

**Seminar at Chiba Institute of Technology**  
November 24th, 2018, Shin-Narashino Campus, Chiba

## Time-Dependent Density Functional Theory for Superfluid Dynamics in the Neutron Star Crust

Kazuyuki Sekizawa

Center for Interdisciplinary Research  
Institute for Research Promotion, Niigata University, Japan

# 自己紹介（略歴）

1988年：埼玉県出身

2006年3月：埼玉県立伊奈学園総合高等学校 卒業

2010年3月：東京理科大学 物理学科 卒業

2012年3月：筑波大学大学院 博士前期課程 修了

2015年3月：筑波大学大学院 博士後期課程 修了（理学博士）

2015年4月～2017年8月：ポーランド・ワルシャワ工科大学（博士研究員）

2017年9月～2017年12月：米国シアトル・ワシントン大学（博士研究員）

2018年1月～現在：新潟大学 研究推進機構 超域学術院（特任助教・テニュアトラック）



幸手権現堂桜堤



## 専門は「原子核理論」



# My recent studies: TDDFT for Nuclear Many-Body Problem

## Multinucleon transfer and quasifission processes in heavy-ion reactions

Tsukuba, Tohoku, Kyushu

PRC96(2017)041601(R),  
PRC96(2017)014615,  
PRC93(2016)054616,  
PRC90(2014)064614,  
PRC88(2013)014614



K. Yabana



K. Hagino



K. Washiyama

BARC, Mumbai, India

B.J. Roy and his coworkers

B.J. Roy *et al.*,  
PRC97(2018)034603,  
PRC92(2015)024603

## Dissipation and fluctuation mechanism in deep-inelastic collisions

ANU, Canberra, Australia  
Texas A&M, USA

E. Williams, K. Sekizawa, D. Hinde *et al.*,  
PRL120(2018)022501



E. Williams



D.J. Hinde



M. Dasgupta



C. Simenel



A. Wakhle

## Superfluid dynamics in fermionic systems

WUT, Warsaw, Poland

PRL120(2018)253002  
PRL119(2017)042501  
PRL117(2016)232701



G. Włazłowski



P. Magierski

UW, Seattle, USA



A. Bulgac



M.M. Forbes

# My recent studies: TDDFT for Nuclear M

Multinucleon transfer and quasifission processes in heavy-ion

Tsukuba, Tohoku, Kyushu

PRC96(2017)041601(R),  
PRC96(2017)014615,  
PRC93(2016)054616,  
PRC90(2014)064614,  
PRC88(2013)014614



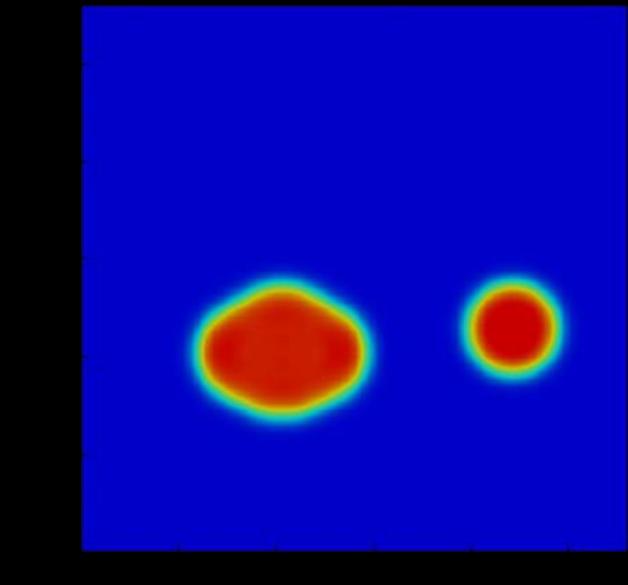
K. Yabana



K. Hagino



K. Washiyama



Dissipation and fluctuation mechanism in deep-inelastic collisions

ANU, Canberra, Australia  
Texas A&M, USA

E. Williams, K. Sekizawa, D. Hinde *et al.*,  
PRL120(2018)022501

Today's talk



E. Williams D.J. Hinde



M. Dasgupta C. Simenel A. Wakhle



Superfluid dynamics in fermionic systems

WUT, Warsaw, Poland

PRL120(2018)253002  
PRL119(2017)042501  
PRL117(2016)232701



G. Wlazłowski



P. Magierski

UW, Seattle, USA



A. Bulgac

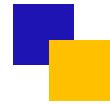


M.M. Forbes

# *Outline*

---

- 1. Method:** DFT, TDDFT, and TDSDLDA
  
  
  
- 2. Dynamics of quantized vortices within TDSDLDA:**  
Topological excitations in spin-imbalanced superfluid Fermi gas
  
  
  
- 3. Application to Neutron Star physics:**  
Vortex-nucleus interaction in the neutron star crust
  
  
  
- 4. Summary**



## DFT, TDDFT, and TDSLDA

---



# What is DFT?

A theory which may provide the exact solution

Equivalent!  
(w/ special EDF)

Kohn-Sham equation

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

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



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

**Quantum Many-Body Problem**



Existence was proved, but “shape” is unknown :(

Energy can also be written as a functional of density



P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964)

## DFT in a nutshell (1/2) - Hohenberg-Kohn theorem

### Assumption:

Two different wave functions  $\Psi$  and  $\Psi'$   
provide the same one-body density  $\rho(\mathbf{r})$

$$\begin{aligned}\hat{H} &= \hat{T} + \hat{W} + \hat{V} & \hat{H}' &= \hat{T} + \hat{W} + \hat{V}' \\ \hat{H}|\Psi\rangle &= E|\Psi\rangle & \hat{H}'|\Psi'\rangle &= E'|\Psi'\rangle\end{aligned}$$

Now, one finds:

$$\begin{aligned}E &= \langle \Psi | \hat{H} | \Psi \rangle < \langle \Psi' | \hat{H} | \Psi' \rangle \\ &= \langle \Psi' | \hat{H}' | \Psi' \rangle + \langle \Psi' | \hat{V} - \hat{V}' | \Psi' \rangle \\ &= E' + \int \rho(\mathbf{r}) [v(\mathbf{r}) - v'(\mathbf{r})] d\mathbf{r} \quad \dots \quad (\text{a})\end{aligned}$$

However, one also gets:

$$\begin{aligned}E' &= \langle \Psi' | \hat{H}' | \Psi' \rangle < \langle \Psi | \hat{H}' | \Psi \rangle \\ &= E + \int \rho(\mathbf{r}) [v'(\mathbf{r}) - v(\mathbf{r})] d\mathbf{r} \quad \dots \quad (\text{b})\end{aligned}$$

(a) + (b)  $E + E' < E + E' \quad ?$  

P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964)

## DFT in a nutshell (1/2) - Hohenberg-Kohn theorem

*Assumption:*

Two different wave functions  $\Psi$  and  $\Psi'$  provide the same one-body density  $\rho(\mathbf{r})$

$$\hat{H} = \hat{T} + \hat{W} + \hat{V}$$

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

$$\hat{H}' = \hat{T} + \hat{W}' + \hat{V}'$$

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

*Our assumption was wrong!*

Now, one finds:

$$E = \langle \Psi | \hat{H} | \Psi \rangle < \langle \Psi' | \hat{H} | \Psi' \rangle \quad \text{"reductio ad absurdum"}$$

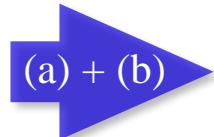
$$= \langle \Psi' | \hat{H}' | \Psi' \rangle + \langle \Psi' | \hat{V} - \hat{V}' | \Psi' \rangle$$

$$= E' + \int \rho(\mathbf{r}) [v(\mathbf{r}) - v'(\mathbf{r})] d\mathbf{r} \quad \dots \dots \text{(a)}$$

However, one also gets:

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

$$= E + \int \rho(\mathbf{r}) [v'(\mathbf{r}) - v(\mathbf{r})] d\mathbf{r} \quad \dots \dots \text{(b)}$$



$$E + E' < E + E' \quad ?$$



P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964)

## DFT in a nutshell (1/2) - Hohenberg-Kohn theorem

Assumptions:

(1st) HK theorem:

There is a one-to-one correspondence between  $\Psi$  and  $\rho$

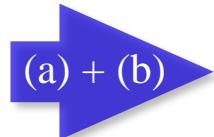
$$\Psi \leftrightarrow \rho(\mathbf{r})$$

Now, one finds:

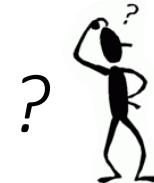
$$\begin{aligned}
 E &= \langle \Psi | \hat{H} | \Psi \rangle < \langle \Psi' | \hat{H} | \Psi' \rangle \quad \text{"reductio ad absurdum"} \\
 &= \langle \Psi' | \hat{H}' | \Psi' \rangle + \langle \Psi' | \hat{V} - \hat{V}' | \Psi' \rangle \\
 &= E' + \int \rho(\mathbf{r}) [v(\mathbf{r}) - v'(\mathbf{r})] d\mathbf{r} \quad \dots \dots \text{(a)}
 \end{aligned}$$

However, one also gets:

$$\begin{aligned}
 E' &= \langle \Psi' | \hat{H}' | \Psi' \rangle < \langle \Psi | \hat{H}' | \Psi \rangle \\
 &= E + \int \rho(\mathbf{r}) [v'(\mathbf{r}) - v(\mathbf{r})] d\mathbf{r} \quad \dots \dots \text{(b)}
 \end{aligned}$$



$$E + E' < E + E'$$



P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964)

KS scheme makes DFT computationally solvable

**(2nd) HK theorem:**

- $\Psi$  can be written as a functional of  $\rho$ :  $\Psi = \Psi[\rho]$
- Any observable can be written as a functional of  $\rho$ :  $\mathcal{O}[\rho] = \langle \Psi[\rho] | \hat{\mathcal{O}} | \Psi[\rho] \rangle$
- Minimization of EDF with respect to  $\rho$  will provide  $E_{\text{g.s.}}$  and  $\rho_{\text{g.s.}}$ :

$$\hat{H} \xleftrightarrow{\text{SE}} \Psi \xleftrightarrow{\text{HK}} \rho(\mathbf{r})$$

$$E_{\text{g.s.}} = E[\rho_{\text{g.s.}}] = \min_{\rho} \left[ \min_{\Psi \rightarrow \rho} E[\rho] \right]$$

$$E[\rho] = \langle \Psi[\rho] | \hat{H} | \Psi[\rho] \rangle : \text{EDF}$$

**Kohn-Sham scheme:**

W. Kohn and L.J. Sham, Phys. Rev. **140**, A1133 (1965)

- ✓ According to the HK theorem, there exists an EDF associated with the exact solution  $\Psi$
- The solution of  $N$  coupled nonlinear equations can be equivalent to the exact solution

$$\hat{h}[\rho]\phi_i(\mathbf{r}) = \varepsilon_i\phi_i(\mathbf{r}) : \text{Kohn-Sham equation}$$

(often called Hartree-Fock eq.)

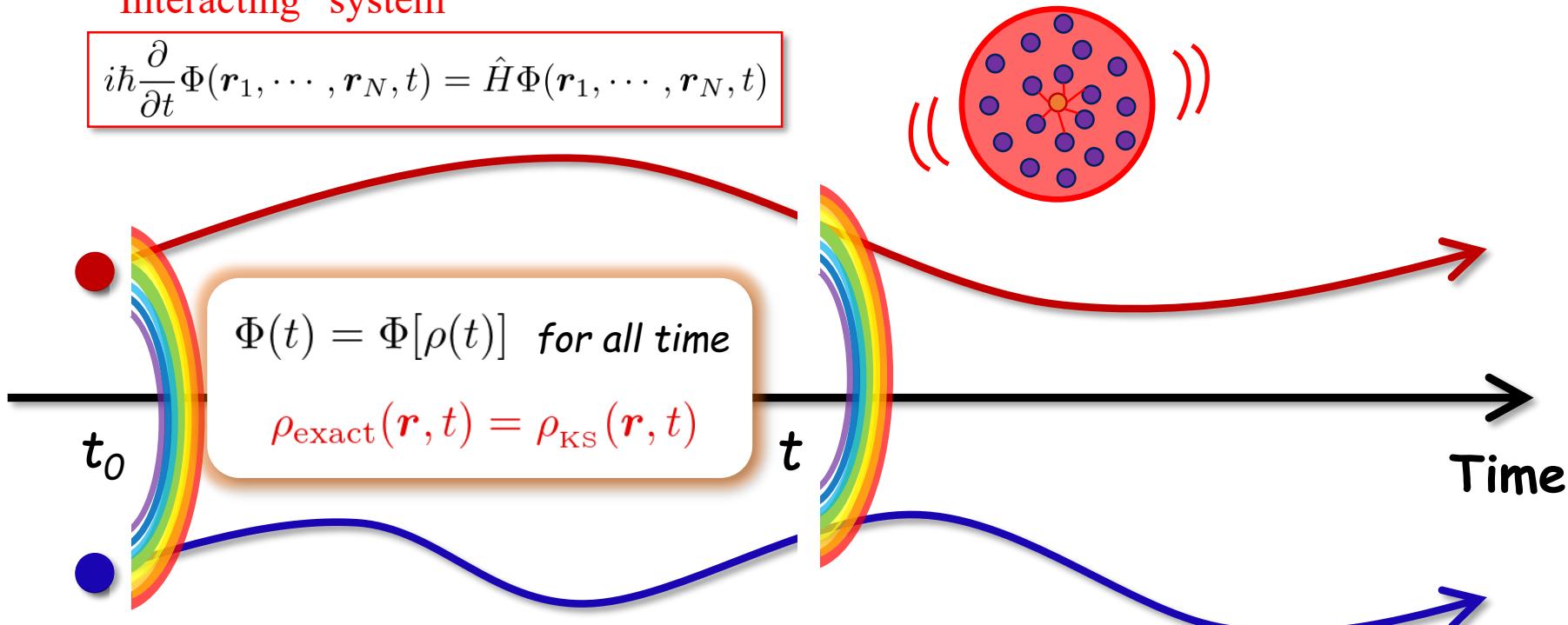
$$\frac{\delta}{\delta\phi_i^*} \left[ E[\rho] - \sum_{kl} \varepsilon_{kl} \left( \langle \phi_k | \phi_l \rangle - \delta_{kl} \right) \right] = 0 \quad \hat{h}[\rho] = \frac{\delta E[\rho]}{\delta\rho} \quad \rho(\mathbf{r}) = \sum_{i=1}^N |\phi_i(\mathbf{r})|^2$$

# What is TDDFT?

TDDFT is a time-dependent extension of DFT

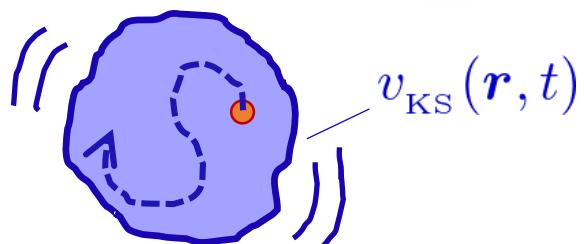
“Interacting” system

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



“Non-interacting” system

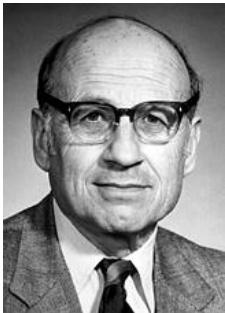
$$i\hbar \frac{\partial \phi_i(\mathbf{r}, t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + v_{\text{KS}}[\rho(\mathbf{r}, t)] \right] \phi_i(\mathbf{r}, t)$$



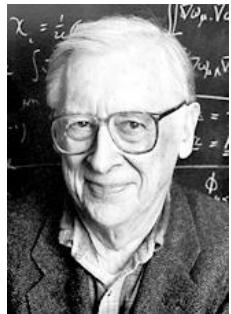
E. Runge and E.K.U. Gross, Phys. Rev. Lett. **52**, 997 (1984); R. van Leeuwen, Phys. Rev. Lett. **82**, 3863 (1999).

# Great success of the Density Functional Theory

## The Nobel Prize in Chemistry 1998



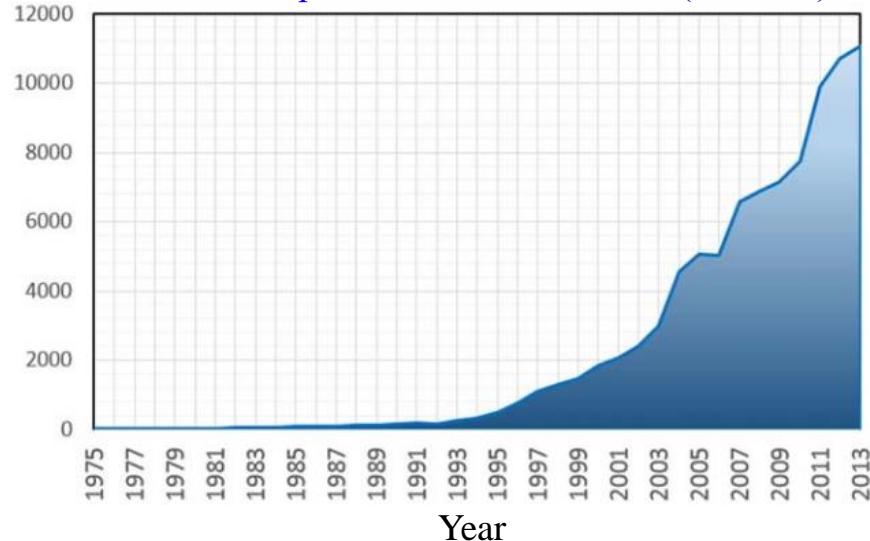
Walter Kohn



John Pople

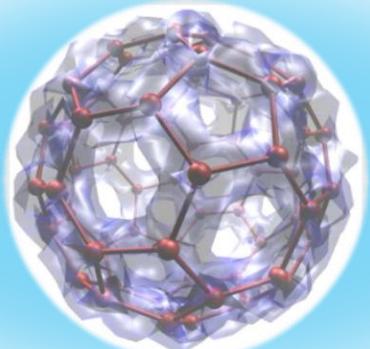


Number of publications with “DFT” (till 2013)



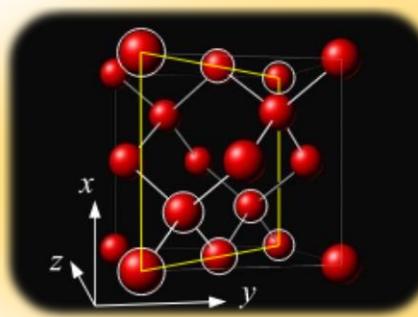
A. Galano and J.R. Alvarez-Idadoy, J. Compt. Chem. **35**, 2019 (2014)

Fullerene:  $C_{60}$

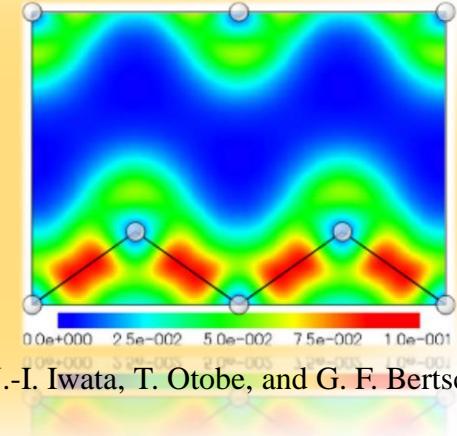


C-Z. Gao et al.,  
J. Phys. B: At. Mol. Opt. Phys. **48**, 105102 (2015)

Si crystal



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



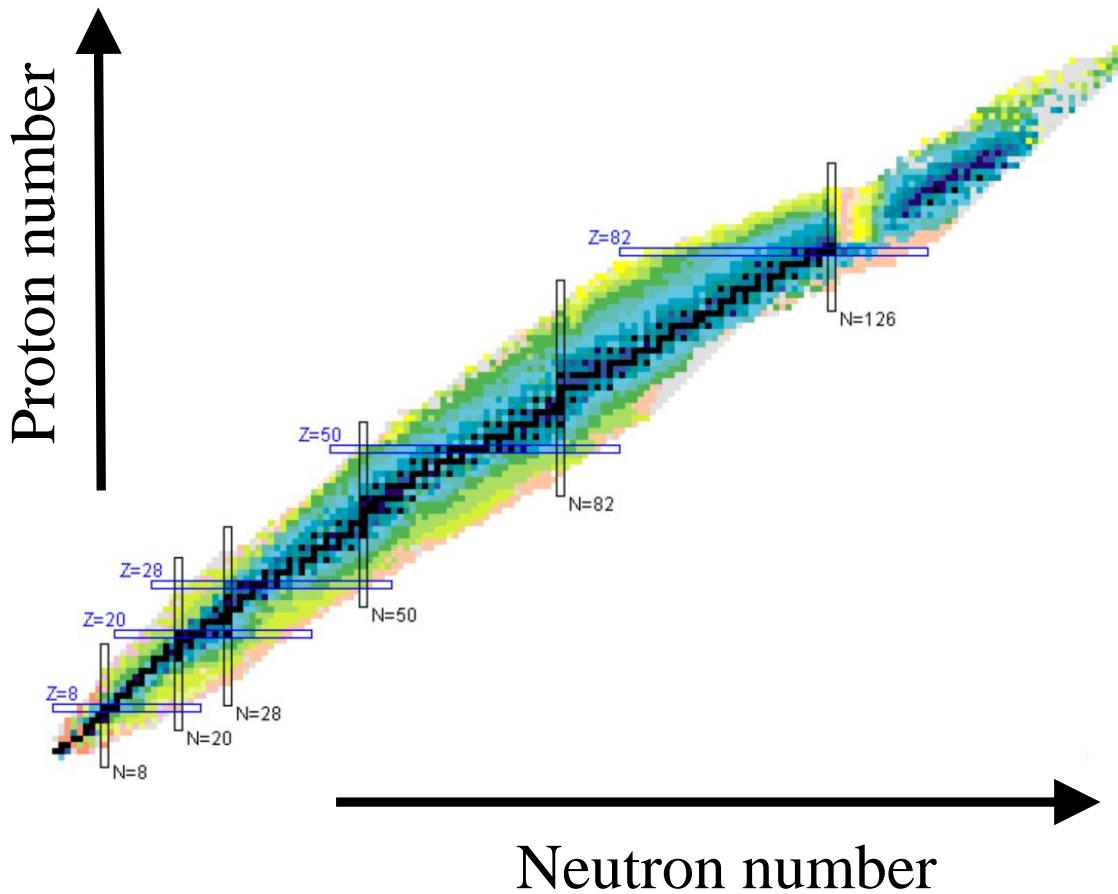
The seminal papers on DFT

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

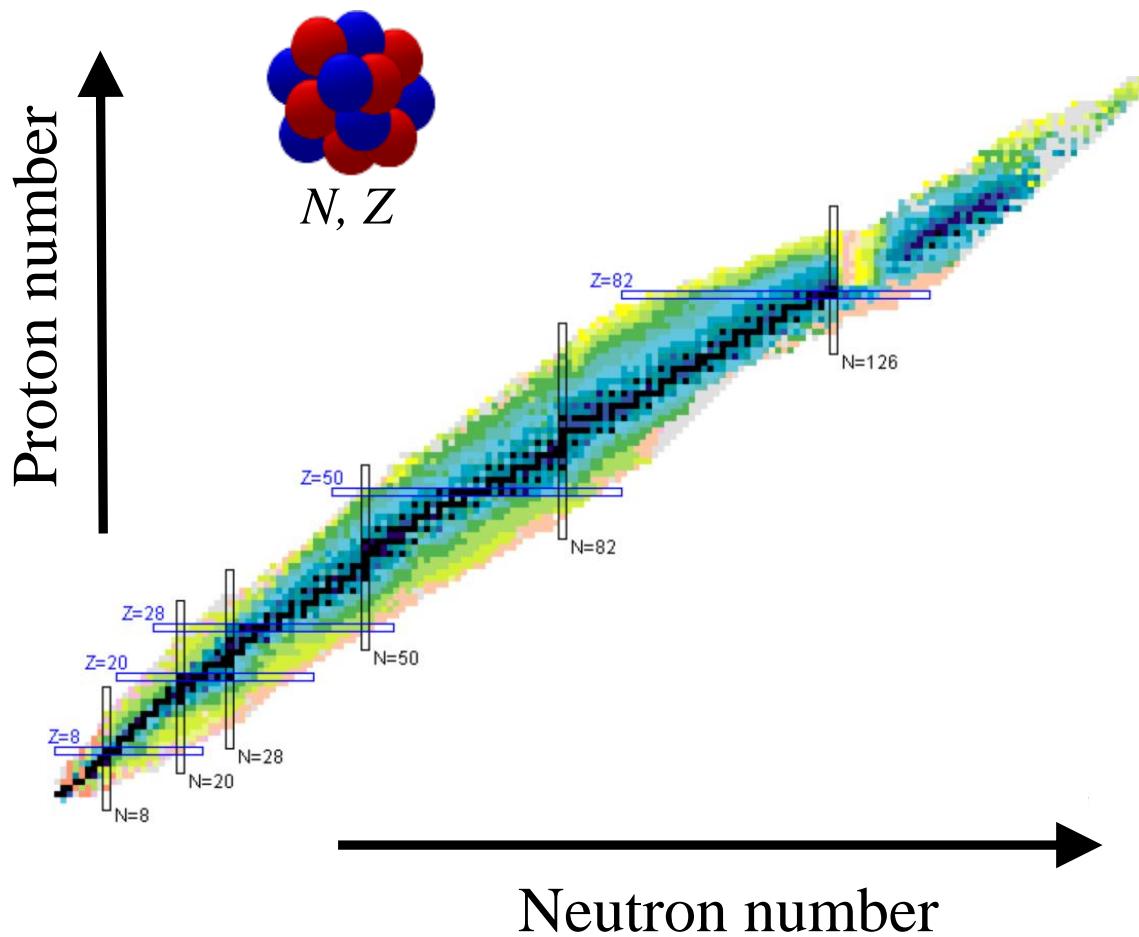
# *DFT in Nuclear Physics*

All nuclei can be described with a single EDF

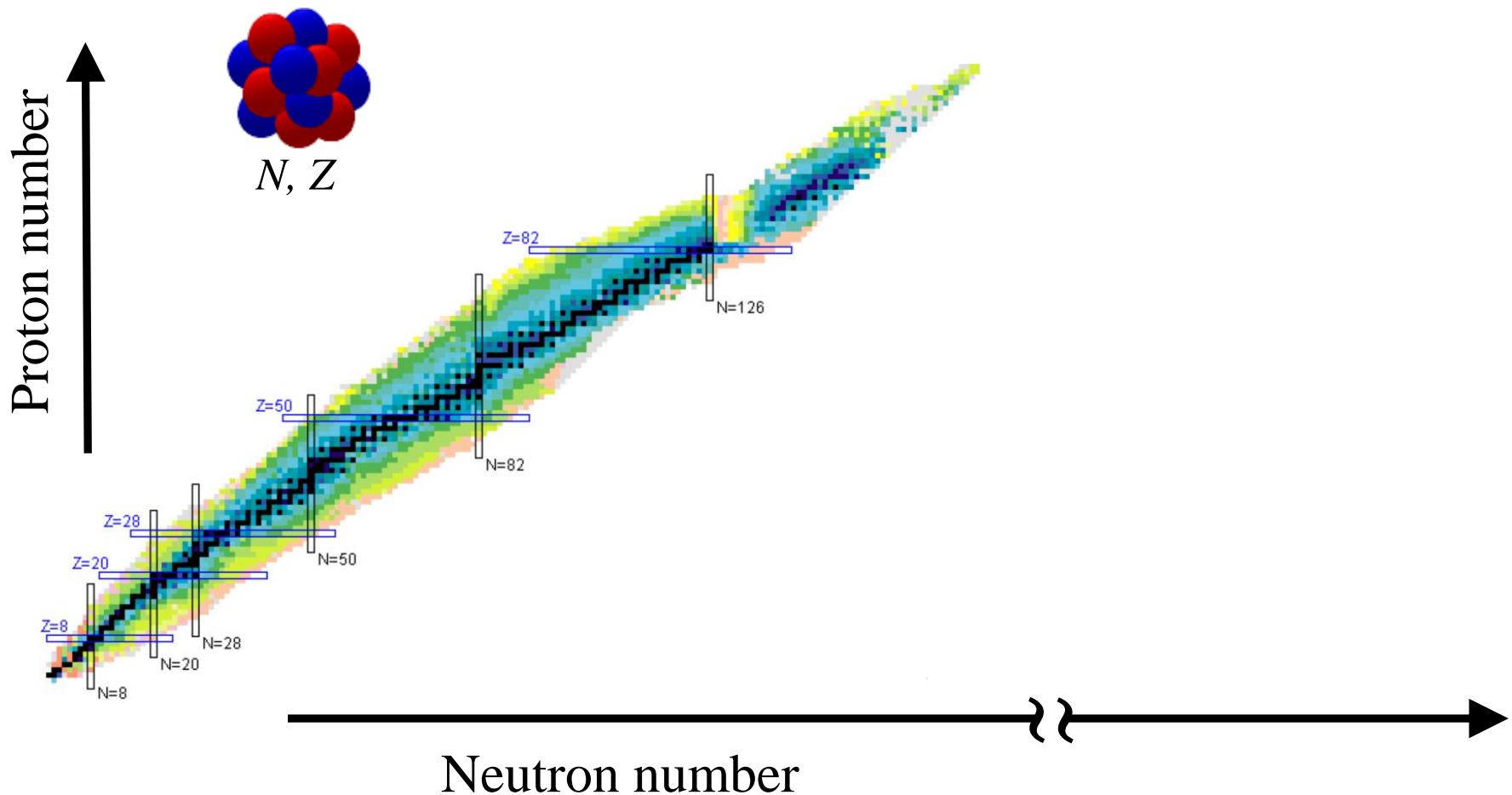
All nuclei can be described with a single EDF



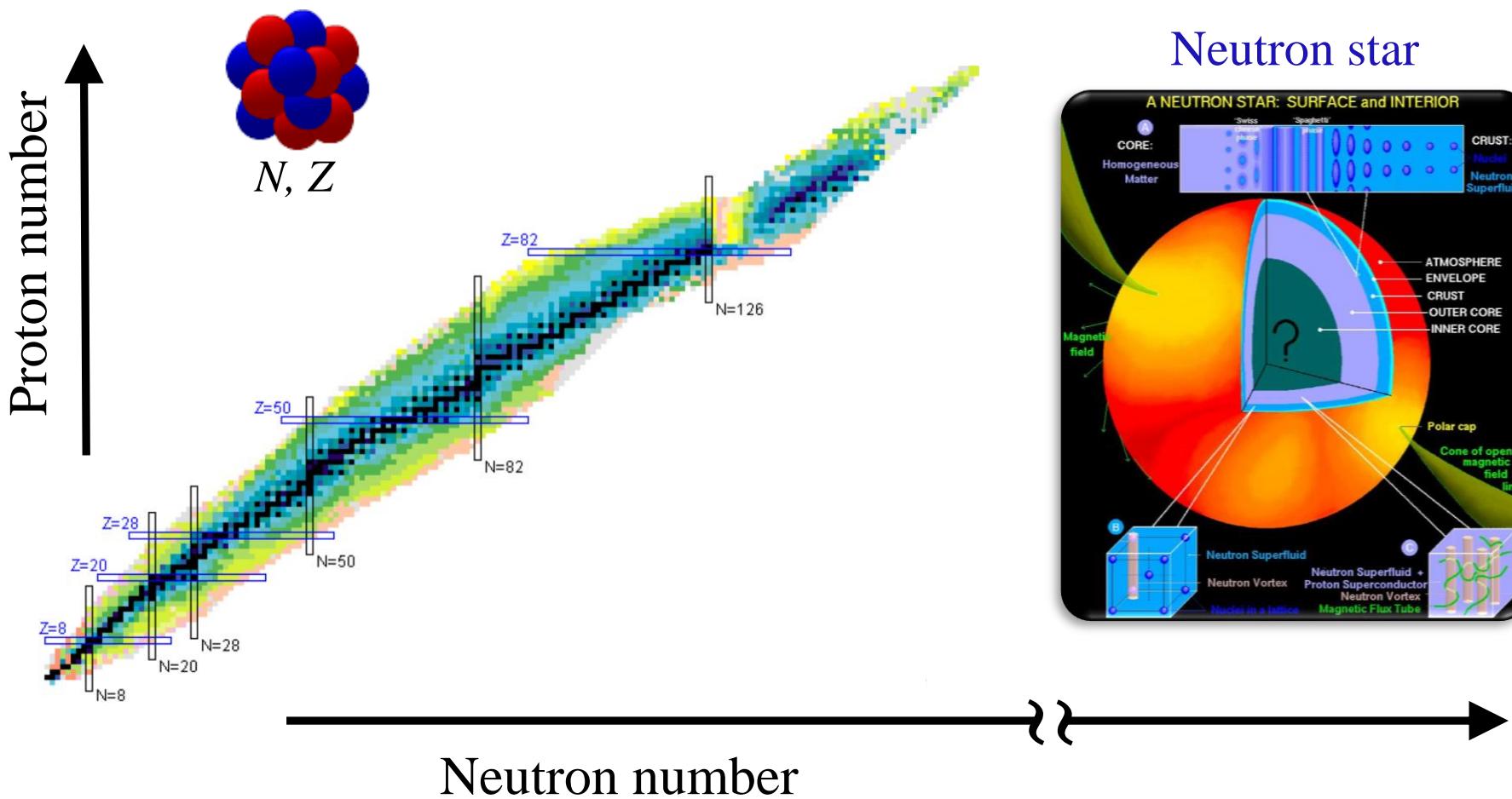
All nuclei can be described with a single EDF



All nuclei can be described with a single EDF



All nuclei can be described with a single EDF



## 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)

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

Supercomputing!!

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

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

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

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

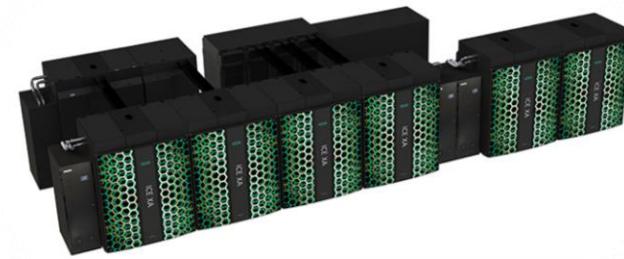
$$\mathbf{j}_\sigma(\mathbf{r}, t) = \hbar \sum_{E_k < E_c} \text{Im}[v_{k,\sigma}^*(\mathbf{r}, t) \nabla v_{k,\sigma}(\mathbf{r}, t)] : \text{current}$$

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

# of qp orbitals ~ # of grid points

\*The number indicates the rank according to the TOP500 list (June 2018)

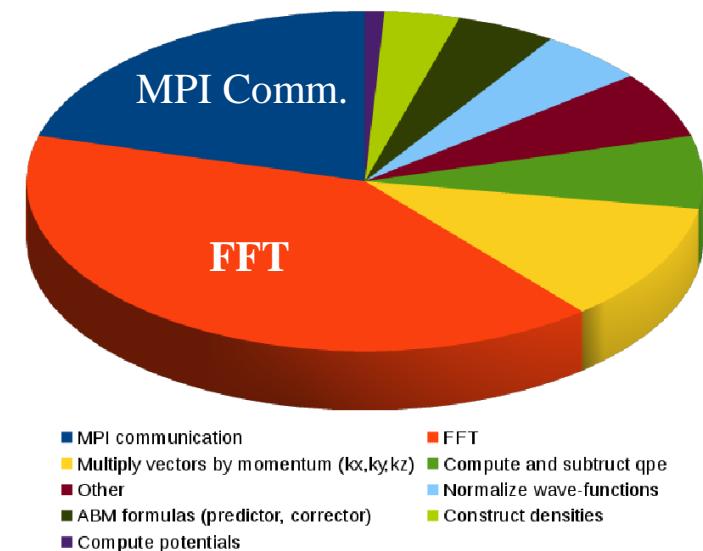
Piz Daint, CSCS, Switzerland (No. 6) TITAN, ORNL, USA (No. 7) TSUBAME3.0, Japan (No. 19)



The fastest machine:  
Summit, ORNL, USA  
GPU, 188 PFlops/s

### Present computing capabilities:

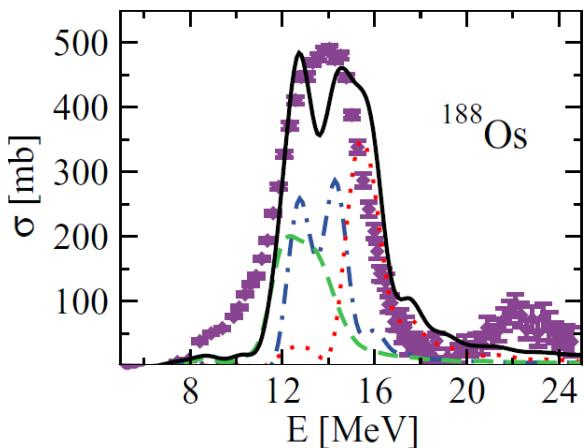
- ✓ Full 3D (w/o symmetry restrictions)
- ✓ Volume as large as  $100^3$  lattice points
- ✓ Evolution up to  $10^6$  time steps (as long as  $10^{-19}$  sec)



# *Applications of TDSLDA: Nuclear systems*

TDSLDA is a versatile tool!!

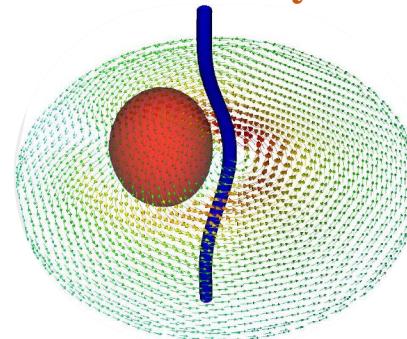
IVGDR



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. Włazłowski, K.S., P. Magierski, A. Bulgac, and M.M. Forbes

Low-energy heavy ion reactions

Time

$$\Delta\varphi = \pi \\ 0$$



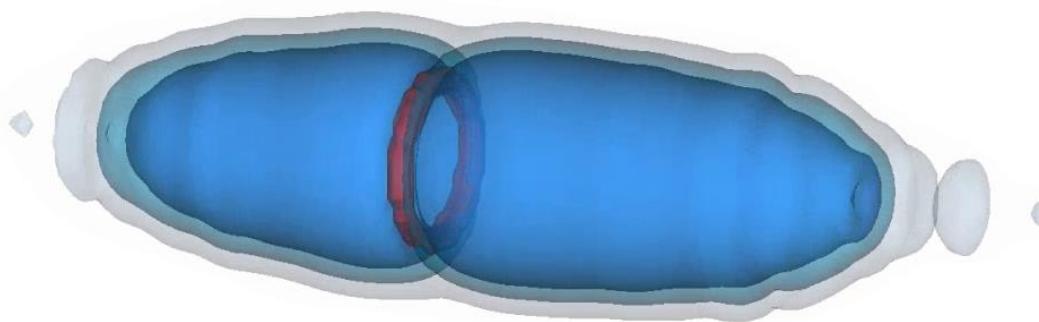
Phys. Rev. Lett. **116**, 122504 (2016)

A. Bulgac, P. Magierski, K.J. Roche, and I. Stetcu

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



## Solitonic cascades in polarized Fermi gas



# *Applications of TDSLDA*

TDSLDA has been successfully applied for both UFG and nuclear systems

## Unitary Fermi Gas (UFG)

$$\left. \begin{array}{l} k_F a \rightarrow \infty, \quad k_F r_{\text{eff}} \rightarrow 0 \\ \qquad \qquad \qquad a : \text{s-wave scattering length} \\ \qquad \qquad \qquad r_{\text{eff}} : \text{effective range} \end{array} \right\}$$

- A. Bulgac and S. Yoon, PRL**102**(2009)085302.
- A. Bulgac *et al.*, Science **332**(2011)1288.
- A. Bulgac *et al.*, PRL**108**(2012)150401.
- A. Bulgac *et al.*, PRL**112**(2014)025301.
- G. Włazłowski *et al.*, PRA**91**(2015)031602(R).

Large-amplitude pairing field dynamics  
Dynamics of quantum vortices  
Quantum shock waves and domain walls  
Dynamics of vortex rings  
Quantum turbulence

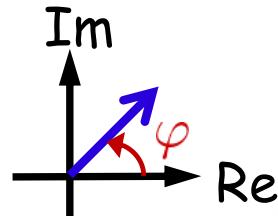
## Nuclear systems

- I. Stetcu *et al.*, PRC**84**(2011)051309(R).
- I. Stetcu *et al.*, PRL**114**(2015)012701.
- A. Bulgac *et al.*, PRL**116**(2016)122504.
- G. Włazłowski *et al.*, PRL**117**(2016)232701.

Isovector giant dipole resonance (IVGDR)  
Relativistic coulomb excitation  
Induced fission of  $^{240}\text{Pu}$   
Vortex-nucleus interaction

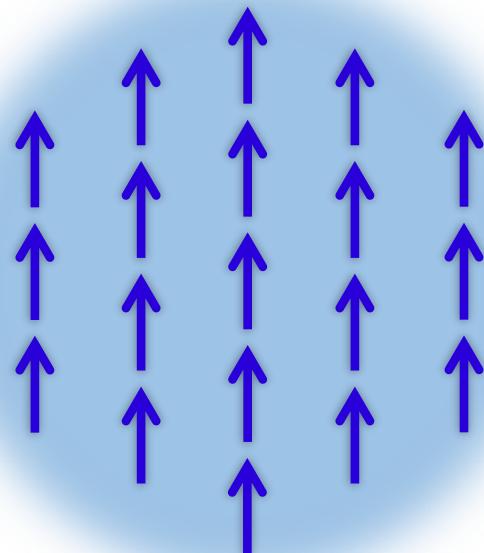
# Dynamic excitations of the pairing field

The **Pairing field** provides a variety of **dynamic** excitation modes

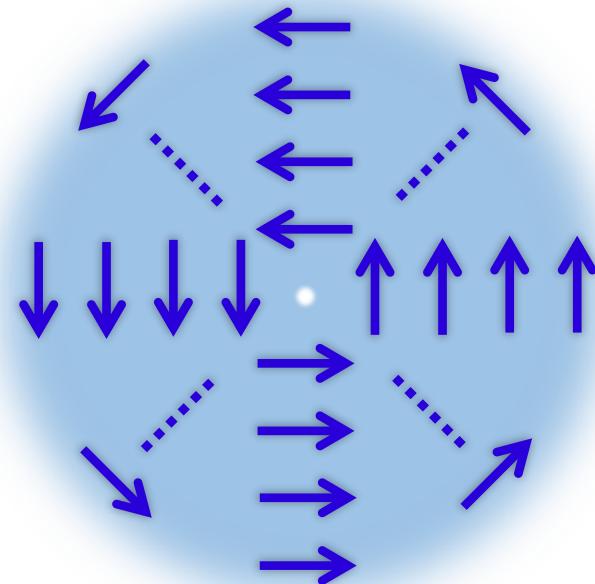


$$|\Delta(\mathbf{r}, t)| e^{i\varphi(\mathbf{r}, t)}$$

\**Superfluid velocity*  
 $v_s(\mathbf{r}, t) \propto \nabla \varphi(\mathbf{r}, t)$



Collective rotation  
(of the phase)



Quantum vortex

# *Applications of TDSLDA: Unitary Fermi Gas*

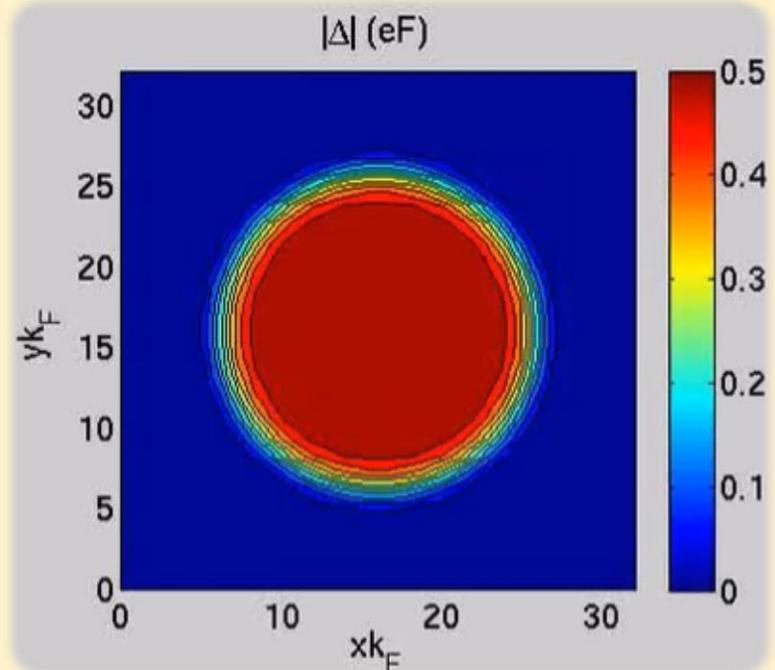
*Real-Time Dynamics of Quantized Vortices in a Unitary Fermi Superfluid*

*A. Bulgac, Y.-L. Luo, P. Magierski, K.J. Roche, Y. Yu  
Science 332, 1288 (2011)*

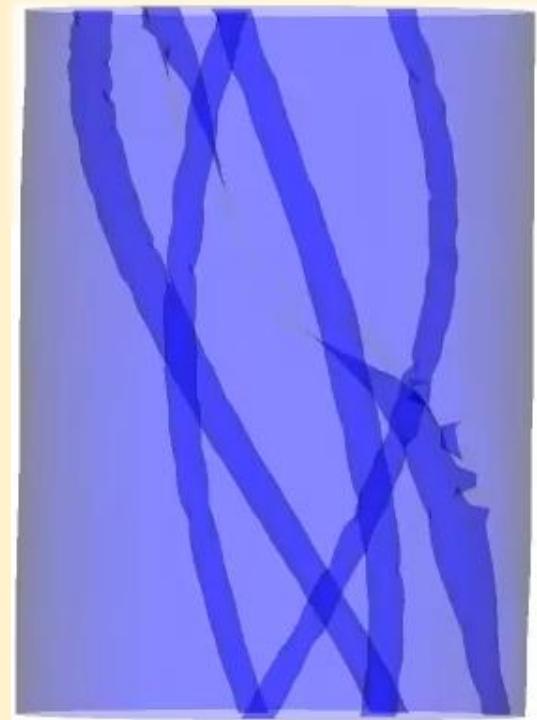
Throwing a spherical projectile  Vortex rings/lines



Stirring  Quantized vortices



Twisted stirring  
  
Vortex crossings  
& reconnections  
(quantum turbulence)

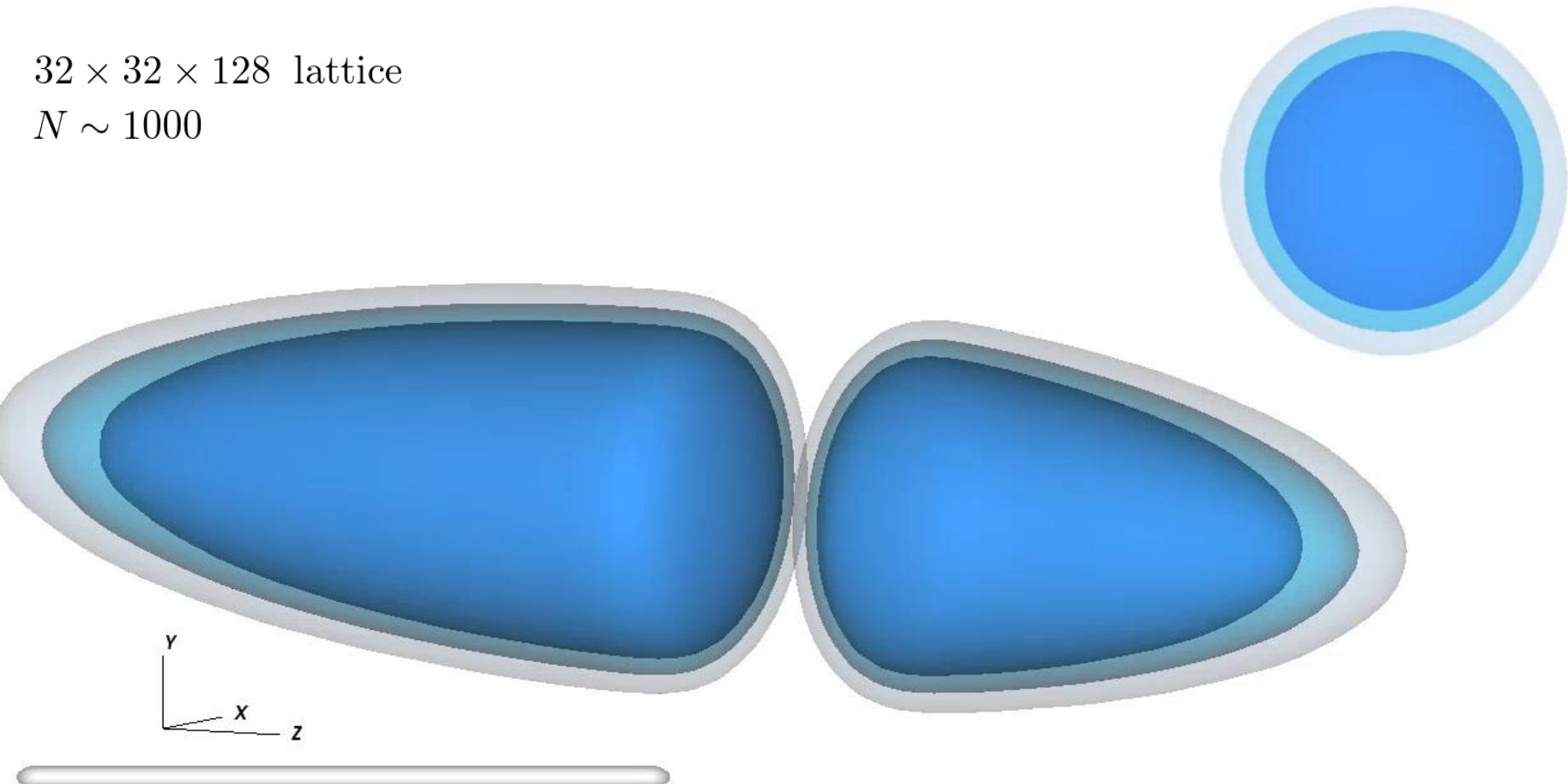


**Result of TDSLDA simulation:**

Phase discontinuity creates a vortex ring which decays into a vortex line

$32 \times 32 \times 128$  lattice

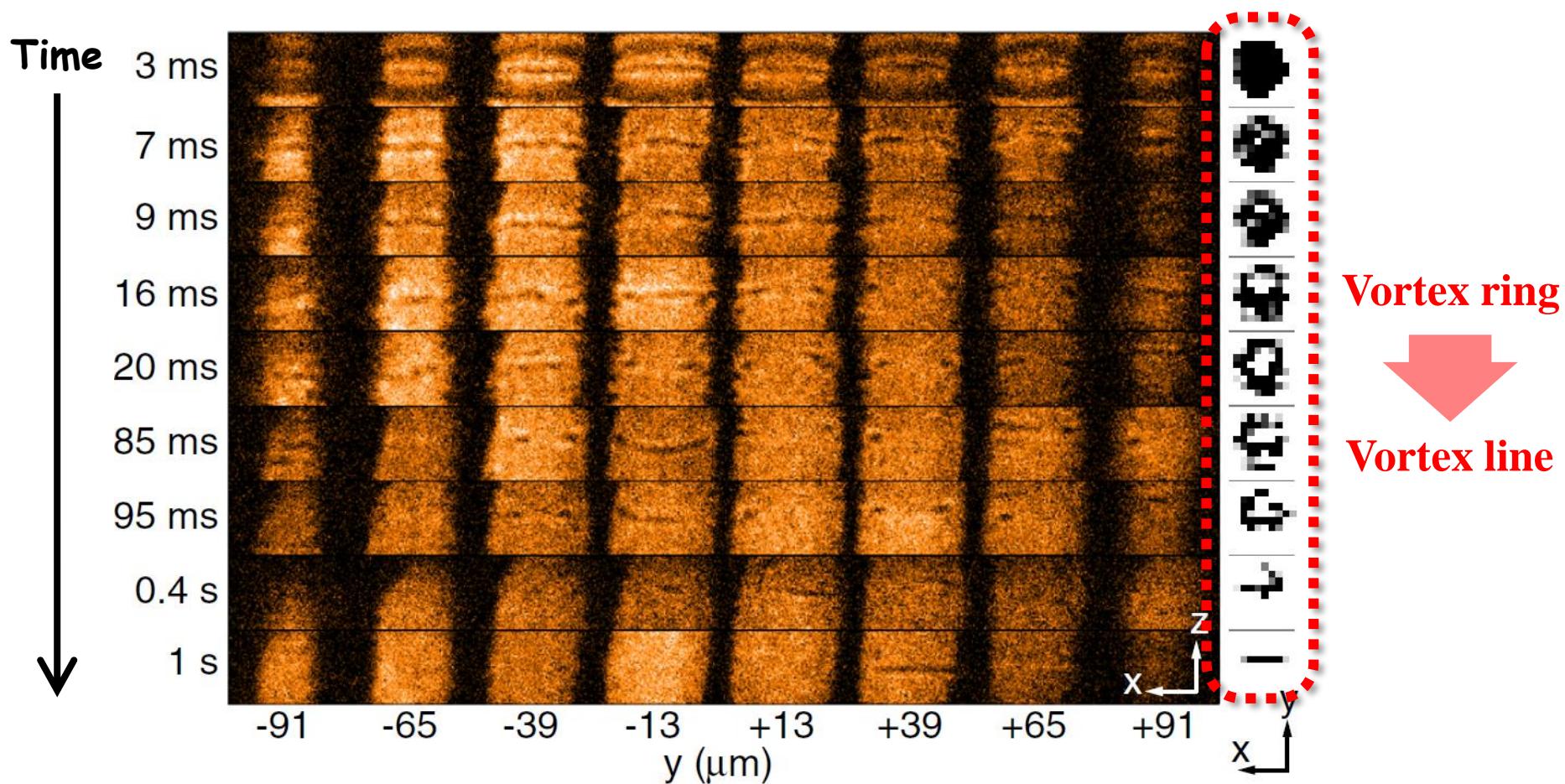
$N \sim 1000$



G. Włazłowski, A. Bulgac, M.M. Forbes, and K.J. Roche, Phys. Rev. A **91**, 031602 (2015)

# Topological excitations in ultracold atomic gases

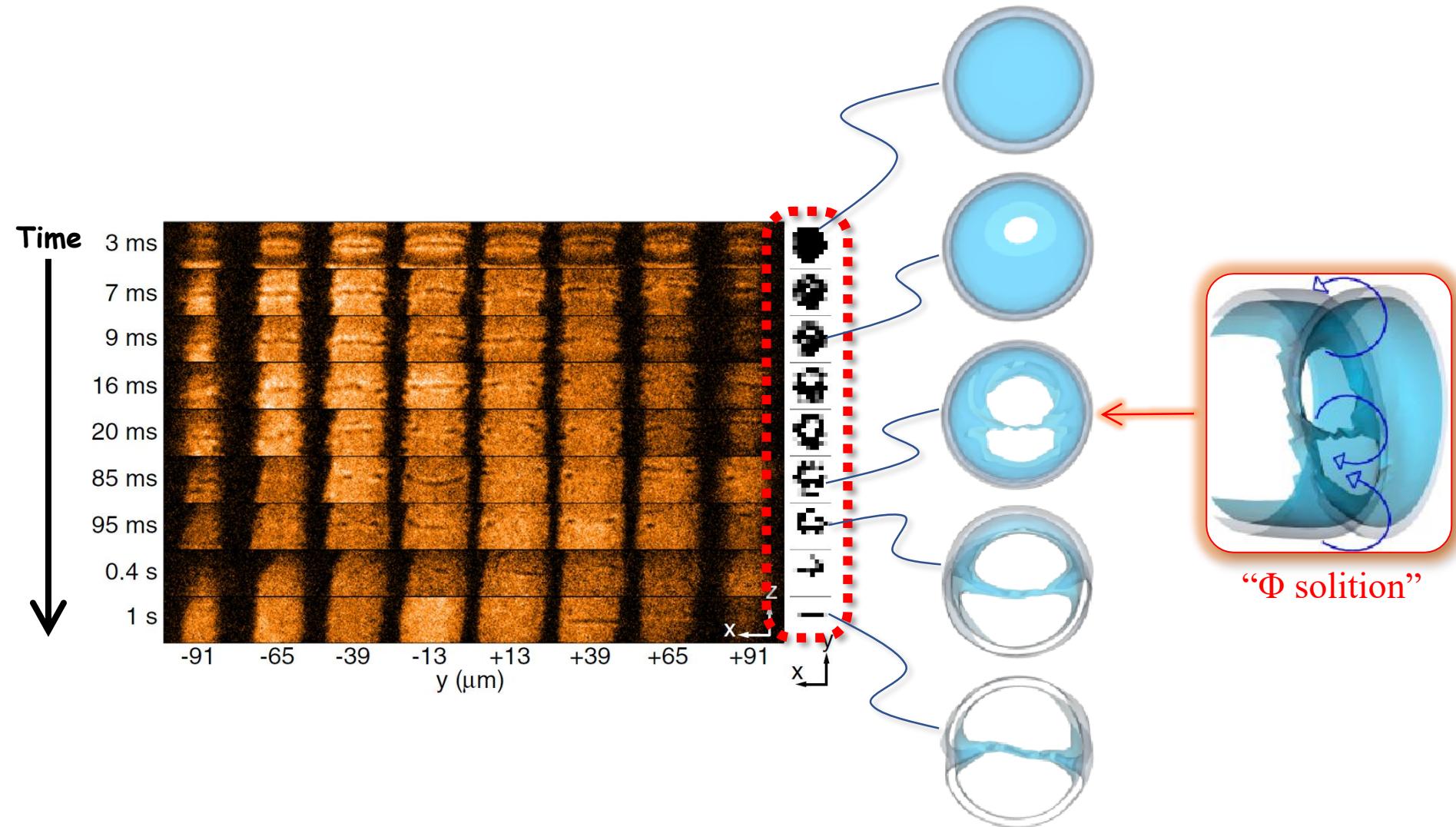
The cascades of solitonic excitations have been identified experimentally



M.J.H. Ku, B. Mukherjee, T. Yefsah, and M.W. Zwierlein, Phys. Rev. Lett. **116**, 045304 (2016)

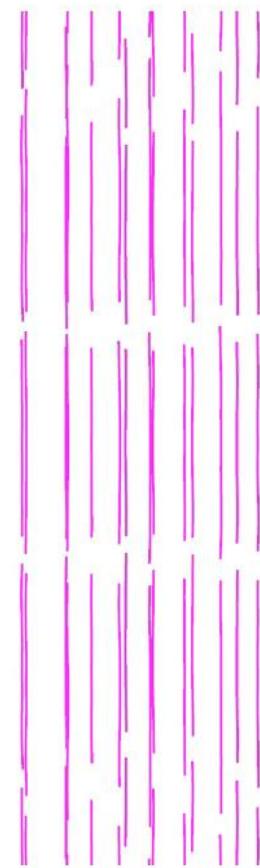
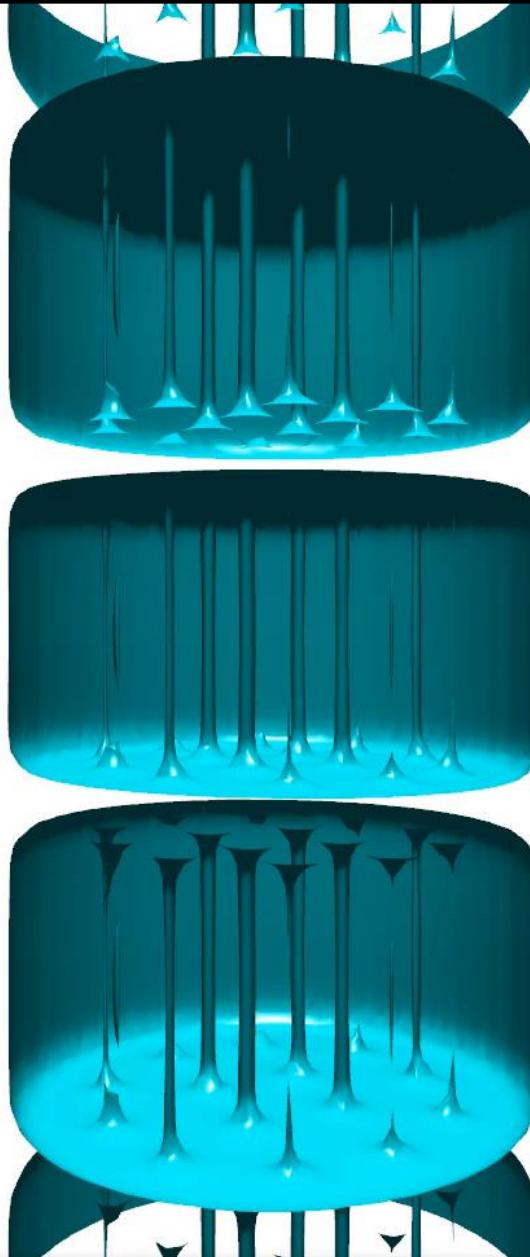
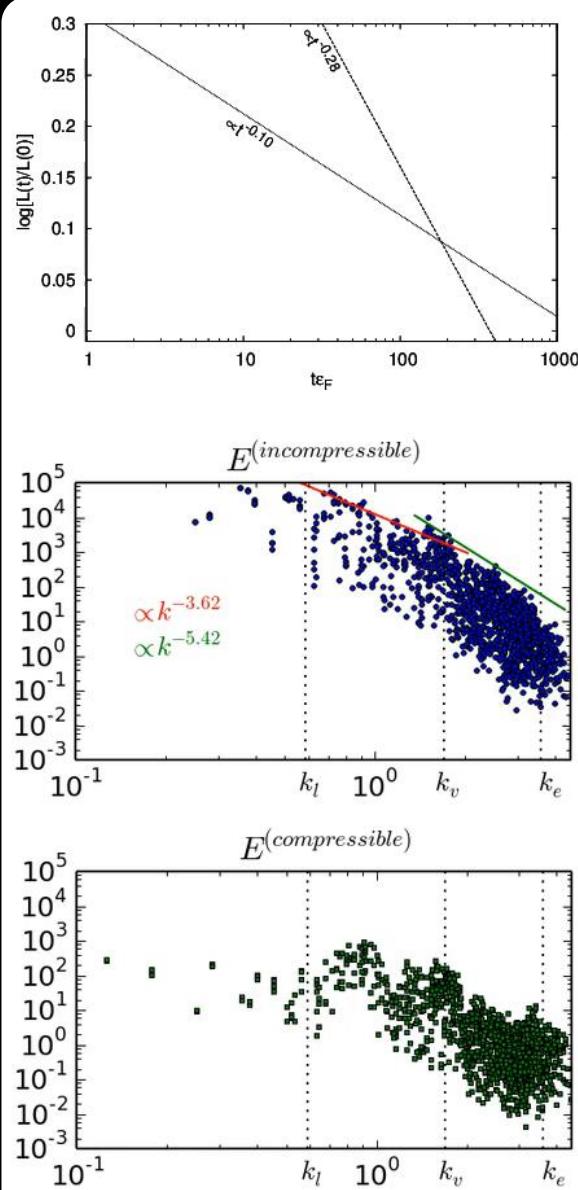
# Topological excitations in ultracold atomic gases

Each stage of solitonic cascade could be reproduced with TDSLDA!



## Computational/theoretical challenge

### *Microscopic simulation of quantum turbulence in superfluid fermi gas*



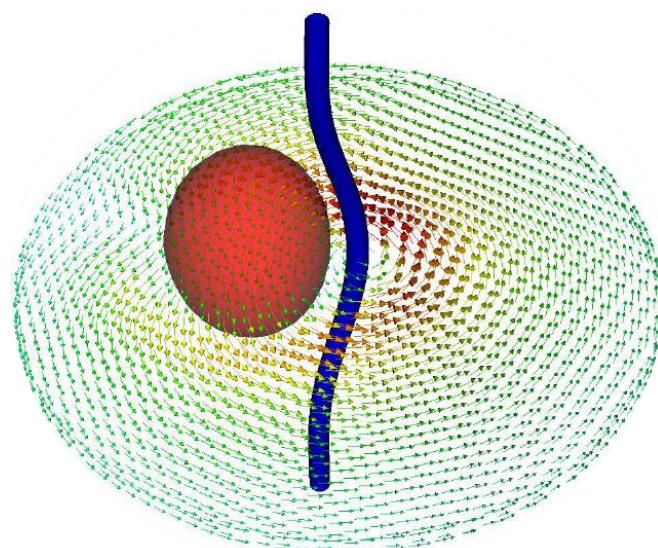
time = 0 [ $\epsilon_F^{-1}$ ]

**Very preliminary**



## Vortex-nucleus dynamics in the NS crust

---

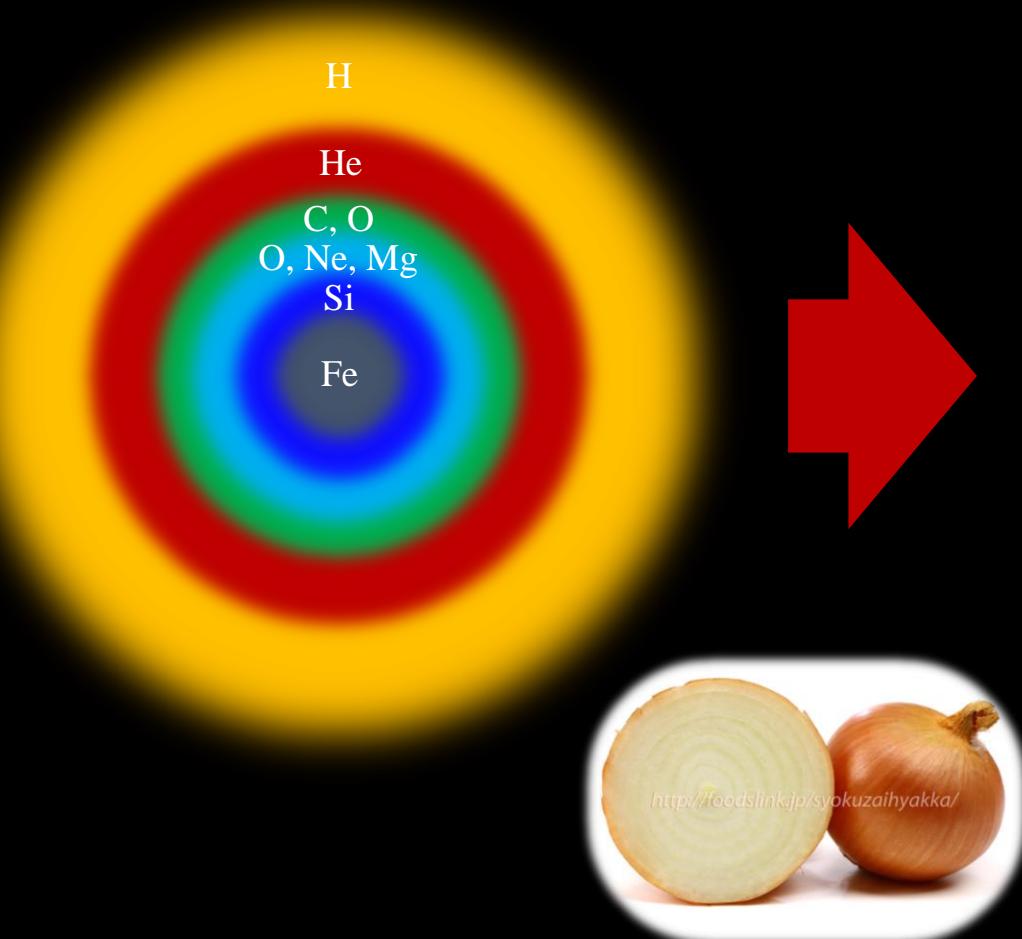


# The fate of a massive star

Nuclear reactions:

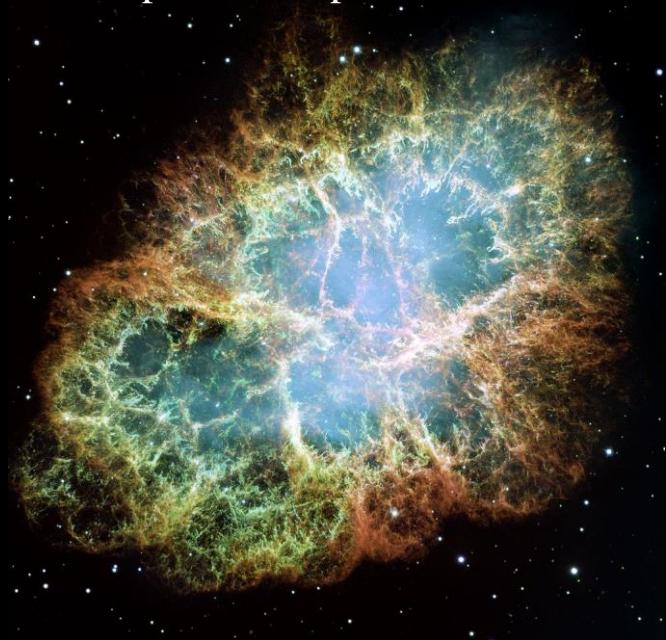


“Onion structure”



After forming the iron core...

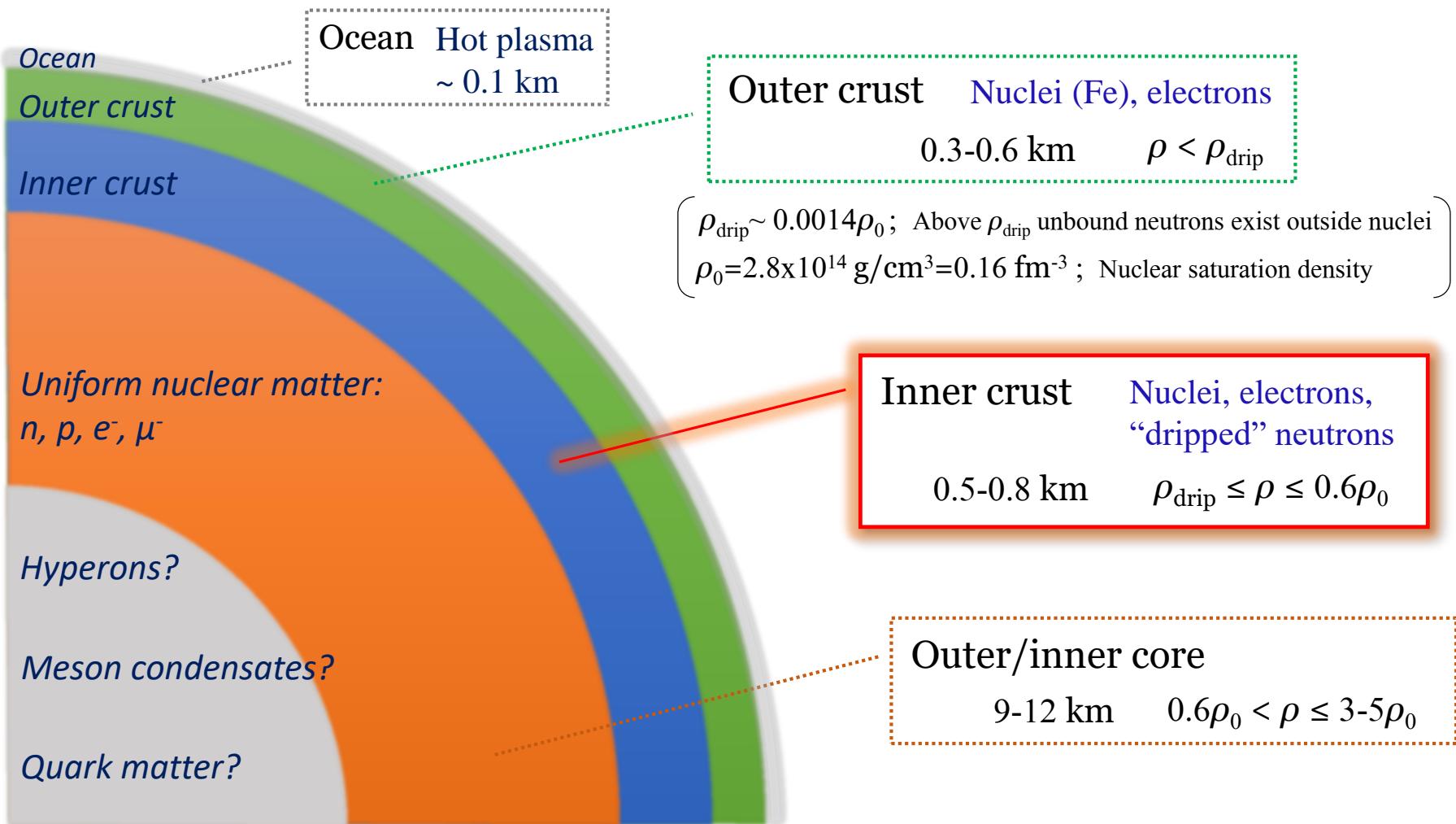
- no more fuel
- gravitational collapse
- supernova explosion



The Crab Nebula  
Remnant of the SN in 1054

# Structure of a neutron star

Neutron star is a great playground for nuclear theorists



# Structure of the inner crust

A lattice of neutron-rich nuclei are imbedded in a sea of electrons.

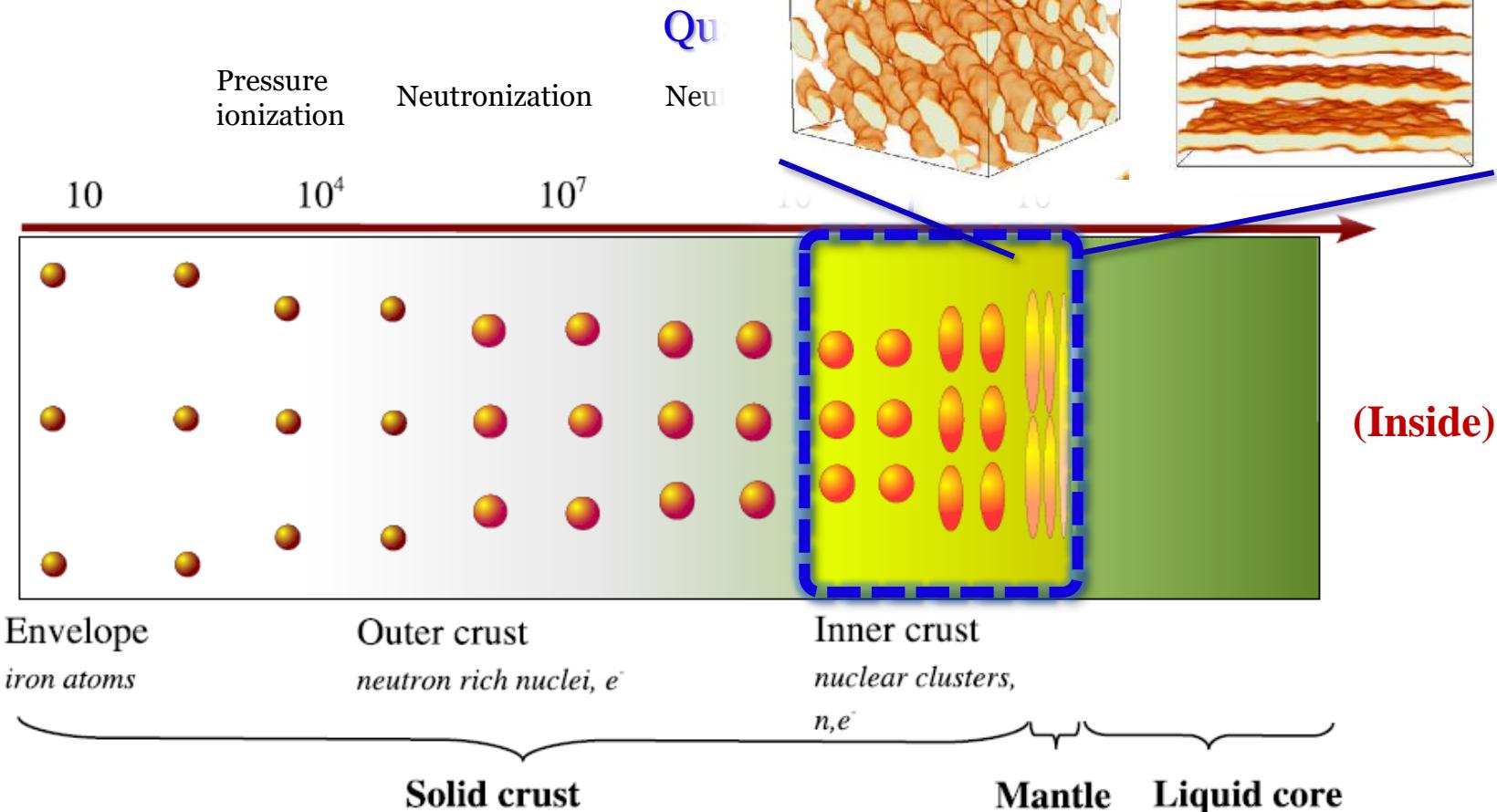


Fig.4 in N. Chamel and P. Haensel, Living Rev. Relativity 11, 10 (2008)

# Quantum vortices

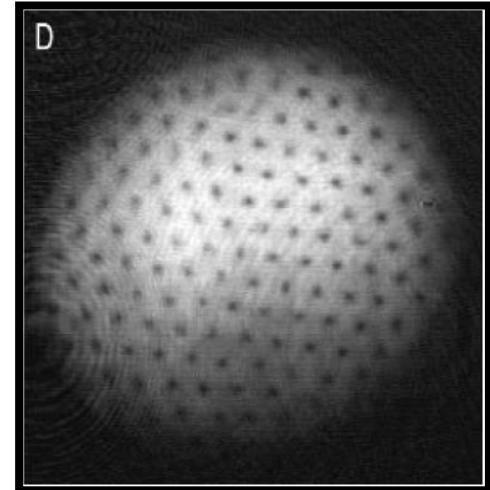
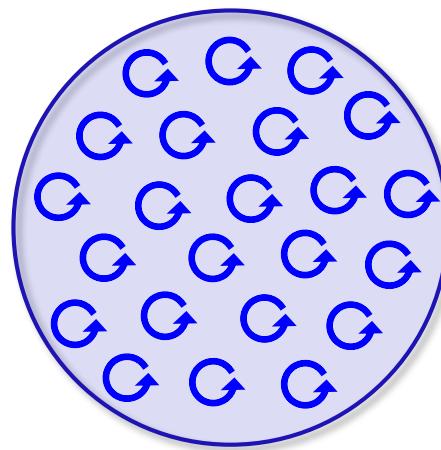
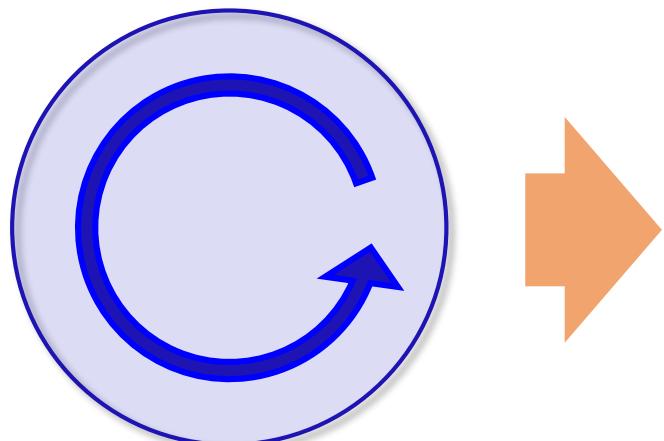
In rotating superfluid, an array

- Observation in ultra-cold atomic gases

## The Nobel Prize in Physics 2003



A.A. Abrikosov V.L. Ginzburg A.J. Leggett



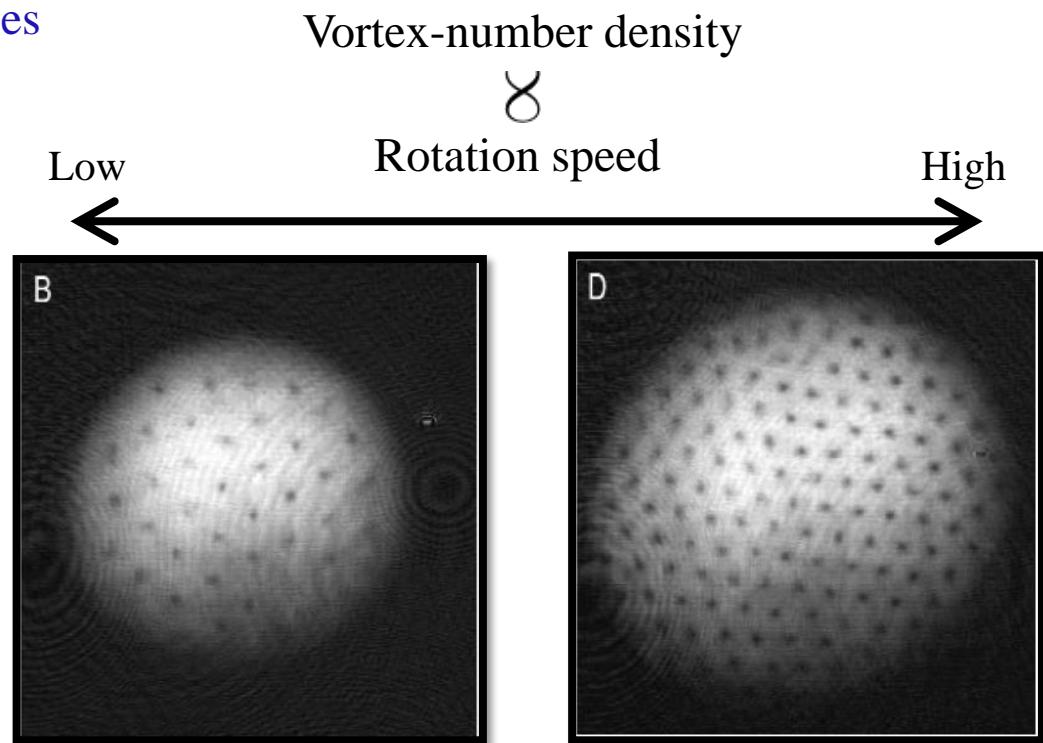
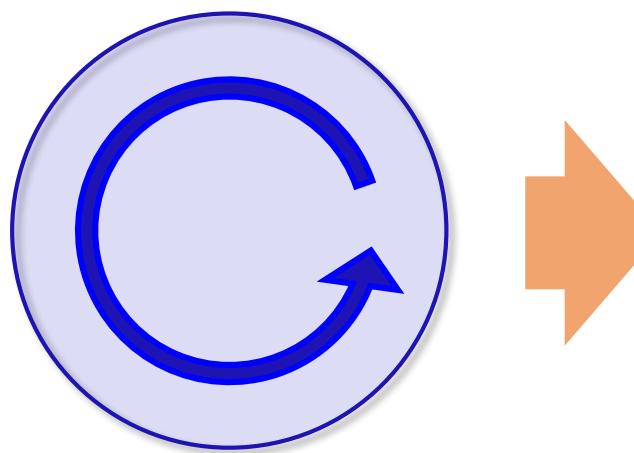
“Abrikosov lattice”

W. Ketterle, MIT Physics Annual. 2001

# Quantum vortices

In rotating superfluid, an array of quantum vortices is generated

## □ Observation in ultra-cold atomic gases

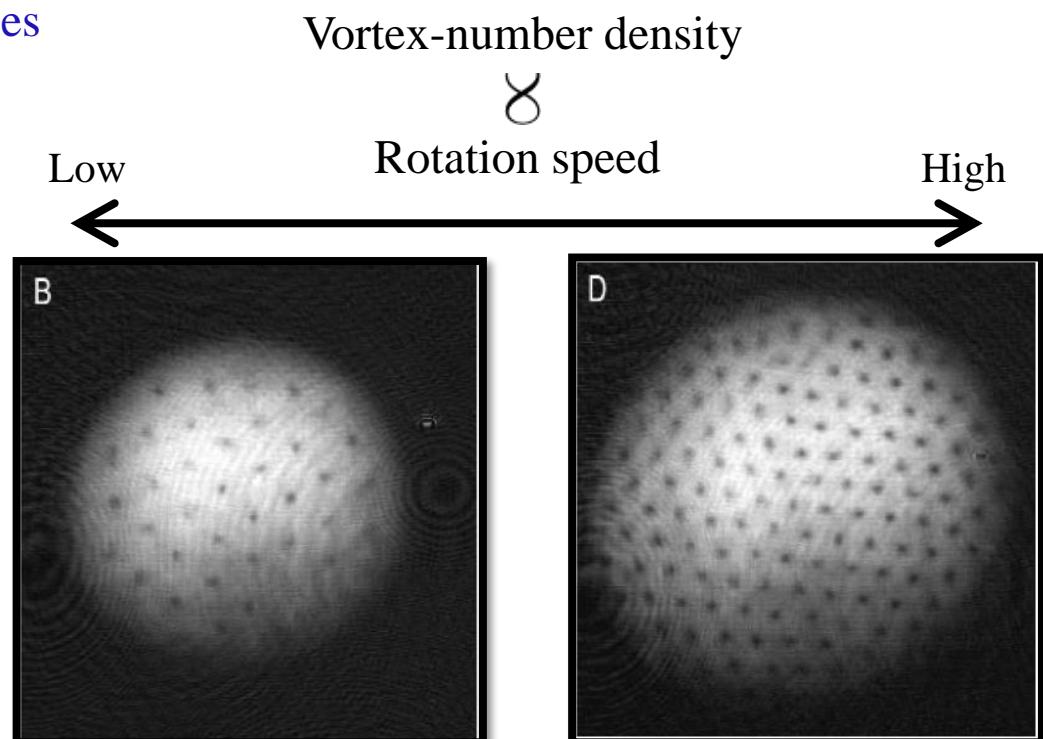
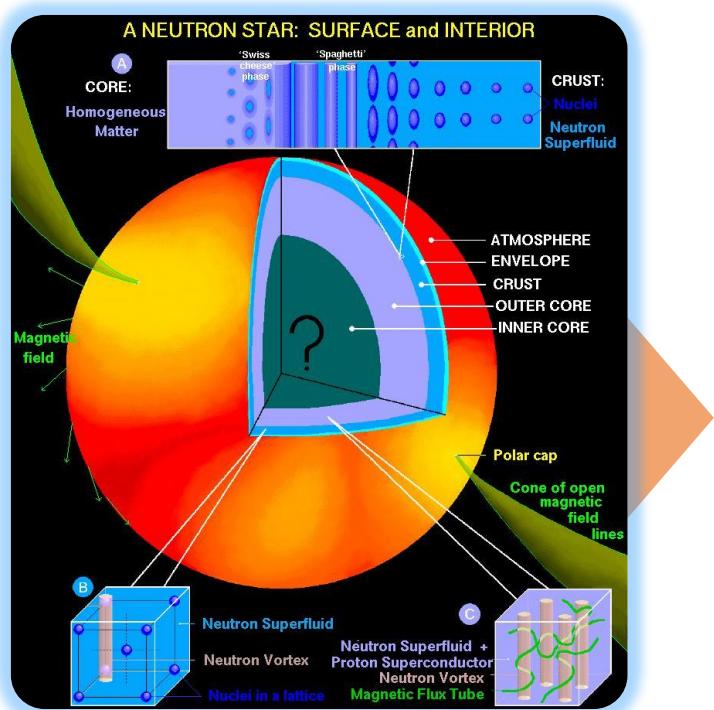


W. Ketterle, MIT Physics Annual. 2001

# Quantum vortices

In rotating superfluid, an array of quantum vortices is generated

## □ Observation in ultra-cold atomic gases

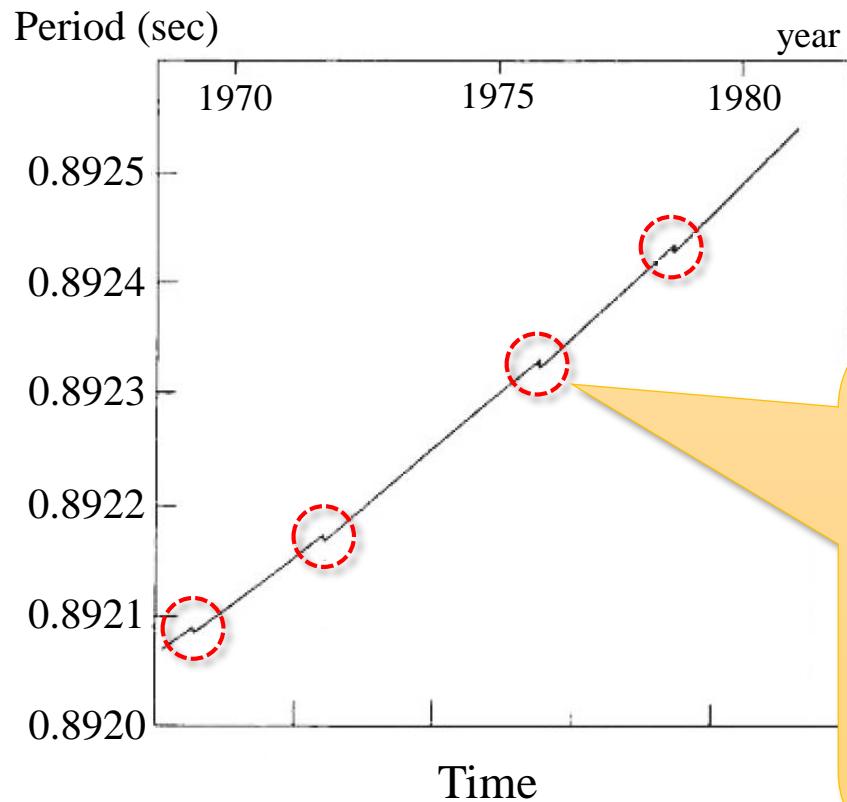


W. Ketterle, MIT Physics Annual. 2001

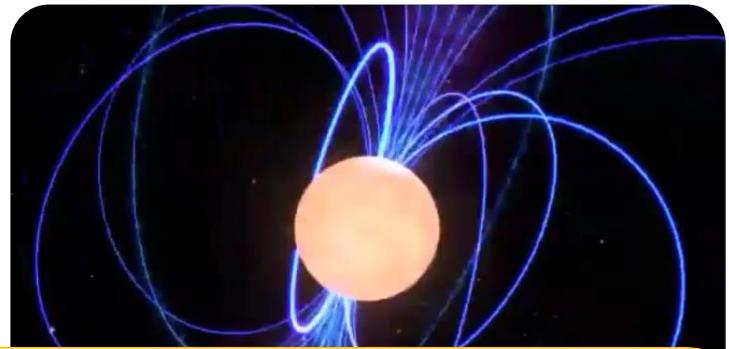
# What is the “glitch”?

Glitch: a sudden increase of the rotational frequency

## □ Glitches in the Vela pulsar

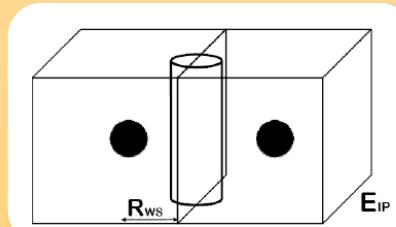


## ➤ Pulsar: a rotating neutron star

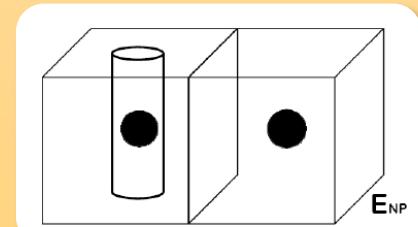


A conjectured scenario:  
Vortex pinning/unpinning in the neutron star crust

Repulsive?



Attractive?



P.W. Anderson and N. Itoh, Nature **256**, 25 (1975)

# *Studies of the pinning force*

## Representative studies of the pinning force

### □ Hartree-Fock-Bogoliubov theory

P. Avogadro, F. Barranco, R.A. Broglia, and E. Vigezzi,  
PRC**75**(2007)012805(R); NPA**788**(2007)130; NPA**811**(2008)378

### □ Thomas-Fermi + LDA

P.M. Pizzochero, L. Viverit, and R. A. Broglia, PRL**79**(1997)3347  
P. Donati and P.M. Pizzochero, PRL**90**(2003)211101; NPA**742**(2004)363; PLB**640**(2006)74  
S. Seveso, P.M. Pizzochero, F. Grill, and B. Haskell, MNRAS**455**(2016)3952

### □ Hydrodynamics + Ginzburg-Landau (for pairing)

M.A. Alpar et al. Astrophys. J. **213**(1977)527; **276**(1984)325  
R.I. Epstein, G. Baym, Astrophys. J. **328**(1988)680  
R.K. Link, R.I. Epstein, Astrophys. J. **373**(1991)592

# Superfluid hydrodynamics

Density dependence and asymptotic behavior of the force are predicted

$$E = E_{\text{tension}} + \frac{1}{2} M^* u^2 + 2\pi R^3 \frac{\rho_{\text{out}}(\rho_{\text{in}} - \rho_{\text{out}})}{2\rho_{\text{out}} + \rho_{\text{in}}} \left( \frac{\kappa}{2\pi r} \right)^2 + \mathcal{O}(1/r^3) \quad (r \gg \xi)$$

Interaction energy between  
a vortex line and an impurity

$\rho_{\text{in}} < \rho_{\text{out}}$  : attraction  
 $\rho_{\text{in}} > \rho_{\text{out}}$  : repulsion

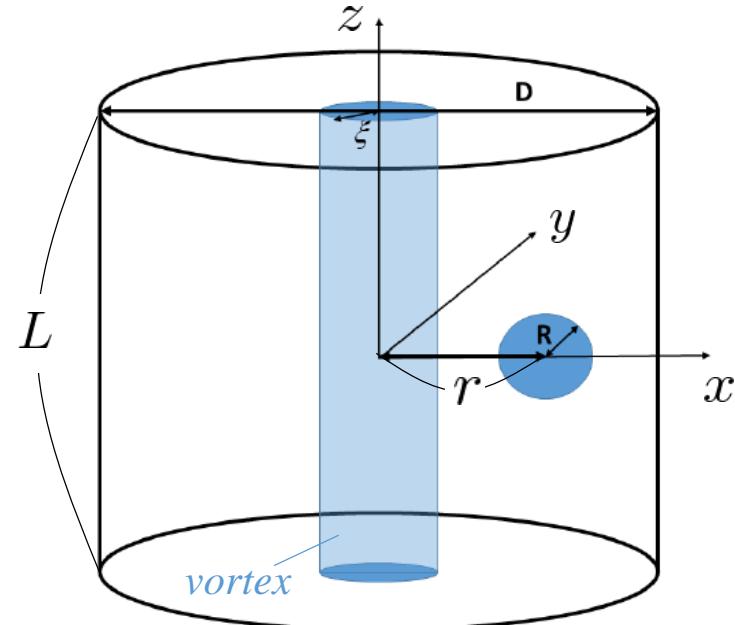
\* $\rho_{\text{in/out}}$  : superfluid density inside/outside a nucleus

$$F = -\frac{dE}{dr} \propto \frac{1}{r^3}$$

$$E_{\text{tension}} = \frac{1}{4\pi} \rho_{\text{out}} \kappa^2 L \ln\left(\frac{D}{2\xi}\right)$$

$$M^* = \frac{4\pi}{3} R^3 \frac{(\rho_{\text{out}} - \rho_{\text{in}})^2}{2\rho_{\text{out}} + \rho_{\text{in}}}$$

$$\kappa = \frac{2\pi\hbar}{2m_n}$$



*What was the state-of-the-art?*

Microscopic, static HFB calculations were performed assuming axial symmetry

$$E_{\text{pin}} = E \left[ \begin{array}{c} \text{Diagram of a cylinder with a central vortex line and a nuclear impurity} \\ - \\ \text{Diagram of a cylinder with a central spherical shell} \end{array} \right] - E \left[ \begin{array}{c} \text{Diagram of a cylinder with three concentric vortex lines} \\ - \\ \text{Diagram of a cylinder with three concentric shells} \end{array} \right]$$

**Energy to create a vortex line  
on a nuclear impurity**

**Energy to create a vortex line  
in a uniform matter**

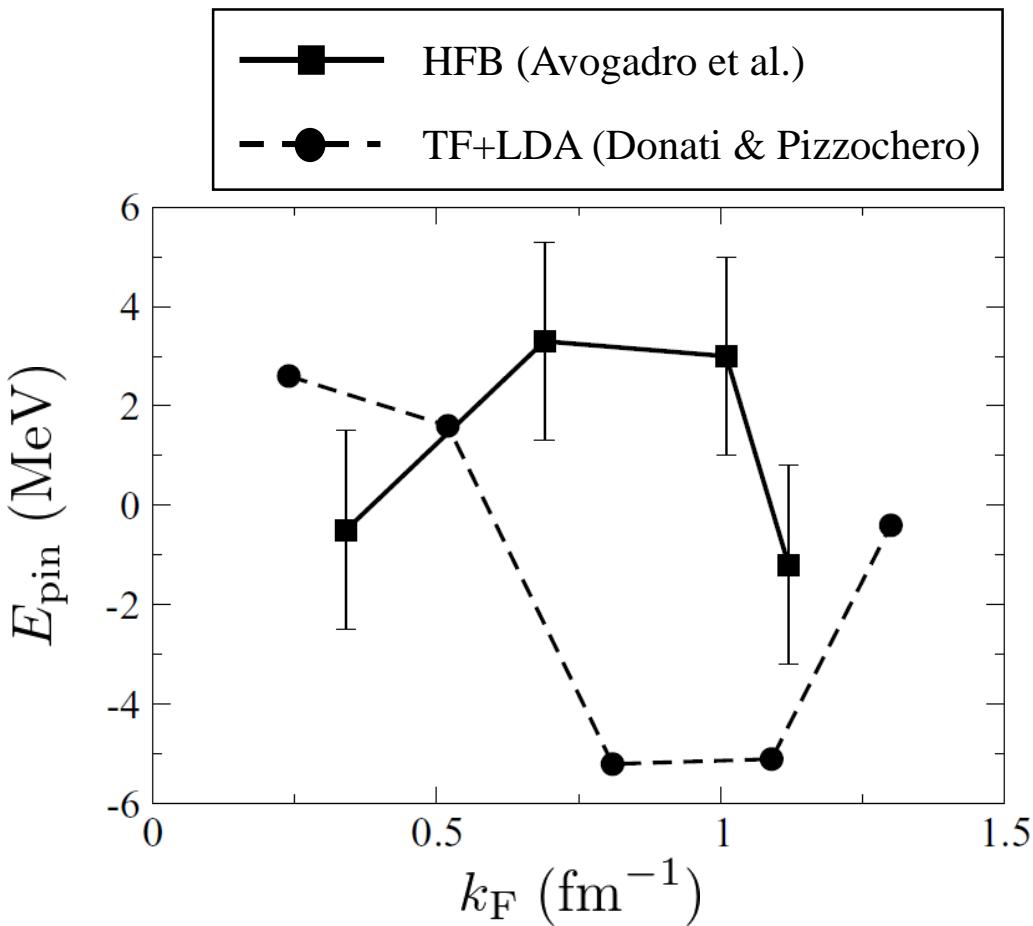
E.g.)  $0.026 \text{ fm}^{-3}$  (SLy4)

6.19 MeV	13058.04	12954.02	13714.88	13617.05
----------	----------	----------	----------	----------

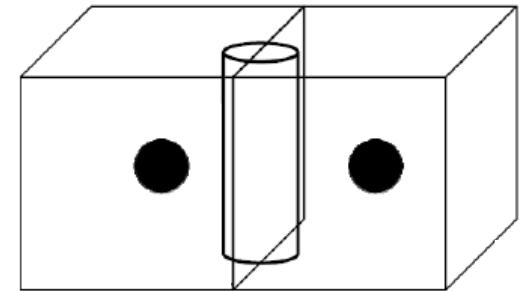
P. Avogadro, F. Barranco, R.A. Broglia, and E. Vigezzi, PRC**75**(2007)012805(R); NPA**788**(2007)130; NPA**811**(2008)378

*What was the state-of-the-art?*

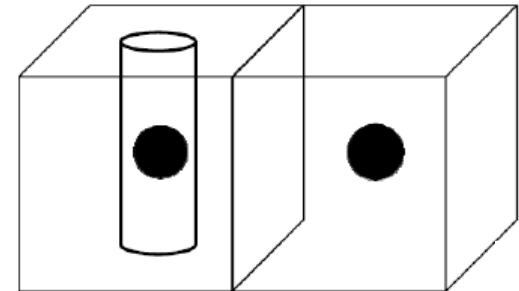
Property of the pinning force was unclear



*Interstitial pinning*

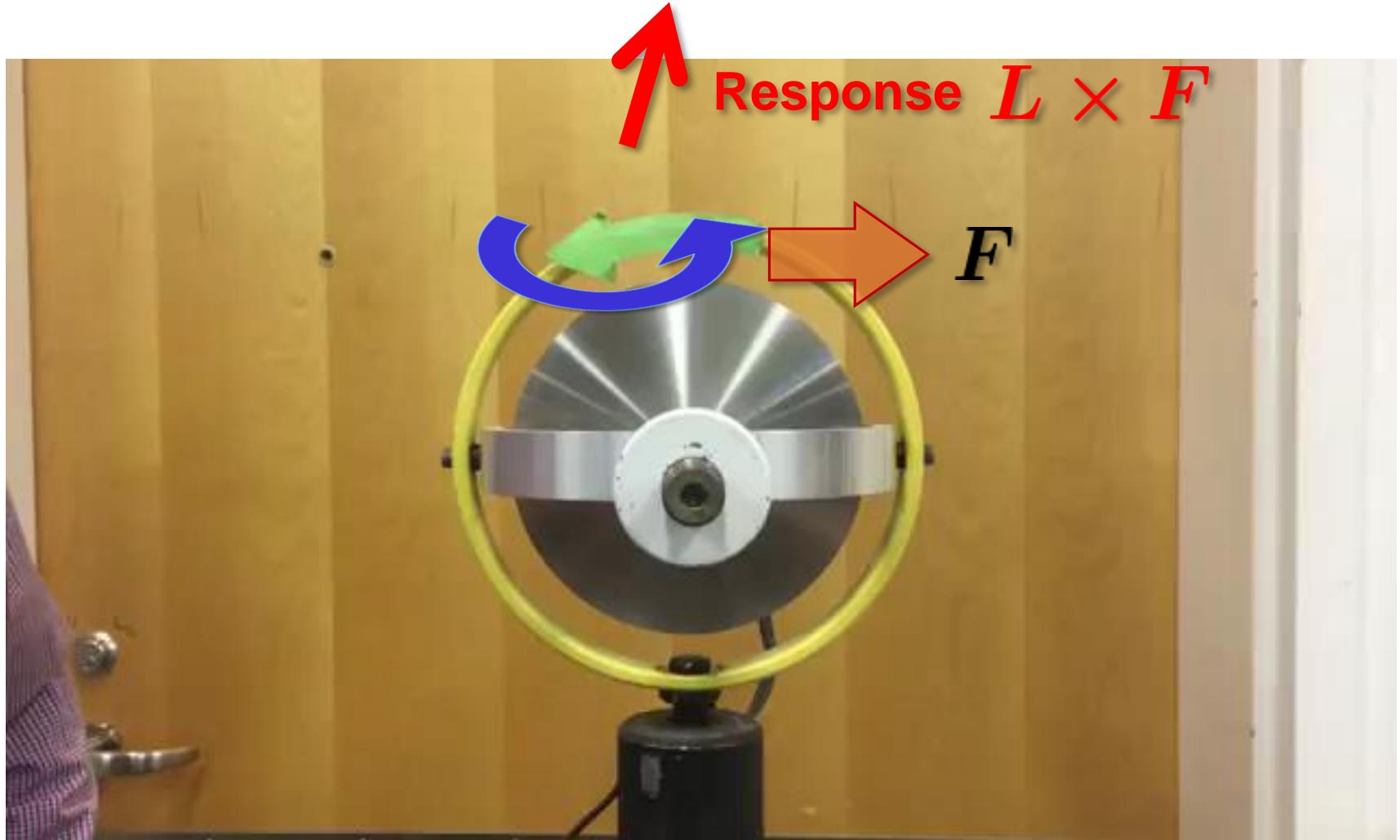


*Nuclear pinning*



## *What we have investigated - Vortex-nucleus dynamics*

Response of a spinning gyroscope when pushed



## Method - TDSLDA

We performed 3D, dynamical simulations by TDDFT with superfluidity

### □ TDSLDA equations (or TDHF, TD-BdG)

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

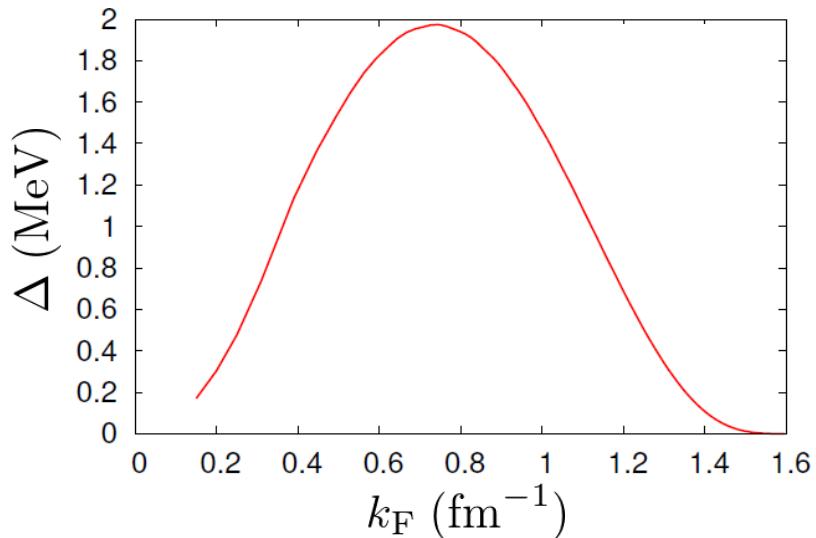
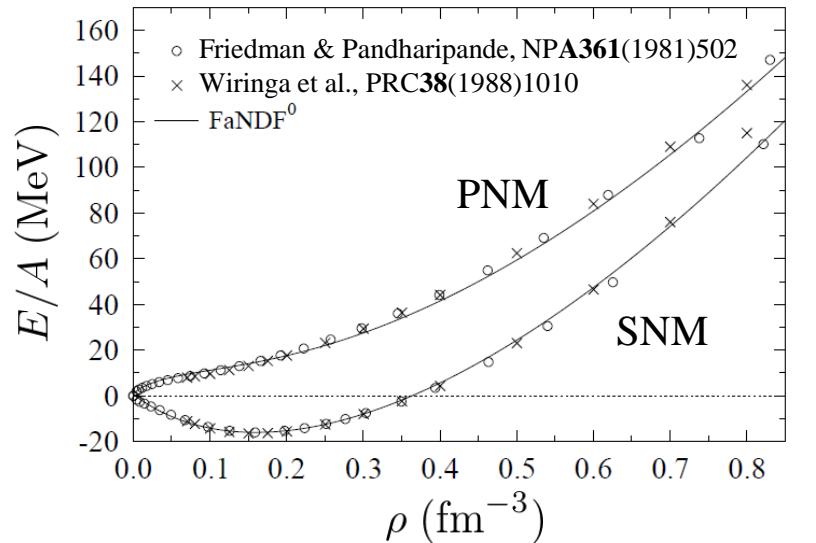
### □ Energy density functional (EDF)

$$\mathcal{E}(\mathbf{r}) = \mathcal{E}_0(\mathbf{r}) + \mathcal{E}_{\text{pair}}(\mathbf{r})$$

$\mathcal{E}_0(\mathbf{r})$  : Fayans EDF (FaNDF<sup>0</sup>) w/o LS

$$\mathcal{E}(\mathbf{r}) = \sum_{q=n,p} g[\rho_q(\mathbf{r})] |\nu_q(\mathbf{r})|^2$$

S.A. Fayans, JETP Lett. **68**, 169 (1998)



## Method - TDSLDA

We performed 3D, dynamical simulations by TDDFT with superfluidity

### □ TDSLDA equations (or TDHF, TD-BdG)

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

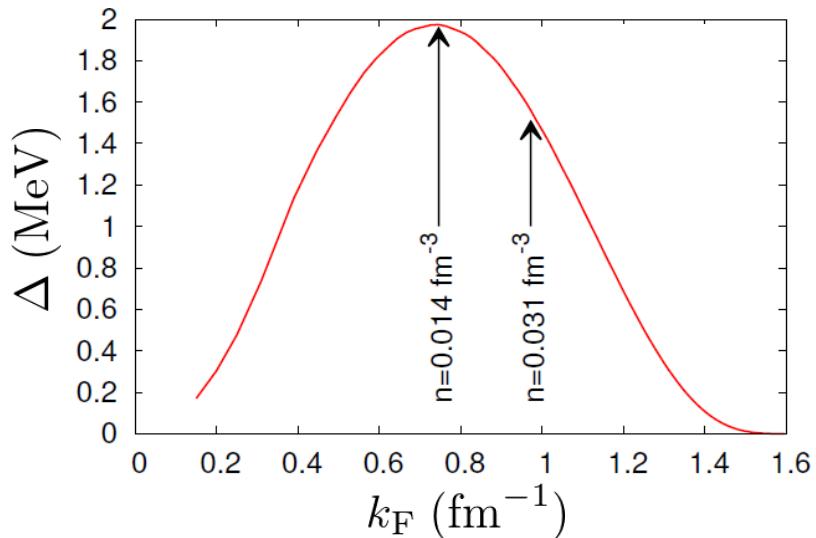
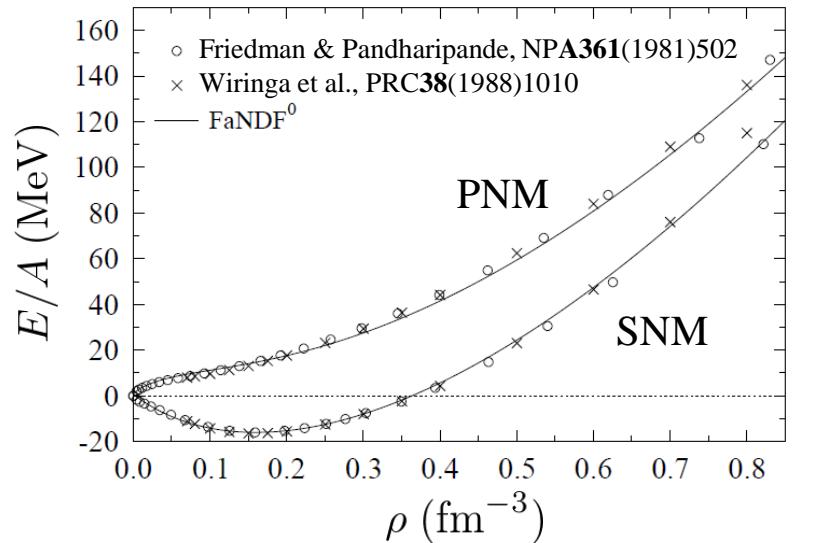
### □ Energy density functional (EDF)

$$\mathcal{E}(\mathbf{r}) = \mathcal{E}_0(\mathbf{r}) + \mathcal{E}_{\text{pair}}(\mathbf{r})$$

$\mathcal{E}_0(\mathbf{r})$  : Fayans EDF (FaNDF<sup>0</sup>) w/o LS

$$\mathcal{E}(r) = \sum_{q=n,p} g[\rho_q(r)] |\nu_q(r)|^2$$

S.A. Fayans, JETP Lett. **68**, 169 (1998)



## Method - TDSLDA

We performed 3D, dynamical simulations by TDDFT with superfluidity

### ■ TDSLDA equations (or TDHF, TD-BdG)

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

### ■ Computational details

75 fm  $\times$  75 fm  $\times$  60 fm

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

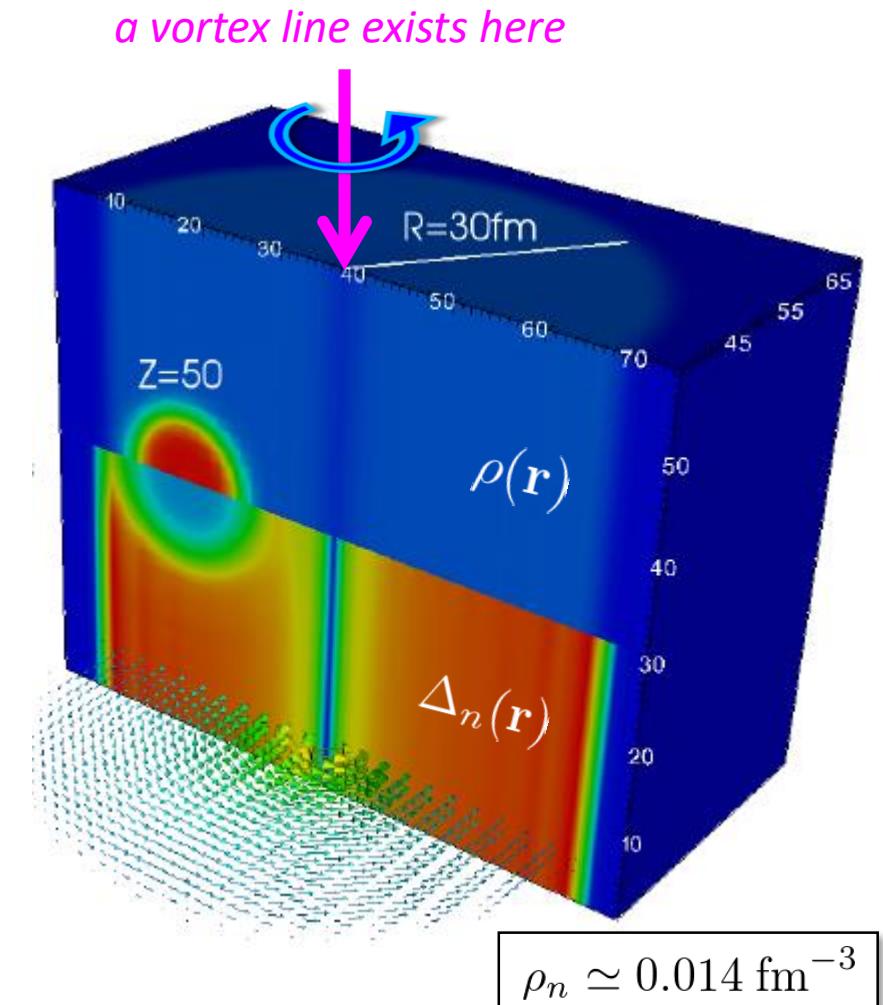
$$k_c = \pi / \Delta x > k_F \quad k_F = (3\pi^2 \rho_n)^{1/3}$$

Nuclear impurity:  $Z = 50$

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

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

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



# Method - TDSLDA

We performed 3D, dynamical simulations by TDDFT with superfluidity

## ■ TDSLDA equations (or TDHF, TD-BdG)

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

## ■ Computational details

75 fm  $\times$  75 fm  $\times$  60 fm

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

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

Nuclear impurity:  $Z = 50$

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

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

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

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



TITAN, Oak Ridge



NERSC Edison, Berkeley



HA-PACS, Tsukuba

## How to extract the force

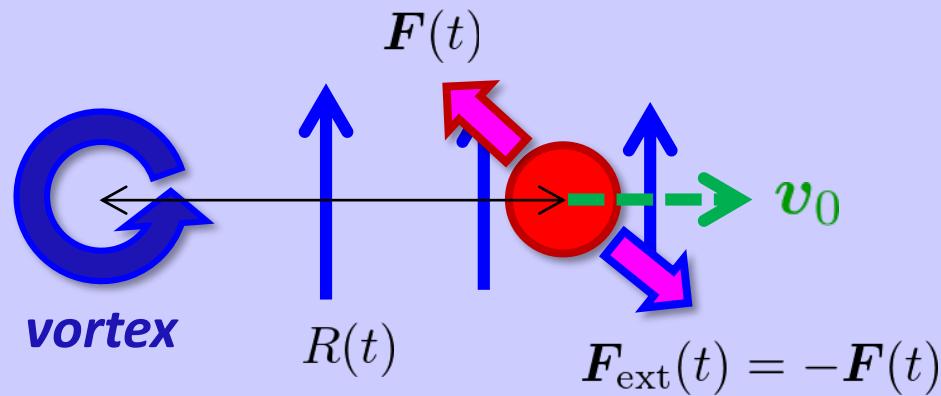
We directly measure the force  $\mathbf{F}(R)$  in dynamical simulation

- Newton's law

$$\mathbf{F} = M \frac{d\mathbf{v}}{dt} \quad \rightarrow \quad \frac{d\mathbf{v}}{dt} = 0 \quad \text{if} \quad \mathbf{F} = 0$$

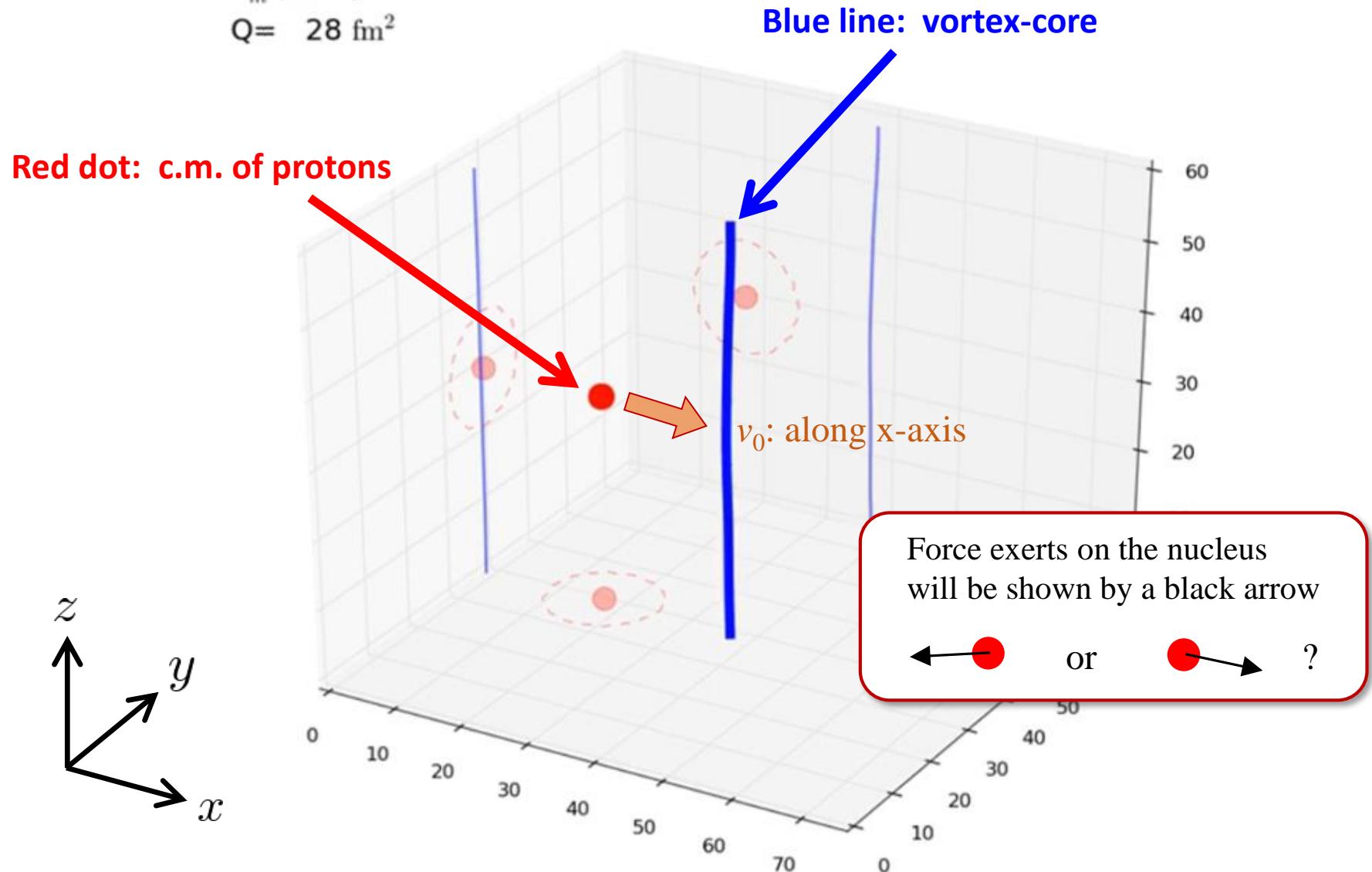
- We keep a nuclear motion in a constant velocity  $v_0$  ( $\ll v_{\text{crit}}$ )

*Superfluid neutrons*



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

time= 0 fm/c  
 $F_m(19.1)$ = unknown  
 $Q= 28 \text{ fm}^2$



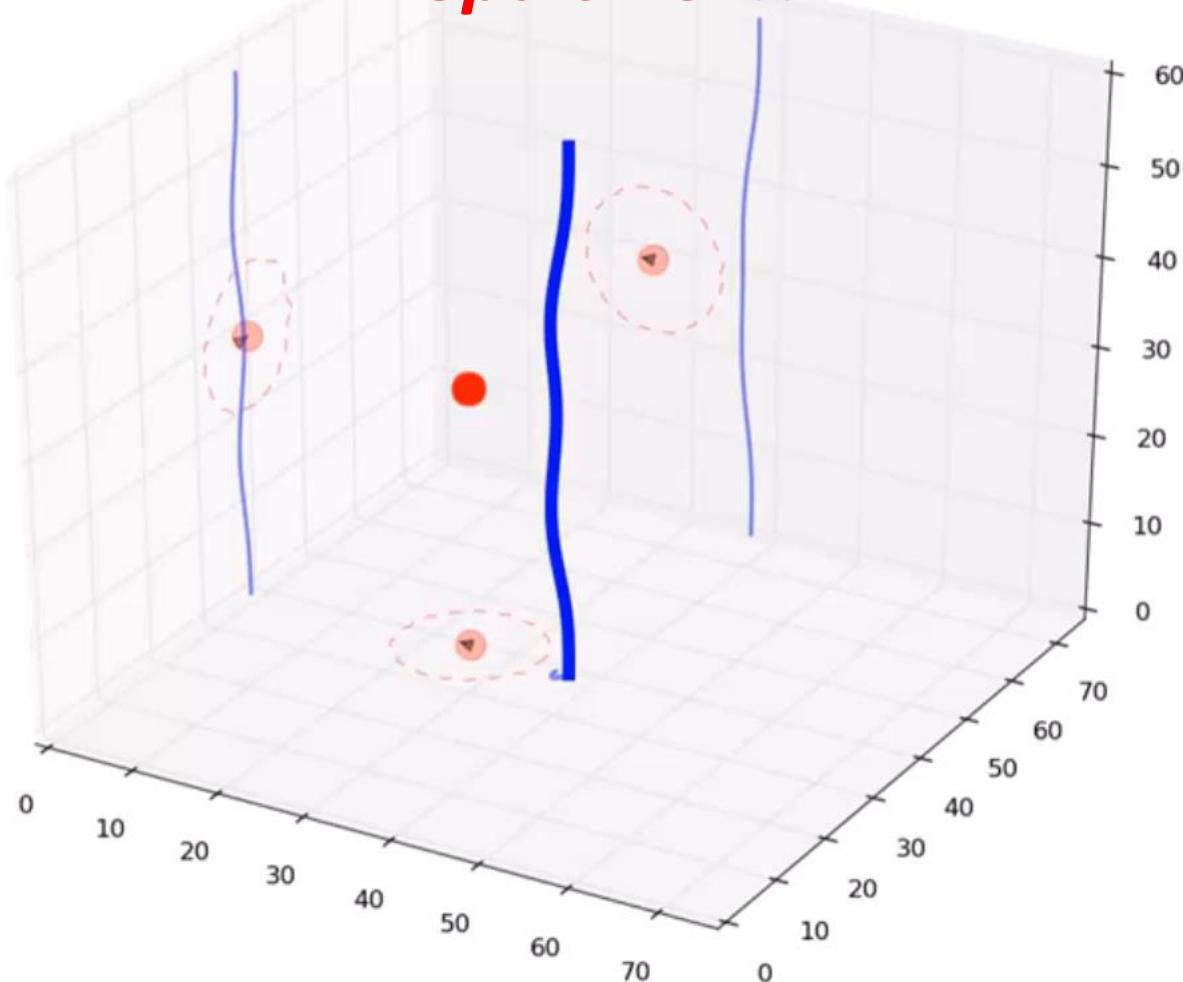
Results of TDSLDA calculation:  $\rho_n \simeq 0.014 \text{ fm}^{-3}$

time= 8032 fm/c

$F_m(10.6) = 0.17 \text{ MeV/fm}$

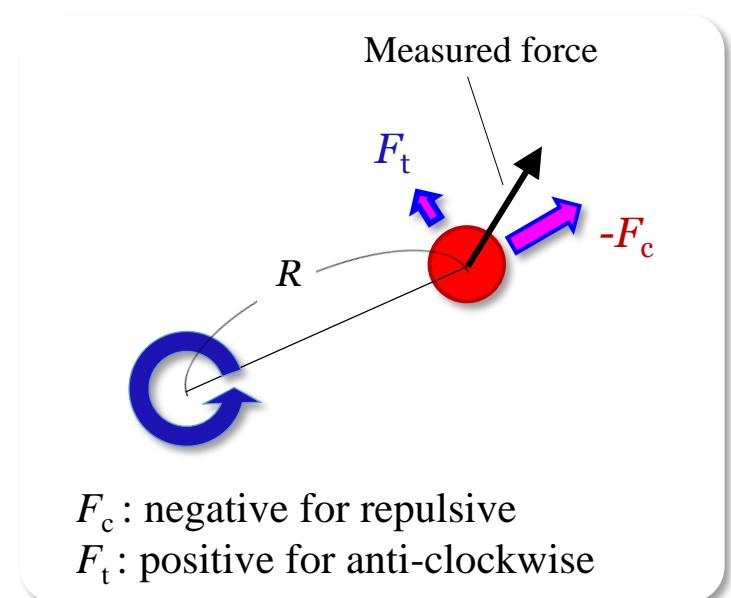
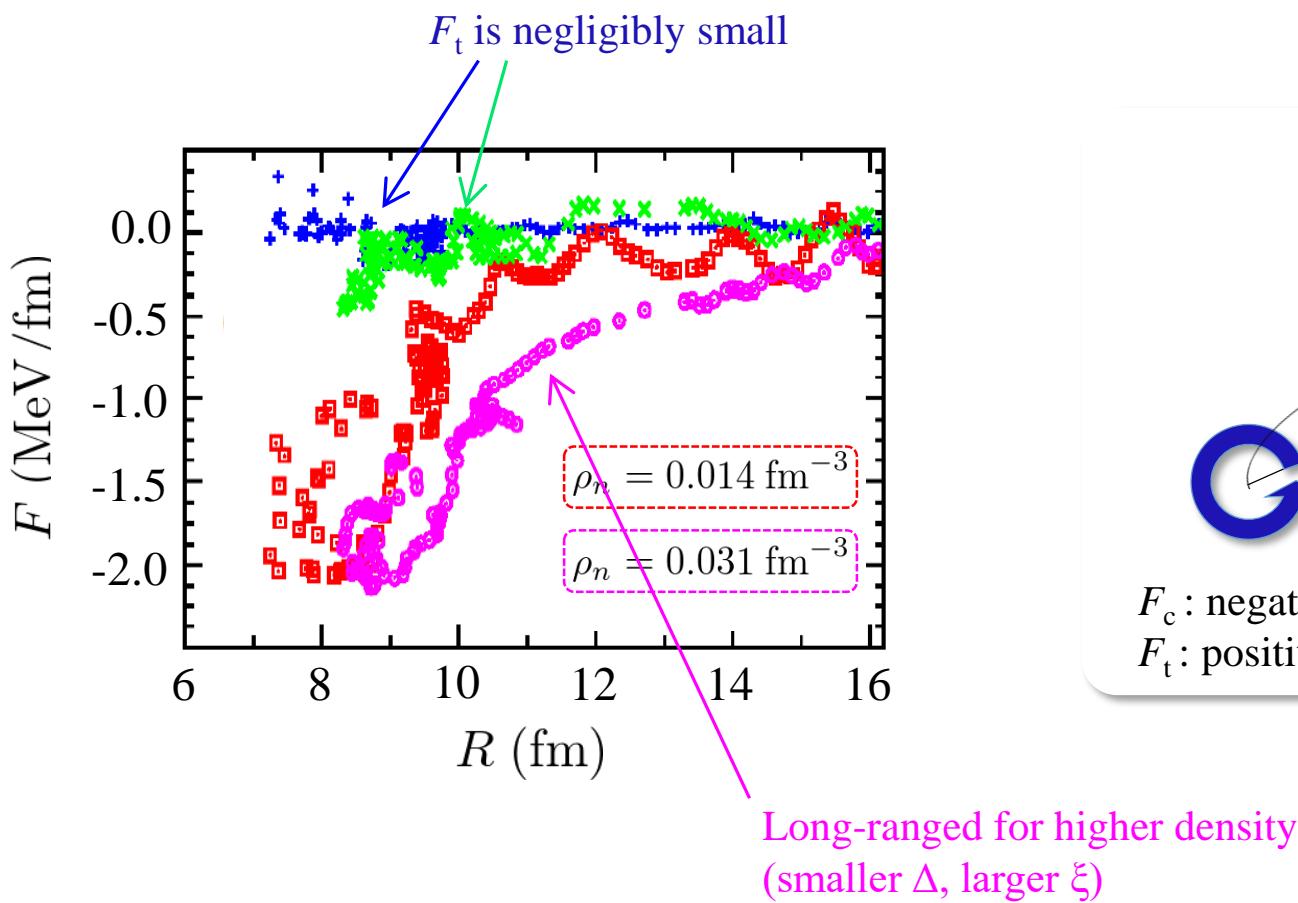
$Q = 13 \text{ fm}^2$

**"Repulsive"!!**



## Measured force

The force is essentially central, not a simple function of  $R$



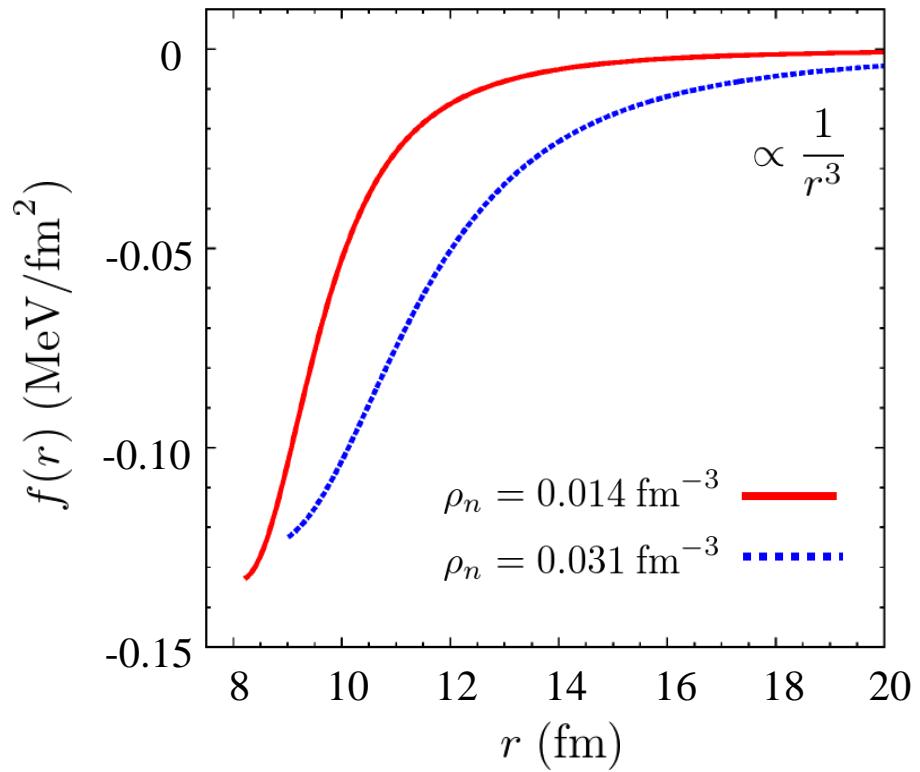
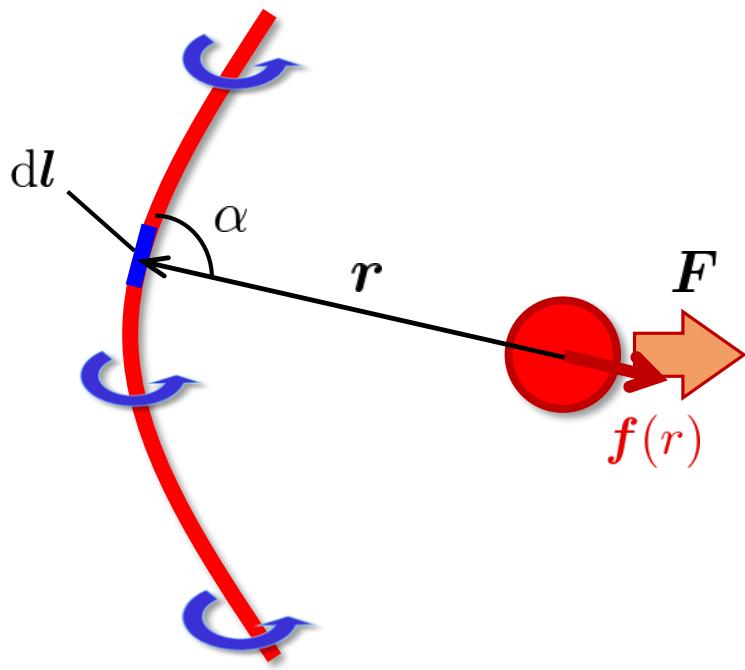
# Force per unit length

We can predict the force for any vortex-nucleus configuration

- Force per unit length

$$\mathbf{F} = \int_L f(r) \sin \alpha \, \mathbf{e}_r \, dl$$

$$f(r) = \frac{\sum_{k=0}^n a_k r^k}{1 + \sum_{k=1}^{n+3} b_k r^k} \quad \text{Padé approximant} \quad (n=2 \text{ was used})$$

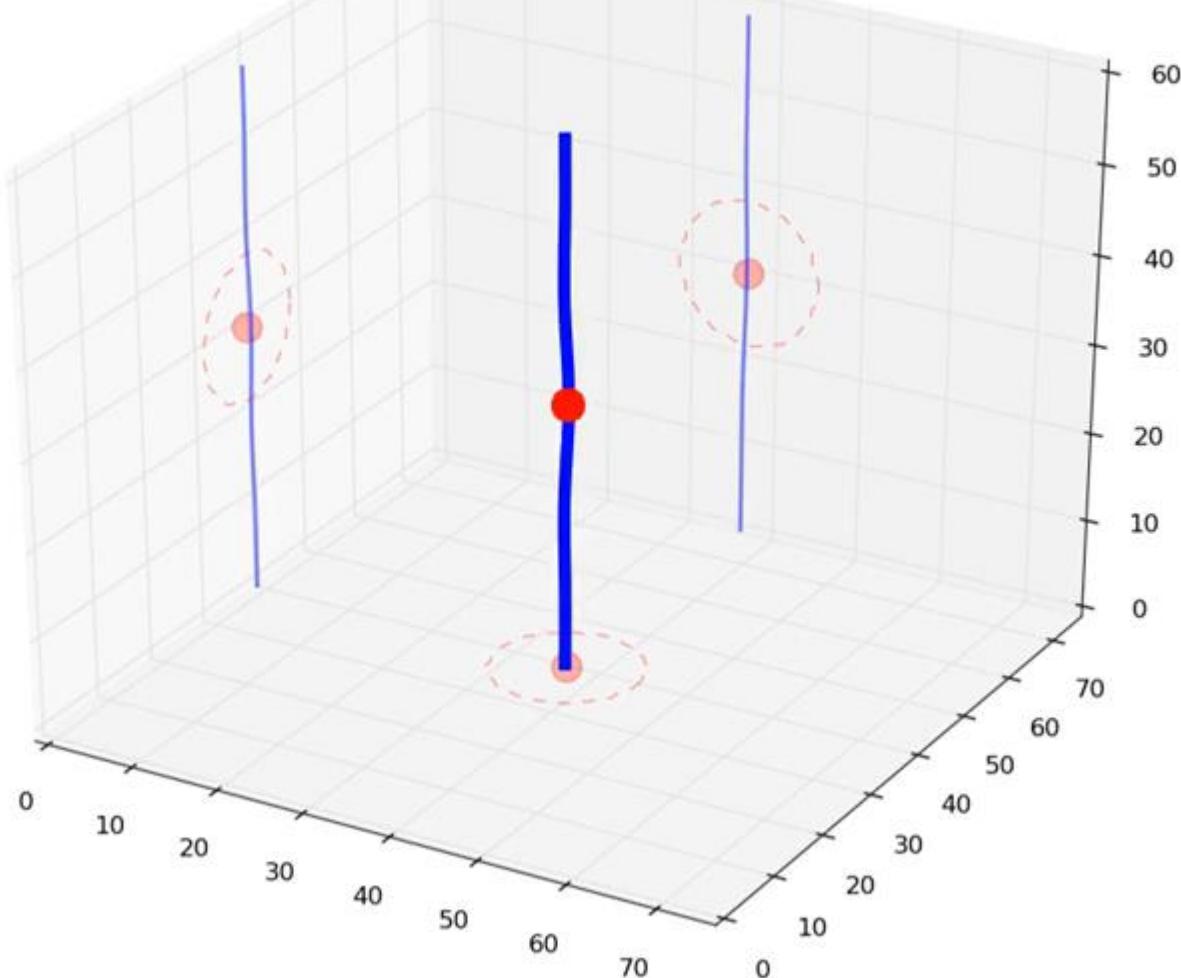


Results of TDSLDA calculation:  $\rho_n \simeq 0.014 \text{ fm}^{-3}$

time= 0 fm/c

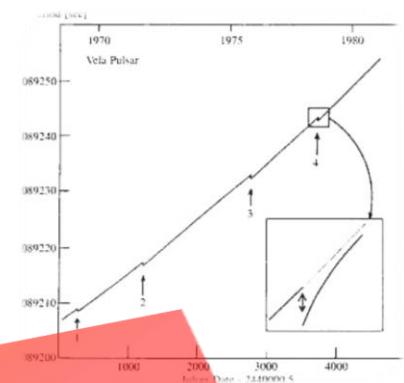
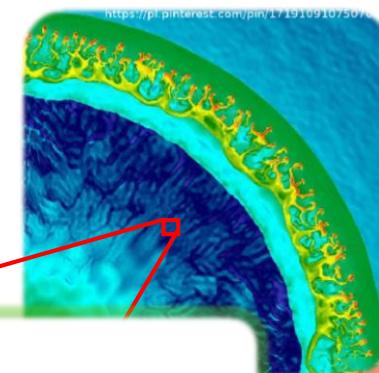
Q= -11 fm<sup>2</sup>

Pinned configuration is dynamically unstable



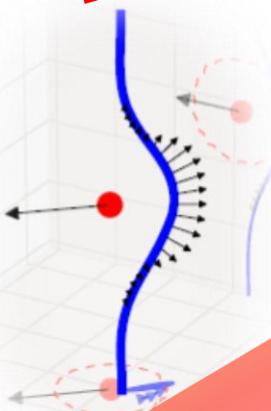
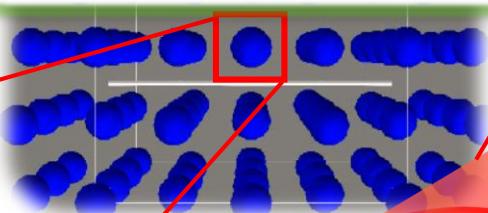
# Our goal and strategy

Goal: Unveil the mechanism of glitches



New collaboration started:

Nicolaus Copernicus Astronomical Centre  
B. Haskell et al.



$10^4 \text{ m}$

**Macroscopic**

- observations
- hydrodynamics

**Mesoscopic**

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

Provide model ingredients

$10^{-15} - 10^{-13} \text{ m}$

**Microscopic**

*Nuclear Physics!!*

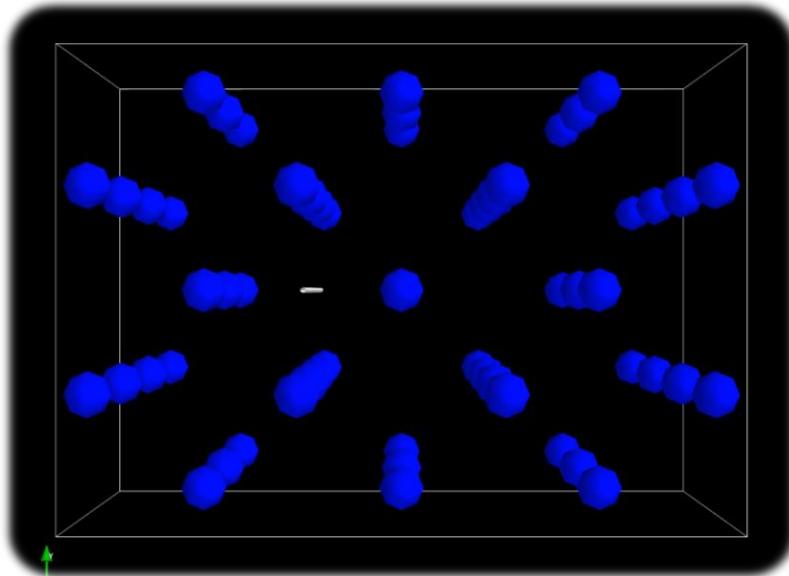
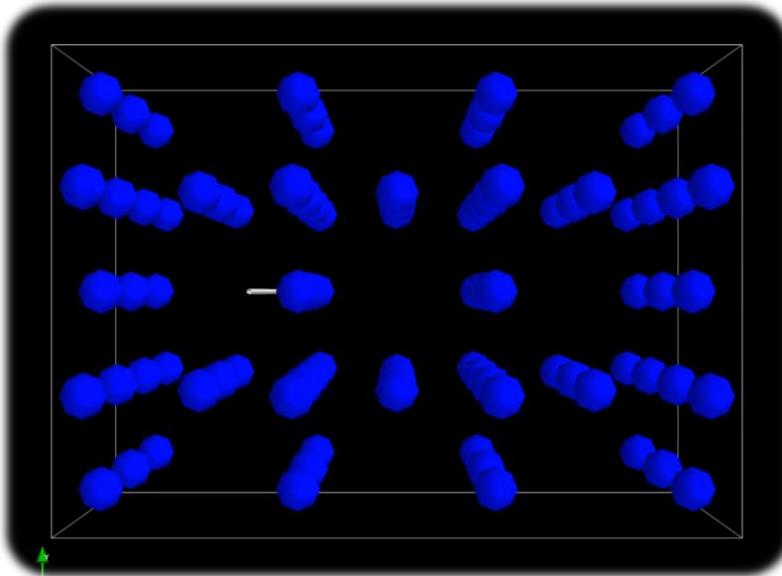
- vortex-nucleus dynamics from *neutrons and protons*

Ongoing project

*Mesoscopic simulation of pinning force with the vortex filament model*

Simulations by K. Kobczewski (PhD student at WUT)

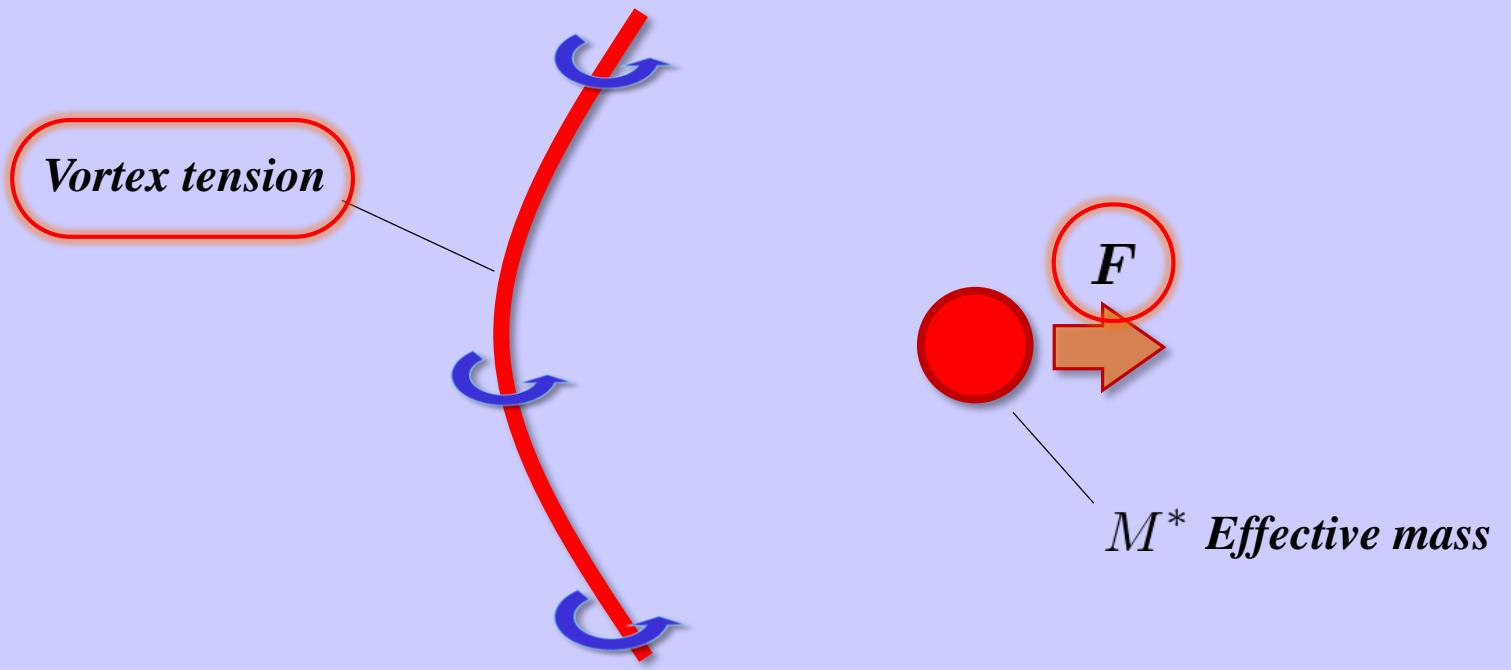
$$n_s \kappa \times (\mathbf{v}_{vor} - \mathbf{v}_{ext}) = \mathbf{f}_{VN} + \mathbf{f}_{tension} + \mathbf{f}_{dissipation}$$



Talk by K. Kobczewski at POLNS18, March 26-28, 2018: <https://indico.camk.edu.pl/event/10/contribution/8>

**Very preliminary**

## *Superfluid neutrons*



## Vortex tension

We can evaluate the vortex tension from the dynamical simulations

$$T \lesssim \frac{E^*}{\Delta L} = \left( E \left[ \begin{array}{c} L_2 \\ \text{---} \\ \text{---} \end{array} \right] - E \left[ \begin{array}{c} L_1 \\ \text{---} \\ \text{---} \end{array} \right] \right) / \Delta L$$

Work done by  $\mathbf{F}_{\text{ext}}$

$$\int_{t_0}^{t_1} \mathbf{F}(t) \cdot \mathbf{v}(t) dt$$

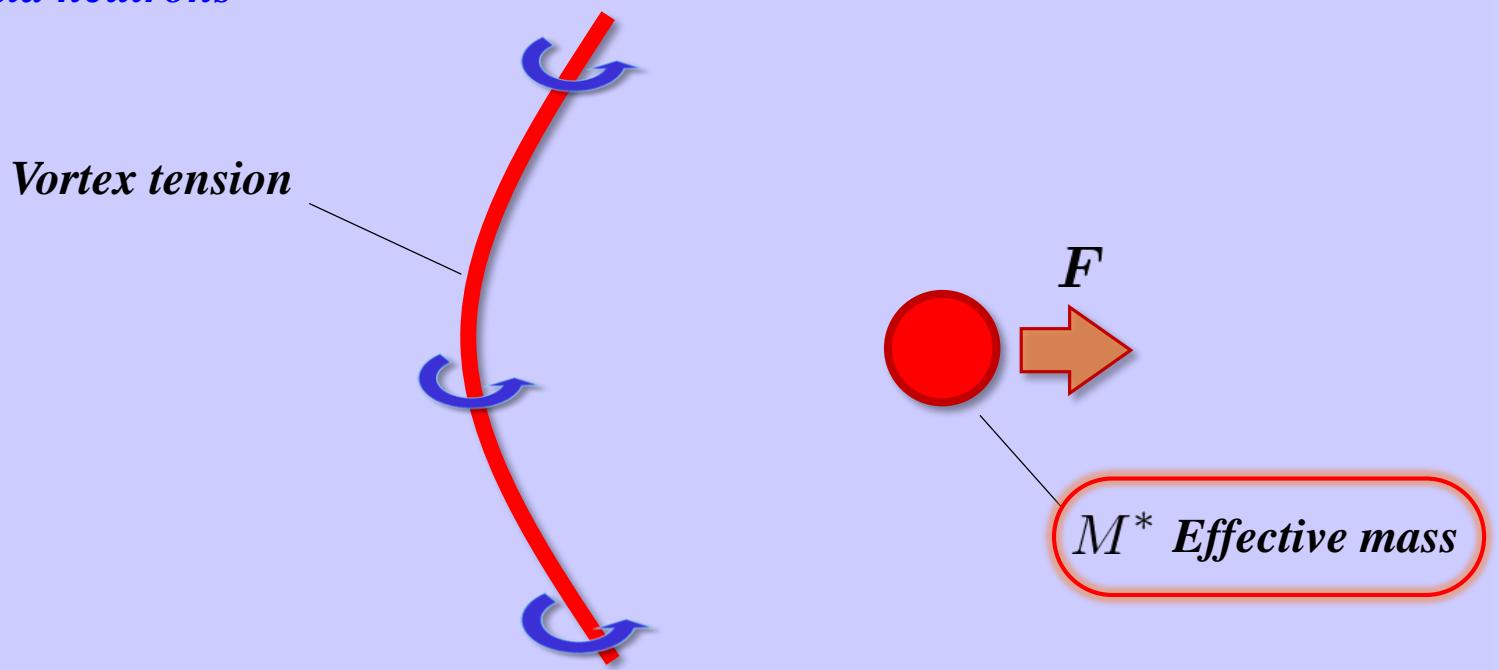


$$T \lesssim \frac{5}{3.5} = 1.4 \text{ MeV/fm} \quad n = 0.014 \text{ fm}^{-3}$$

$$T \lesssim \frac{11}{1.5} = 7.3 \text{ MeV/fm} \quad n = 0.031 \text{ fm}^{-3}$$

$$\frac{1.4}{7.3} = 0.19 \quad \text{cf. hydrodynamic approx.: } 0.77$$

## *Superfluid neutrons*



# How to extract the effective mass

Dragging by a constant force provides the effective mass

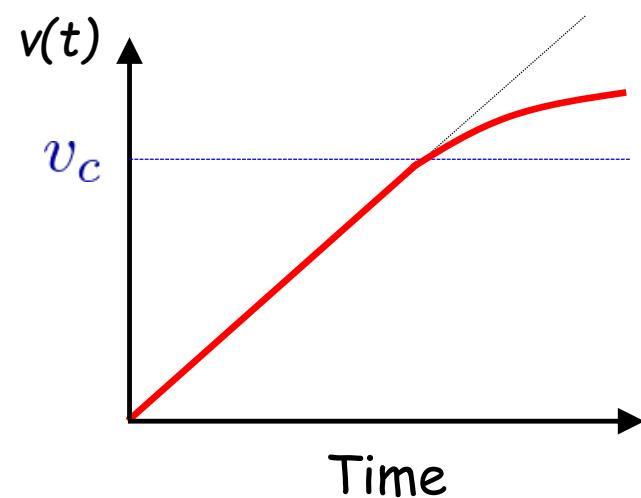
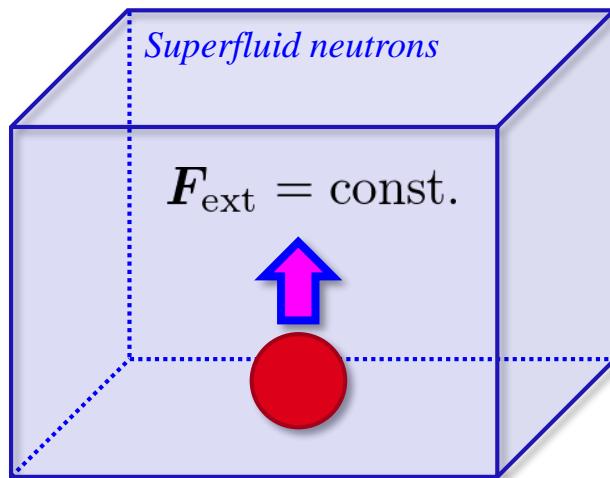
- Newton's law

$$\mathbf{F} = M \frac{d\mathbf{v}}{dt}$$



$$M = F \left( \frac{d\mathbf{v}}{dt} \right)^{-1}$$

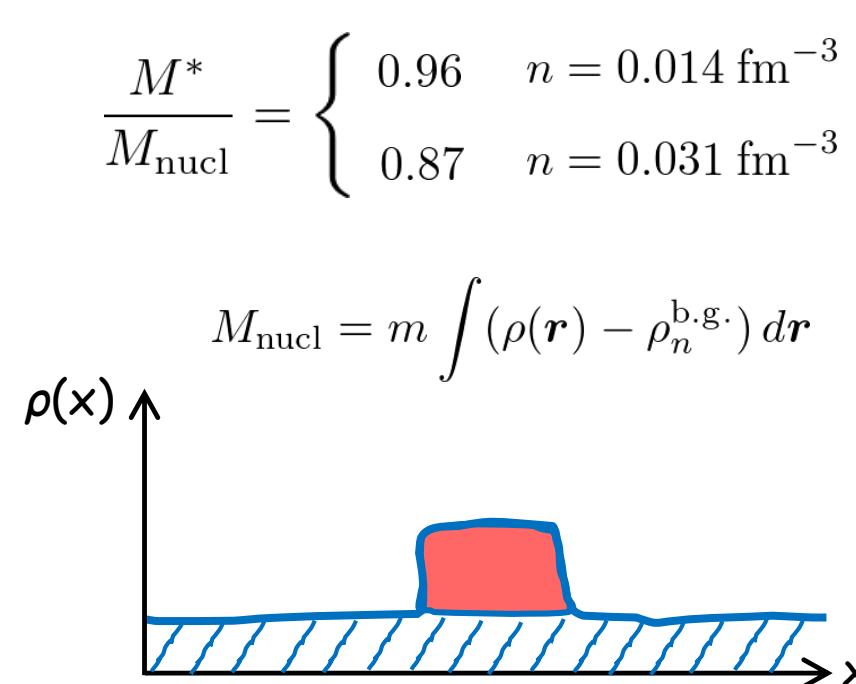
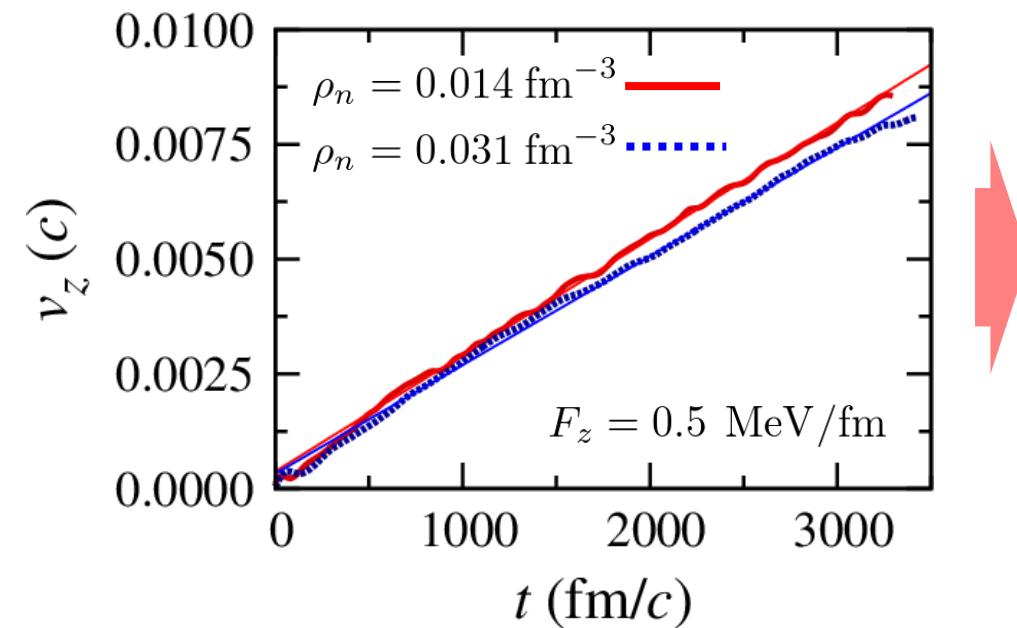
- We accelerate a nuclear impurity by a constant force



# Effective mass

Dynamical effects may reduce the effective mass

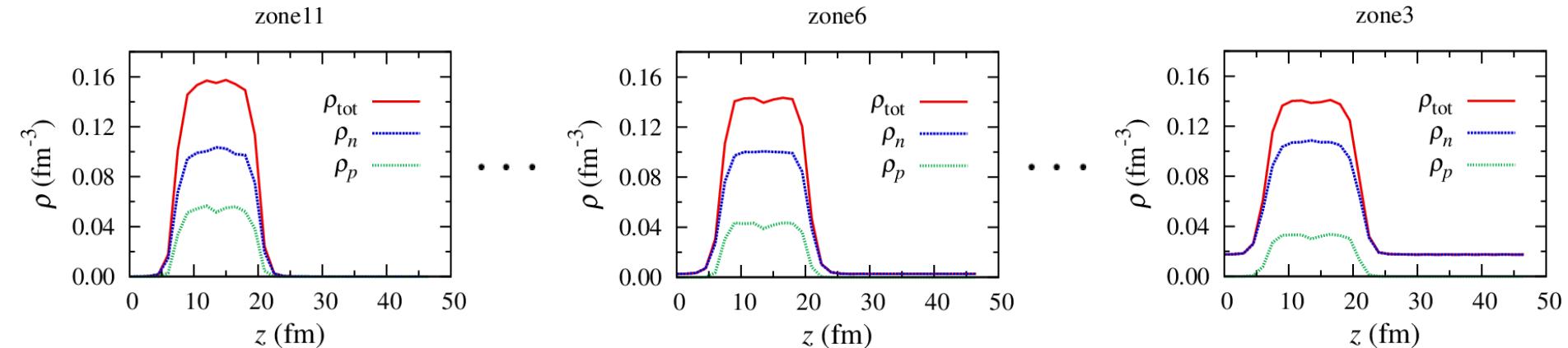
*Very preliminary*



## Effective mass: future work

We are going to calculate  $M^*$  and  $v_c$  through out the inner crust

- ✓ We have prepared initial states for dynamical simulations

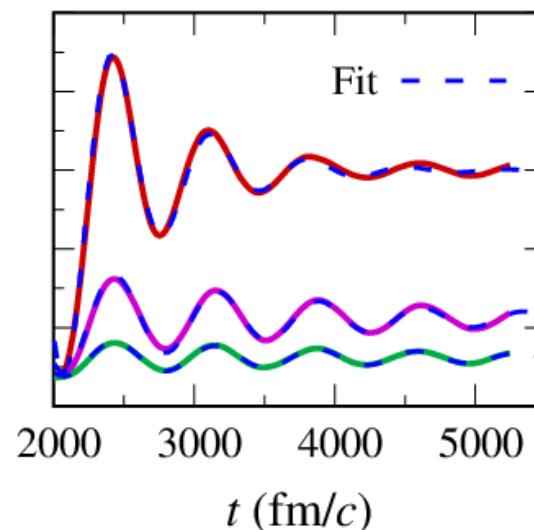
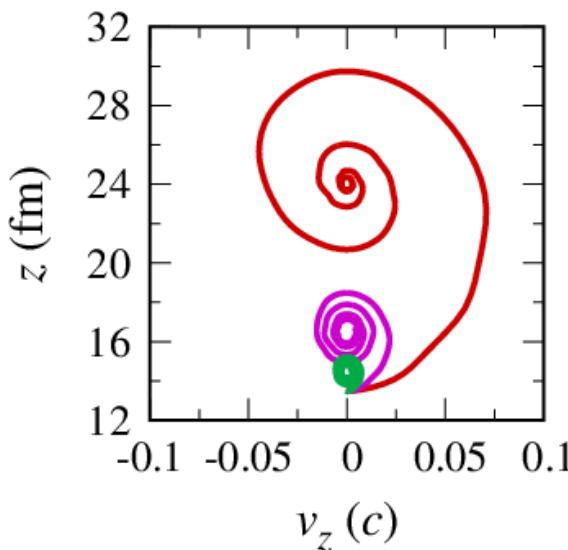


# Crust oscillation

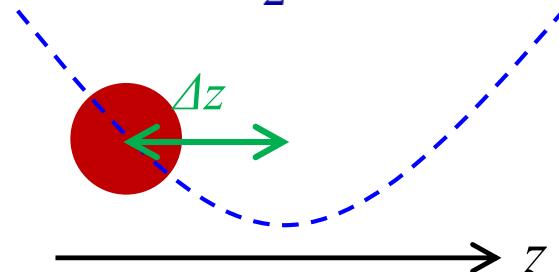
Coupling between the nuclear lattice and superfluid may be extracted

$$\rho_n \sim 0.024 \text{ fm}^{-1}; Z=50, R_{WS}=33 \text{ fm}$$

*Very preliminary*



$$V(z) = \frac{1}{2} M^* \omega_p^2 z^2$$



$$\omega_p = \sqrt{\frac{3Z^2e^2}{M^* R_{WS}^3}}$$

$$\Gamma = 0.330 \text{ MeV}; \tau = 598.46 \text{ fm}/c$$

$$\begin{aligned} \Gamma &= 0.123 \text{ MeV}; \tau = 1600.09 \text{ fm}/c \\ \Gamma &= 0.083 \text{ MeV}; \tau = 2370.53 \text{ fm}/c \end{aligned}$$



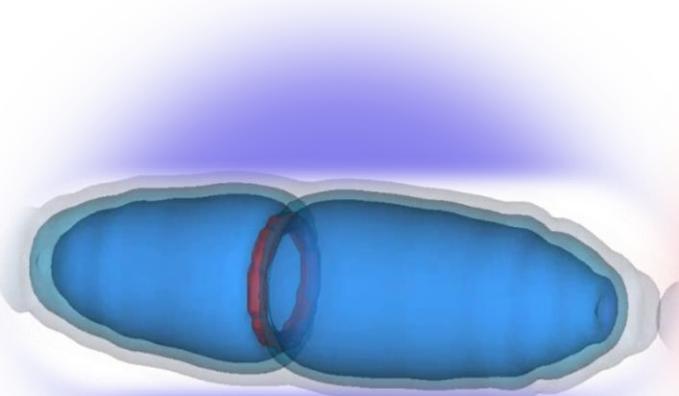
## Conclusion

---

# Conclusion

## Takeaway message

- ✓ TDSLDA is a powerful tool to study a variety of dynamics in superfluid Fermi systems!

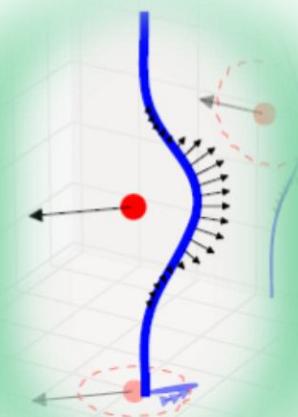


### *Cold atoms:* **UFG**

- solitonic cascades
- quantum turbulence

### *Atomic nuclei:* **Nuclear dynamics**

- solitonic excitations
- fusion hindrance



### *Neutron star:* **Inner crust**

- vortex-nucleus interaction
- tension,  $M^*$ , dissipations

*Kazuyuki Sekizawa*

*Specially Appointed Assistant Professor*

*Center for Transdisciplinary Research*

*Institute for Research Promotion, Niigata University*

*8050, Ikarashi Ninoho, Nishi-ku, Niigata City, Niigata 950-2181, Japan*

*sekizawa @ phys.sc.niigata-u.ac.jp*

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