Vortex pinning and dynamics in the neutron star crust

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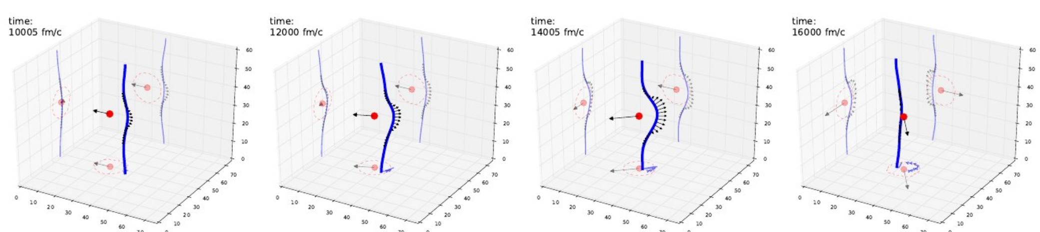
Reference: arXiv:1606.04847



Supported by:
• Polish National Science Center (NCN) grant under decision No. DEC-2014/13/D/ST3/01940.

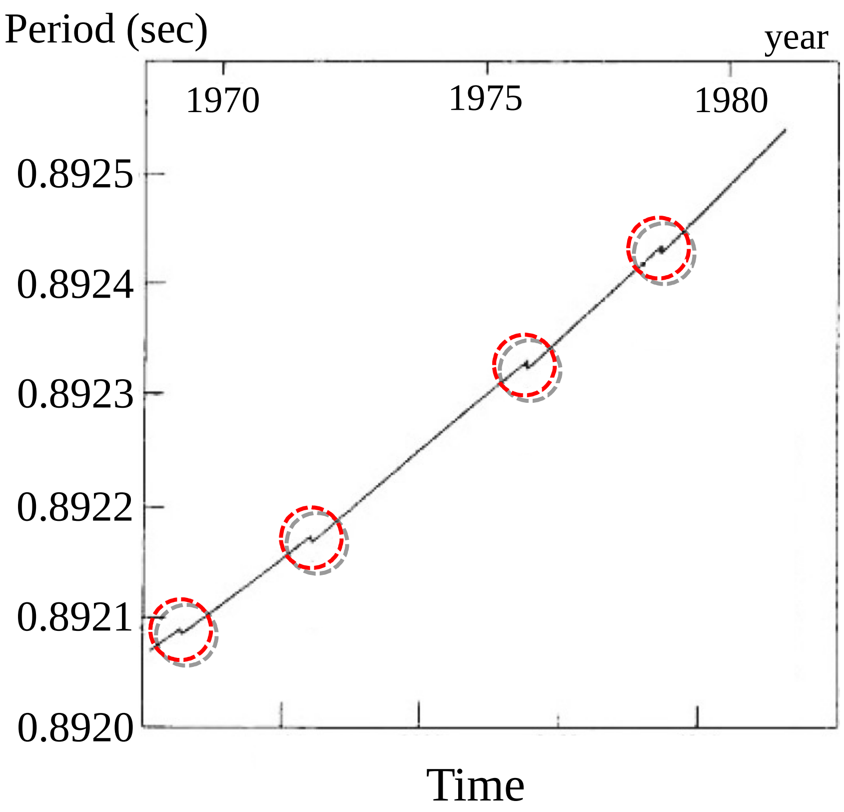
•Polish National Science Center (NCN) grant under decision No. DEC-2013/08/A/ST3/00708.

•U.S. DOE Office of Science Grant DE-FG02-97ER4101

INT Program INT-16-2b: *The Phases of Dense Matter,* July 21, 2016, Seattle

Glitch: a sudden increase of the rotational frequency

- Glitches in the Vela pulsar

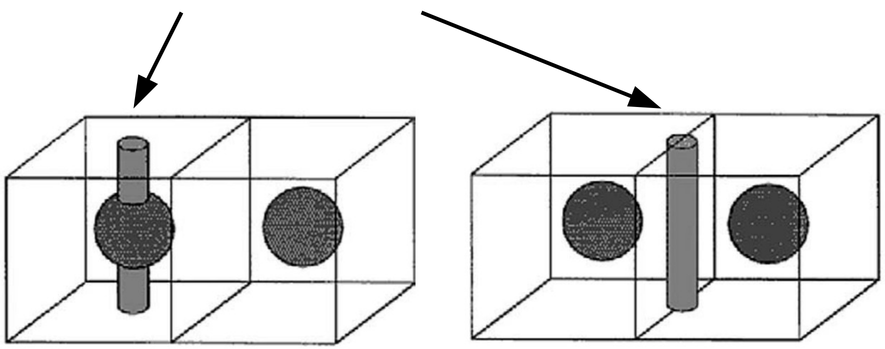


V.B. Bhatia, A Textbook of Astronomy and Astrophysics with Elements of Cosmology, Alpha Science, 2001.

➢ Vortex model

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

- Presently the standard picture for pulsar glitches
- Can explain: post-glitch relaxation, statistics of the glitching populations...
- Idea:
  - Superfluid interior contains quantized vortices pinned to the crustal lattice
  - Glitches are believed to occur when a large number of vortices simultaneously unpin and move outward
- Open problem: **Nuclear** or **Interstitial** pinning



Figs from: P. Donati et al., Nuclear Physics A 742 (2004) 363

First observed in 1969: V. Radhakrishnan and R. N. Manchester, Nature 222, 228–229 (1969);
P. E. Reichley and G. S. Downs, Nature 222, 229–230 (1969);

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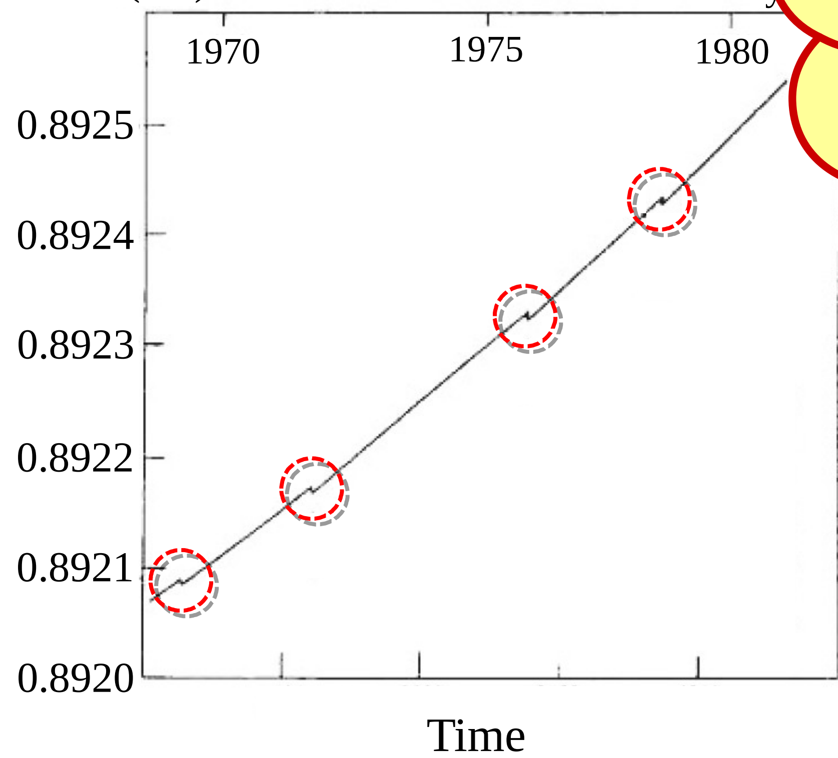
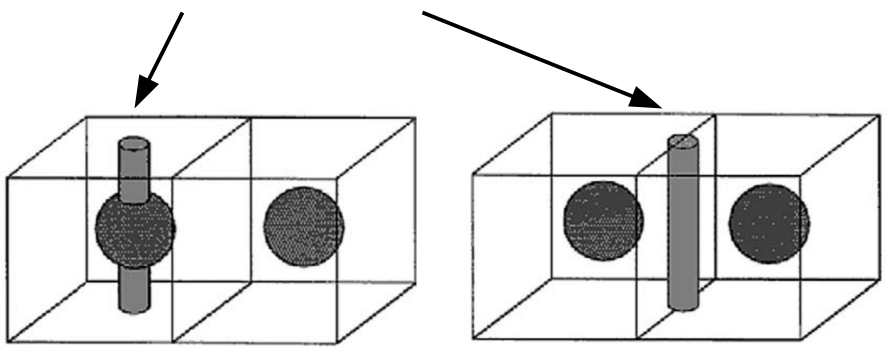


V.B. Bhatia, A Textbook of Astronomy and Astrophysics with Elements of Cosmology, Alpha Science, 2001.

Note:
Type of pinning can affect dynamics dramatically...
(in case of interstitial the vortex moves around the lattice avoiding impurities)

- Open problem:
  Nuclear or **Interstitial** pinning



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First observed in 1969: V. Radhakrishnan and R. N. Manchester, Nature 222, 228–229 (1969); P. E. Reichley and G. S. Downs, Nature 222, 229–230 (1969);

Predictions for “pinning force”:

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

} Hydrodynamics + GL (for pairing)

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

} TF + LDA

P. Avogadro, F. Barranco, R. A. Broglia, and E. Vigezzi, Phys. Rev. C 75, 012805(R) (2007)
P. Avogadro, F. Barranco, R.A. Broglia, E. Vigezzi, Nucl. Phys. A 788, 130 (2007)
P. Avogadro, F. Barranco, R.A. Broglia, E. Vigezzi, Nucl. Phys. A 811, 378 (2008)

} HFB

So far there is no consensus concerning the character of vortex pinning

Irrotational hydrodynamics

$$\Phi_{out}(r,\phi) = \frac{\kappa}{2\pi}\phi + A\frac{(\boldsymbol{r}-\boldsymbol{s})\cdot(\frac{\nu}{s}\boldsymbol{e}_y - \boldsymbol{u})}{|\boldsymbol{r}-\boldsymbol{s}|^3},$$

$$\Phi_{in}(r,\phi) = B_0 + B_1(\boldsymbol{r}-\boldsymbol{s})\cdot\frac{\kappa}{2\pi s}\boldsymbol{e}_y + B_2(\boldsymbol{r}-\boldsymbol{s})\cdot\boldsymbol{u},$$

$$\Phi_{in}|_R = \Phi_{out}|_R,$$

$$\rho_{in}(\frac{\partial\Phi_{in}}{\partial r} - \vec{u})|_R = \rho_{out}(\frac{\partial\Phi_{out}}{\partial r} - \vec{u})|_R,$$

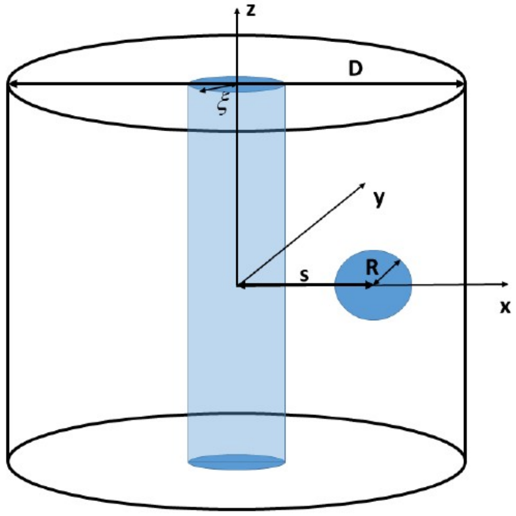


FIG. 9. (Color online) Schematic picture showing the mutual arrangement of the vortex (of radius ξ) and the impurity (of radius R) together with a cylinder of diameter D ($D \to \infty$) defining the boundary of the system.

$$E = \frac{1}{2}\rho_{in}\int_{V_i}(\nabla\Phi_{in})^2 d^3r + \frac{1}{2}\rho_{out}\int_{V-V_i-V_{vor}}(\nabla\Phi_{out})^2 d^3r,$$

tension

effective mass

$$E = \frac{1}{4\pi}\rho_{out}\kappa^2 H\ln\left(\frac{D}{2\xi}\right) + \frac{1}{2}\left(\frac{4\pi}{3}R^3\frac{(\rho_{out}-\rho_{in})^2}{2\rho_{out}+\rho_{in}}\right)u^2$$
$$+\left(2\pi R^3\frac{\rho_{out}(\rho_{in}-\rho_{out})}{2\rho_{out}+\rho_{in}}\right)\left(\frac{\kappa}{2\pi s}\right)^2 + O(1/s^3) \quad (24)$$

vortex-nucleus interaction

$$F = -\frac{\partial E}{\partial s} \propto 1/s^3$$

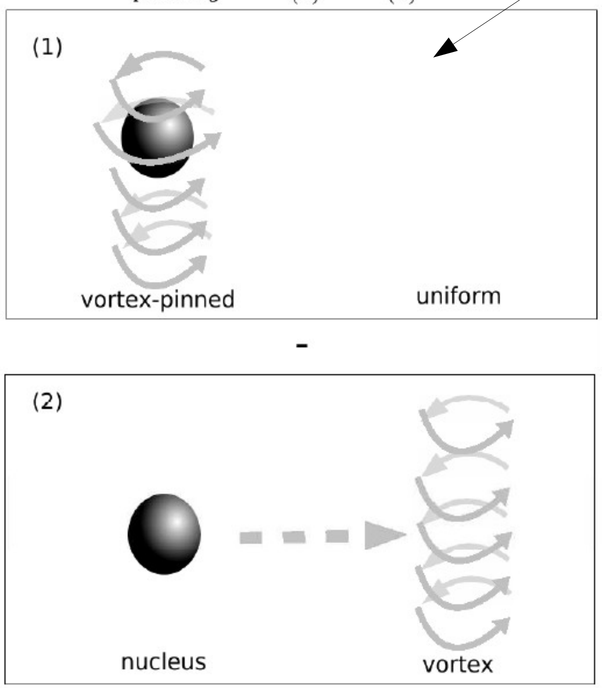
Vortex-impurity interaction – present status

only calculations of *pinning energy*...

only symmetric configurations have been considered with energies of order 10,000 MeV

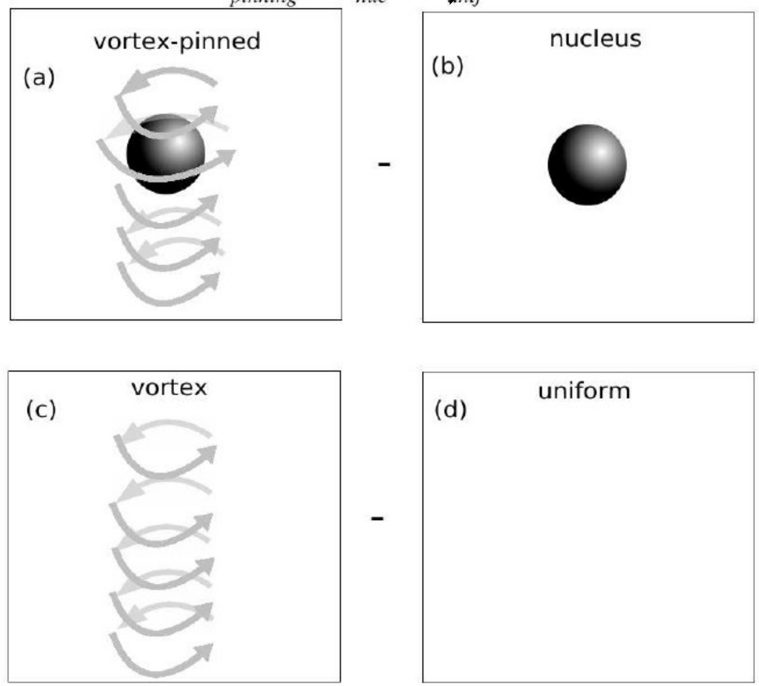
~1 MeV ~10,000 MeV

$$E_{pinning} = E_{(1)} - E_{(2)}$$



Calculations for fixed chemical potential + correction $\Delta E = \mu \Delta N$

$$E_{pinning} = E^{vor}_{nuc} - E^{vor}_{unif}$$



$$E^{vor}_{nuc} = (a) - (b)$$

$$E^{vor}_{unif} = (c) - (d)$$

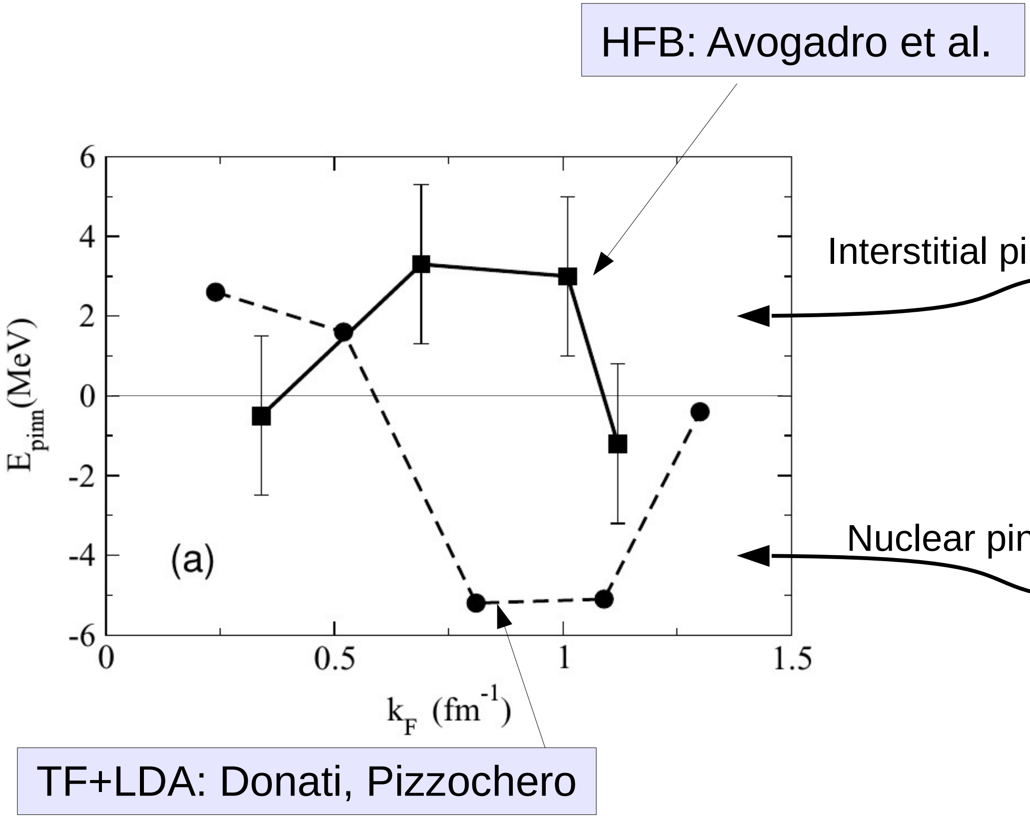
Fixed chemical potential or neutron background density?

Volume: tube of radius 30fm and height of 40fm

SLy4 $n_\infty = 0.026\ \mathrm{fm}^{-3}$

[MeV]	Chem.pot	energy
Pinned	8.55	12956.57
Nucleus	8.50	12954.02
Vortex	8.55	13712.91
Uniform	8.50	13617.05

Figures and numbers from:
P. Avogadro, F. Barranco, R.A. Broglia, E. Vigezzi Nucl. Phys. A811, 378-412 (2008)



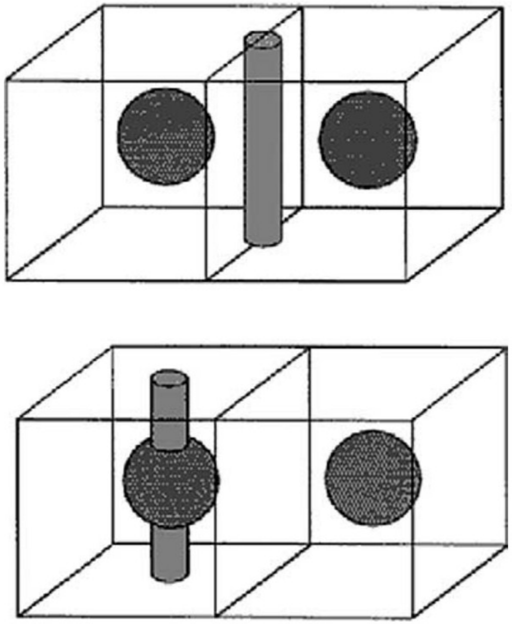


Fig. from: P. Avogadro et al.,
Phys. Rev. C 75, 012805(R) (2007)

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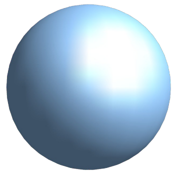
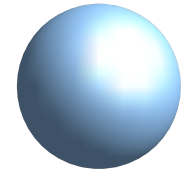
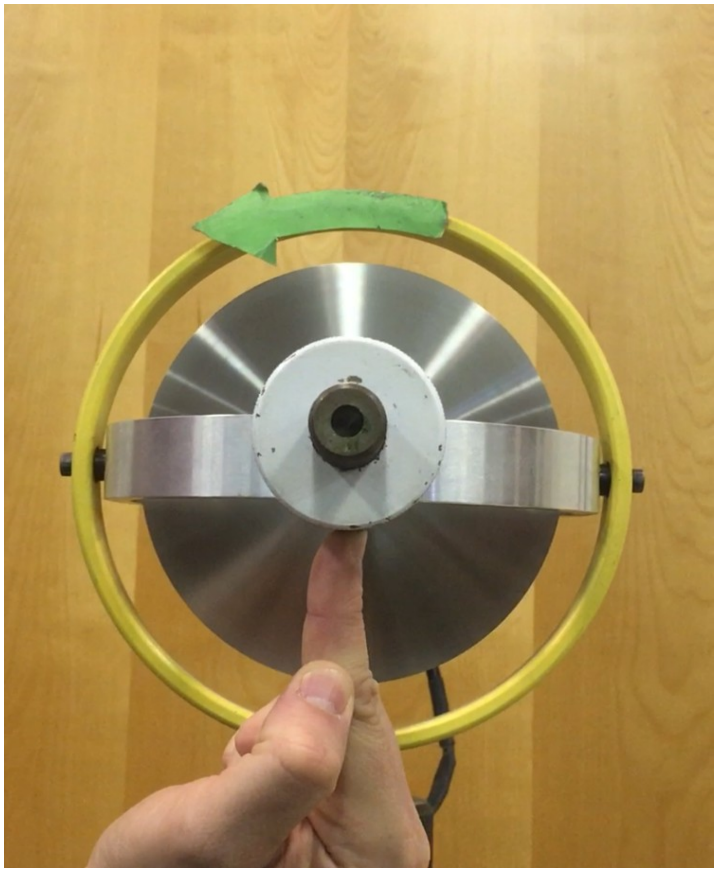
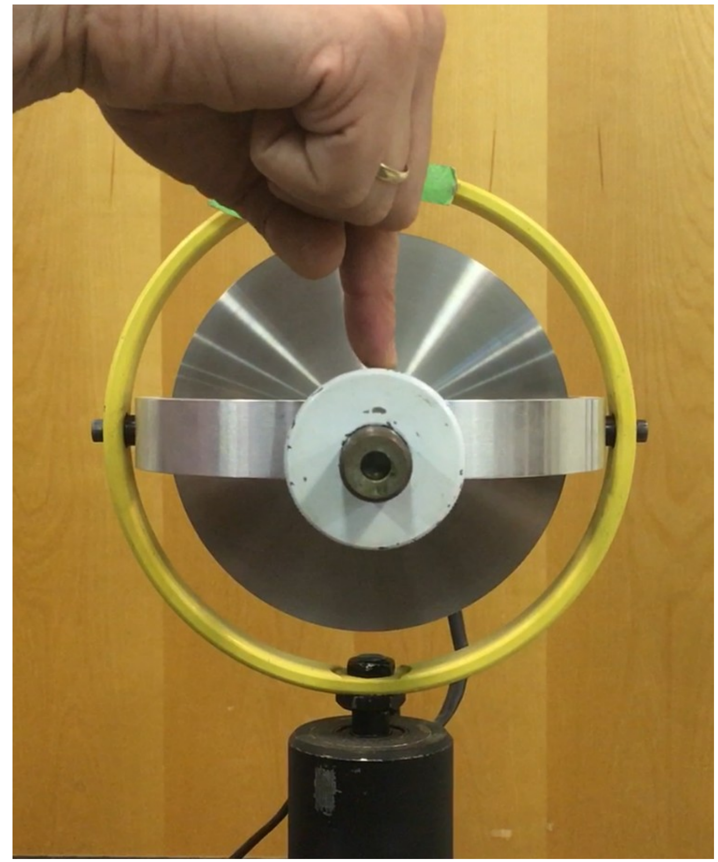


attracted by nucleus



repelled by nucleus





What is response of the gyroscope when pushed?

Our strategy ...

Instead of solving
static problem...

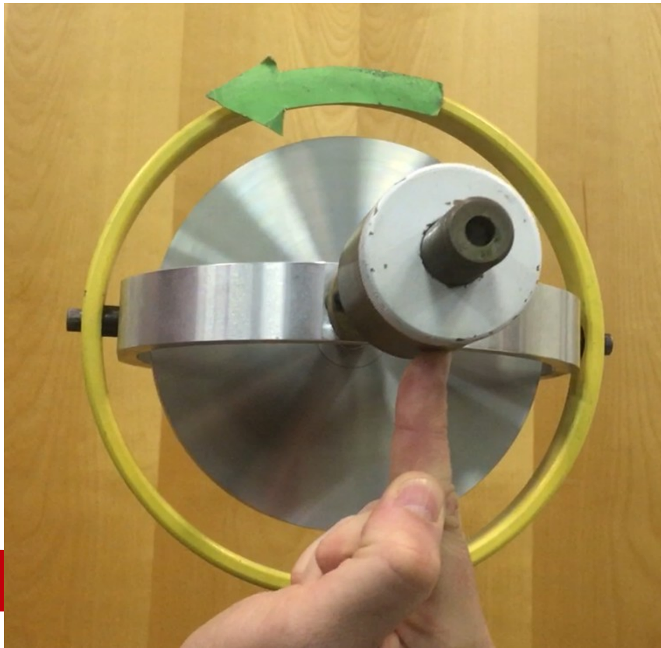
$$\hat{H}\psi = E\psi$$

… we solve
time-dependent problem...

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi$$

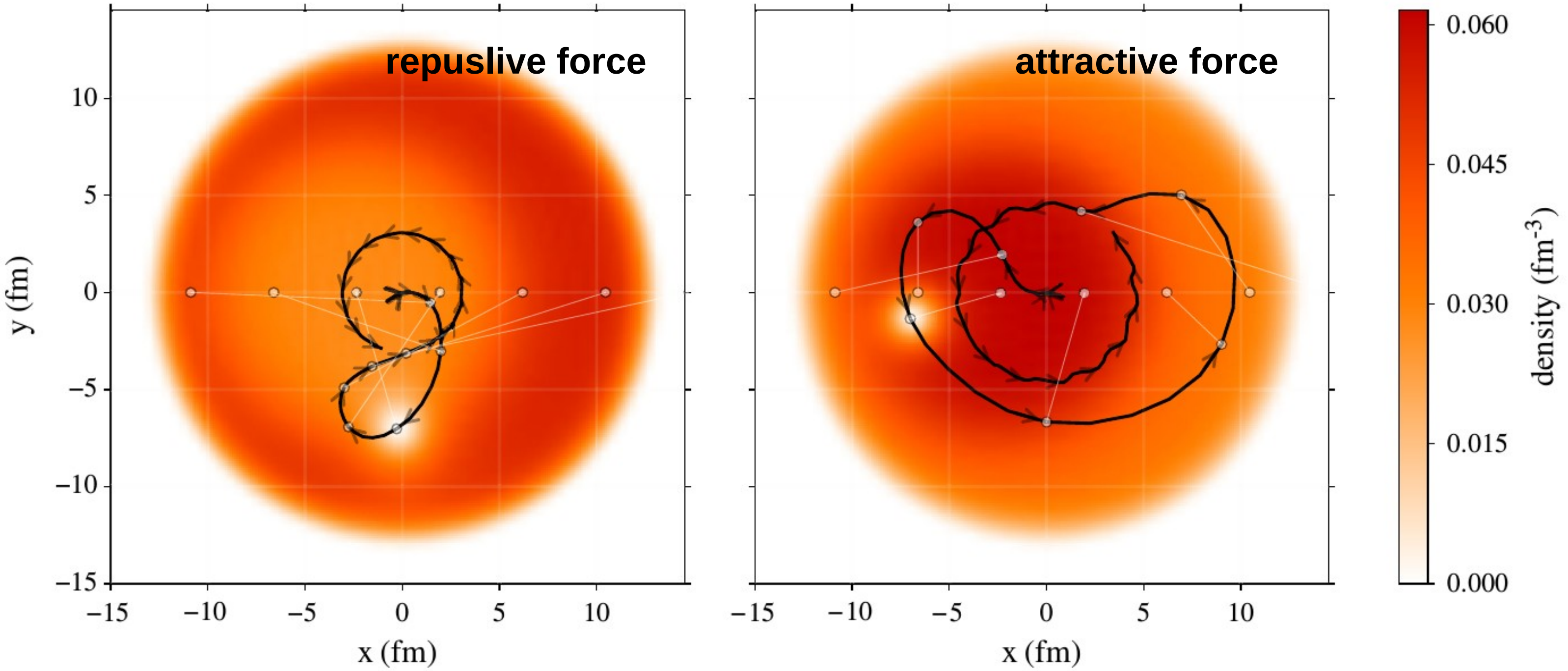
… and observing dynamics of the system
we determine the forces.

Unambiguous determination of the force sign...



Idea introduced in:
Aurel Bulgac, Michael McNeil Forbes, and Rishi Sharma
Phys. Rev. Lett. 110, 241102 (2013)

2D simulations with GP



Equation of motion:

$$M\ddot{\vec{r}}_v - \vec{f}_{qp} = \rho_s \vec{\kappa} \times (\dot{\vec{r}}_v - \vec{v}_s) + \vec{F}_v$$

negligible

repulsive **attractive** PHYSICS.WUT

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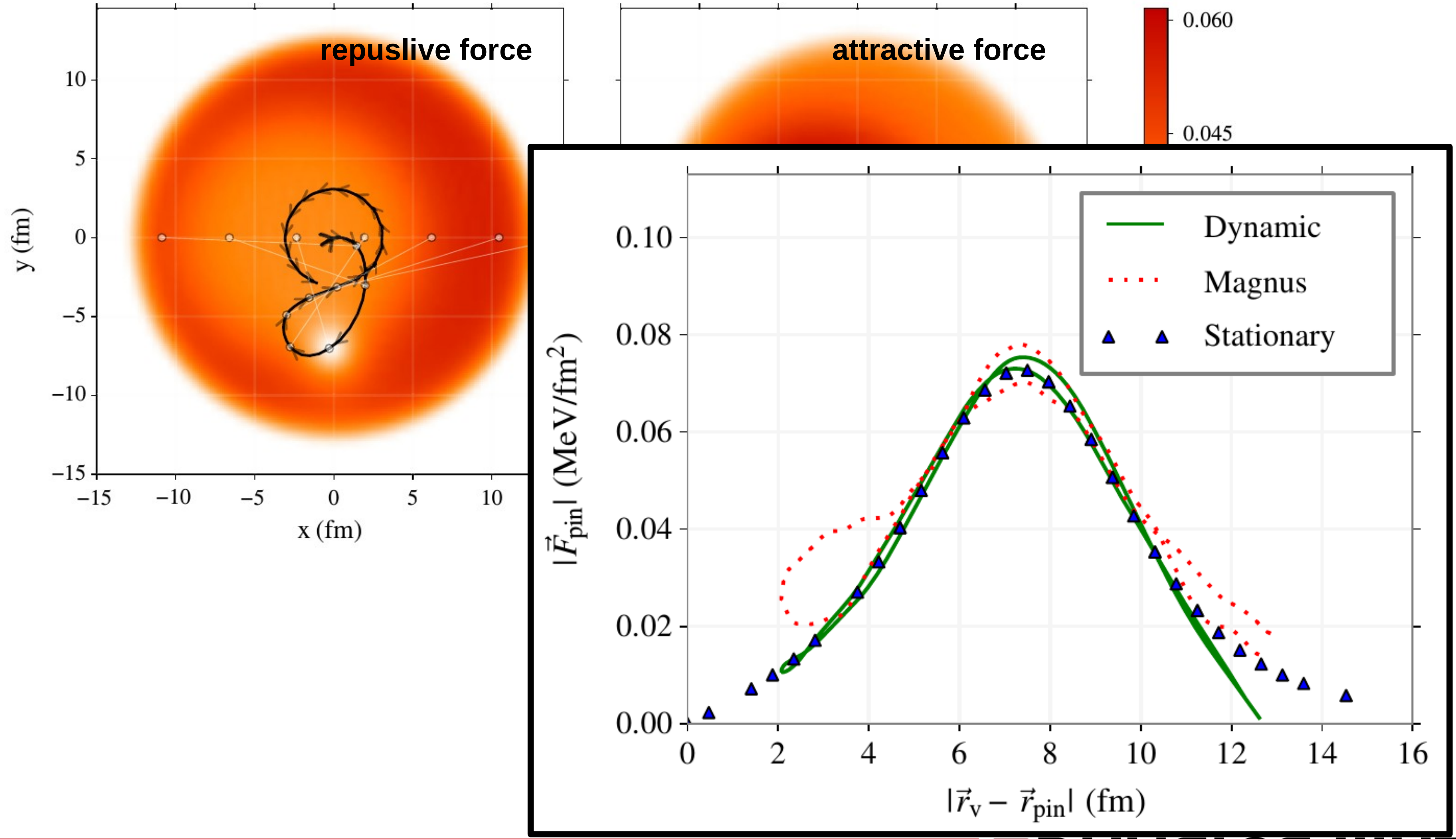


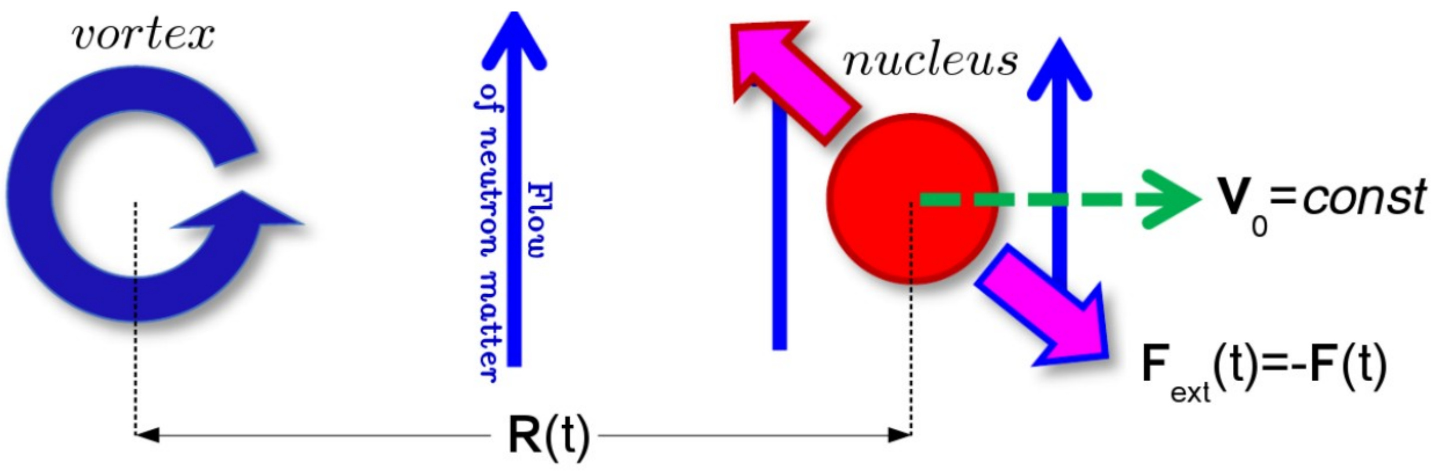
3D case

In 3D one should consider the equation of motion for the vortex line...

We use Newton's 3rd law and extract the force from motion of the nucleus.....

Vortex-nucleus interaction

$$M\frac{d\boldsymbol{v}}{dt} = \boldsymbol{F}_{\text{tot.}} = \boldsymbol{F} + \boldsymbol{F}_{\text{ext.}} = 0 \Leftrightarrow \boldsymbol{v} = \text{const}$$



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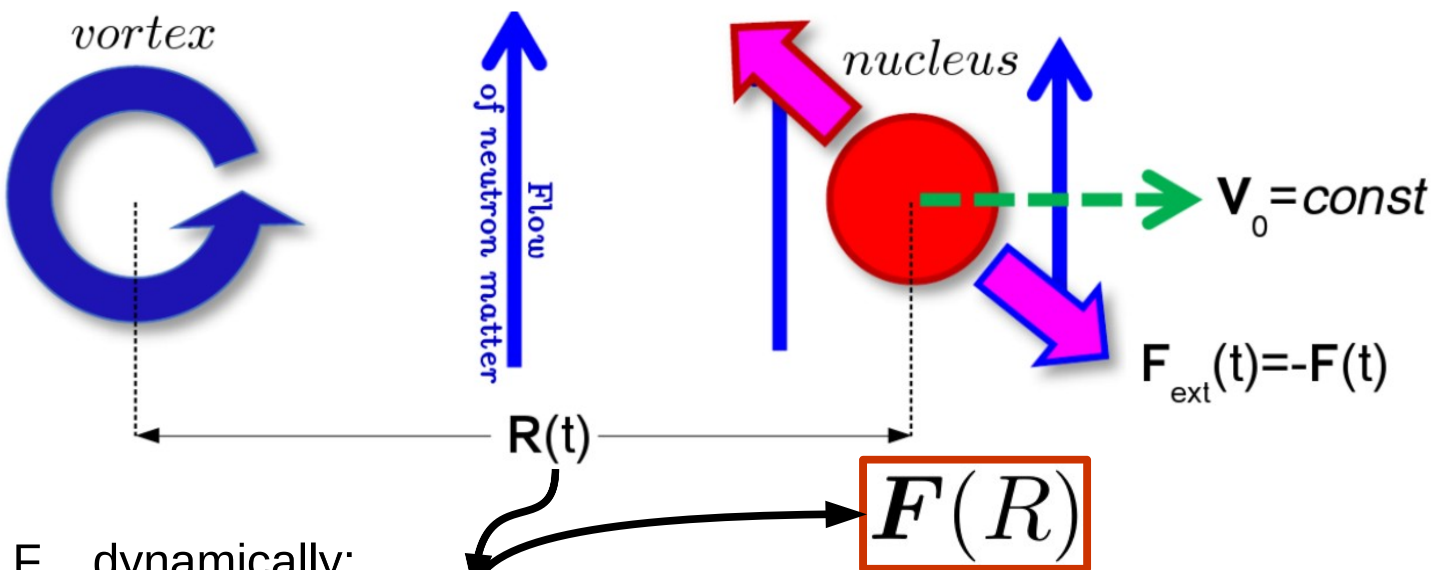


We construct F_{ext} dynamically:

$$\boldsymbol{F}_{\text{ext}}(t+\Delta t) = \boldsymbol{F}_{\text{ext}}(t) - \alpha\left[\boldsymbol{v}(t) - \boldsymbol{v}_0\right]$$

We performed 3D, dynamical simulations by TDDFT with superfluidity

- TDSLDA equations (similar to TDHFB, TD-BdG)

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_k \\ v_k \end{pmatrix} = \begin{pmatrix} h & \Delta \\ \Delta^* & -h \end{pmatrix}\begin{pmatrix} u_k \\ v_k \end{pmatrix}$$

- Energy density functional (EDF)

$$\mathcal{E} = \mathcal{E}_0 + \mathcal{E}_{\text{pair}}$$

$\mathcal{E}_0$: Fayans EDF (FaNDF^0) w/o LS

S.A. Fayans, JETP Letters 68, 169 (1998);

- Potentials

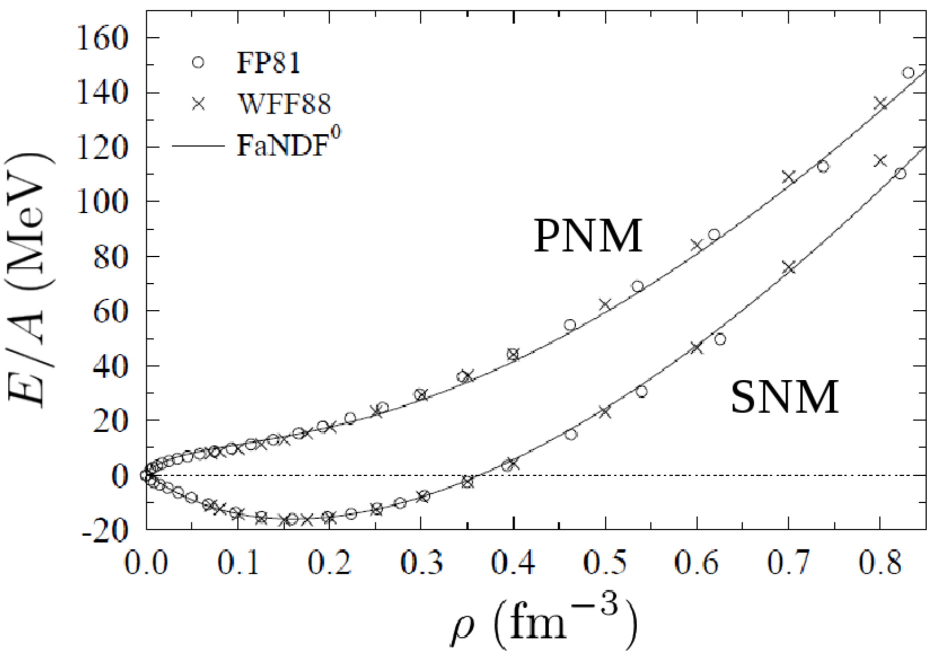
$$h = \frac{\delta\mathcal{E}}{\delta n}, \quad \Delta = \frac{\delta\mathcal{E}}{\delta\nu^*}$$

$$n(\boldsymbol{r}) = \sum_{0<E_k<E_c} |v_k(\boldsymbol{r})|^2$$

$$\nu(\boldsymbol{r}) = \sum_{0<E_k<E_c} u_k(\boldsymbol{r})v_k^*(\boldsymbol{r})$$

FP81: B. Friedman and V. R. Pandharipande, Nucl. Phys. A 361, 502 (1981)

WFF88: R. B. Wiringa, V. Fiks, and A. Fabrocini, Phys. Rev. C 38, 1010 (1988).



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- Energy density functional (EDF)

$$\mathcal{E} = \mathcal{E}_0 + \mathcal{E}_{\rm pair}$$

$$\mathcal{E}_{\rm pair}(\boldsymbol{r}) = g(n(\boldsymbol{r}))\left[|\nu_n(\boldsymbol{r})|^2 + |\nu_p(\boldsymbol{r})|^2\right]$$

The coupling constant g is chosen to reproduce the neutron pairing gap in pure neutron matter.

- Potentials

$$h = \frac{\delta\mathcal{E}}{\delta n},\quad \Delta = \frac{\delta\mathcal{E}}{\delta\nu^*}$$

$$n(\boldsymbol{r}) = \sum_{0<E_k<E_c} |v_k(\boldsymbol{r})|^2$$

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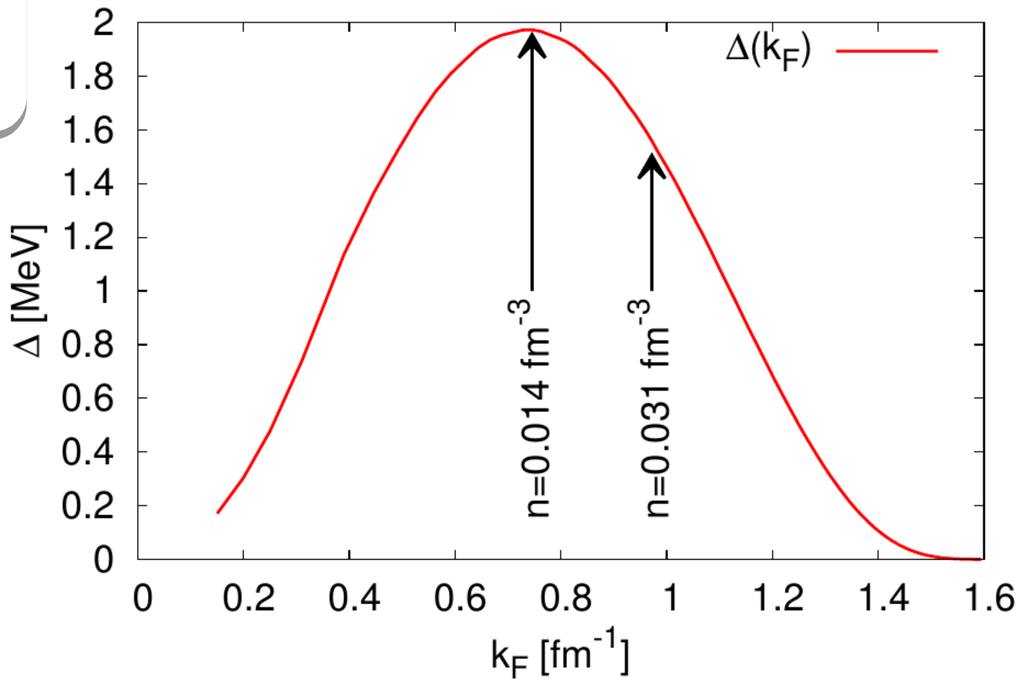


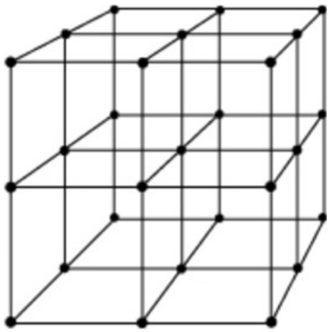
Numerical details

Determined self-consistently in each moment

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

HFB matrix=$200{,}000^2$

- The system is placed on a large 3D spatial lattice of size 50 x 50 x 40 with lattice spacing 1.5fm



  - Discrete Variable Representation (DVR) - solid framework (see for example: Bulgac, Forbes, Phys. Rev. C 87, 051301(R) (2013))
  - No symmetry restrictions

- Number of PDEs is of the order of the number of spatial lattice points [Typically: 10^5 – 10^6]

  ...106,000 to evolve...

Numerical details

Determined sel

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_k(\boldsymbol{r},t) \\ v_k(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} h(\boldsymbol{r}, \\ \Delta^*(\boldsymbol{r} \end{pmatrix}$$

OLCF Oak Ridge Titan (DOE Contract DE-AC05-00OR22725)

NERSC Edison (DOE Contract No. DE-AC02-05CH11231)

HA-PACS (PACS-VIII) system Interdisciplinary Computational Science Program in Center for Computational Sciences, University of Tsukuba

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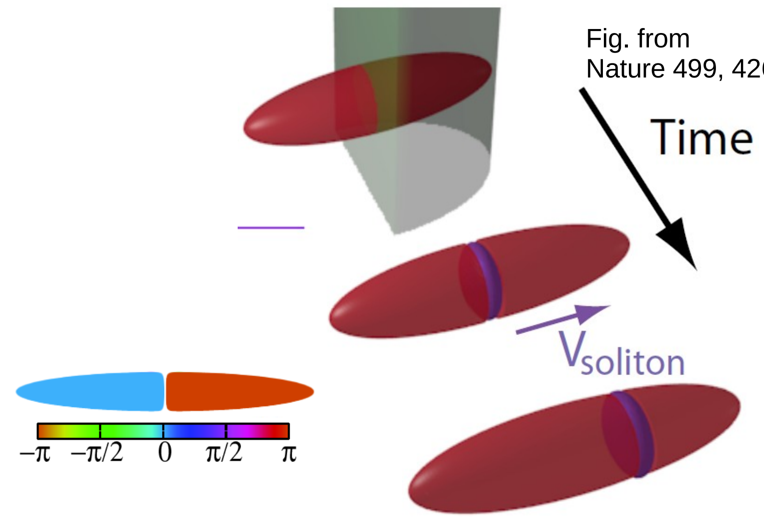
  - Discrete Variable Representat solid framework (see for example: B Phys. Rev. C 87, 051301(R) (2013))
  - No symmetry restrictions
- Number of PDEs is of the or spatial lattice points [Typically ...106,000 to evolve...
- parallelization (MPI) + acceleration (GPU)

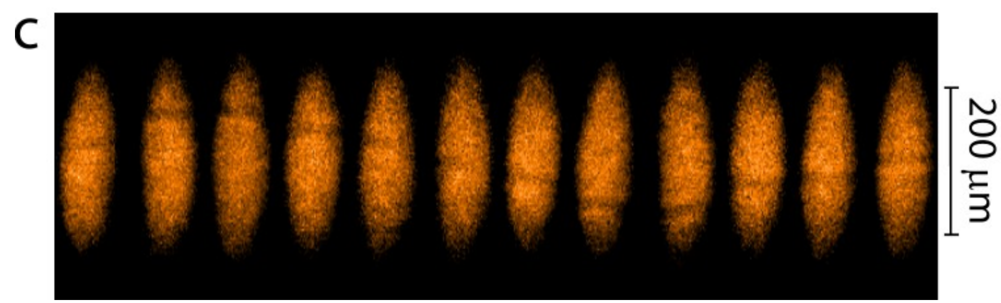
Validation against dynamical properties of the system

MIT experiments: T. Yefsah et al., Nature 499, 426 (2013)

- ^{6}Li atoms near a Feshbach resonance ($N \approx 10^6$) cooled in harmonic trap
- Step potential used to imprint a soliton (evolve to π phase shift)
- Let system evolve...
- Take picture (subtle imaging with tomography)

Fig. from
Nature 499, 426 (2013)





Our method predicted quantum vortex ring and corrected the initial interpretation as a heavy soliton...

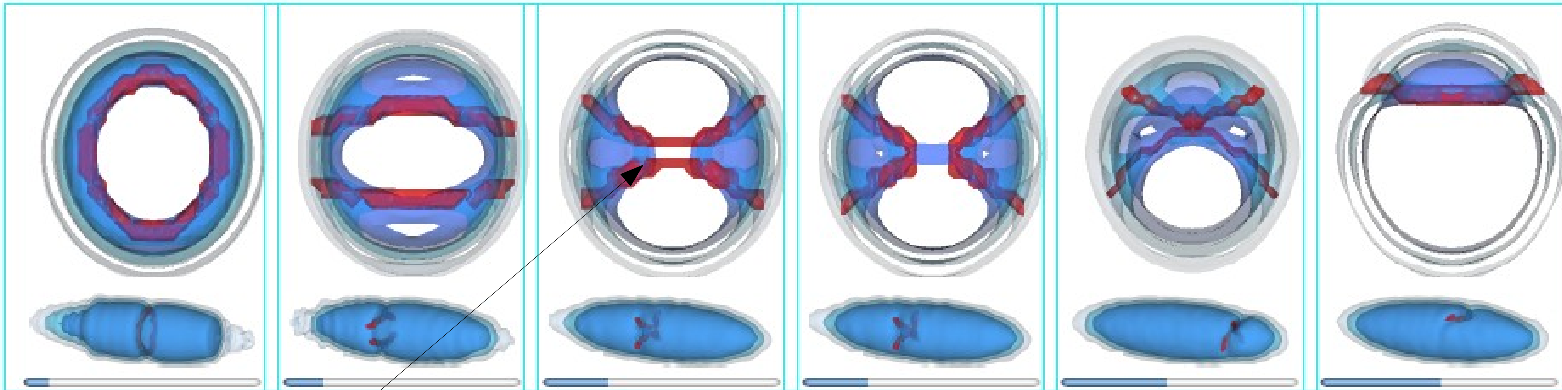
What do fully 3D simulations reveal?

Phys. Rev. A 91, 031602 (2015)

Cold atoms 1

$$\delta \approx 10\%$$

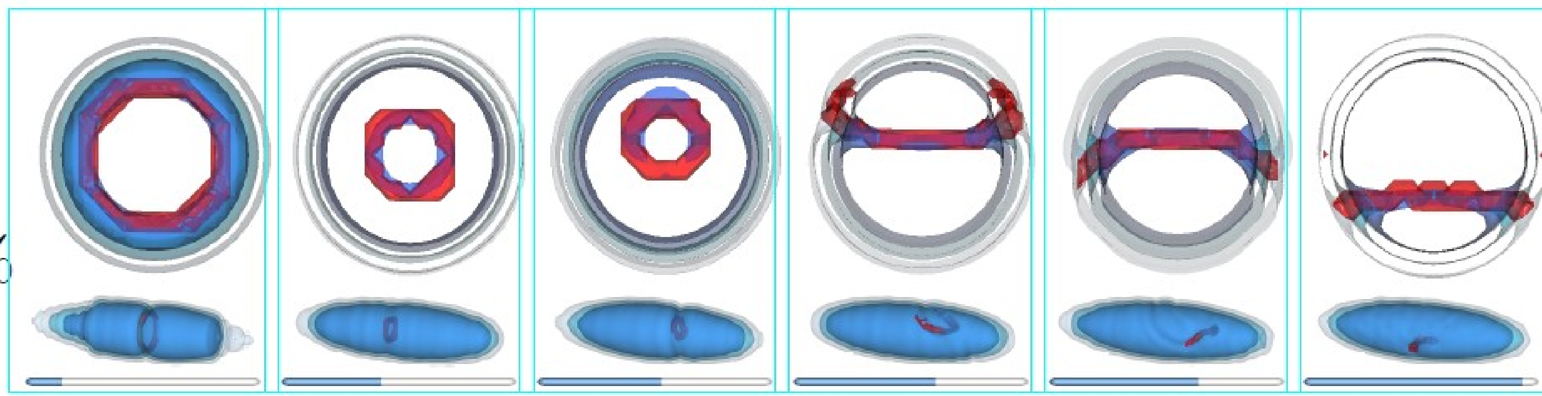
$$\frac{C}{C_0} \approx 3\%$$



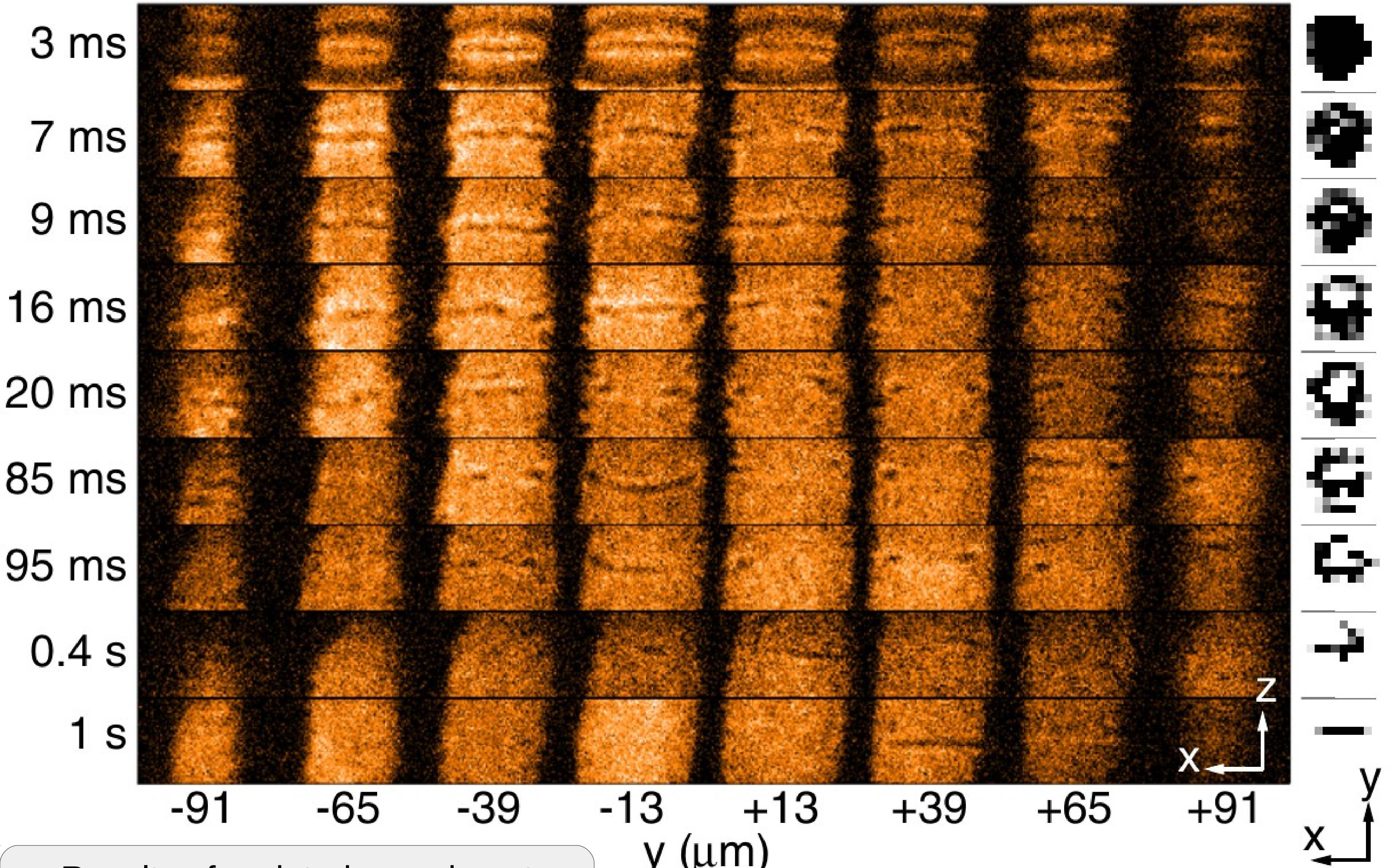
Crossing and reconnection!

$$\delta \approx 0.5\%$$

$$\frac{C}{C_0} \approx 0.15\%$$



Cold atoms 2



Results of updated experiment agree with our predictions...

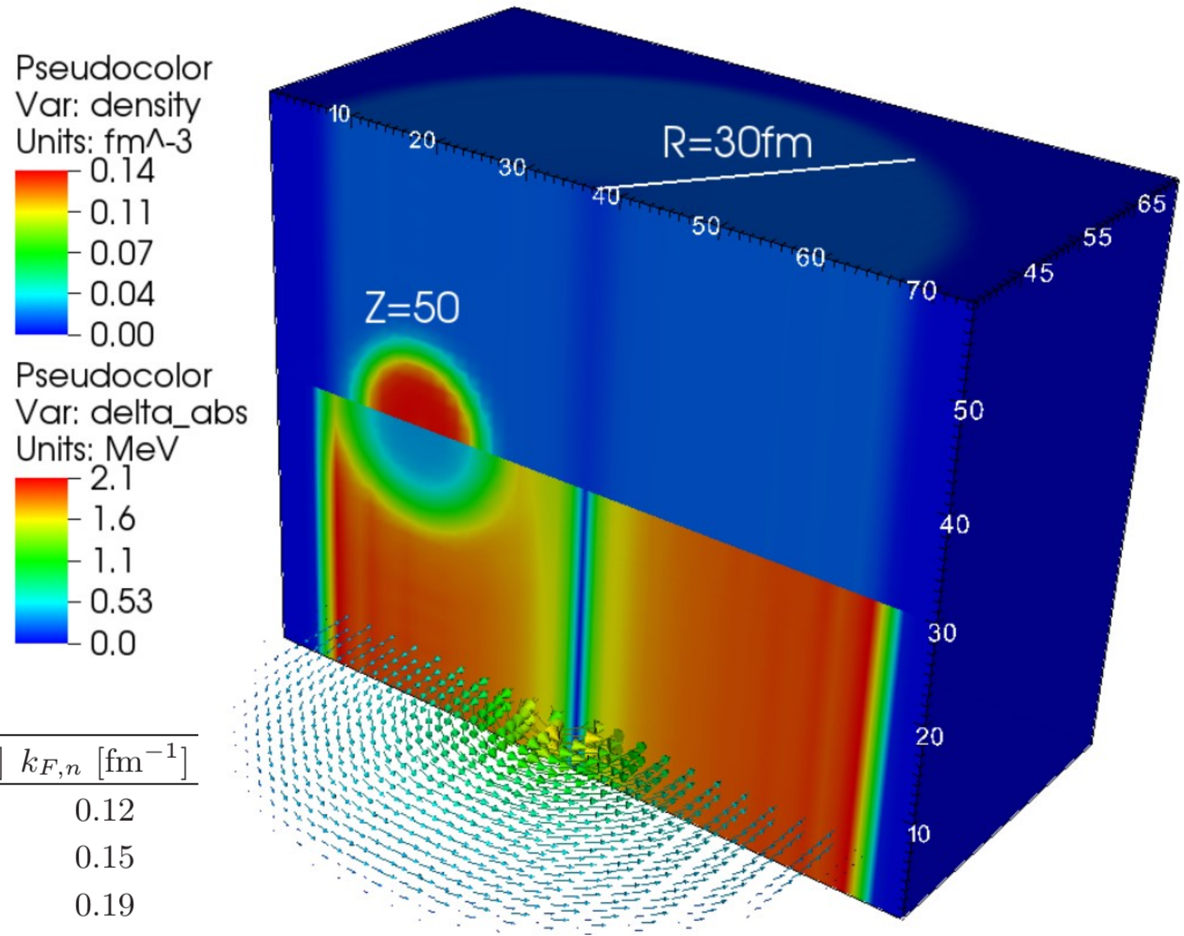
Mark J. H. Ku, Biswaroop Mukherjee, Tarik Yefsah, and Martin W. Zwierlein, Phys. Rev. Lett. 116, 045304 (2016)

Initial state

Self-consistent solution
of static problem

$$\begin{pmatrix} h & \Delta \\ \Delta^* & -h \end{pmatrix} \begin{pmatrix} u_k \\ v_k \end{pmatrix} = \varepsilon_k \begin{pmatrix} u_k \\ v_k \end{pmatrix}$$

J. Negele and D. Vautherin,
Nucl. Phys. A 207, 298 (1973)

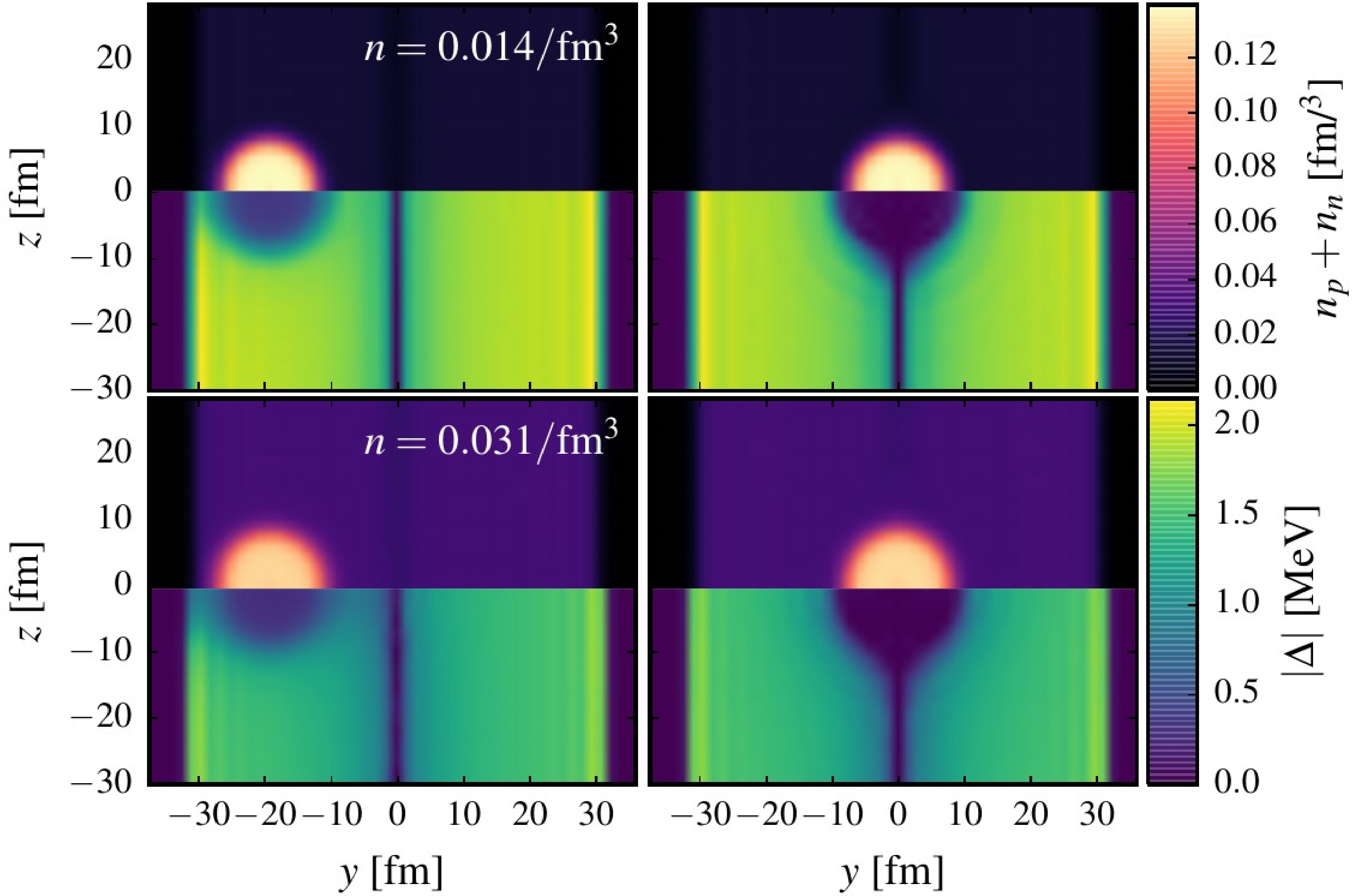


$$75\ \mathrm{fm} \times 75\ \mathrm{fm} \times 60\ \mathrm{fm}$$

3D lattice – no symmetry restrictions

Zone	Element	Z	N	R_{WS} [fm]	ρ_b [g · cm^{-3}]	$k_{F,n}$ [fm^{-1}]
11	^{180}Zr	40	140	53.6	$4.67 \cdot 10^{11}$	0.12
10	^{200}Zr	40	160	49.2	$6.69 \cdot 10^{11}$	0.15
9	^{250}Zr	40	210	46.4	$1.00 \cdot 10^{12}$	0.19
8	^{320}Zr	40	280	44.4	$1.47 \cdot 10^{12}$	0.23
7	^{500}Zr	40	460	42.2	$2.66 \cdot 10^{12}$	0.31
6	^{950}Sn	50	900	39.3	$6.24 \cdot 10^{12}$	0.43
5	^{1100}Sn	50	1050	35.7	$9.65 \cdot 10^{12}$	0.51
4	^{1350}Sn	50	1300	33.0	$1.49 \cdot 10^{13}$	0.60
3	^{1800}Sn	50	1750	27.6	$3.41 \cdot 10^{13}$	0.80
2	^{1500}Zr	40	1460	19.6	$7.94 \cdot 10^{13}$	1.08
1	^{982}Ge	32	950	14.4	$1.32 \cdot 10^{14}$	1.33

Simulations for background density:
k_F=0.75 fm^{-1} and k_F=0.97 fm^{-1}



Static solutions: $E_{unpinned}$ < E_{pinned}

Dragging force

external time-dependent potential couples only to protons and it is constant in space.

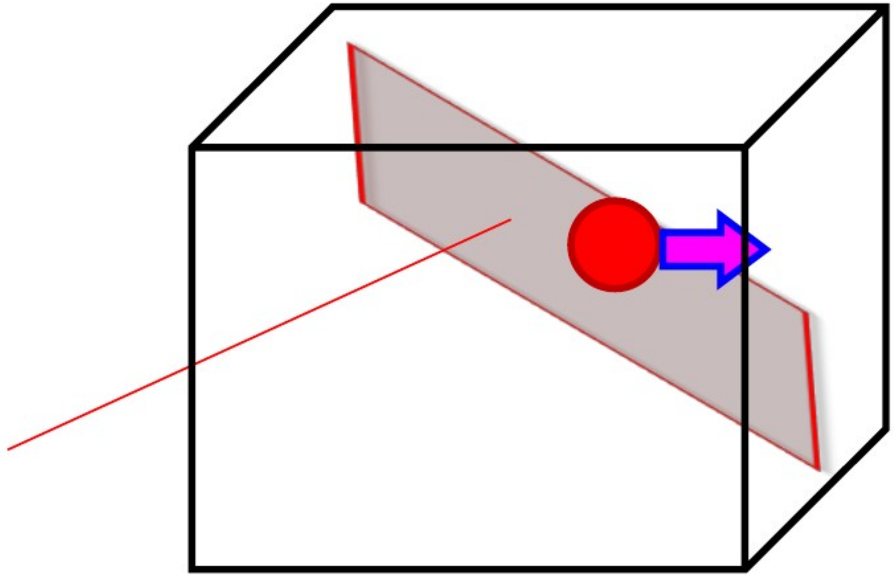
Dragging speed:

$$v_0 = 0.001c \ll v_{\mathrm{crit}}$$

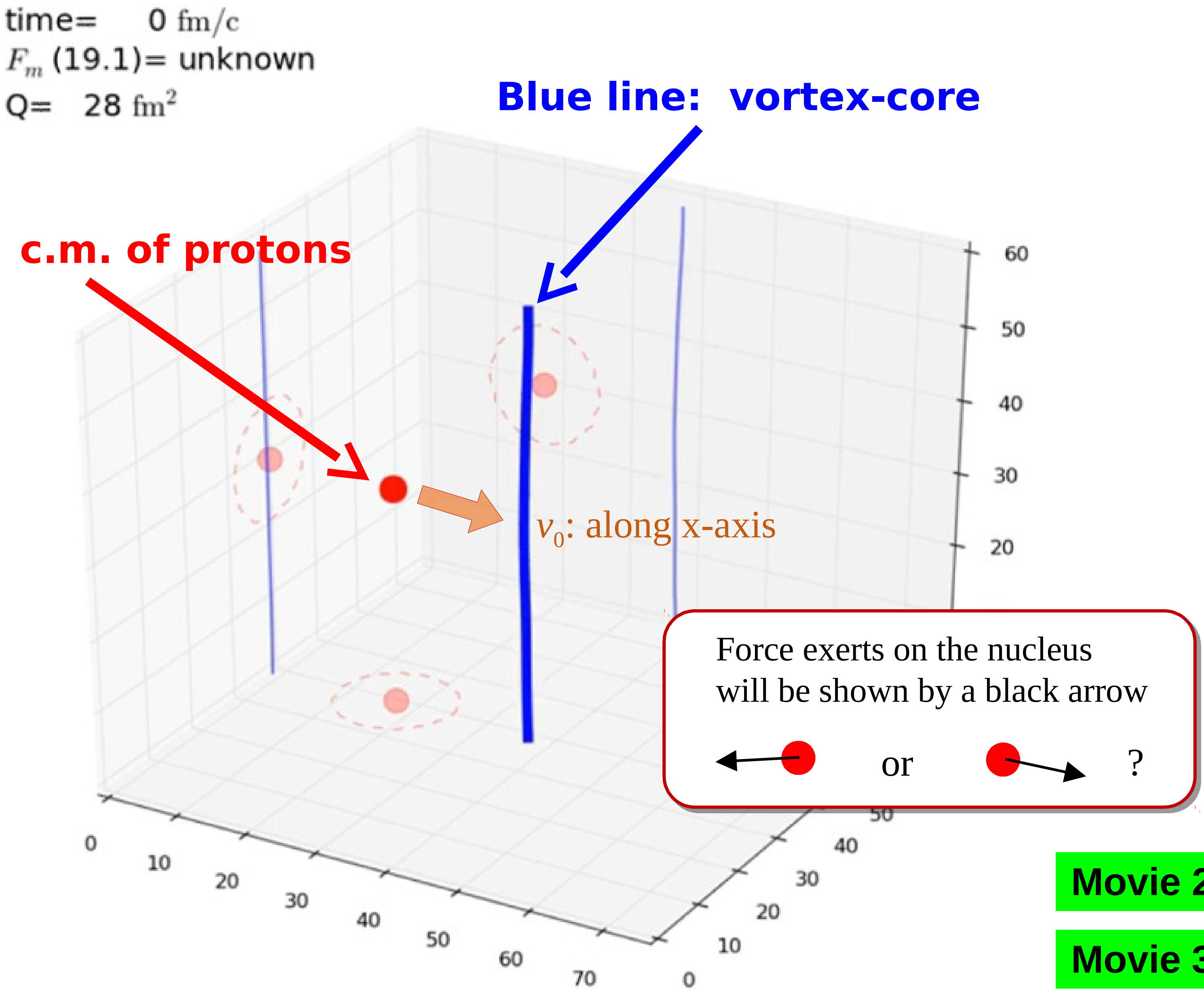
$$U_{\mathrm{ext}}(\boldsymbol{r},t) = -\frac{1}{Z}\boldsymbol{F}_{\mathrm{ext}}(t)\cdot\boldsymbol{r}$$

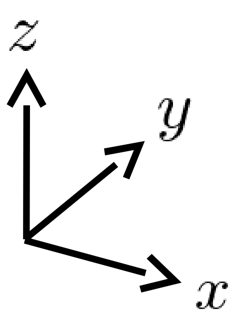
$$\frac{d\,\langle\hat{\boldsymbol{p}}\rangle}{dt} = -\left\langle\boldsymbol{\nabla}U_{\mathrm{ext}}(\boldsymbol{r},t)\right\rangle = \boldsymbol{F}_{\mathrm{ext}}(t)$$

This force moves the center of mass of the protons together with those neutrons bound (entrained) in the nucleus without significantly modifying the internal structure of the nucleus and surrounding neutron medium



Results

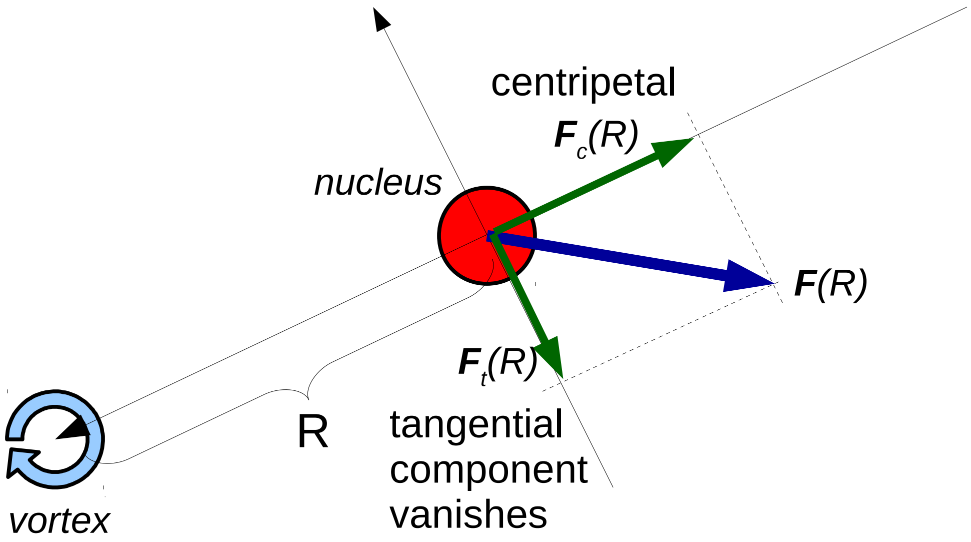




Movie 2

Movie 3

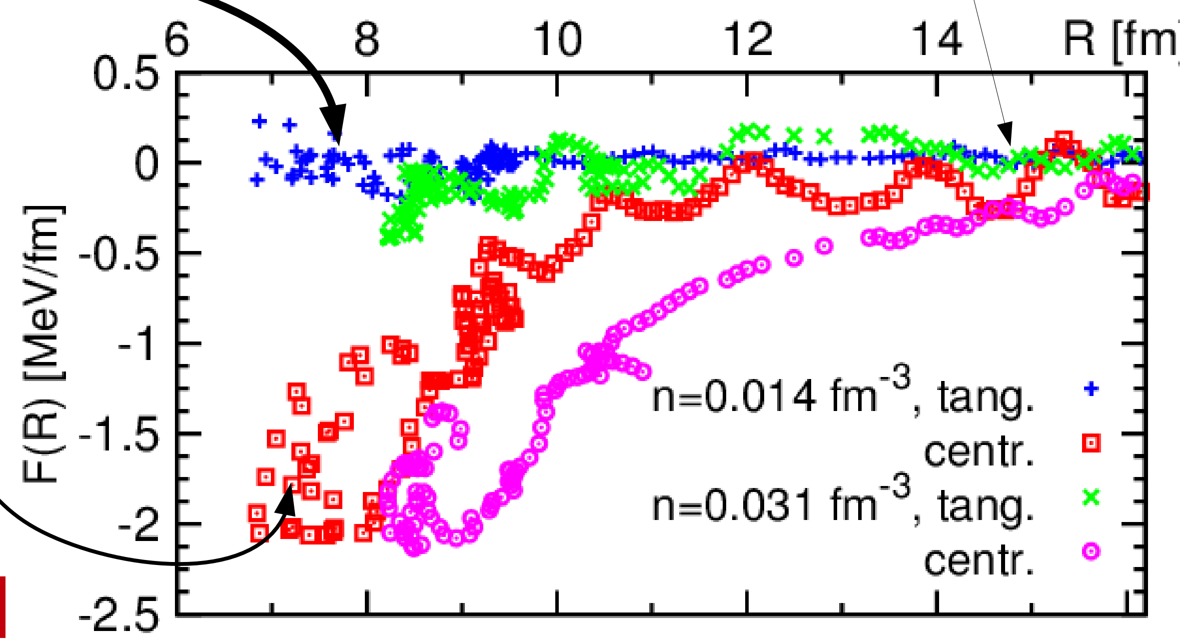
Force decomposition



Range:
10-15 fm

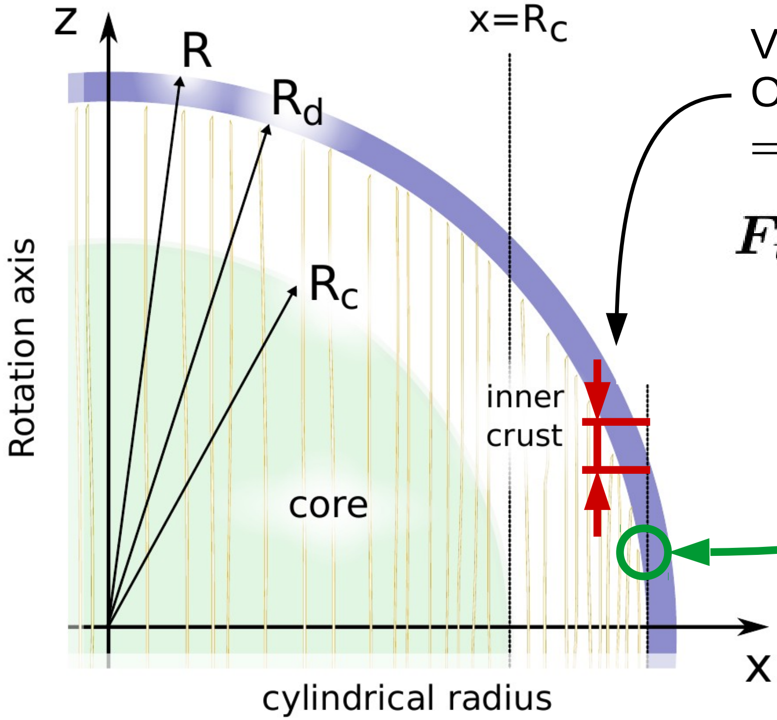
Force is
central

At close separation
the force is not a function
of distance R only



Pinning force – what is needed?

Example of hydrodynamical description (M. Antonelli, P. Pizzochero, arXiv:1603.02838)



Vortex is divided in elements of length dl.
One needs to consider forces acting on each element
⇒ *force per unit length **f***

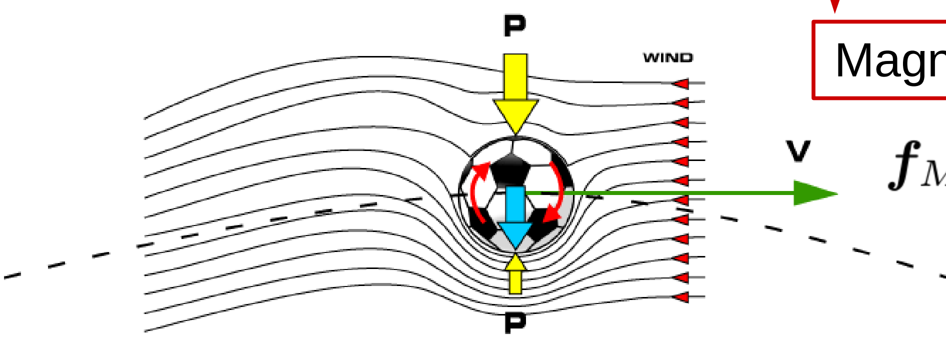
$$\boldsymbol{F}_{tot} = \int_L dl(\boldsymbol{x}) \left[\boldsymbol{f}_M(\boldsymbol{x}) + \boldsymbol{f}_D(\boldsymbol{x}) + \boldsymbol{f}_P(\boldsymbol{x}) \right] = 0$$

Drag force exert on vortices due to mutual friction with outer crust (normal component)

"Pinning force" between vortex and lattice

$$\boldsymbol{f}_D = -\eta(\boldsymbol{x})(\boldsymbol{v}_L(\boldsymbol{x}) - \boldsymbol{v}_p(\boldsymbol{x}))$$

Magnus force



$$\boldsymbol{f}_M = \rho_n(\boldsymbol{x})\boldsymbol{\kappa} \times (\boldsymbol{v}_L(\boldsymbol{x}) - \boldsymbol{v}_n(\boldsymbol{x}))$$

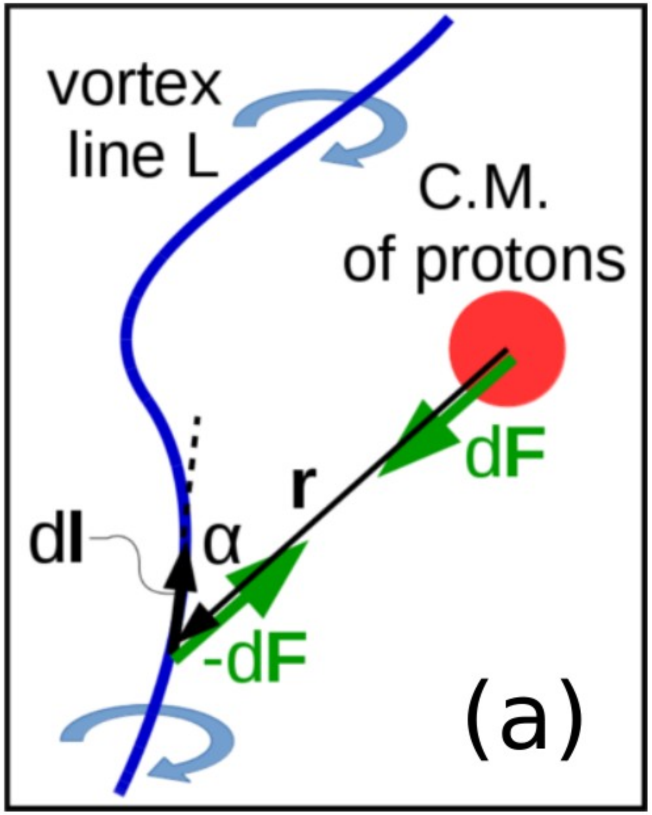
Force per unit length

Inspired by the vortex filament model (describes vortex-vortex Interaction)

$$\mathrm{d}\boldsymbol{F} = f(r)\sin\alpha\,\hat{\boldsymbol{r}}\,\mathrm{d}l \qquad \hat{\boldsymbol{r}} = \boldsymbol{r}/r$$

$$\boldsymbol{F} = \int_L \mathrm{d}\boldsymbol{F}$$

Total force acting on nucleus



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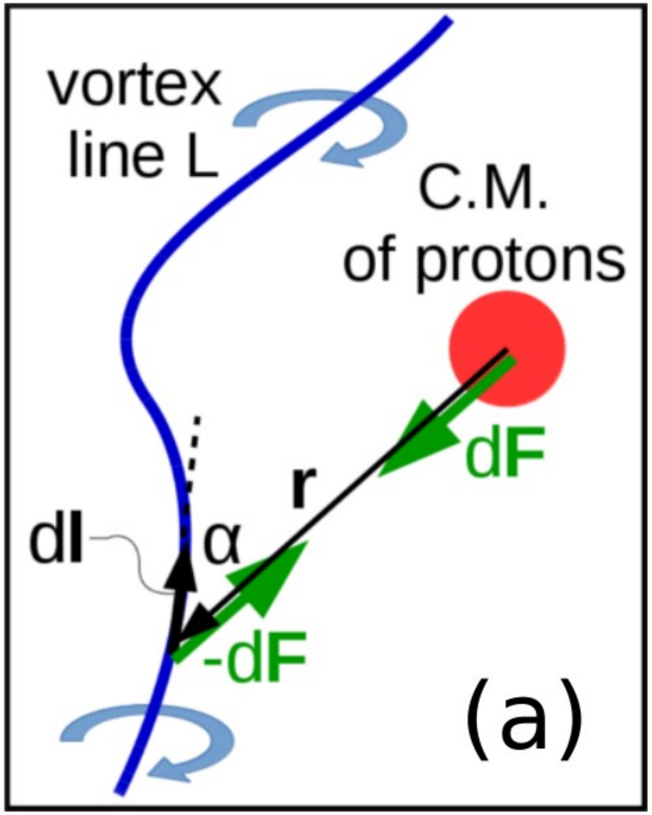


Ansatz for f(r) - Pade approximant

$$f(r) = \frac{\sum_{k=0}^{n} a_k r^k}{1 + \sum_{k=1}^{n+3} b_k r^k}$$

$$f(r \to \infty) \propto 1/r^3$$

from irrotational and incompressible hydrodynamics

We minimize chi2 with respect of $\{a_k, b_k\}$

$$\chi_w^2 = \sum_{i=1}^{N} w(|\boldsymbol{F}_i|)\left(\boldsymbol{F}_i - \boldsymbol{F}_i^{(f)}(\{a_k, b_k\})\right)^2$$

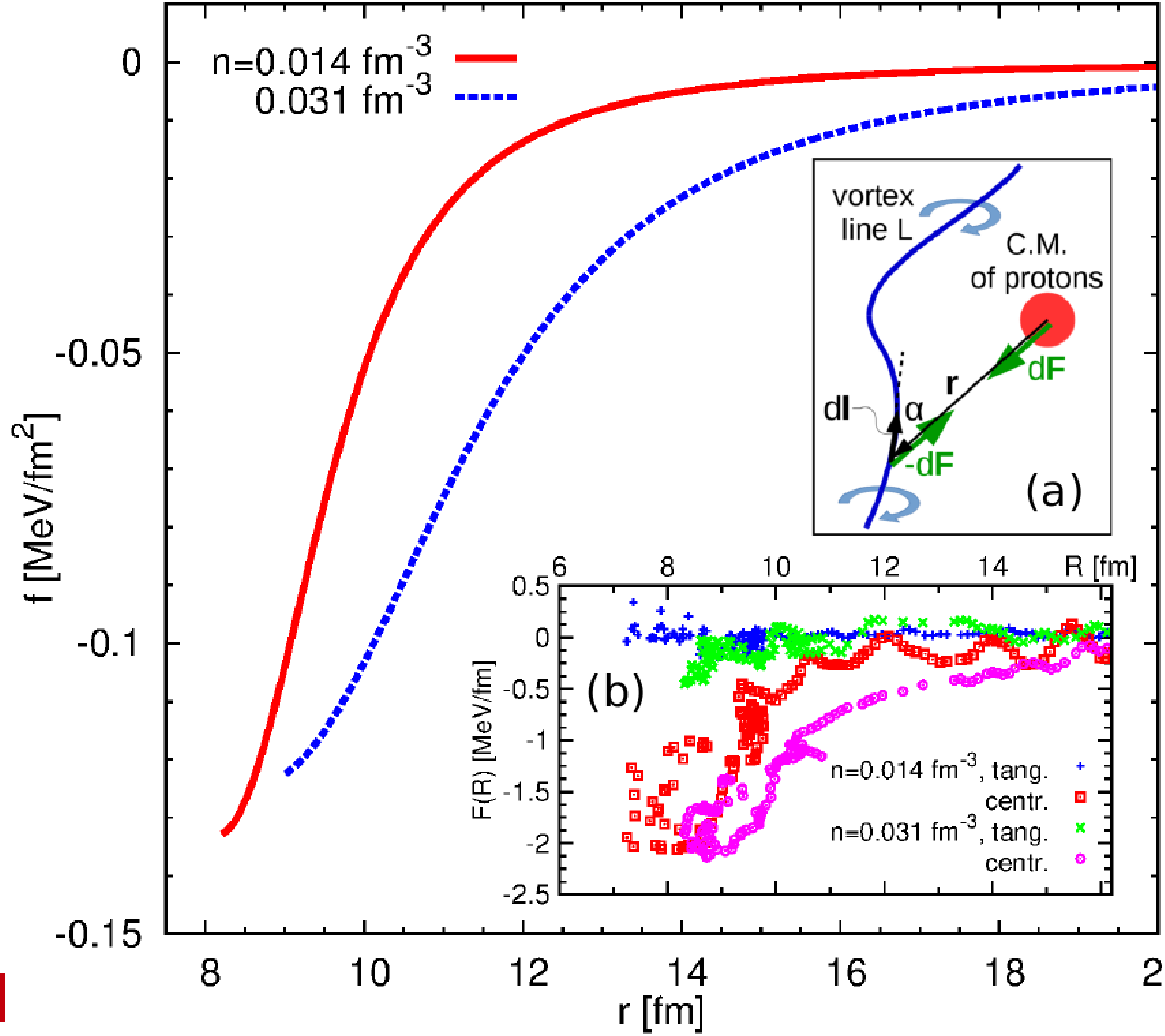
"frames of movie"

Measured force

Predicted for given set $\{a_k, b_k\}$

$$\boldsymbol{F}_i^{(f)} = \int_{L_i} f(r; \{a_k, b_k\}) \sin\alpha\, \boldsymbol{e}_r\, dl$$

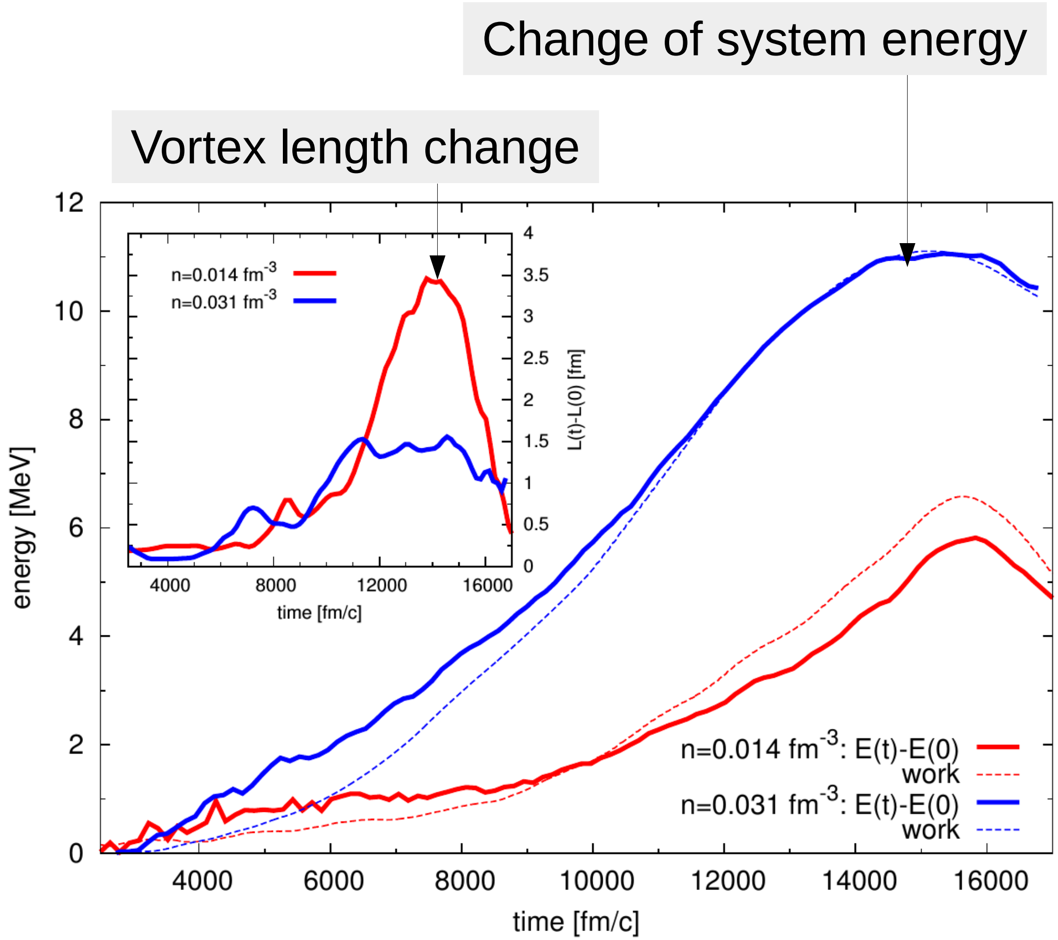
Force per unit length



Movie 4

Vortex tension

Tension: energy needed to increase vortex length by unit

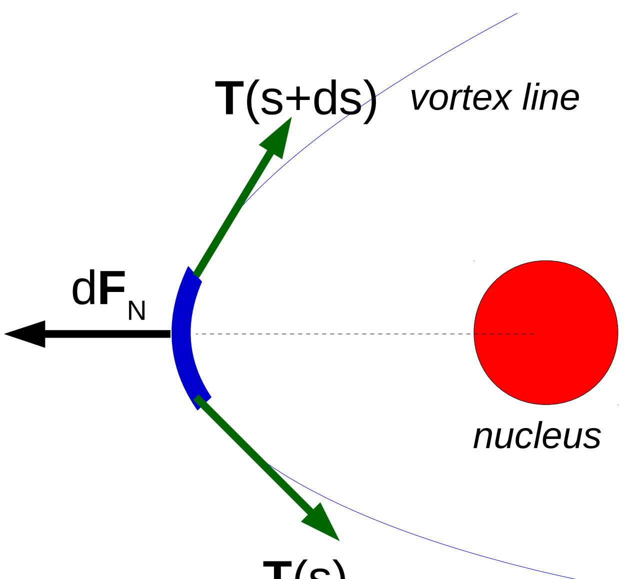


$T \lesssim 1.4\ \mathrm{MeV/fm}$ and $7.3\ \mathrm{MeV/fm}$

n=0.014 fm^{-3} n=0.031 fm^{-3}

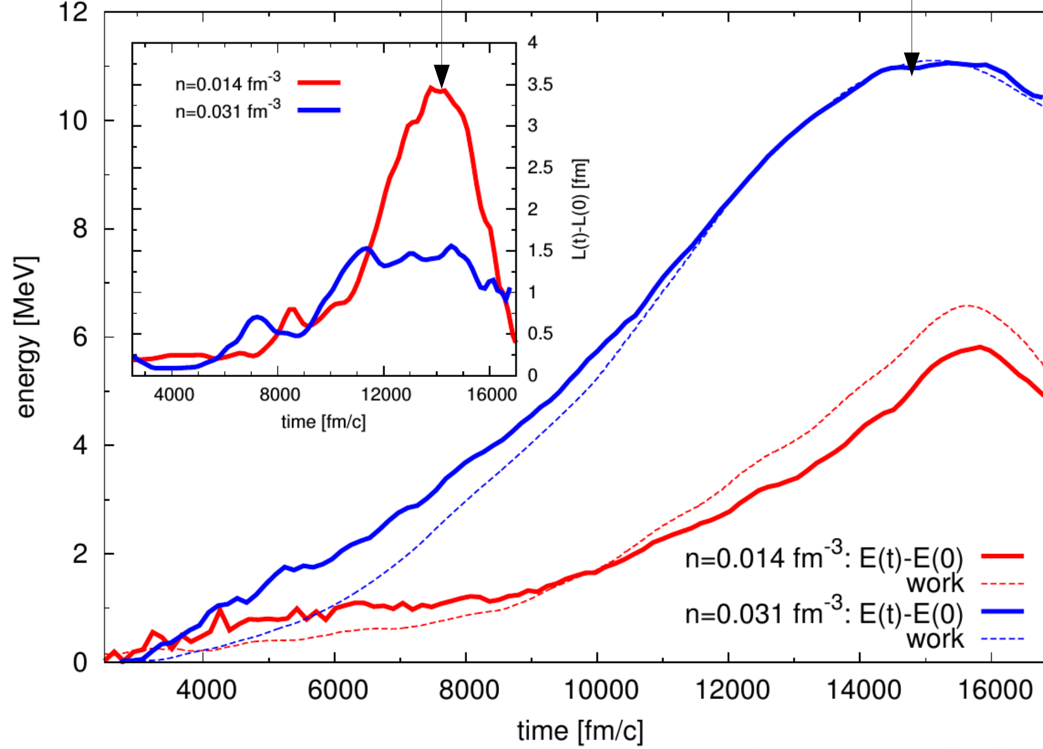
Vortex tension

Tension: energy needed to increase vortex length by unit



Change of system energy

Vortex length change



$$\mathrm{d}\boldsymbol{F}_M = \mathrm{d}\boldsymbol{F}_N + \boldsymbol{T}(s+\mathrm{d}s) - \boldsymbol{T}(s)$$

By inverting equations of motion for vortex elements we can gain detailed information about tension

CONCLUSIONS:

- Using a **qualitatively new approach**, we follow the dynamics as superfluid **vortices** move in **response** to the presence of **“nuclei”**

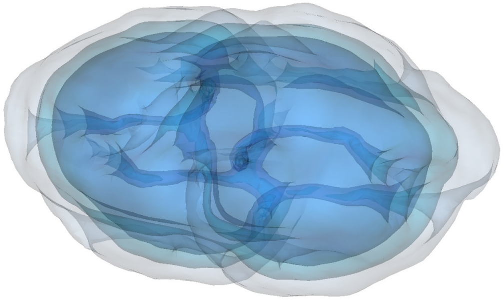
- **Nuclei repel vortices** in the neutron star crust,
  leading thus to **interstitial** vortex **pinning**

- The approach can provide **detailed** insight into vortex-nuclues interaction

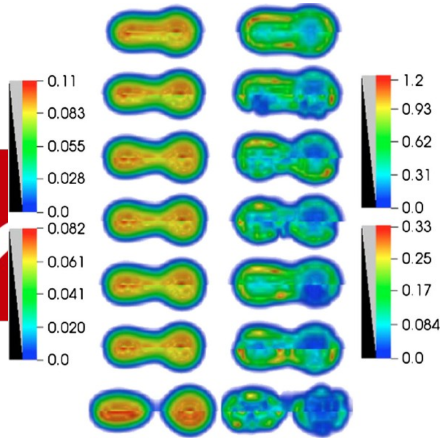
- Time-dependent simulations can be used to extract **various** quantities.

  - Dynamics in ultracold atoms
    vortex dynamics (Phys. Rev. Lett. 112, 025301 (2014))
    quantum turbulence (Phys. Rev. A 91, 031602(R) (2015))
    shock waves (Phys. Rev. Lett. 108, 150401 (2012))

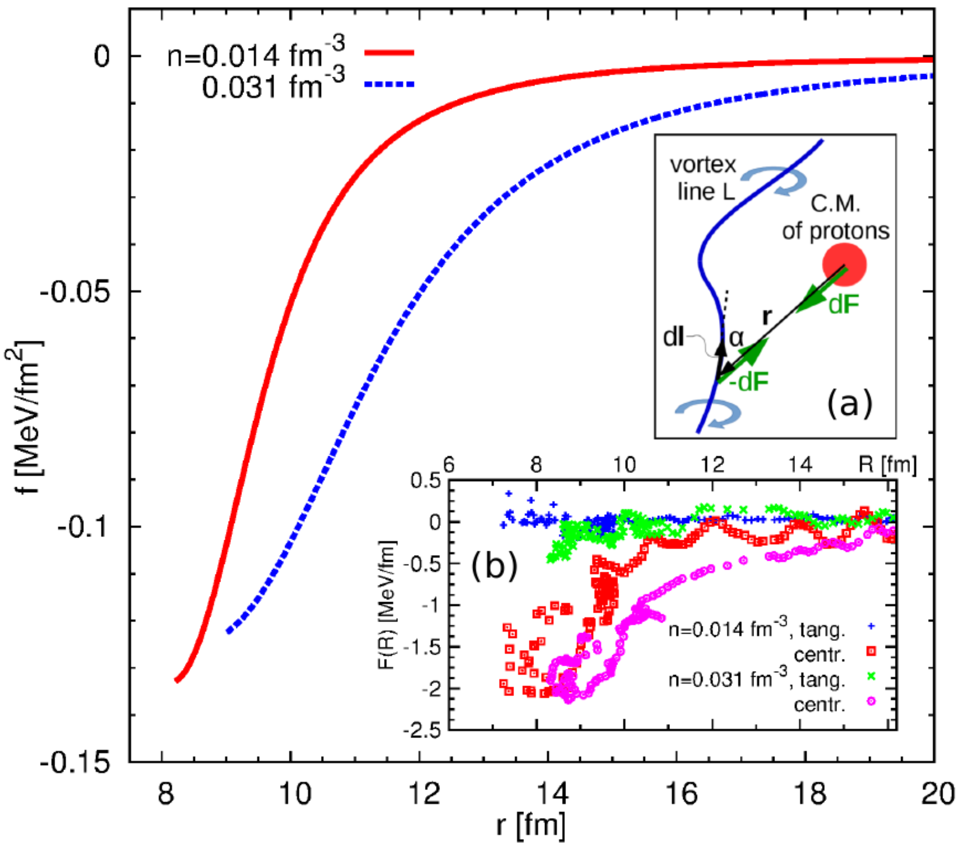
  - Dynamics of nuclear systems
    fission (Phys. Rev. Lett. 116, 122504 (2016))
    relativistic coulomb excitation (Phys. Rev. Lett. 114, 012701 (2015))
    isovector giant dipole resonance(Phys. Rev. C 84, 051309(R) (2011))

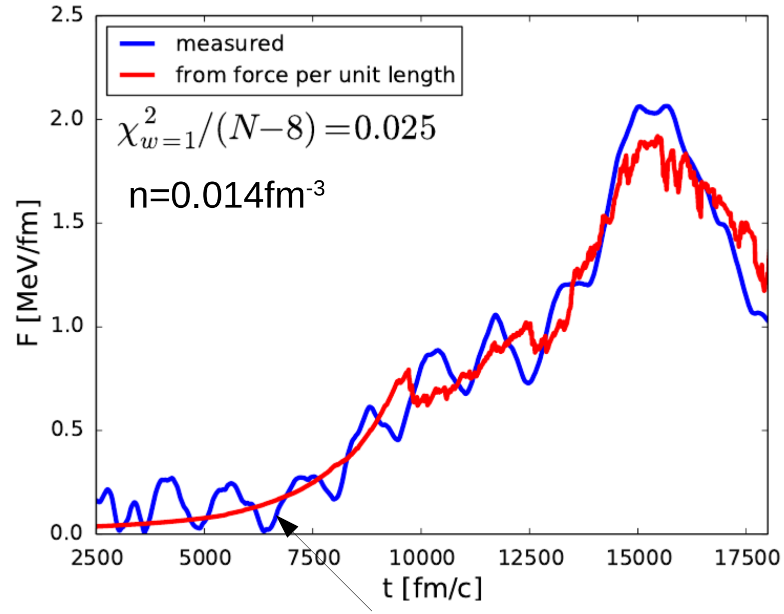


Thank you



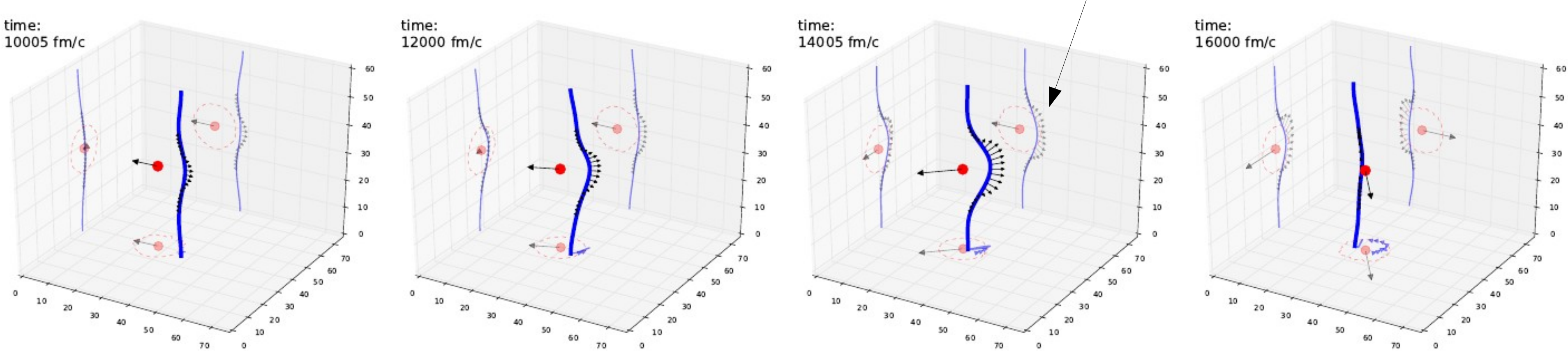
Force per unit length



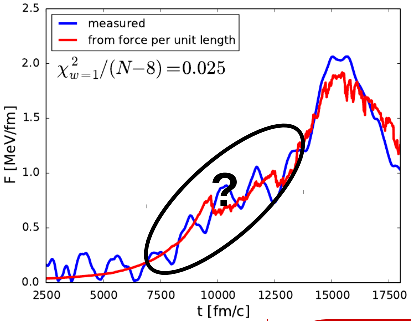


Fluctuations?

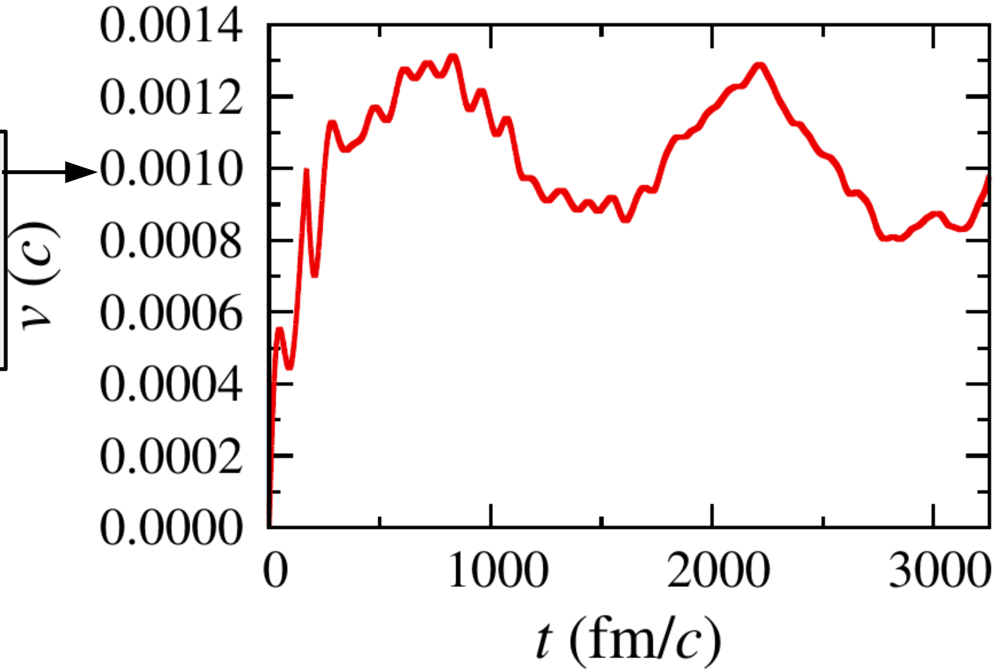
Only part close to nucleus surface contributes...



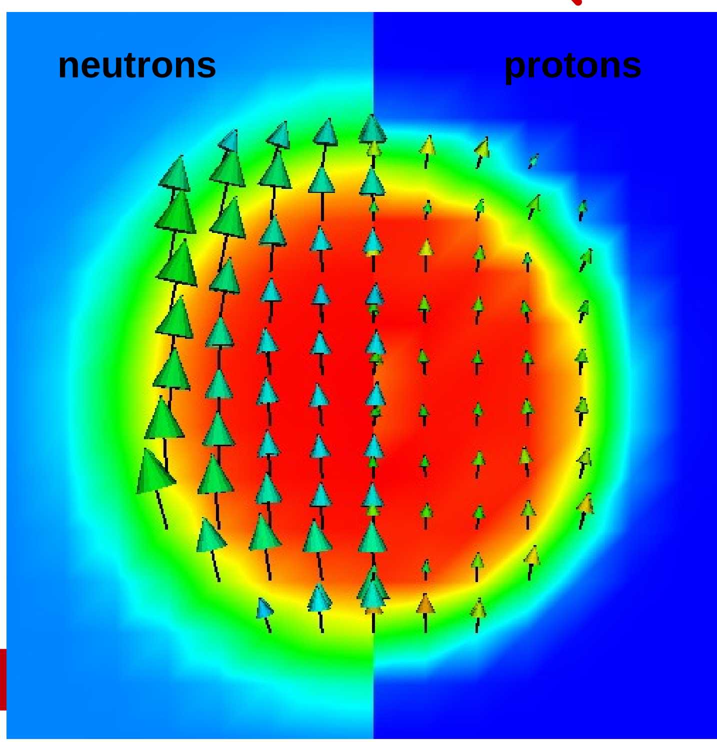
Force fluctuations

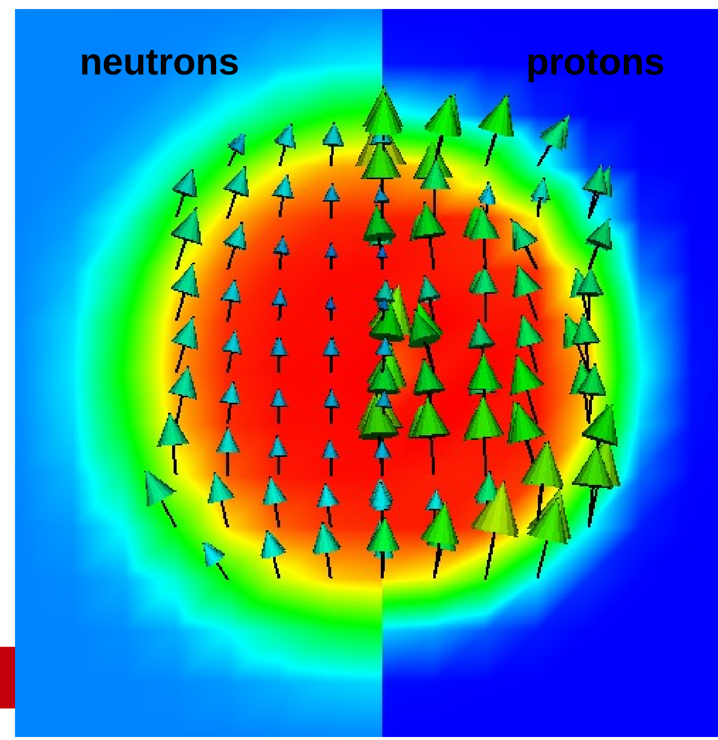


We accelerated nucleus to v_0
(by dragging protons)
and let it go...



We induce giant dipole oscillations

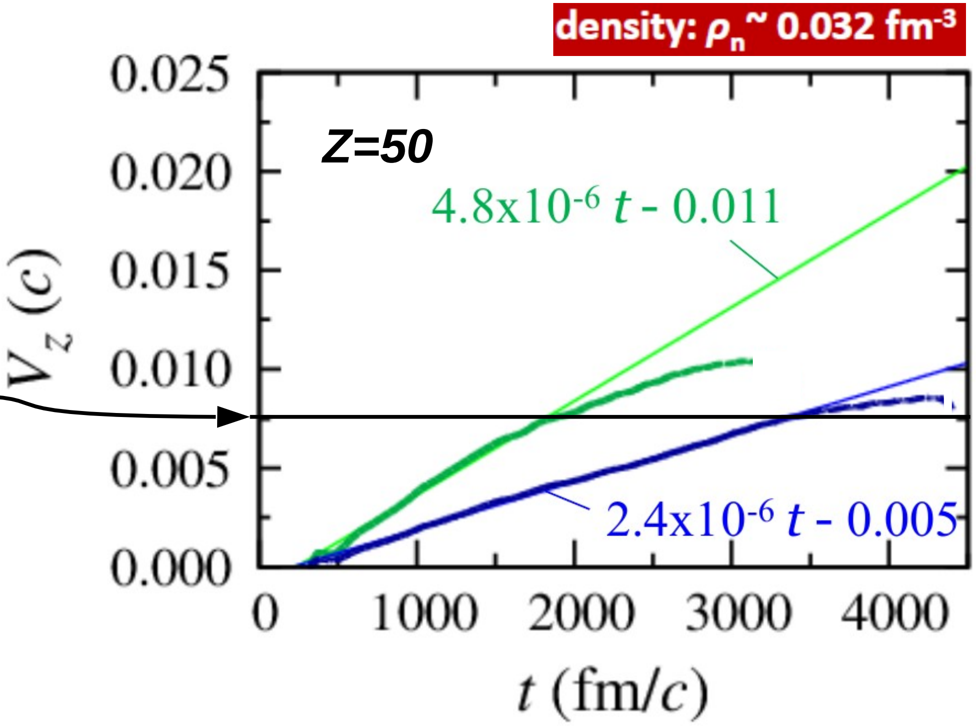




$$\boldsymbol{F} = M^* \boldsymbol{a}$$

$$M^* \simeq 218 m_N$$

“critical” velocity



Vortex model - idea

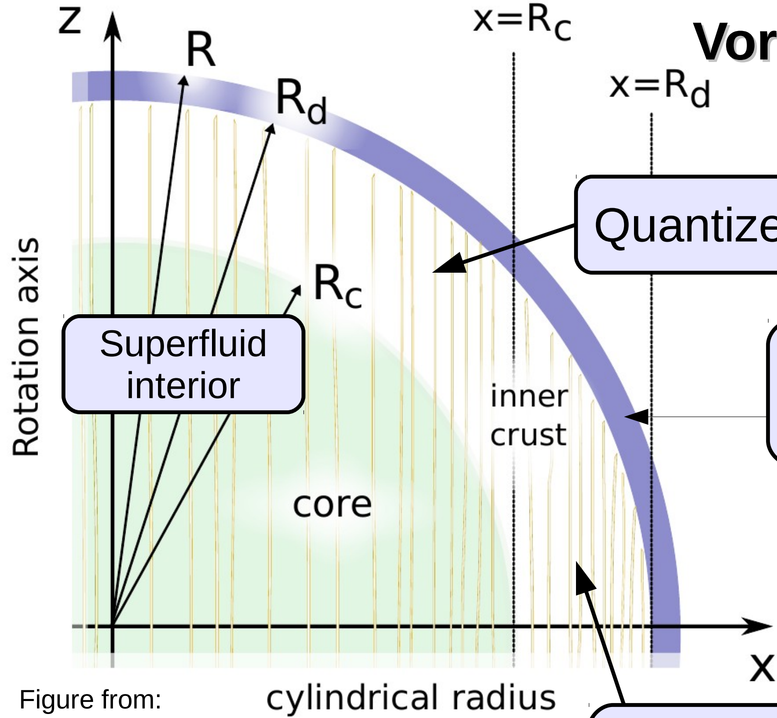


Figure from:
M. Antonelli, P. Pizzochero,
arXiv:1603.02838

Quantized vortices

Superfluid interior

Outer crust sets observed rotation period

Glitches are believed to occur when a large number of vortices simultaneously **unpin** and move outward (vortex avalanches)

When vortex “hits” outer crust: Transfer of angular momentum from interior to the crust

Vortices can “**pin**” to lattice of nuclear defects in inner crust

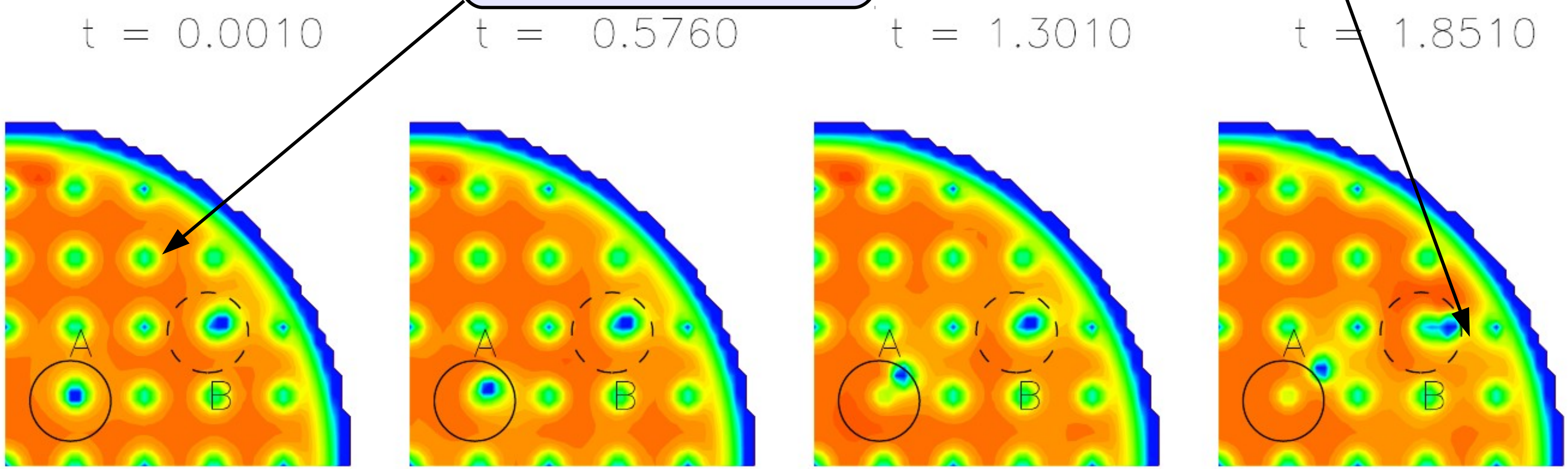
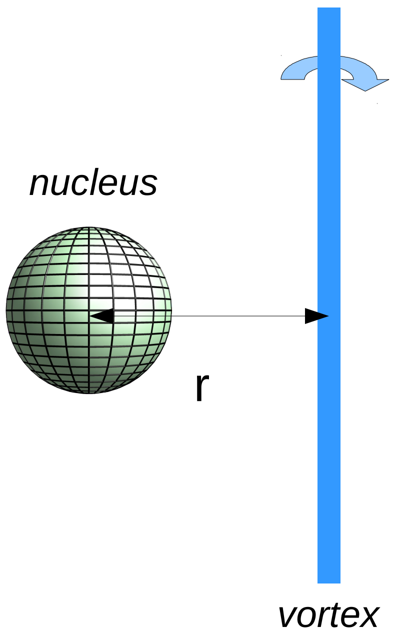


Figure from: L. Warszawski, A. Melatos, N. G. Berloff, Phys. Rev. B 85, 104503 (2012)

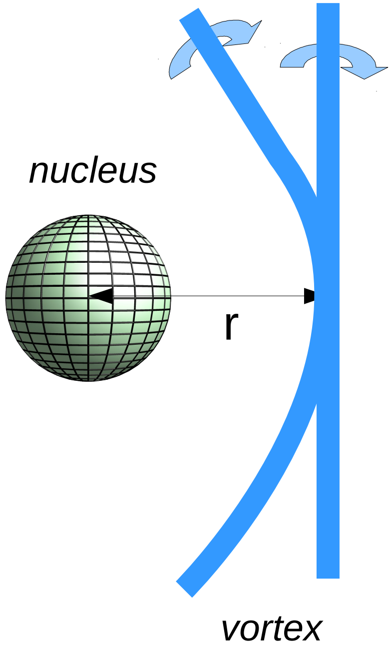
Force per unit length

From pinning energy the average force can be deduced: $F_{\text{pin}} \approx -\dfrac{\Delta E}{\Delta r}$

One should consider energy change as
a function of separation r...



… as well as function of deformation



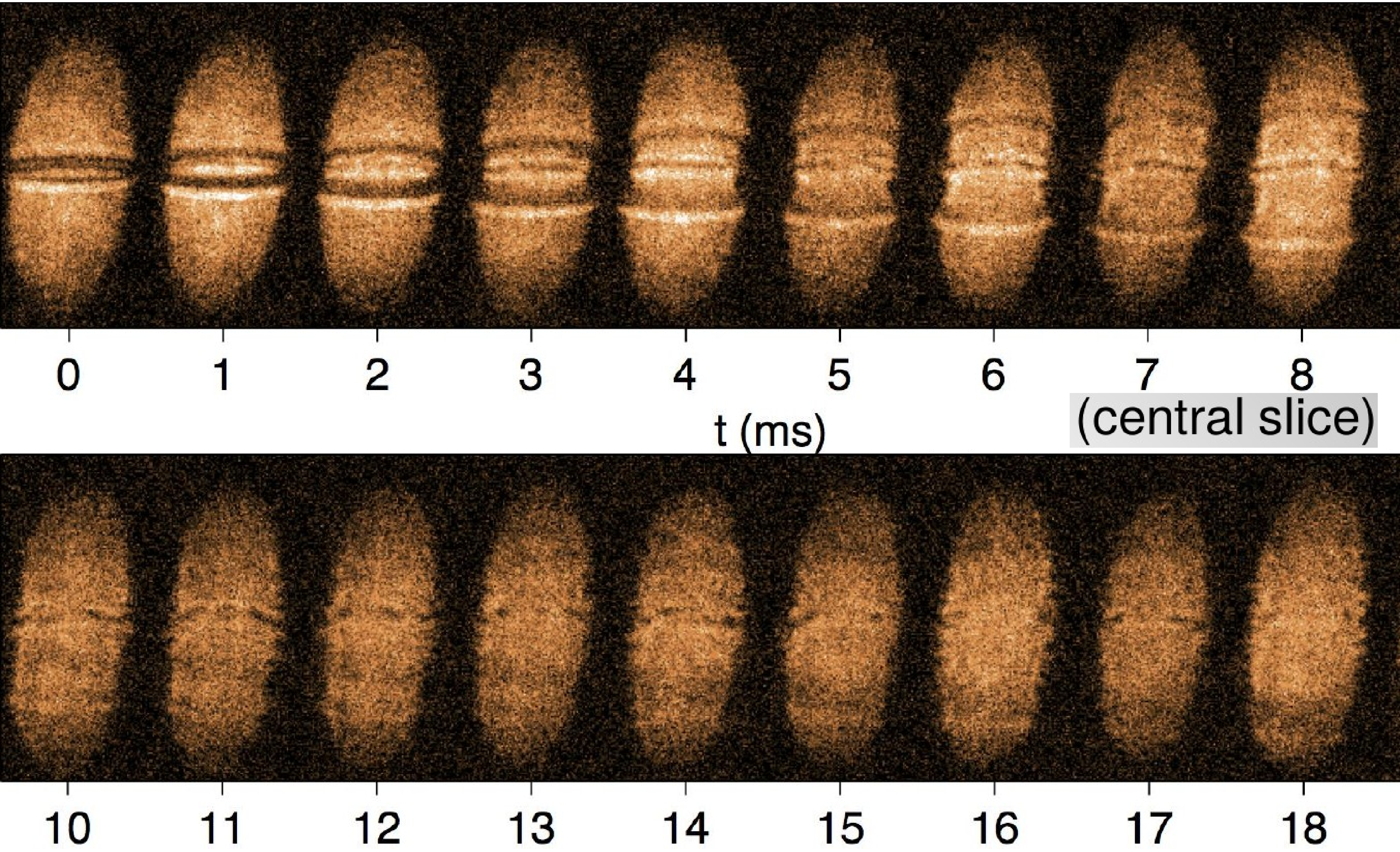
<u>Note:</u>
Vortex impurity
is not a function
of distance r only!!!

Very problematic within static calculations...

Experimental results – Cascade of Solitary Waves

Figures taken from: M. Zwierlein talk, (http://en.sif.it/activities/fermi_school/mmxiv)
School of Physics E. Fermi – Quantum Matter at Ultralow Temperatures Varenna, July 9th , 2014

See also: Mark J.H. Ku, et al., Phys. Rev. Lett. 116, 045304 (2016)



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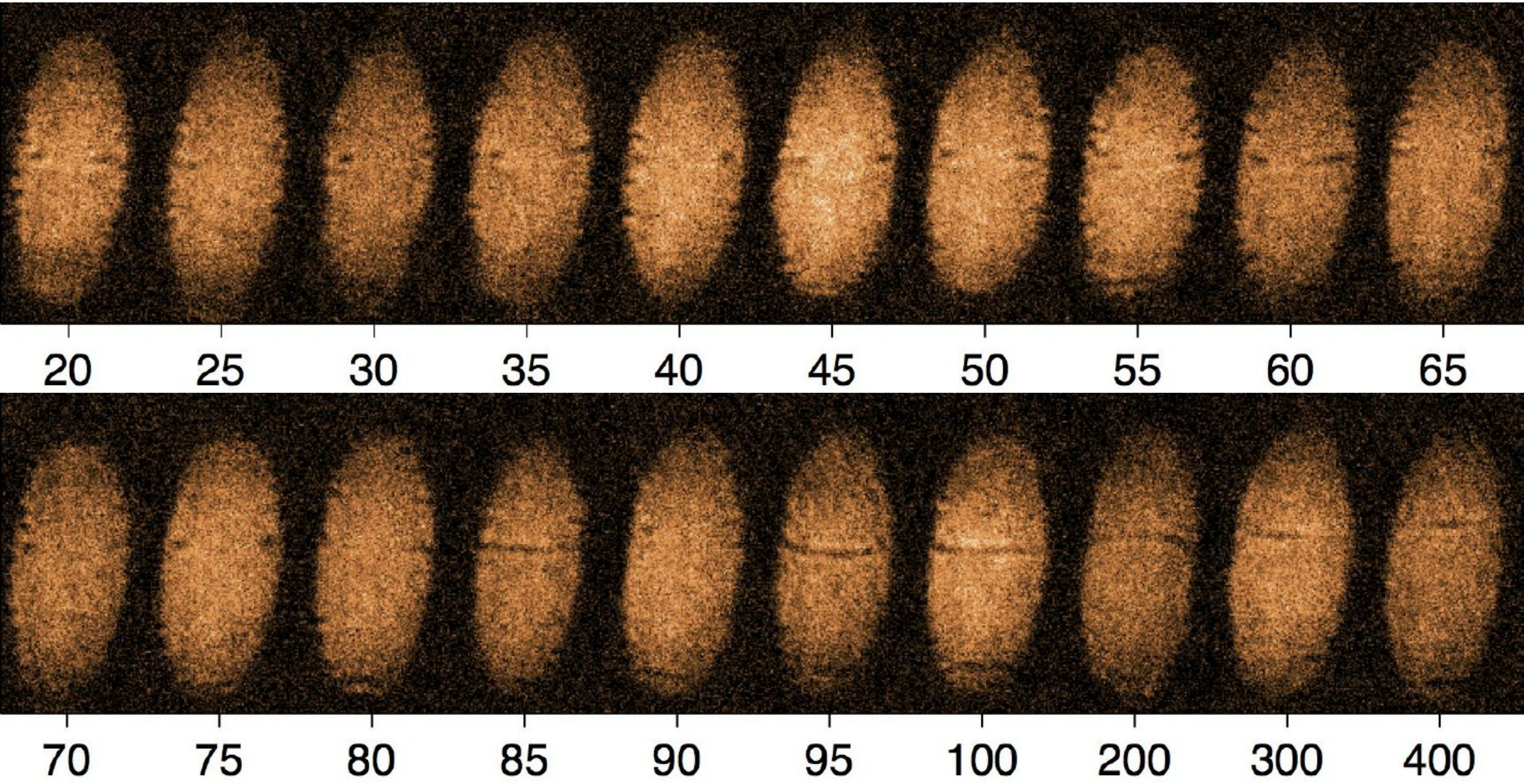

Experimental results – Cascade of Solitary Waves

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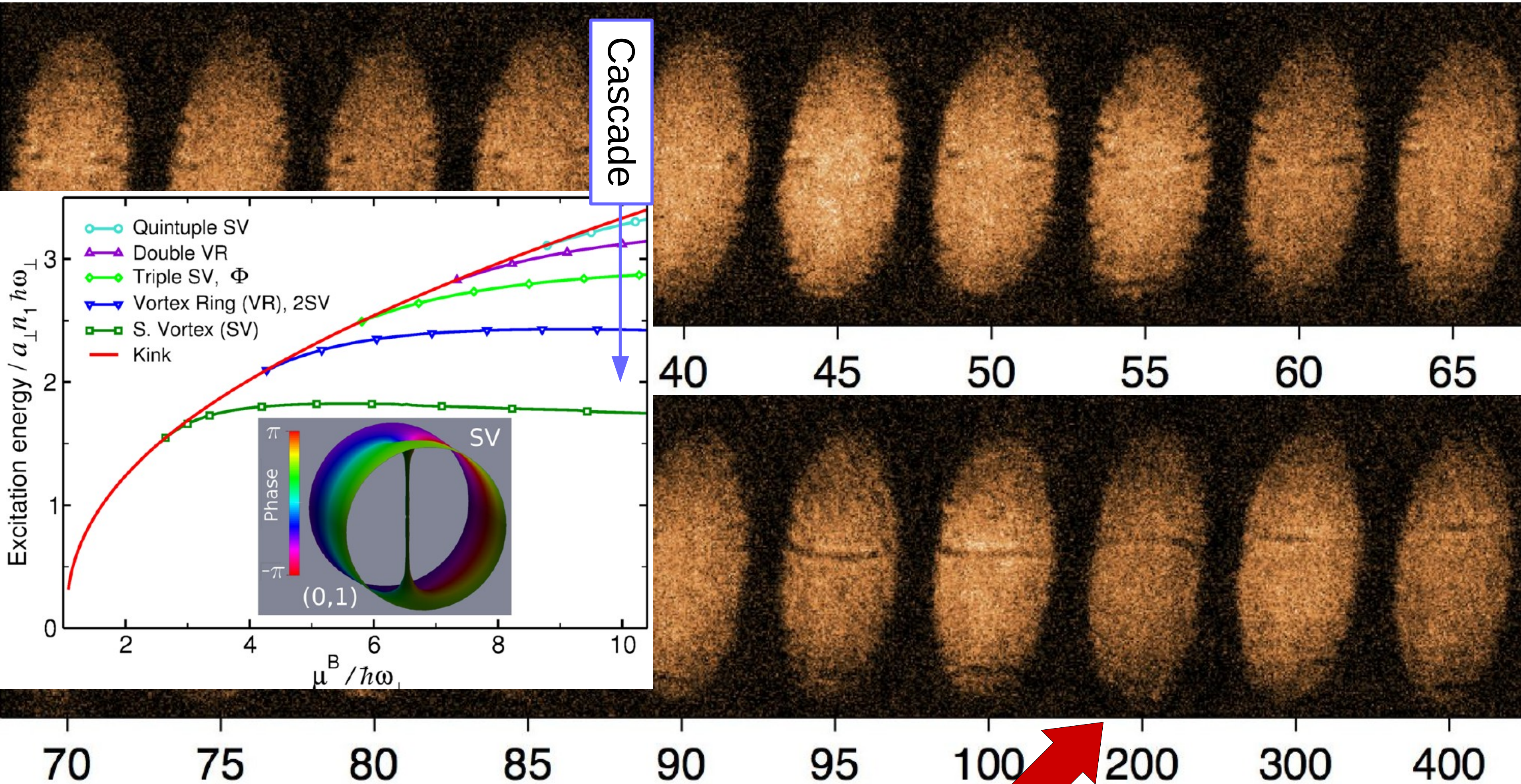
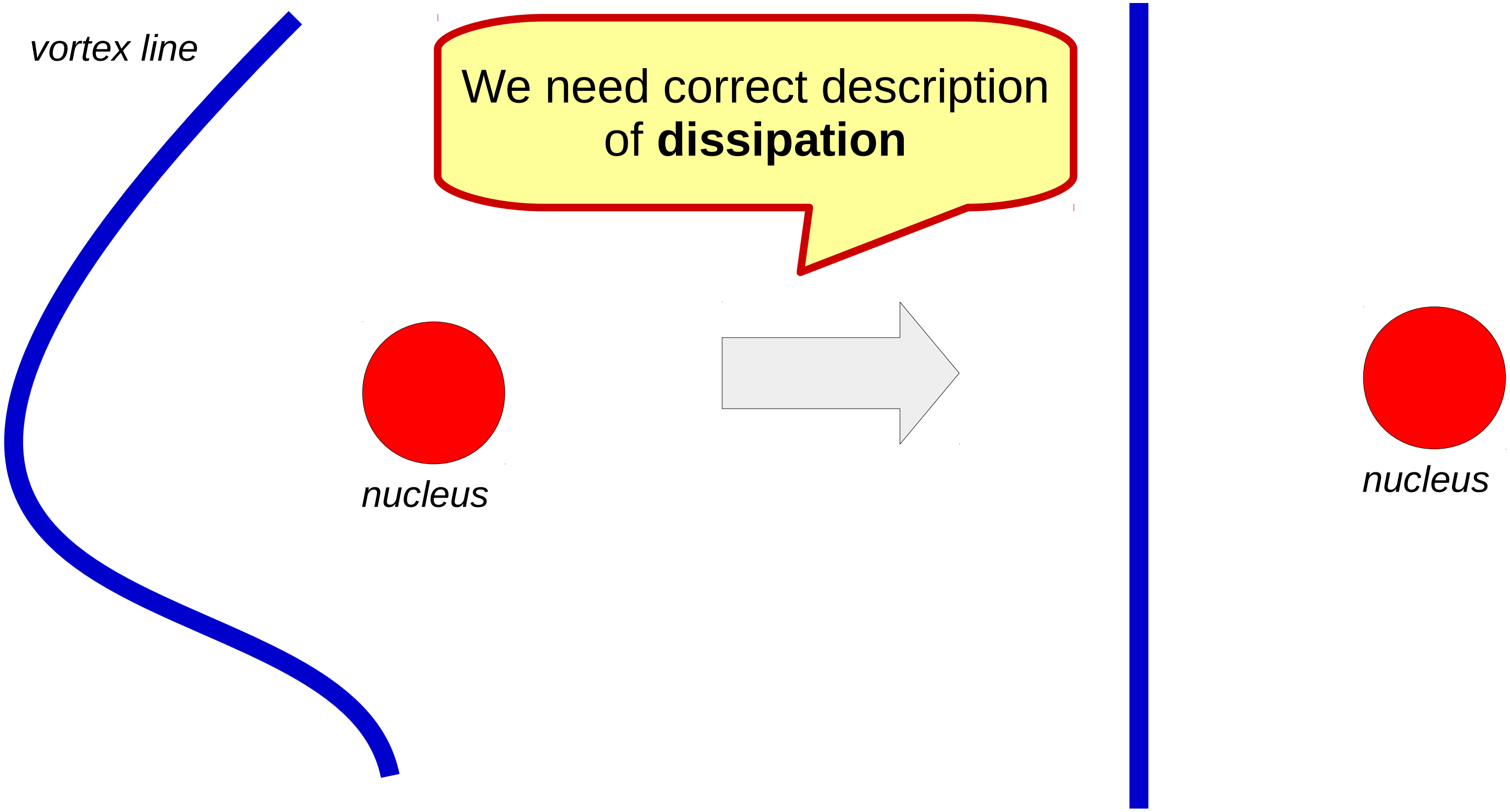


Challenge for theory to describe all stages of the cascade! Dissipation is crucial...

Dissipation



adiabatic approximation $\Rightarrow$ Memory effects are usually neglected

Result: dissipation effects are not correctly taken into account except for one-body dissipation

...but our system is superfluid...

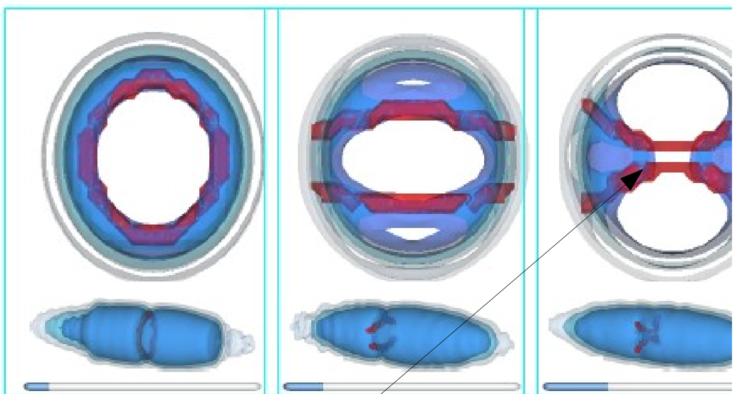
… and one-body dissipation sufficient to describe dynamics of vortex in ultra-cold atoms...

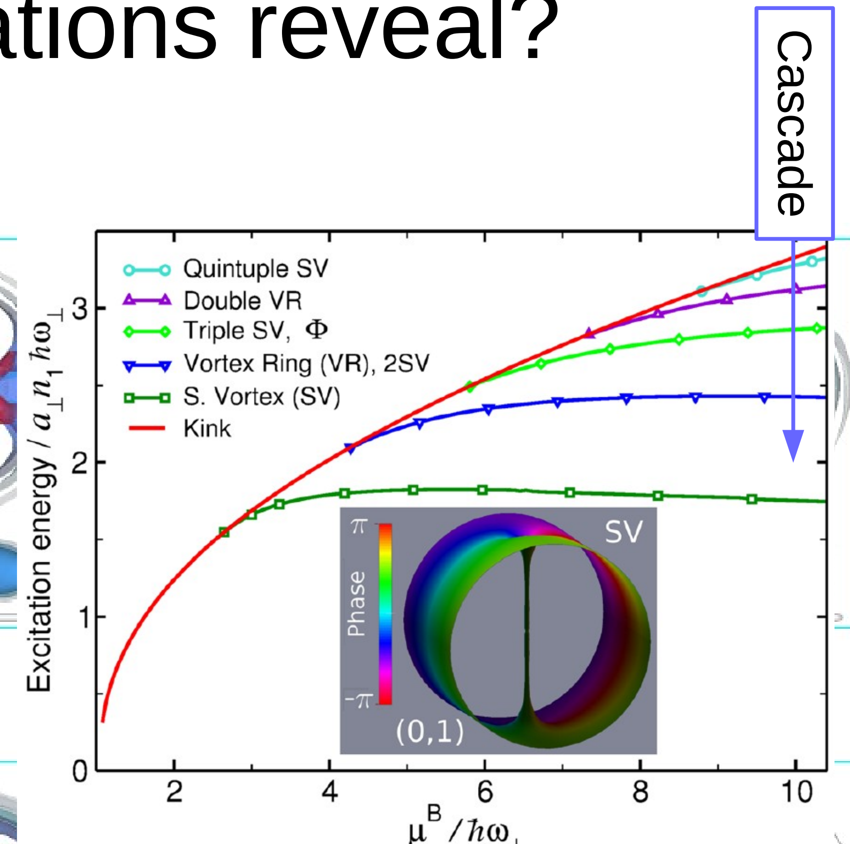
What do fully 3D simulations reveal?

Phys. Rev. A 91, 031602 (2015)

$\delta \approx 10\%$

$\frac{C}{C_0} \approx 3\%$

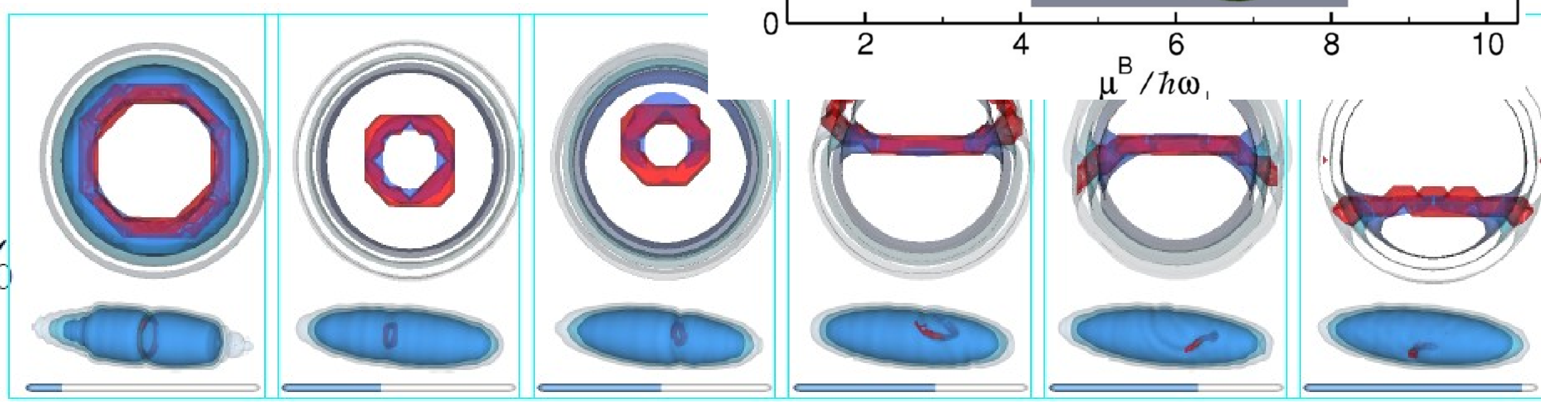




Crossing and reconnection!

$\delta \approx 0.5\%$

$\frac{C}{C_0} \approx 0.15\%$



Density Functional Theory – Idea

It can be shown that **instead of *wave function*** one may use a **density** distribution:

contains vastly more information than the one needed

$$\rho_1(\mathbf{x}_1,\mathbf{x}_1') = N \int \Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N)\Psi(\mathbf{x}_1',\ldots,\mathbf{x}_N)^* d\mathbf{x}_2 \cdots d\mathbf{x}_N$$

reduced object - sufficient to extract one body observables

Theorem (Hohenberg & Kohn):
The energy of the nondegenerate ground state of the Fermi system is uniquely determined by its density distribution.

$$\Psi \overset{1\text{–}1}{\longleftrightarrow} \rho \quad \Rightarrow \quad E[\rho] = \left\langle \Psi[\rho] \middle| \hat{H} \middle| \Psi[\rho] \right\rangle$$

The energy is a functional of the density

In general:

$$\langle O \rangle = \langle \Psi[\rho] | O | \Psi[\rho] \rangle = O[\rho]$$

"Universal" part

External field

$$E[\rho] = F[\rho] + \int d\mathbf{x}\, v_{\text{ext}}(\mathbf{x})\rho(\mathbf{x})$$

Formally rigorous way of approaching any **interacting problem** by **mapping** it exactly to a much easier-to-solve **noninteracting system**.

Kohn-Sham method:

easy, if Energy Density Functional (EDF) is known...

interacting system

non-interacting system

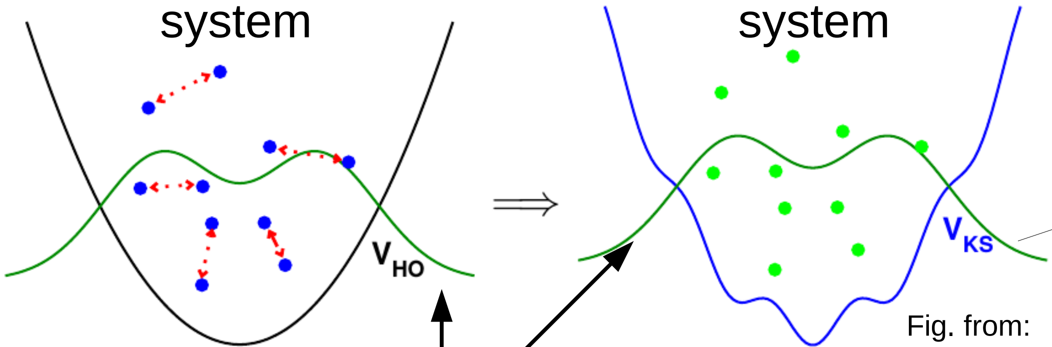


Fig. from: Prog.Part.Nucl.Phys.64:120-168,2010

$$v_{KS} = \frac{\delta F}{\delta \rho} + v_{ext}$$

Both systems described by the same density

$$[-\nabla^2/2m + v_{\text{KS}}(\mathbf{x})]\phi_i(\mathbf{x}) = \varepsilon_i \phi_i(\mathbf{x})$$

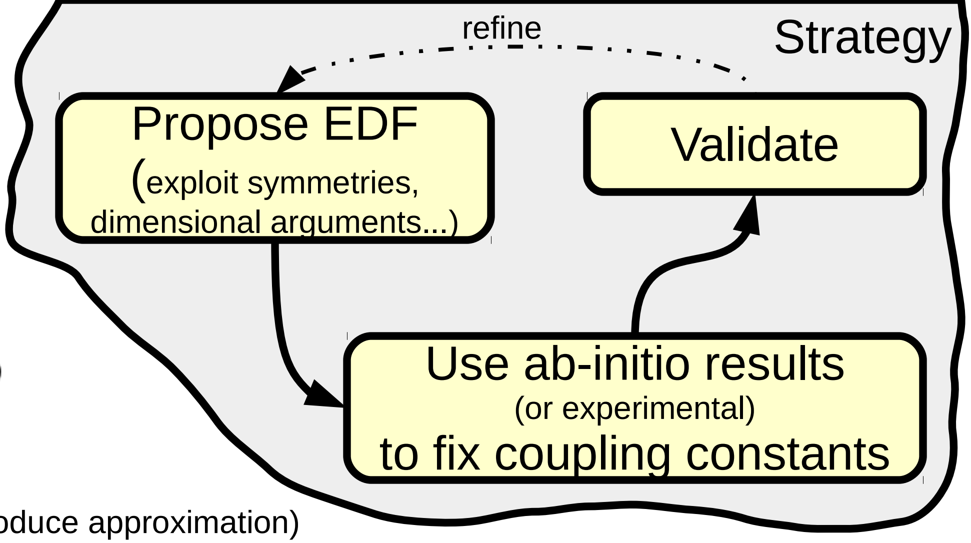
$$\rho(\mathbf{x}) = \sum_i n_i |\phi_i(\mathbf{x})|^2 \quad n_i = \theta(\varepsilon_{\text{F}} - \varepsilon_i)$$

More general:

Interacting System ⇨ System of non-interacting quasiparticles

Note: There are easy and difficult observables in DFT.
In general: **easy** observables are **one-body** observables. They are easily extracted and reliable.

Energy density functional



How to derive EDF?

$$E[\rho] = T[\rho] + V[\rho] + v_{ext}\rho$$

We build models of EDF (typically here we introduce approximation)

$$E[\rho_i, \tau_i, \ldots] = \int d\mathbf{x}\, \mathcal{E}(\rho_i(\mathbf{x}), \tau_i(\mathbf{x}), \ldots)$$

Example:
Local Density Approximation
(only dependence on diagonal parts of densities $\rho(\boldsymbol{x}) \equiv \rho(\boldsymbol{x}, \boldsymbol{x})$)

$$[-\boldsymbol{\nabla}^2/2m + v_{\mathrm{KS}}(\mathbf{x})]\phi_i(\mathbf{x}) = \varepsilon_i \phi_i(\mathbf{x})$$

$$\rho(\mathbf{x}) = \sum_{i=1}^{A} |\phi_i(\mathbf{x})|^2$$

$$\tau(\boldsymbol{x}) = \sum_{i=1}^{A} |\nabla\phi_i(\boldsymbol{x})|^2$$

From orbitals
we build other densities
(correlated with ρ)

$$T_s[\rho] = -\frac{1}{2m}\sum_{i=1}^{A}\int d\mathbf{x}\, \phi_i^\dagger(\mathbf{x})\nabla^2\phi_i(\mathbf{x})$$

$$= \int d\boldsymbol{x}\, \frac{1}{2m}\tau(\boldsymbol{x})$$

Ultracold atoms are superfluid!

Normal system

$$\begin{cases} [-\nabla^2/2m + v_{\rm KS}(\mathbf{x})]\phi_i(\mathbf{x}) = \varepsilon_i\phi_i(\mathbf{x}) \\ v_{KS} = \dfrac{\delta F}{\delta\rho} + v_{ext} \end{cases}$$

pairing (anomalous) density

$$F[\rho,\tau,\ldots] \rightarrow F[\rho,\tau,\nu,\ldots]$$

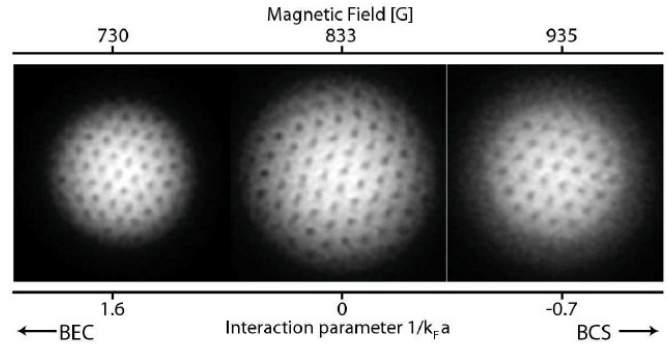


FIG. 36 Vortex lattice in a rotating gas of ^{6}Li precisely at the Feshbach resonance and on the BEC and BCS side. Reprinted with permission from Zwierlein *et al.* (2005).

$$\begin{cases} [h(\mathbf{r})-\mu]u_k(\mathbf{r}) + \Delta(\mathbf{r})v_k(\mathbf{r}) = E_k u_k(\mathbf{r}), \\ \Delta^*(\mathbf{r})u_k(\mathbf{r}) - [h(\mathbf{r})-\mu]v_k(\mathbf{r}) = E_k v_k(\mathbf{r}), \end{cases}$$

BCS-like

$$h(\mathbf{r}) = -\nabla^2/2m + v_{\rm KS}(\mathbf{x})$$

$$\Delta = -\frac{\delta F}{\delta\nu^*}$$

$$n(\mathbf{r}) = 2\sum_k |v_k(\mathbf{r})|^2, \quad \tau(\mathbf{r}) = 2\sum_k |\nabla v_k(\mathbf{r})|^2,$$

$$\nu(\mathbf{r}) = \sum_k v_k^*(\mathbf{r})u_k(\mathbf{r}),$$

Note: diagonal part
of pairing density is divergent
Regularization required!

We use prescription given in:
Bulgac, Yu, Phys. Rev. Lett. 88 (2002) 042504
Bulgac, Phys. Rev. C65 (2002) 051305

Extension to time-dependent case

$$i\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi, \quad \psi_0 = \psi(t_0) \qquad \text{and} \qquad \frac{\partial \rho}{\partial t} + \nabla\cdot\vec{j} = 0$$

$$\mathbf{j}(\mathbf{r}) = -\frac{iN}{2}\int d\mathbf{r}_2\cdots d\mathbf{r}_N \Psi(\mathbf{r},\ldots,\mathbf{r}_N)^*\nabla\Psi(\mathbf{r},\ldots,\mathbf{r}_N) - \Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)\nabla\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)^* \,.$$

Runge & Gross theorem

$$\left.\begin{matrix}\rho(\vec{r},t) \\ \psi(\ldots,t_0)\end{matrix}\right\} \leftrightarrow e^{i\alpha(t)}\psi(\ldots,t)$$

Up to arbitrary function α(t)

… and consequently density functional exists...
NOTE: in general this functional:
- is initial state dependent
- at time t depends on densities in previous times (memory effect)

Very little is known about the memory terms, but in principle it can be long ranged (see eg. Dobson, Brunner, Gross, Phys. Rev. Lett. 79 (1997) 1905)

Memory effects are usually neglected = adiabatic approximation
[Result: dissipation effects are not correctly taken into account except for one-body dissipation]

...but our system is superfluid...

van Leeuwen's Theorem:

Time evolution of interacting system

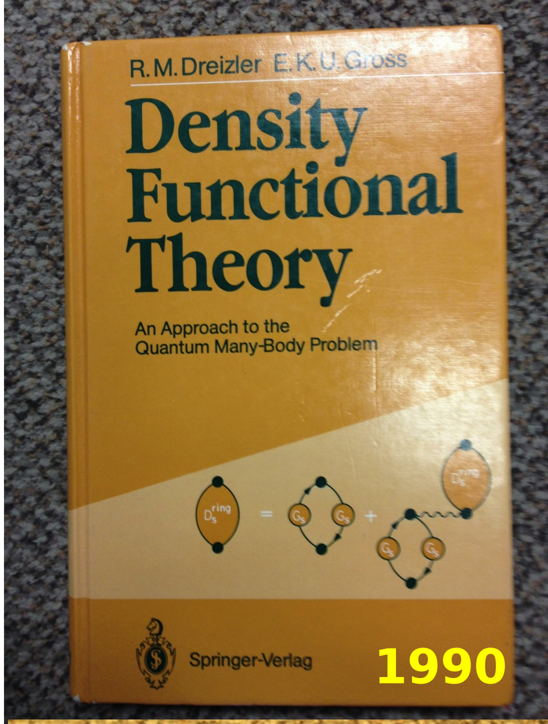
⇩

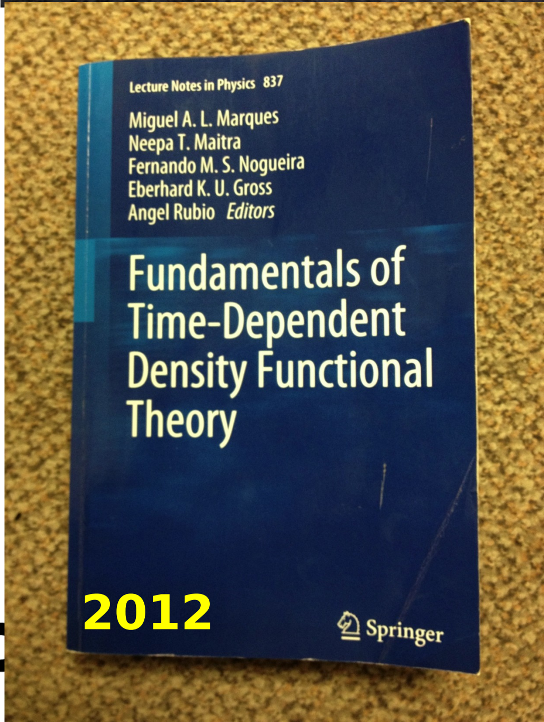
Time evolution of non-interacting system

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

DFT: workhorse for electronic structure simulations

- The Hohenberg-Kohn theorem assures that the theory can reproduce exactly the ground state energy if the “exact” Energy Density Functional (EDF) is provided
- Often called as *ab initio* method
- Extension to Time-Dependent DFT is straightforward
- Can be extended to superfluid systems... (numerical cost increases dramatically)
- **Very successful** – DFT industry (commercial codes for quantum chemistry and solid-state physics)





Solving time-dependent problem...

The real-time dynamics is given by equations, which are formally equivalent to the Time-Dependent HFB (TDHFB) or Time-Dependent Bogolubov-de Gennes (TDBdG) equations:

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{n,a}(\boldsymbol{r},t) \\ u_{n,b}(\boldsymbol{r},t) \\ v_{n,a}(\boldsymbol{r},t) \\ v_{n,b}(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} h_a(\boldsymbol{r},t) & 0 & 0 & \Delta(\boldsymbol{r},t) \\ 0 & h_b(\boldsymbol{r},t) & -\Delta(\boldsymbol{r},t) & 0 \\ 0 & -\Delta^*(\boldsymbol{r},t) & -h_a^*(\boldsymbol{r},t) & 0 \\ \Delta^*(\boldsymbol{r},t) & 0 & 0 & -h_b^*(\boldsymbol{r},t) \end{pmatrix} \begin{pmatrix} u_{n,a}(\boldsymbol{r},t) \\ u_{n,b}(\boldsymbol{r},t) \\ v_{n,a}(\boldsymbol{r},t) \\ v_{n,b}(\boldsymbol{r},t) \end{pmatrix}$$

The mean field potentials $h_i(\boldsymbol{r},t)$ are derived from the EDF as functional derivative $h_i = \frac{\delta E}{\delta n_i}$ and they explicitly depends on local densities $n(\boldsymbol{r})$, $\tau(\boldsymbol{r})$, etc. The set of 4-component "wave functions" is in turn related to the densities and the pairing field $\Delta(r)$

$$\begin{aligned} n_i(\boldsymbol{r}) &= \sum_{E_n<E_c} |v_{n,i}(\boldsymbol{r})|^2, \\ \tau_i(\boldsymbol{r}) &= \sum_{E_n<E_c} |\nabla v_{n,i}(\boldsymbol{r})|^2, \\ \nu(\boldsymbol{r}) &= \sum_{E_n<E_c} u_{n,a}(\boldsymbol{r}) v_{n,b}^*(\boldsymbol{r}), \\ \Delta(\mathbf{r}) &= -g_{\text{eff}}(\mathbf{r})\nu(\mathbf{r}). \end{aligned}$$

nonlinear coupled 3D Partial Differential Equations

Supercomputing

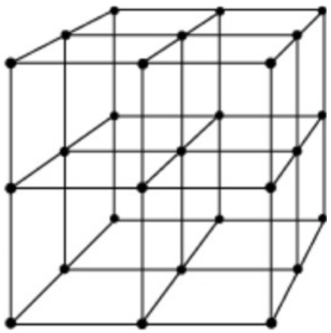
We simulate fermionic systems consisting of $10^3 - 10^4$ particles (**cold atoms**, neutron stars)

… also nuclear reactions (spin-orbit term required)

Solving...

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{n,a}(\boldsymbol{r},t) \\ u_{n,b}(\boldsymbol{r},t) \\ v_{n,a}(\boldsymbol{r},t) \\ v_{n,b}(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} h_a(\boldsymbol{r},t) & 0 & 0 & \Delta(\boldsymbol{r},t) \\ 0 & h_b(\boldsymbol{r},t) & -\Delta(\boldsymbol{r},t) & 0 \\ 0 & -\Delta^*(\boldsymbol{r},t) & -h_a^*(\boldsymbol{r},t) & 0 \\ \Delta^*(\boldsymbol{r},t) & 0 & 0 & -h_b^*(\boldsymbol{r},t) \end{pmatrix} \begin{pmatrix} u_{n,a}(\boldsymbol{r},t) \\ u_{n,b}(\boldsymbol{r},t) \\ v_{n,a}(\boldsymbol{r},t) \\ v_{n,b}(\boldsymbol{r},t) \end{pmatrix}$$

- The system is placed on a large 3D spatial lattice of size $N_x \times N_y \times N_z$



  - Discrete Variable Representation (DVR) - solid framework (see for example: Bulgac, Forbes, Phys. Rev. C 87, 051301(R) (2013))
  - Errors are well controlled – exponential convergence
  - No symmetry restrictions
- Number of PDEs is of the order of the number of spatial lattice points
  - Typically (without spin-orbit term): 10^5 - 10^6

Solving...

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}u_{n,a}(\boldsymbol{r},t)\\u_{n,b}(\boldsymbol{r},t)\\v_{n,a}(\boldsymbol{r},t)\\v_{n,b}(\boldsymbol{r},t)\end{pmatrix}=\begin{pmatrix}h_a(\boldsymbol{r},t) & 0 & 0 & \Delta(\boldsymbol{r},t)\\0 & h_b(\boldsymbol{r},t) & -\Delta(\boldsymbol{r},t) & 0\\0 & -\Delta^*(\boldsymbol{r},t) & -h_a^*(\boldsymbol{r},t) & 0\\\Delta^*(\boldsymbol{r},t) & 0 & 0 & -h_b^*(\boldsymbol{r},t)\end{pmatrix}\begin{pmatrix}u_{n,a}(\boldsymbol{r},t)\\u_{n,b}(\boldsymbol{r},t)\\v_{n,a}(\boldsymbol{r},t)\\v_{n,b}(\boldsymbol{r},t)\end{pmatrix}$$

- Derivatives are computed with FFT
  - insures machine accuracy
  - very fast

It sets scaling
(N-number of lattice points)

$$O(N\,N\log N)\Rightarrow \#O(N^2)$$

Number of wave-functions

FFT

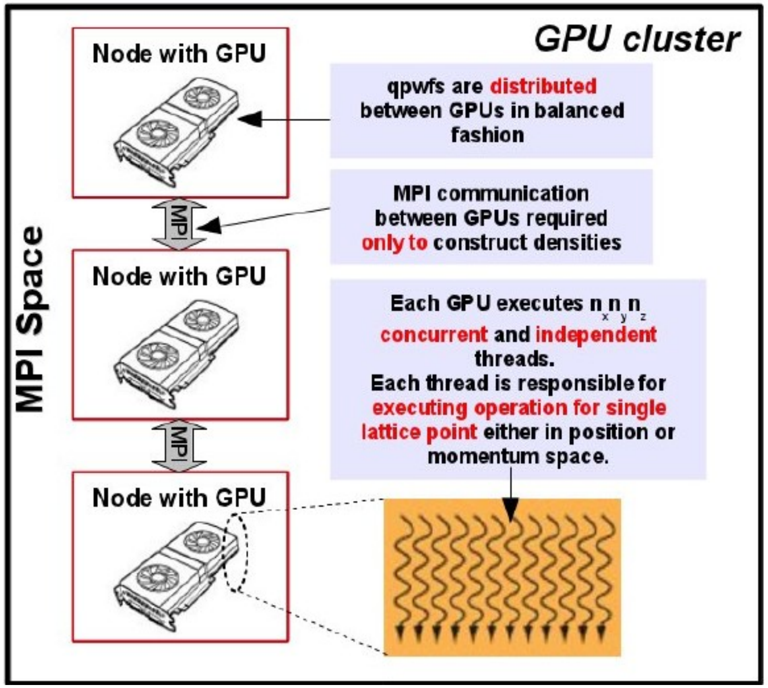
for large lattice

- Integration methods:
  - Adams-Bashforth-Milne fifth order predictor-corrector-modifier integrator – very accurate but memory intensive
  - Split-operator method that respects time-reversal invariance (third order) – very fast, but can work with simple EDF

If non local densities
N^3!!!
(beyond our reach)

The spirit of SLDA is to exploit only <u>local densities</u>...

- Suitable for efficient parallelization (MPI)
- Excellent candidate for utilization multithreading computing units like GPUs



Lattice	# of GPUs	# of qpwfs	time per step [s]
24x24x96	64	24425	0.33
24x24x96	128	24425	0.17
24x24x96	256	24425	0.09
24x24x96	512	24425	0.06
32x32x128	256	57849	0.32
32x32x128	313	57849	0.25
48x48x128	512	129881	0.95
48x48x128	1024	129881	0.50
48x48x128	2048	129881	0.27
48x48x128	4096	129881	0.16
48x48x128	8192	129881	0.10

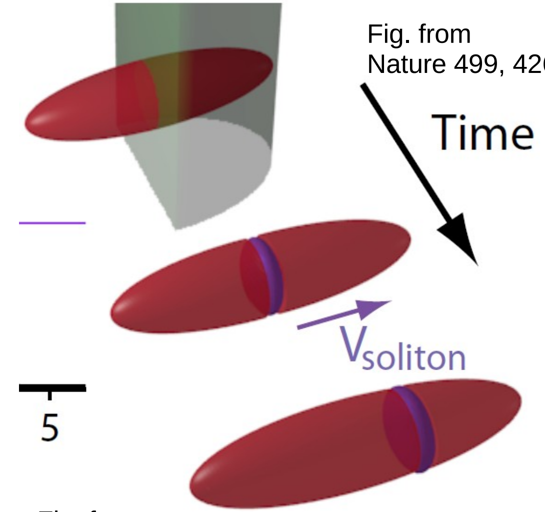
Lattice 64^3, 137,062 (2-component) wave functions, ABM
CPU version running on 16x4096=65,536 cores
GPU version running on 4096 GPUs

15 times Speed-up!!!

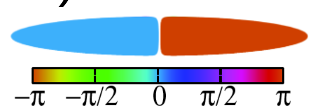
Validation against dynamical properties of the system

Recent MIT experiments: Nature 499, 426 (2013), PRL 113, 065301(2014)

Fig. from
Nature 499, 426 (2013)

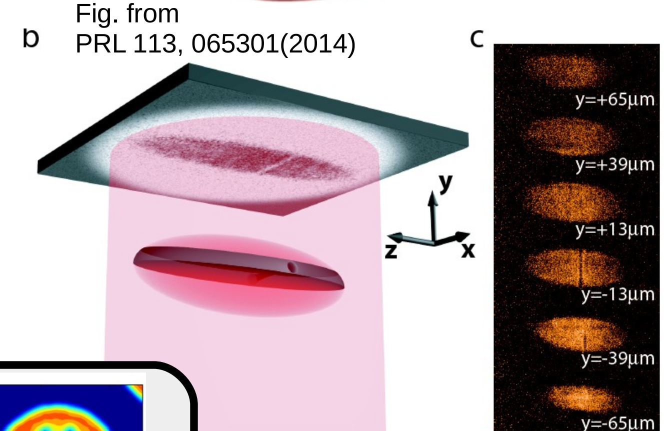


- ^{6}Li atoms near a Feshbach resonance ($N \approx 10^6$) cooled in harmonic trap
- Step potential used to imprint a soliton (evolve to π phase shift)

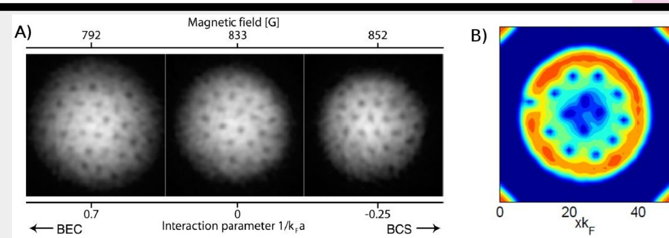


- Let system evolve...
- Take picture (subtle imaging with tomography)

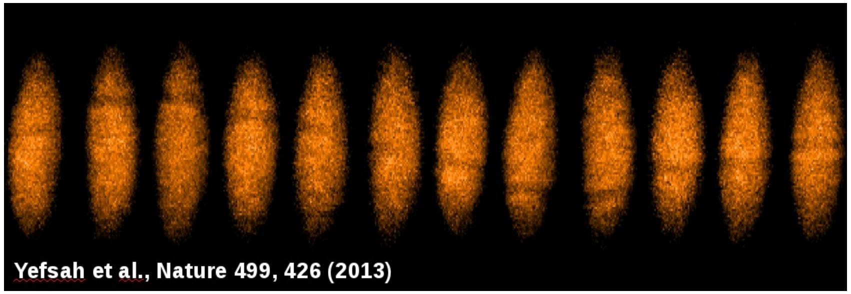
Fig. from
PRL 113, 065301(2014)

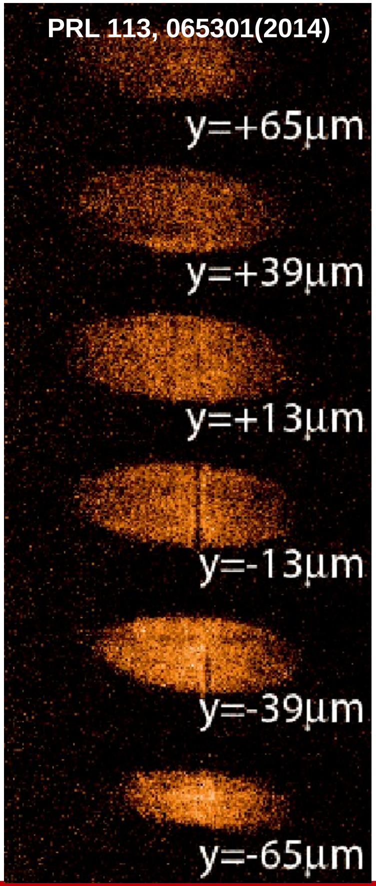


NOTE:
We did tests against other dynamical properties



Experimental results





RESULTS:

- In the final state: Observe an oscillating **vortex line** with long period
- Intertial mass 200 times larger than the free fermion mass
- Precessional motion
- ...