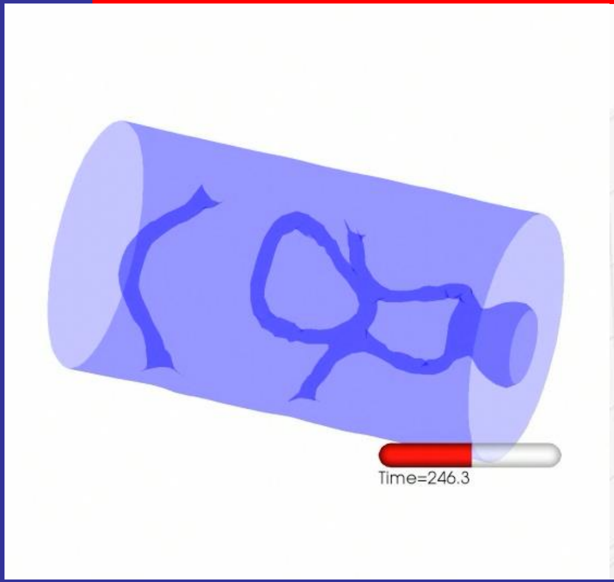
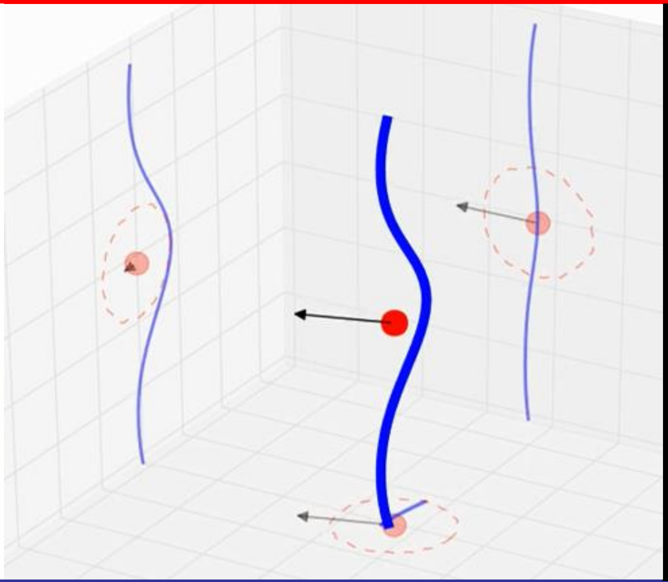
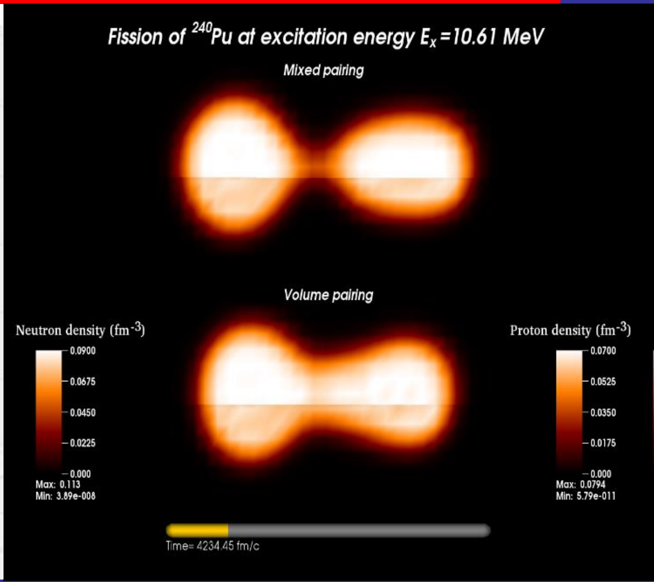
Dynamics of superfluid neutron matter and ultracold fermionic atoms within TDDFT







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GOAL:

Description of superfluid dynamics far from equilibrium within the framework of Time Dependent Density Functional Theory (TDDFT).

We would like to describe the time evolution of (externally perturbed) spatially inhomogeneous, superfluid Fermi system and in particular such phenomena as:

- **Vortex dynamics in ultracold Fermi gases and neutron matter.**
- **Vortex impurity interaction, vortex reconnections.**
- **Quantum turbulence.**
- **Atomic cloud collisions.**
- **Nuclear dynamics: large amplitude collective motion, induced nuclear fission, reactions, fusion, excitation of nuclei with gamma rays and neutrons.**

Runge Gross mapping

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle, \quad \left|\psi_0\right\rangle = \left|\psi(t_0)\right\rangle$$

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

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

Up to an arbitrary function α(t)

and consequently the functional exists:

$$F[\psi_0,\rho] = \int_{t_0}^{t_1}\left\langle\psi[\rho]\right|\left(i\hbar\frac{\partial}{\partial t} - \hat{H}\right)\left|\psi[\rho]\right\rangle dt$$

E. Runge, E.K.U Gross, PRL 52, 997 (1984)
B.-X. Xu, A.K. Rajagopal, PRA 31, 2682 (1985)
G. Vignale, PRA77, 062511 (2008)

Kohn-Sham approach

Suppose we are given the density of an interacting system.
There exists a unique noninteracting system with the same density.

Interacting system

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = (\hat{T}+\hat{V}(t)+\hat{W})\left|\psi(t)\right\rangle$$

Noninteracting system

$$i\hbar\frac{\partial}{\partial t}\left|\varphi(t)\right\rangle = (\hat{T}+\hat{V}_{KS}(t))\left|\varphi(t)\right\rangle$$

$$\rho(\vec{r},t) = \left\langle\psi(t)\right|\hat{\rho}(\vec{r})\left|\psi(t)\right\rangle = \left\langle\varphi(t)\right|\hat{\rho}(\vec{r})\left|\varphi(t)\right\rangle$$

<u>**Hence the DFT approach is essentially exact.**</u>

However as always there is a price to pay:

- **Kohn-Sham potential in principle depends on the past (memory).** **Very little is known about the memory term and usually it is disregarded (adiabatic TDDFT).**
- **Only one body observables can be reliably evaluated within standard DFT.**

Pairing correlation in DFT

One may extend DFT to superfluid systems by defining the pairing field:

$$\Delta(\mathbf{r}\sigma,\mathbf{r}'\sigma') = -\frac{\delta E(\rho,\chi)}{\delta\chi^*(\mathbf{r}\sigma,\mathbf{r}'\sigma')}.$$

L. N. Oliveira, E. K. U. Gross, and W. Kohn, Phys. Rev. Lett. 60 2430 (1988).
O.-J. Wacker, R. Kümmel, E.K.U. Gross, Phys. Rev. Lett. 73, 2915 (1994).

and introducing anomalous density $\chi(\mathbf{r}\sigma,\mathbf{r}'\sigma') = \langle\hat{\psi}_{\sigma'}(\mathbf{r}')\hat{\psi}_{\sigma}(\mathbf{r})\rangle$

However in the limit of the local field these quantities diverge unless one renormalizes the coupling constant:

$$\begin{aligned}\Delta(\mathbf{r}) &= g_{eff}(\mathbf{r})\chi_c(\mathbf{r})\\ \frac{1}{g_{eff}(\mathbf{r})} &= \frac{1}{g(\mathbf{r})} - \frac{mk_c(\mathbf{r})}{2\pi^2\hbar^2}\left(1 - \frac{k_F(\mathbf{r})}{2k_c(\mathbf{r})}\ln\frac{k_c(\mathbf{r})+k_F(\mathbf{r})}{k_c(\mathbf{r})-k_F(\mathbf{r})}\right)\end{aligned}$$

which ensures that the term involving the kinetic and the pairing energy density is finite:

$$\frac{\tau_c(r)}{2m} - \Delta(r)\chi_c(r)$$

Bulgac, Yu, Phys. Rev. Lett. 88 (2002) 042504
Bulgac, Phys. Rev. C65 (2002) 051305

Formalism for Time Dependent Phenomena: TDSLDA

Local density approximation (no memory terms)

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

Density functional contains normal densities, anomalous density (pairing) and currents:

$$E(t) = \int d^3r \left[\varepsilon(n(\vec{r},t), \tau(\vec{r},t), \nu(\vec{r},t), \underline{\vec{j}(\vec{r},t)}) + V_{ext}(\vec{r},t)n(\vec{r},t) + \ldots \right]$$

- **The system is placed on a large 3D spatial lattice.**
- **No symmetry restrictions**
- **Number of PDEs is of the order of the number of spatial lattice points**

Current capabilities of the code:

- **volumes of the order of ($L = 80^3$) capable of simulating time evolution of 42000 neutrons at saturation density (natural application: neutron stars)**
- **capable of simulating up to times of the order of 10^{-19} s (a few million time steps)**
- **CPU vs GPU on Titan ≈ 15 speed-up** (likely an additional factor of 4 possible)

Eg. for 137062 two component wave functions:

CPU version (4096 nodes x 16 PEs) - 27.90 sec for 10 time steps

GPU version (4096 PEs + 4096GPU) - 1.84 sec for 10 time step

SLDA energy density functional at unitarity

$$\varepsilon(\vec{r}) = \left[\alpha\frac{\tau_c(\vec{r})}{2} - \Delta(\vec{r})\nu_c(\vec{r})\right] + \beta\frac{3(3\pi^2)^{2/3}n^{5/3}(\vec{r})}{5}$$

$$n(\vec{r}) = 2\sum_{0<E_k<E_c}\left|\mathrm{v}_k(\vec{r})\right|^2, \quad \tau_c(\vec{r}) = 2\sum_{0<E_k<E_c}\left|\vec{\nabla}\mathrm{v}_k(\vec{r})\right|^2,$$

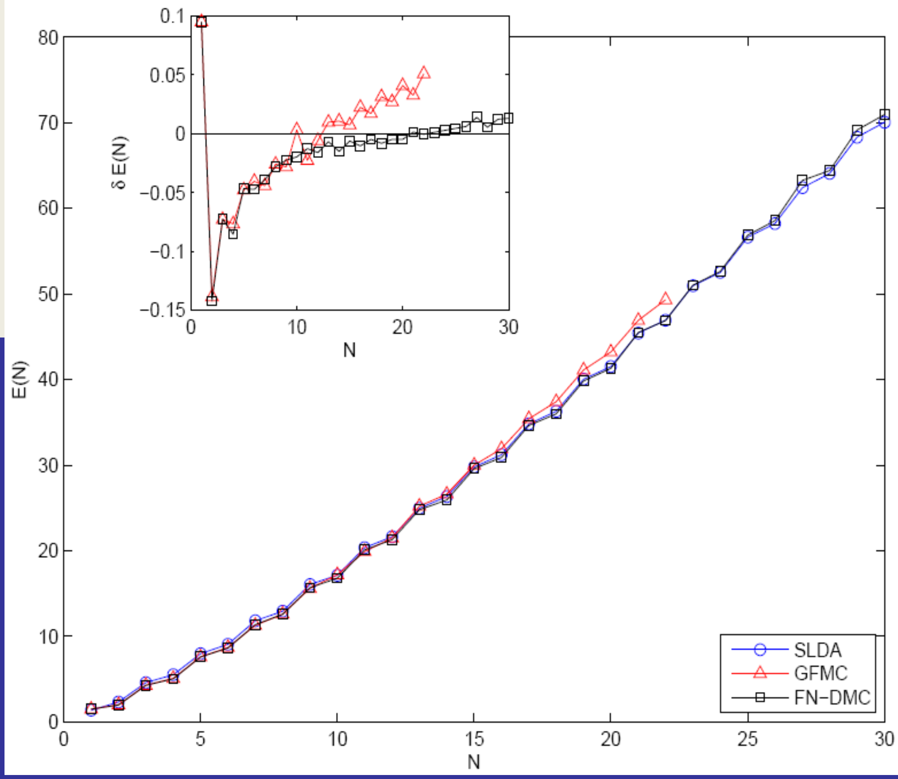
$$\nu_c(\vec{r}) = \sum_{0<E<E_c}\mathrm{u}_k(\vec{r})\mathrm{v}_k^*(\vec{r})$$

$$U(\vec{r}) = \beta\frac{(3\pi^2)^{2/3}n^{2/3}(\vec{r})}{2} - \frac{\left|\Delta(\vec{r})\right|^2}{3\gamma n^{2/3}(\vec{r})} + V_{ext}(\vec{r})$$

$$\Delta(\vec{r}) = -g_{eff}(\vec{r})\nu_c(\vec{r})$$

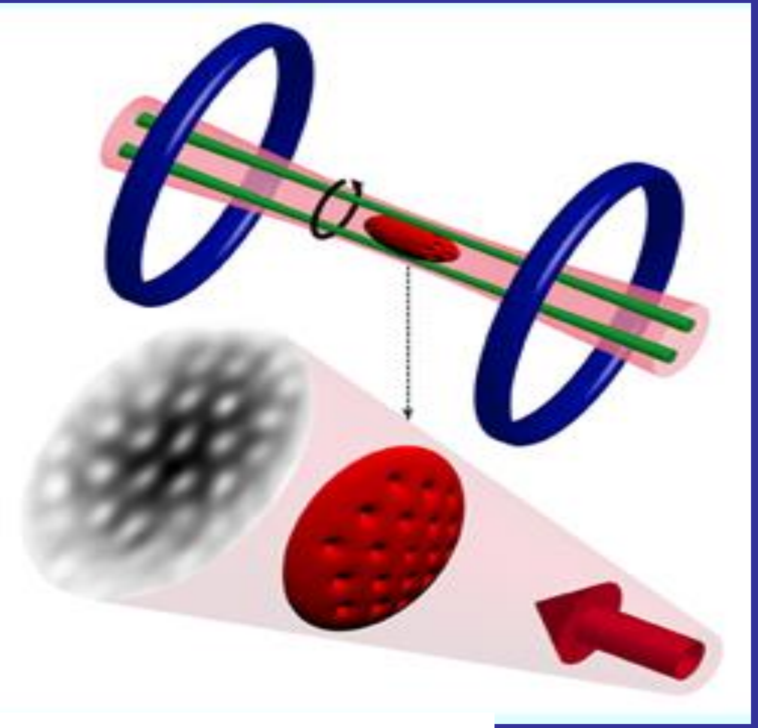
Bulgac, PRA 76, 040502(R) (2007)

Fermions at unitarity in a harmonic trap
Total energies E(N)



GFMC - Chang and Bertsch, Phys. Rev. A 76, 021603(R) (2007)
FN-DMC - von Stecher, Greene and Blume, PRL 99, 233201 (2007)
PRA 76, 053613 (2007)

Vortex generation in ultracold Fermi gases

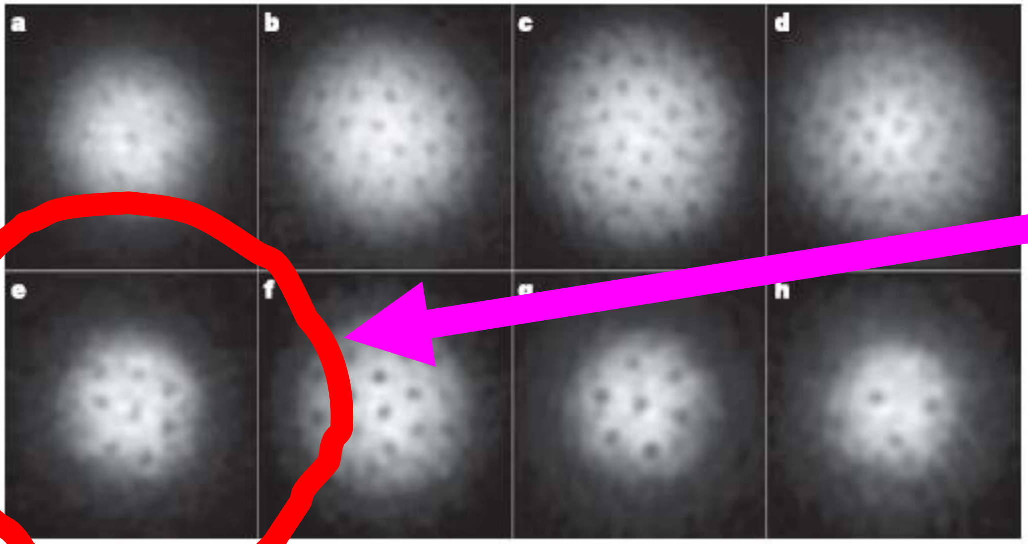


system of fermionic ^6Li atoms

Feshbach resonance: B=834G

BEC side: a>0

BCS side: a<0

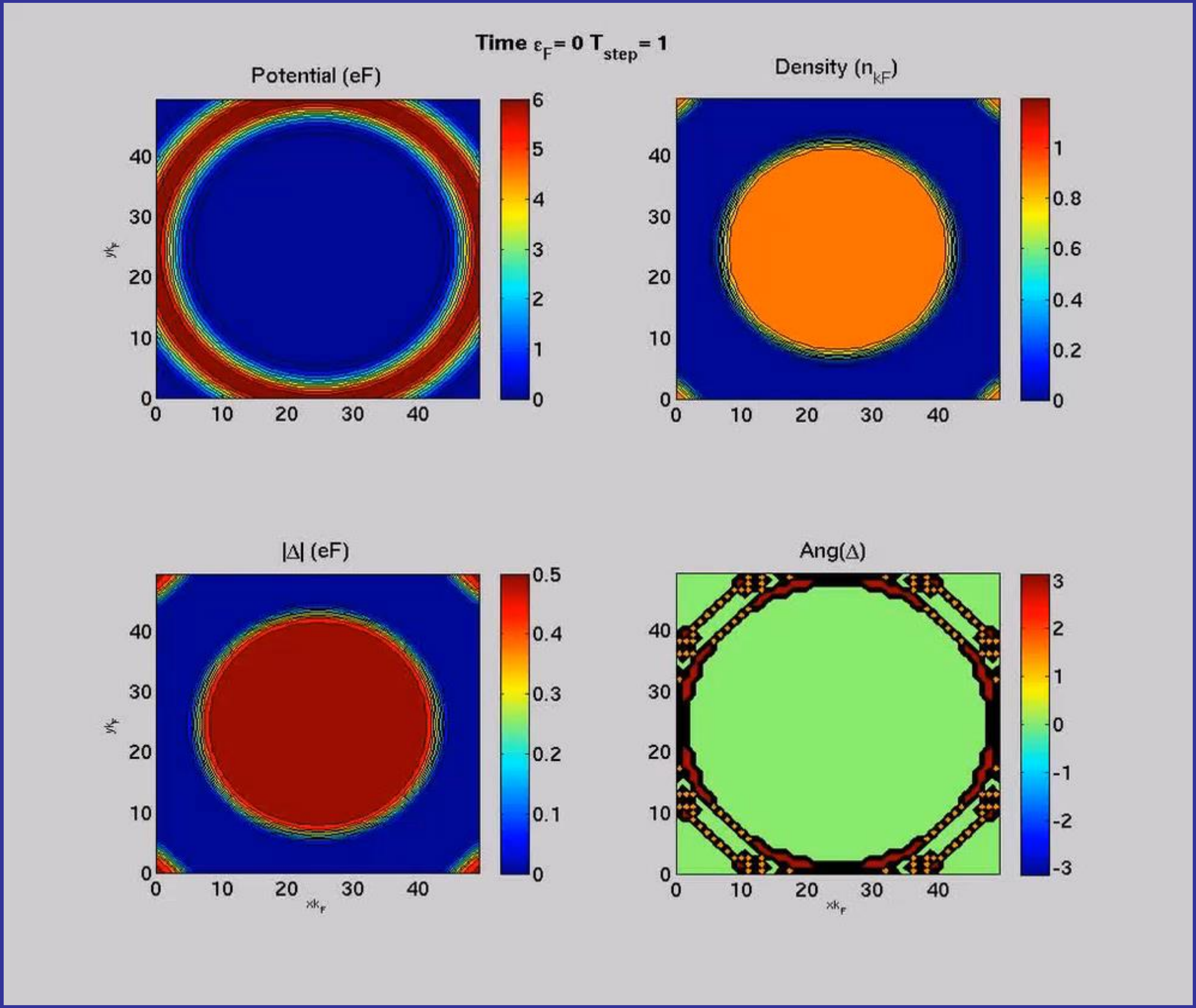


UNITARY REGIME

Figure 2 | Vortices in a strongly … fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (**a**) or 500 ms (**b–h**) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, the magnetic field was ramped to 735 G for imaging (… magnetic fields were 740 G (**a**), 766 G (**b**), 792 G (**c** … 843 G (**f**), 853 G (**g**) and 863 G (**h**). The field of vie… 880 μm × 880 μm.

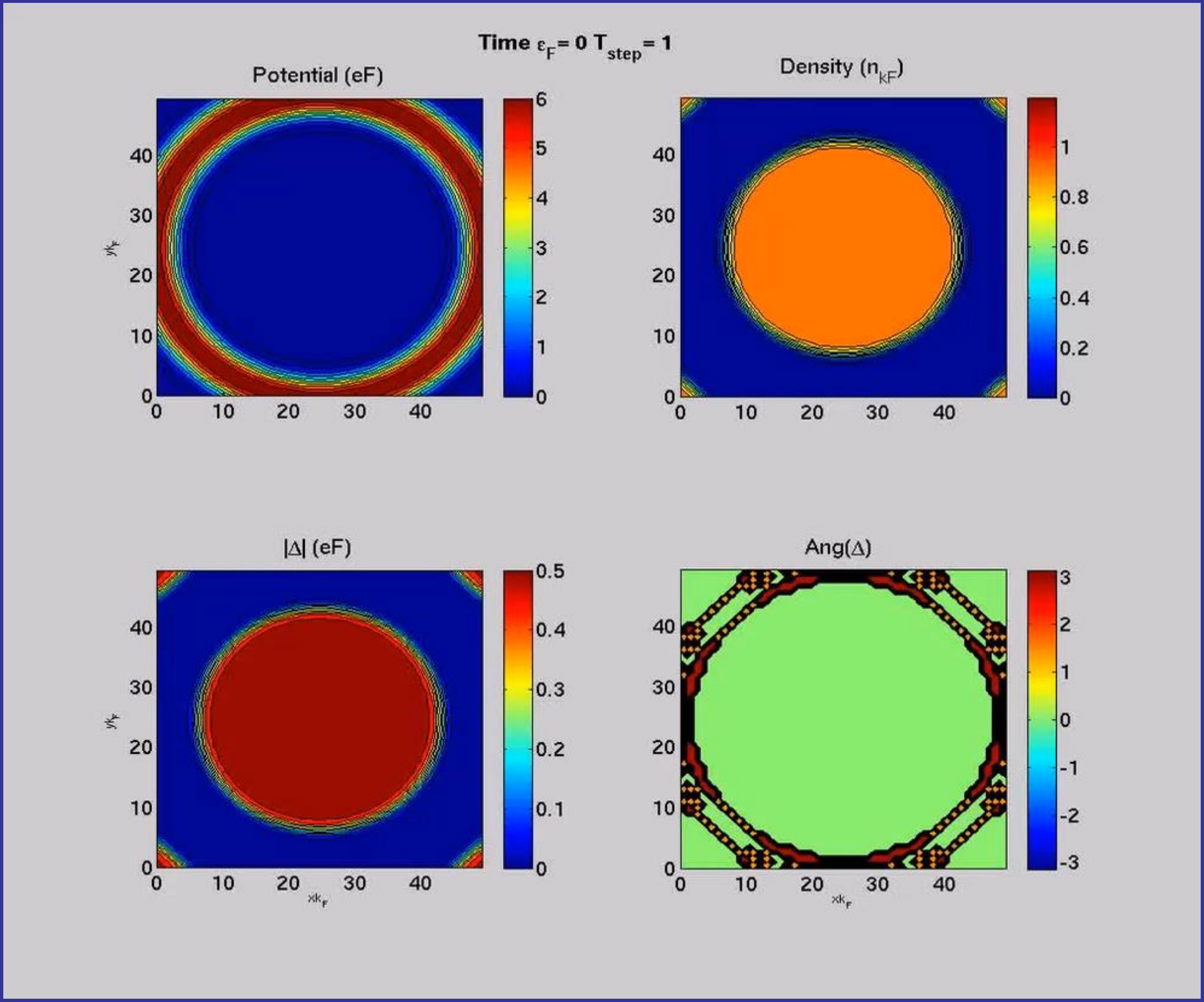
M.W. Zwierlein *et al*., Nature, 435, 1047 (2005)

Stirring the atomic cloud with stirring velocity **lower** than the critical velocity



Bulgac, Luo, Magierski, Roche, Yu, *Science* 332, 1288 (2011)

Stirring the atomic cloud with stirring velocity **exceeding** the critical velocity



Bulgac, Luo, Magierski, Roche, Yu, *Science* 332, 1288 (2011)

Vortex reconnections

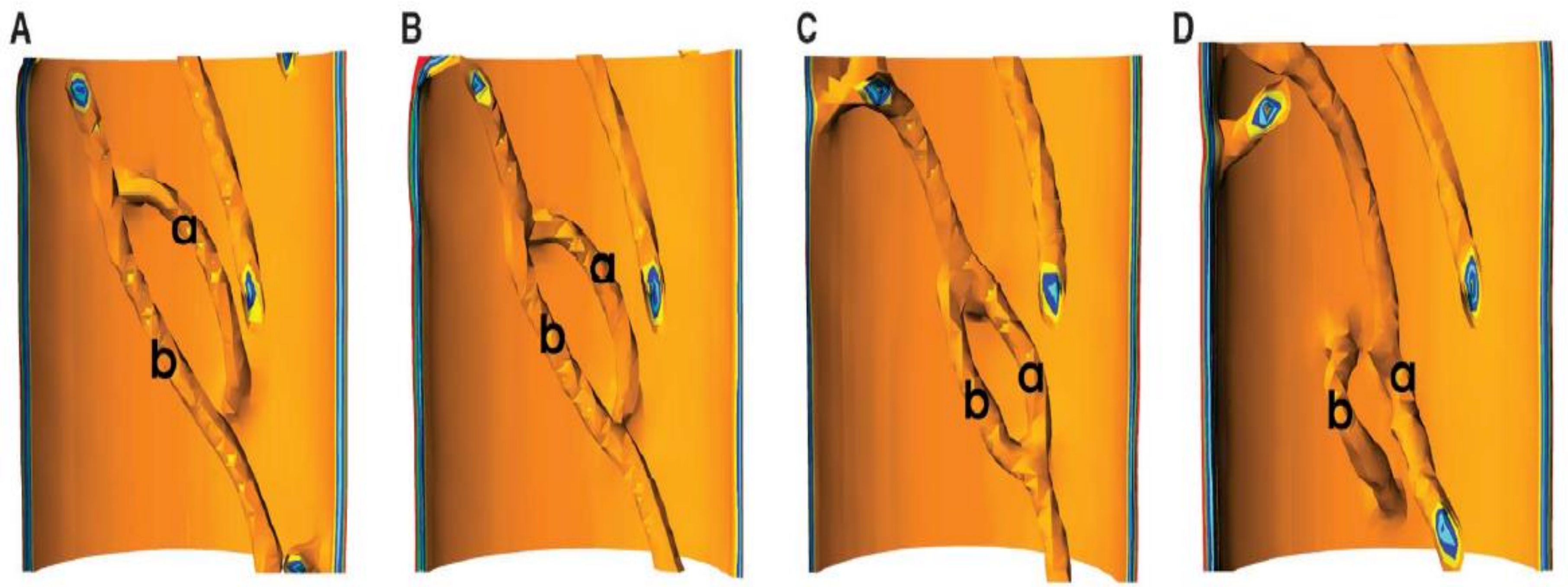
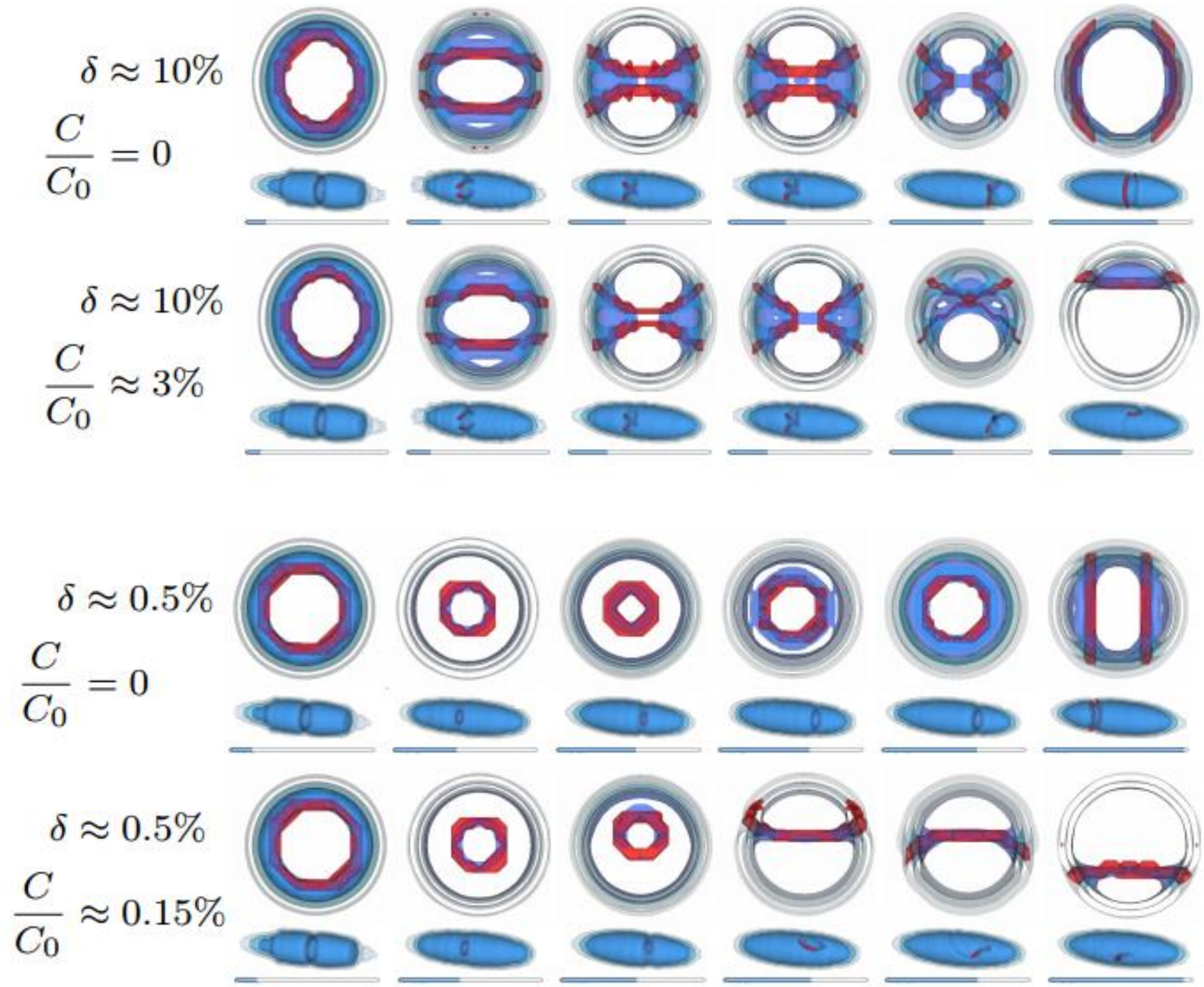


Fig. 3. (**A** to **D**) Two vortex lines approach each other, connect at two points, form a ring and exchange between them a portion of the vortex line, and subsequently separate. Segment (a), which initially belonged to the vortex line attached to the wall, is transferred to the long vortex line (b) after reconnection and vice versa.

Vortex reconnections are important for the energy dissipation mechanism in quantum turbulence.

TDSLDA can describe these processes as well as the energy transfer between collective and single particle degrees of freedom (which is a problem for simplified treatments based e.g. on Gross-Pitaevskii equation)

Bulgac, Luo, Magierski, Roche, Yu, *Science* 332, 1288 (2011)



Moreover with TDDFT we can reproduce the sequence of topological excitations observed experimentally (M.H.J. Ku et al. Phys. Rev. Lett. 113, 065301 (2014)).

Wlazłowski, et al., Phys. Rev. A91, 031602 (2015)

Effective mass of a nucleus in superfluid neutron environment

Suppose we would like to evaluate an effective mass of a heavy particle immersed in a Fermi bath.
Can one come up with the effective (classical) equation of motion of the type:

$$M\frac{d^2q}{dt^2} - F_D\left(\frac{dq}{dt},\ldots\right) + \frac{dE}{dq} = 0 \quad ?$$

In general it is a complicated task as the first and the second term may not be unambiguously separated.

However for the superfluid system it can be done as for sufficiently slow motion (below the critical velocity) the second term may be neglected due to the presence of the pairing gap.

Energy density functional without spin-orbit (Fayans):

$$E = \int d^3r \mathcal{H}(\mathbf{r})$$

where

$$\begin{aligned}
\mathcal{H}(\mathbf{r}) &= \frac{2}{3}\epsilon_F^0 \rho_0 \left(a_+^v \frac{1 - h_{1+}^v x_+^\sigma(\mathbf{r})}{1 + h_{2+}^v x_+^\sigma(\mathbf{r})} x_+^2(\mathbf{r}) + a_-^v \frac{1 - h_{1-}^v x_+(\mathbf{r})}{1 + h_{2-}^v x_+(\mathbf{r})} x_-^2(\mathbf{r}) + \frac{a_+^s r_0^2 (\nabla x_+(\mathbf{r}))^2}{1 + h_+^s x_+^\sigma(\mathbf{r}) + h_\nabla^s r_0^2 (\nabla x_+(\mathbf{r}))^2} \right) \\
&+ \frac{1}{2} e \rho_0 \Phi(\mathbf{r}) \left(x_+(\mathbf{r}) - x_-(\mathbf{r}) \right)
\end{aligned}$$

where

$$\begin{aligned}
x_\pm(\mathbf{r}) &= \frac{1}{2\rho_0} (\rho_n(\mathbf{r}) \pm \rho_p(\mathbf{r})) \\
\epsilon_F^0 &= \left(\frac{9\pi}{8} \right)^{2/3} \frac{\hbar^2}{2mr_0^2} \\
r_0 &= (3\pi\rho_0/8)^{1/3} \\
\rho_0 &= 0.08 fm^{-3} \\
\sigma &= 1/3
\end{aligned}$$

Single particle potential without spin-orbit (Fayans):

$$\begin{aligned}
h_i(\mathbf{r}) &= -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{3}\epsilon_F^0 \left(a_+^v x_+(\mathbf{r}) A(\mathbf{r}) - a_-^v x_-(\mathbf{r}) B_i(\mathbf{r}) \right) + \\
&- \frac{1}{3}\epsilon_F^0 a_+^s r_0^2 \left(\frac{h_+^s (\vec{\nabla} x_+(\mathbf{r}))^2 \sigma x_+^{\sigma-1}(\mathbf{r})}{C^2(\mathbf{r})} + 2\vec{\nabla} \cdot \left(\vec{\nabla} x_+(\mathbf{r}) \frac{1 + h_+^s x_+^\sigma(\mathbf{r})}{C^2(\mathbf{r})} \right) \right) + e\Phi(\mathbf{r})\delta_{ip}
\end{aligned}$$

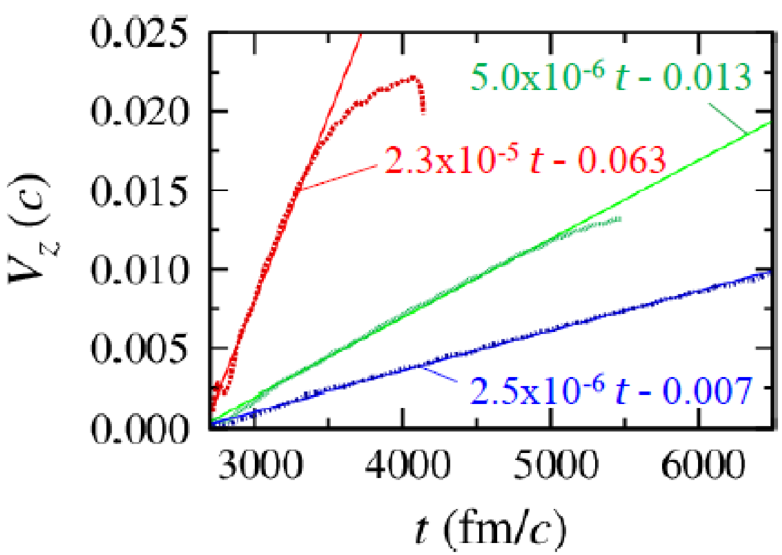
S. Fayans, Pis’ma Zh. Eks. Teor. Fiz. 70, 235 (1999) [JETP Lett. 70, 240 (1999)]; S.A. Fayans et al., Nucl. Phys. A 676, 49 (2000).

Effective mass of a nucleus immersed in superfluid neutron matter:

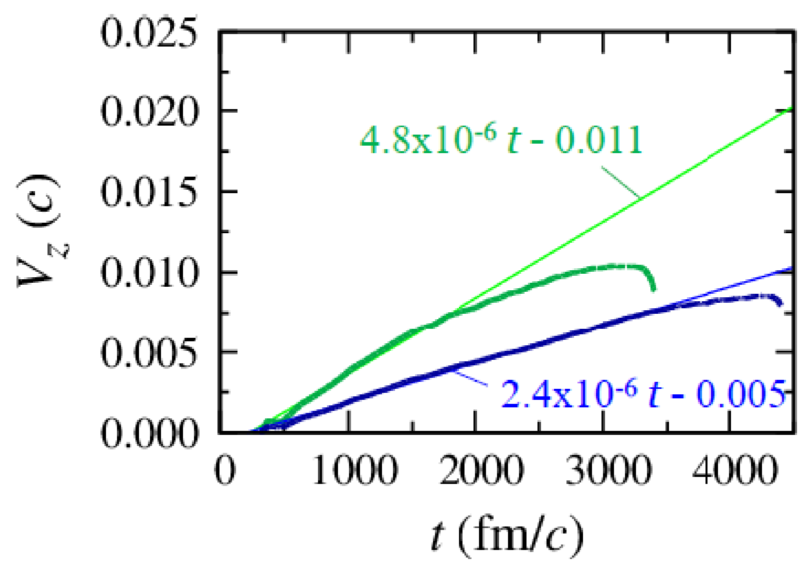
We apply the external potential for protons (50) of the form: $V_{EXT}(\vec{r}) = -\vec{F}\cdot\vec{r}$

and measure the C.M. velocity of the system

Lower density: ρ_n~ 0.016 fm^{-3}



Higher density: ρ_n~ 0.032 fm^{-3}

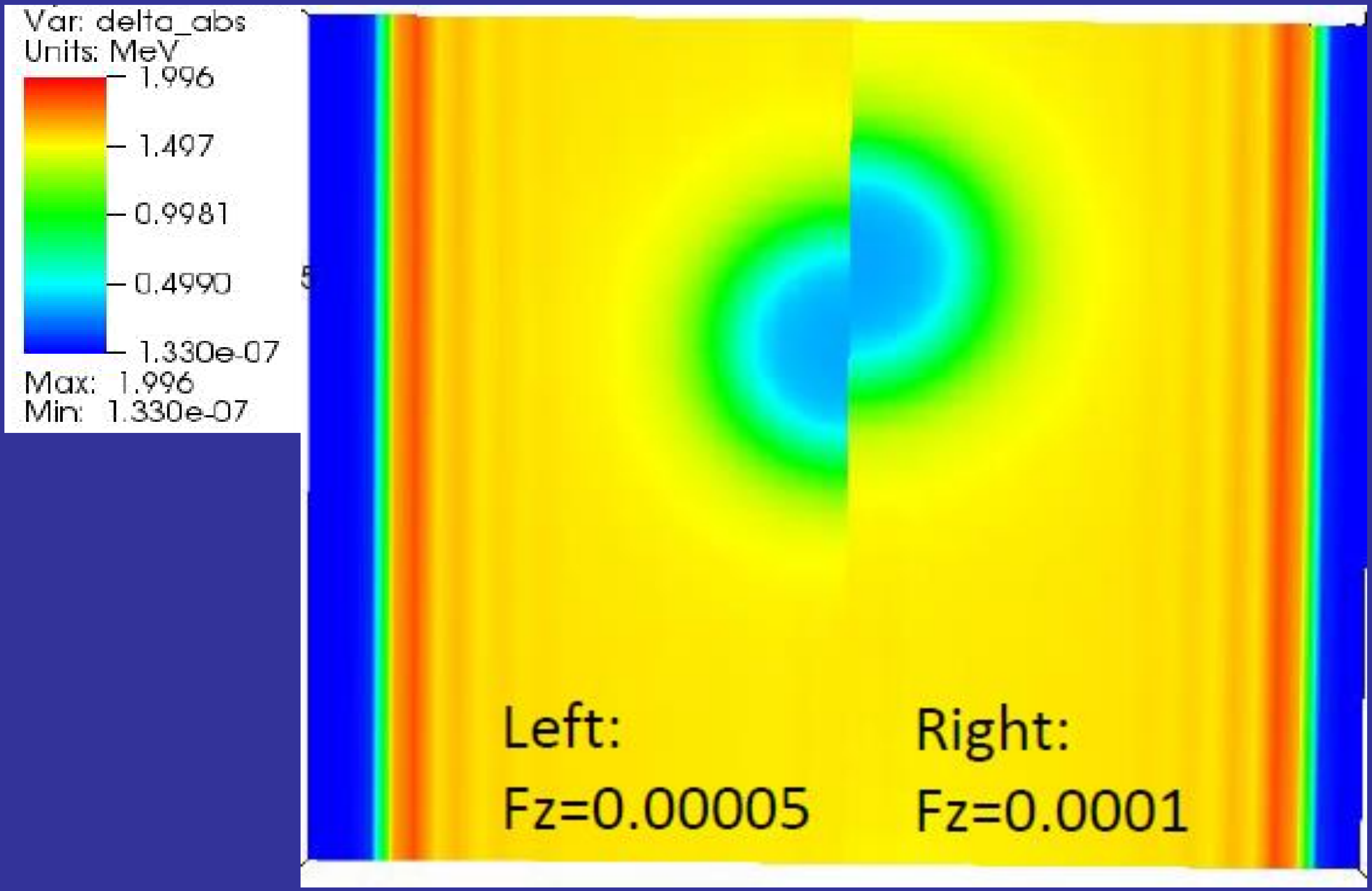


At low velocities: $v(t) \sim t$

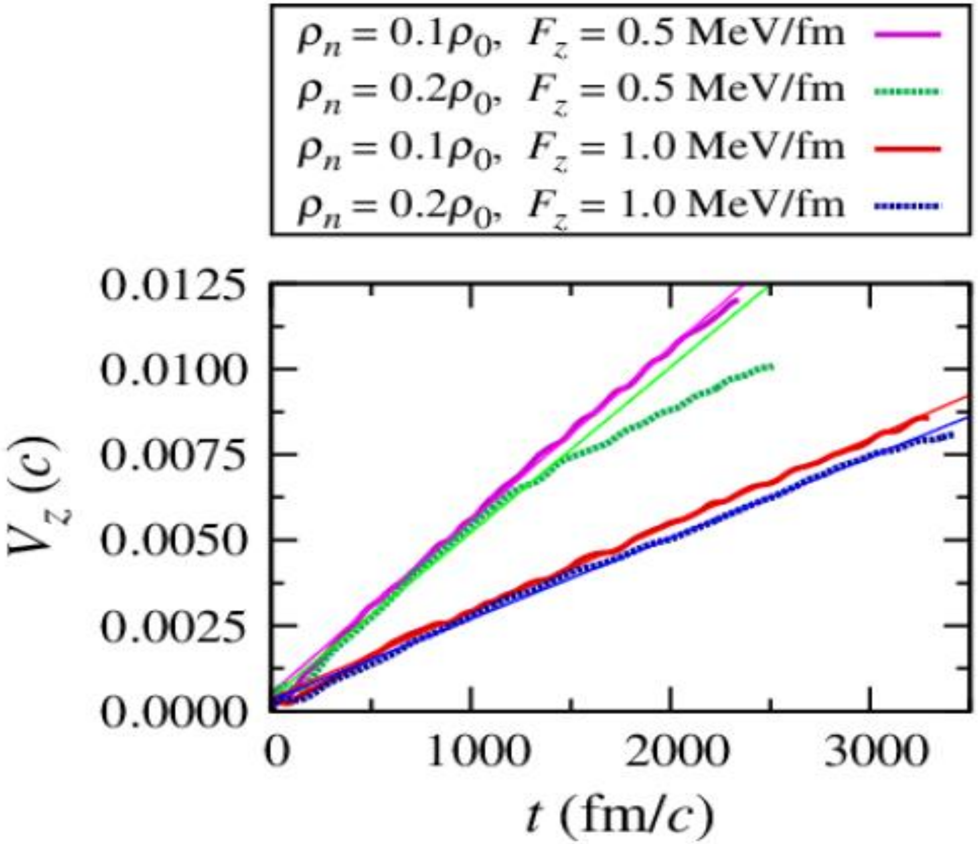
The deviations for higher velocities indicate excitations of other modes

K. Sekizawa, G. Wlazłowski, P. Magierski (preliminary results)

At low velocity the motion is almost adiabatic



Interestingly the effective mass weakly depends on the density of the neutron environment



Dragging 50 protons the effective mass corresponds to dragging about 207 nucleons for lower density and about 228 nucleons for higher density.

This invalidates a simple irrotational hydrodynamic estimation:

$$M \sim \frac{\left(\frac{\rho_{out}}{\rho_{in}} - 1\right)^2}{2\frac{\rho_{out}}{\rho_{in}} + 1}$$

K. Sekizawa, G. Wlazlowski, P. Magierski (preliminary results)

Vortex dynamics and vortex-impurity interaction

The effective equations of motion for the vortex dynamics (per unit length of the vortex):

$$M_{vor}\frac{d^2\vec{r}}{dt^2} = \vec{F}_M + \vec{F}_D + \vec{F}_{vor-impurity}$$

The mass of the vortex (per unit length) is unknown.
Sometimes it is neglected, although some arguments indicate that an unambiguous vortex mass may not exist in a sense it depends on the process by which it is measured.

$\vec{F}_M = \rho_s\vec{\Gamma}\times\left(\frac{d\vec{r}}{dt} - \vec{v}_s\right)$ - Magnus force; $\vec{\Gamma}$ – local vorticity;

$\frac{d\vec{r}}{dt}$ - local vortex velocity, ρ_s – superfluid density, $\vec{v}_s$ – superfluid velocity

$\vec{F}_D$ – frictional force (negligible at small T)

$\vec{F}_{vor-impurity}$ - vortex-impurity force

To date the impurity-vortex interaction has been extracted from static calculations (Ginzburg-Landau, local density, HFB) with several severe approximations:

- Vortex is always straight
- Nucleus is spherical
- Only very symmetric configurations are considered:
    - nucleus on vortex
    - vortex inbetween two nuclei (intersitial configuration)
    - nucleus at infinity

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)
P.Pizzochero et al. PRL 79,3347(1997)
R.Broglia et al.PRD50,4781(1994)
M.Baldo et al. Nucl.Phys.515,409(1990)
P.Donati,P.Pizzochero, PRL90,211101(2003);
PLB640,74(2006);Nucl.Phys.A742,363(2004)
P.Avogadro et al. PRC75,012805(2007);NPA811,378(2008)

From these assumptions the average force can be deduced and the energetically favorable configuration may be determined.

However, there is still no agreement whether the pinned or unpinned configuration is preferred.

We will use approach based on TDDFT which allow to extract the force from dynamics.

It has the following advantages:

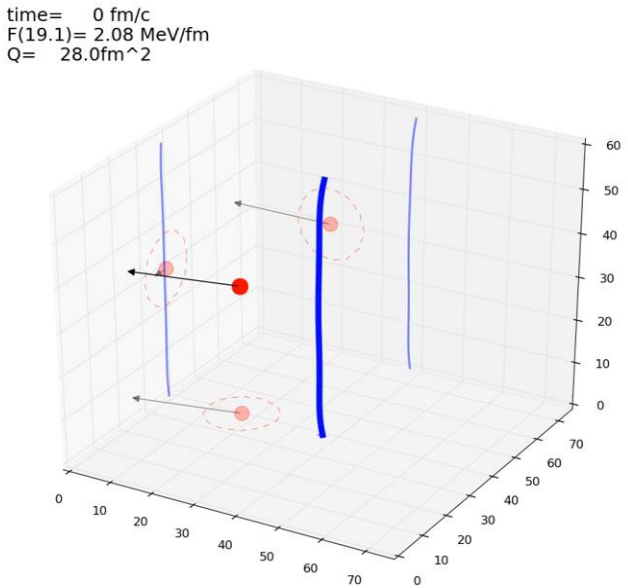
- We can extract the force at various nonsymmetric configurations
- All degrees of freedom are treated on the same footing and in particular those associated with the vortex (bending) and nucleus (deformations) are taken into account
- One can get a better insight into the dynamics of the vortex-impurity system at various energy scales.

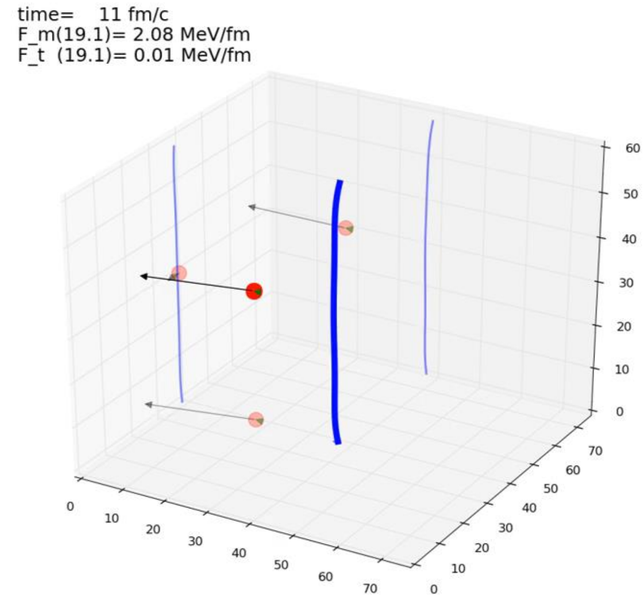
The procedure consists of dragging protons through the neutron medium with the vortex.
Such an approach has been shown to give the same force as extracted from static configurations (Bulgac,Forbes,Sharma, PRL 110,241102(2013)).

Note also that this approach is much cheaper numerically than searching for stationary solutions at various vortex-impurity configurations.

Vortex – impurity interaction

The extrenal potential: $V_{EXT}(\vec{r}) = -\vec{F}\cdot\vec{r}$ keeps the nucleus moving along the straight Line with a constant velocity below the critical velocity.

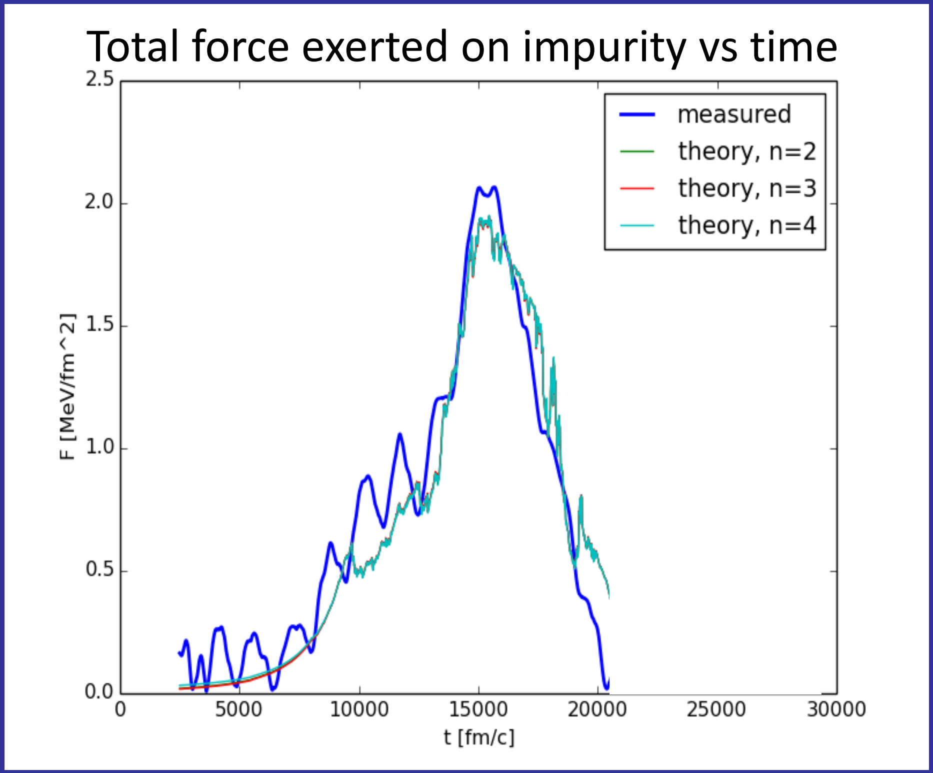




One can extract the total force and also the force exerted on each part of the vortex. Assuming that the force behaves asymptotically as $1/r^3$ (superfluid hydrodynamic estimate) one can extract the force per unit length by fitting the expression :

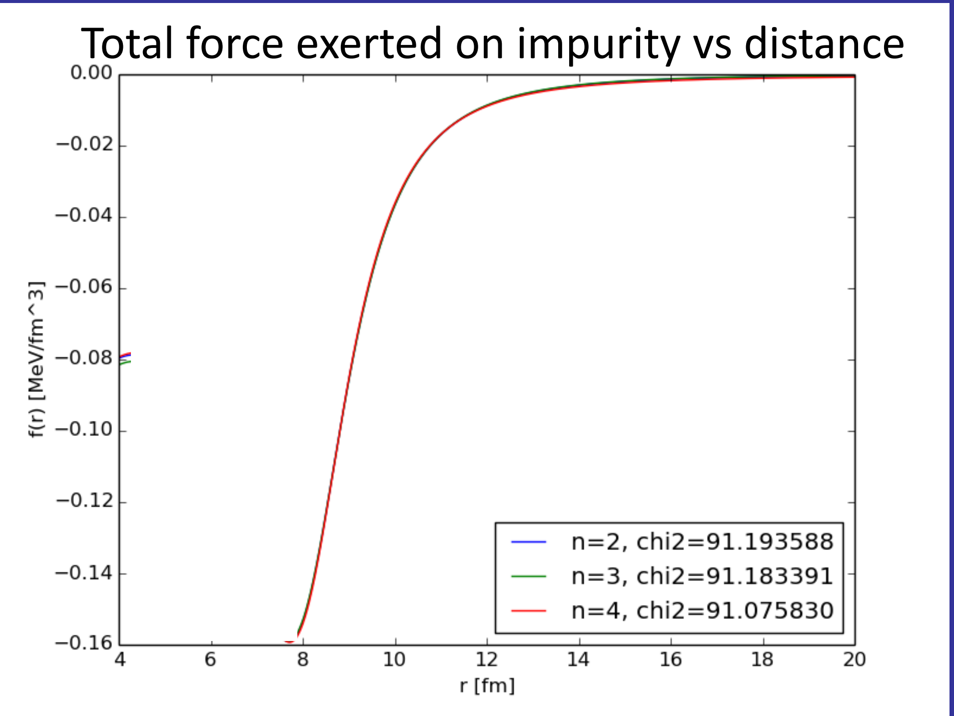
$$f(r) = \frac{\sum_{k=0}^{n} a_n r^n}{\sum_{k=0}^{n+3} b_n r^n}; \quad f(r) \sim 1/r^3; \; b_0 = 1$$

K. Sekizawa, G. Wlazlowski, P. Magierski (preliminary results)



The force is repulsive as nucleus approaches the vortex and practically vanishes at distances of the order of 20fm.

The force weakly depends on the neutron density.



The force has centripetal character.
Its tangent component is practically zero.

K. Sekizawa, G. Wlazlowski, P. Magierski (preliminary results)

Summary:

- ***We have applied superfluid TDDFT in the form of superfluid local density approximation (TDSLDA) to study dynamics of vortices in ultracold atoms and neutron matter.***

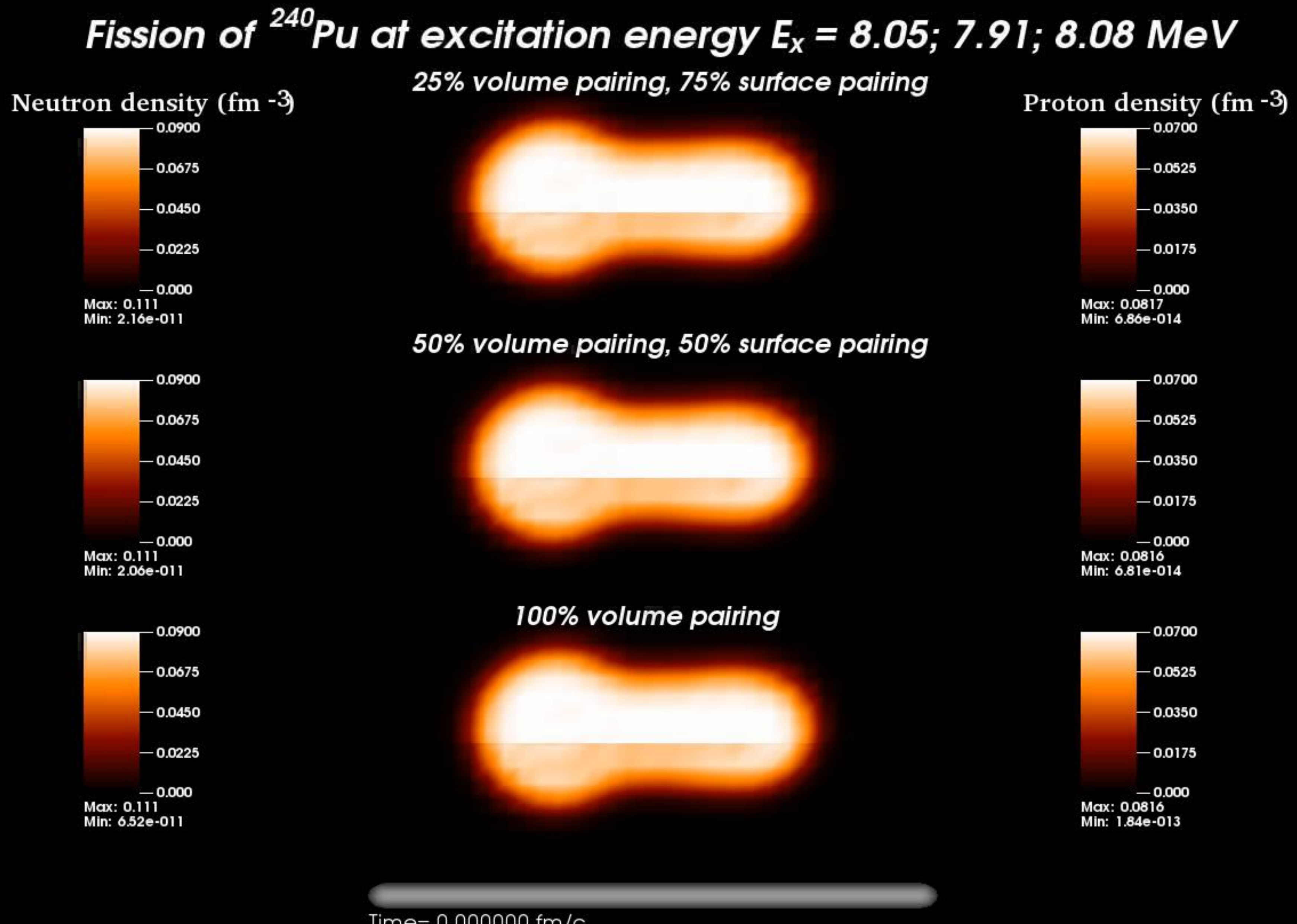
- ***In ultracold atomic system TDSLDA correctly describe the dynamics of vortices contrary to simpler approaches based on Gross-Pitaevski eq.***

- ***For neutron matter we were able to extract the effective mass of impurity (nucleus) immersed in the neutron environment. It turns out to be weakly dependent on the density of neutron matter.***

- ***We were able to describe nucleus-vortex interaction from the dynamics without any symmetry constraints, taking into account internal degrees freedom of the nucleus and the vortex.***

- ***We exctracted the force per unit of the vortex length, which can be used as an input for simplified large scale calculations for the neutron star crust (eg. based on filament model).***
- ***We have found that the force weakly depends on the neutron density and is repulsive when nucleus is approaching the vortex.***

Slightly offtopic but interesting…



Bulgac,Magierski,Roche,Stetcu, PRL (in press)

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