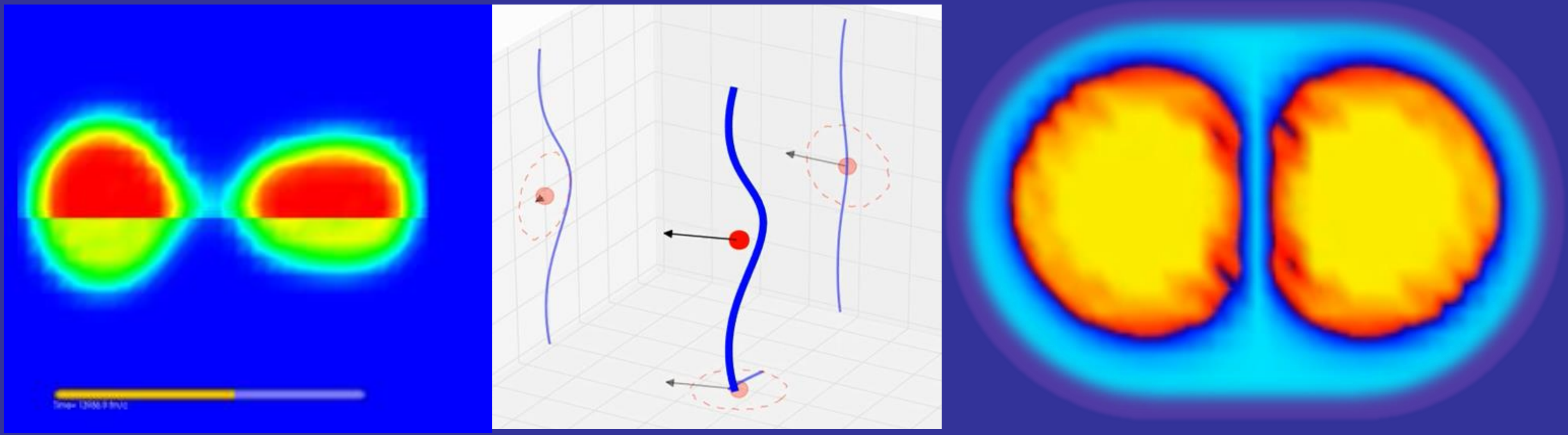
Towards exascale simulations of quantum superfluids – new prospects for modelling nuclear processes



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GOAL:

Description of superfluid dynamics of fermionic systems far from equilibrium based on microscopic theoretical framework.

Microscopic framework = explicit treatment of fermionic degrees of freedom.

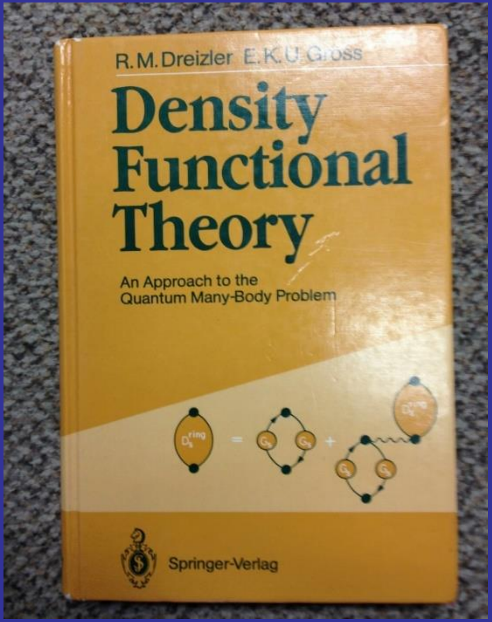
Why Time Dependent Density Functional Theory (TDDFT)?

We need to describe the time evolution of (externally perturbed) spatially inhomogeneous, superfluid Fermi system.

Within current computational capabilities TDDFT allows to describe real time dynamics of strongly interacting, superfluid systems of hundred of thousands fermions.

Main Theoretical Tool

THEOREM: There exist an universal density functional of particle density.



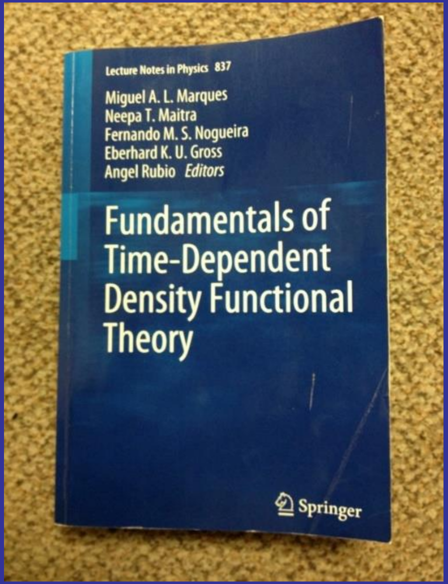
R. M. Dreizler E. K. U. Gross

Density Functional Theory

An Approach to the Quantum Many-Body Problem

Springer-Verlag

1990



Lecture Notes in Physics 837

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Fundamentals of Time-Dependent Density Functional Theory

Springer

2012

DFT has been developed and used mainly to describe normal (non-superfluid) electron systems – more than <u>50 years old theory</u>:

DFT - Kohn and Hohenberg, 1964
LDA - Kohn and Sham, 1965
Extension for superconductors/superfluids: DFT - Oliveira, Gross, Kohn (1988),
TDDFT - Wacker, Kummel, Gross (1994)
SLDA, TDSLDA – Bulgac (2002)

TDDFT equations with local pairing field (TDSLDA):

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

The form of $h(r,t)$ and $\Delta(r,t)$ is determined by EDF (Energy Density Functional)

- 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.

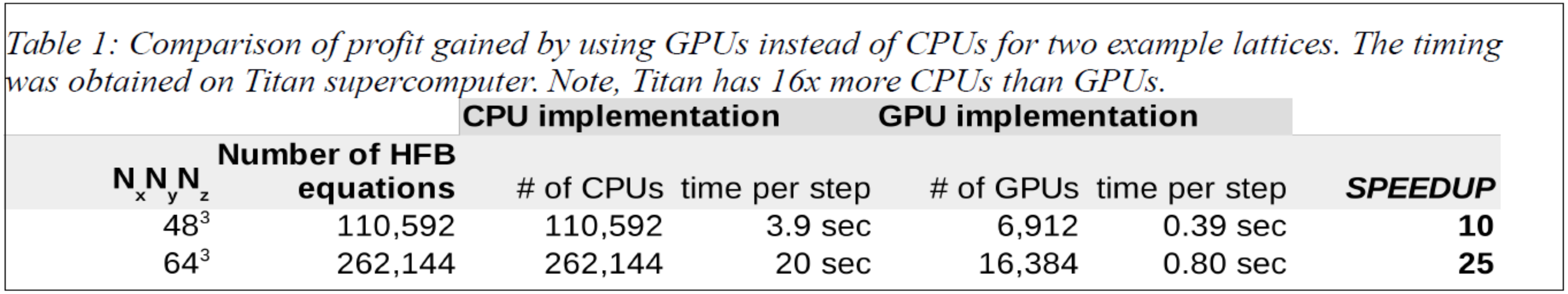


Table 1: Comparison of profit gained by using GPUs instead of CPUs for two example lattices. The timing was obtained on Titan supercomputer. Note, Titan has 16x more CPUs than GPUs.

		CPU implementation		GPU implementation		
$N_xN_yN_z$	Number of HFB equations	# of CPUs	time per step	# of GPUs	time per step	*SPEEDUP*
48^3	110,592	110,592	3.9 sec	6,912	0.39 sec	**10**
64^3	262,144	262,144	20 sec	16,384	0.80 sec	**25**

The main advantage of TDSLDA over TDHF (+TDBCS) is related to the fact that in TDSLDA the pairing correlations are described as a true complex field which has its own modes of excitations, which include spatial variations of both amplitude and phase. Therefore in TDSLDA description the evolution of nucleon Cooper pairs is treated consistently with other one-body degrees of freedom.

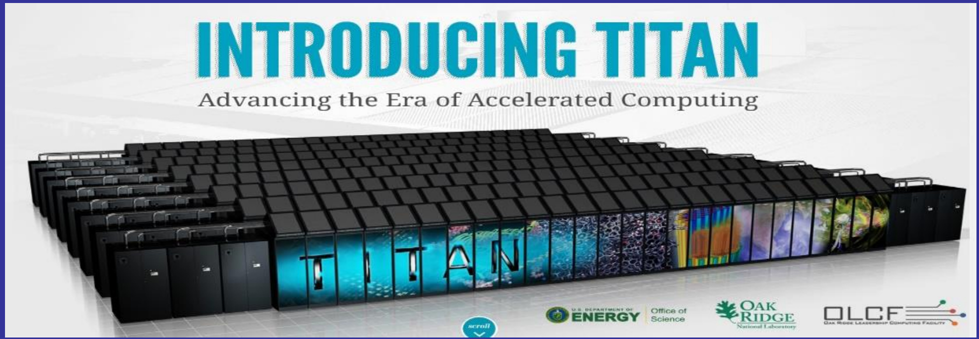
Selected supercomputers (CPU+GPU) currently in use:

Piz Daint: 25.3 PFlops
(Swiss National Supercomputing Centre)

HA-PACS: 0.802 PFlops
(University of Tsukuba)

Tsubame: 5.7 PFlops
(Tokyo Institute of Technology)

Titan: 27 PFlops
(ORNL Oak Ridge)



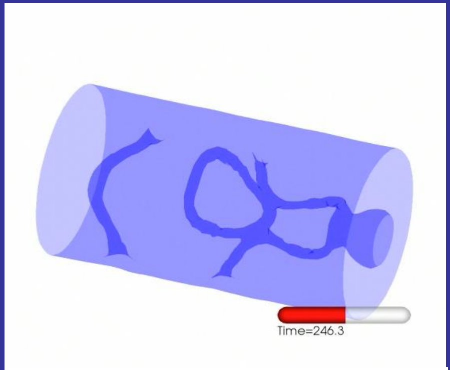
Areas of applications

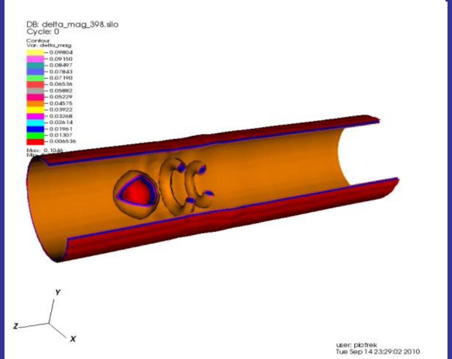
$$\frac{\Delta}{\varepsilon_F} \leq 0.5$$

Ultracold atomic (fermionic) gases.

Unitary regime.

Dynamics of quantum vortices, solitonic excitations, quantum turbulence.

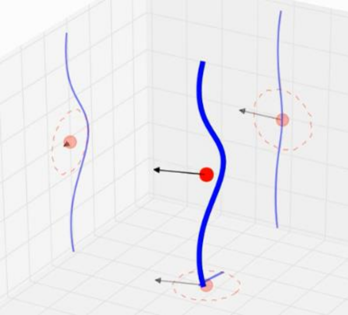


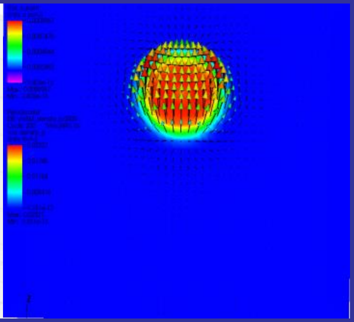


$$\frac{\Delta}{\varepsilon_F} \leq 0.1-0.2$$

Astrophysical applications.

Modelling of neutron star interior (glitches): vortex dynamics, dynamics of inhomogeneous nuclear matter (in strong magnetic fields).

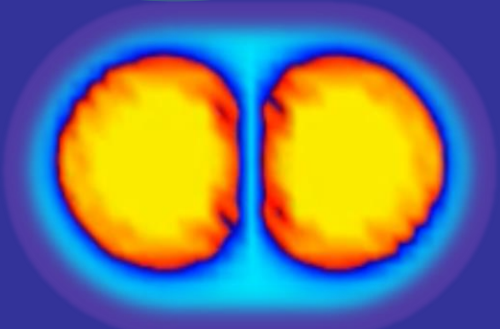


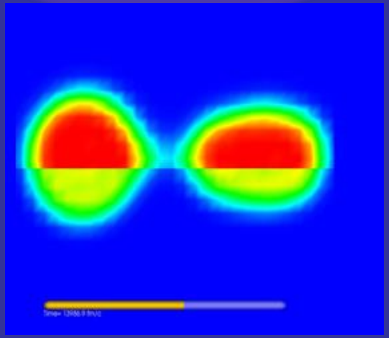


$$\frac{\Delta}{\varepsilon_F} \leq 0.03$$

Nuclear physics.

Induced nuclear fission, fusion, collisions.



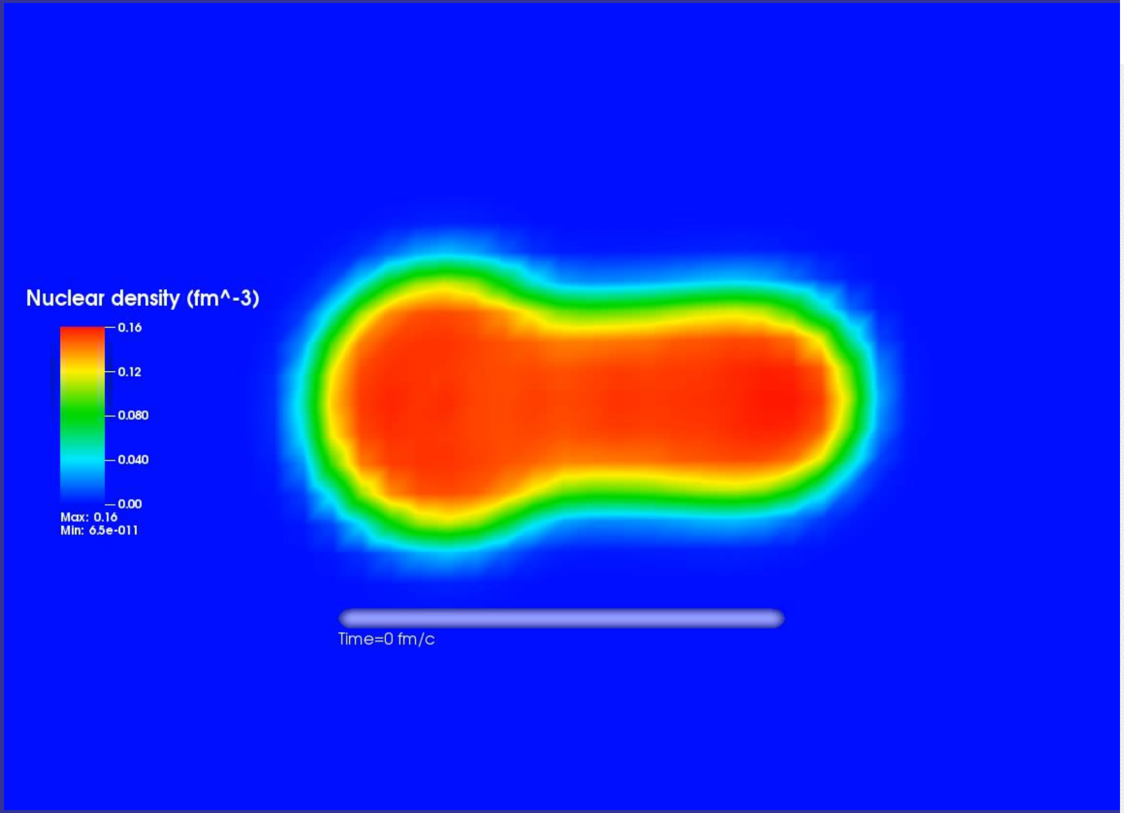


Examples of applications:

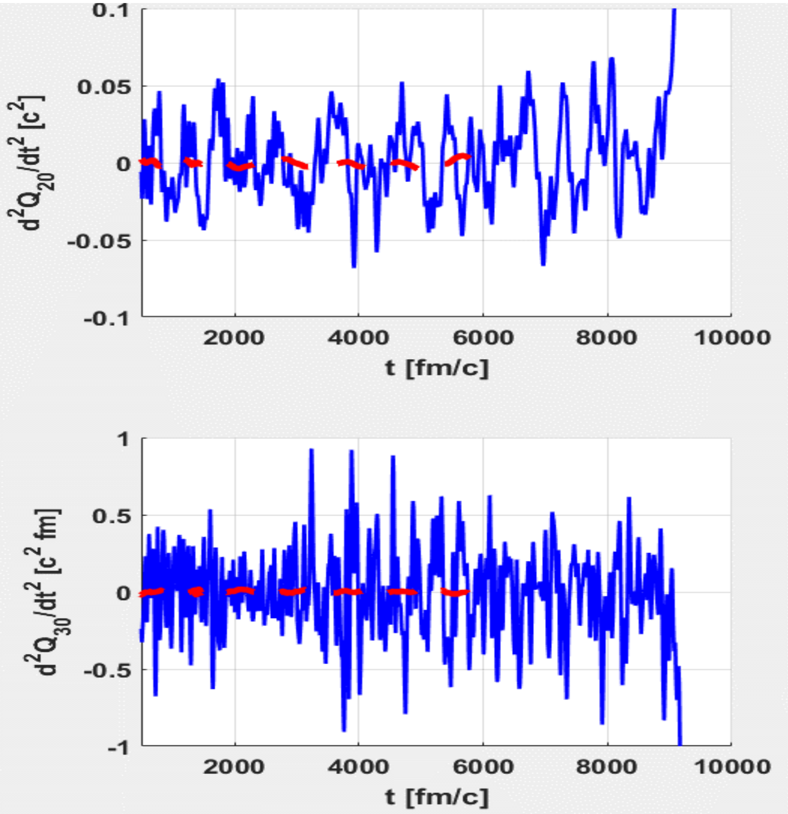
- Nuclear induced fission
- Collisions of medium or heavy superfluid nuclei
- Dynamics of inhomogeneous nuclear matter in neutron stars
- Dynamics of topological excitations in ultracold fermionic gases (both unpolarized and spin-imbalanced)

Fission dynamics of ^{240}Pu

Initial configuration of ^{240}Pu is prepared beyond the barrier at quadrupole deformation *Q=165b* and excitation energy *E=8.08 MeV*:

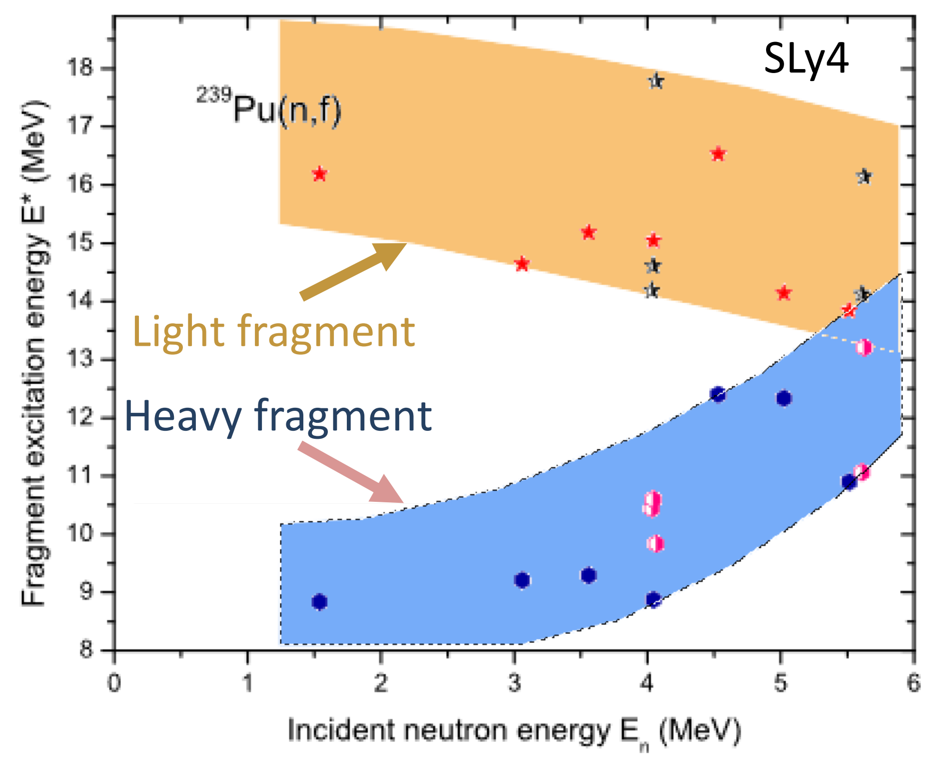


Accelerations in quadrupole and octupole moments along the fission path



Note that despite the fact that nucleus is already beyond the saddle point the collective motion on the time scale of 1000 fm/c and larger is characterized by the constant velocity (*see red dashed line for an average acceleration*) till the very last moment before splitting. On times scales, of the order of 300 fm/c and shorter, the collective motion is a subject to random-like kicks indicating strong coupling to internal d.o.f

Induced fission of 240Pu



E^* (MeV)	E_n (MeV)	$t_{fission}$ (fm/c)	TKE (MeV)	Z_L	N_L
8.08	1.542	8517	173.81	40.825	62.246
9.60	3.063	9215	174.73	40.500	61.536
10.10	3.560	9287	179.09	41.625	62.783
10.57	4.032	7243	173.67	40.092	61.256
10.58	4.043	7287	173.39	40.146	61.388
10.58	4.047	7134	175.11	40.313	61.475
10.60	4.065	7737	174.75	40.904	62.611
11.07	4.534	6444	176.46	41.495	63.134
11.56	5.024	6261	175.15	40.565	61.894
12.05	5.515	5898	176.75	40.412	61.809
12.15	5.610	6100	176.36	40.355	61.695
12.16	5.626	7404	176.10	41.386	62.764

The lighter fragment is more excited (and strongly deformed) than the heavier one.

Energies are not shared proportionally to mass numbers of the fragments!

$$\mathrm{TKE} = 177.80 - 0.3489 E_n \quad [\text{in MeV}],$$

Nuclear data evaluation, Madland (2006)

Calculated total kinetic energies (TKE) of the fragments slightly underestimate the observed values by no more than: 1 - 3 MeV !

J. Grineviciute, et al. (in preparation)

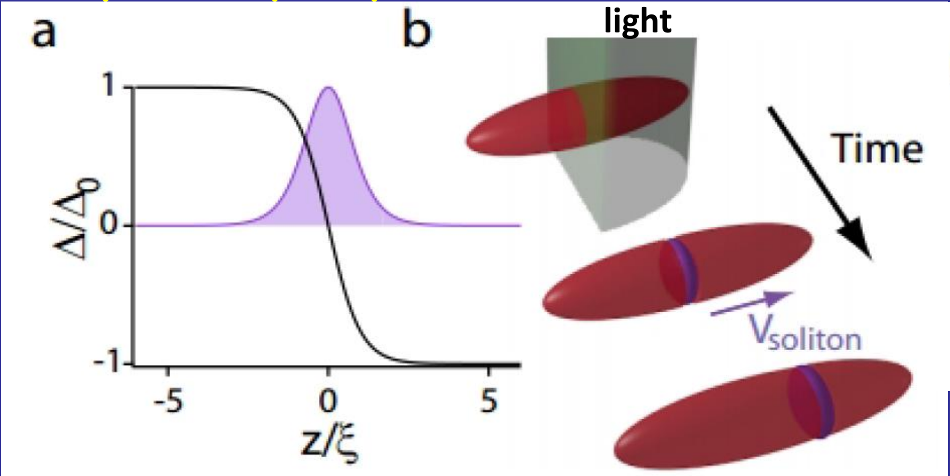
see also:

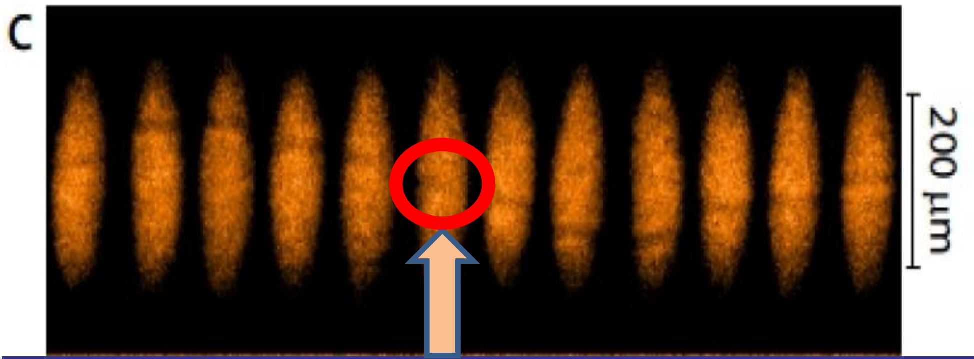
A. Bulgac, P. Magierski, K.J. Roche, and I. Stetcu, Phys. Rev. Lett. 116, 122504 (2016)

Nuclear collisions

Collisions of superfluid nuclei having different phases of the pairing fields

Inspired by experiments on ultracold atomic gases: merging two 6Li clouds



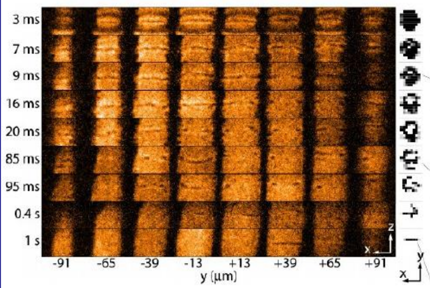


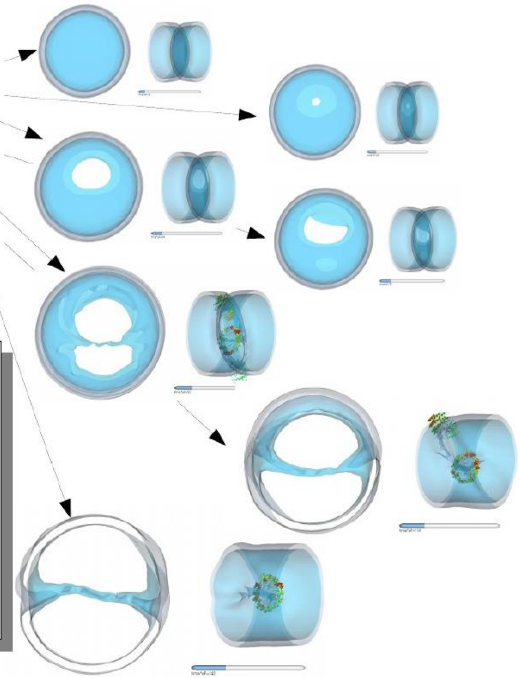
Creation of a „**heavy soliton**" after merging two superfluid atomic clouds.

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

And recently detailed analysis of **solitonic cascade** has been performed in experiment at MIT:

M.J.H. Ku et al. Phys. Rev. Lett. 116, 045304 (2016)





We can reproduce all stages of the experiment within unified framework without any ajusting parameters!

From Gabriel Wlazłowski talk

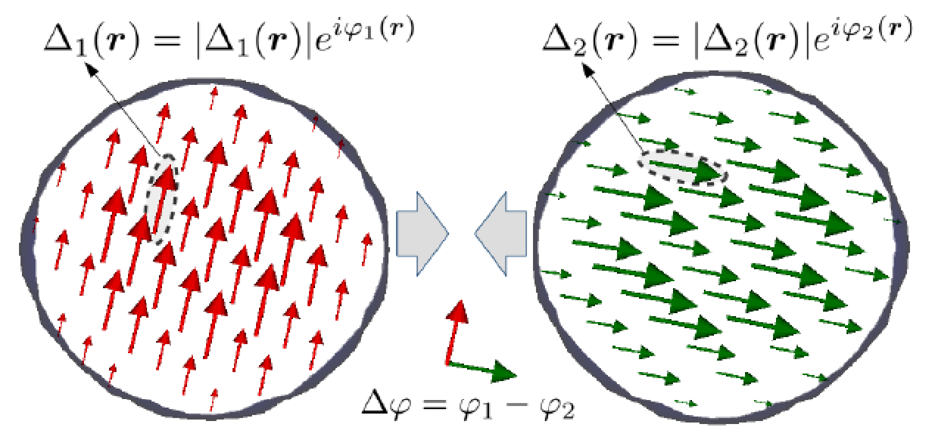
Wlazłowski, Sekizawa, Magierski (in preparation)

In the context of nuclear systems the main questions are:

-how a possible solitonic structure can be manifested in nuclear system?

-what observable effect it may have on heavy ion reaction:
kinetic energies of fragments, capture cross section, etc.?

Clearly, we cannot control phases of the pairing field in nuclear experiments and the possible signal need to be extracted after averaging over the phase difference.



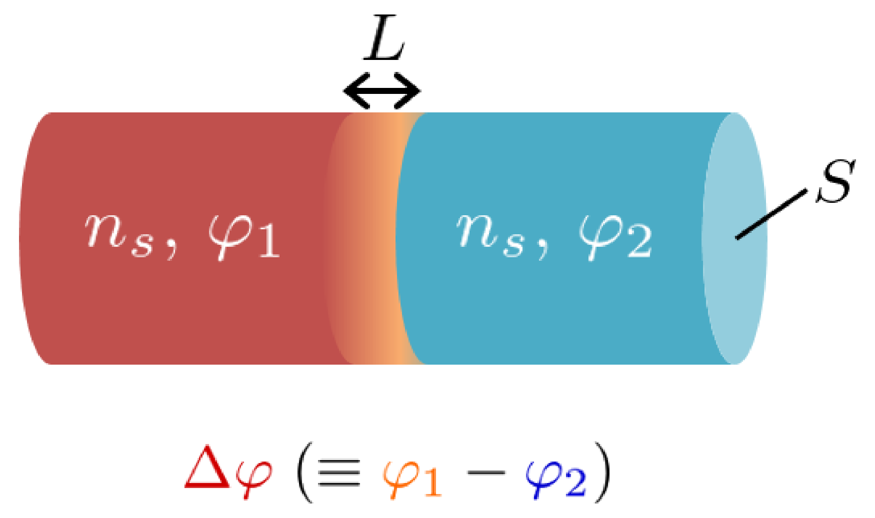
Y. Hashimoto, G. Scamps, Phys. Rev. C94, 014610(2016) – TDHFB studies of small systems: 20O+20O reaction produced negligible effect.

Estimates for the magnitude of the effect

At first one may think that the magnitude of the effect is determined by the nuclear pairing energy which is of the order of MeV's in atomic nuclei (according to the expression):

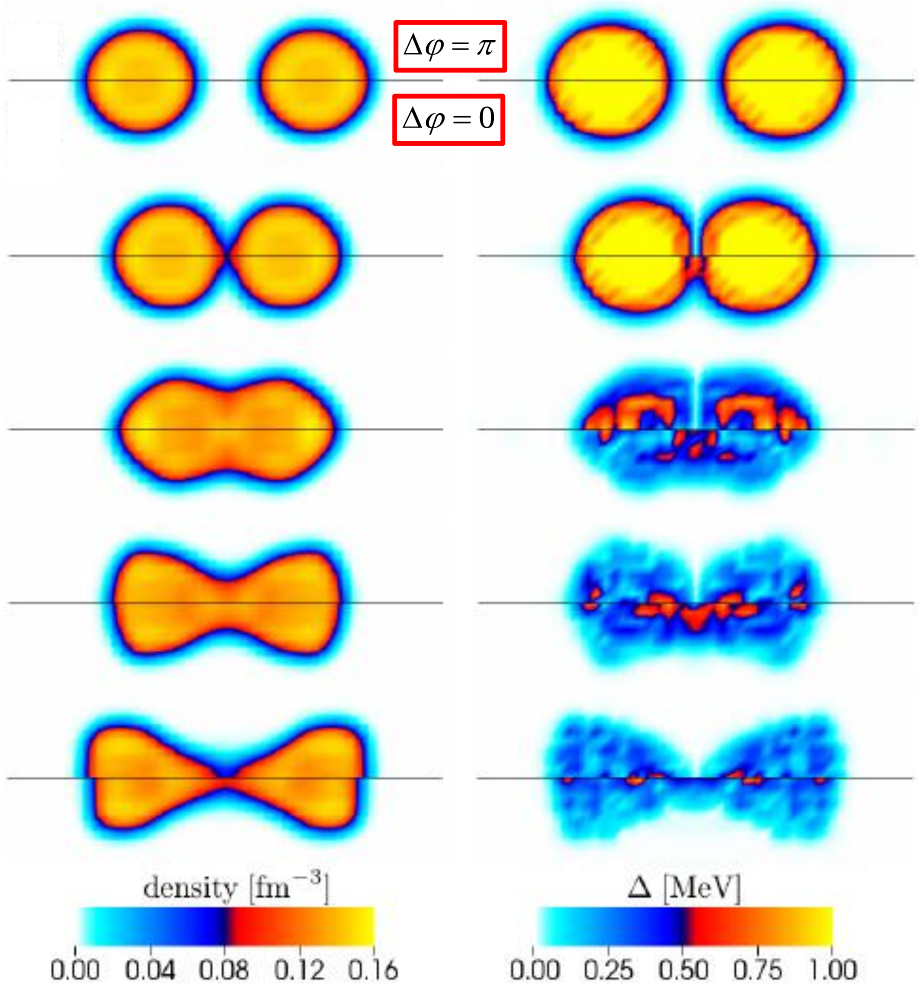
$$\frac{1}{2}g(\varepsilon_F)|\Delta|^2; \quad g(\varepsilon_F) \text{ - density of states}$$

On the other hand the energy stored in the junction can be estimated from Ginzburg-Landau (G-L) approach:

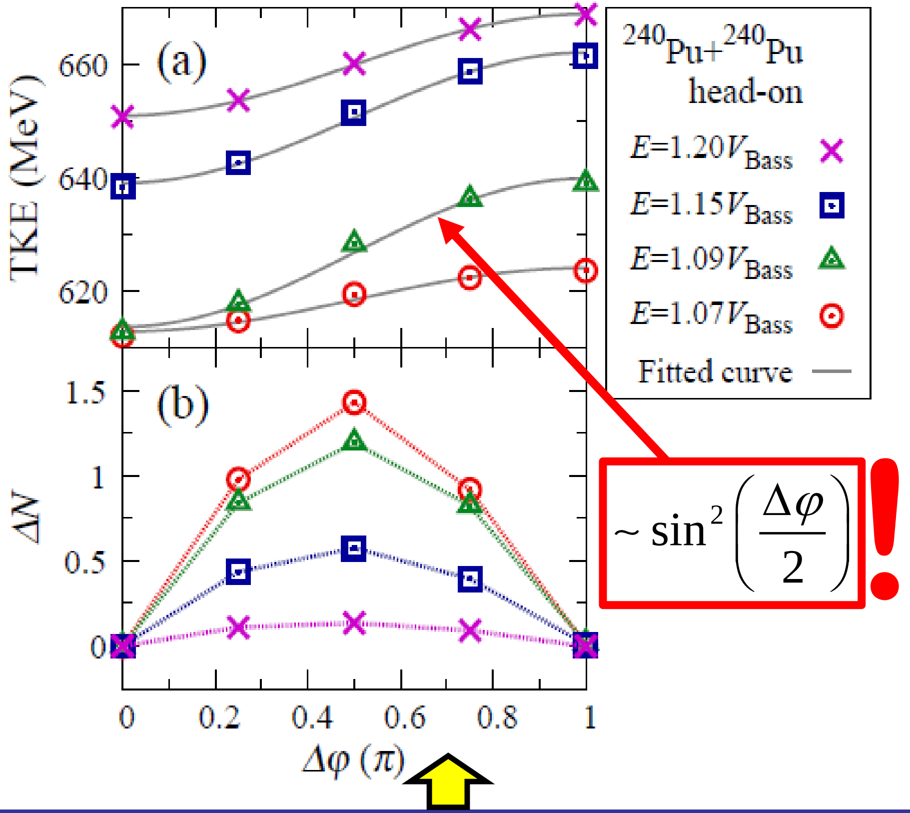


$$\boxed{E_j = \frac{S}{L}\frac{\hbar^2}{2m}n_s \sin^2\frac{\Delta\varphi}{2}}$$

For typical values characteristic for two heavy nuclei: $E_j \approx 30MeV$



Total kinetic energy of the fragments (TKE)



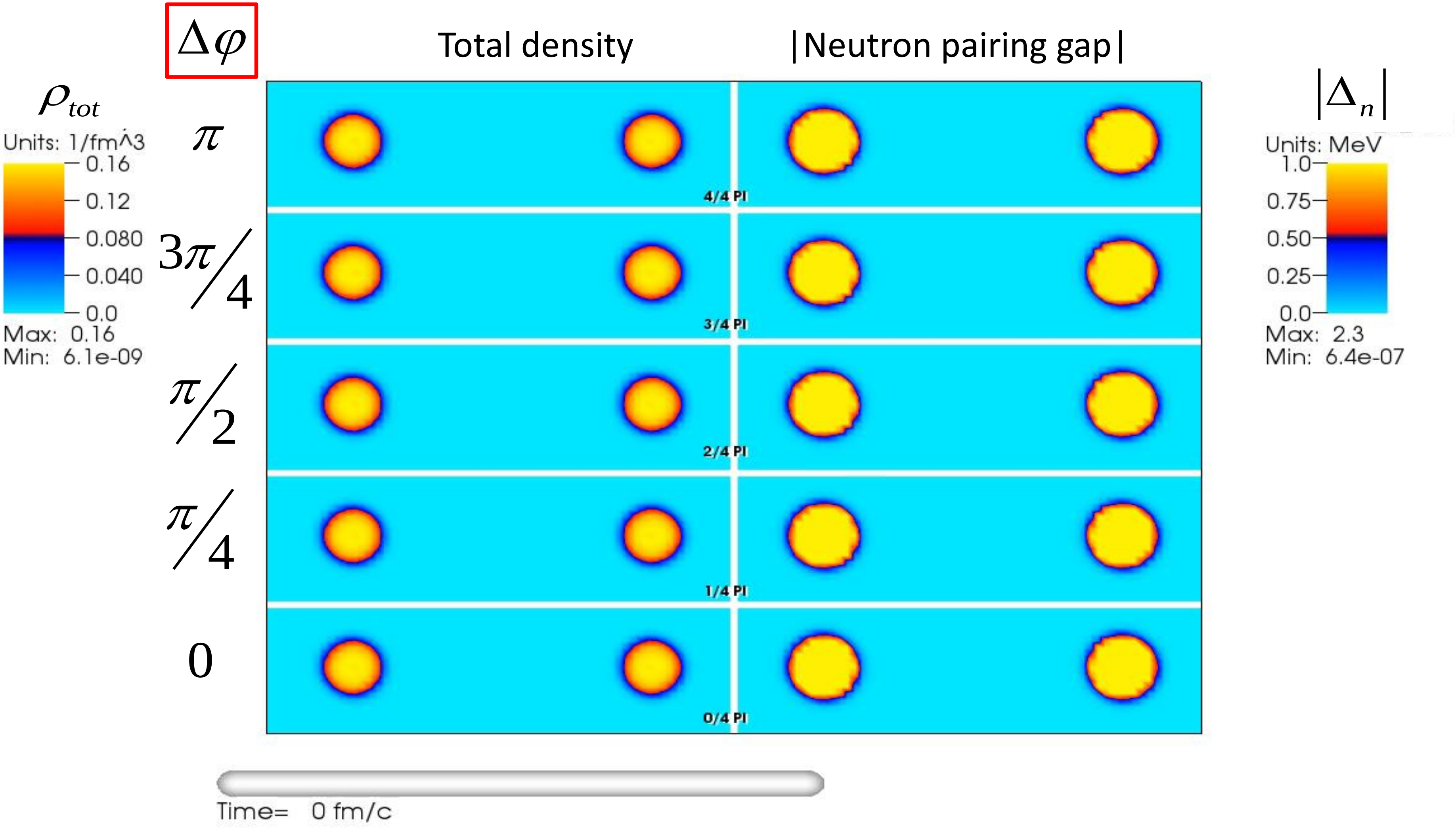
$\sim \sin^2\left(\frac{\Delta\varphi}{2}\right)$!

Average particle transfer between fragments.

Creation of the solitonic structure between colliding nuclei prevents energy transfer to internal degrees of freedom and consequently enhances the kinetic energy of outgoing fragments.

Surprisingly, the gauge angle dependence from the G-L approach is perfectly well reproduced in the kinetic energies of outgoing fragments!

$^{90}Zr + {}^{90}\mathrm{Zr}$ at energy $E \simeq V_{Bass}$



Modification of the capture cross section!

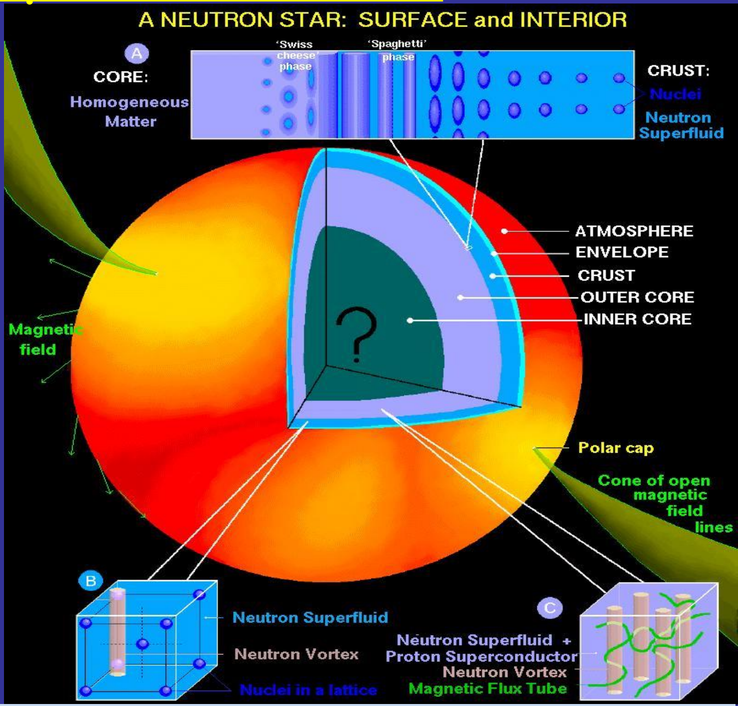
P. Magierski, K. Sekizawa, G. Wlazłowski, Phys. Rev. Lett. 119 042501 (2017)

Modelling neutron star interior – towards microscopic foundations of the neutron star crust dynamics

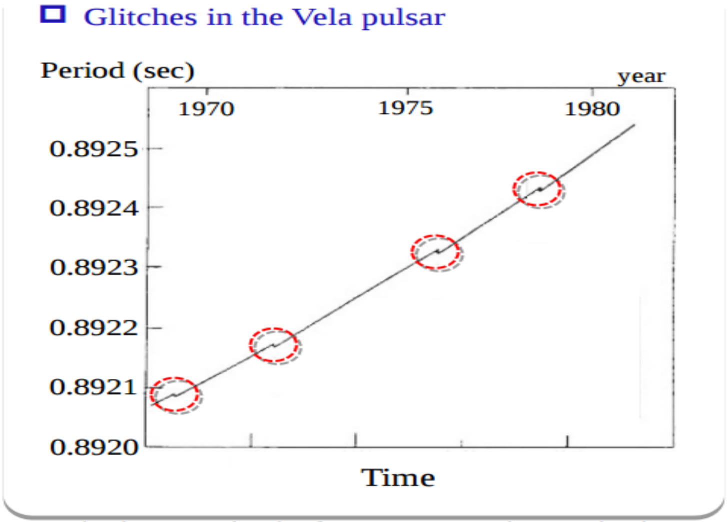
GOAL: Construct large scale model of neutron star interior (in particular neutron star crust), based on microscopic input from nuclear theory.

MICROSCOPIC INPUTS NEEDED:

- vortex-impurity interaction,
- effective masses of nuclear impurities,
- couplings between lattice vibrations and neutron superfluid medium,
- ...



Glitch: a sudden increase of the rotational frequency



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

glitch phenomenon=a sudden speed up of rotation. To date more than 300 glitches have been detected in more than 100 pulsars

Glitch phenomenon is commonly believed to be related to rearrangement of vortices in the interior of neutron stars (Anderson,Itoh,Nature 256,25 (1975))
It would require however a correlated behavior of huge number of quantum vortices and the mechanism of such collective rearrangement is still a mystery.

Vortex – impurity interaction

Static approach

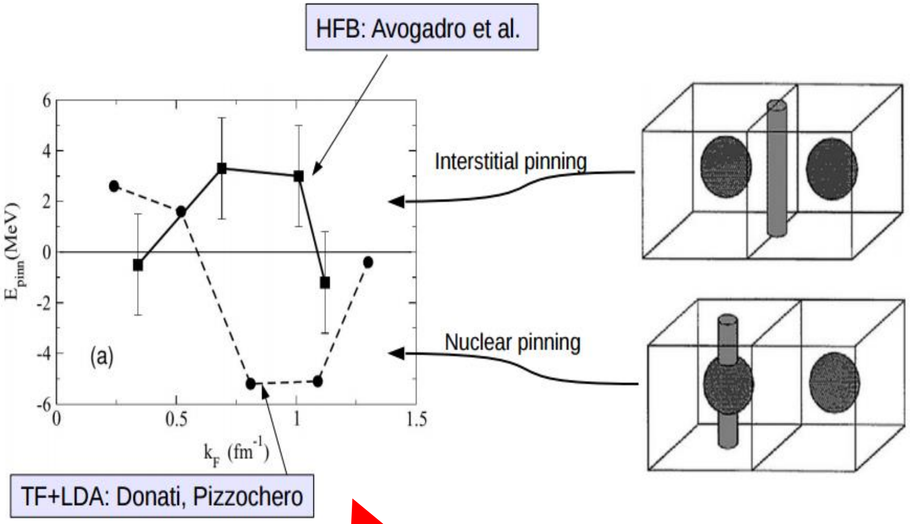
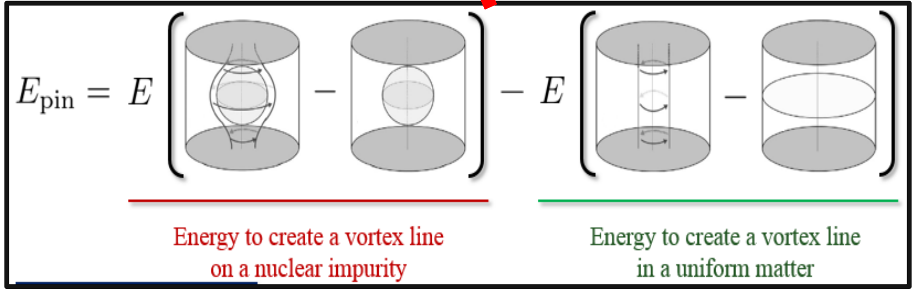


Fig. from: P. Avogadro et al.,
Phys. Rev. C 75, 012805(R) (2007)

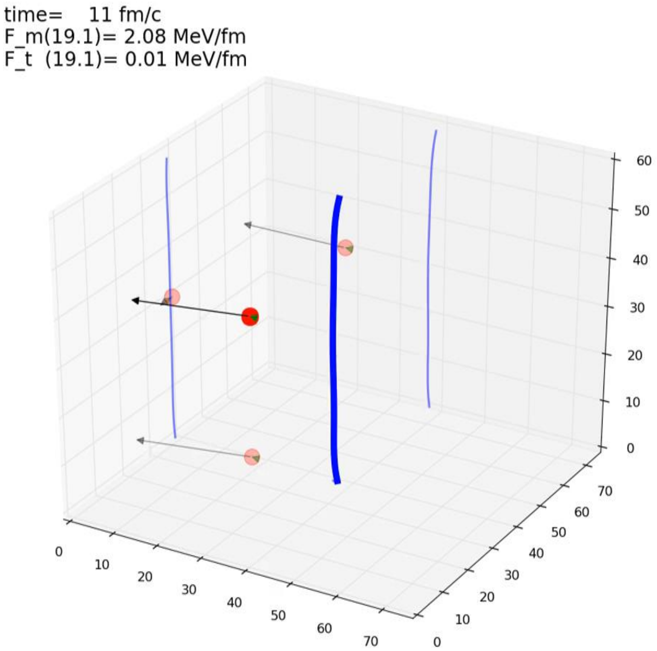
Figs from: P. Donati et al.,
Nuclear Physics A 742 (2004) 363



Pinning energy is obtained as a result of substraction of two large numbers!

Dynamic approach

The external potential keeps the nucleus moving along the straight line with a constant velocity below the critical velocity.



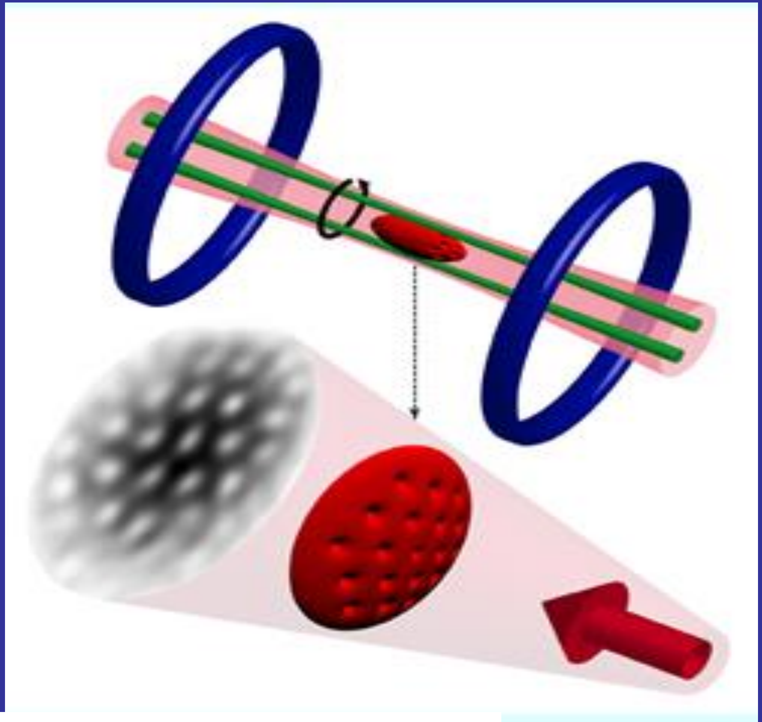
G. Wlazłowski, K. Sekizawa, P. Magierski,
A. Bulgac, M.M. Forbes,
Phys. Rev. Lett. 117, 232701(2016)

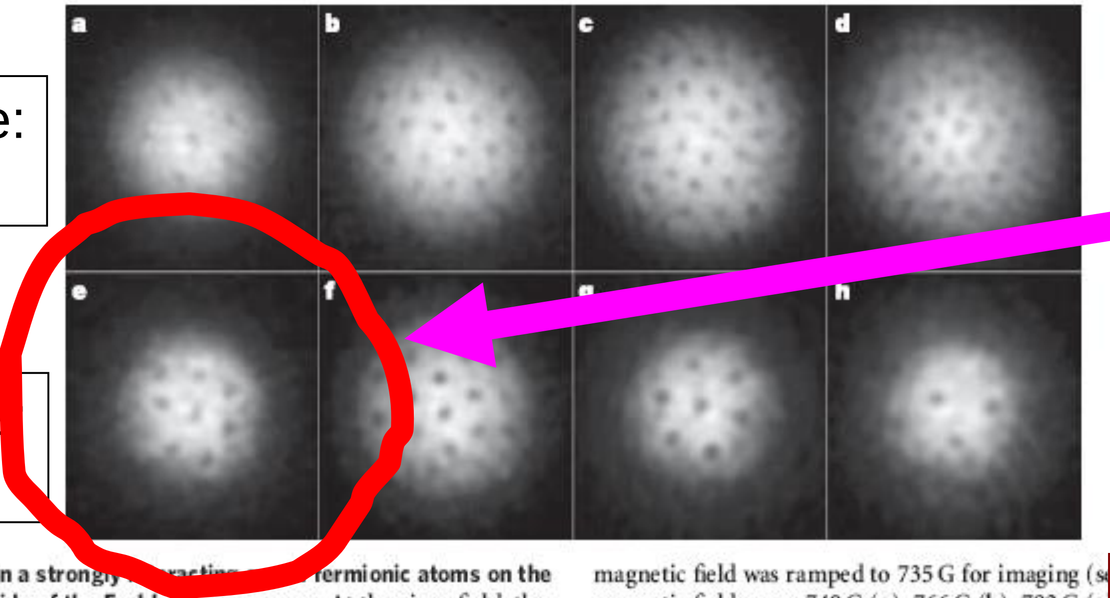
Dynamics of ultracold atomic (fermionic) gases

- ✓In 1999 DeMarco and Jin created a degenerate atomic Fermi gas.
- ✓In 2005 Zwierlein/Ketterle group observed quantum vortices which survived when passing from BEC to unitarity – evidence for superfluidity!

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 interacting [illegible] 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 (s 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)

What is a unitary gas?

A gas of interacting fermions is in the unitary regime if the average separation between particles is large compared to their size (range of interaction), but small compared to their scattering length.

$n\, r_0^3 << 1$ $n\, |a|^3 >> 1$

n - particle density
a - scattering length
r_0 - effective range

$$\text{i.e. } r_0 \to 0, a \to \pm\infty$$

NONPERTURBATIVE REGIME

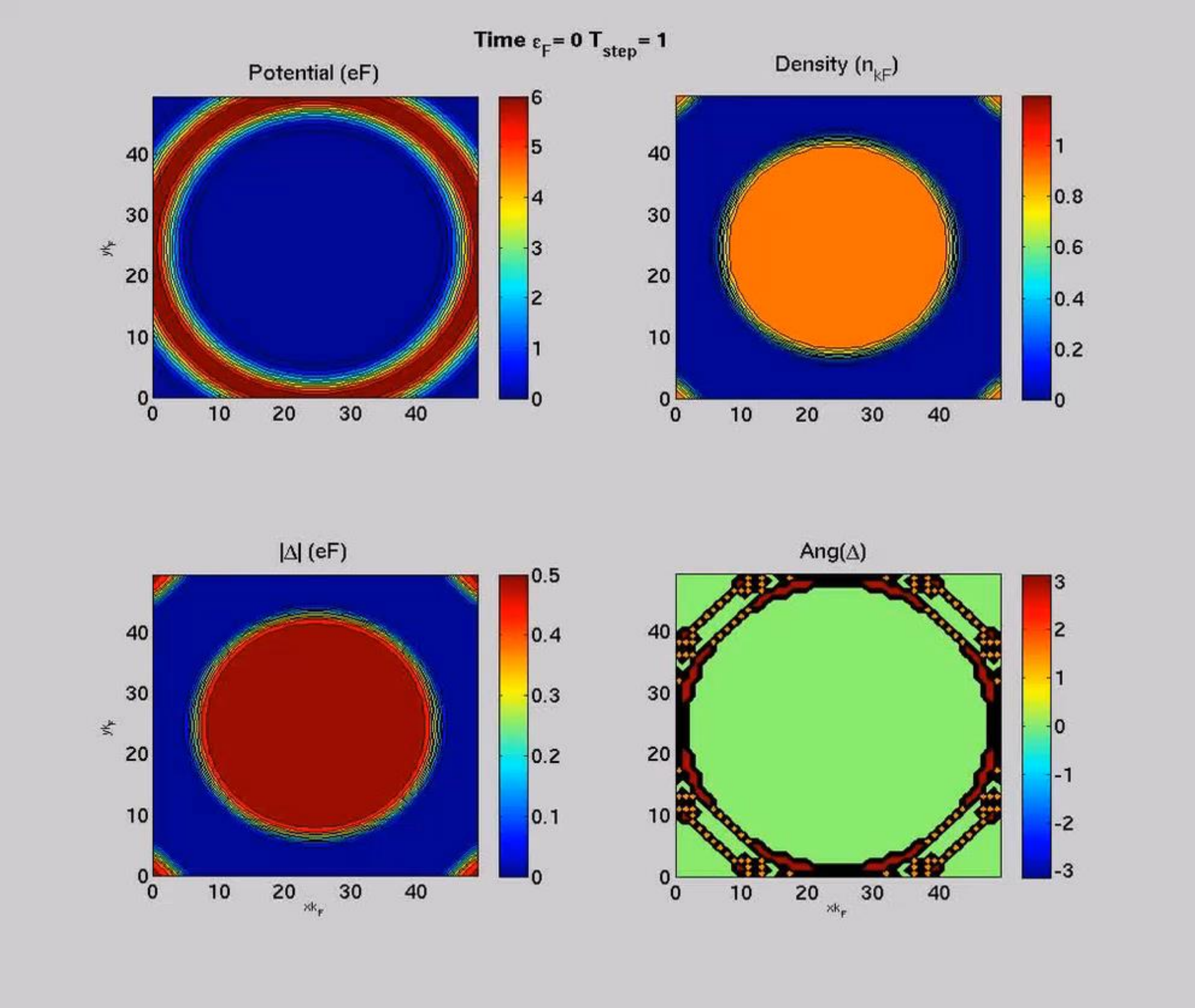
System is dilute but strongly interacting!

Universality: $E(x) = \xi(x) E_{FG}$; $x = T / \varepsilon_F$

$\xi(0) = 0.37(1)$ - **Exp. estimate**

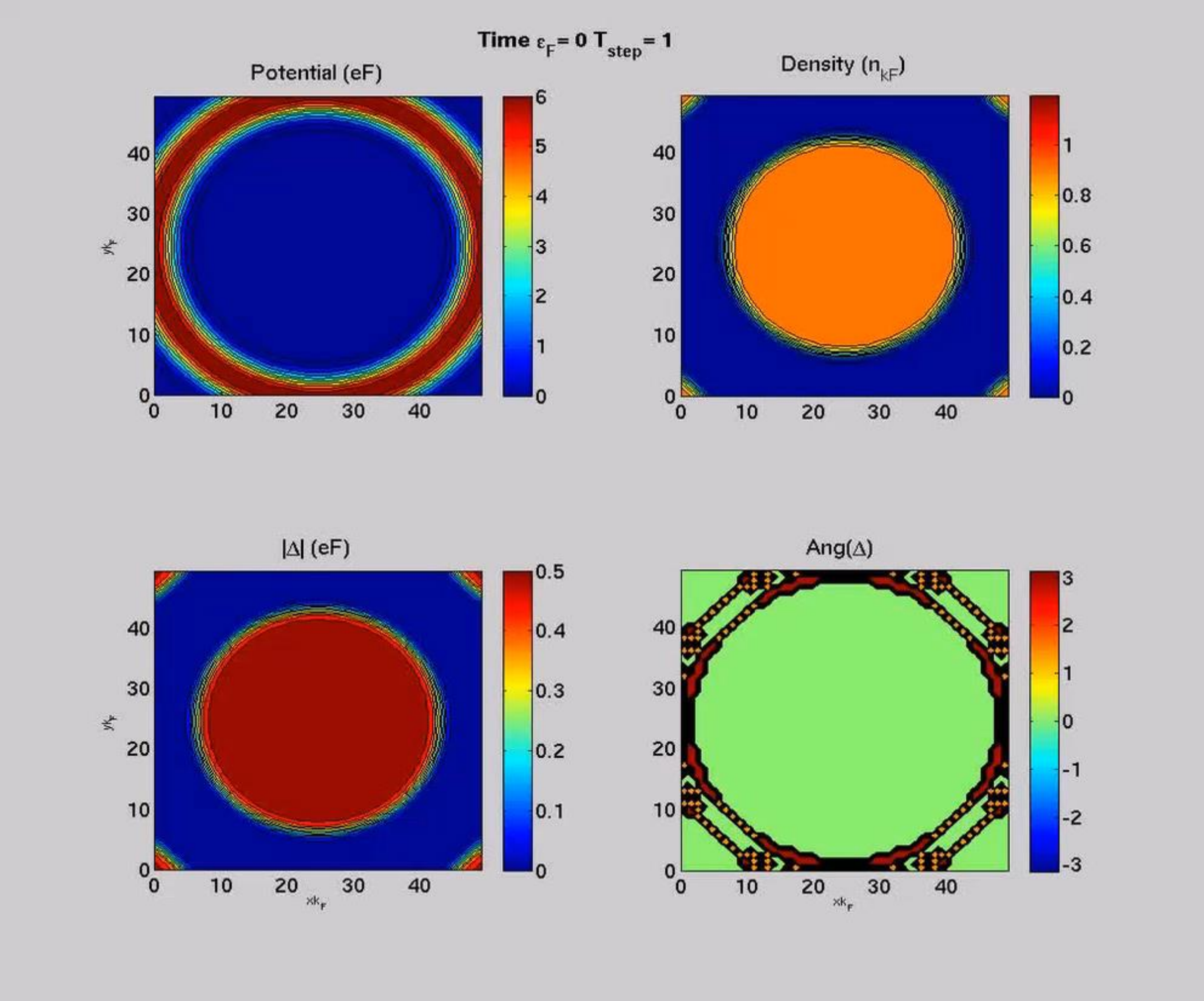
E_{FG} - **Energy of noninteracting Fermi gas**

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

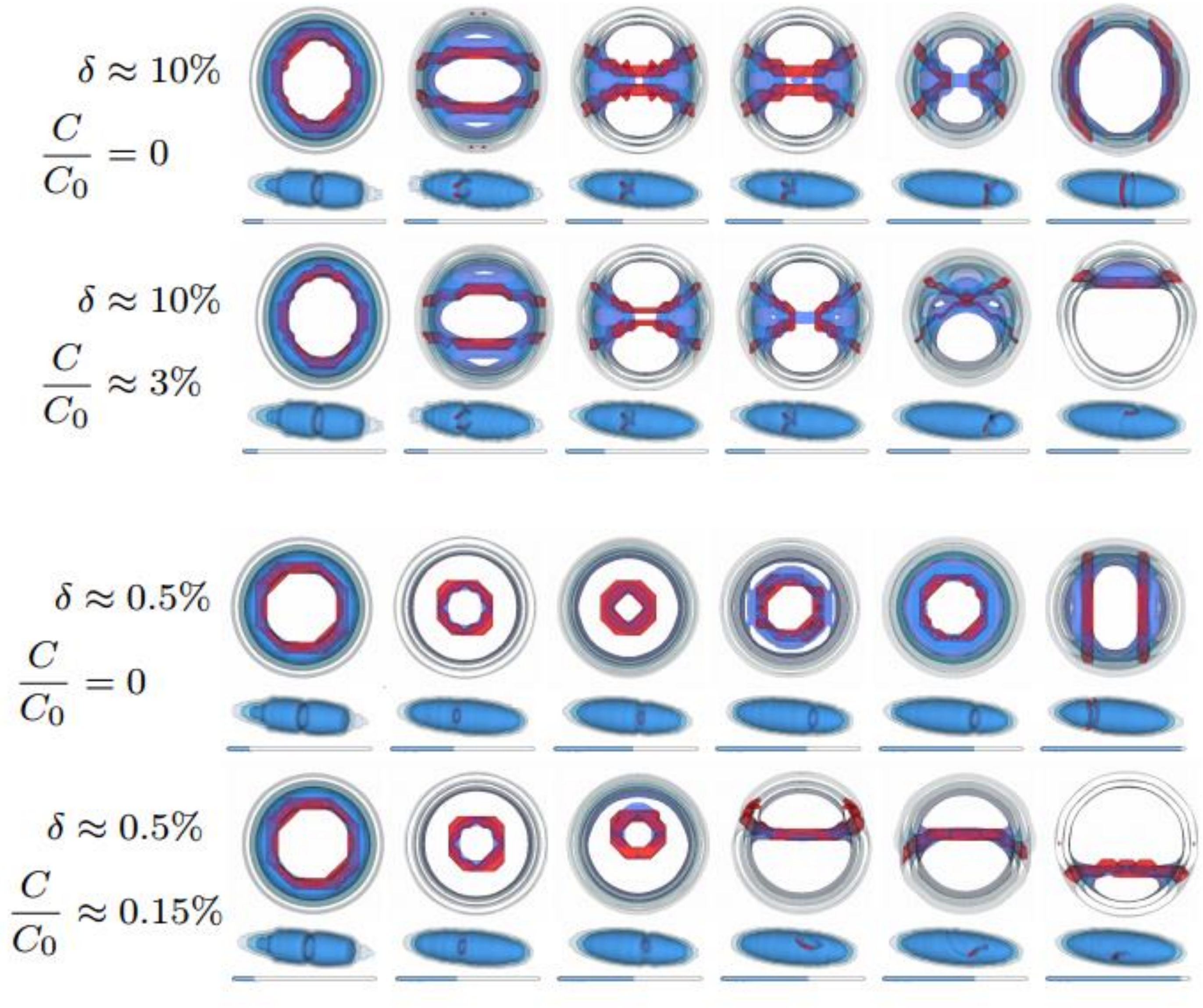


Bulgac, Luo, Magierski, Roche, Yu, *Science* 332, 1288 (2011)

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



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



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)

Summarizing

- TDDFT extended to superfluid systems and based on the local densities offers a flexible tool to study quantum superfluids far from equilibrium.

- Future plans:

- Ultracold atoms: investigation of quantum turbulence in Fermi systems;
  topological excitations in spin-polarized atomic gases in the presence of LOFF phase.
- Neutron star: Provide a link between large scale models of neutron stars and microscopic studies;
  towards the first simulation of the glitch phenomenon based on microscopic input.
- Nuclear physics: induced fission and fusion processes – *from more phenomenology and adjusted parameters to more fundamental theory and increased predictive power;*
  search for new effects related to pairing dynamics in nuclear nuclear processes.
  Extension of TDDFT (account for dissipation and fluctuations of one-body observables):
  - stochastic extension of TDDFT
  - Baranger-Veneroni prescription