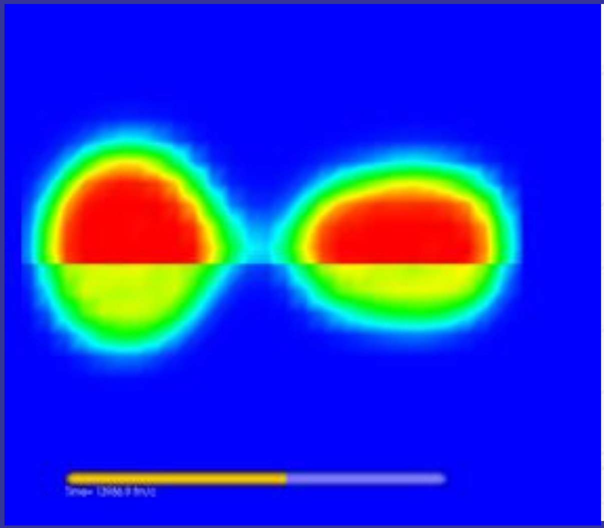
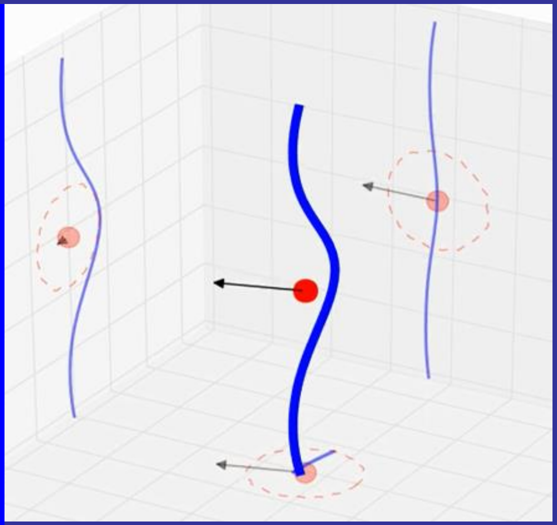
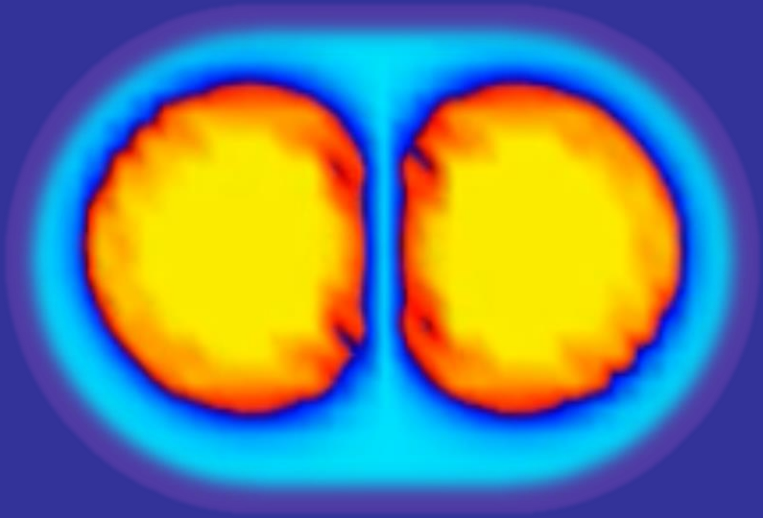
# *Towards exascale simulations of quantum superfluids – new perspectives for modelling nuclear processes*







***Piotr Magierski (Warsaw University of Technology)***

Collaborators:

<u>Warsaw Univ. of Technology</u>

| | |
|---|---|
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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.

# Superfluid extension of (TD)DFT

Triggered initially by the discovery of high-Tc supercondutors:

DFT for superconductors:
L. N. Oliveira, E. K. U. Gross, and W. Kohn, Phys. Rev. Lett. 60 2430 (1988).
TDDFT for supercondutors:
O.-J. Wacker, R. Kummel, E.K.U. Gross, Phys. Rev. Lett. 73, 2915 (1994).

Extensions required to introduce an anomalous density:

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

***Problem***:
*Such formulation results in Kohn-Sham equations in a form of integro-differential equations of enormous computational complexity.*

**However: local pairing approximation is possible!**

A. Bulgac, Phys. Rev.A, 040502(R) (2007)

# TDSLDA equations:

Local density approximation

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

**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**

**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.**

# Current capabilities of the code:

- volumes of the order of ($L = 100^3$) capable of simulating time evolution of about 150000 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 (16 CPUs per 1 GPU)

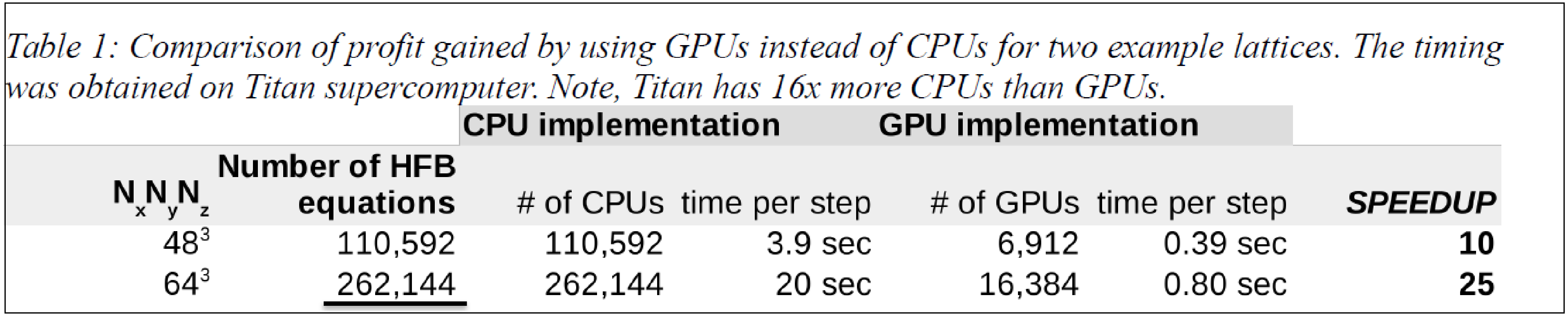


*Table 1: Comparison of profit gained by using GPUs instead of CPUs for two example lattices. The timing was obtained on Titan supercomputer. Note, Titan has 16x more CPUs than GPUs.*

| | | **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** |

Over 1 million time-dependent 3D nonlinear complex coupled PDEs

***Cray XK7, ranked at peak ≈ 27 Petaflops (Peta – $10^{15}$)***

*On Titan there are 18,688 GPUs which provide 24.48 Petaflops !!!*
*and 299,008 CPUs which provide only 2.94 Petaflops.*

**A single GPU on Titan performs the same amount of FLOPs as approximately 134 CPUs.**

# Areas of applications

**Ultracold atomic (fermionic) gases. Unitary regime.**

Dynamics of vortices, solitonic excitations, quantum turbulence.

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

**Astrophysical applications.**

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

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

**Nuclear physics.**

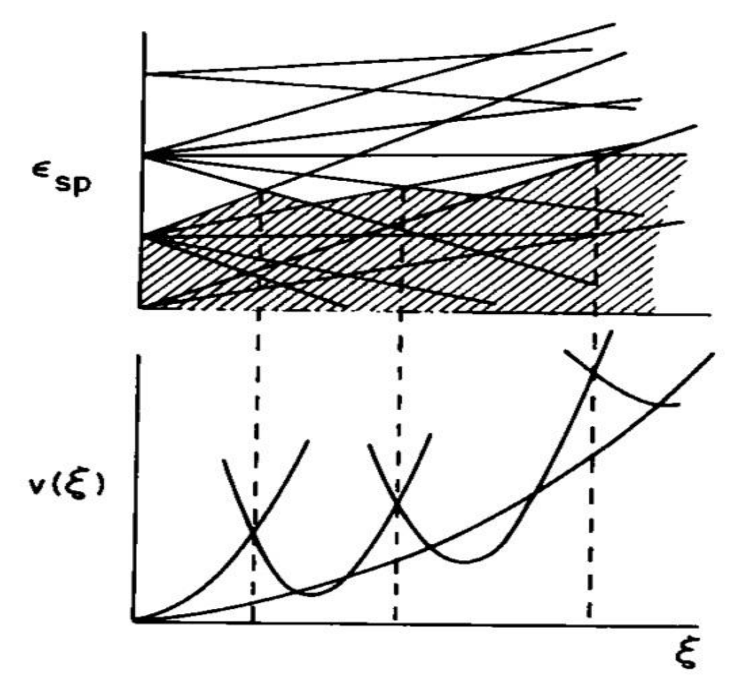
Induced nuclear fission, fusion, collisions.

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

# Nuclear physics applications: Induced Fission

## Physics of nuclear superfluid dynamics

**What is the mechanism of nuclear shape evolution during the fission process?**



**From Barranco, Bertsch, Broglia, and Vigezzi**
**Nucl. Phys. A512, 253 (1990)**

- **While a nucleus elongates its Fermi surface becomes oblate and its sphericity must be restored**
  **Hill and Wheeler, PRC, 89, 1102 (1953)**
  **Bertsch, PLB, 95, 157 (1980)**

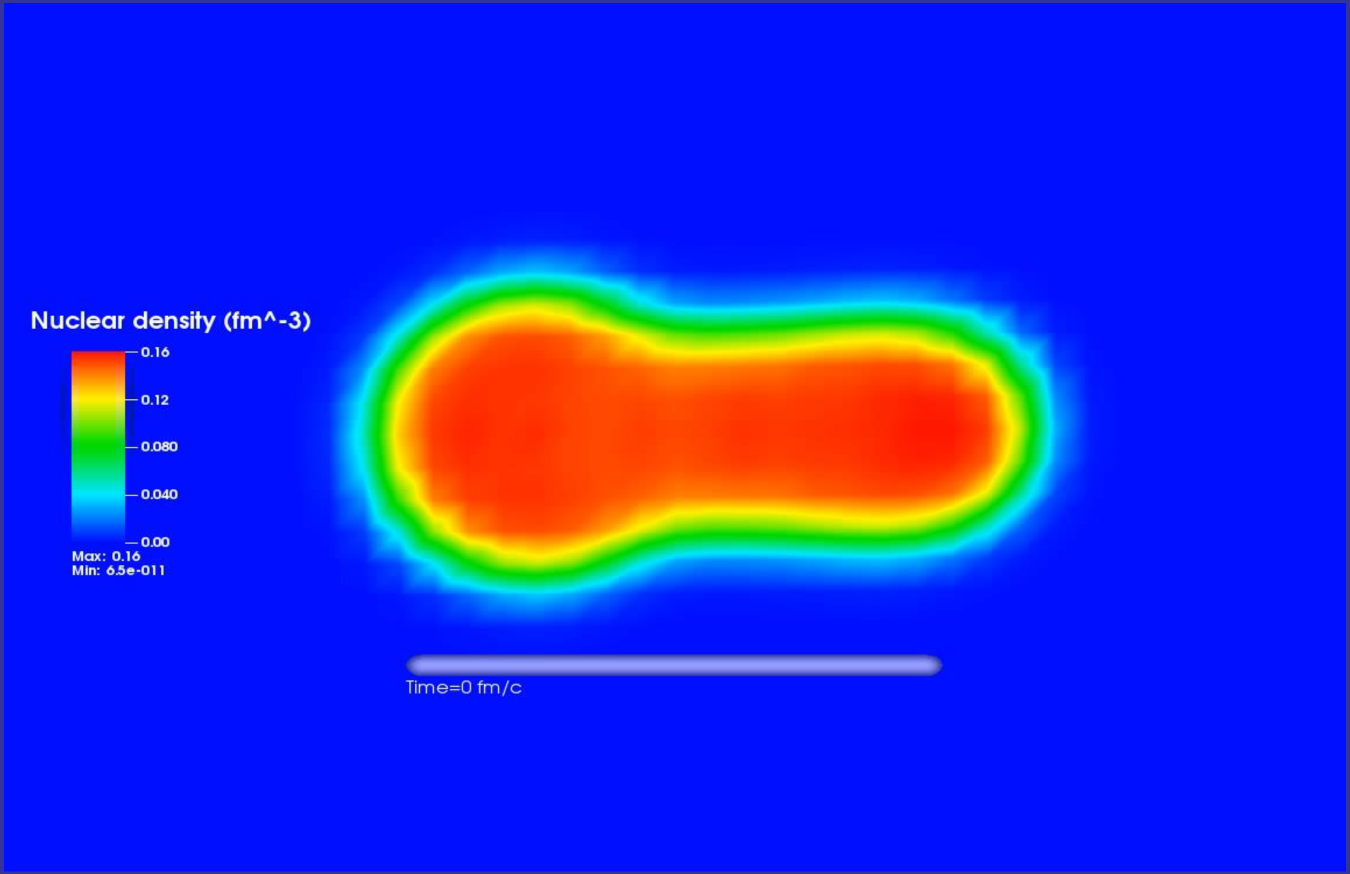
- **Each single-particle level is double degenerate (Kramers' degeneracy) and at each level crossing <u>two nucleons must jump simultaneously</u>!**

**(m,-m) => (m',-m')**
**"Cooper pair" => "Cooper pair"**

- **<u>Pairing interaction/superfluidity is the most effective mechanism at performing shape changes.</u>**

# Complexity of fission dynamics

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



During the process shown, the exchange of about 2 neutrons and 3 protons occur between fragments before the actual fission occurs.
Interestingly the fragment masses seem to be relatively stiff with respect to changes of the initial conditions.

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

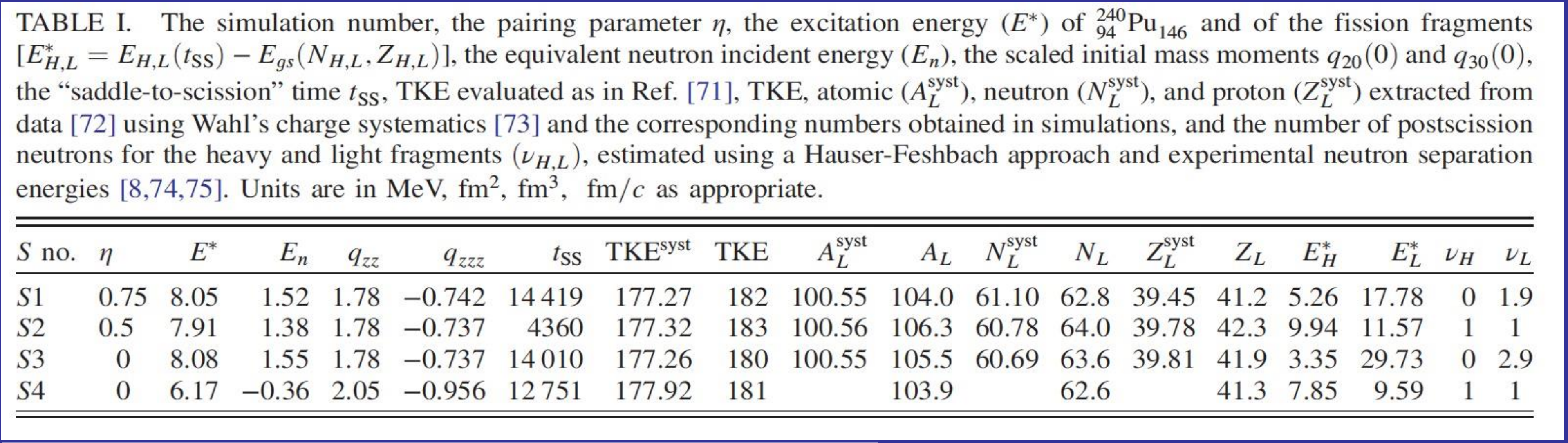
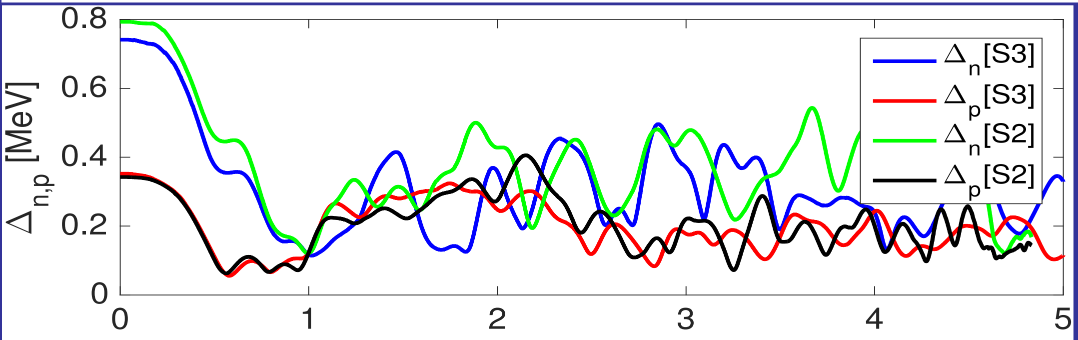
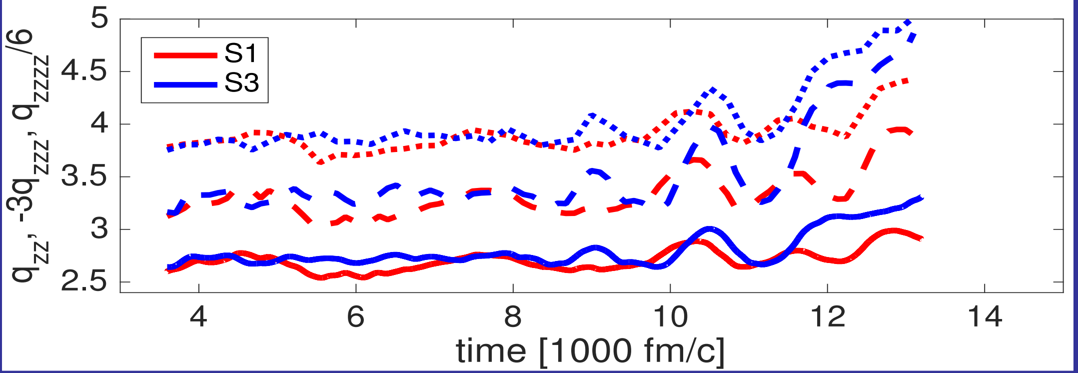


TABLE I. The simulation number, the pairing parameter $\eta$, the excitation energy ($E^*$) of ${}^{240}_{94}\mathrm{Pu}_{146}$ and of the fission fragments $[E^*_{H,L} = E_{H,L}(t_{SS}) - E_{gs}(N_{H,L}, Z_{H,L})]$, the equivalent neutron incident energy ($E_n$), the scaled initial mass moments $q_{20}(0)$ and $q_{30}(0)$, the "saddle-to-scission" time $t_{SS}$, TKE evaluated as in Ref. [71], TKE, atomic ($A_L^{\mathrm{syst}}$), neutron ($N_L^{\mathrm{syst}}$), and proton ($Z_L^{\mathrm{syst}}$) extracted from data [72] using Wahl's charge systematics [73] and the corresponding numbers obtained in simulations, and the number of postscission neutrons for the heavy and light fragments ($\nu_{H,L}$), estimated using a Hauser-Feshbach approach and experimental neutron separation energies [8,74,75]. Units are in MeV, fm$^2$, fm$^3$, fm$/c$ as appropriate.

| $S$ no. | $\eta$ | $E^*$ | $E_n$ | $q_{zz}$ | $q_{zzz}$ | $t_{SS}$ | TKE$^{\mathrm{syst}}$ | TKE | $A_L^{\mathrm{syst}}$ | $A_L$ | $N_L^{\mathrm{syst}}$ | $N_L$ | $Z_L^{\mathrm{syst}}$ | $Z_L$ | $E_H^*$ | $E_L^*$ | $\nu_H$ | $\nu_L$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $S1$ | 0.75 | 8.05 | 1.52 | 1.78 | −0.742 | 14 419 | 177.27 | 182 | 100.55 | 104.0 | 61.10 | 62.8 | 39.45 | 41.2 | 5.26 | 17.78 | 0 | 1.9 |
| $S2$ | 0.5 | 7.91 | 1.38 | 1.78 | −0.737 | 4360 | 177.32 | 183 | 100.56 | 106.3 | 60.78 | 64.0 | 39.78 | 42.3 | 9.94 | 11.57 | 1 | 1 |
| $S3$ | 0 | 8.08 | 1.55 | 1.78 | −0.737 | 14 010 | 177.26 | 180 | 100.55 | 105.5 | 60.69 | 63.6 | 39.81 | 41.9 | 3.35 | 29.73 | 0 | 2.9 |
| $S4$ | 0 | 6.17 | −0.36 | 2.05 | −0.956 | 12 751 | 177.92 | 181 | | 103.9 | | 62.6 | | 41.3 | 7.85 | 9.59 | 1 | 1 |

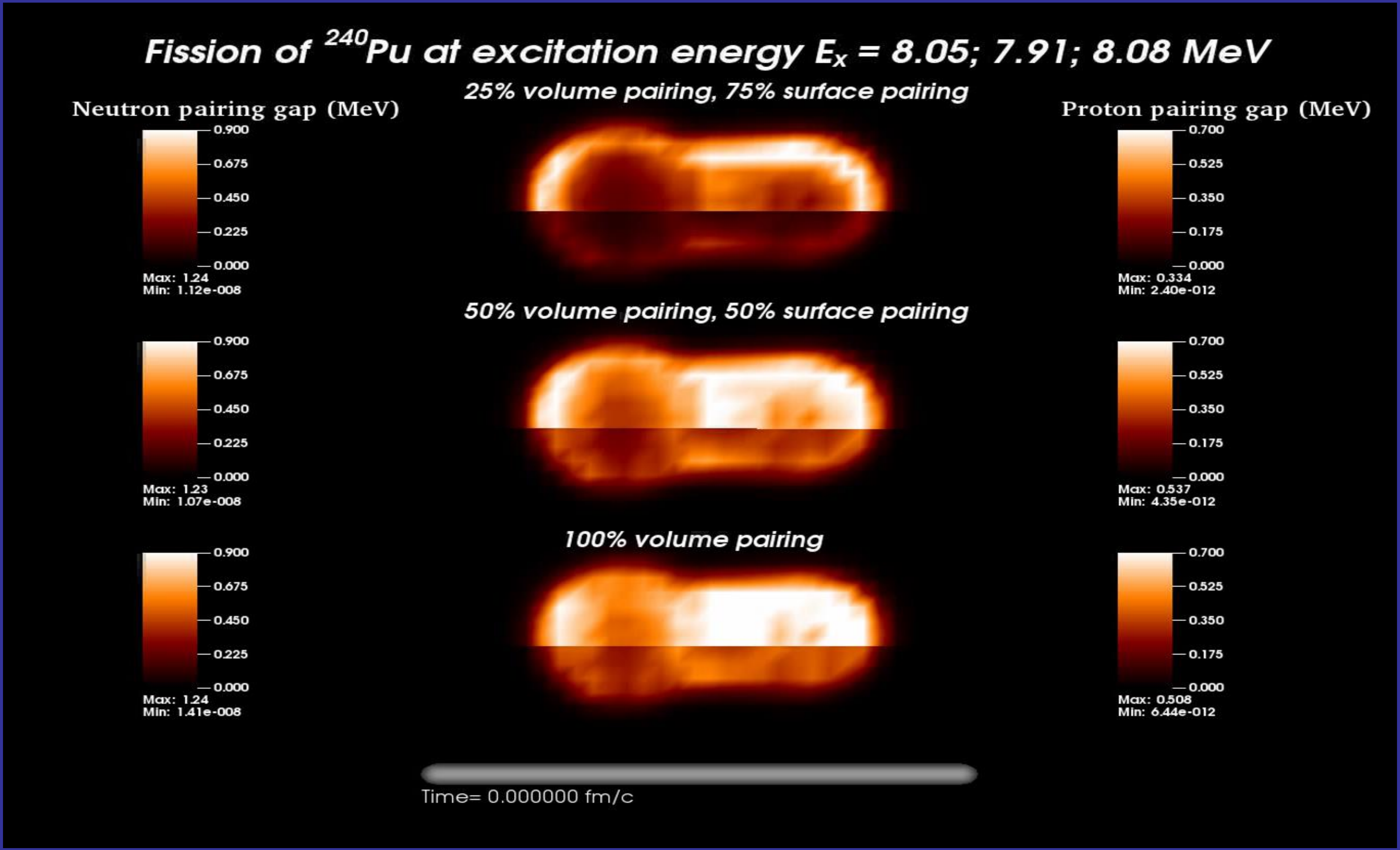


**Evolution of the average magnitude of the pairing fields.**



**Hexadecapole (dashed), octupole (dotted), and quadrupole (solid) mass moments.**

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



Fission of $^{240}$Pu at excitation energy $E_x$ = 8.05; 7.91; 8.08 MeV

25% volume pairing, 75% surface pairing

50% volume pairing, 50% surface pairing

100% volume pairing

$1\ \text{zs} = 10^{-21}\ \text{sec.} = 300\ \text{fm/c}$

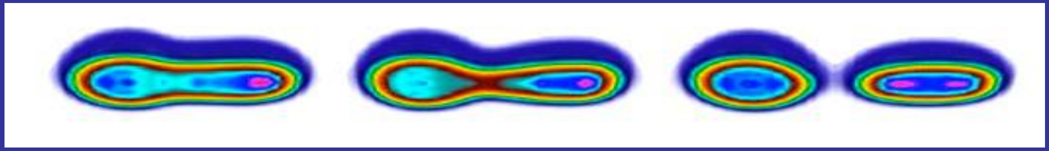
**A. Bulgac, P.Magierski, K.J. Roche, and I. Stetcu, Phys. Rev. Lett. 116, 122504 (2016)**

- TDSLDA will offer insights into nuclear processes and quantities which are either not easy or impossible to obtain in the laboratory:
  fission fragments excitation energies and angular momenta distributions,
  element formation in astrophysical environments, other nuclear reactions …

- The quality of the agreement with experimental observations is surprisingly good, especially taking into account the fact that we made no effort to reproduce any measured data.

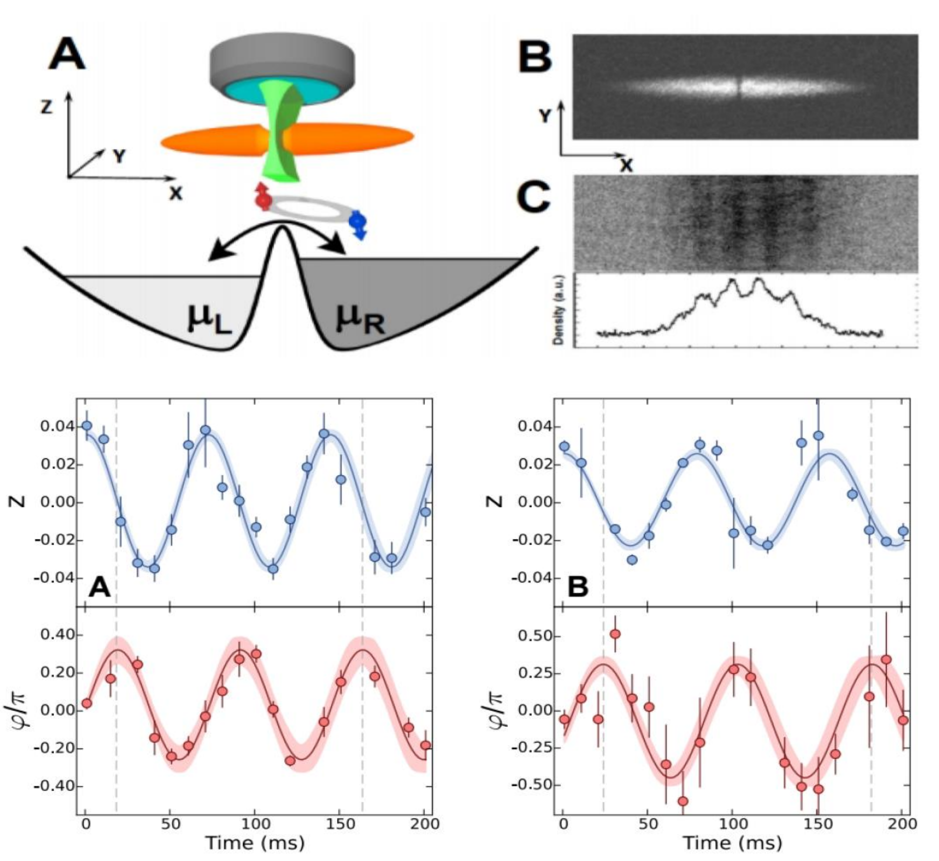
- TDSLDA predicts long saddle-to-scission time scales and the systems behaves superficially as a very viscous one, while at the same time the collective motion is not overdamped. There is no thermalization and the "temperatures" of the fission fragments are not equal.

- It is straightforward to implement the Balian and Vénéroni recipe to compute two-body observables: fission fragments mass, charge, angular momenta, excitation energy widths, …



# Ultracold atomic gases: two regimes for realization of the Josephson junction

## Weak coupling (weak link)



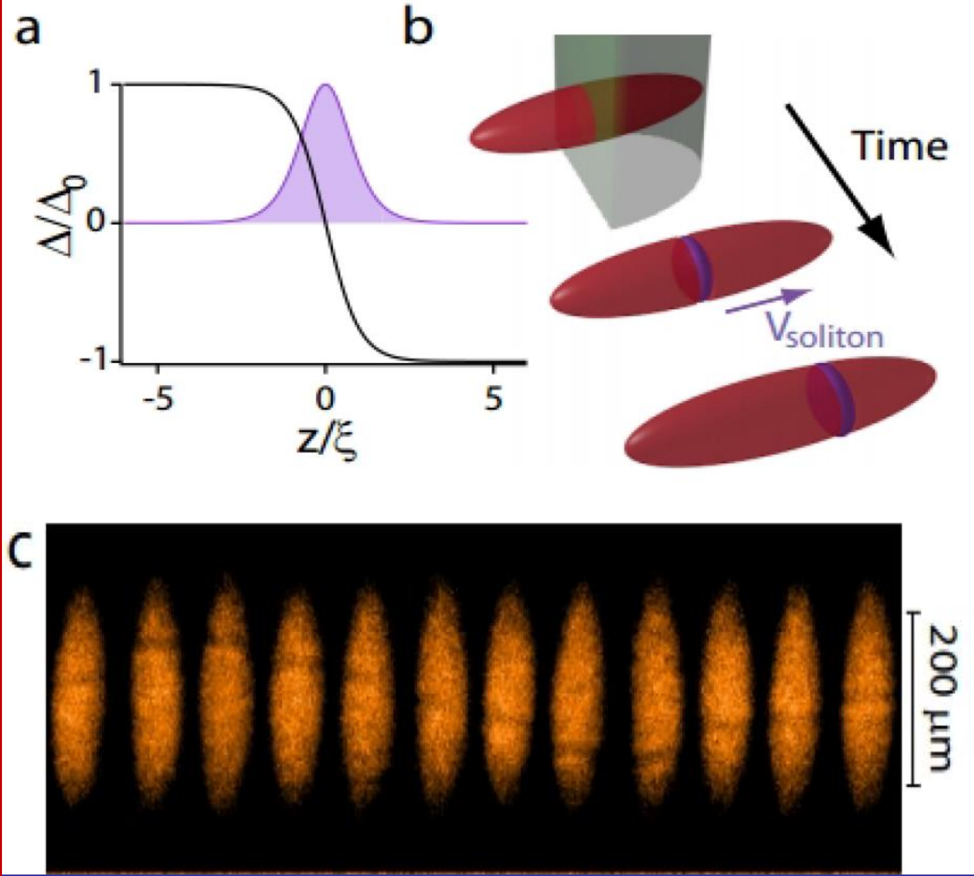
Observation of ***AC Josephson effect*** between two 6Li atomic clouds.

$$J(t) = J_c \sin\left(\Delta\varphi(t)\right)$$

$$\frac{d\left(\Delta\varphi\right)}{dt} = \frac{2eU}{\hbar}$$

G. Valtolina et al., Science 350, 1505 (2015).

## Strong coupling



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

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

Usually, nuclear applications are limited to the first regime (weak link) and focused on the detection of the Josephson current in the form of enhanced cross section for pair transfer.

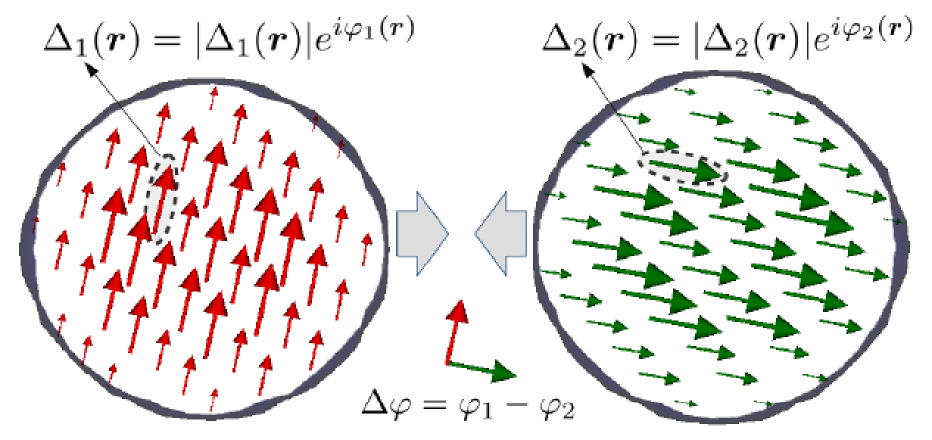
We are, however, interested **in the second regime** and nuclear collisions ABOVE the barrier.

Consequently **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.



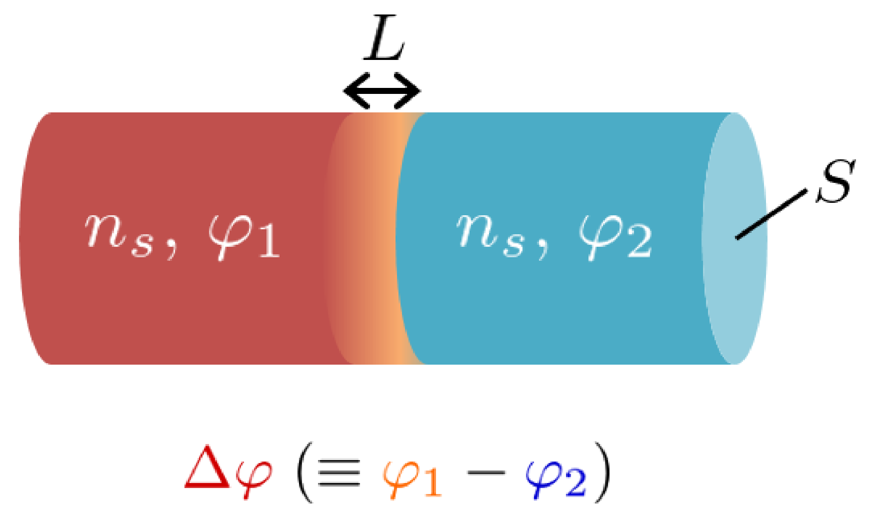
Y. Hashimoto, G. Scamps, Phys. Rev. C94, 014610(2016) – TDHFB studies of 20O+20O reaction produced negligible effect.

# 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):

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

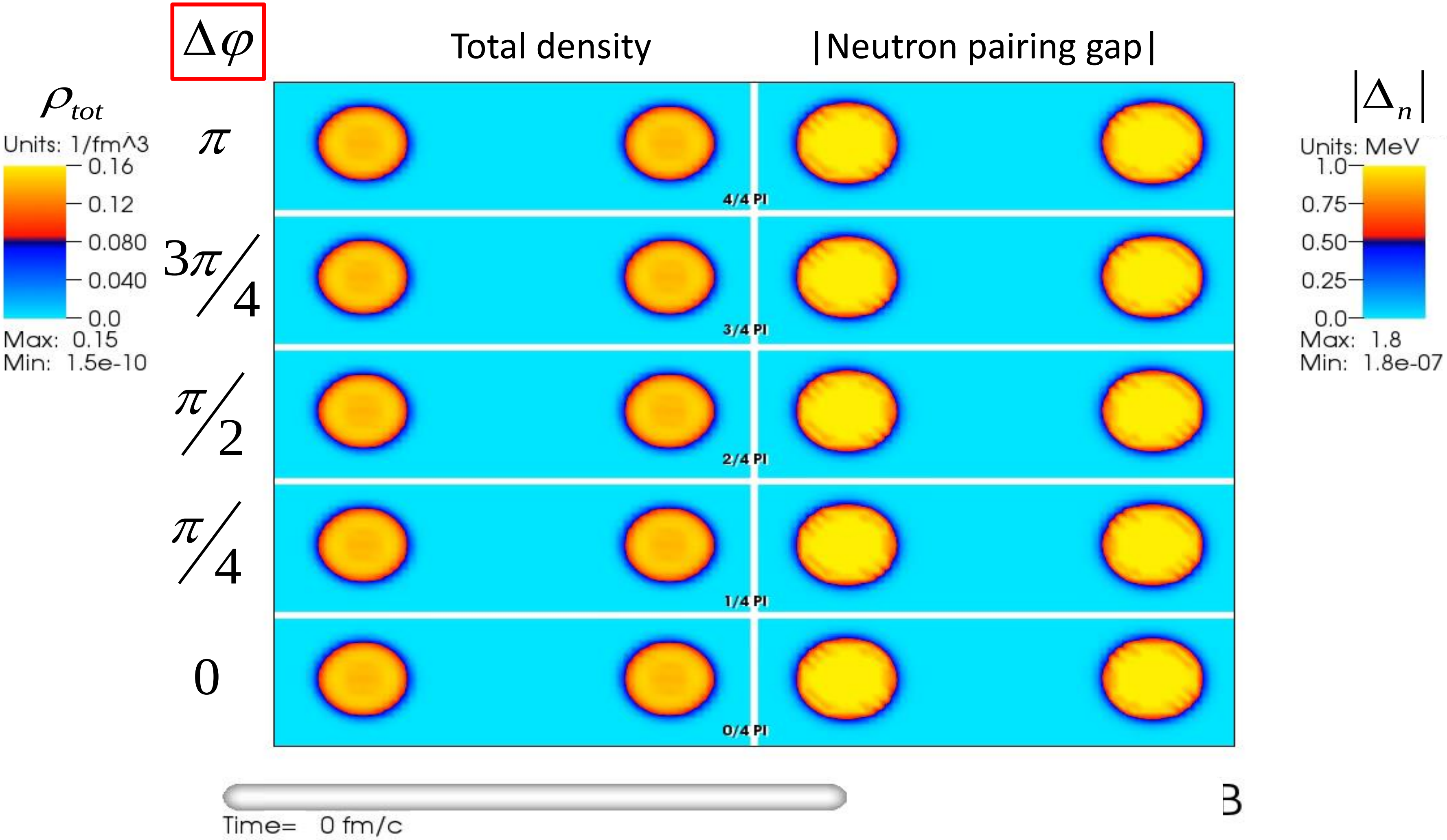
On the other hand the energy stored in the junction can be estimated from Ginzburg-Landau (G-L) approach:



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

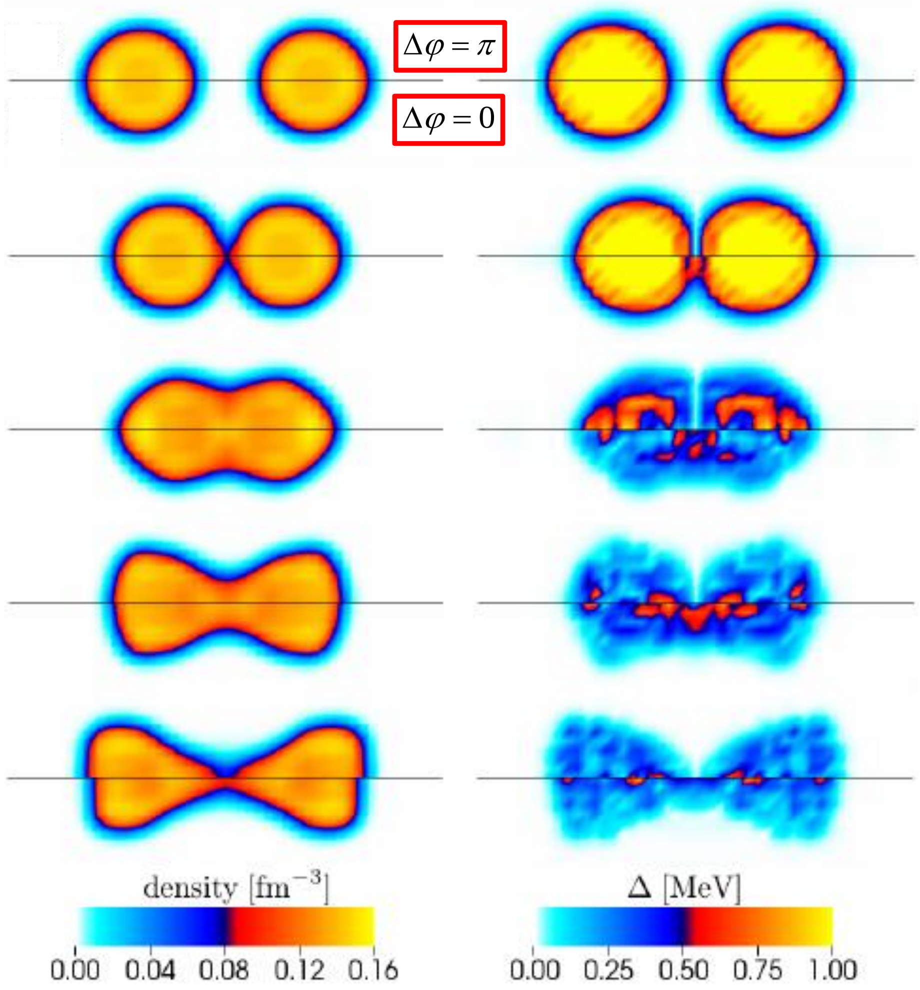
For typical values characteristic for two heavy nuclei: $E_j \approx 30 MeV$

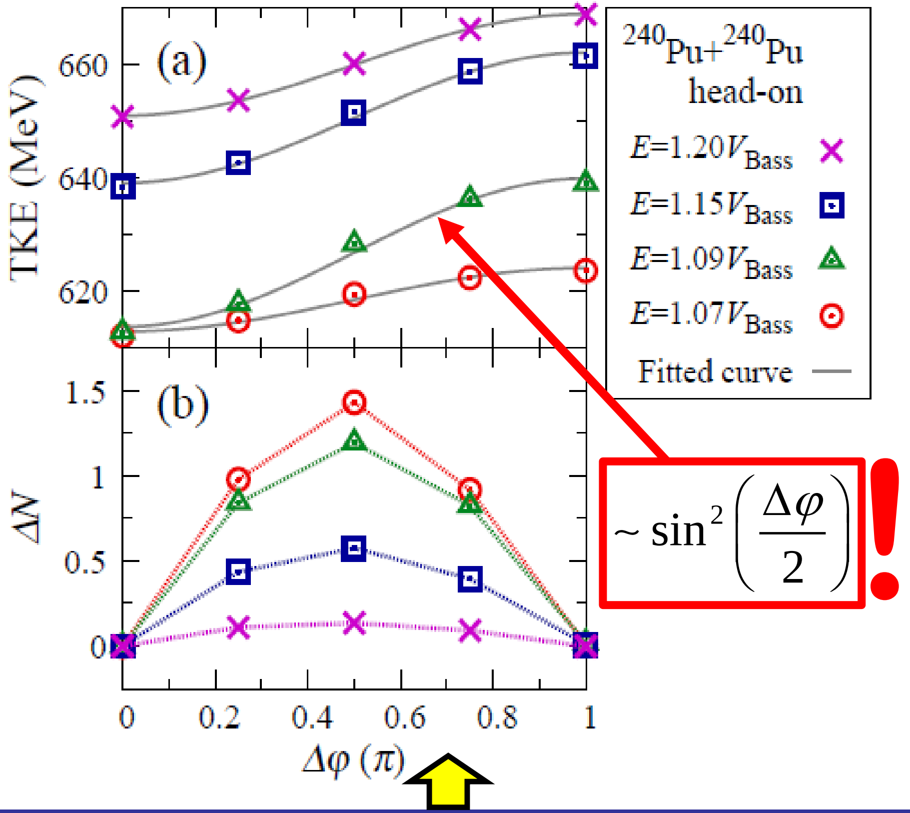
# $^{240}Pu + {}^{240}Pu$ at energy $E \simeq 1.1V_{Bass}$



P.Magierski, K.Sekizawa, G.Wlazłowski, Phys. Rev. Lett. (2017) – in press

## Total kinetic energy of the fragments (TKE)



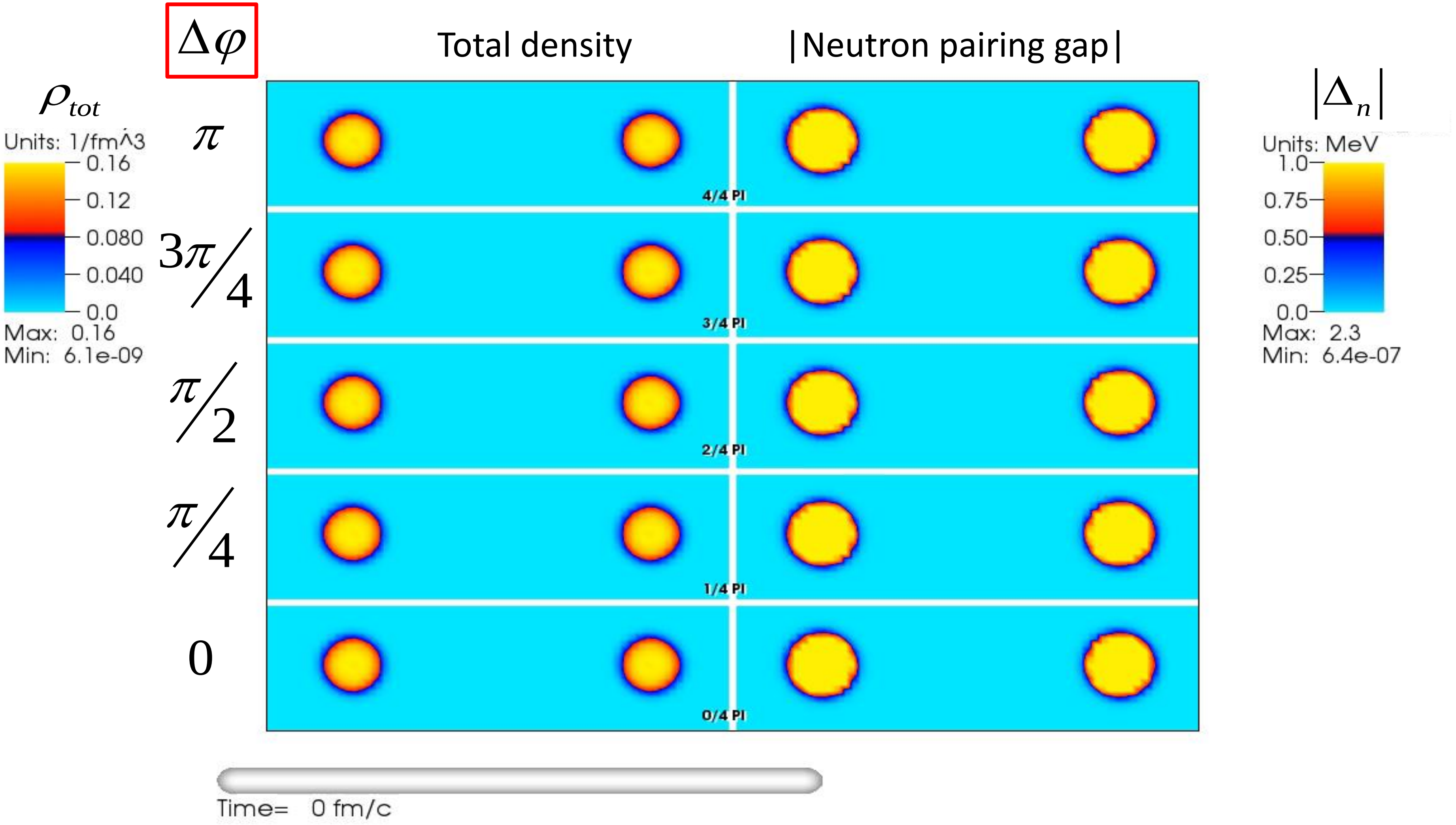


$\sim \sin^2\left(\frac{\Delta\varphi}{2}\right)$ !

Average particle transfer between fragments.

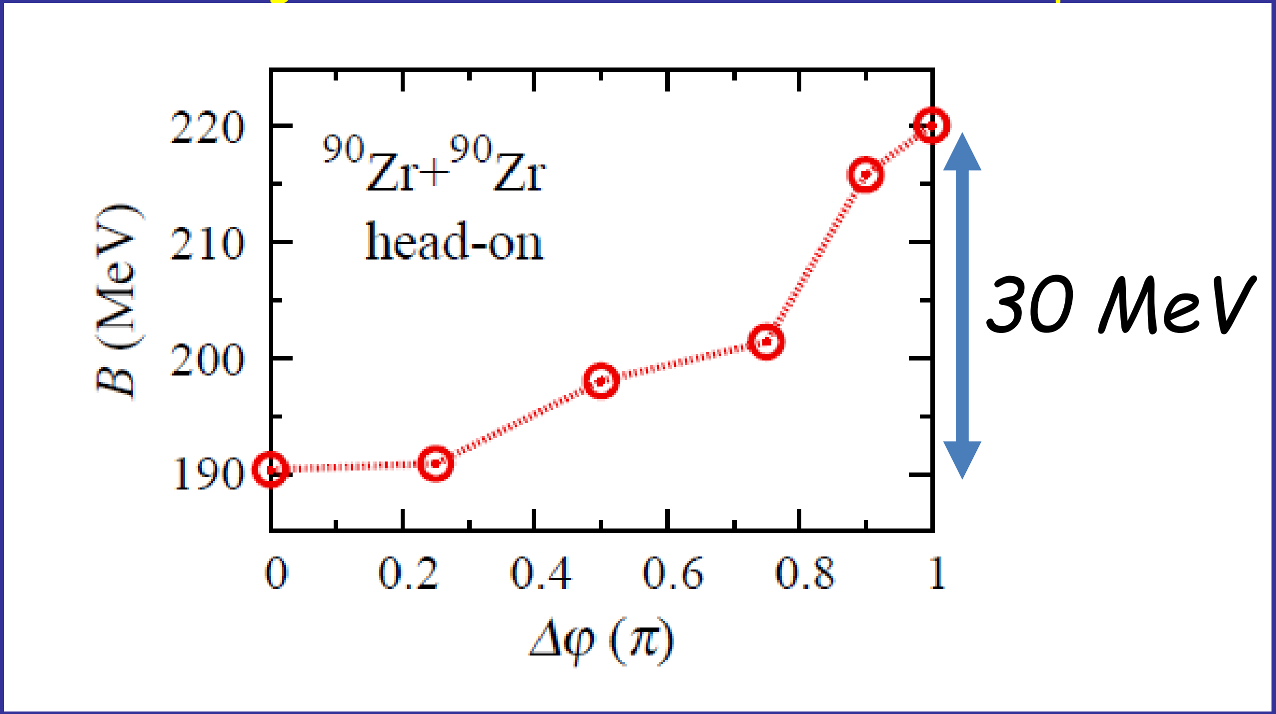
Creation of the solitonic structure between colliding nuclei prevents energy transfer to internal degrees of freedom and consequently enhances the kinetic energy of outgoing fragments.
Surprisingly, the gauge angle dependence from the G-L approach is perfectly well reproduced in the kinetic energies of outgoing fragments!

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



**Modification of the capture cross section!**

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



What is an average extra energy needed for the capture?

$$\boxed{E_{extra}=\frac{1}{\pi}\int_{0}^{\pi}\left(B(\Delta\varphi)-V_{Bass}\right)d(\Delta\varphi)\approx 10MeV}$$

How the angle dependence affects the shape of the excitation function?

$$\boxed{\frac{d}{dE}\left(E\sigma(E)\right)\propto\Delta\varphi_{tr}+\ldots}$$

P. Magierski, K. Sekizawa, G. Wlazłowski, Phys. Rev. Lett. (2017) – in press

# Summarizing

Pairing field dynamics play an important role in nuclear dynamics including both induced fission and collisions.

Clearly the aforementioned effects CANNOT be grasped by any version of simplified (and commonly used) TDHF+BCS approach.

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.

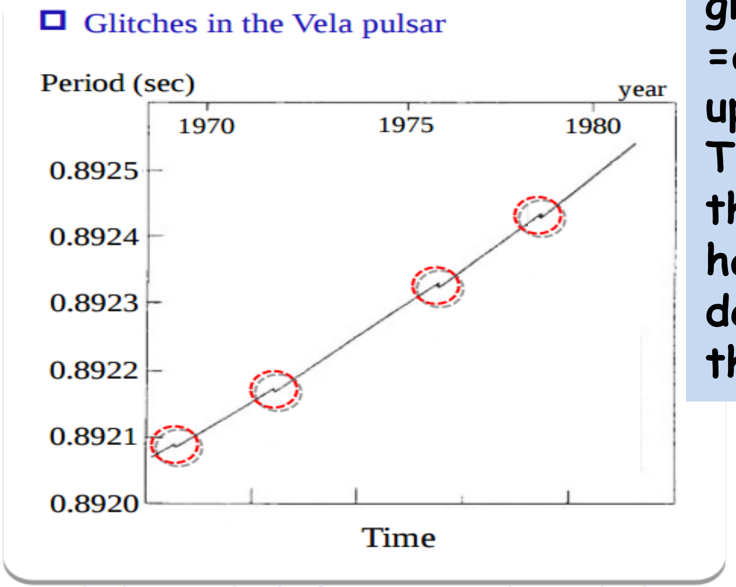
The energy stored in the created junction is subsequently released giving rise to an increased kinetic energy of the fragments and modifying their trajectories. The effect is found to be of the order of 30MeV for heavy nuclei and occur for energies up to 20-30% of the barrier height.

Consequently the effective barrier for the capture of medium nuclei is enhanced by about 10MeV.

Josephson current is weak and DOES NOT contribute noticeably to collision dynamics (consistent with other studies).

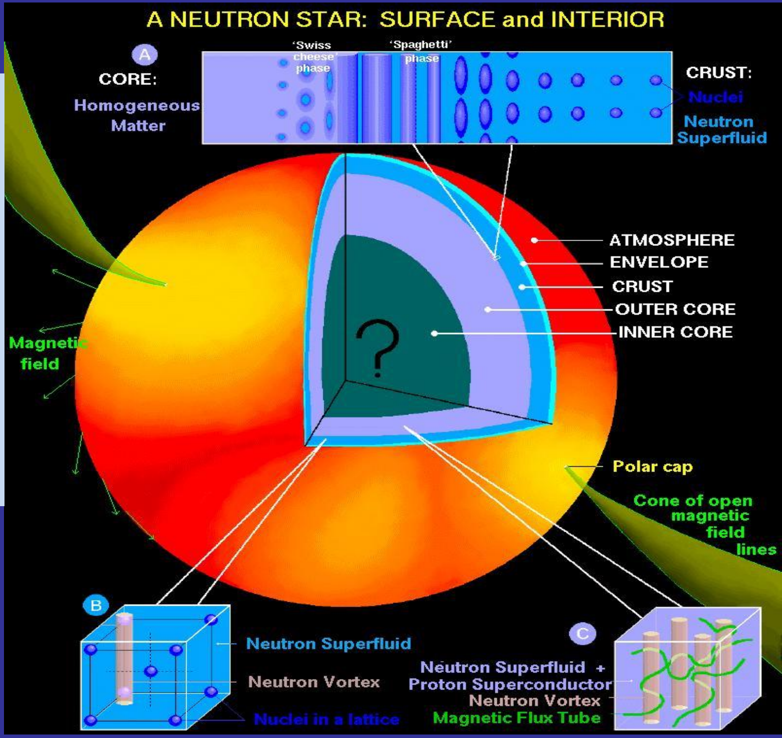
# Modelling neutron star interior

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.

Large scale dynamical model of neutron star interior (in particular neutron star crust), based on microscopic input from nuclear theory, is required.
In particular: vortex-impurity interaction, deformation modes of nuclear lattice, effective masses of nuclear impurities and couplings between lattice vibrations and neutron superfluid medium, need to be determined.

# Vortex – impurity interaction

## Static approach

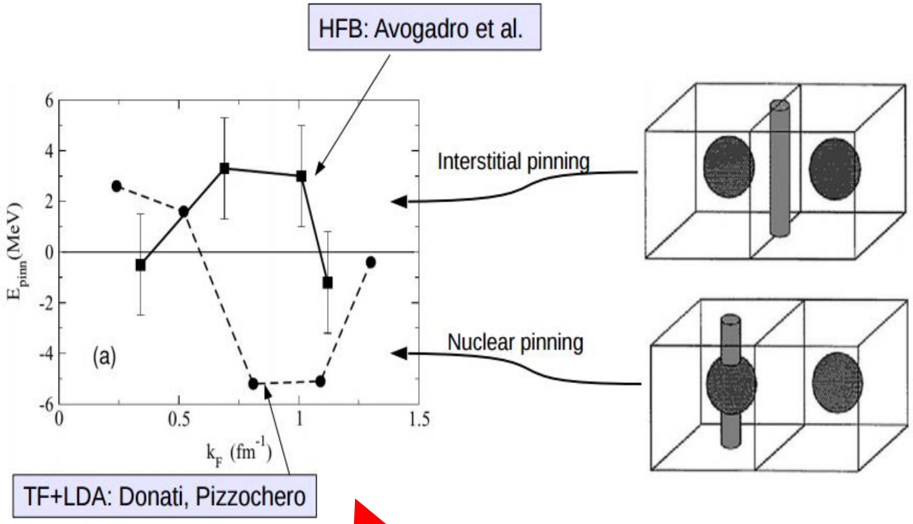
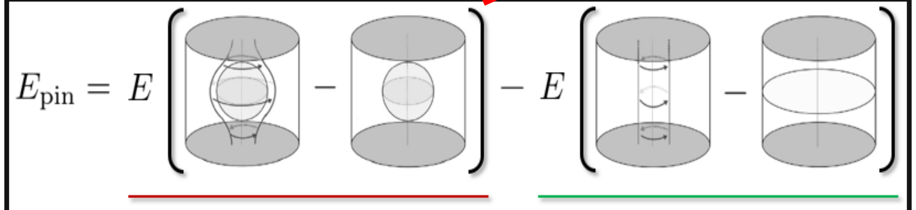


Fig. from: P. Avogadro et al.,
Phys. Rev. C 75, 012805(R) (2007)

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



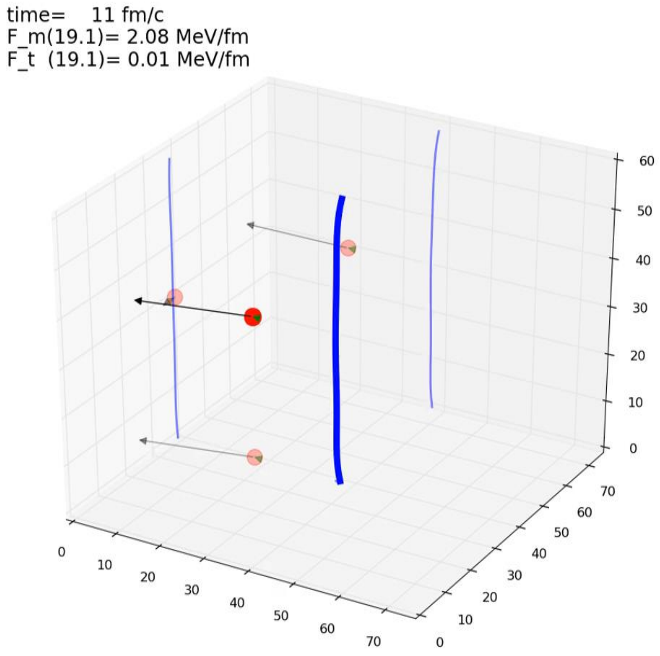
Energy to create a vortex line on a nuclear impurity

Energy to create a vortex line in a uniform matter

**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)

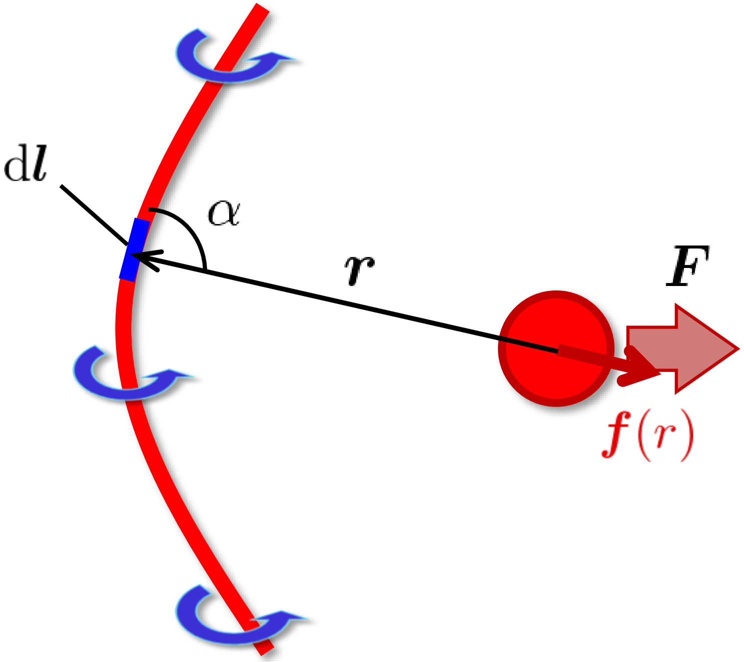
# *Force per unit length*

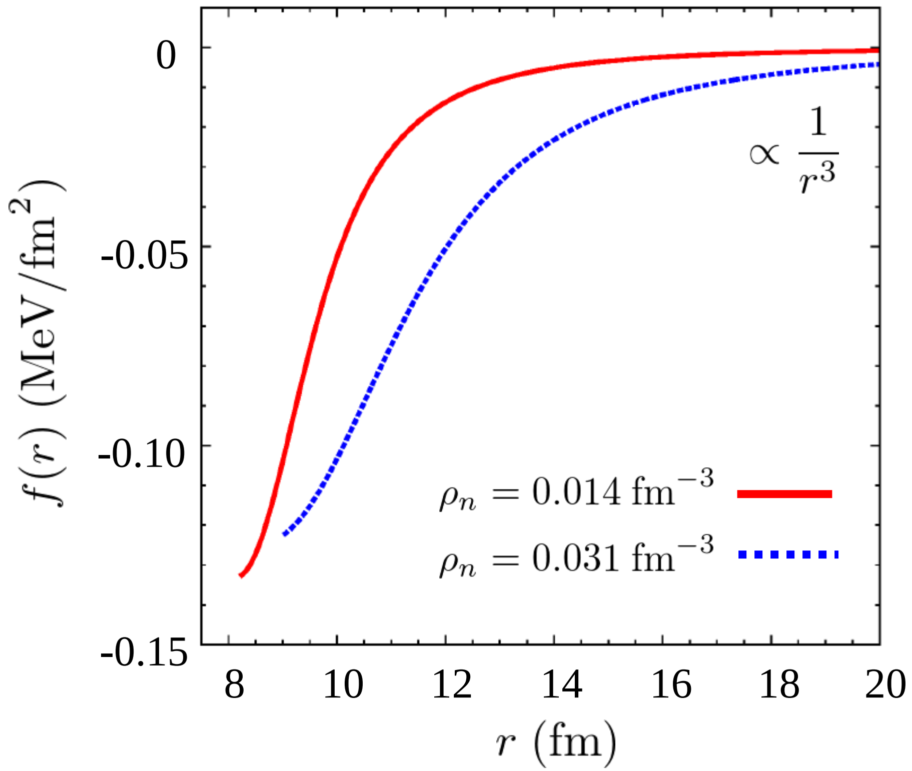
We can predict the force for any vortex-nucleus configuration

- Force per unit length

$$\boldsymbol{F} = \int_L f(r)\sin\alpha\, \boldsymbol{e}_r\, \mathrm{d}l \qquad f(r) = \frac{\sum_{k=0}^{n} a_k r^k}{1+\sum_{k=1}^{n+3} b_k r^k}$$

Padé approximant
($n$=2 was used)





# Summarizing

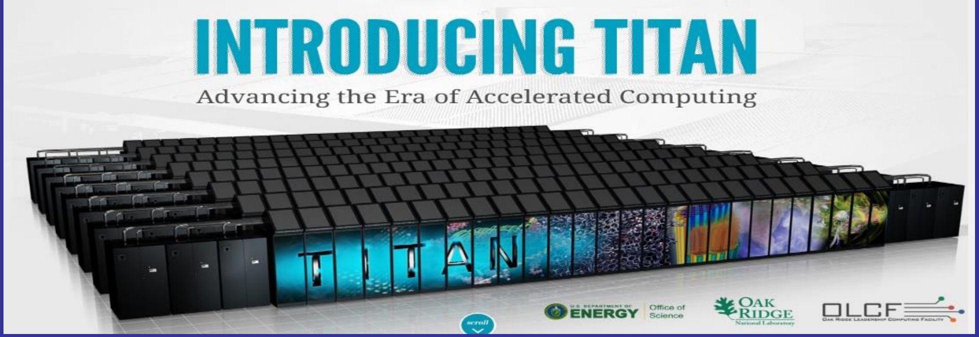
- TDDFT extended to superfluid systems and based on the local densities offers a flexible tool to study quantum superfluids far from equilibrium.

  In nuclear systems TDSLDA 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:

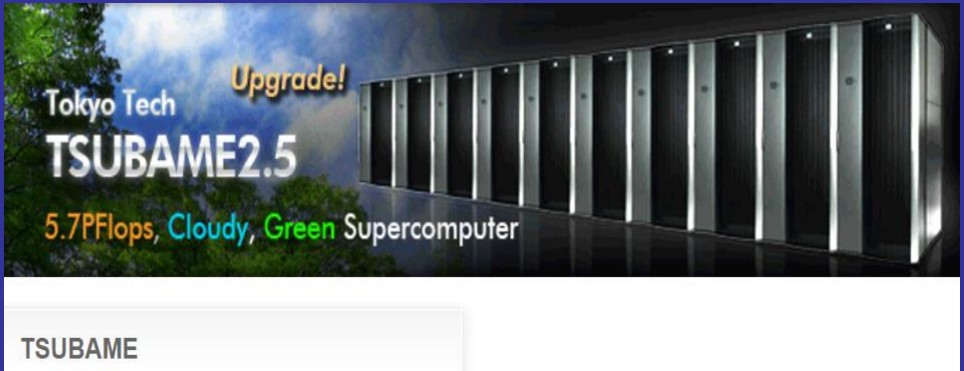
- Ultracold atoms: investigation of quantum turbulence in Fermi systems; topological excitations in spin-polarized atomic gases in the presence of LOFF phase.
- Neutron star: Provide a link between large scale models of neutron stars and microscopic studies; towards the first simulation of the glitch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

# Selected supercomputers (CPU+GPU) currently in use:



**Titan: 27 PFlops**
**(ORNL Oak Ridge)**

**HA-PACS: 0.802 PFlops**
**(University of Tsukuba)**



**Tsubame: 5.7 PFlops**
**(Tokyo Institute of Technology)**

**Piz Daint: 7.787 PFlops**
**(Swiss National Supercomputing Centre)**