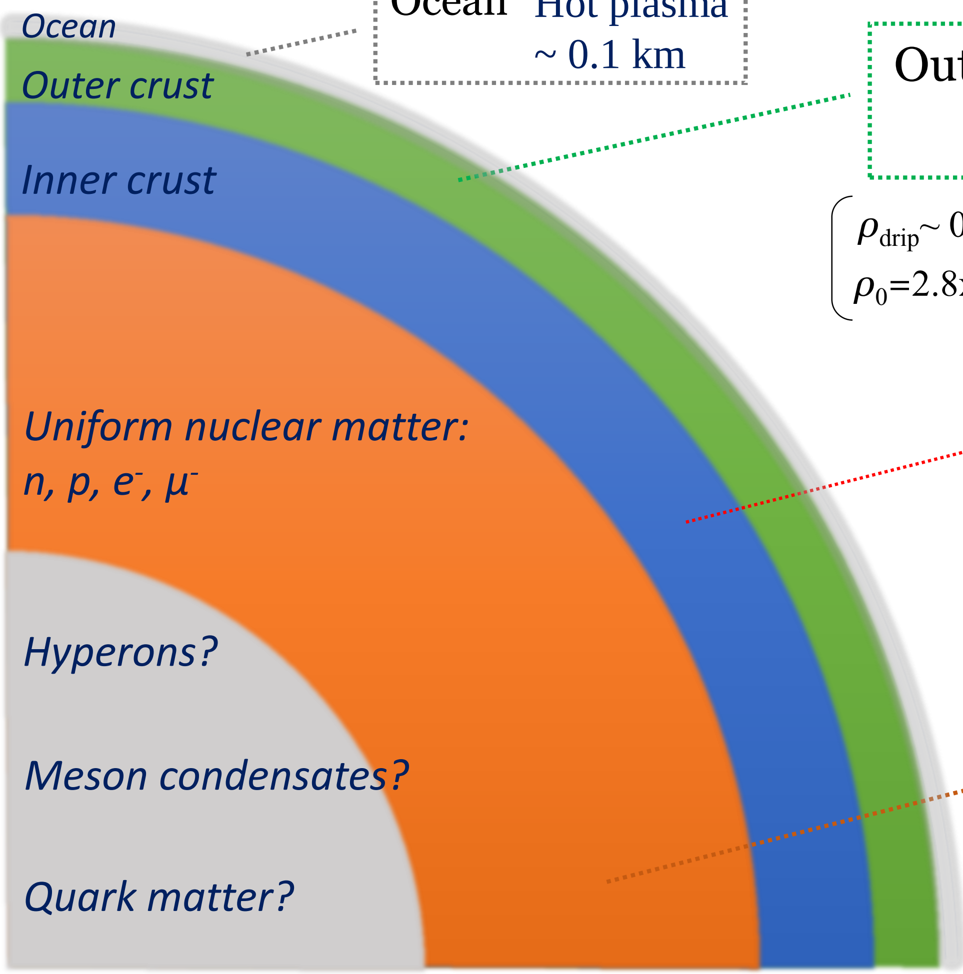
Life cyc
An ultra-heavy, super-N-rich "nucleus"
→ Paradise for nuclear physicists! :D
The size is like Earth,
but with the solar mass
※The Sun will be a WD
after 5 billion years
White dwarf
Planetary nebula
Interstellar gas
Protostar
$M \lesssim M_\odot$
$M \sim 8-20M_\odot$
Neutron star
SN remnant
Black hole
Star
$M \sim 1-7M_\odot$
$M \gtrsim 10-20M_\odot$
H
He
C, O
Red giant
Supernova
Red supergiant
$M \gtrsim 8M_\odot$
$1.3M_\odot \lesssim M \lesssim 8M_\odot$
H
He
CNO cycle, 3α, p-p chain
$M \lesssim 1.3M_\odot$
p-p chain
Picture: https://www.astroarts.co.jp/products/stlnav7/spec/plane_list-j.shtml

What’s inside a neutron star?

Structure of a neutron star

Neutron star is a great playground for nuclear physicists

✓ **It offers extreme situations which can not be realized in terrestrial experiments!**



Ocean — Hot plasma ~ 0.1 km

Outer crust — Nuclei (Z=26-42), electrons
0.3-0.6 km $\rho < \rho_{\text{drip}}$

$\rho_{\text{drip}} \sim 0.0014\rho_0$; Above ρ_{drip} unbound neutrons exist outside nuclei
$\rho_0 = 2.8\text{x}10^{14}\ \text{g/cm}^3 = 0.16\ \text{fm}^{-3}$; Nuclear saturation density

Inner crust — Nuclei, electrons, "dripped" neutrons
0.5-0.8 km $\rho_{\text{drip}} \leq \rho \leq 0.6\rho_0$

Outer/inner core
9-12 km $0.6\rho_0 < \rho \leq 3\text{-}5\rho_0$

How can we understand NS structure from nucleons?

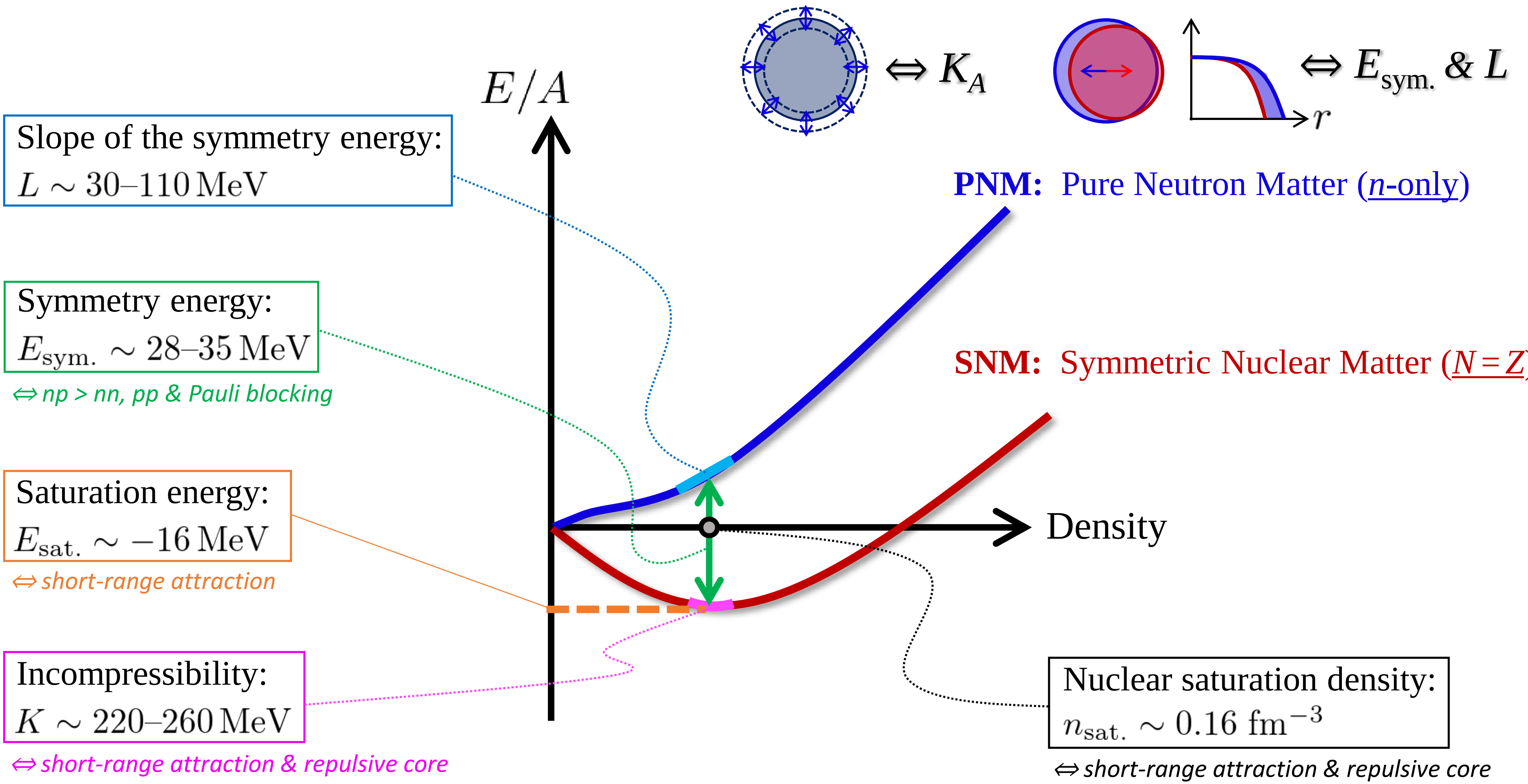
from nuclear force to neutron stars

Equation of state (EoS) of nuclear matter

➢ EoS characterizes the nuclear matter properties

✓ From low-energy nuclear experiments, one may extract information in the vicinity of the saturation density

E.g.) ISGMR: U. Grag and G. Colò, PPNP**101**(2018)55; Electric dipole (E1) polarizability → skin thickness: A. Tamii *et al.*, EPJA**50**(2014)28



cf. Frontiers in Physics Vol. 21, Understanding the World of Supernova Explosion from Atomic Nuclei (原子核から読み解く超新星爆発の世界), K. Sumiyoshi (Kyoritsu printing Co., Ltd.)

➢ An EoS defines a Mass-Radius relation of neutron stars

◻ Equation of state, $E(n)$
→ A relation between pressure and density:

$$P(n) = -\frac{dE}{dV} = n^2 \frac{dE/A}{dn}$$

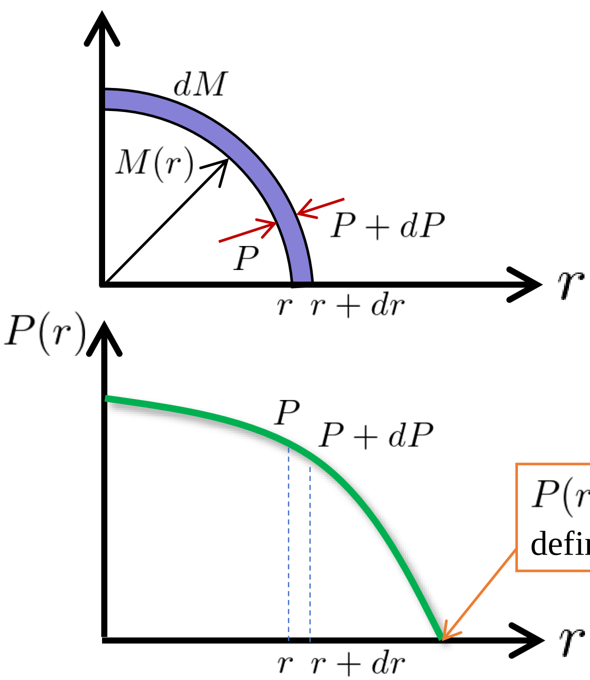
◻ Tolman-Oppenheimer-Volkoff (TOV) equation:

$$\frac{dP(r)}{dr} = -\frac{GM(r)\rho(r)}{r^2}\left(1+\frac{P(r)}{\rho(r)c^2}\right)\left(1+\frac{4\pi r^3 P(r)}{M(r)c^2}\right)\left(1-\frac{2GM(r)}{rc^2}\right)^{-1}$$

correction from General Relativity (GR)

where $\frac{dM(r)}{dr} = 4\pi r^2 \rho(r)$ $\quad M(r)$: Integrated mass within radius r

Equilibrium condition:
Gravitational force (inward) + Pressure (outward) = 0



$P(r) = 0$
defines the NS radius

Mass-radius relation

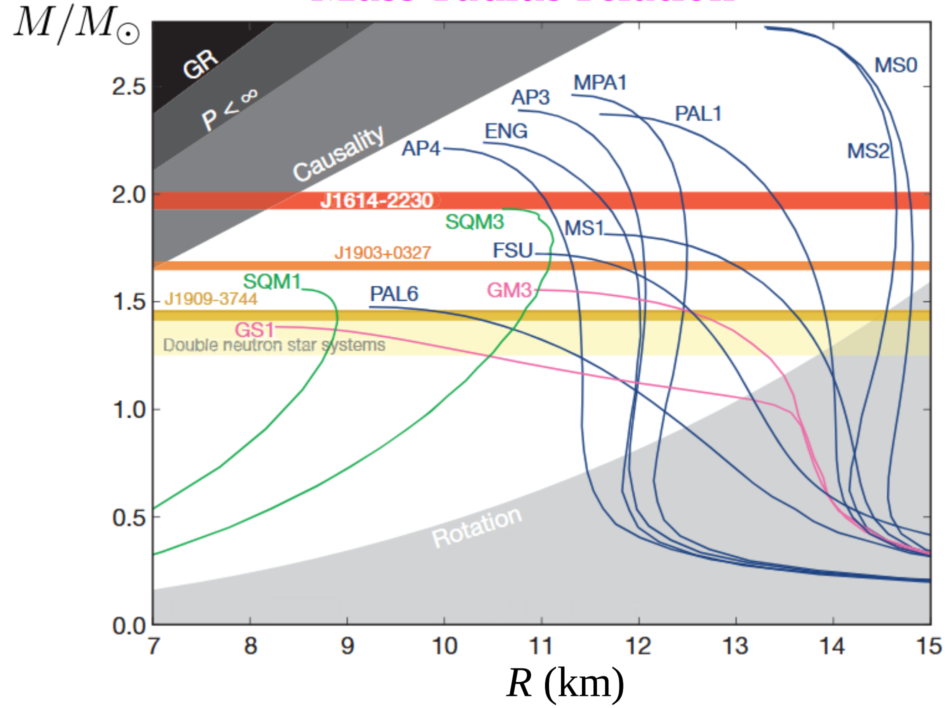


Figure: P.B. Demorest *et al.*, Nature **467**, 1081 (2010)

In an outer (low-density) region of neutron stars,
nuclear matter is *not* actually *homogeneous*

The nuclear interaction “clusterize” neutrons and protons,
akin to finite nuclei, which form a Coulomb lattice
(*i.e.* a crystal, like a solid)

Let’s see: from the outer crust to the inner crust

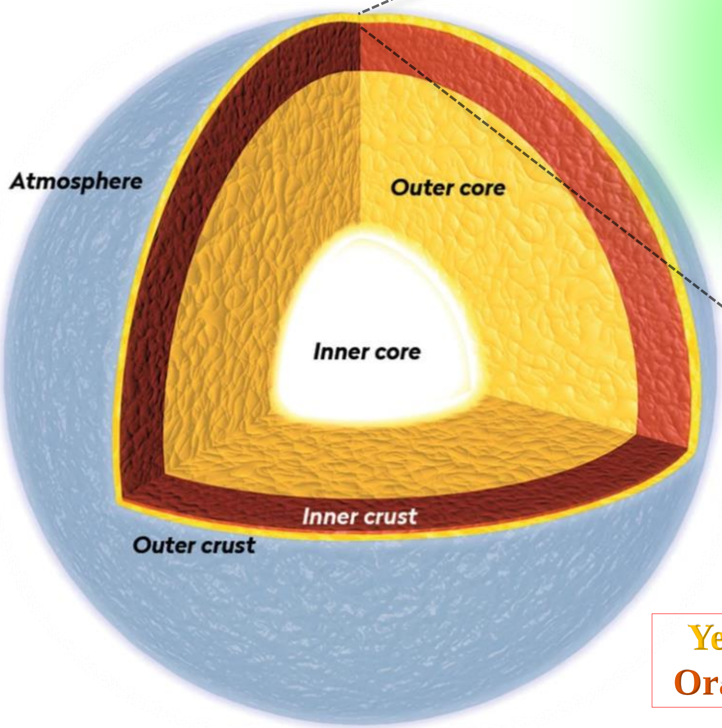
Note:
In the figure showing nuclides composition, the **bold** font indicates known-mass nuclei.

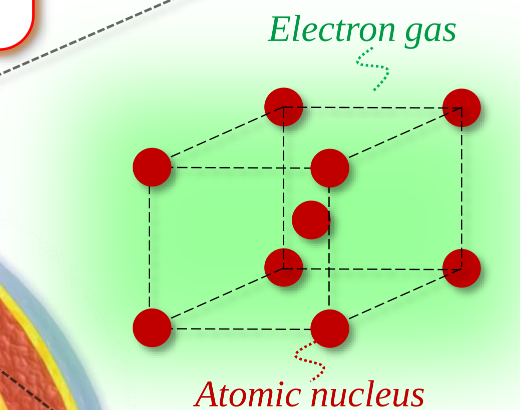
Structure of the outer crust is “similar” to that of a white dwarf

but, nuclei are different and become neutron-rich!

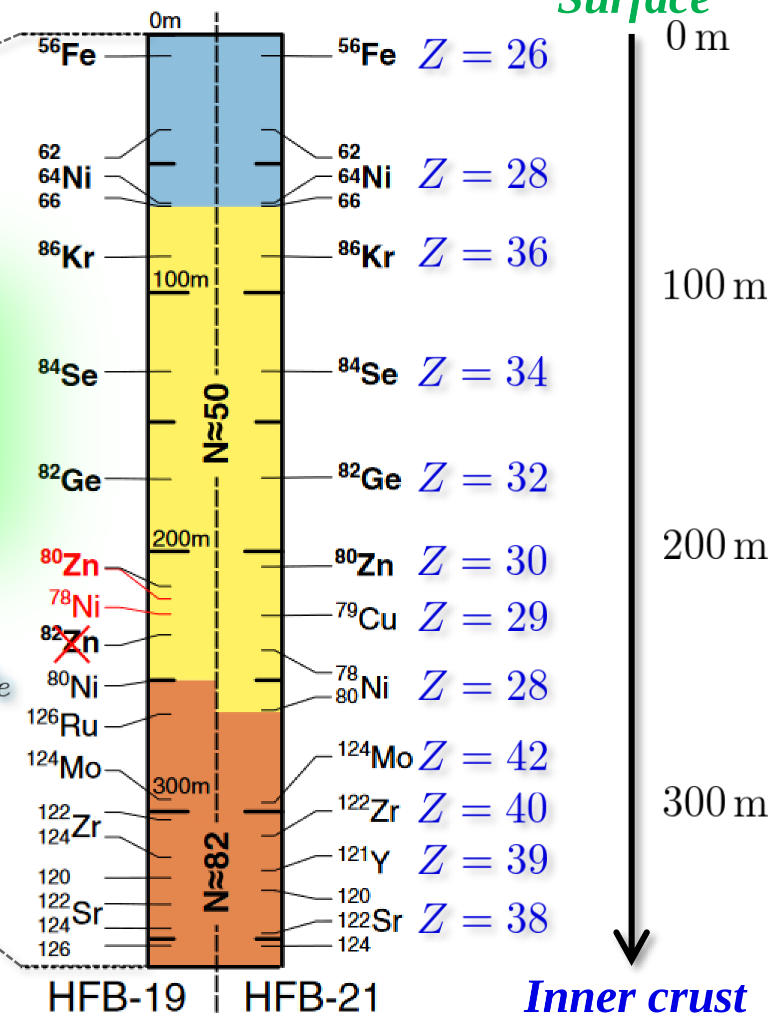
Composition of the outer crust:

✓ Coulomb lattice of nuclei
+ Electron gas





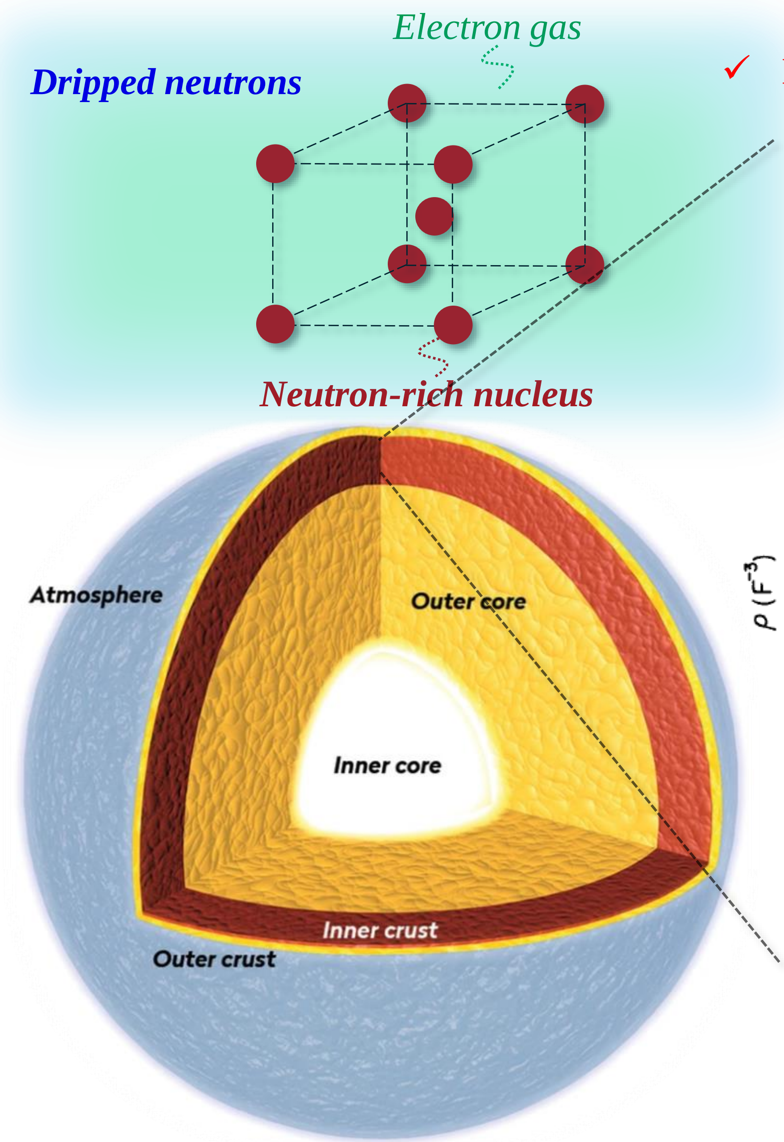
$$p + e^- \to n + \nu_e$$



Yellow region: $N \approx 50$
Orange region: $N \approx 82$

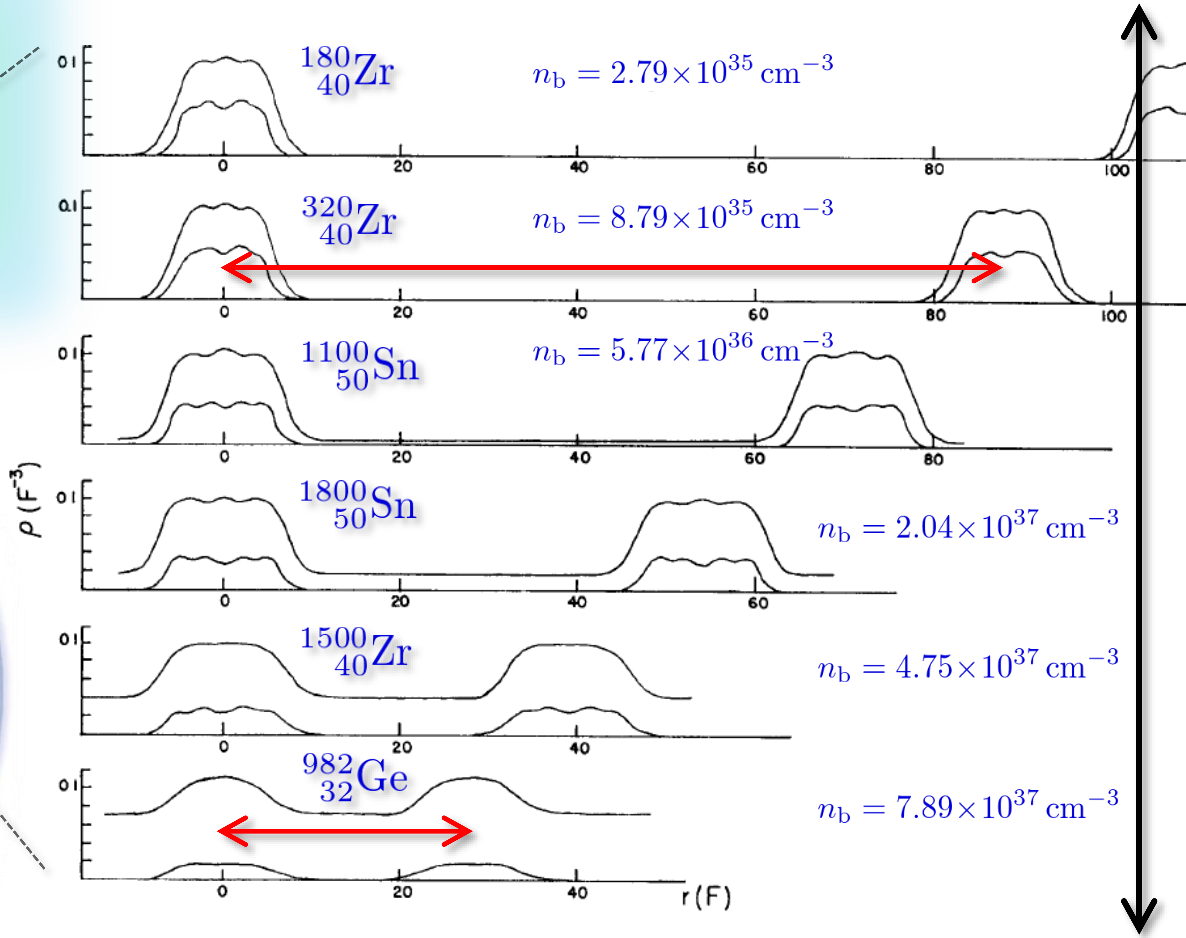
Figure: R.N. Wolf et al., Phys. Rev. Lett. **110**, 041101 (2013)
Neutron star: https://www.skyatnightmagazine.com/space-science/neutron-star/

In the inner crust, a sea of "dripped neutrons" permeates the Coulomb lattice



✓ Distance between nuclei decreases with increasing density

Outer crust



Outer core

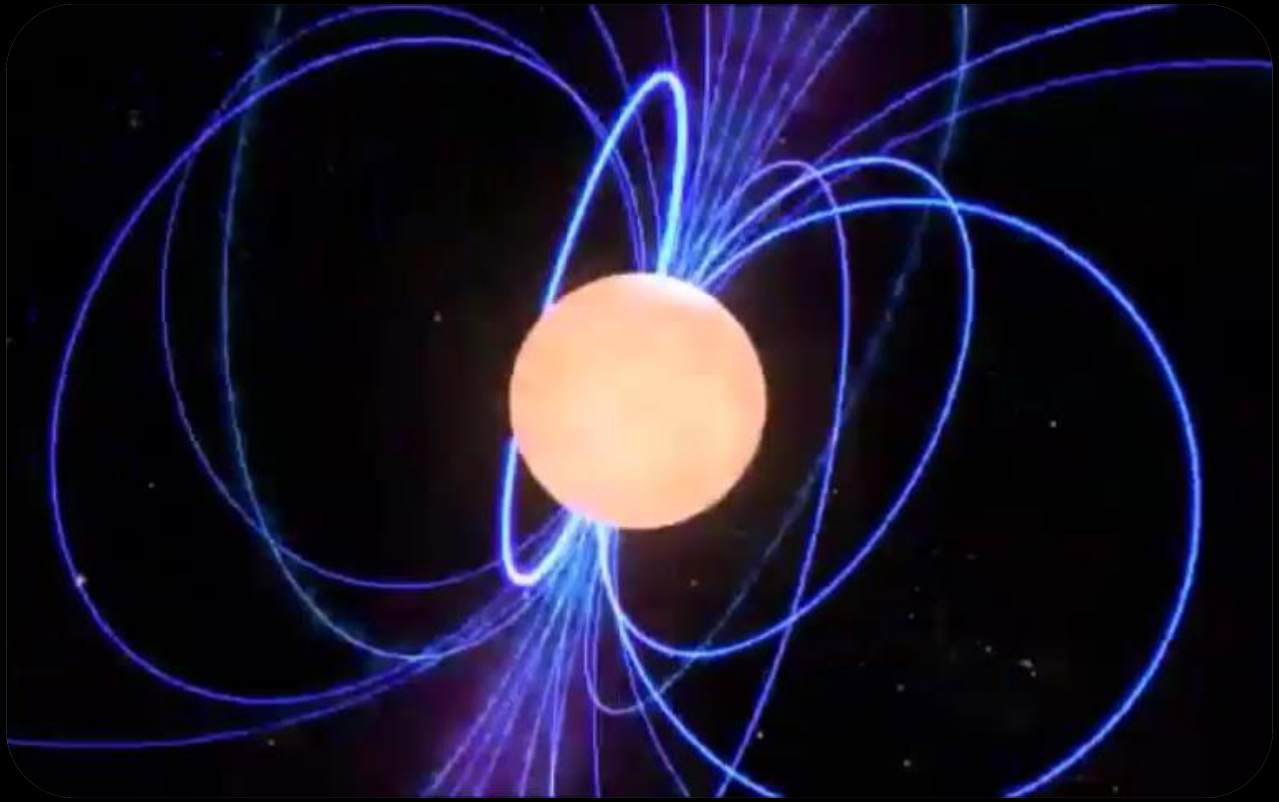
Figure: J.W. Negele and D. Vautherin, Nucl. Phys. **A207**, 298 (1978)
Neutron star: https://www.skyatnightmagazine.com/space-science/neutron-star/

Neutron-star “glitch”

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

Pulsar - a rotating neutron star

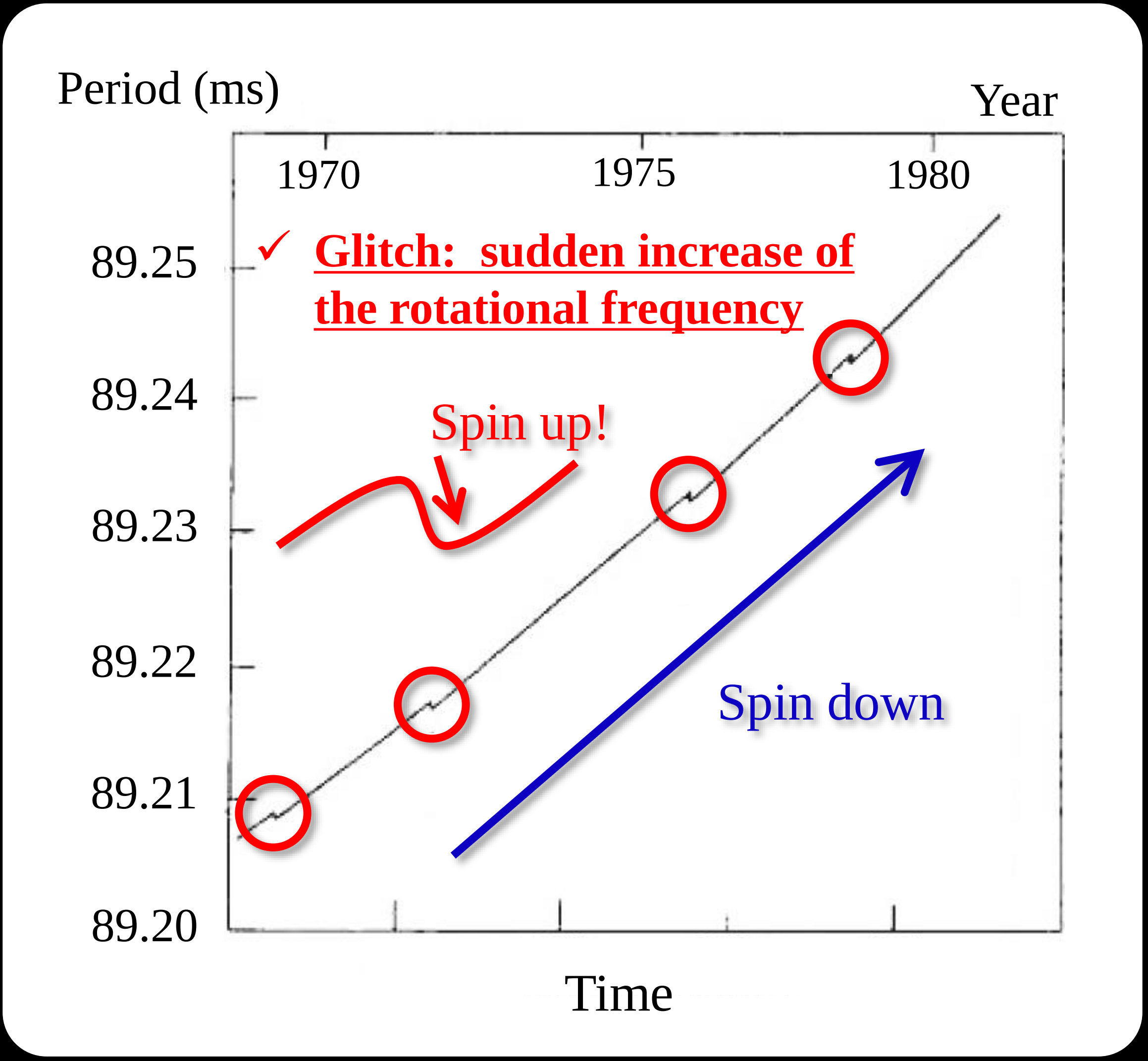
- ✓ First discovery in August 1967 → "Little Green Man" LGM-1 → PSR B1919+21
- ✓ Since then, more than 2650 pulsars have been observed
- ✓ It gradually spins down due to the EM radiation



What is the glitch?

Typical example: the Vela pulsar

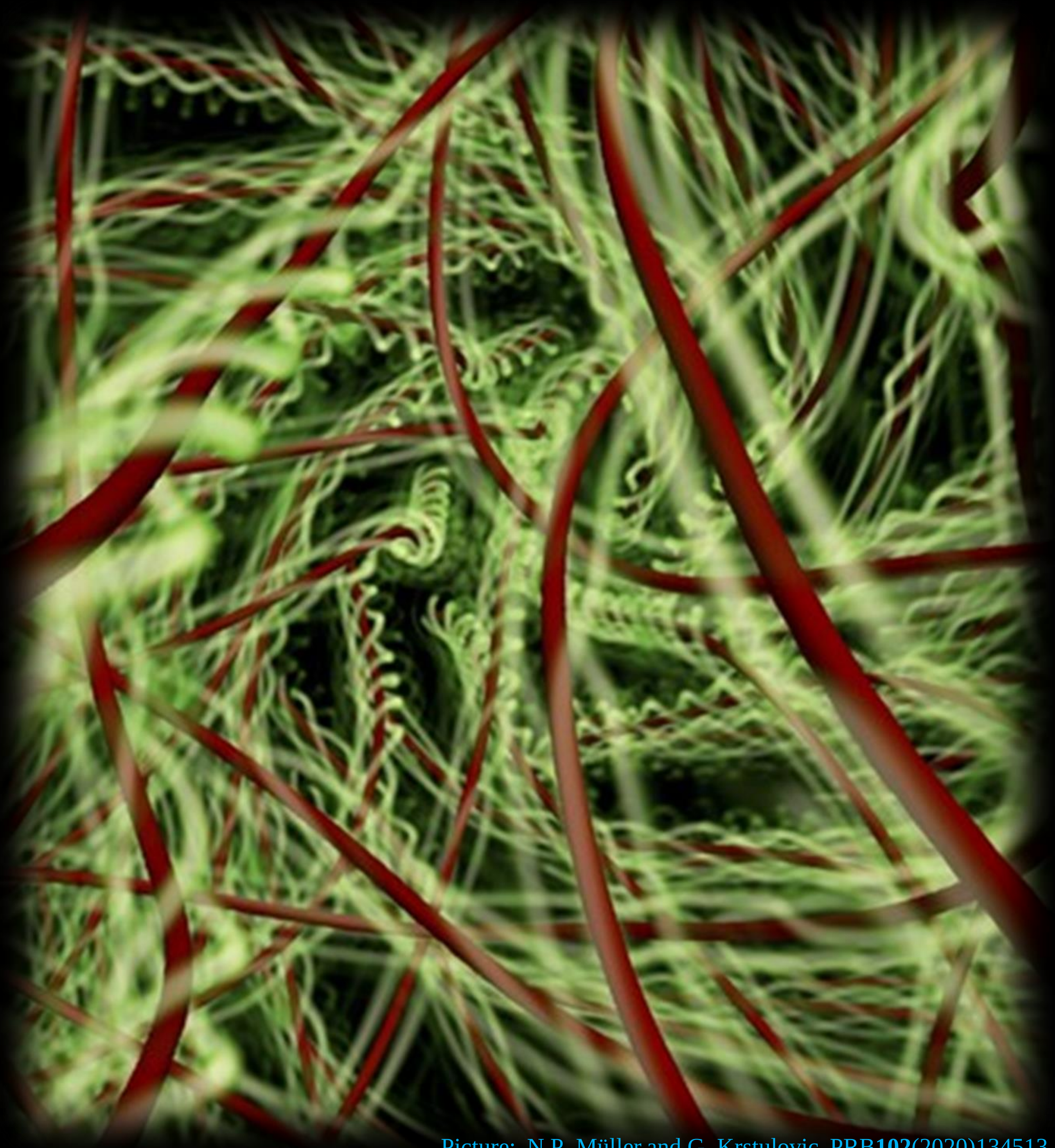
- *Irregularity* has been observed from continuous monitoring of the pulsation period



What happened?

- Dynamics of superfluid *“quantized vortices”* play a key role! **!?**

Quantum vortices



Picture: N.P. Müller and G. Krstulovic, PRB**102**(2020)134513

In superfluid, vortices are quantized!

Superfluid order parameter:

$$\Delta(\boldsymbol{r},t) = |\Delta(\boldsymbol{r},t)|e^{i\phi(\boldsymbol{r},t)}$$

Superfluid velocity:

$$\boldsymbol{v}_s(\boldsymbol{r},t) = \frac{\hbar}{m}\nabla\phi(\boldsymbol{r},t)$$

Vorticity:

$$\boldsymbol{\omega} = \nabla \times \boldsymbol{v}_s = 0$$

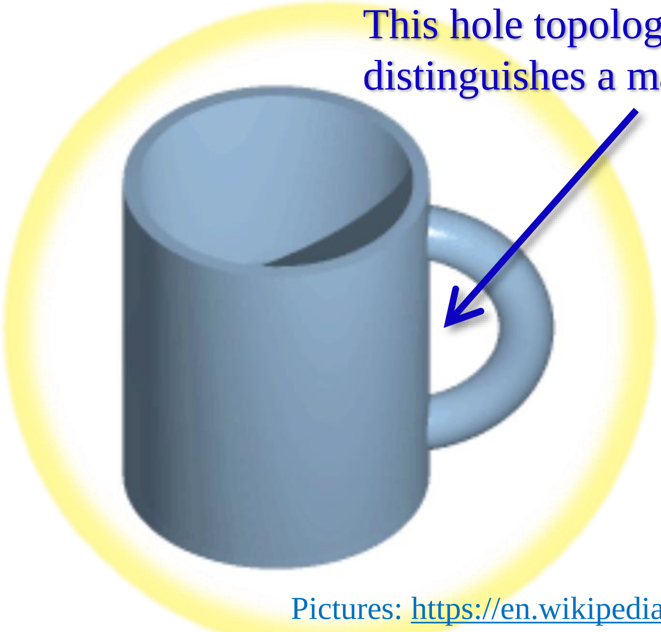
superfluid is irrotational

Circulation:

$$\kappa = \int_S (\nabla \times \boldsymbol{v}_s)\cdot d\boldsymbol{S} = 0$$

*Unless, there is no topological defect

This hole topologically distinguishes a mag from a cow



Pictures: https://en.wikipedia.org/wiki/Topology

What is a quantum vortex?

In superfluid, vortices are quantized!

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*Unless, there is no topological defect

If there is a defect:

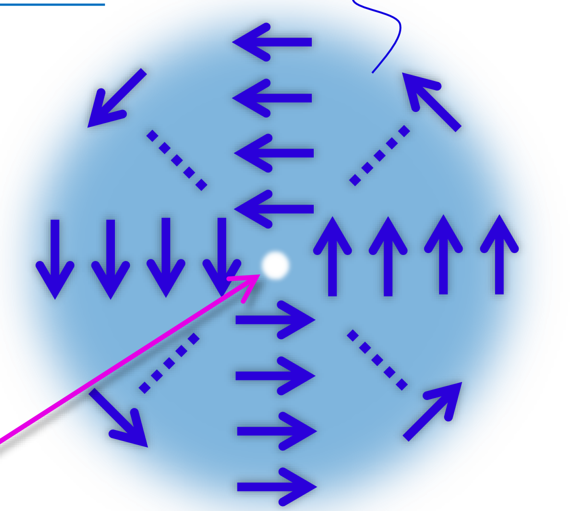
$$\kappa = \oint_C \boldsymbol{v}_s \cdot d\boldsymbol{l} = \frac{\hbar}{m}\oint_C \nabla\phi\cdot d\boldsymbol{l} = \frac{\hbar}{m}2\pi n$$

Quantization of circulation

*the phase $\phi(\boldsymbol{r})$ at the same point must be equivalent!

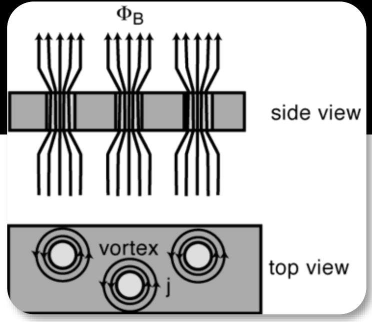
Flow velocity of rotation shall be quantized!

Superfluid



A hole at which superfluidity is lost

Quantum vortex



In superconductor, magnetic flux is quantized!

Magnetic flux:

Meissner effect

$$\Phi = \int_S \boldsymbol{B}\cdot d\boldsymbol{S} = \int_S (\nabla\times\boldsymbol{A})\cdot d\boldsymbol{S} = 0$$

$$\boldsymbol{j}_s = -\frac{n_s e_s^2}{m_s}\boldsymbol{A} + \frac{n_s e_s \hbar}{m_s}\nabla\phi$$: the London equation

If there is a defect:

$$\Phi = \oint_C \boldsymbol{A}\cdot d\boldsymbol{l} \approx \frac{\hbar}{e_s}\oint_C \nabla\phi\cdot d\boldsymbol{l} = \frac{\hbar}{e_s}2\pi n$$

n_s, m_s, e_s: density, mass, and charge of a carrier (Cooper pair)

Quantization of magnetic flux (fluxtube, fluxoid, or fluxon)

Circulation:

$$\kappa = \int_S (\nabla\times\boldsymbol{v}_s)\cdot d\boldsymbol{S} = 0$$

*Unless, there is no topological defect

If there is a defect:

$$\kappa = \oint_C \boldsymbol{v}_s\cdot d\boldsymbol{l} = \frac{\hbar}{m}\oint_C \nabla\phi\cdot d\boldsymbol{l} = \frac{\hbar}{m}2\pi n$$

Quantization of circulation

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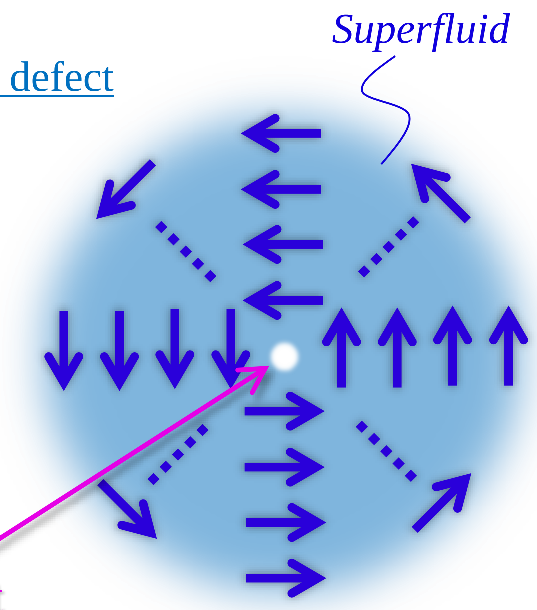


A hole at which superfluidity is lost

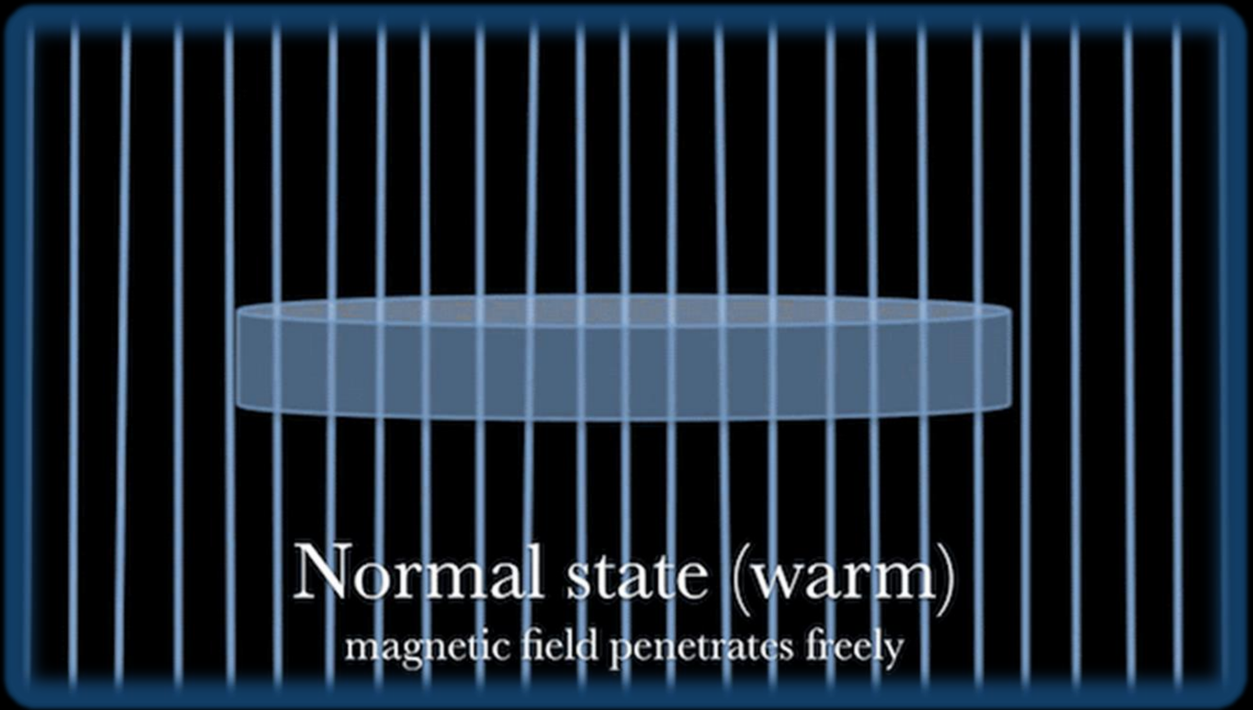
Quantum vortex

Comment on flux tube generation in neutron stars

Supernova

A hot, "proto" neutron star resides as a remnant.

It would cool down form $T > T_c$ to below T_c :



A similar situation should have happened inside the neutron star core!

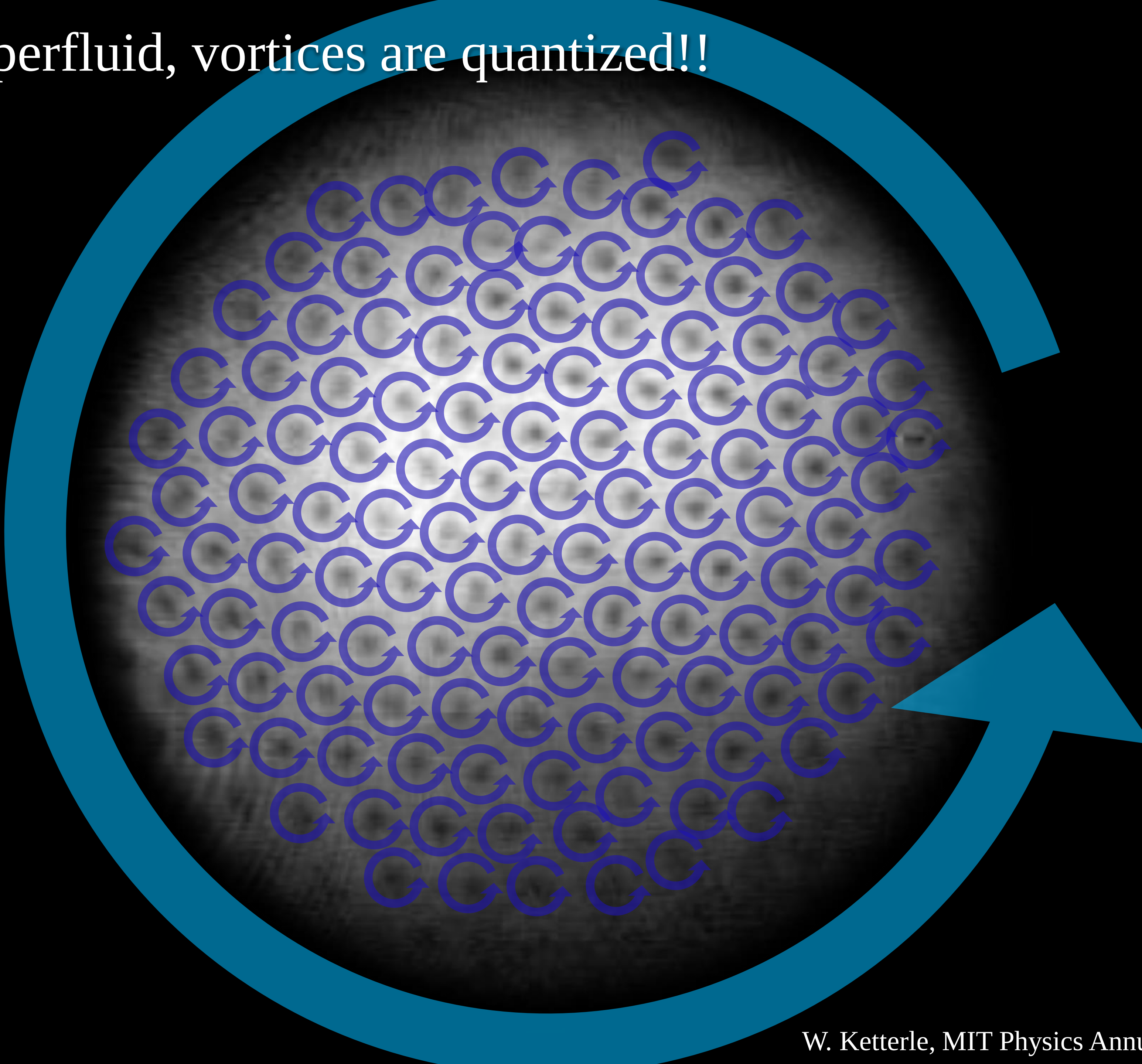
***Protons** are supposed to be **type-II superconductor** via $^1S_0$ pairing inside the neutron-star core.

Animation: https://i.imgur.com/gROHZnG.gifv

Supernova: https://www.forbes.com/sites/jamiecartereurope/2021/09/15/a-zombie-supernova-that-stunned-stargazers-in-the-year-1181-has-finally-been-found-welcome-to-parkers-star/

In daily life, a vortex is continuous..

In superfluid, vortices are quantized!!



W. Ketterle, MIT Physics Annual. 2001

G.P. Bewley, D.P. Lathrop, and K.R. Sreenivasan, Nature **441**, 588 (2006)

A movie from a talk by W. Guo (available from https://youtu.be/P2ckefSAN20) at
INT Program 19-1a “Quantum Turbulence: Cold Atoms, Heavy Ions, and Neutron Stars”
March 18 - April 19, 2019

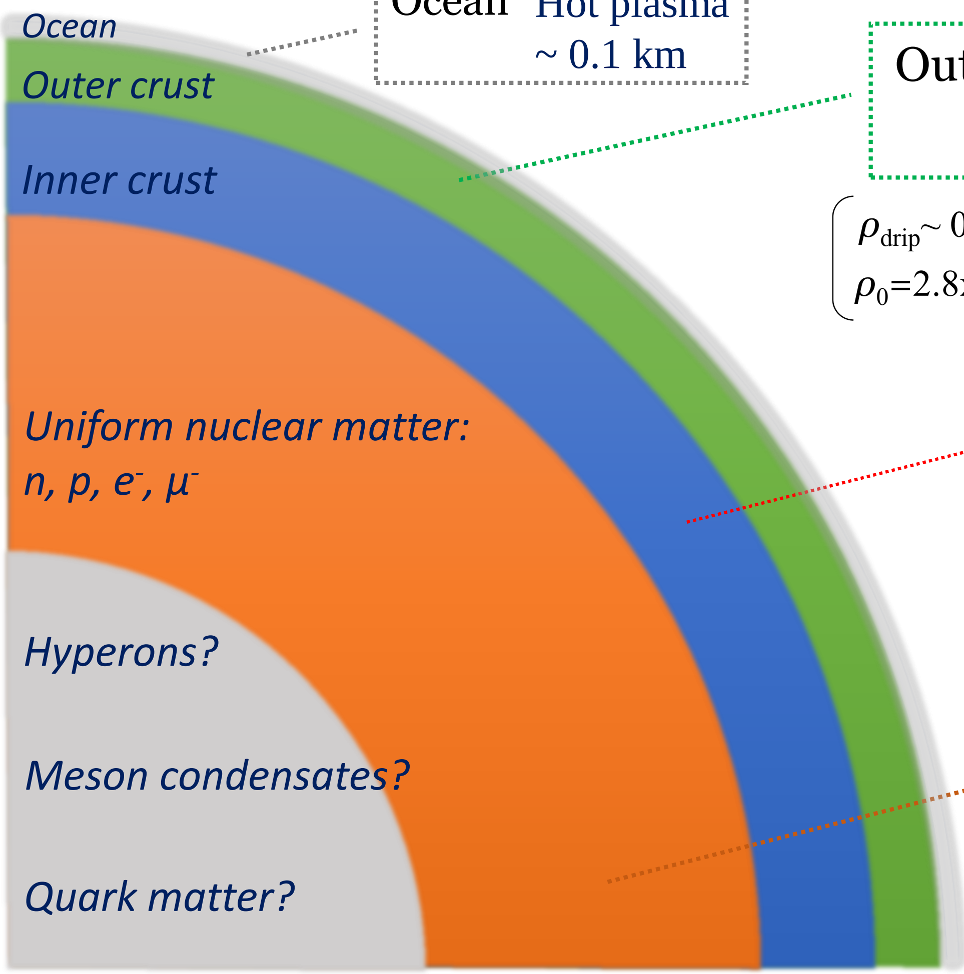
Direct visualization of quantized vortices

Hydrogen particles were trapped in the vortex core, then worked as a tracer

Structure of a neutron star

Neutron star is a great playground for nuclear physicists

✓ **It offers extreme situations which can not be realized in terrestrial experiments!**



Ocean Hot plasma
~ 0.1 km

Outer crust Nuclei (Z=26-42), electrons
0.3-0.6 km $\rho < \rho_{\mathrm{drip}}$

$\rho_{\mathrm{drip}} \sim 0.0014\rho_0$; Above ρ_{drip} unbound neutrons exist outside nuclei
$\rho_0 = 2.8\times10^{14}$ g/cm^3 = 0.16 fm^{-3} ; Nuclear saturation density

Inner crust Nuclei, electrons, "dripped" neutrons
0.5-0.8 km $\rho_{\mathrm{drip}} \le \rho \le 0.6\rho_0$

Outer/inner core
9-12 km $0.6\rho_0 < \rho \le 3\text{-}5\rho_0$

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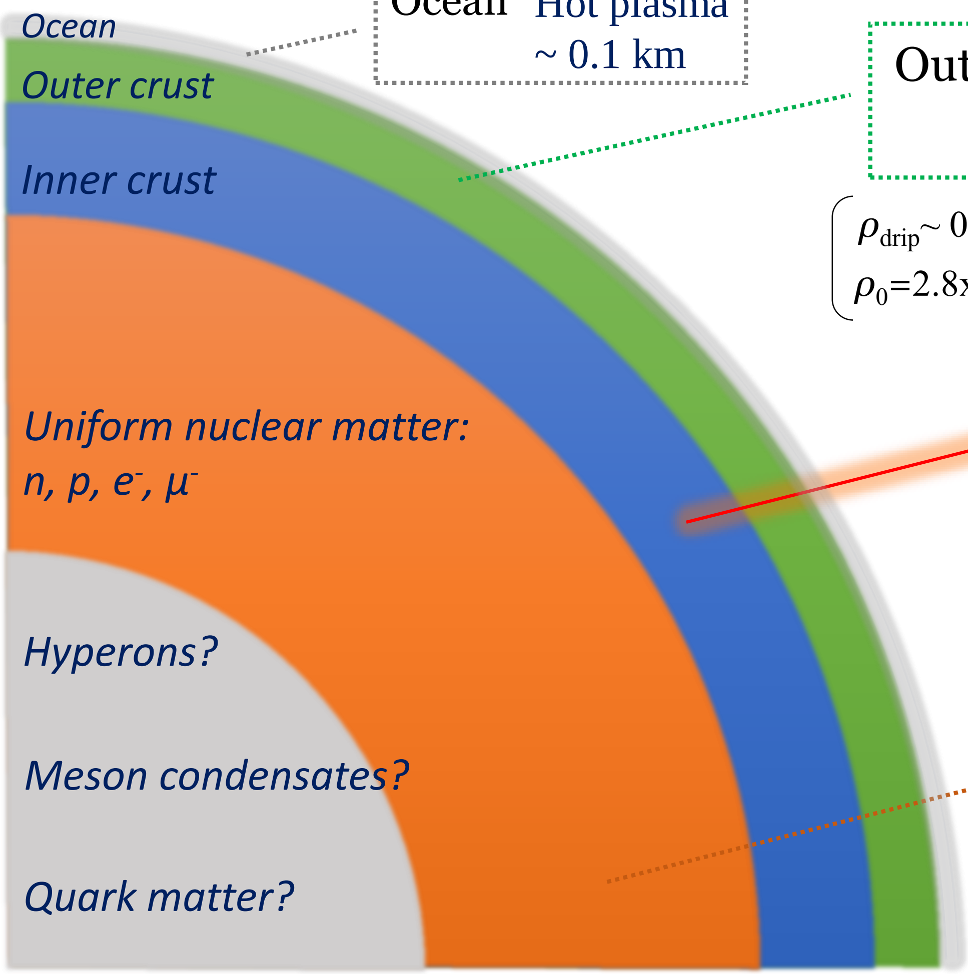

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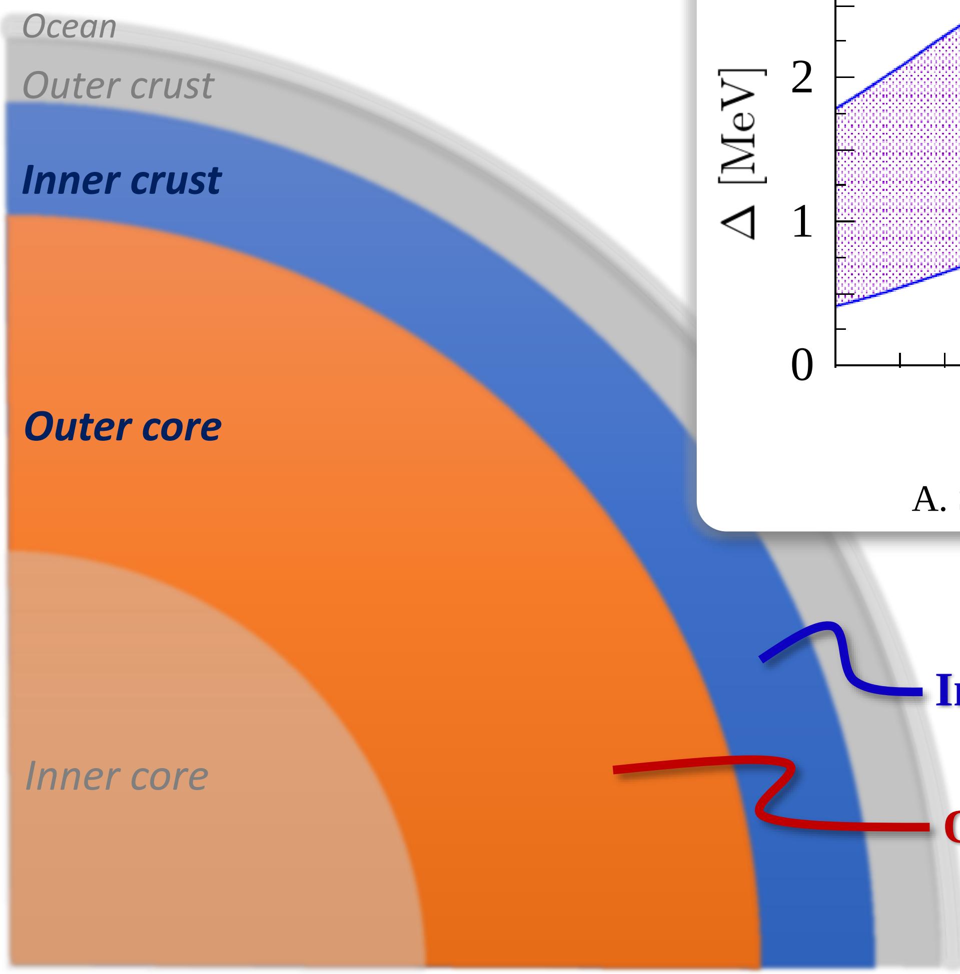
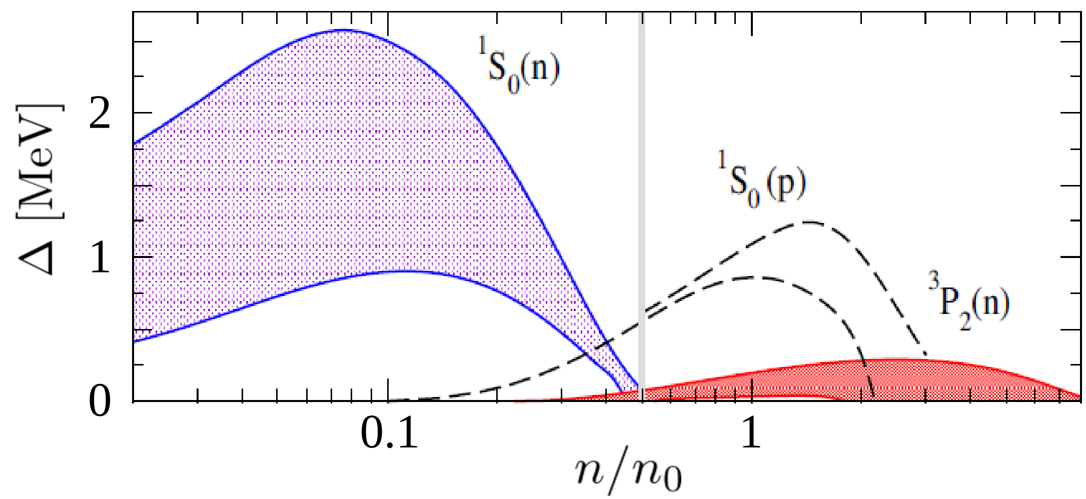
$T < T_c \sim 10^{10}\,\mathrm{K} \quad B < B_c \sim 10^{17}\,\mathrm{G}$

Neutrons (protons) are superfluid (superconducting) in neutron stars!





A. Sedrakian and J.W. Clark, Eur. Phys. J. A **55**, 167 (2019)

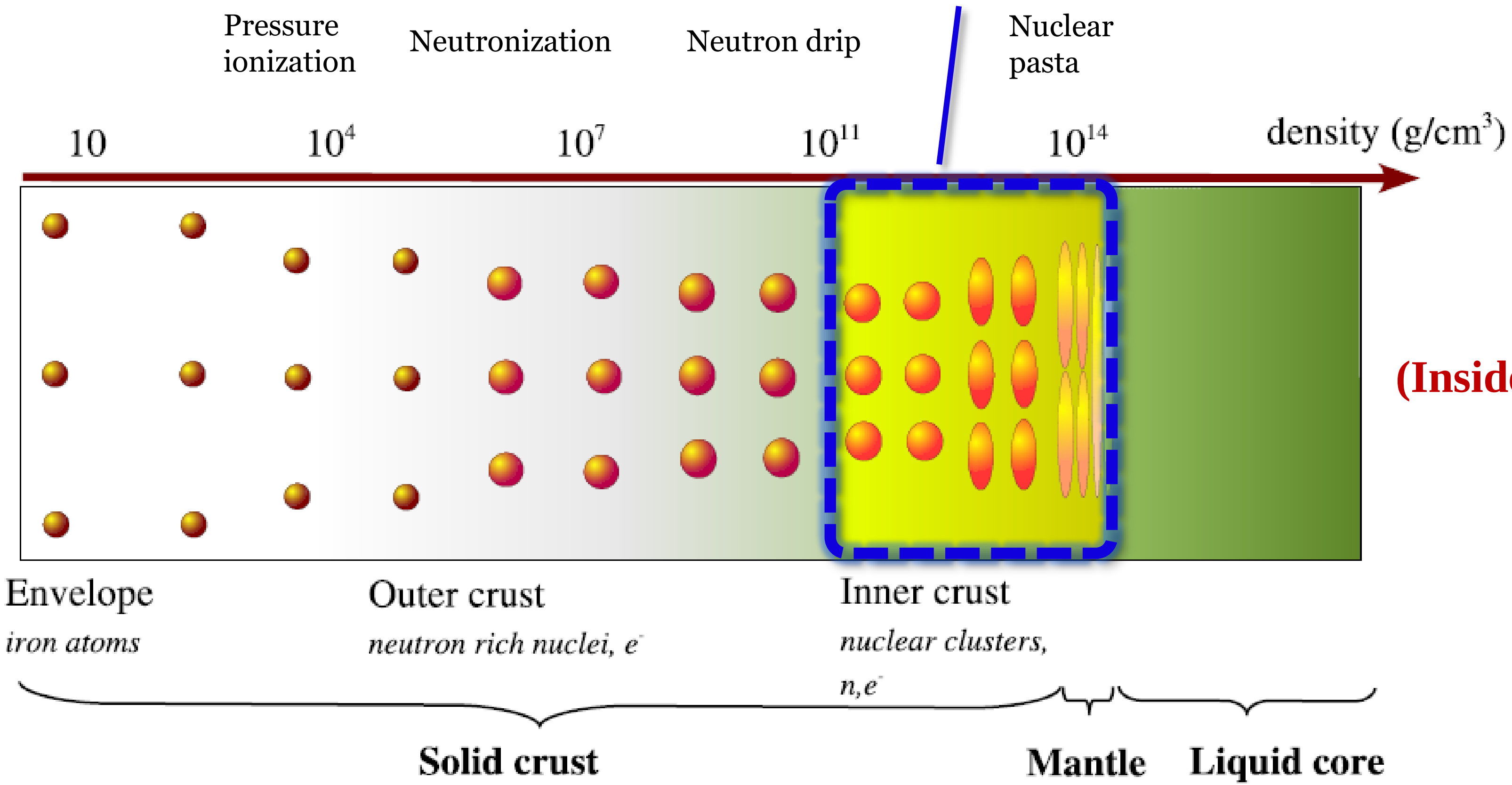
Inner crust: S-wave neutron superfluid

Outer core: S-wave proton superconductor (+ P-wave neutron superfluid)

A lattice of neutron-rich nuclei are immersed in a neutron superfluid

Quantum vortices can exist!

(Outside)



(Inside)

Fig.4 in N. Chamel and P. Haensel, Living Rev. Relativity **11**, 10 (2008)

Quantum vortices in a neutron star

In rotating superfluid, an array of quantum vortices is generated

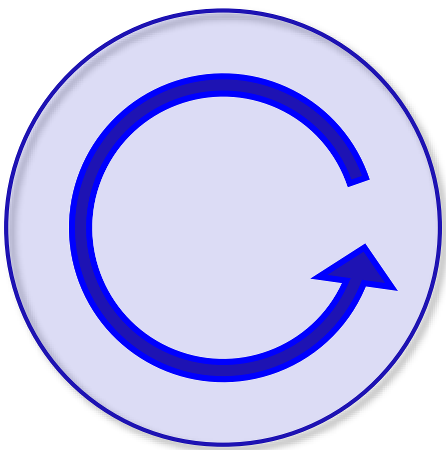
- Observation in ultra-cold atomic gases

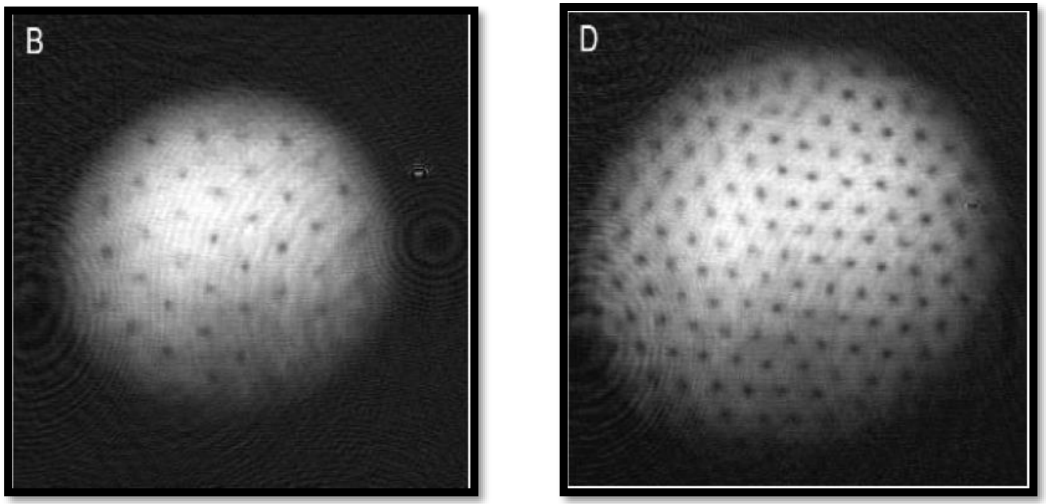
Vortex-number density

$\propto$

Rotation speed

Low ⟷ High





W. Ketterle, MIT Physics Annual. 2001

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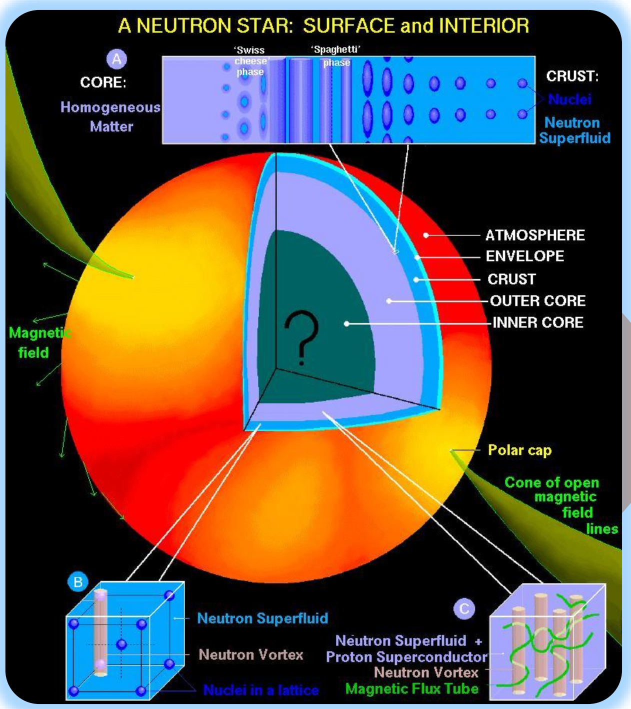

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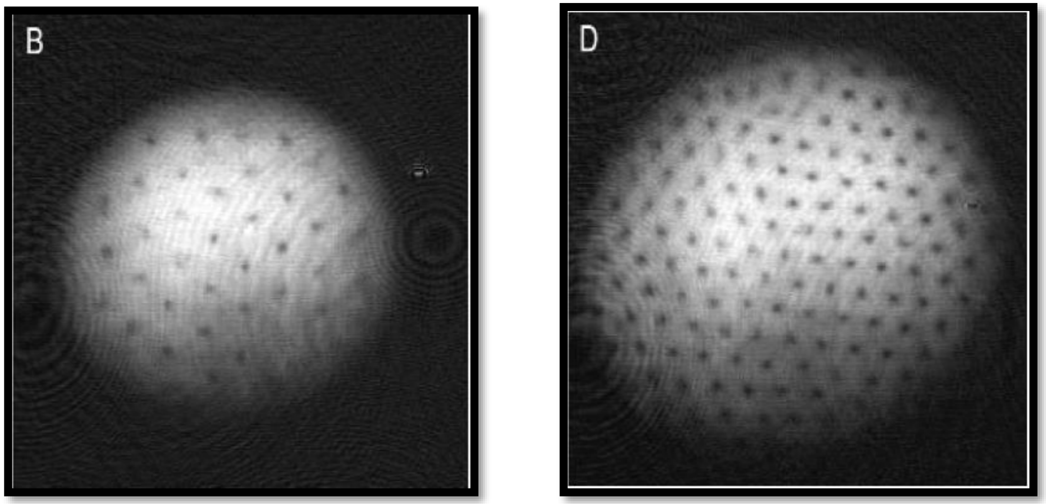
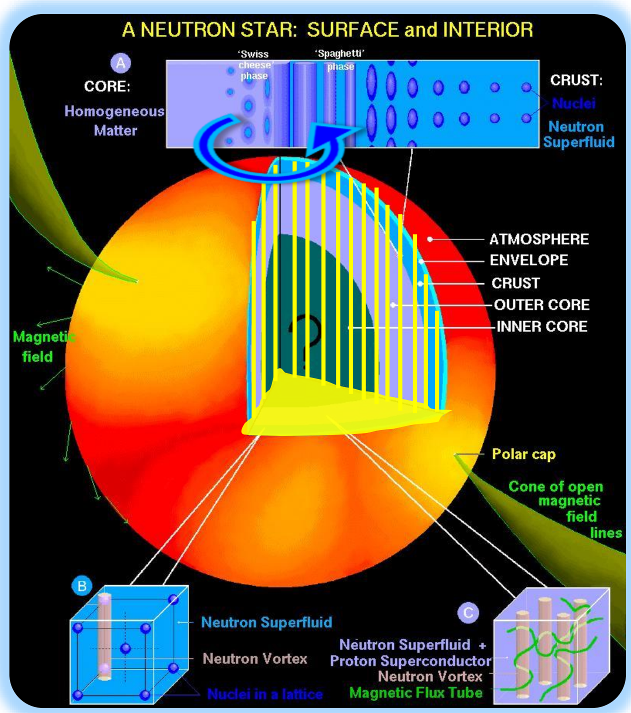


W. Ketterle, MIT Physics Annual. 2001

There must be a huge number (~10^{18}) of vortices inside a neutron star!!



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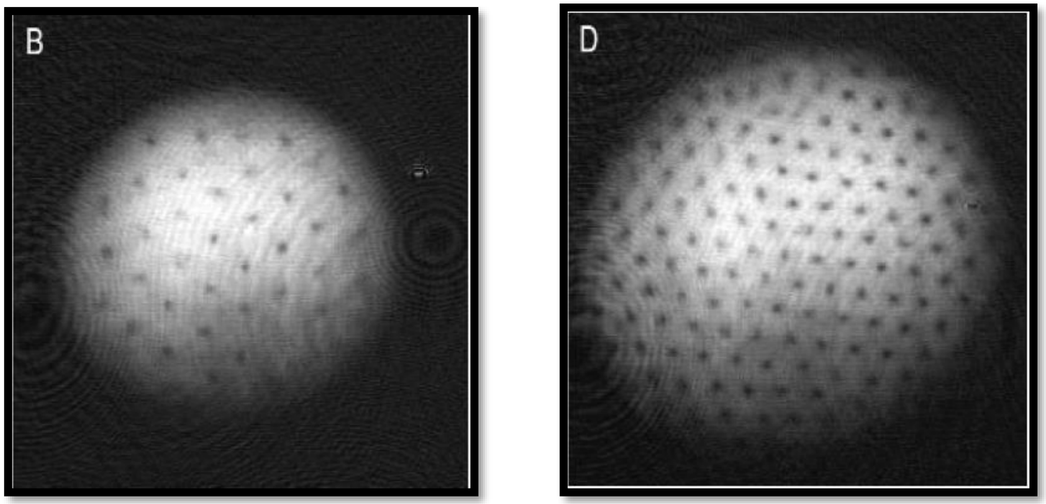
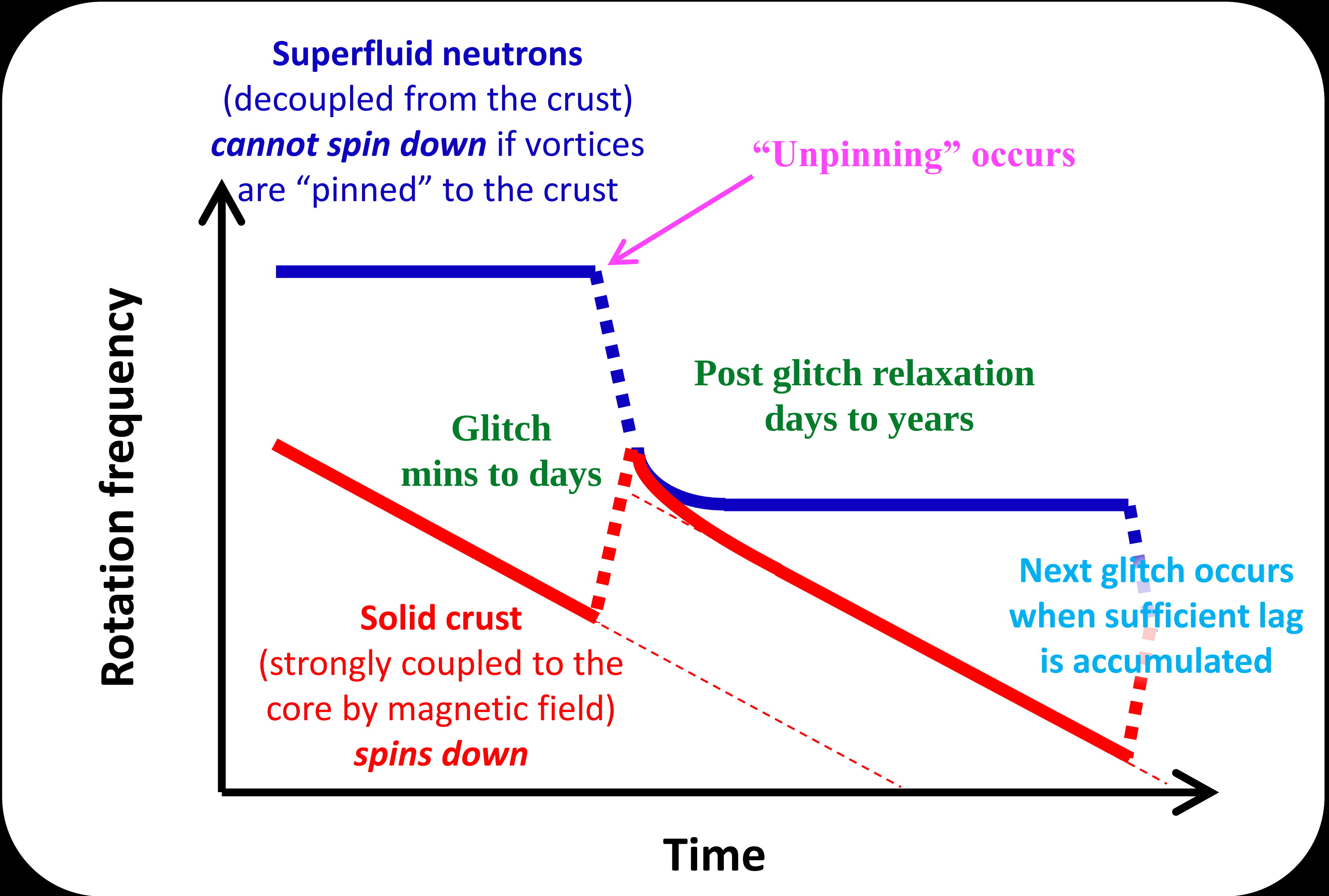


W. Ketterle, MIT Physics Annual. 2001

The vortex mediated glitch: Naive picture



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: 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)

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

$$h_\sigma = \frac{\delta E}{\delta n_\sigma} \quad : \text{ s.p. Hamiltonian}$$

$$\Delta = -\frac{\delta E}{\delta \nu^*} \quad : \text{ pairing field}$$

$$n_\sigma(\boldsymbol{r},t) = \sum_{E_k<E_c} |v_{k,\sigma}(\boldsymbol{r},t)|^2 \quad : \text{ number density}$$

$$\nu(\boldsymbol{r},t) = \sum_{E_k<E_c} u_{k,\uparrow}(\boldsymbol{r},t)v^*_{k,\downarrow}(\boldsymbol{r},t) \quad : \text{ anomalous density}$$

$$\boldsymbol{j}_\sigma(\boldsymbol{r},t) = \hbar\sum_{E_k<E_c} \mathrm{Im}[v^*_{k,\sigma}(\boldsymbol{r},t)\boldsymbol{\nabla} v_{k,\sigma}(\boldsymbol{r},t)] \quad : \text{ current}$$

A large number (10^4-10^6) of 3D coupled non-linear PDEs have to be solved!!

# of qp orbitals ~ # of grid points

TDSLDA (Time-Dependent Superfluid Local Density Approximation)

TDSLDA: TDDFT with local treatment of pairing

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Supercomputing!!

$$h_\sigma = \frac{\delta E}{\delta n_\sigma}$$: s.p. Hamiltonian

$$\Delta = -\frac{\delta E}{\delta \nu^*}$$: pairing field

$$n_\sigma(\boldsymbol{r},t) = \sum_{E_k<E_c} |v_{k,\sigma}(\boldsymbol{r},t)|^2$$: number density

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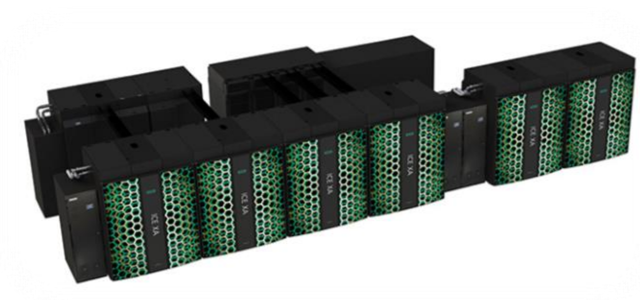
# of qp orbitals ~ # of grid points

*The number indicates the rank according to the TOP500 list (June 2022)

Piz Daint, CSCS, Switzerland (No. 23)

TITAN, ORNL, USA

TSUBAME3.0, Japan (No. 64)



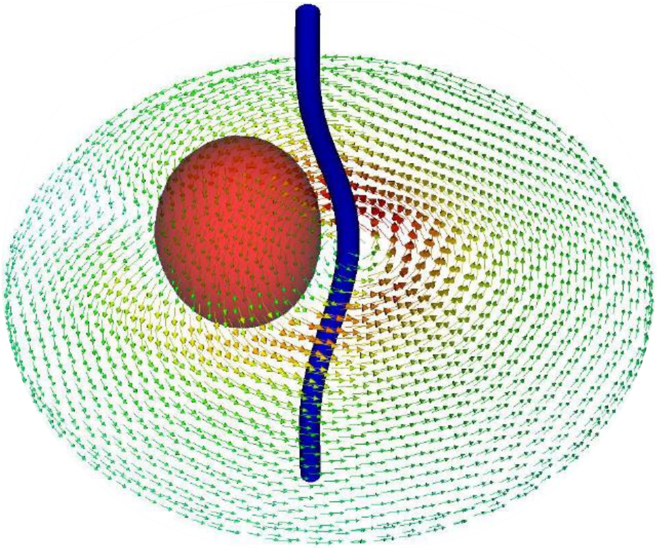
Summit, ORNL, USA (No. 4)
GPU, 200 PFlops/s

GPU machines within Nos. 1-20

No.4: Summit, ORNL, USA
No.5: Sierra, LLNL, USA
No.7: Perlmutter, NERSC, USA
No.8: Selene, NVIDIA Co., USA
No.11: JUWELS Booster Module, FZJ, Germany
No.12: HPC5, Eni S. p. A., Italy
No.13: Voyager-EUS2, Azure East US 2, USA
No.14: Polaris, ANL, USA
No.15: SSC-21, Samsung Electronics, South Korea
No.18: Damman-7, Saudi Aramco, Saudi Arabia
No.19: ABCI 2.0, AIST, Japan

Certainly, GPU is competing with CPU machines!!

Vortex-nucleus dynamics within TDSLDA



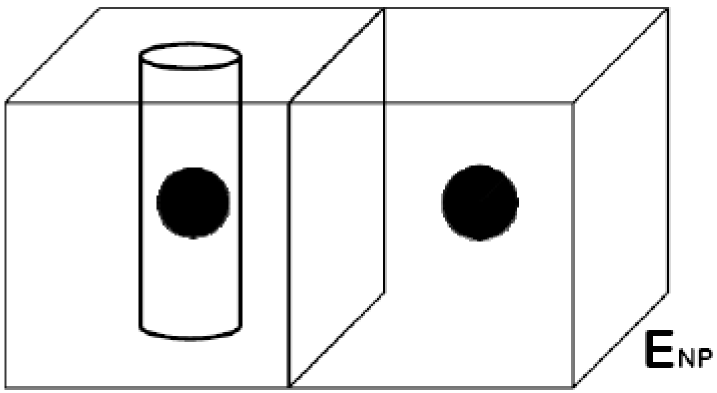
G. Wlazłowski, K. Sekizawa, P. Magierski, A. Bulgac, and M.M. Forbes,
Phys. Rev. Lett. **117**, 232701 (2016)

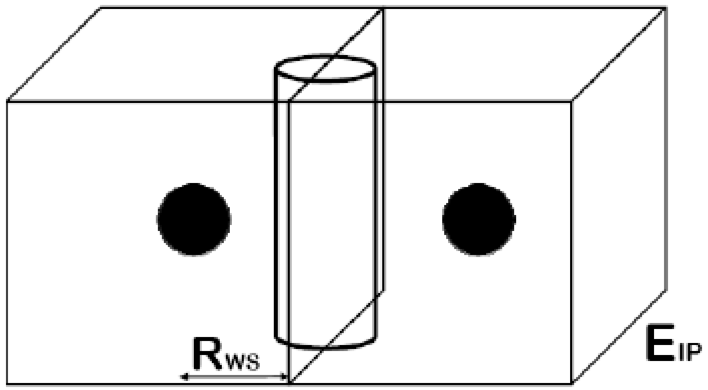
A key to understand the glitches is:

Vortex pinning mechanism in the inner crust of neutron stars

Q. Is the vortex-nucleus interaction

Attractive? or Repulsive?





"Nuclear pinning"

"Interstitial pinning"

We performed 3D, dynamical simulations by TDDFT with superfluidity

TDSLDA equations (or TDHFB, TD-BdG)

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Computational details

$75 \text{ fm} \times 75 \text{ fm} \times 60 \text{ fm}$

$(50 \times 50 \times 40,\ \Delta x = 1.5 \text{ fm})$

$k_c = \pi/\Delta x > k_F \qquad k_F = (3\pi^2 \rho_n)^{1/3}$

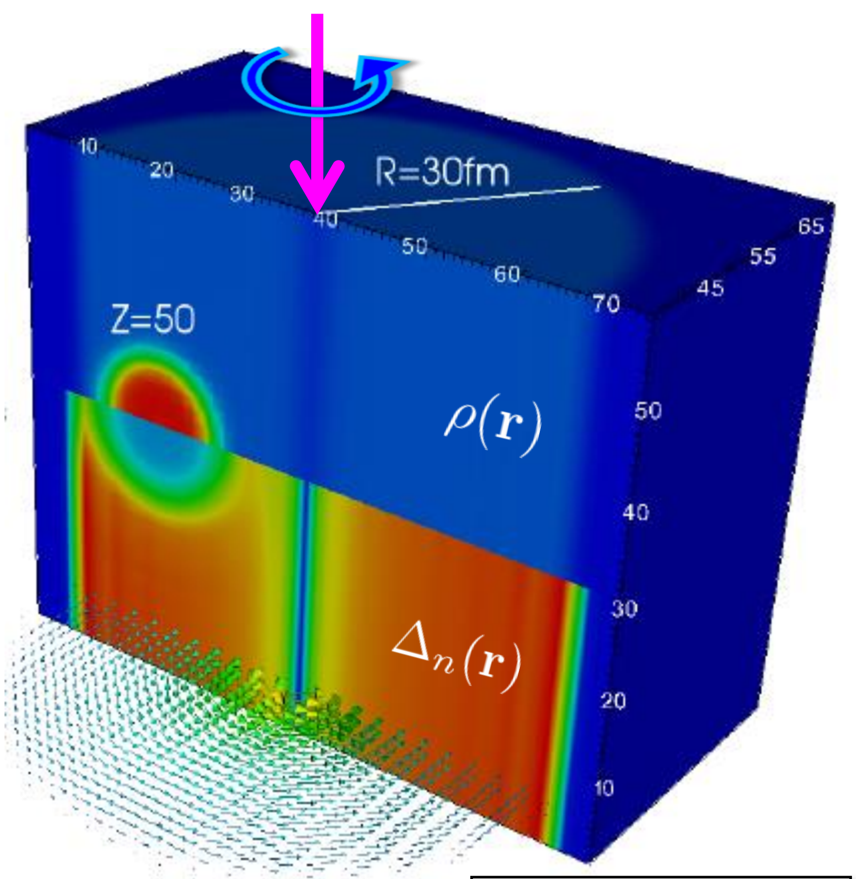
Nuclear impurity: $Z = 50$

$\rho_n \simeq 0.014 \text{ fm}^{-3}$ $(N \simeq 2{,}530)$

$\rho_n \simeq 0.031 \text{ fm}^{-3}$ $(N \simeq 5{,}714)$

# of quasi-particle w.f. $\approx 100,000$

a vertex line exists here



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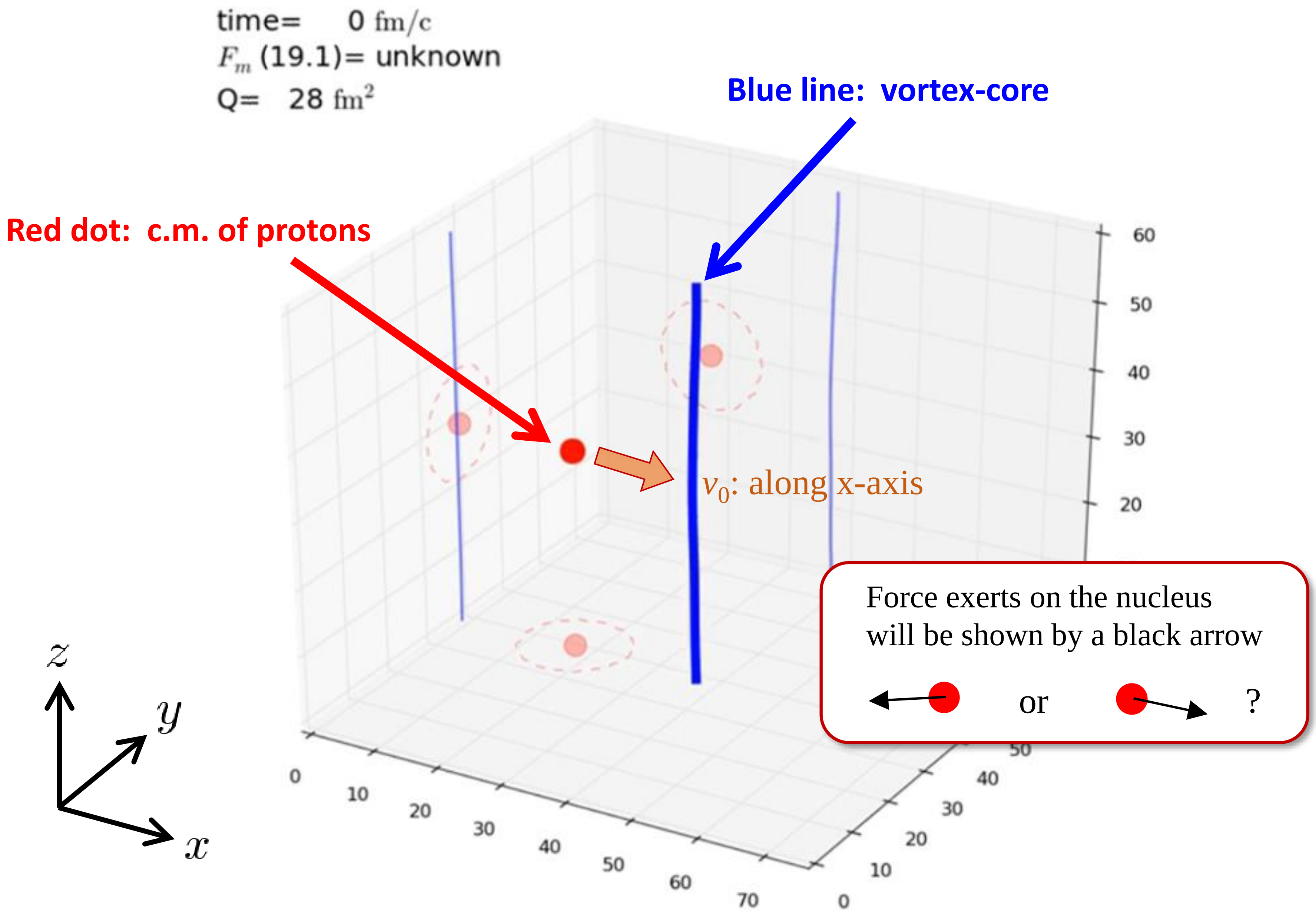
MPI+GPU
→ 48h w/ 200GPUs
for 10,000 fm/c

TITAN, Oak Ridge

NERSC Edison, Berkeley

HA-PACS, Tsukuba

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



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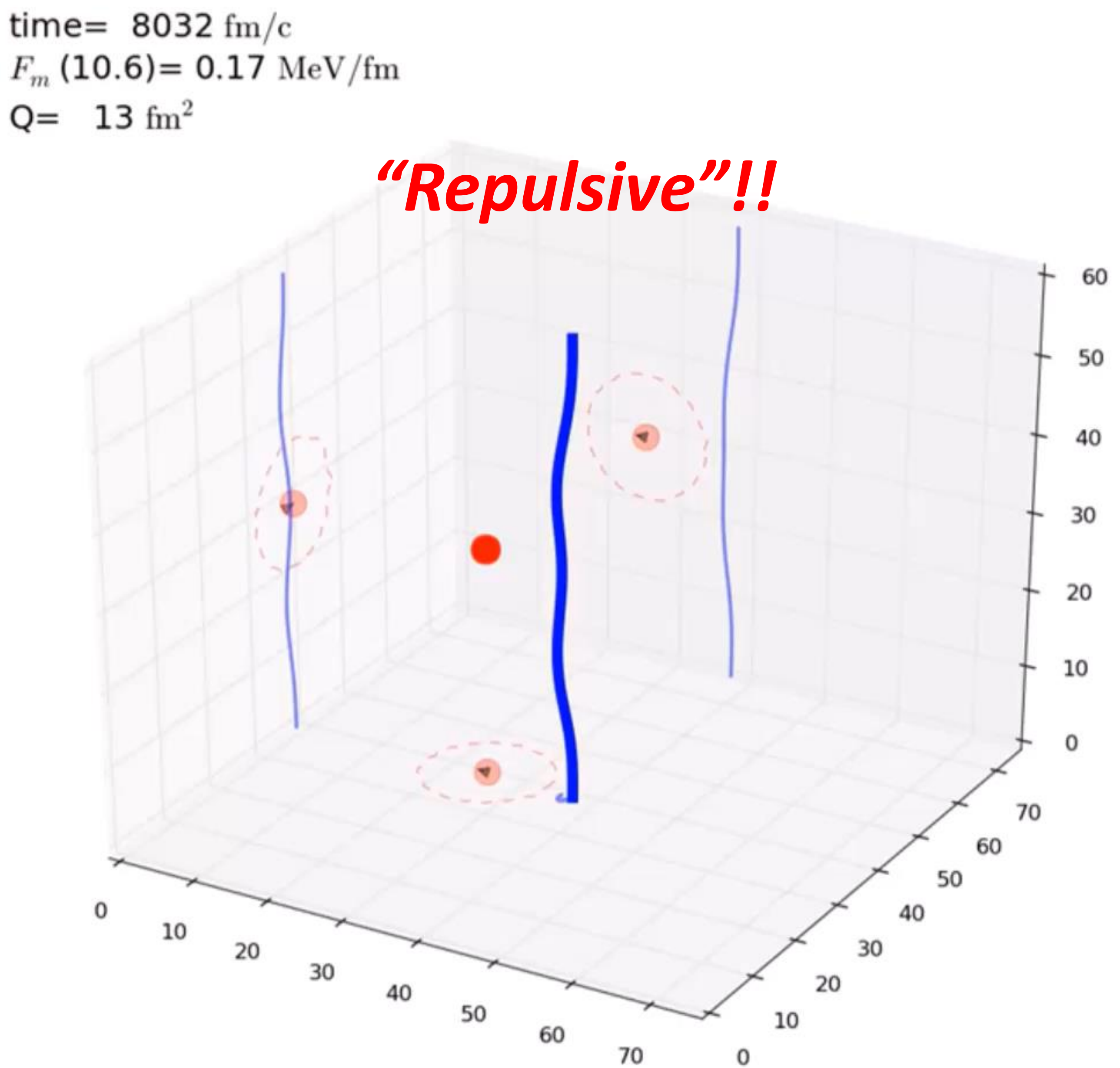

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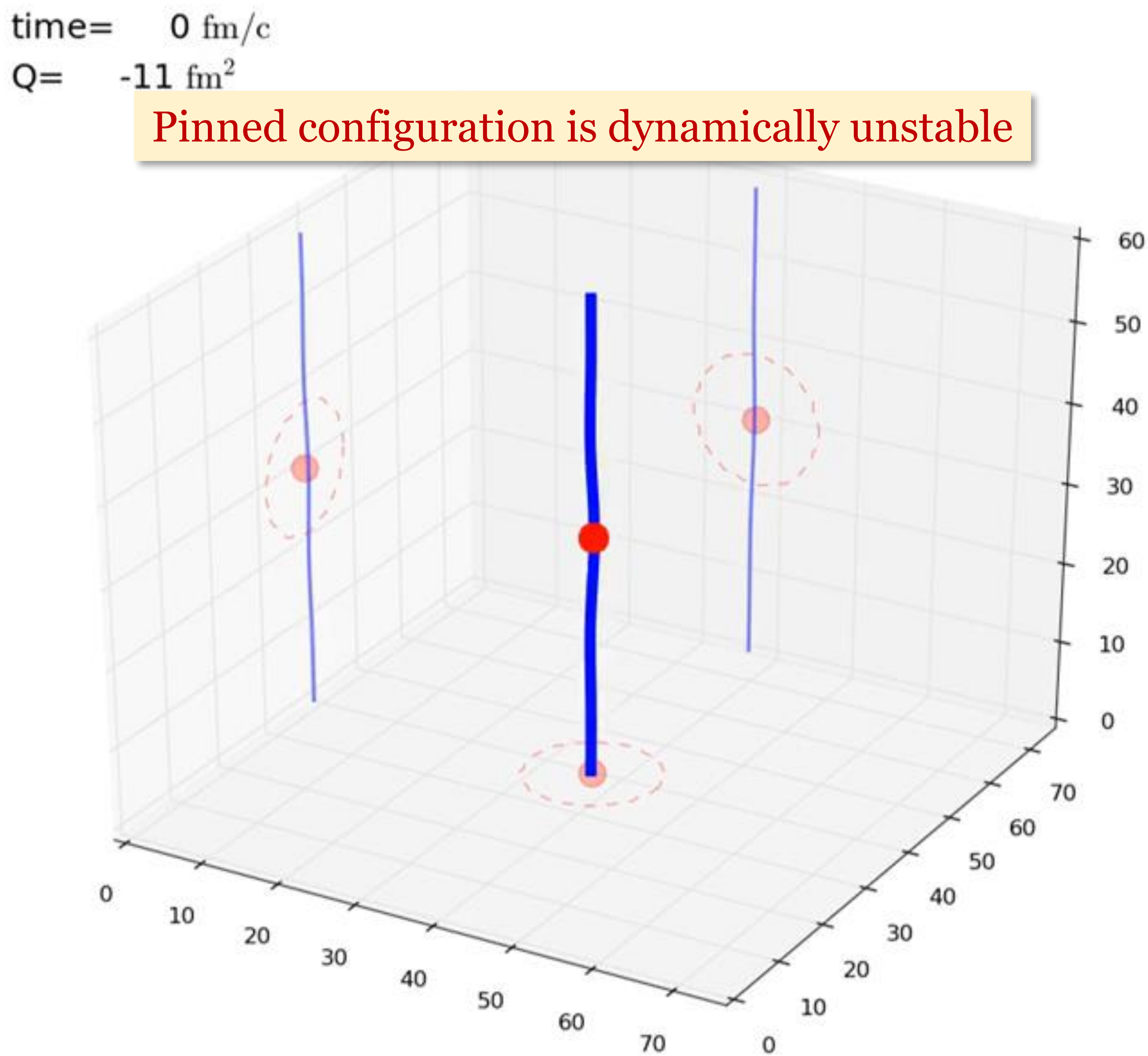
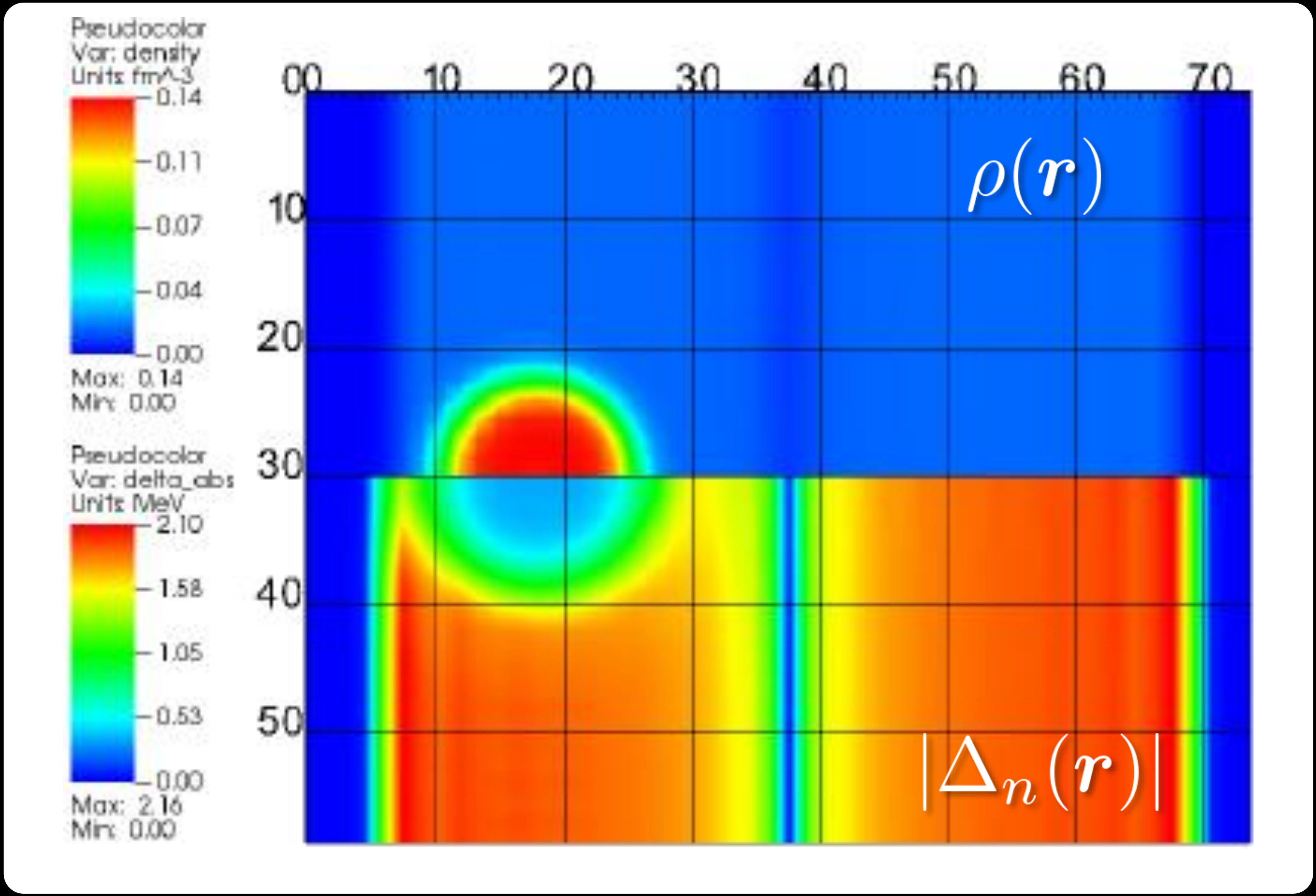
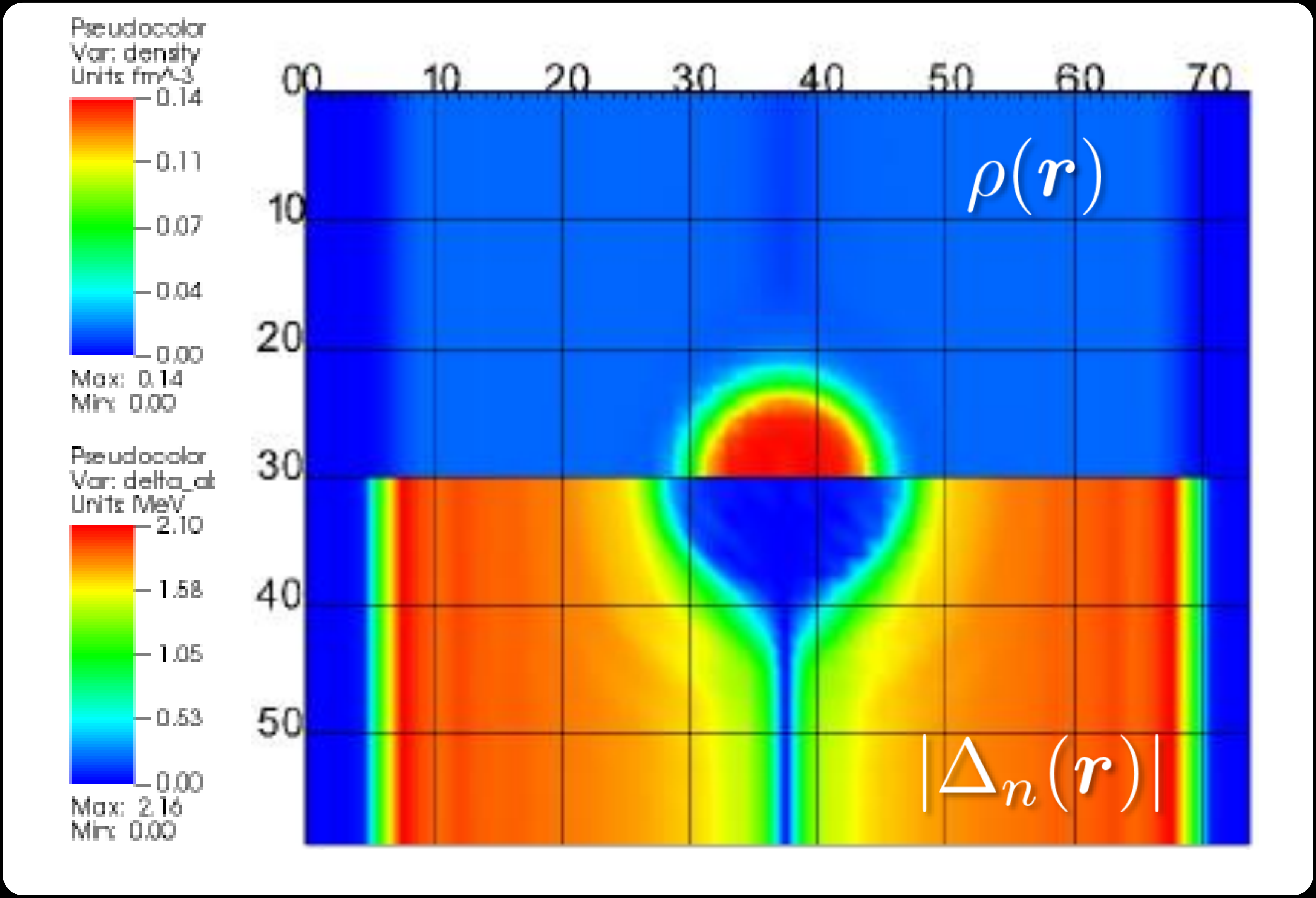


Pinned configuration is dynamically unstable

"Unpinned configuration"

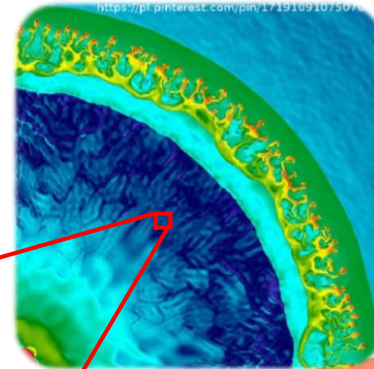


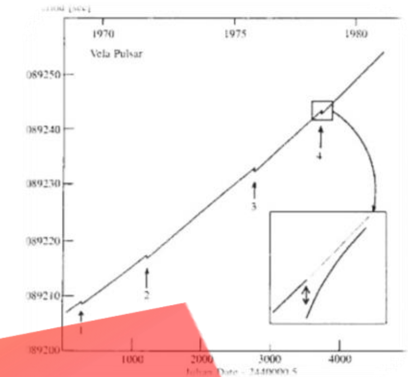
"Pinned configuration"

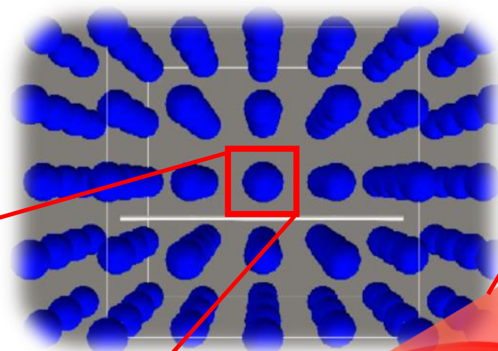


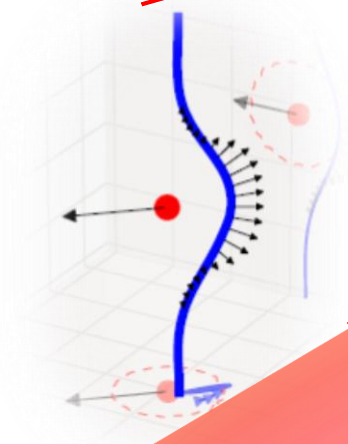
Our goal and strategy

Goal: Unveil the mechanism of glitches









10^{4}m

Macroscopic

- observations
- hydrodynamics

$\sim 10^{-10}$m

Mesoscopic

- dynamics of *vortices* in a lattice of *nuclei* (e.g. filament model)

Provide model ingredients

10^{-15}-10^{-13}m

Microscopic

Nuclear Physics!!

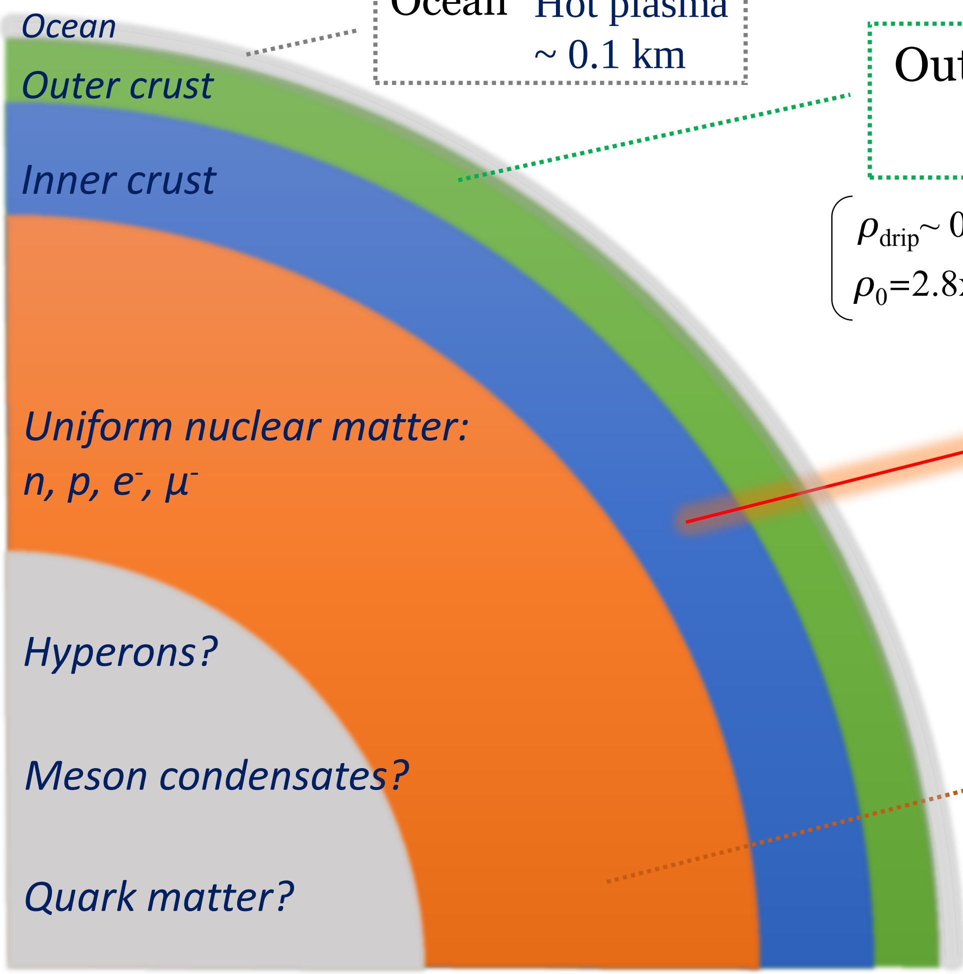
- vortex-nucleus dynamics from *neutrons and protons*

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

https://www.newsweek.com/nuclear-pasta-neutron-star-strongest-material-universe-1127491

Structure of a neutron star

Neutron star is a great playground for nuclear physicists



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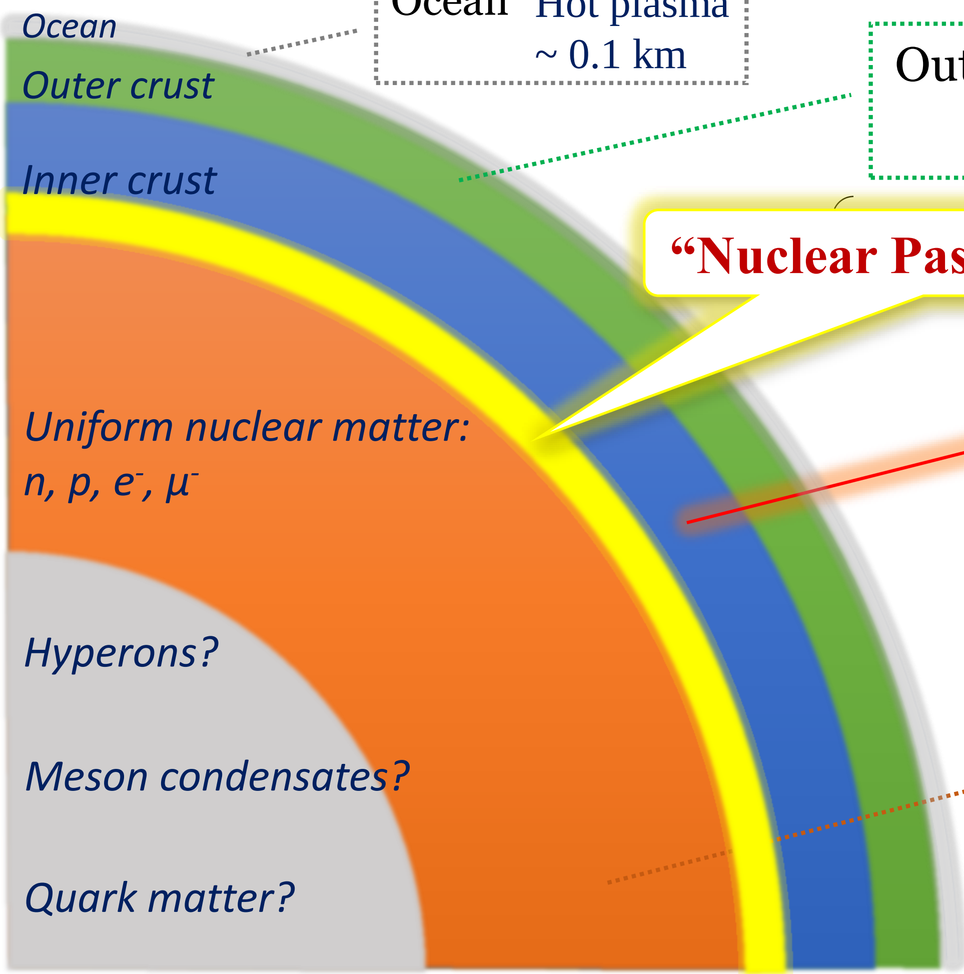

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; Nuclear saturation density

"Nuclear Pasta" may exist!

Inner crust Nuclei, electrons, "dripped" neutrons
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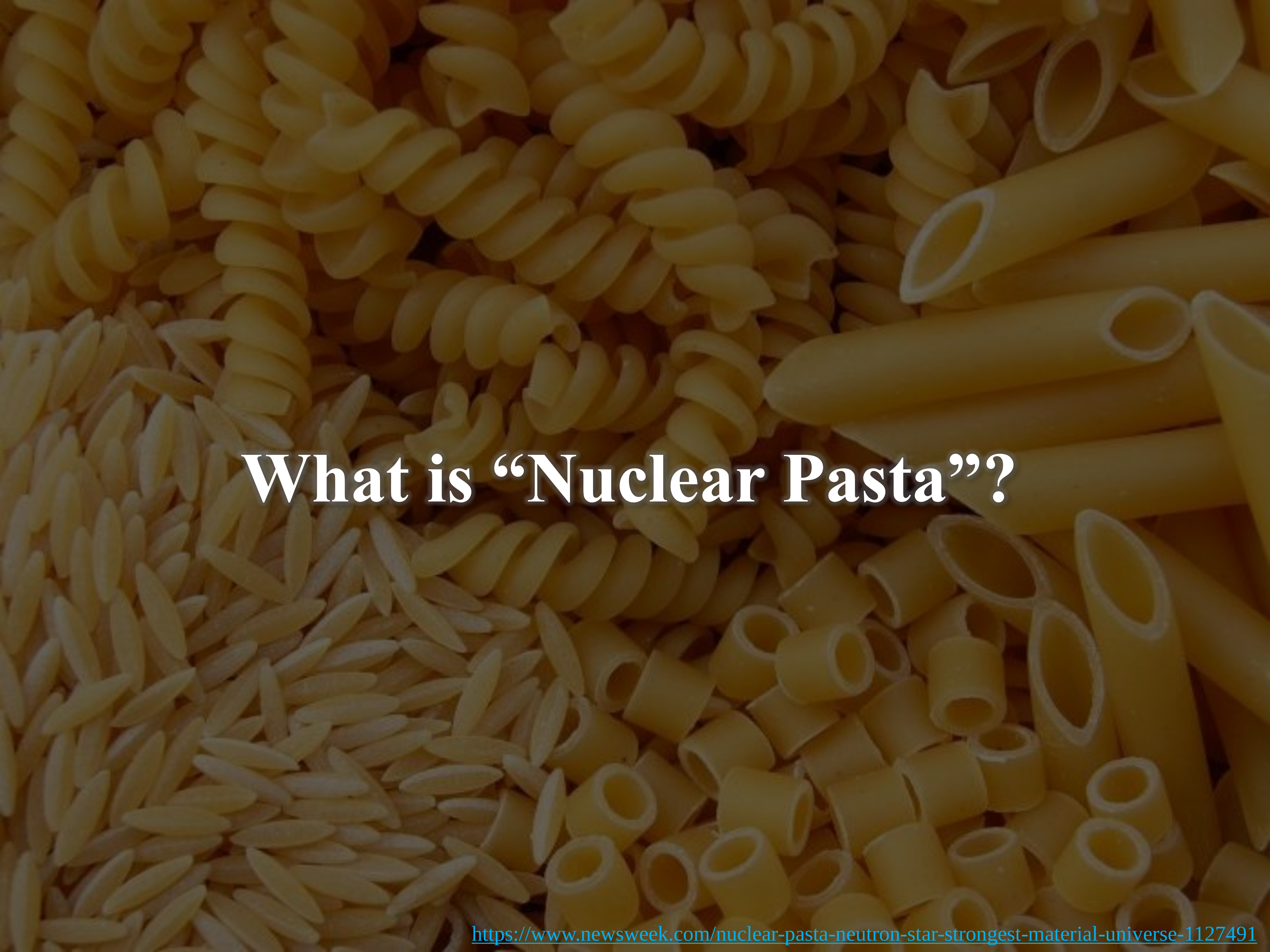
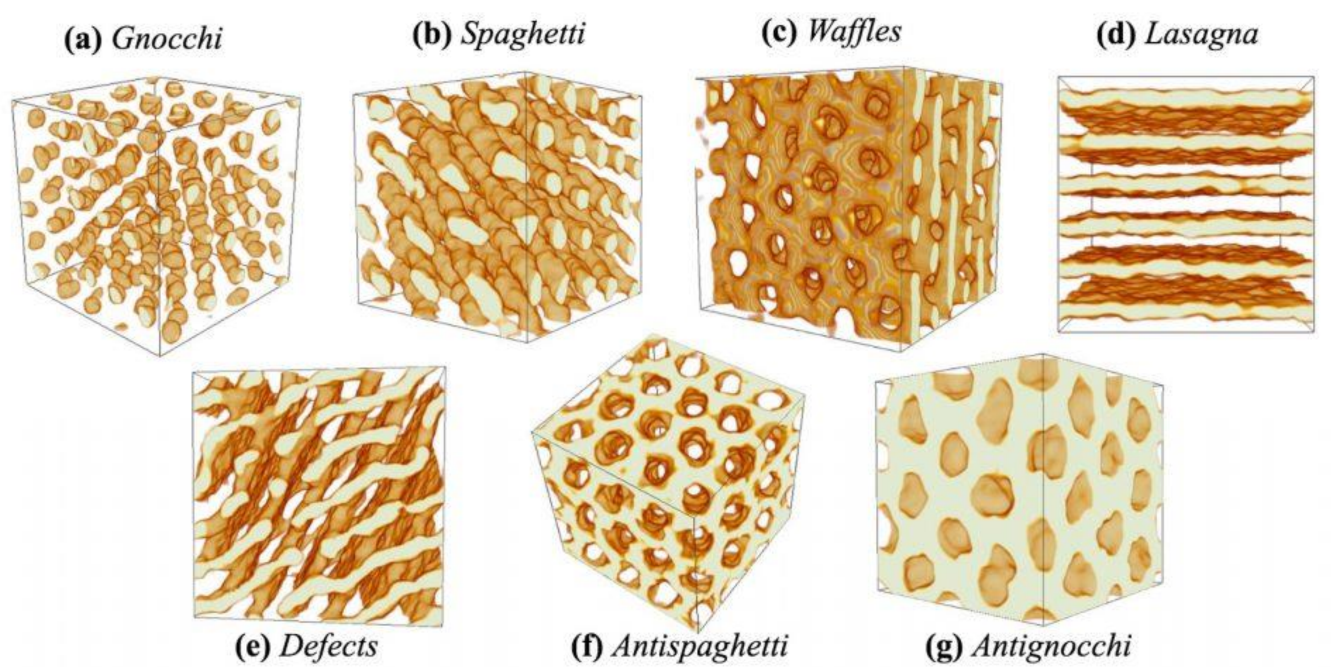
Outer/inner core
9-12 km $0.6\rho_0 < \rho \leq 3\text{-}5\rho_0$



What is “Nuclear Pasta”?

https://www.newsweek.com/nuclear-pasta-neutron-star-strongest-material-universe-1127491

What is Nuclear Pasta?



M. E. Caplan and C. J. Horowitz, Rev. Mod. Phys. **89**, 041002 (2017)

This is 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

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[2]*Nuclear Physics Division, Center for Computational Sciences, University of Tsukuba, Ibaraki 305-8577, Japan*
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[4]*Department 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)

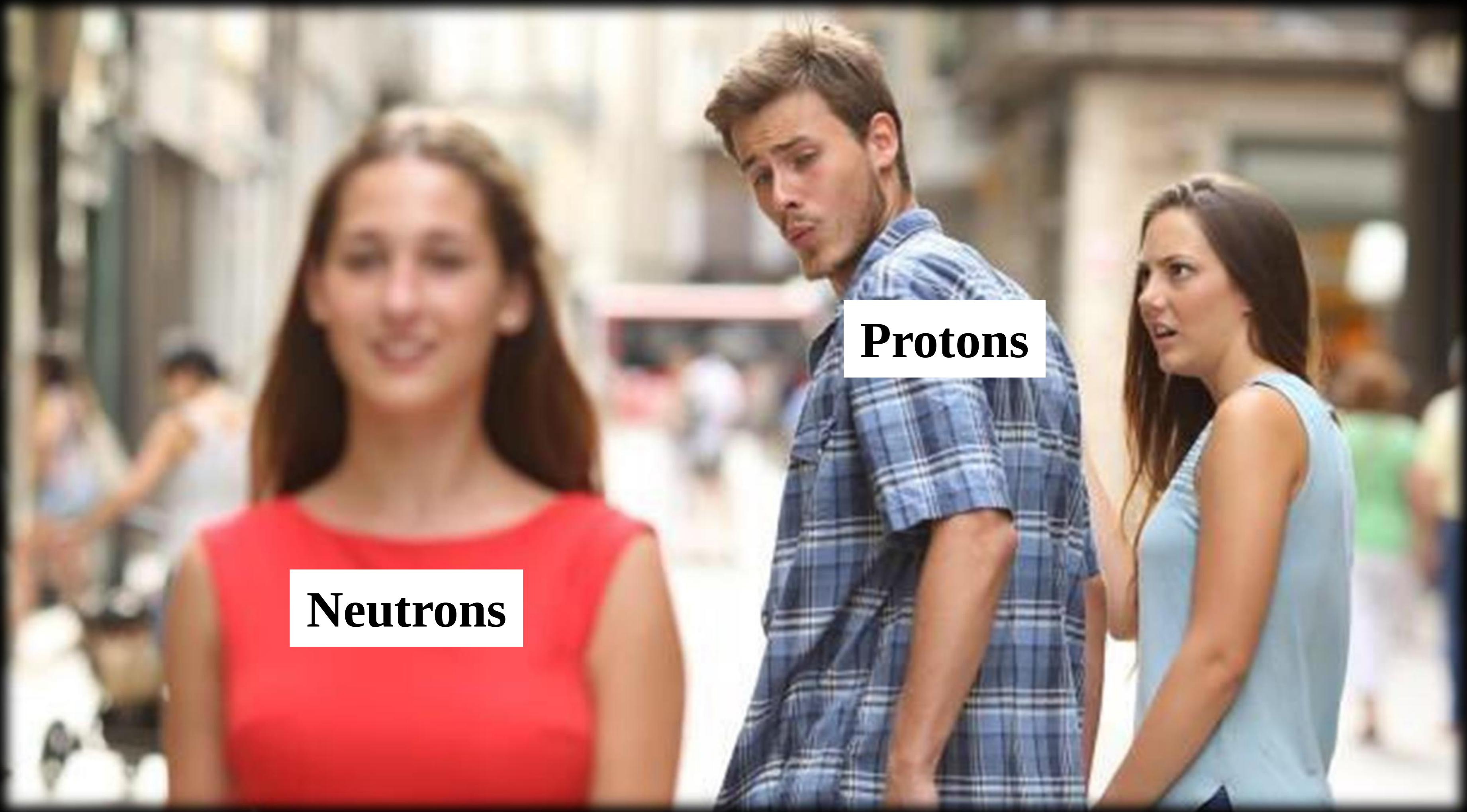
真の強さを学ぶ。
新潟大學
NIIGATA UNIVERSITY

東京工業大学
Tokyo Institute of Technology

Superfluid extension: Dec. 12 (Mon)

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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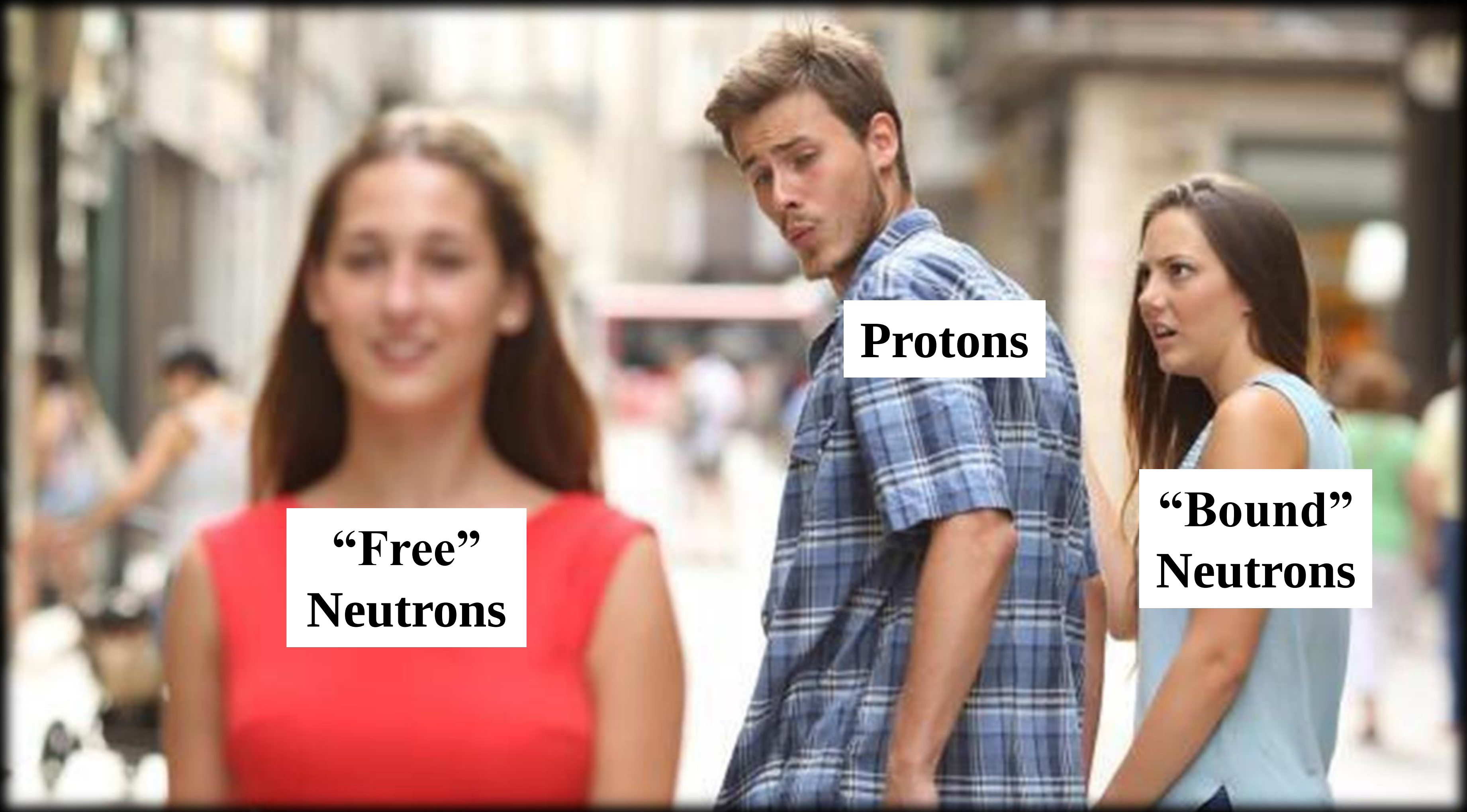


"Entrainment" in the inner crust

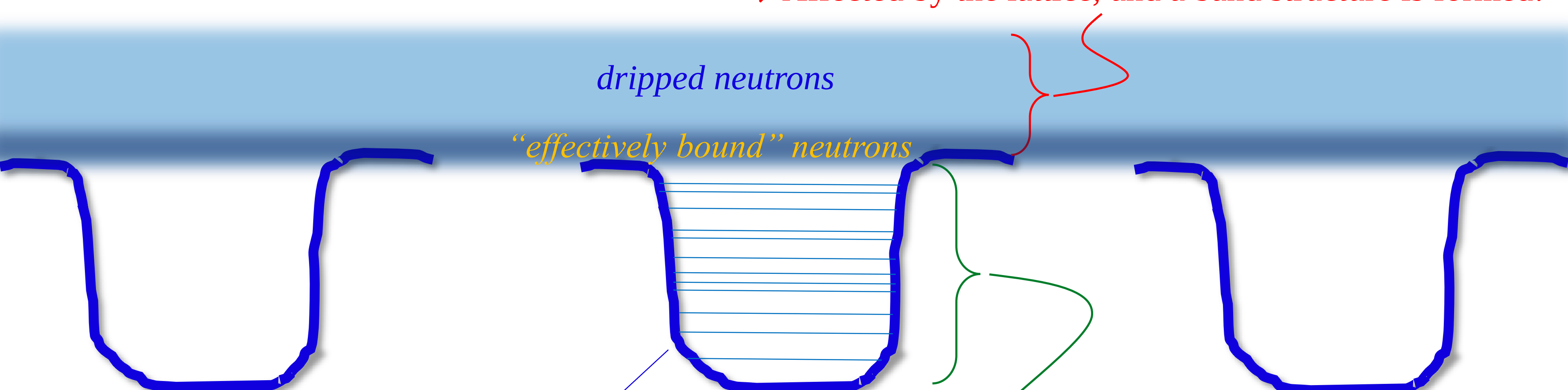
- **Part of dripped neutrons are "effectively bound" (immobilized) by the periodic structure (due to Bragg scatterings), resulting in a larger effective mass**

$$m_{\mathrm{n}} n_{\mathrm{n}}^{\mathrm{f}} = m_{\mathrm{n}}^{\star} n_{\mathrm{n}}^{\mathrm{c}}$$

$n_{\mathrm{n}}^{\mathrm{c}}$: Conduction neutron number density (neutrons that can actually flow)

$m_{\mathrm{n}}^{\star}$: (Macroscopic) Effective mass

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



Potential for neutrons

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

Entrainment leads:
→ reduction of n_c
→ enhancement of m^*

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:

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

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

  N. Chamel, 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:

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

- 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:

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

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

New!

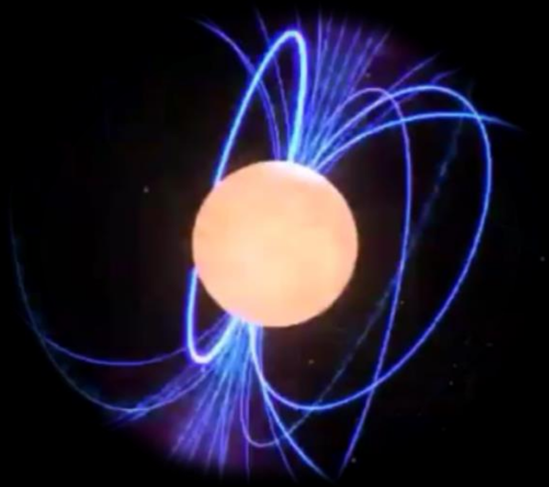
- **Time-dependent extension of the self-consistent band theory (based on TDDFT with a Skyrme EDF)**

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

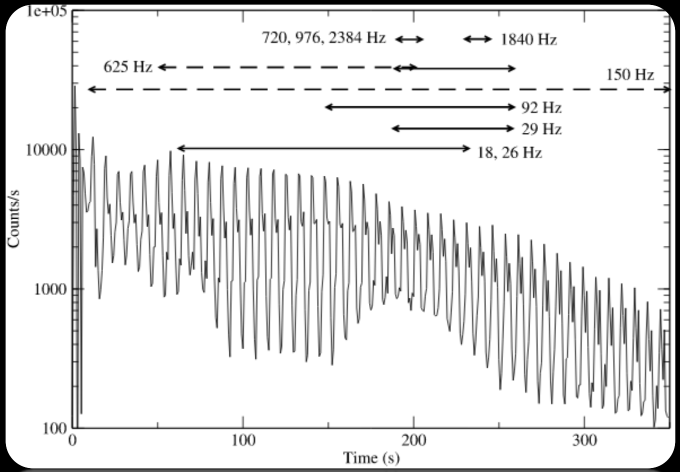
  K. Sekizawa, S. Kobayashi, and M. Matsuo, PRC**105**(2022)045807

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

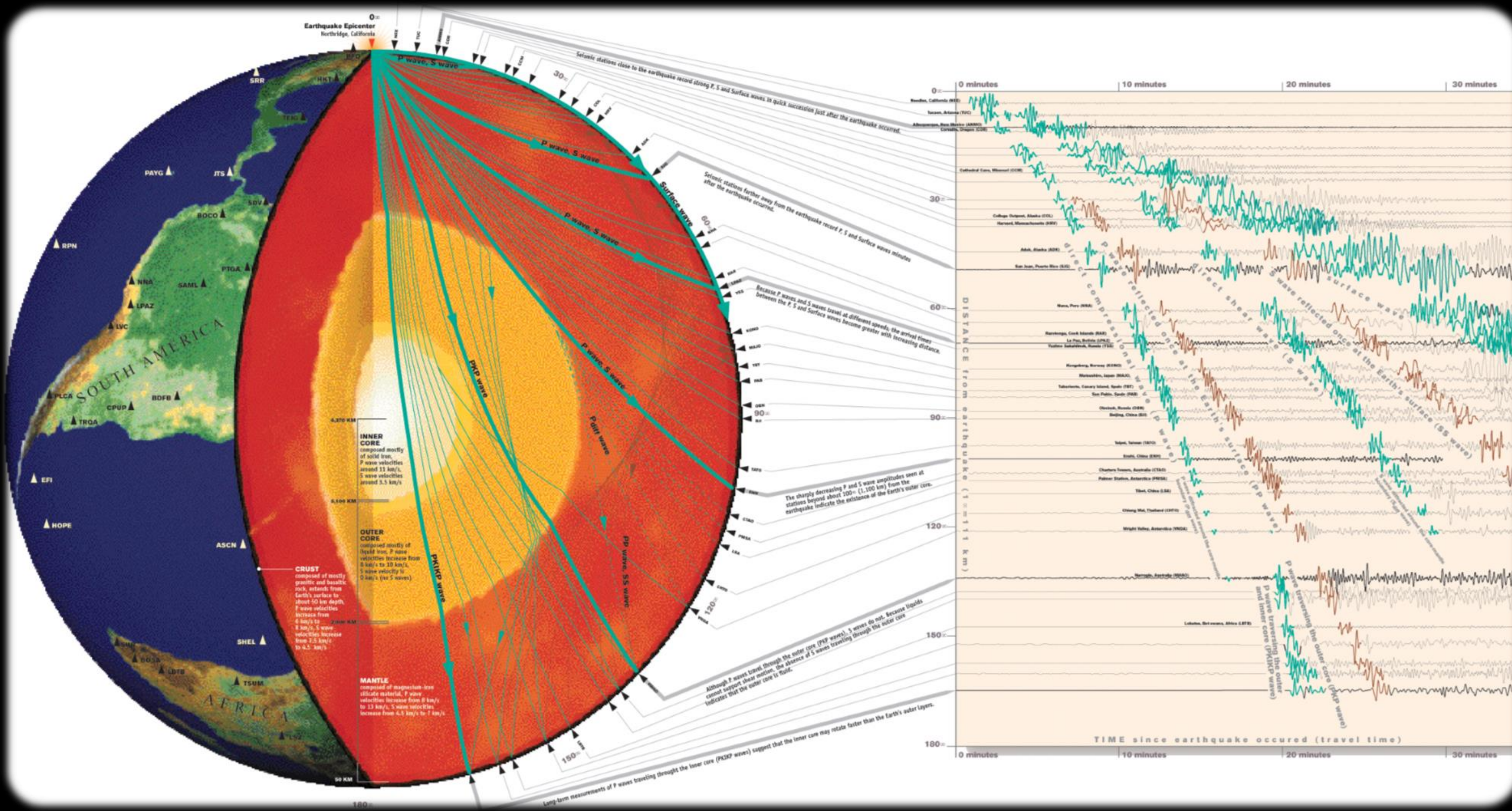
Neutron-star glitch



Quasi-periodic oscillation



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



Picture taken from AusPass by Australian National University

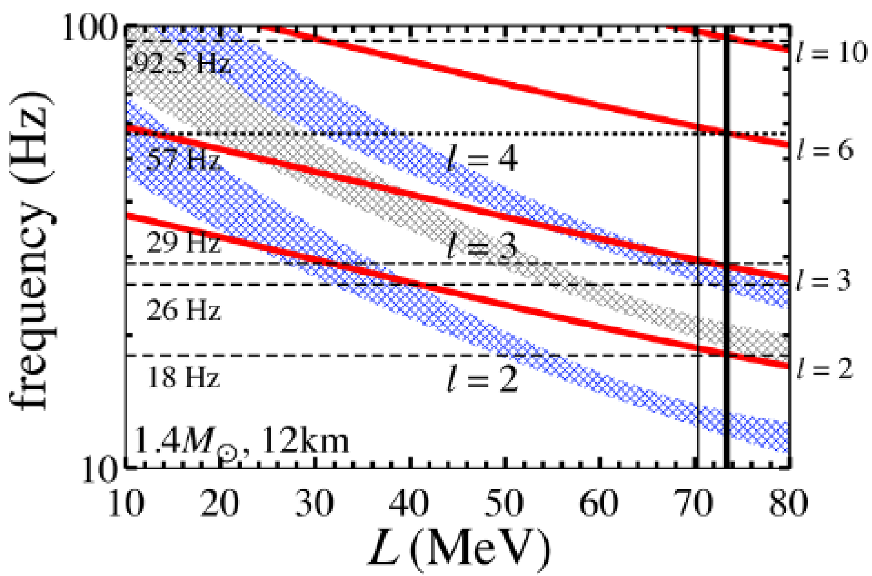
Monthly Notices of the ROYAL ASTRONOMICAL SOCIETY

MNRAS **489**, 3022–3030 (2019) doi:10.1093/mnras/stz2385
Advance Access publication 2019 August 29

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

Hajime Sotani,[1★] Kei Iida[2] and Kazuhiro Oyamatsu[3]

[1] *Division of Science, National Astronomical Observatory of Japan, 2-21-1 Osawa, Mitaka, Tokyo 181-8588, Japan*
[2] *Department of Mathematics and Physics, Kochi University, 2-5-1 Akebono-cho, Kochi 780-8520, Japan*
[3] *Department 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

QPOs as "asteroseismology"

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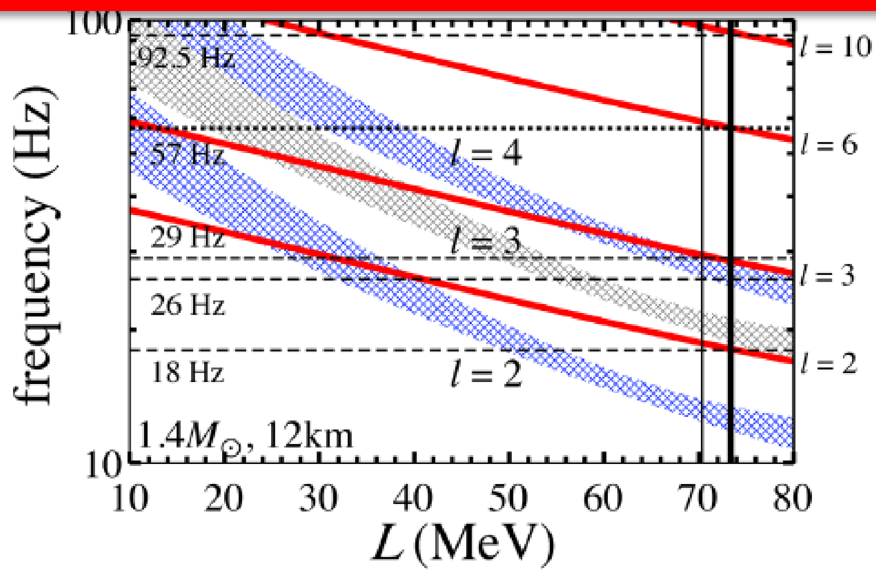
The interpretation could be affected by the entrainment effects!



- 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

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

✓ The Bloch boundary condition for single-particle orbitals

$$\psi^{(q)}_{\alpha\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{V}} u^{(q)}_{\alpha\boldsymbol{k}}(z) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \qquad \underbrace{u^{(q)}_{\alpha\boldsymbol{k}}(z+na) = u^{(q)}_{\alpha\boldsymbol{k}}(z)}_{\text{Periodicity of the slabs}}$$

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

✓ Skyrme EDF

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

Number density:

$$n_q(z) = 2\sum_{\alpha,\boldsymbol{k}}^{\mathrm{occ.}} \left|\psi^{(q)}_{\alpha\boldsymbol{k}}(\boldsymbol{r})\right|^2$$

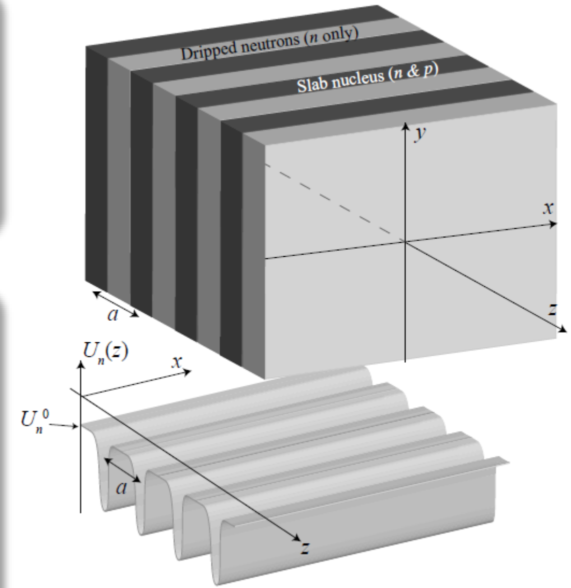
Kinetic density:

$$\tau_q(z) = 2\sum_{\alpha,\boldsymbol{k}}^{\mathrm{occ.}} \left|\nabla\psi^{(q)}_{\alpha\boldsymbol{k}}(\boldsymbol{r})\right|^2$$

Current (momentum) density:

$$\boldsymbol{j}_q(z) = 2\sum_{\alpha,\boldsymbol{k}}^{\mathrm{occ.}} \mathrm{Im}\left[\psi^{(q)*}_{\alpha\boldsymbol{k}}(\boldsymbol{r})\nabla\psi^{(q)}_{\alpha\boldsymbol{k}}(\boldsymbol{r})\right]$$

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



Picture from PRC**100**(2019)035804

✓ Skyrme-Kohn-Sham equations

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

$$\hat{h}^{(q)}(z)\psi^{(q)}_{\alpha\boldsymbol{k}}(\boldsymbol{r}) = \varepsilon^{(q)}_{\alpha\boldsymbol{k}}\psi^{(q)}_{\alpha\boldsymbol{k}}(\boldsymbol{r}) \quad \Rightarrow \quad \left(\hat{h}^{(q)}(z) + \hat{h}^{(q)}_{\boldsymbol{k}}(z)\right)u^{(q)}_{\alpha\boldsymbol{k}}(z) = \varepsilon^{(q)}_{\alpha\boldsymbol{k}} u^{(q)}_{\alpha\boldsymbol{k}}(z)$$

Ordinary single-particle Hamiltonian:

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

Additional (k-dependent) term:

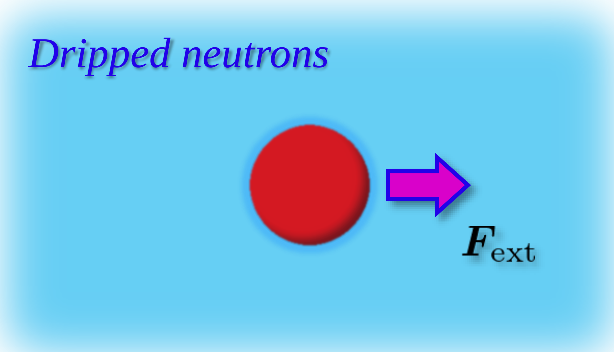
$$\hat{h}^{(q)}_{\boldsymbol{k}}(z) = \frac{\hbar^2\boldsymbol{k}^2}{2m_q^\oplus(z)} + \hbar\boldsymbol{k}\cdot\hat{\boldsymbol{v}}^{(q)}(z)$$

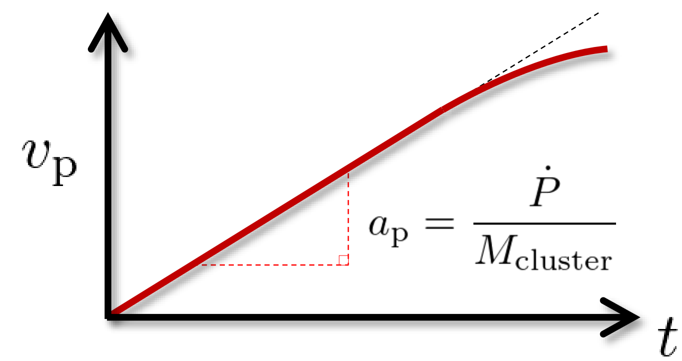
Velocity operator:

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

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

The real-time method: Idea





How to introduce spatially-uniform electric field

✓ TDKS equation in a "velocity gauge"

Spatially-uniform Vector potential

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

Gauge transformation for the Bloch orbitals:

$$\widetilde{u}^{(q)}_{\alpha\boldsymbol{k}}(z,t) = \exp\Big[-\frac{ie}{\hbar c}A_z(t)z\Big]u^{(q)}_{\alpha\boldsymbol{k}}(z,t)$$

Electric field:

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

k-dependent term:

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

Velocity operator:

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

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

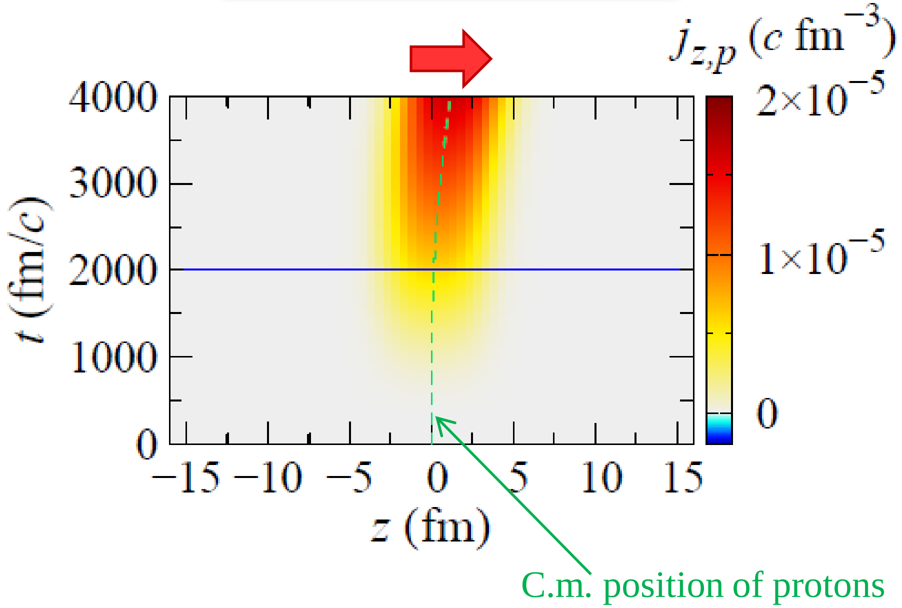
K.S., S. Kobayashi, and M. Matsuo, PRC**105**(2022)045807

Current density:

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

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

Proton current density



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

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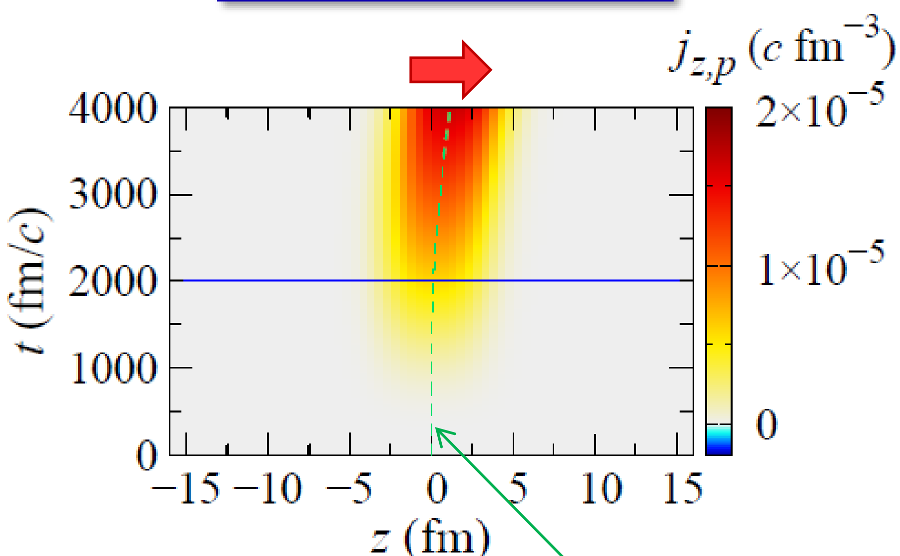
✓ Dripped neutrons outside the slab move toward the opposite direction!

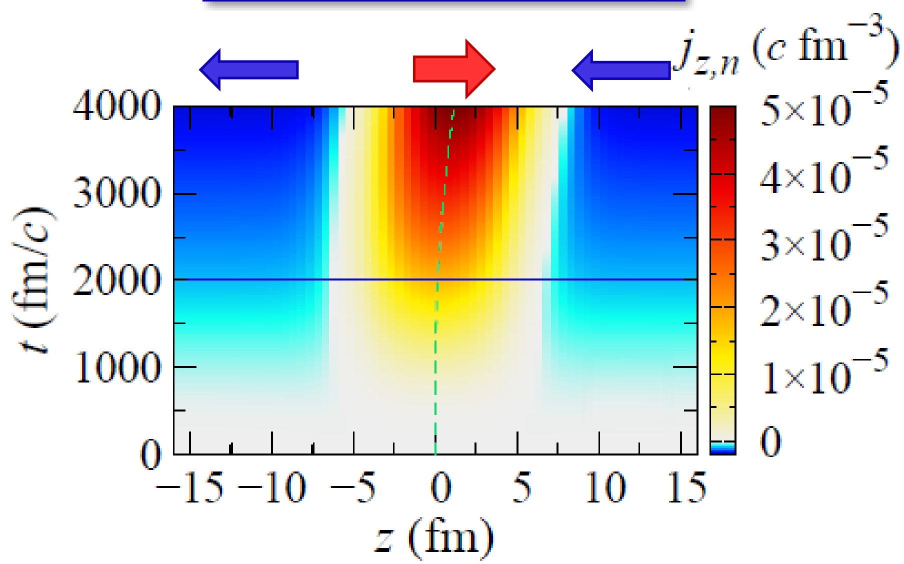
Since it reduces P_{tot} and $\dot{P}_{\mathrm{tot}}$, $M_{\mathrm{slab}} = \dot{P}_{\mathrm{tot}}/a_{\mathrm{p}}$ is reduced

Proton current density



C.m. position of protons

Neutron current density



$$\left(m^{\star\,-1}_{\mathrm{n},\alpha\boldsymbol{k}}\right)_{\mu\nu} = \frac{1}{\hbar^2}\frac{\partial^2\varepsilon^{(\mathrm{n})}_{\alpha\boldsymbol{k}}}{\partial k_\mu\partial k_\nu}$$

Current density:

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

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

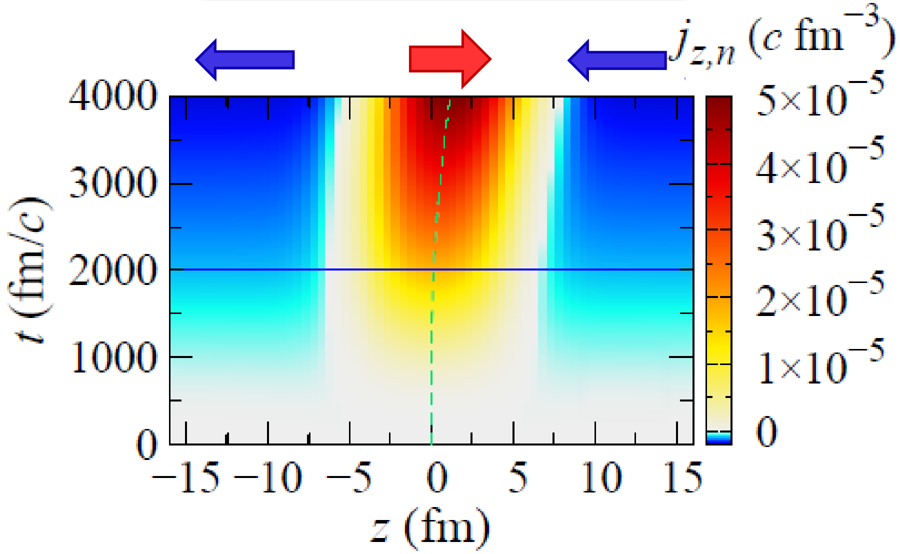
Since it reduces $P_{\rm tot}$ and $\dot{P}_{\rm tot}$, $M_{\rm slab} = \dot{P}_{\rm tot}/a_{\rm p}$ is reduced

Reduction of $M_{\rm slab}$
→ enhancement of $n_{\rm c}$
→ reduction of m^*

We interpret it as an "anti-entrainment" effect

$Y_{\rm p}$	$n_{\rm n}^{\rm f}/\bar{n}_{\rm n}$	Static		Dynamic
		$n_{\rm n}^{\rm c}/\bar{n}_{\rm n}$	$m_{\rm n}^{\star}/m_{\rm n}$	$n_{\rm n}^{\rm c}/\bar{n}_{\rm n}$
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

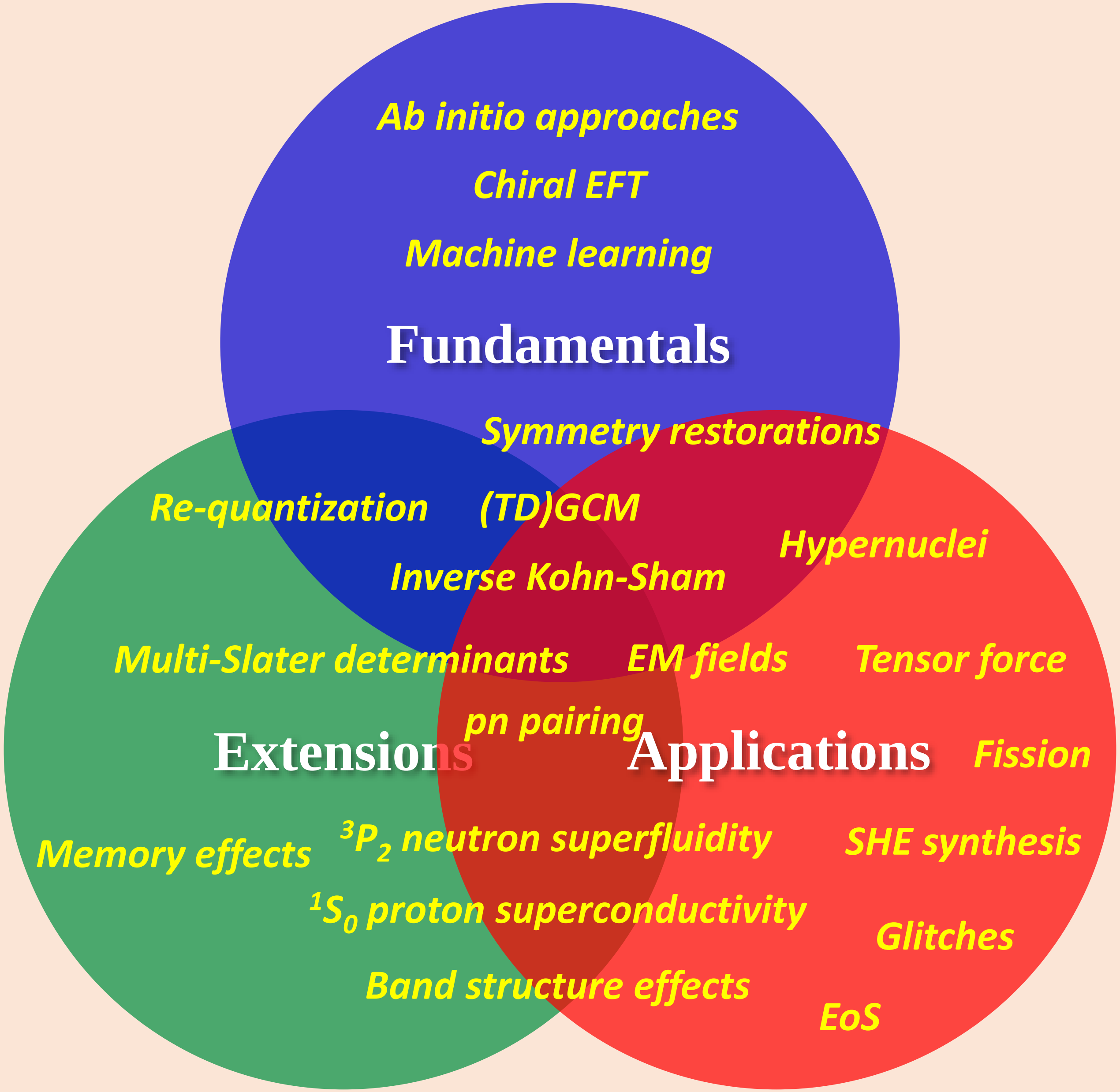
Neutron current density



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

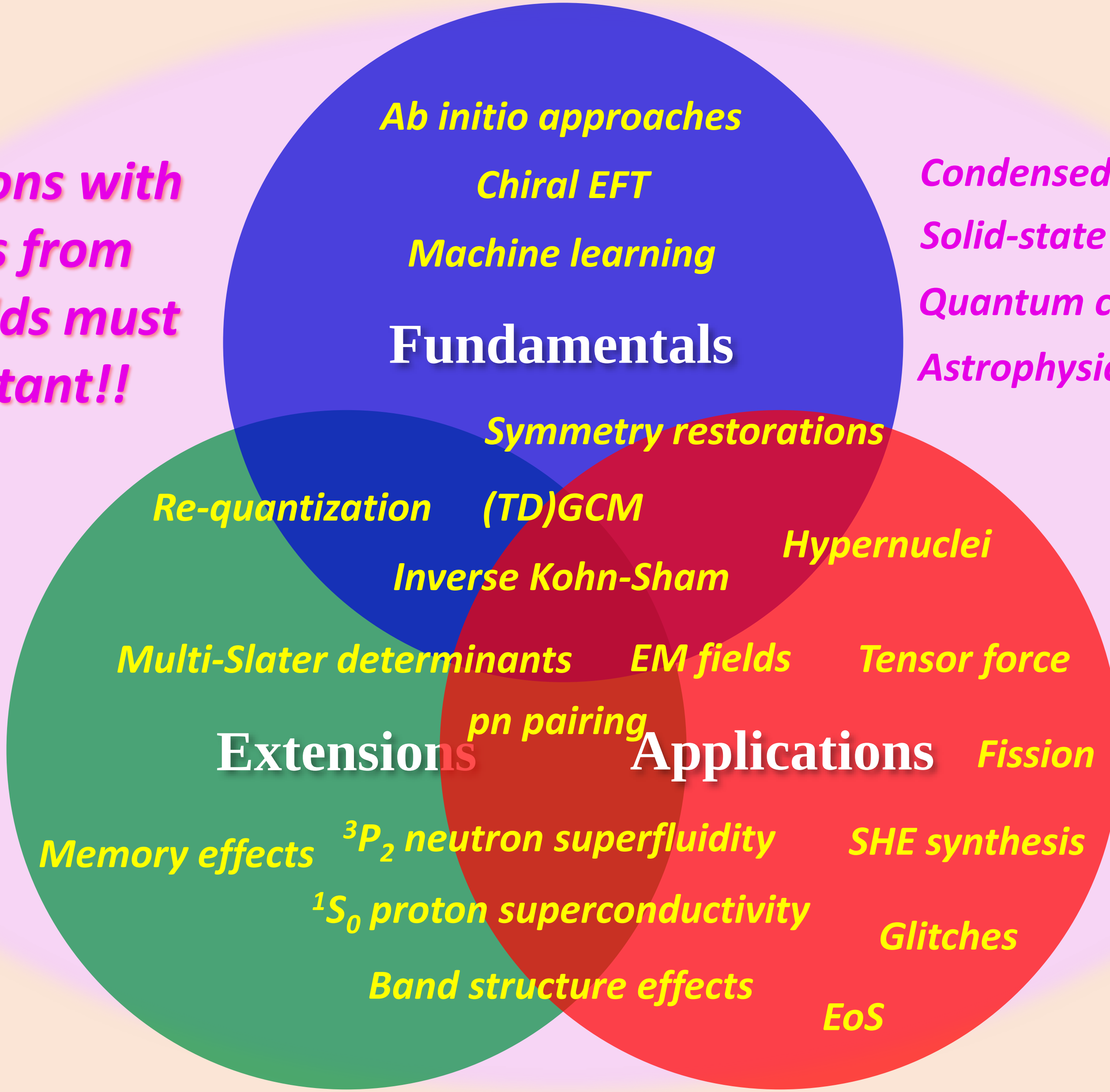
Summary

Future of nuclear (TD)DFT - a personal look



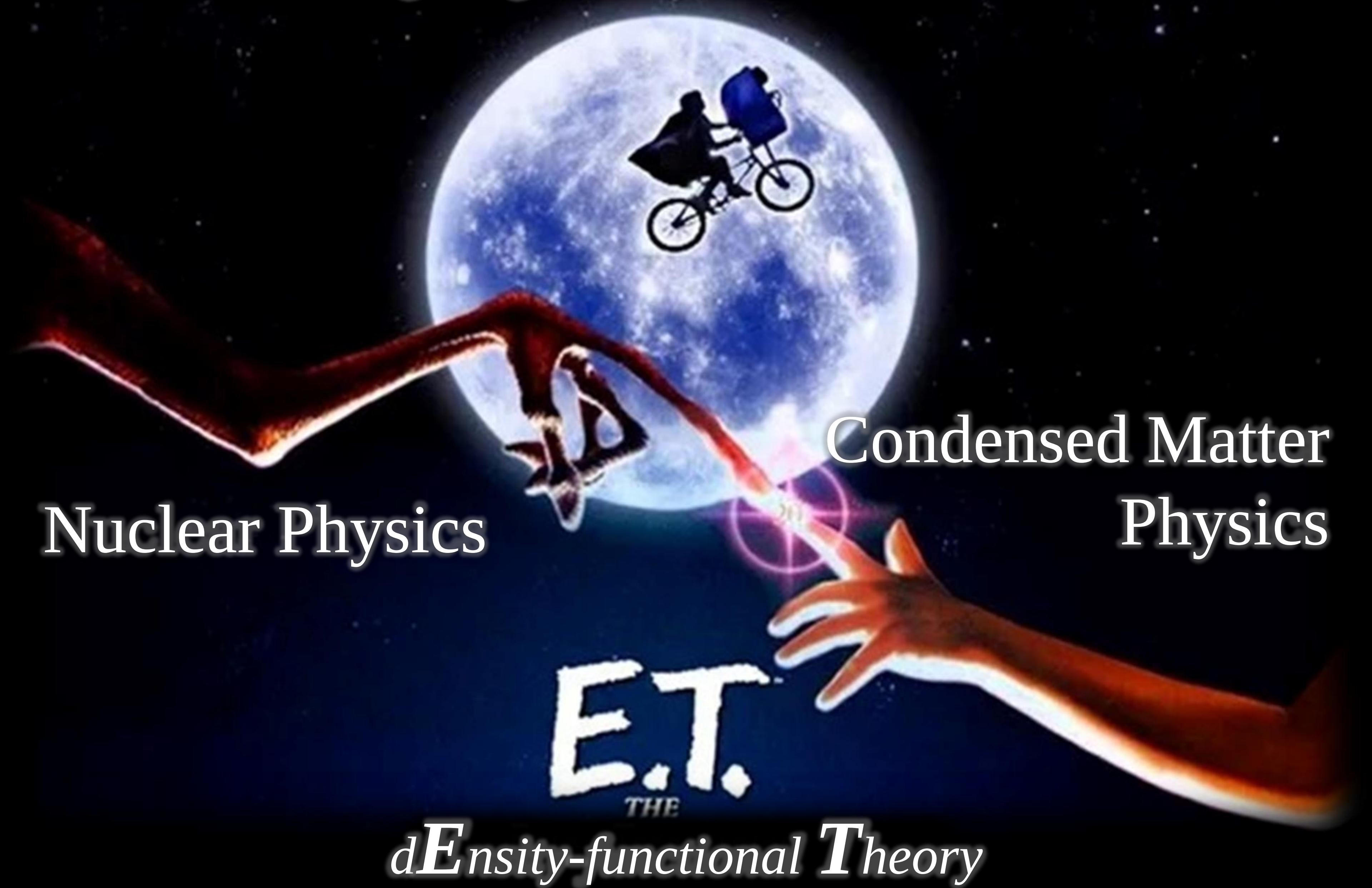
Future of nuclear (TD)DFT - a personal look

Interactions with physicists from other fields must be important!!



Condensed-matter physics
Solid-state physics
Quantum chemistry
Astrophysics

..and we should go together for the future of DFT..



"End Credits" from "E.T.": https://youtu.be/YuhZ80YHFns

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