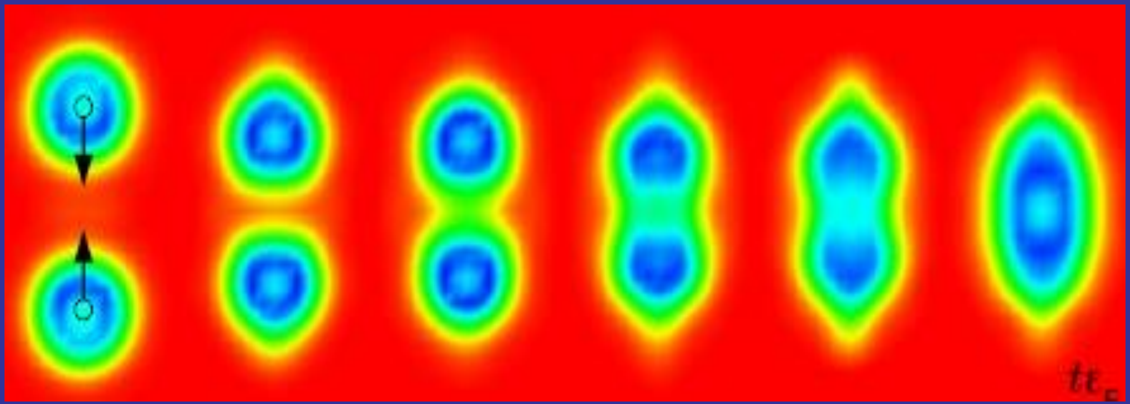
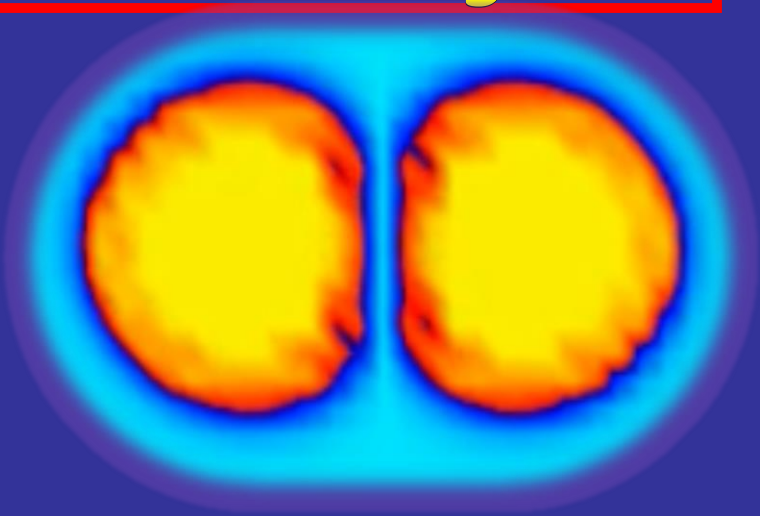
New features of superfluidity far from equilibrium: nuclear reactions, dynamics of ferrons and quantum vortices in ultracold gases





Piotr Magierski
Warsaw University of Technology (WUT)

Collaborators:

Matthew Barton (WUT)
Aurel Bulgac (UoW)
Shi Jin (UoW)
Konrad Kobuszewski (WUT – Ph.D. student)
Paweł Kuliński (WUT – student)
Kenneth Roche (PNNL)
Kazuyuki Sekizawa (WUT -> Niigata U.)
Buğra Tüzemen (WUT - Ph.D. student)
Gabriel Wlazłowski (WUT)

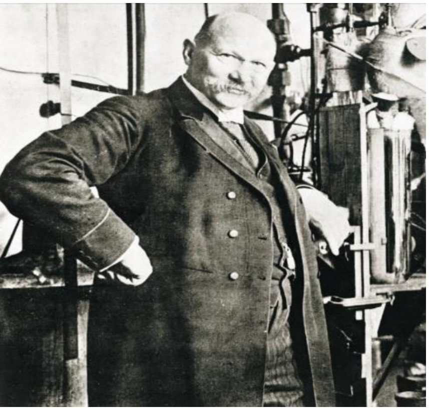
SUPERCOMPUTING FRONTIERS EUROPE 2020

icm

UNIWERSYTET WARSZAWSKI

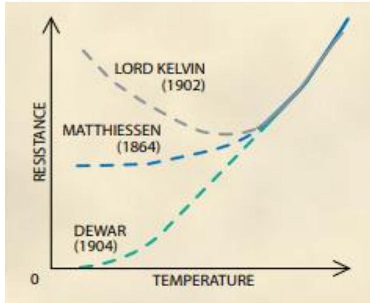
Discovery of superconductivity

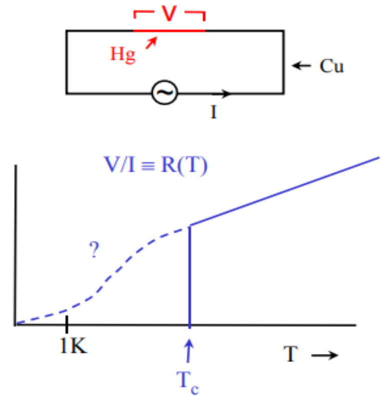
1911 – Heike Kamerlingh Onnes



Heike Kamerlingh Onnes (Leiden Institute of Physics)

Theretical predictions before 1911





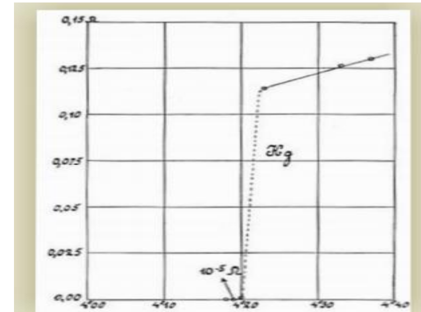
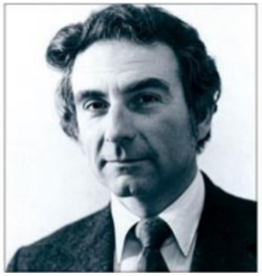


Figure 4. Historic plot of resistance (ohms) versus temperature (kelvin) for mercury from the 26 October 1911 experiment shows the superconducting transition at 4.20 K. Within 0.01 K, the resistance jumps from unmeasurably small (less than $10^{-6}\ \Omega$) to 0.1 Ω. (From ref. 9.)

BCS THEORY (1957)

J. Bardeen



L. Cooper

J.R. Schrieffer

Superconductivity critical temperatures for various physical systems:

- ✓ **Dilute atomic Fermi gases:** $T_c \approx 10^{-12} - 10^{-9}$ eV
- ✓ **Liquid ^{3}He:** $T_c \approx 10^{-7}$ eV
- ✓ **Metals, composite materials:** $T_c \approx 10^{-3} - 10^{-2}$ eV
- ✓ **Atomic nuclei and neutron stars:** $T_c \approx 10^{5} - 10^{6}$ eV
- ▪ **Quark superconductivity :** $T_c \approx 10^{7} - 10^{8}$ eV

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.

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.

Density Functional Theory (DFT):

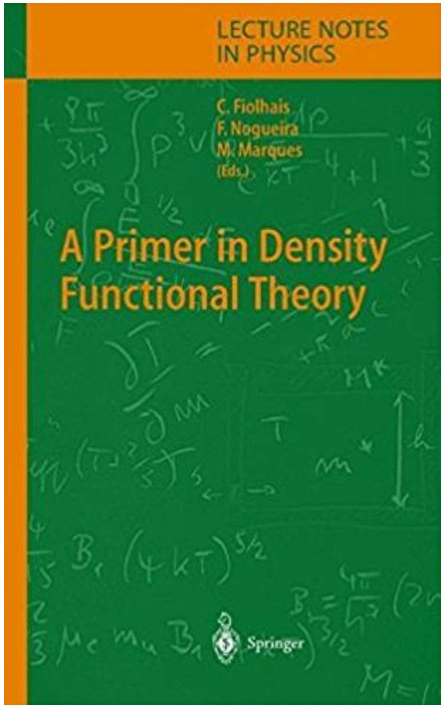
Quantitatively accurate

Unified description of static and dynamic properties of **large Fermi systems**

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

We know what Eq. should be solved...
The only problem:
How to do it in practice?

Input:
energy density functional



Methods:

- QMC (static)
- *DFT* (static and *dynamic*)
- ...

feed

Solving time-dependent problem (TDDFT) for superfluids...

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

$$h \sim f_1(n,\nu,\ldots)\nabla^2 + \boldsymbol{f}_2(n,\nu,\ldots)\cdot\nabla + f_3(n,\nu,\ldots)$$

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

We explicitly track fermionic degrees of freedom!

where *h* and Δ depends on "densities":

$$n_\sigma(\boldsymbol{r},t) = \sum_{E_n<E_c} |v_{n,\sigma}(\boldsymbol{r},t)|^2, \qquad \tau_\sigma(\boldsymbol{r},t) = \sum_{E_n<E_c} |\nabla v_{n,\sigma}(\boldsymbol{r},t)|^2,$$

$$\nu(\boldsymbol{r},t) = \sum_{E_n<E_c} u_{n,\uparrow}(\boldsymbol{r},t)v^*_{n,\downarrow}(\boldsymbol{r},t), \qquad \boldsymbol{j}_\sigma(\boldsymbol{r},t) = \sum_{E_n<E_c} \mathrm{Im}[v^*_{n,\sigma}(\boldsymbol{r},t)\nabla v_{n,\sigma}(\boldsymbol{r},t)],$$

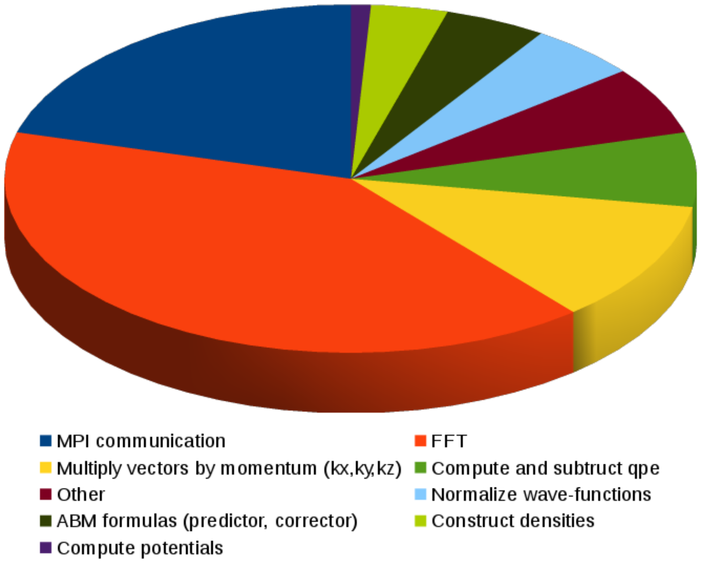
huge number of nonlinear coupled 3D Partial Differential Equations
(in practice n=1,2,…, 10^5 - 10^6)

Present computing capabilities:

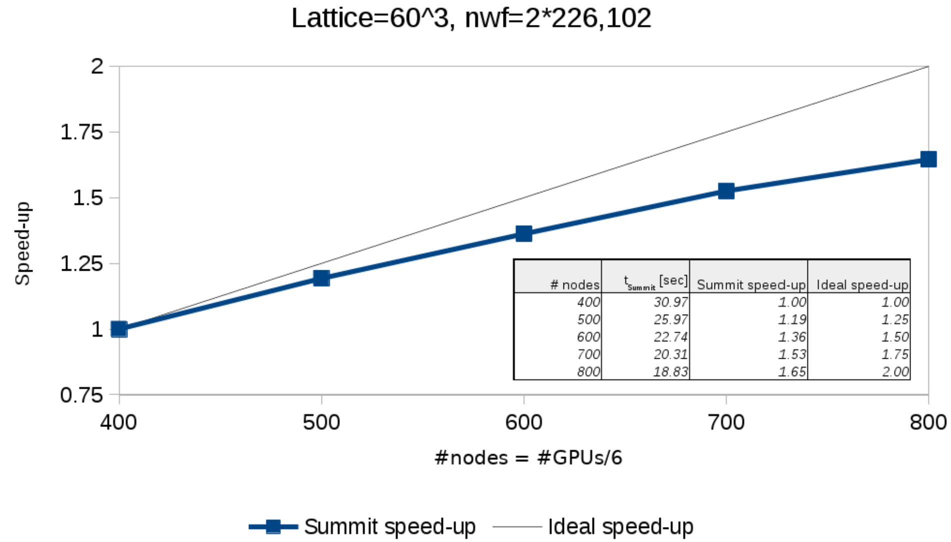
- full 3D (unconstrained) superfluid dynamics
- spatial mesh up to 100^3
- max. number of particles of the order of 10^4
- up to 10^6 time steps

(for cold atomic systems – time scale: a few ms
for nuclei – time scale: 100 zs)

Performance on supercomputers (Piz Daint & Summit)



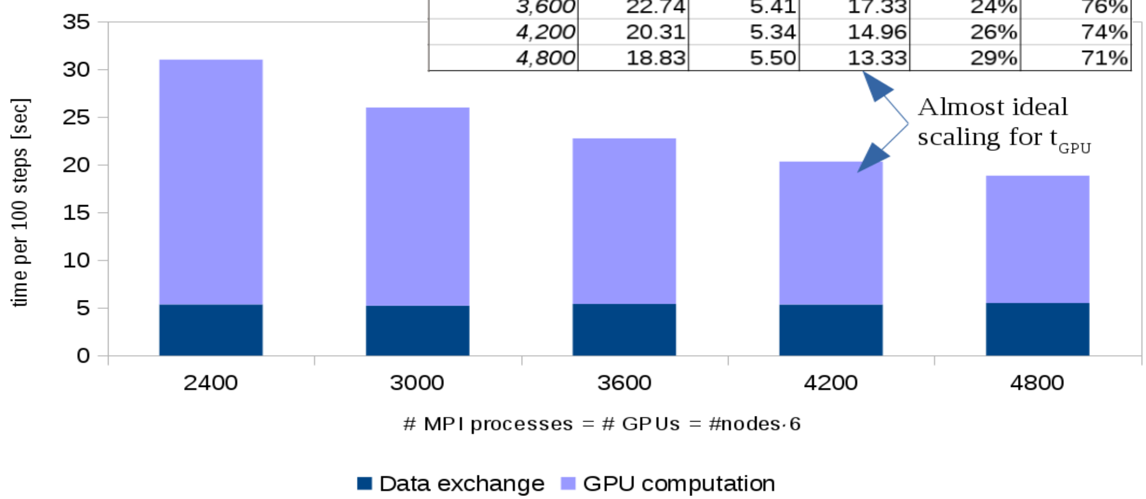
Profiling of TDDFT code executed on 512GPUs (Piz Daint)



# nodes	t_{Summit} [sec]	Summit speed-up	Ideal speed-up
400	30.97	1.00	1.00
500	25.97	1.19	1.25
600	22.74	1.36	1.50
700	20.31	1.53	1.75
800	18.83	1.65	2.00

Strong scaling of TDDFT code (Summit)

# GPUs	t_{total} [sec]	t_{comm} [sec]	t_{GPU} [sec]	t_{comm} [%]	t_{GPU} [%]
2,400	30.97	5.36	25.61	17%	83%
3,000	25.97	5.22	20.75	20%	80%
3,600	22.74	5.41	17.33	24%	76%
4,200	20.31	5.34	14.96	26%	74%
4,800	18.83	5.50	13.33	29%	71%



Comparison of GPU computing time and MPI exchange time (Summit)

Example1: Nuclear collisions

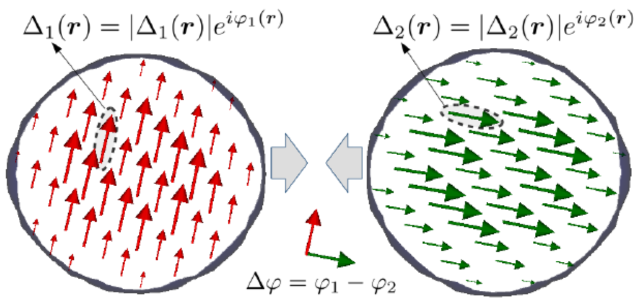
Collisions of superfluid nuclei having <u>different phases</u> of the <u>pairing fields</u>

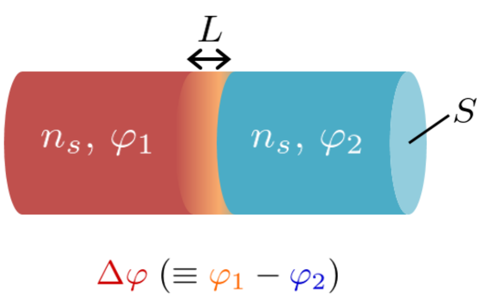
<u>The main questions are:</u>

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

-what observable effect it may have on heavy ion reaction:
kinetic energy distribution 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.



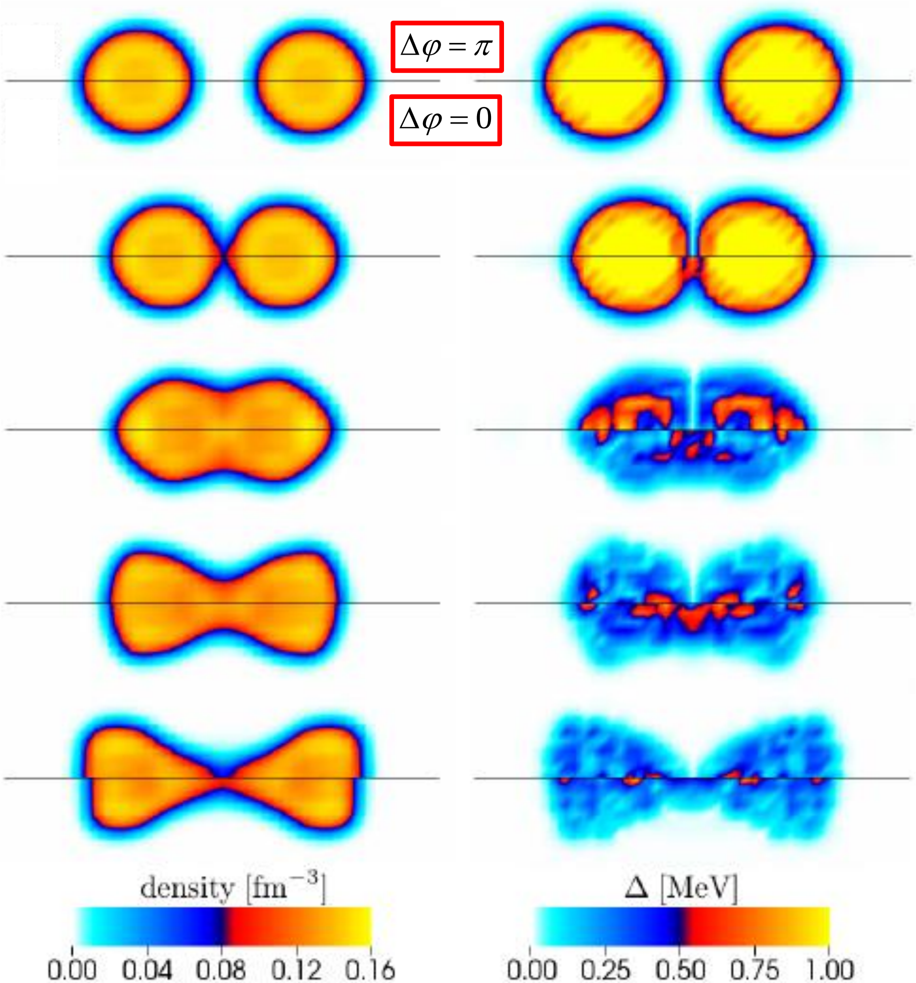


From Ginzburg-Landau (G-L) approach:

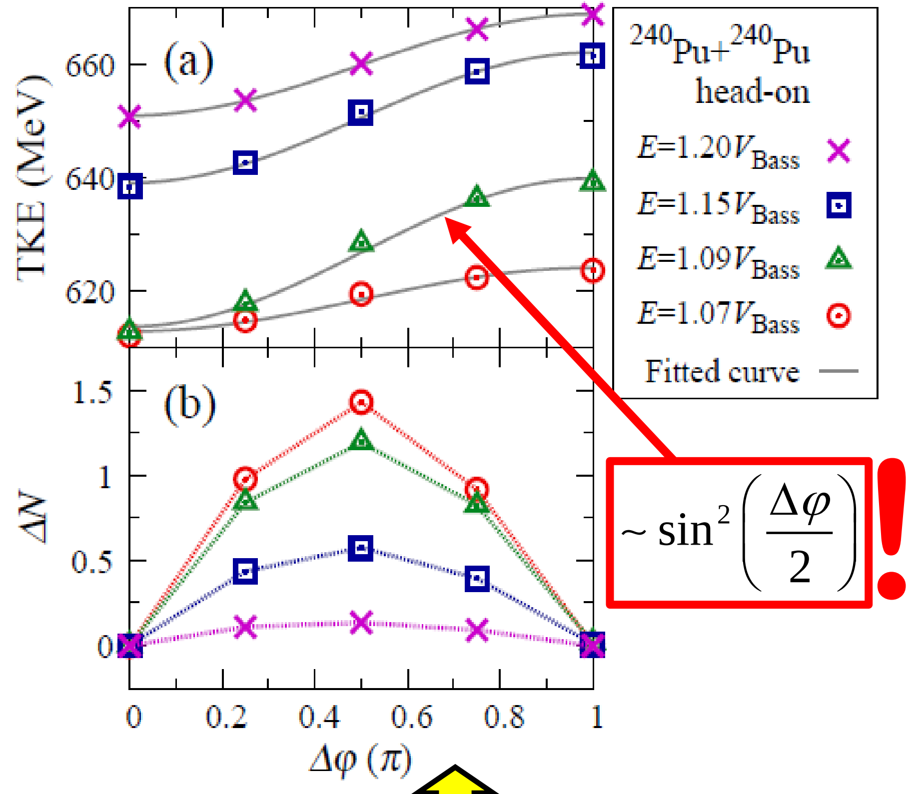
$$E_j = \frac{S}{L}\frac{\hbar^2}{2m} n_s \sin^2 \frac{\Delta\varphi}{2}$$

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

Total kinetic energy of the fragments (TKE)



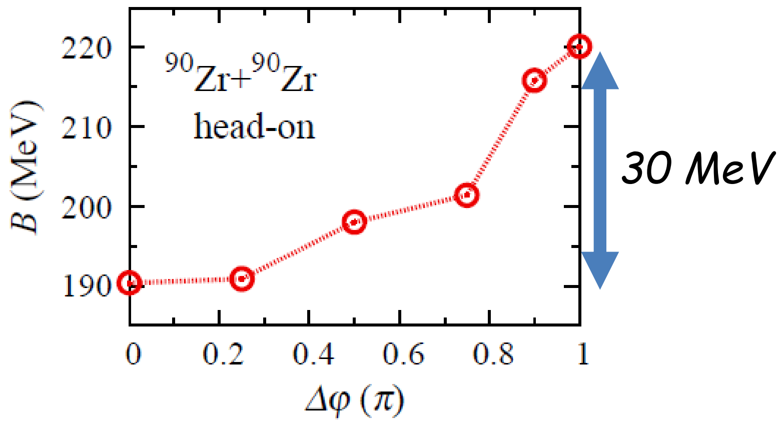
$^{240}Pu + ^{240}Pu$ at energy $E \simeq V_{Bass}$



Average particle transfer between fragments.

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

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



What is an average extra energy needed for the capture?

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

The effect is found (within TDDFT) to be of the order of <u>30MeV</u> for medium nuclei and occur for <u>energies up to 20-30% of the barrier height</u>.

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

G. Scamps, Phys. Rev. C 97, 044611 (2018): barrier fluctuations extracted from experimental data indicate that the effect exists although is weaker than predicted by TDDFT

Recent simulations including spin-orbit term: M.C. Barton, et al. Acta Phys. Pol. B (in press)

Example 2: Spin-imbalanced Fermi superfluid

Larkin-Ovchinnikov (LO): $\Delta(r) \sim cos(\vec{q} \cdot \vec{r})$

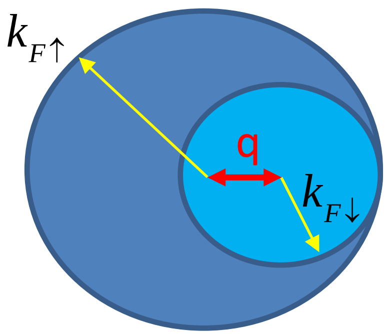
Fulde-Ferrell (FF): $\Delta(r) \sim \exp(i\vec{q} \cdot \vec{r})$

Predictions for exotic phases
in spin-imbalnced Fermi superfluid

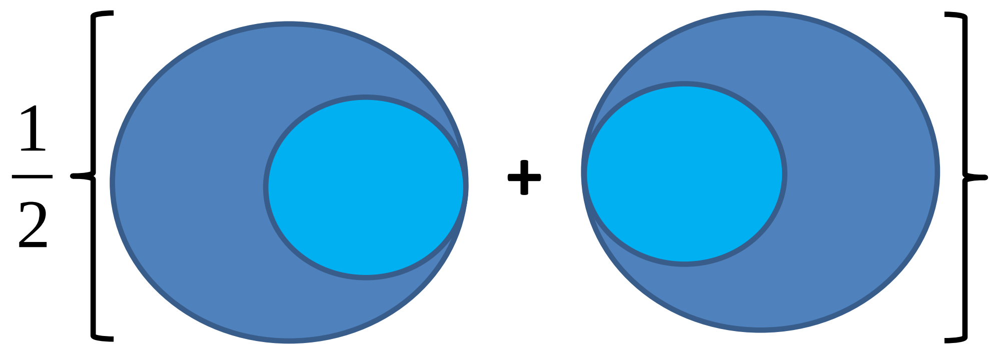
A.I. Larkin and Y. N. Ovchinnikov, Sov. Phys. JETP 20, 762 (1965)
P. Fulde and R. A. Ferrell, Phys. Rev. 135, A550 (1964)

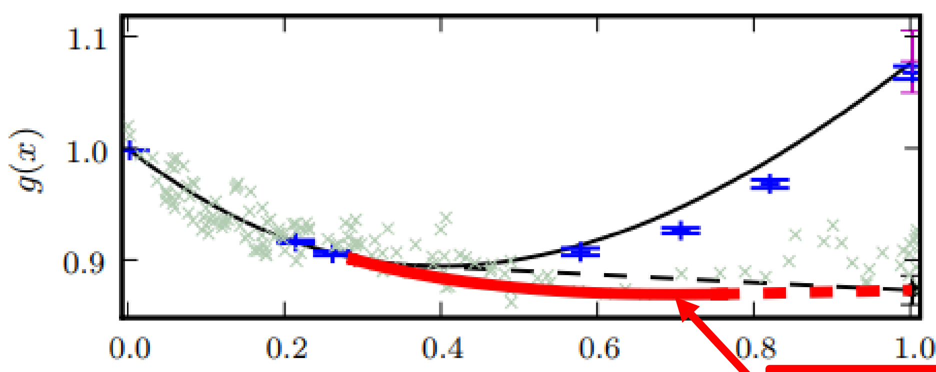
Spatial modulation of the pairing field costs energy proportional to q^2 but may be compensated by an increased pairing energy due to the mutual shift of Fermi spheres:

FF:



LO:





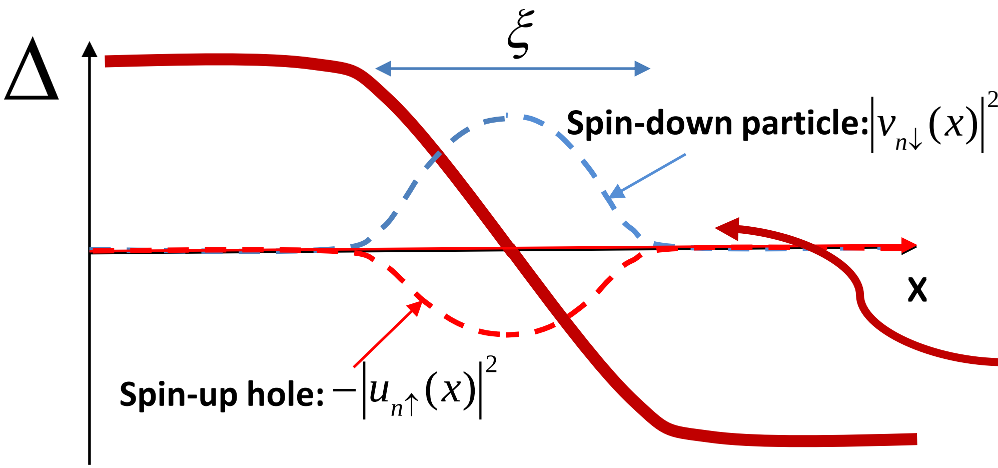
$E \sim [n_a g(x)]^{5/3}$

Bulgac & Forbes have shown, within DFT, that Larkin-Ovchinnikov (LO) phase may exist in the unitary Fermi gas (UFG) (realized experimentally in ultracold atomic clouds)

LO configuration – supersolid state

A. Bulgac, M.M.Forbes, Phys. Rev. Lett. 101,215301 (2008)
See also review of mean-field theories : Radzihovsky,Sheehy, Rep.Prog. Phys.73,076501(2010)

Andreev states and stability of pairing nodal points



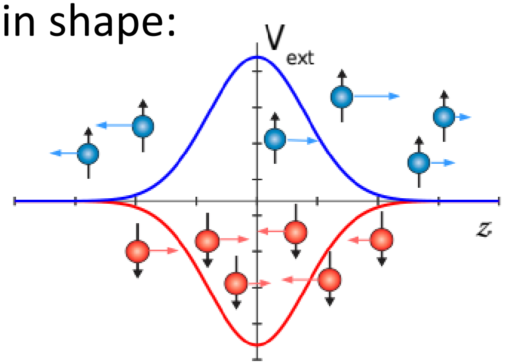
Due to quasiparticle scattering the localized Andreev states appear at the nodal point. These states induce local spin-polarization

BdG in the Andreev approx. ($\Delta \ll k_F^2$)

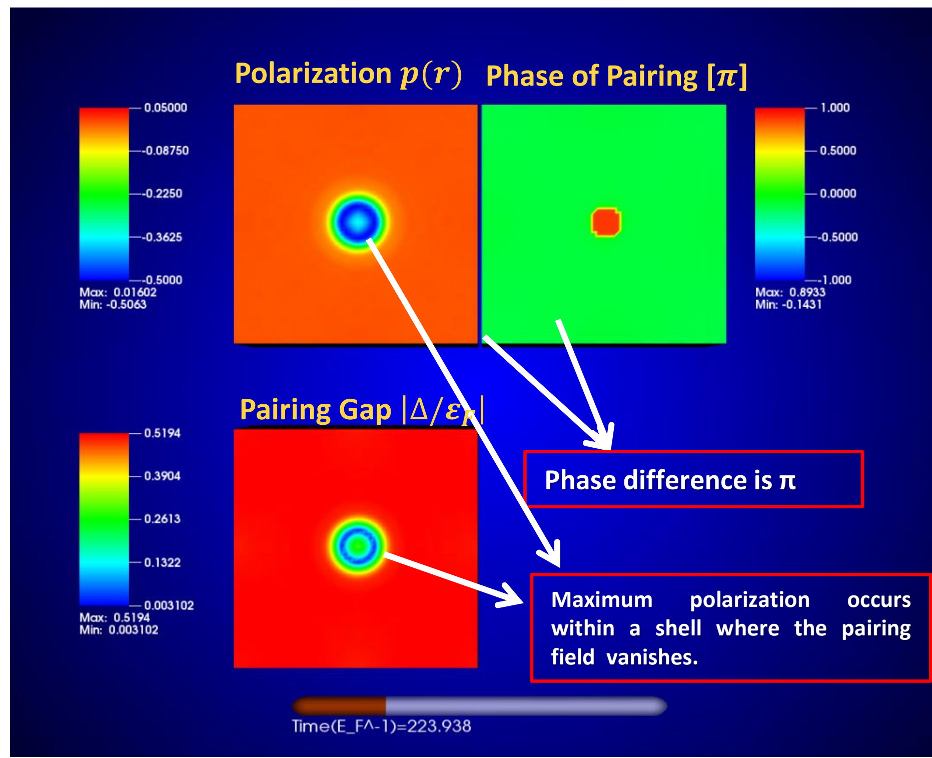
$$\begin{bmatrix} -2ik_F \frac{d}{dx} & \Delta(x) \\ \Delta^*(x) & 2ik_F \frac{d}{dx} \end{bmatrix} \begin{bmatrix} u_{n\uparrow}(x) \\ v_{n\downarrow}(x) \end{bmatrix} = E_n \begin{bmatrix} u_{n\uparrow}(x) \\ v_{n\downarrow}(x) \end{bmatrix}$$

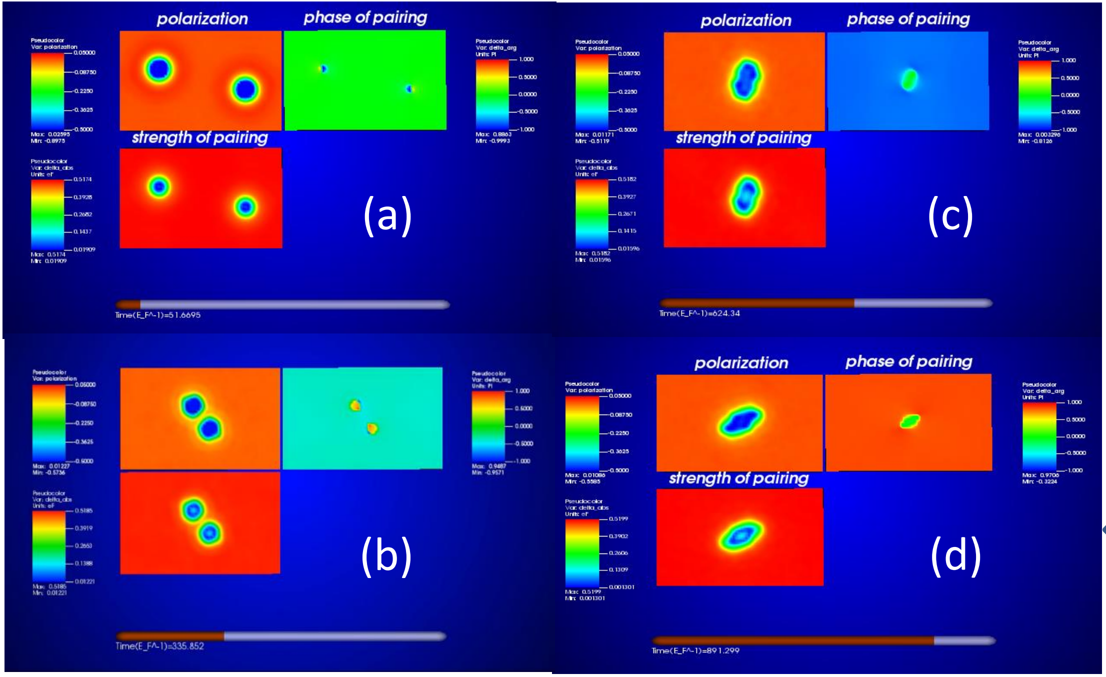
Engineering the structure of nodal surfaces

Apply the spin-selective potential of a certain shape:



Wait until the proximity effects of the pairing field generate the nodal structure and remove the potential.





Moving impurity:

From Larkin-Ovchinnikov towards Fulde-Ferrell limit:

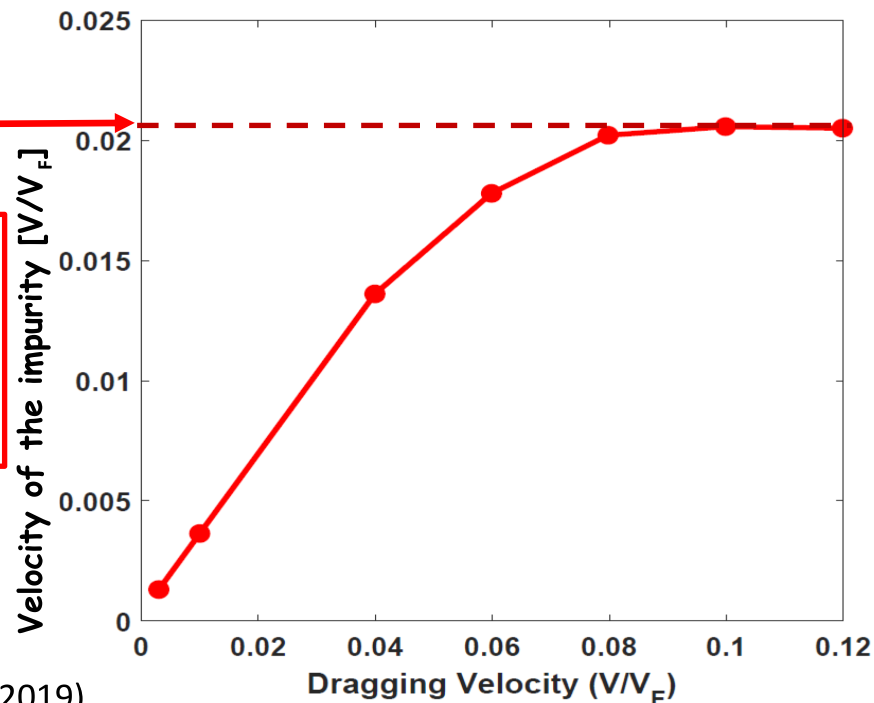
$$\Delta(r) : cos(qr) \Rightarrow \exp(iqr)$$

Surprisingly, the nodal structure remains stable even during collisions

The velocities of impurites are about 30% of the velocity of sound.

Limiting velocity with respect to superfluid background

Note that the Fulde-Ferrell limit defines the **critical velocity** which is associated with the maximum spin current that can flow through the impurity $(\sim q \sim |k_{F\uparrow} - k_{F\downarrow}|)$.

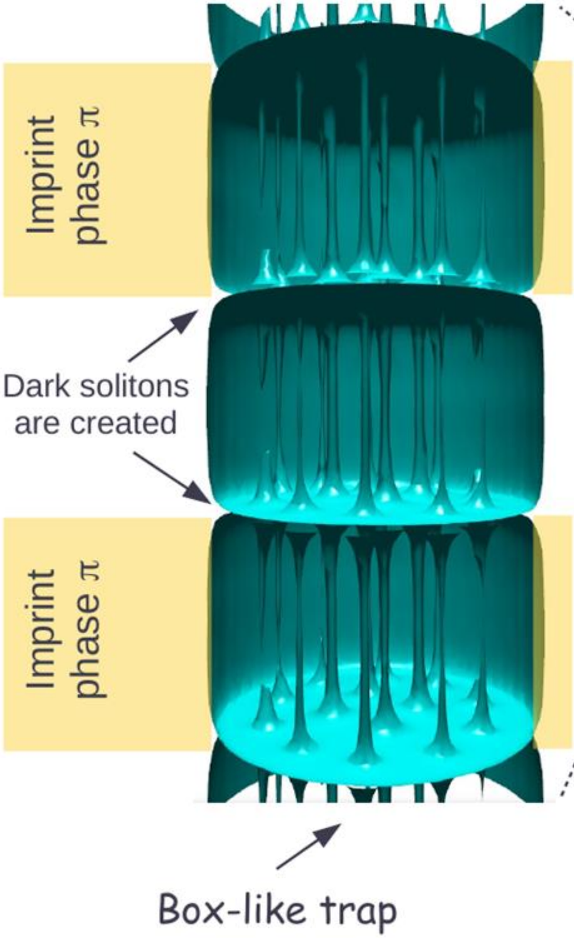


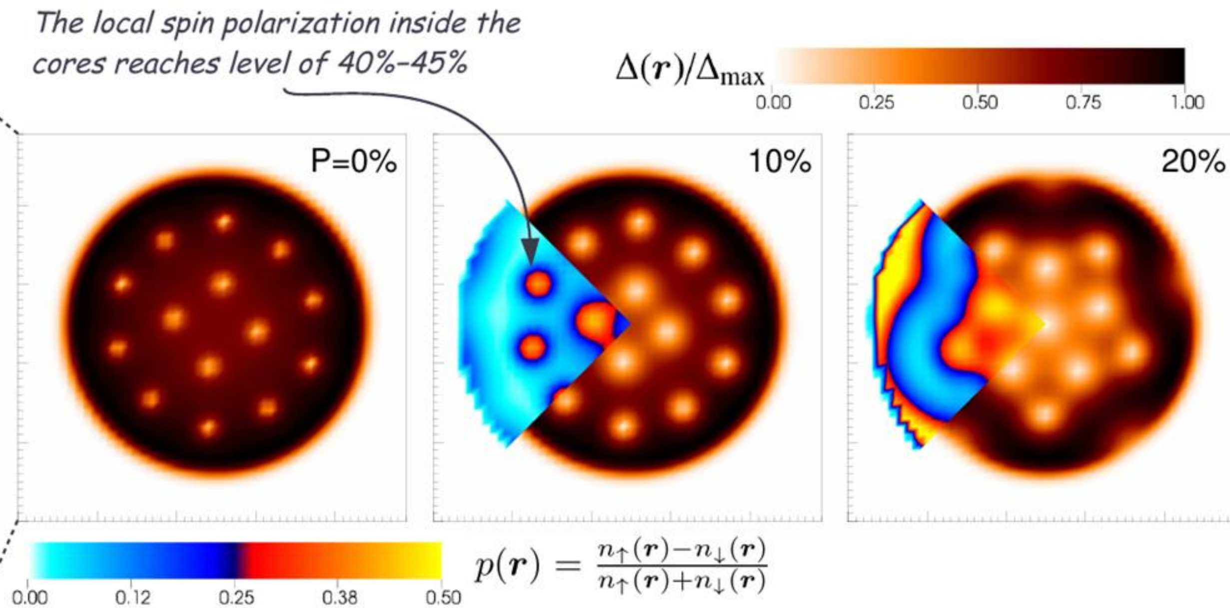
P.Magierski, B.Tüzemen , G.Wlazłowski, Phys. Rev. A100, 033613 (2019)

Example 3: Quantum turbulence in Fermi superfluid

Problem 1: how to generate the turbulence?

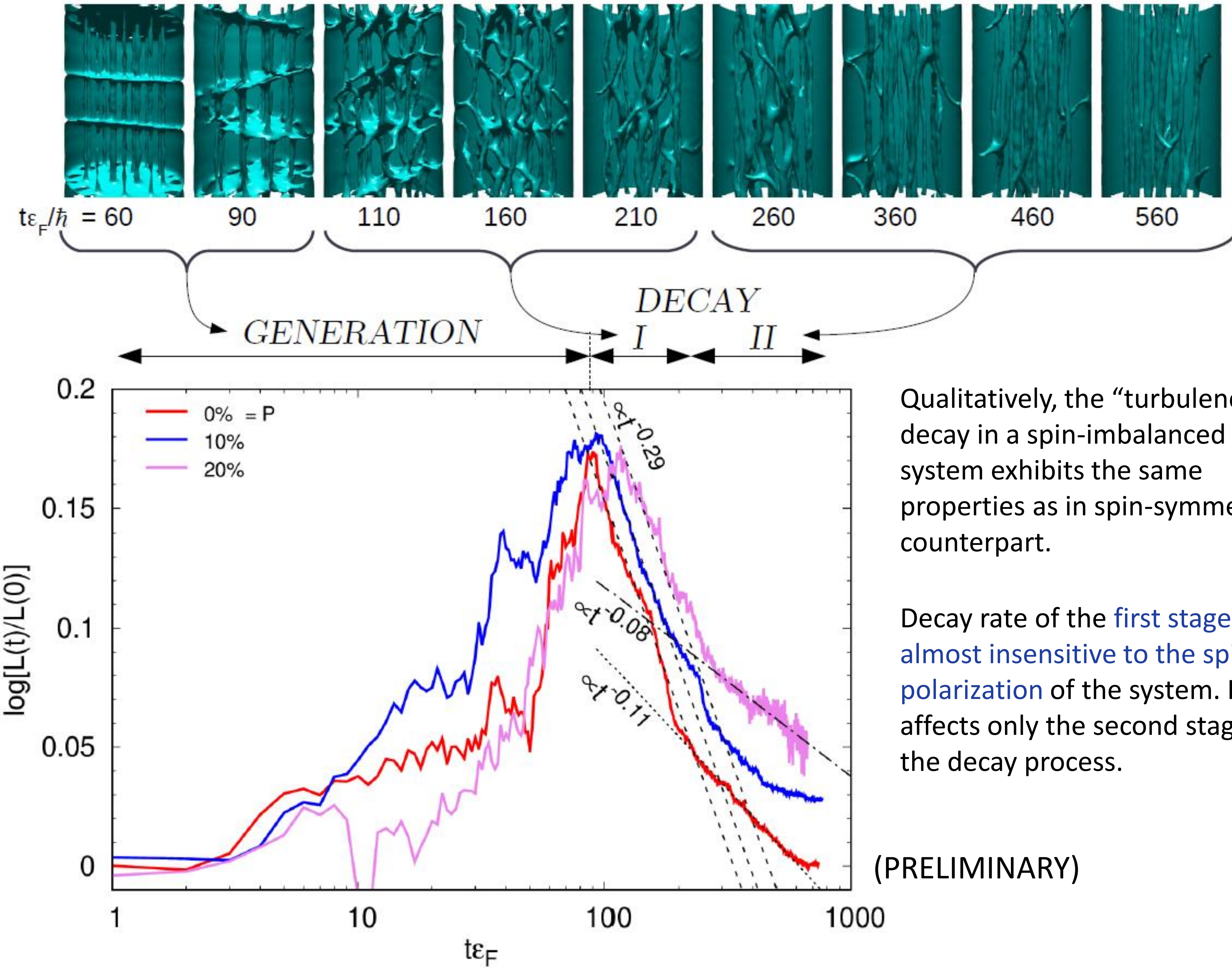
→ Our suggestion: *imprint few dark solitons on existing vortex lattice*
→ *rotating turbulence* *(nonzero total angular momentum)*





Interesting questions:

- *What are differences and similarities of turbulence in Fermi and Bose superfluids?*
- *What type of quantum turbulence is present in the fermionic systems?*
- *Turbulence in spin-imbalanced systems?*

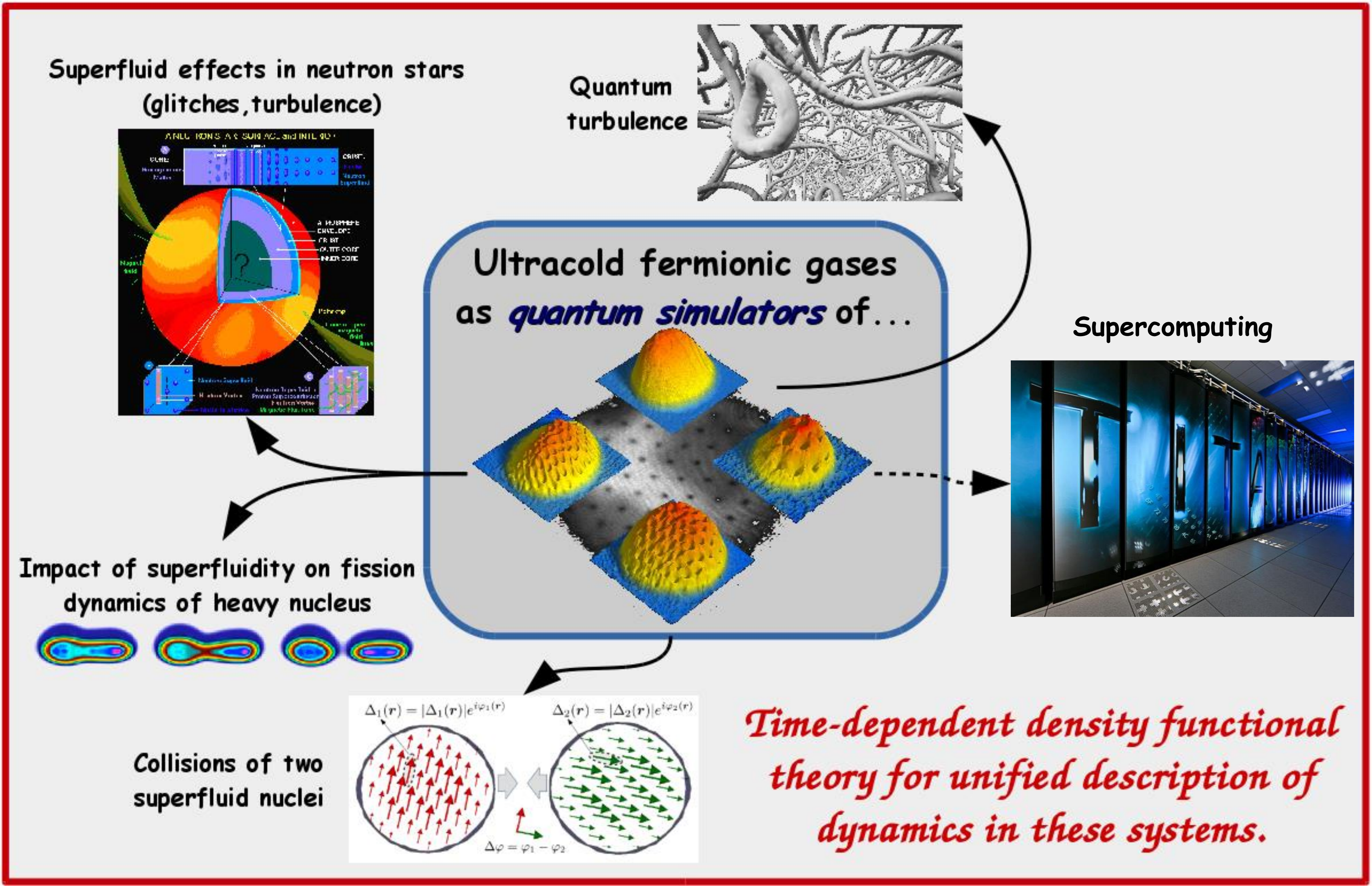


Qualitatively, the "turbulence" decay in a spin-imbalanced system exhibits the same properties as in spin-symmetric counterpart.

Decay rate of the first stage is almost insensitive to the spin-polarization of the system. It affects only the second stage of the decay process.

(PRELIMINARY)

Wlazłowski, Kobuszewski, Sekizawa, Magierski, in preparation


Superfluid effects in neutron stars (glitches, turbulence)
Quantum turbulence
Ultracold fermionic gases as *quantum simulators* of...
Supercomputing
Impact of superfluidity on fission dynamics of heavy nucleus
Collisions of two superfluid nuclei
$\Delta_1(\boldsymbol{r}) = |\Delta_1(\boldsymbol{r})|e^{i\varphi_1(\boldsymbol{r})}$
$\Delta_2(\boldsymbol{r}) = |\Delta_2(\boldsymbol{r})|e^{i\varphi_2(\boldsymbol{r})}$
$\Delta\varphi = \varphi_1 - \varphi_2$
Time-dependent density functional theory for unified description of dynamics in these systems.

Thank you