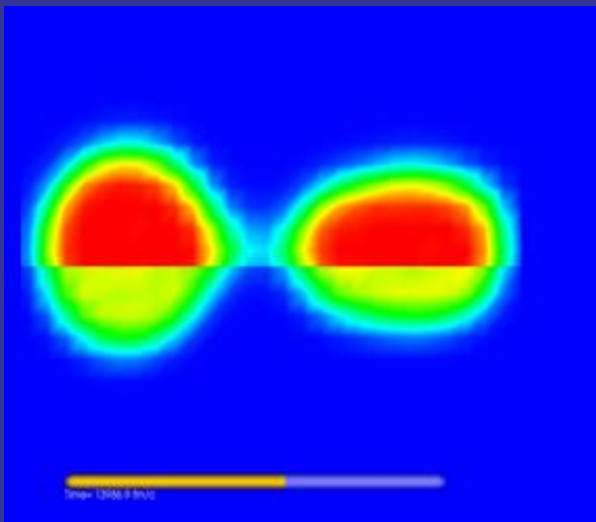
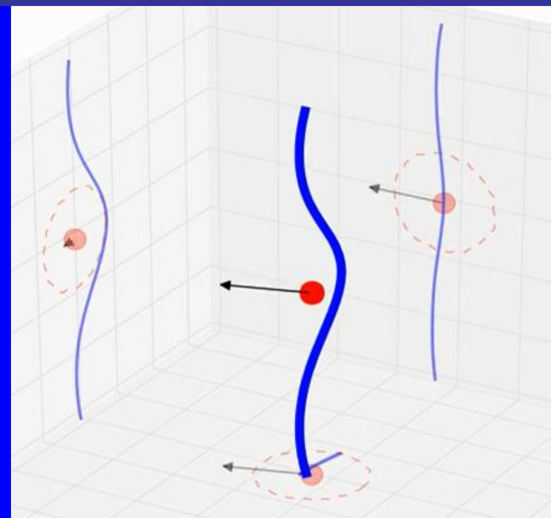
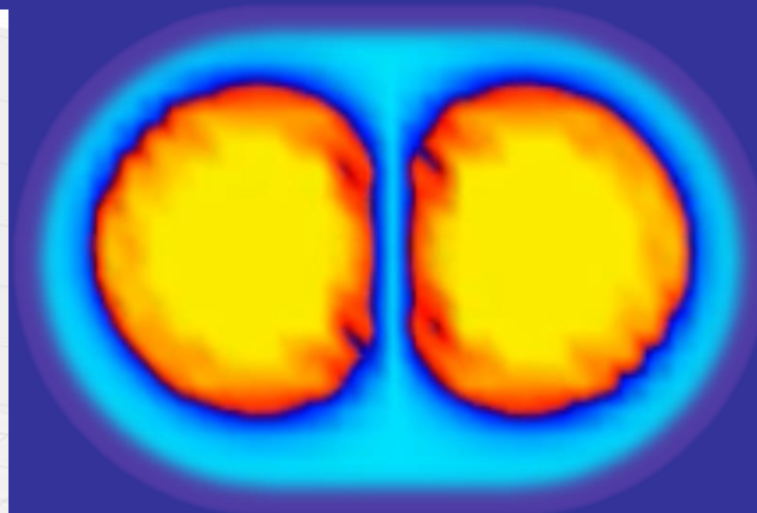
Time Dependent Density Functional Theory for nuclear fission and reactions.







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GOAL:
Unified 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)?

See review talk by Nicolas Schunck and talk on TDDFT (TDHF) by Sait Umar.

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.

Runge Gross mapping

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

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

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

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

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

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

Hence the DFT approach is essentially exact.

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.
- Only one body observables can be reliably evaluated within standard DFT.

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 <u>complex field which has its own modes of excitations</u>, 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.

Advantages of TDDFT

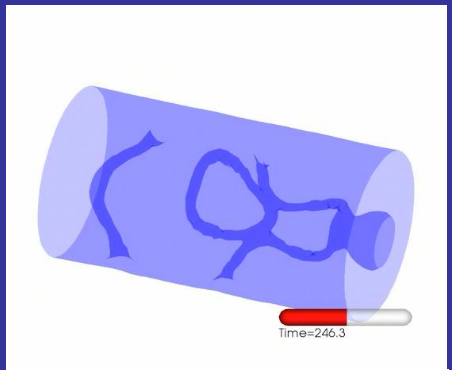
- The same framework describes various limits: eg. linear and highly nonlinear regimes, adiabatic and nonadiabatic (dynamics far from equilibrium).
- Simulations follow closely the way how experiments are conducted.
- TDDFT does not require introduction of hard-to-define collective degrees of freedom and there are no ambiguities arising from defining potential energy surfaces and inertias.
- In principle it offers consistent way to reconstruct the energy spectrum through re-quantization of TDDFT trajectories (No need for considering off-diagonal matrix elements which have vague meaning in the DFT framework)
- One-body dissipation, the window and wall dissipation mechanisms are automatically incorporated into the theoretical framework.
- All shapes are allowed and the nucleus chooses dynamically the path in the shape space, the forces acting on nucleons are determined by the nucleon distributions and velocities, and the nuclear system naturally and smoothly evolves into separated fission fragments.
- There is no need to introduce such unnatural quantum mechanical concepts as "rupture" and there is no worry about how to define the scission configuration.

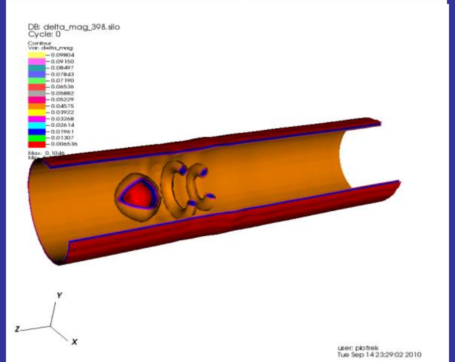
Areas of applications

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

Ultracold atomic (fermionic) gases. Unitary regime.

Dynamics of quantum vortices, solitonic excitations, quantum turbulence.

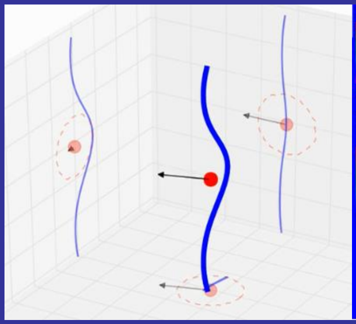


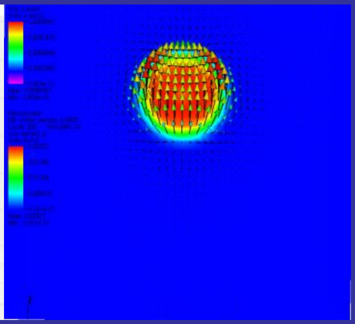


$$\frac{\Delta}{\varepsilon_F} \leq 0.1-0.2$$

Astrophysical applications.

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

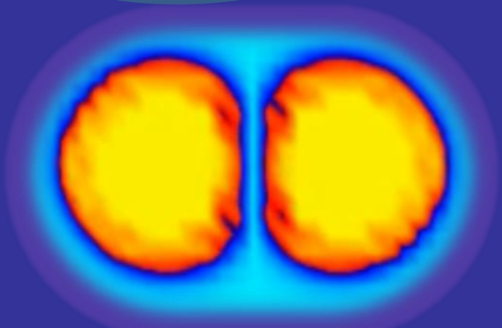


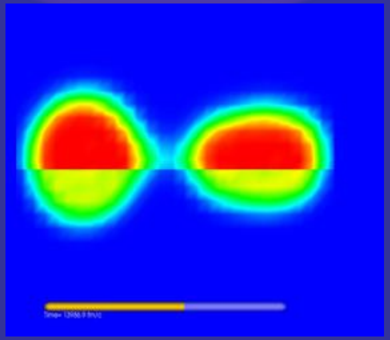


$$\frac{\Delta}{\varepsilon_F} \leq 0.03$$

Nuclear physics.

Induced nuclear fission, fusion, collisions.



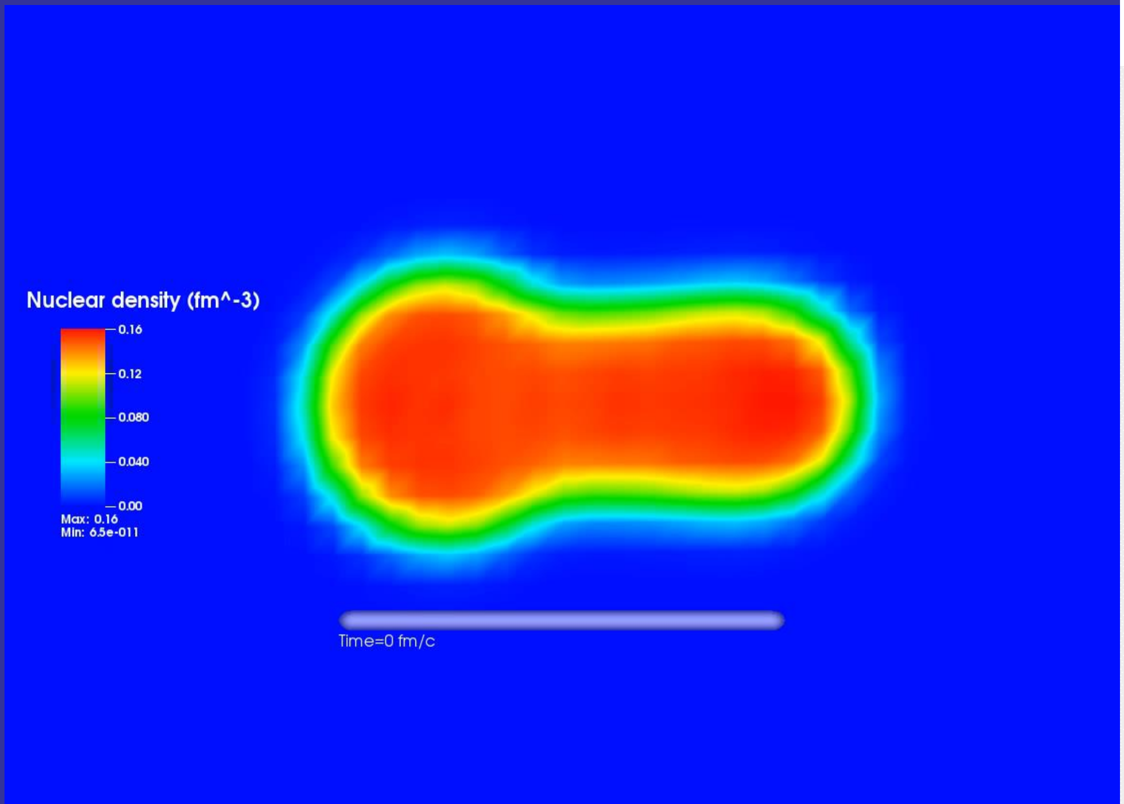


Examples of applications:

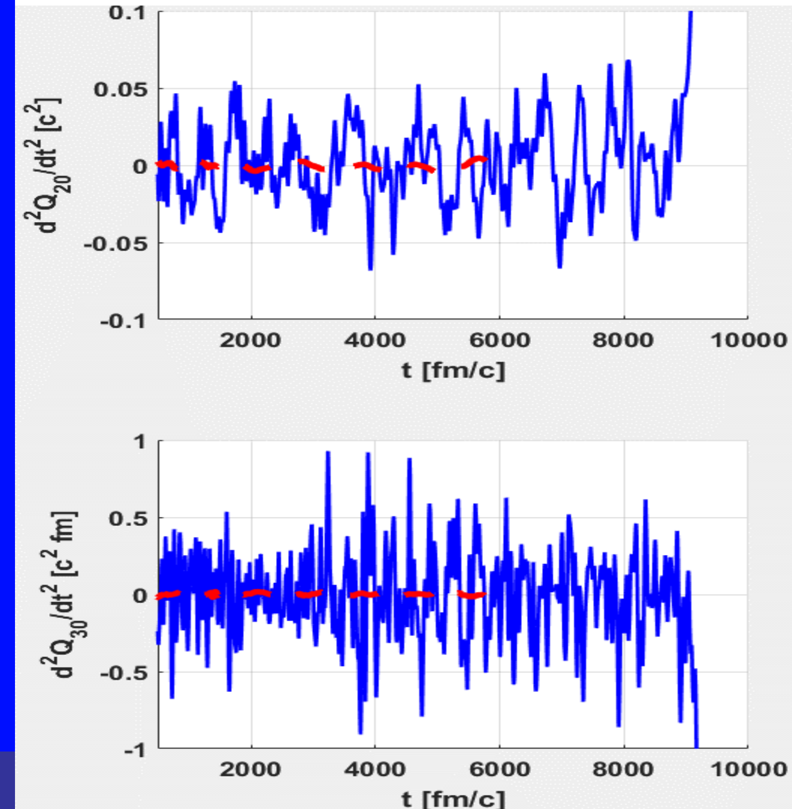
- Nuclear induced fission
- Collisions of medium or heavy superfluid nuclei

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*:



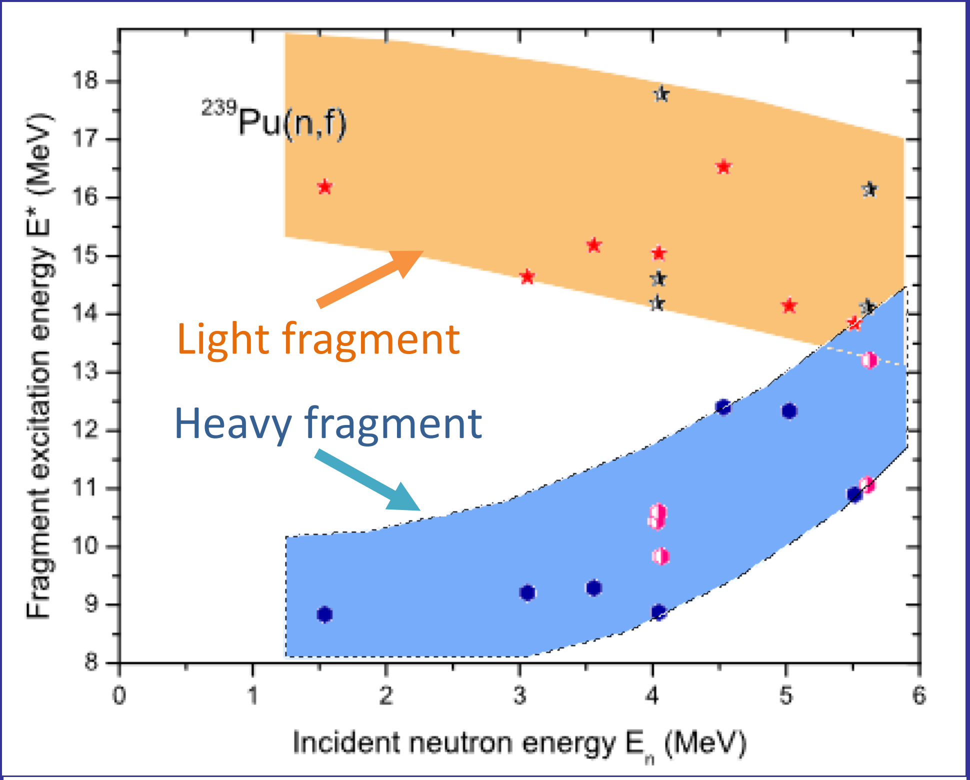
Accelerations in quadrupole and octupole moments along the fission path



During the process shown, the exchange of about 2 neutrons and 3 protons occur between fragments before the actual fission occurs.

Interestingly <u>the fragment masses seem to be relatively stiff</u> with respect to changes of the initial conditions.

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



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

Excitation energy of the fragments from TDDFT

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

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

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

Nuclear data evaluation, Madland (2006)

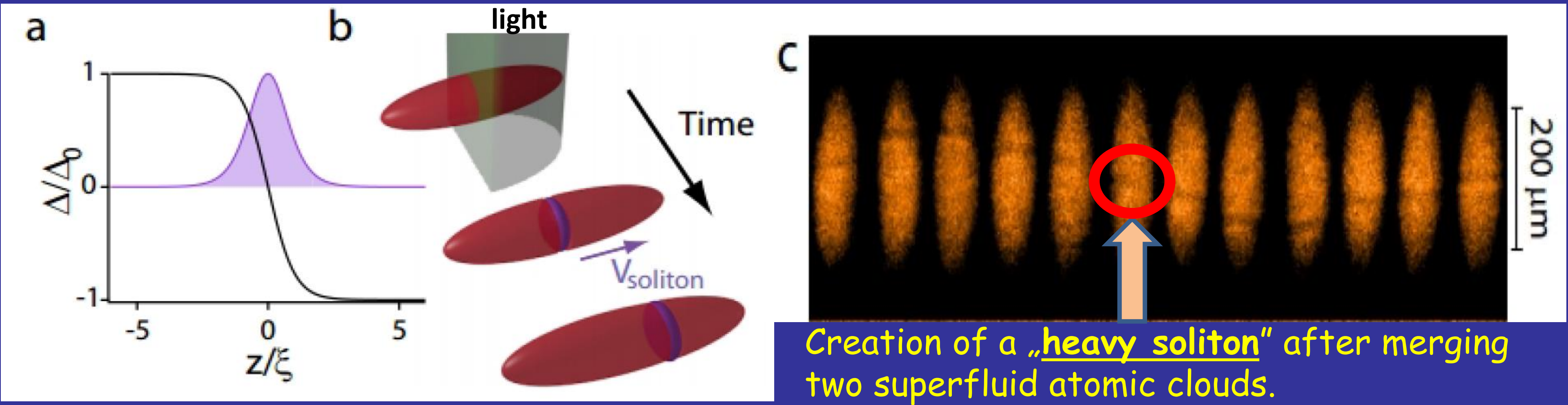
Calculated TKEs slightly underestimate the observed values by no more than: 1 - 3 MeV !

J. Grineviciute et al. (in preparation)

Nuclear collisions

Collisions of superfluid nuclei having different phases of the pairing fields

Motivated 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).

Sequence of decays of topological excitations is reproduced byTDSLDA:
Wlazłowski, et al.,Phys. Rev. A91, 031602 (2015)

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.?

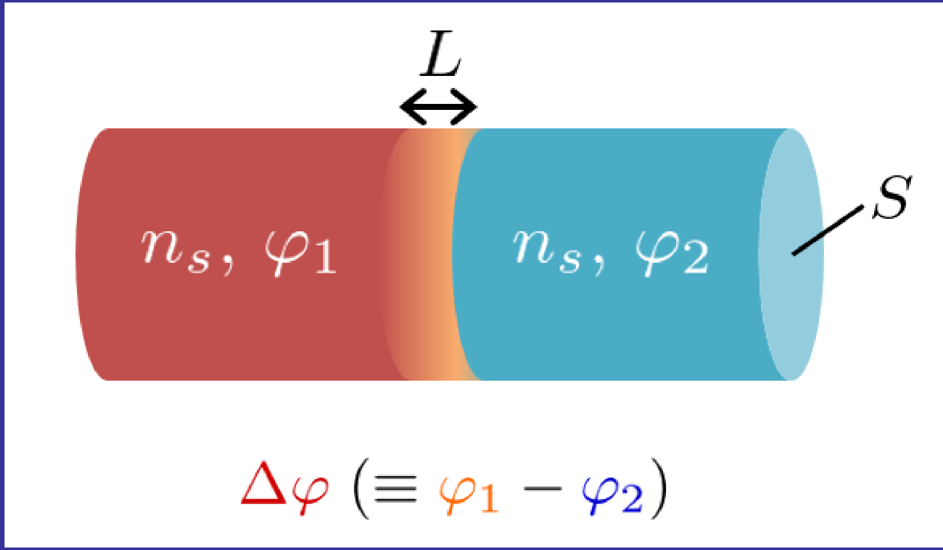
Clearly, we cannot control phases of the pairing field in nuclear experiments and the possible signal need to be extracted after averaging over the phase difference.

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):

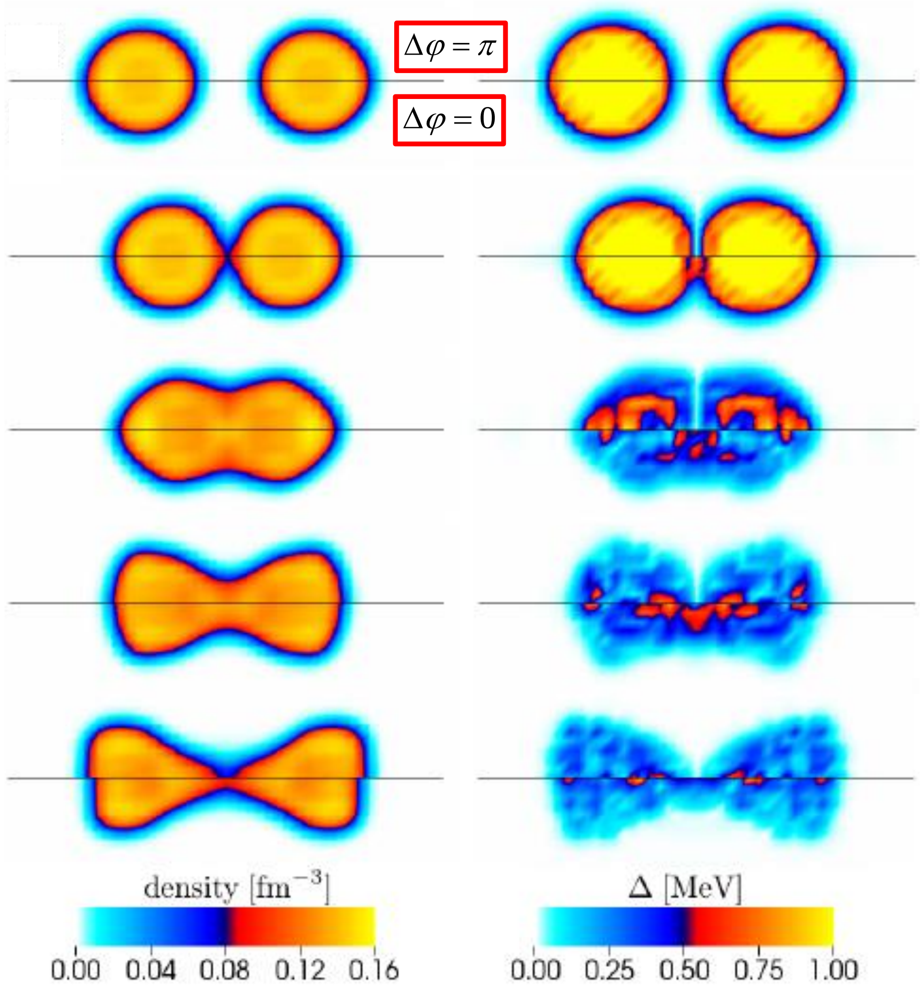
$$\frac{1}{2} g(\varepsilon_F)|\Delta|^2; \quad g(\varepsilon_F) \text{ - density of states}$$

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

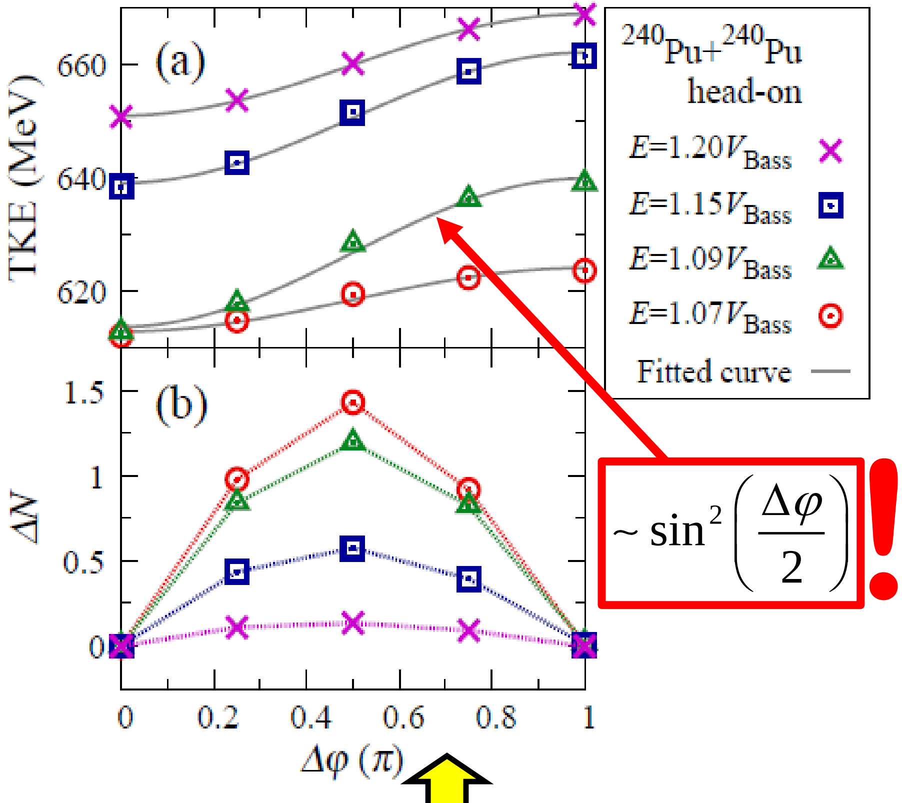


$$E_j = \frac{S}{L}\frac{\hbar^2}{2m} n_s \sin^2 \frac{\Delta\varphi}{2}$$

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



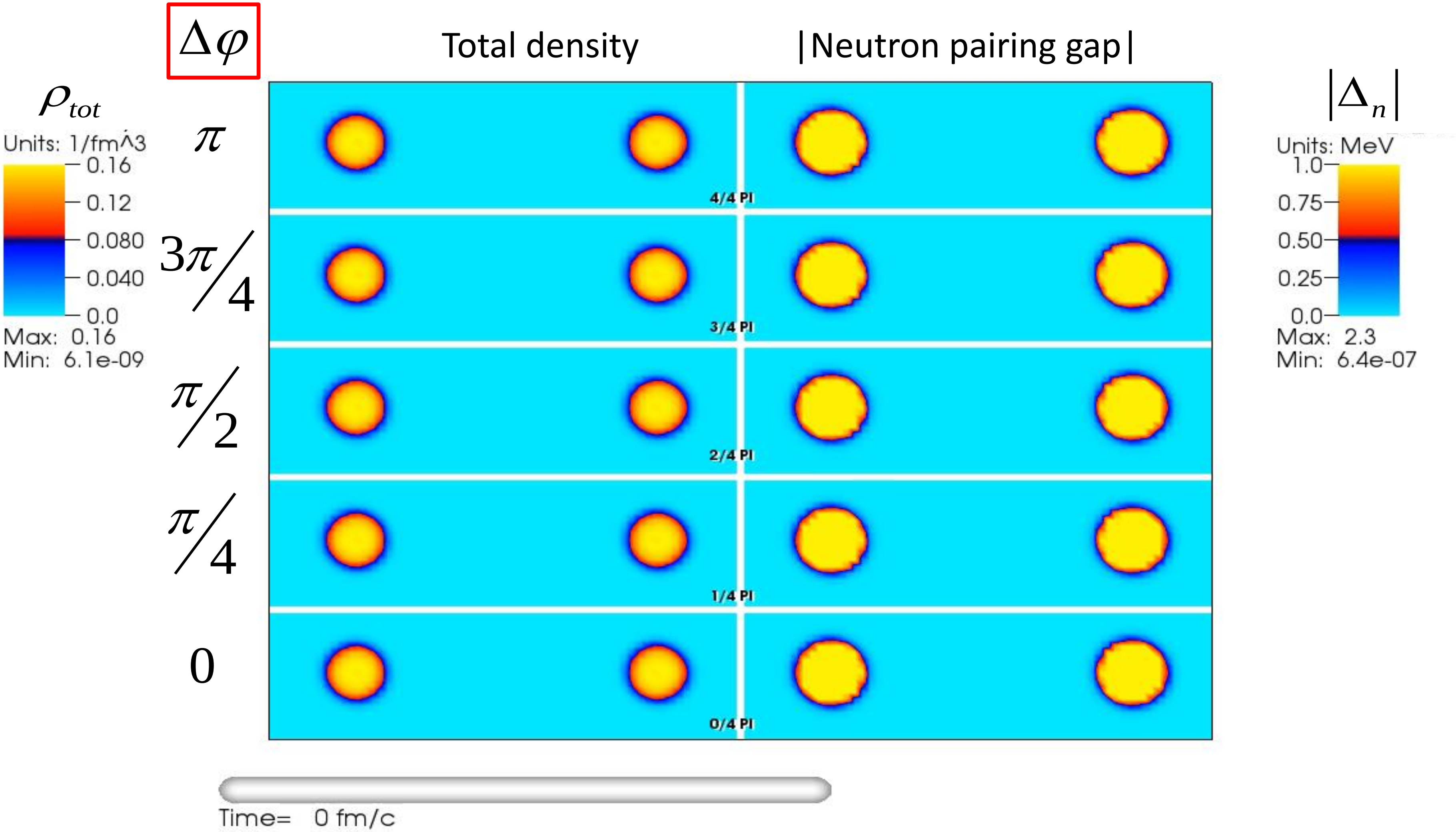
Total kinetic energy of the fragments (TKE)



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!

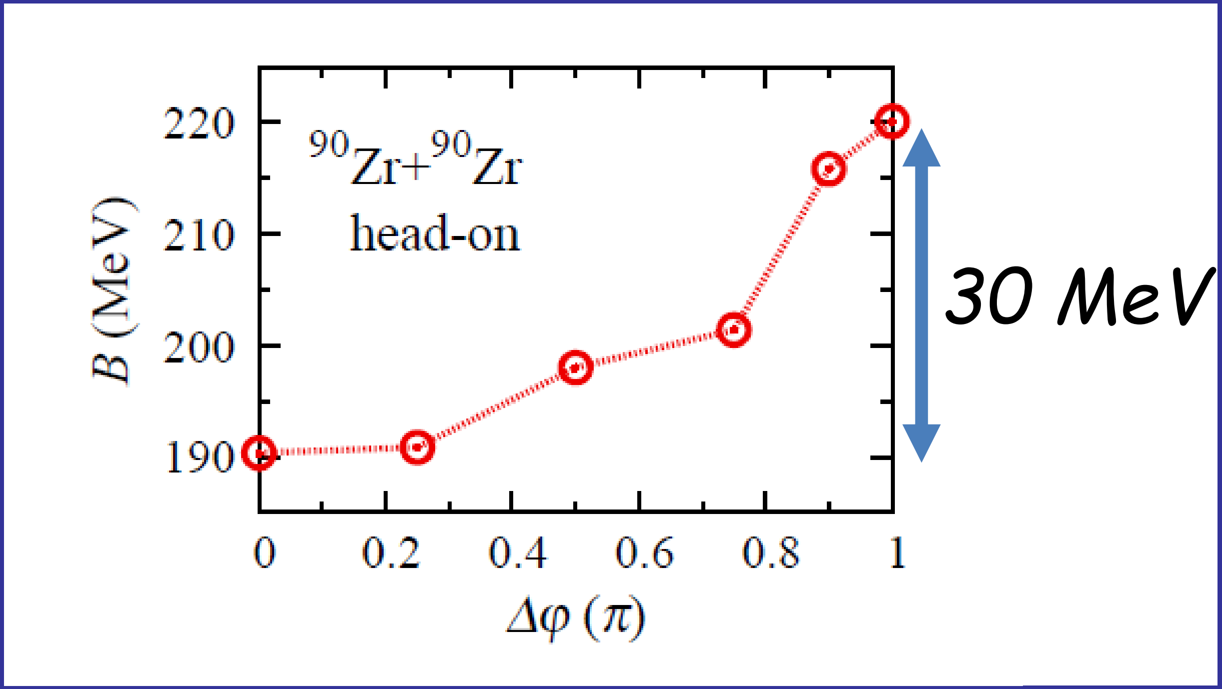
$^{90}Zr + {}^{90}Zr$ at energy $E \simeq V_{Bass}$



Modification of the capture cross section!

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

Effective barrier height for fusion as a function of the phase difference



What is an average extra energy needed for the capture?

$$E_{extra} = \frac{1}{\pi}\int_0^{\pi}\left(B(\Delta\varphi) - V_{Bass}\right) d(\Delta\varphi) \approx 10 MeV$$

The phase difference of the pairing fields of colliding medium or heavy nuclei produces a similar solitonic structure as the system of two merging atomic clouds.
The energy stored in the created junction is subsequently released giving rise to an increased kinetic energy of the fragments. The effect is found to be of the order of 30MeV for heavy nuclei and occur for energies up to 20-30% of the barrier height.

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

Summarizing

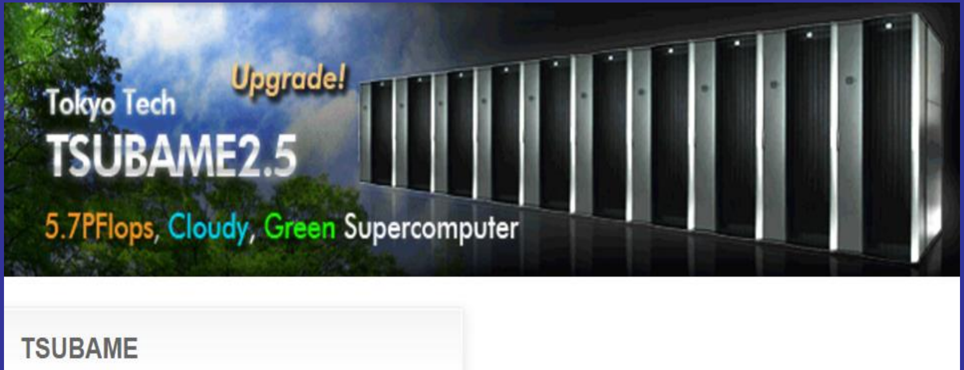
- TDDFT extended to superfluid systems and based on the local densities offers a flexible tool to study quantum superfluids far from equilibrium.
- TDDFT offers an unprecedented opportunity to test the nuclear energy density functional for large amplitude collective motion, non-equilibrium phenomena, and in new regions of the collective degrees of freedom.

- **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 based directly on EDF. search for new effects related to pairing dynamics in nuclear processes.

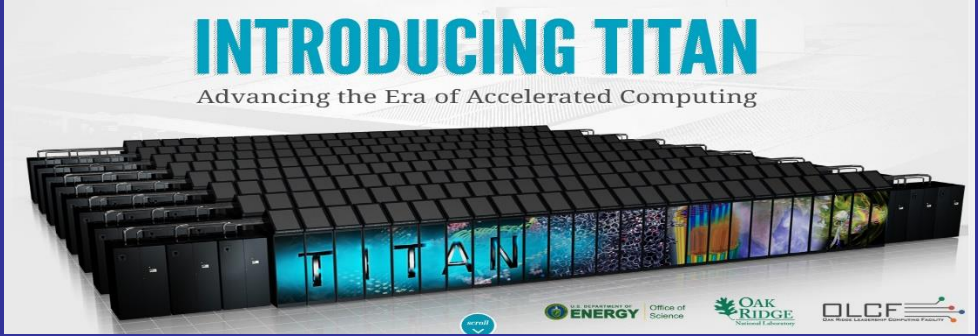
Selected supercomputers (CPU+GPU) currently in use:

Piz Daint: 7.787 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)