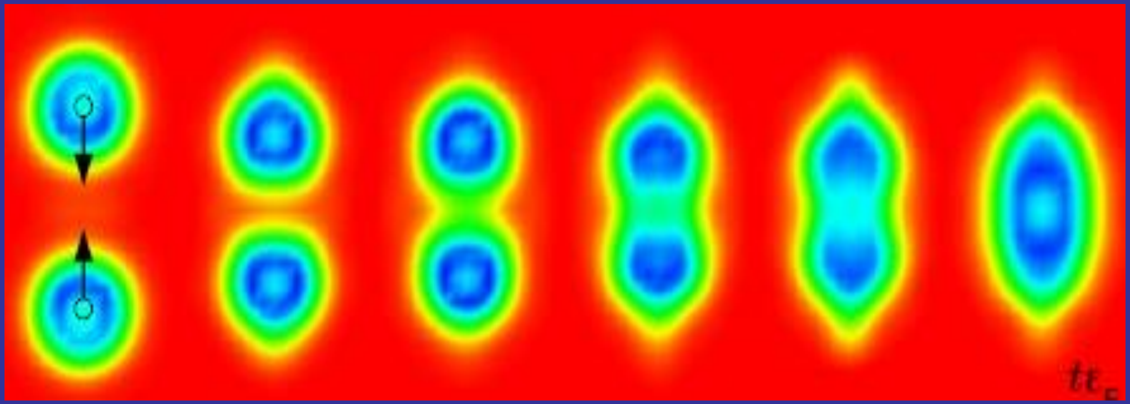
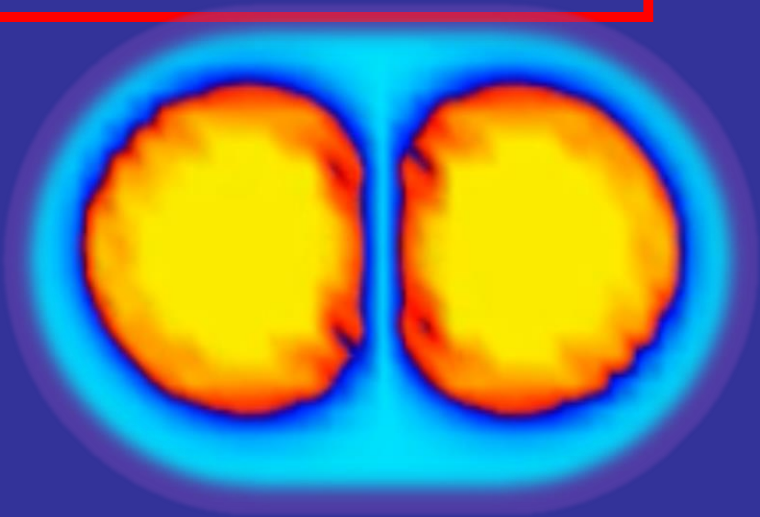
Exotic features of superfluidity far from equilibrium





Piotr Magierski
Warsaw University of Technology (WUT)

Collaborators:

Matthew Barton (WUT)
Aurel Bulgac (UoW)
Janina Grineviciute (WUT)
Konrad Kobuszewski (WUT – Ph.D. student)
Kenneth Roche (PNNL)
Kazuyuki Sekizawa (WUT -> Niigata U.)
Ionel Stetcu (LANL)
Buğra Tüzemen (WUT - Ph.D. student)
Gabriel Wlazłowski (WUT)

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)?

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.

Pairing correlations 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).
Triggered by discovery of high-Tc superconductors

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:

$$\frac{\tau_c(r)}{2m} - \Delta(r)\chi_c(r), \qquad \tau_c(r) = \nabla\cdot\nabla'\rho_c(r,r')|_{r=r'}$$

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

It allows to reduce the size of the problem for static calculations by introducing the energy cutoff

Pairing correlations in time-dependent superfluid local density approximation (TDSLDA)

$$S = \int_{t_0}^{t_1} \left(\left\langle 0(t) \left| i \frac{d}{dt} \right| 0(t) \right\rangle - E[\rho(t), \chi(t)] \right) dt$$

Stationarity requirement produces the set of equations:

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} U_\mu(\mathbf{r},t) \\ V_\mu(\mathbf{r},t) \end{pmatrix} = \begin{pmatrix} h(\mathbf{r},t) & \Delta(\mathbf{r},t) \\ \Delta^*(\mathbf{r},t) & -h^*(\mathbf{r},t) \end{pmatrix} \begin{pmatrix} U_\mu(\mathbf{r},t) \\ V_\mu(\mathbf{r},t) \end{pmatrix}$$

$$B(t) = \begin{pmatrix} U(t) & V^*(t) \\ V(t) & U^*(t) \end{pmatrix} = \exp[iG(t)] \qquad G(t) = \begin{pmatrix} h(t) & \Delta(t) \\ \Delta^\dagger(t) & -h^*(t) \end{pmatrix}$$

Orthogonality and completeness has to be fulfilled: $B^\dagger(t)B(t) = B(t)B^\dagger(t) = I$,

In order to fulfill the completenes relation of Bogoliubov transform all states need to be evolved!
Otherwise Pauli principle is violated, i.e. the evolved densities do not describe a fermionic system (spurious bosonic effects are introduced).

Consequence: the computational cost increases considerably.

P. Magierski, *Nuclear Reactions and Superfluid Time Dependent Density Functional Theory*, Frontiers in Nuclear and Particle Physics vol. 2, 57 (2019)
A. Bulgac, *Time-Dependent Density Functional Theory and Real-Time Dynamics of Fermi Superfluids*, Ann. Rev. Nucl. Part. Sci. 63, 97 (2013)

Solving time-dependent problem 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)

How reliably can we describe superfluid dynamics in various Fermi systems within TDSLDA?

Areas of applications

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

Ultracold atomic (fermionic) gases. Unitary regime.

Dynamics of quantum vortices, solitonic excitations, quantum turbulence.

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

Astrophysical applications.

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

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

Nuclear physics.

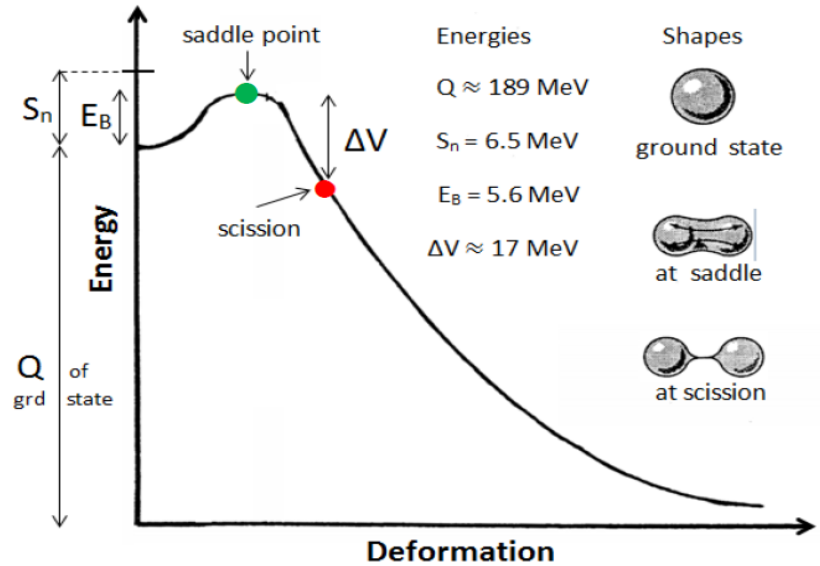
Induced nuclear fission, fusion, collisions.

Example 1: nuclear fission dynamics

Potential energy versus deformation

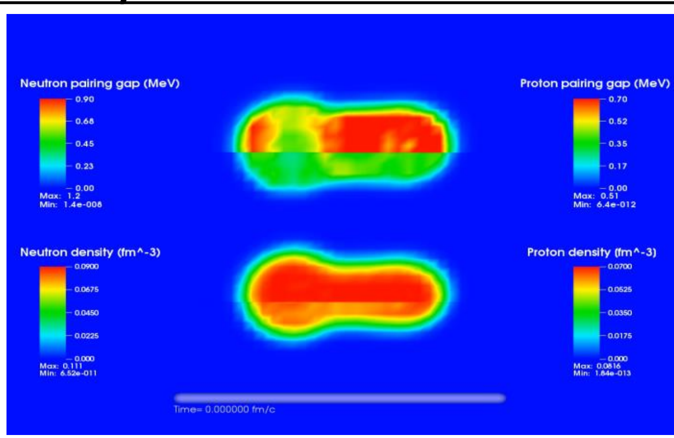
Estimation of characteristic time scales for low energy fission (<10MeV):

Ground state to saddle	-	1 000 000 zs
Saddle to scission	-	10-100 zs
Acceleration of fission fragments to 90% of their final velocity	-	10 zs
Neutron evaporation	-	1 000 zs



From F. Gonnenwein FIESTA2014

Fission dynamics of ^{240}Pu within TDSLDA



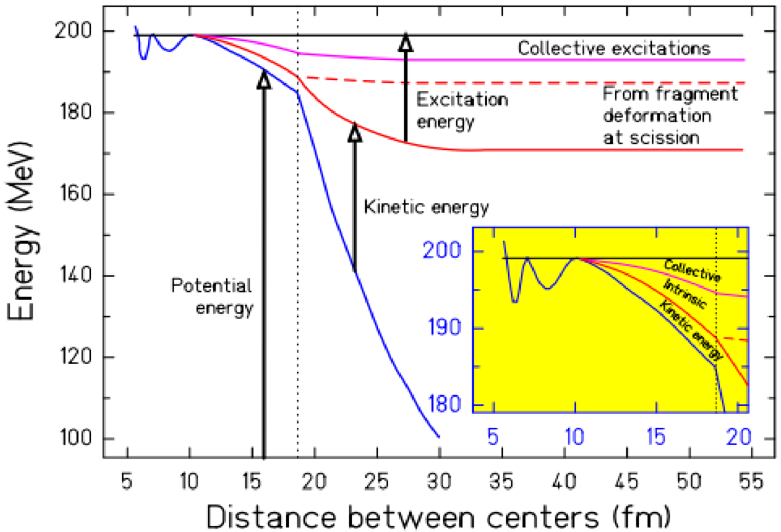
Total kinetic energy of the fragments

E^* (MeV)	E_n (MeV)	TKE_{TDSLDA} (MeV)	TKE_{syst} (MeV)	err (%)	Z_L	N_L
8.08	1.542	173	177.26	1.95	40.825	62.246
9.60	3.063	174	176.73	1.13	40.500	61.536
10.10	3.560	179	176.56	1.43	41.625	62.783
10.57	4.032	173	176.39	1.55	40.092	61.256
10.58	4.043	173	176.39	1.70	40.146	61.388
10.58	4.047	175	176.39	0.72	40.313	61.475
10.60	4.065	174	176.38	0.92	40.904	62.611
11.07	4.534	176	176.22	0.14	41.495	63.134
11.56	5.024	175	176.05	0.51	40.565	61.894
12.05	5.515	176	175.88	0.49	40.412	61.809
12.15	5.610	176	175.84	0.29	40.355	61.695
12.16	5.626	176	175.84	0.15	41.386	62.764

Calculated TKEs reproduce experimental data with accuracy < 2%

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

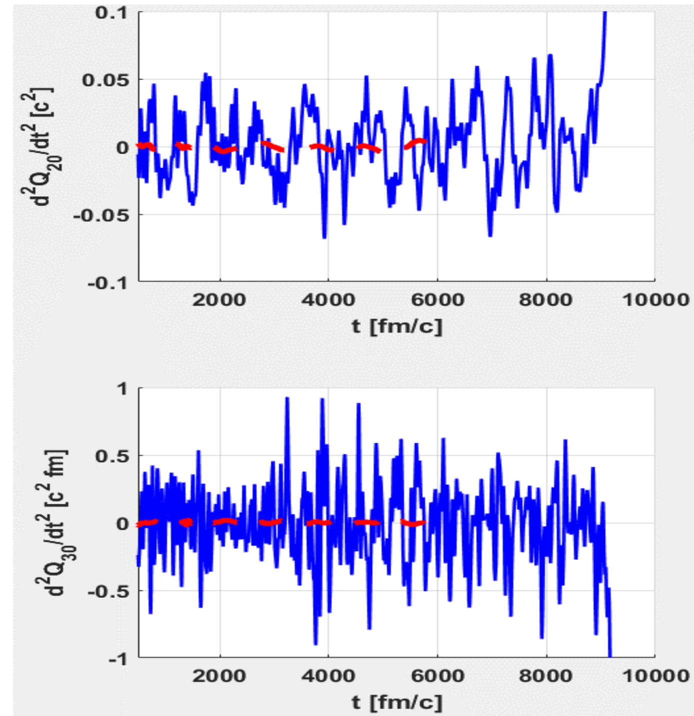
Q: Excitation energy sharing of the fragments



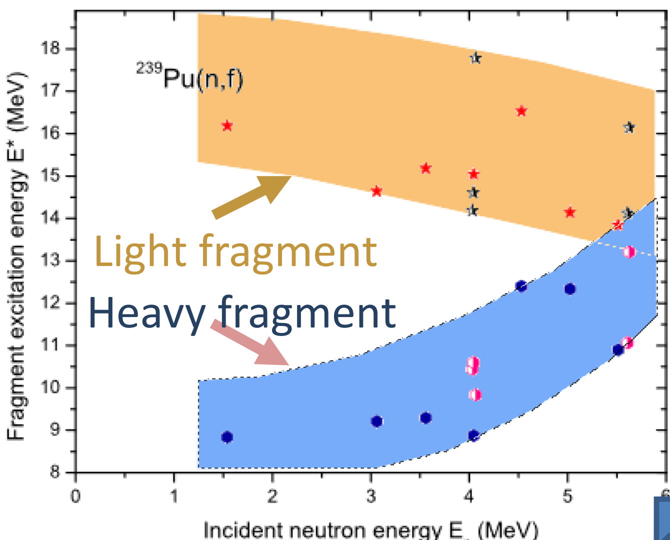
Schmidt&Jurado:Phys.Rev.C83:061601,2011

Character of nuclear motion along the fission path – from TDSLDA

Accelerations in quadrupole and octupole moments



TDSLDA energy sharing between fragments



J. Grineviciute et al. – in preparation

It is important to realize that these results indicate that the motion <u>is not adiabatic, although it is slow.</u>

Although the average collective velocity is constant till the very last moment before scission, the system heats up as the energy flows <u>irreversibly from collective to intrinsic degrees of freedom</u>.

Severe test for the theory – unfortunately no exp. data are available yet.

Example 2: spin-imbalanced unitary Fermi gas

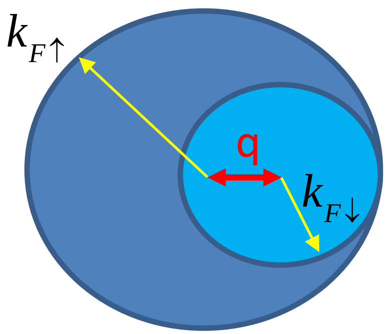
Larkin-Ovchinnikov (LO): $\Delta(r) \sim \cos(\vec{q}\cdot\vec{r})$

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

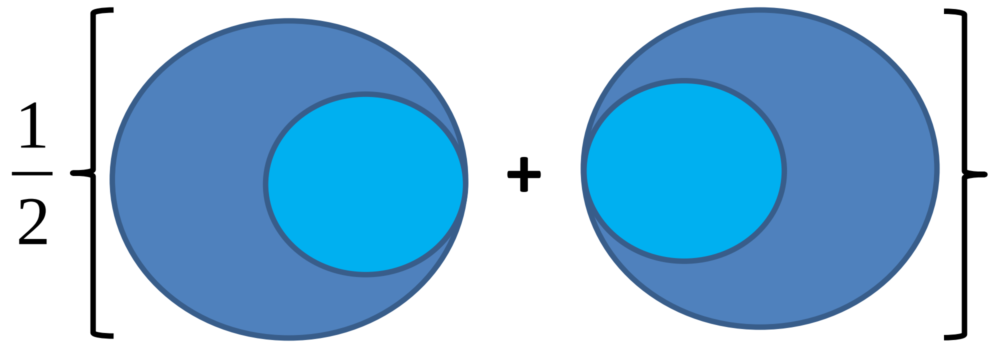
A.I. Larkin and Y. N. Ovchinnikov, Sov. Phys. JETP 20, 762 (1965)
P. Fulde and R. A. Ferrell, Phys. Rev. 135, A550 (1964)

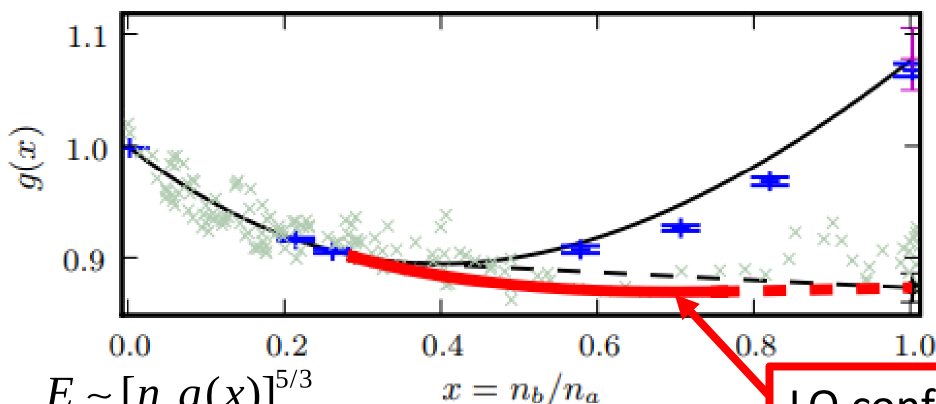
Spatial modulation of the pairing field costs energy proportional to q^2 but may be compensated by an increased pairing energy due to the mutual shift of Fermi spheres:

FF:



LO:





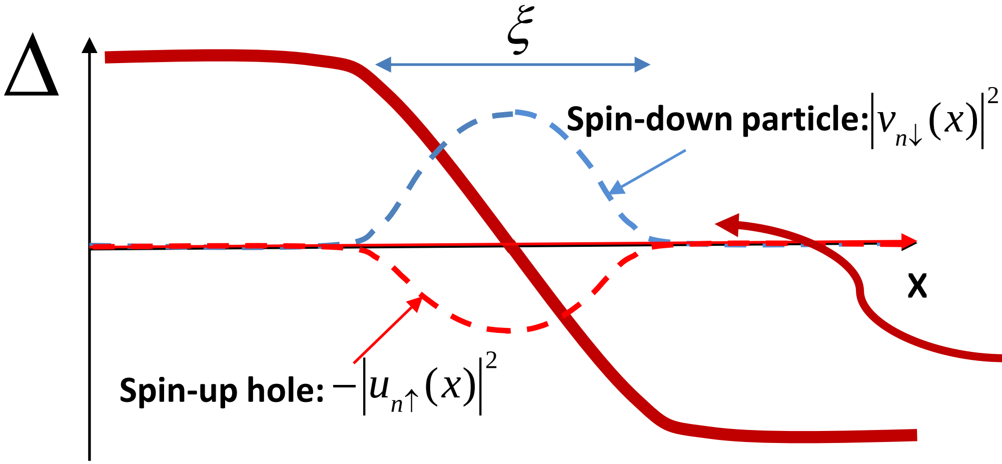
$E \sim [n_a g(x)]^{5/3}$

LO configuration – supersolid state

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)

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



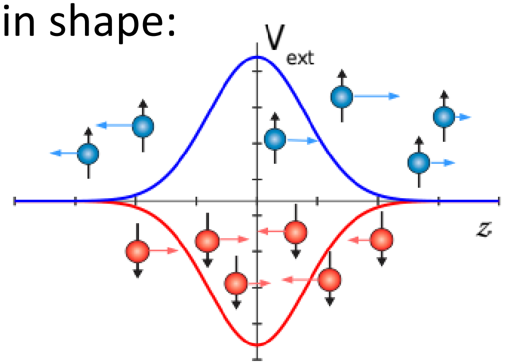
Due to quasiparticle scattering the localized Andreev states appear at the nodal point. These states induce local spin-polarization

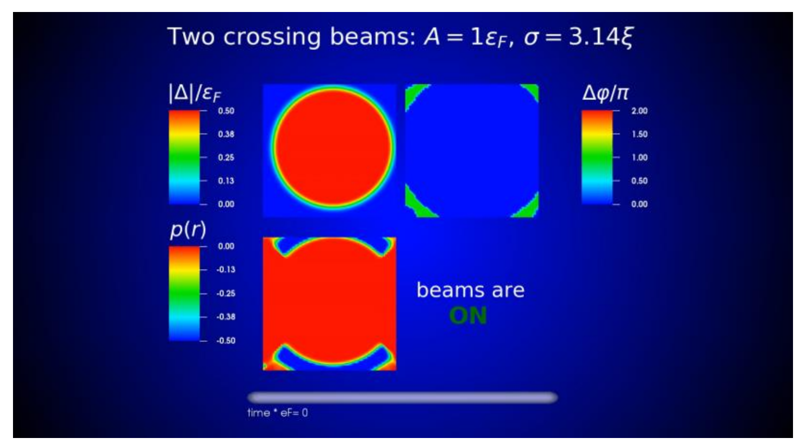
BdG in the Andreev approx. ($\Delta \ll k_F^2$)

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

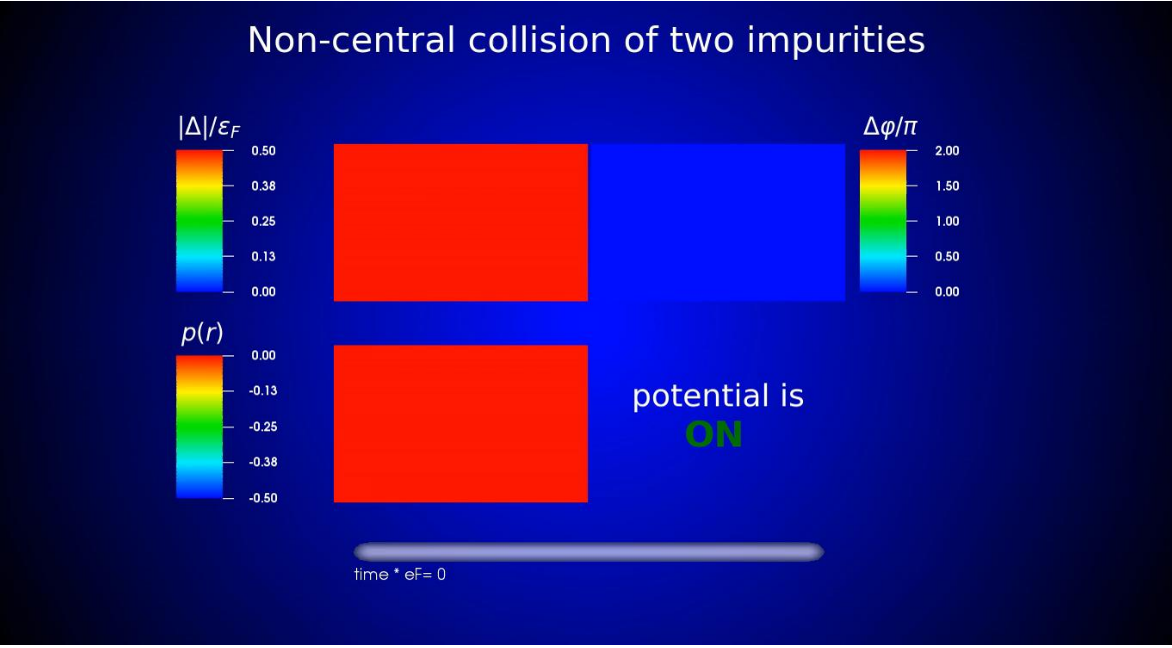
Engineering the structure of nodal surfaces

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:

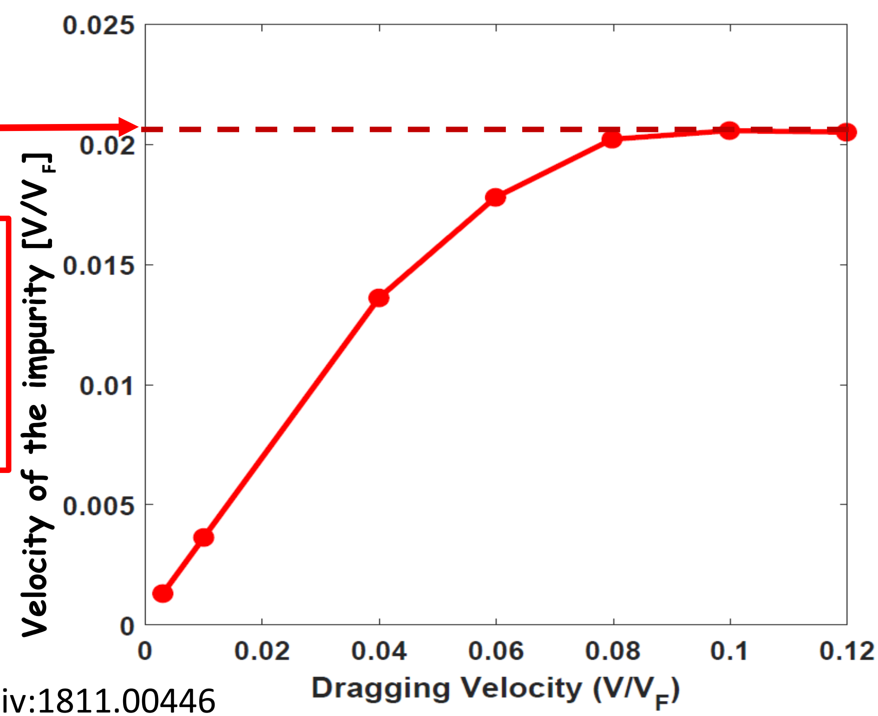
$$\Delta(r) : \cos(qr) \Rightarrow \exp(iqr)$$

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 ($\sim q \sim |k_{F\uparrow} - k_{F\downarrow}|$).

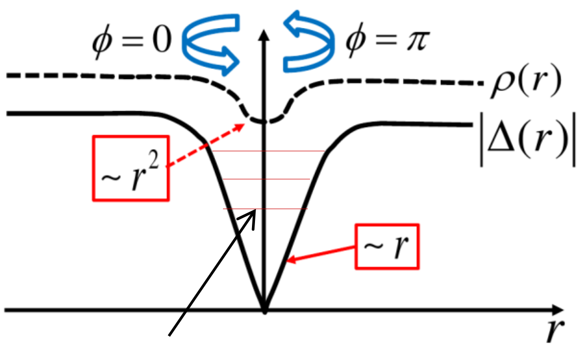


P.Magierski, B.Tüzemen , G.Wlazłowski, Phys. Rev. A (in press) arXiv:1811.00446

Andreev states and anatomy of the vortex core

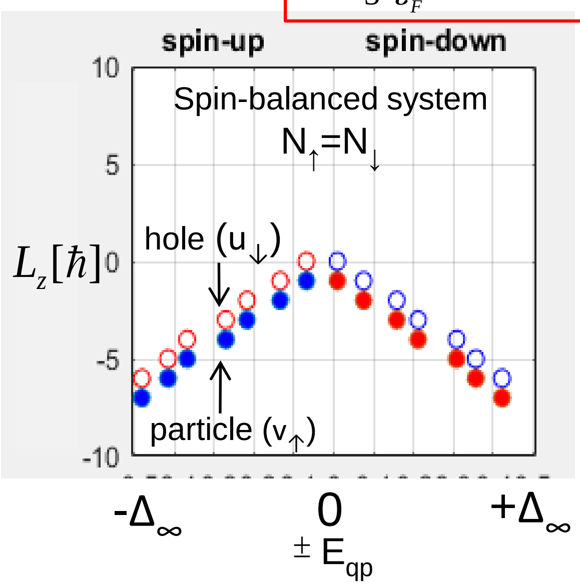
FERMIONS:

Vortex structure: Fermi gas → BdG eq.



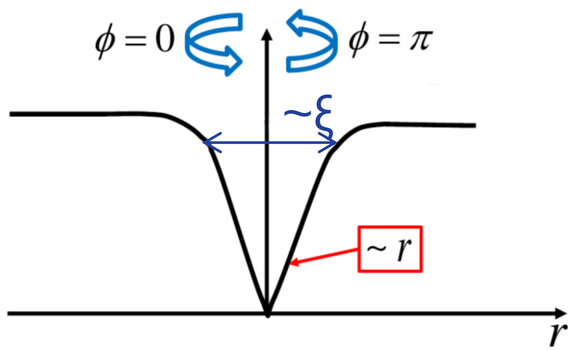
Andreev states inside the core give rise to **anomalous branch of excitations (of chiral fermions):**

$$E_m \approx \frac{4}{3}\frac{|\Delta|^2}{\varepsilon_F} m \;\; ; \;\; |m| = 1, 2, \ldots$$



BOSONS:

Vortex structure: Bose gas → Gross-Pitaevskii eq. (GPE)



Order parameter:

$$\Psi = \sqrt{\rho(r)}e^{i\phi}$$

$$\boldsymbol{v}_s = \frac{\hbar}{M}\boldsymbol{\nabla}\phi$$

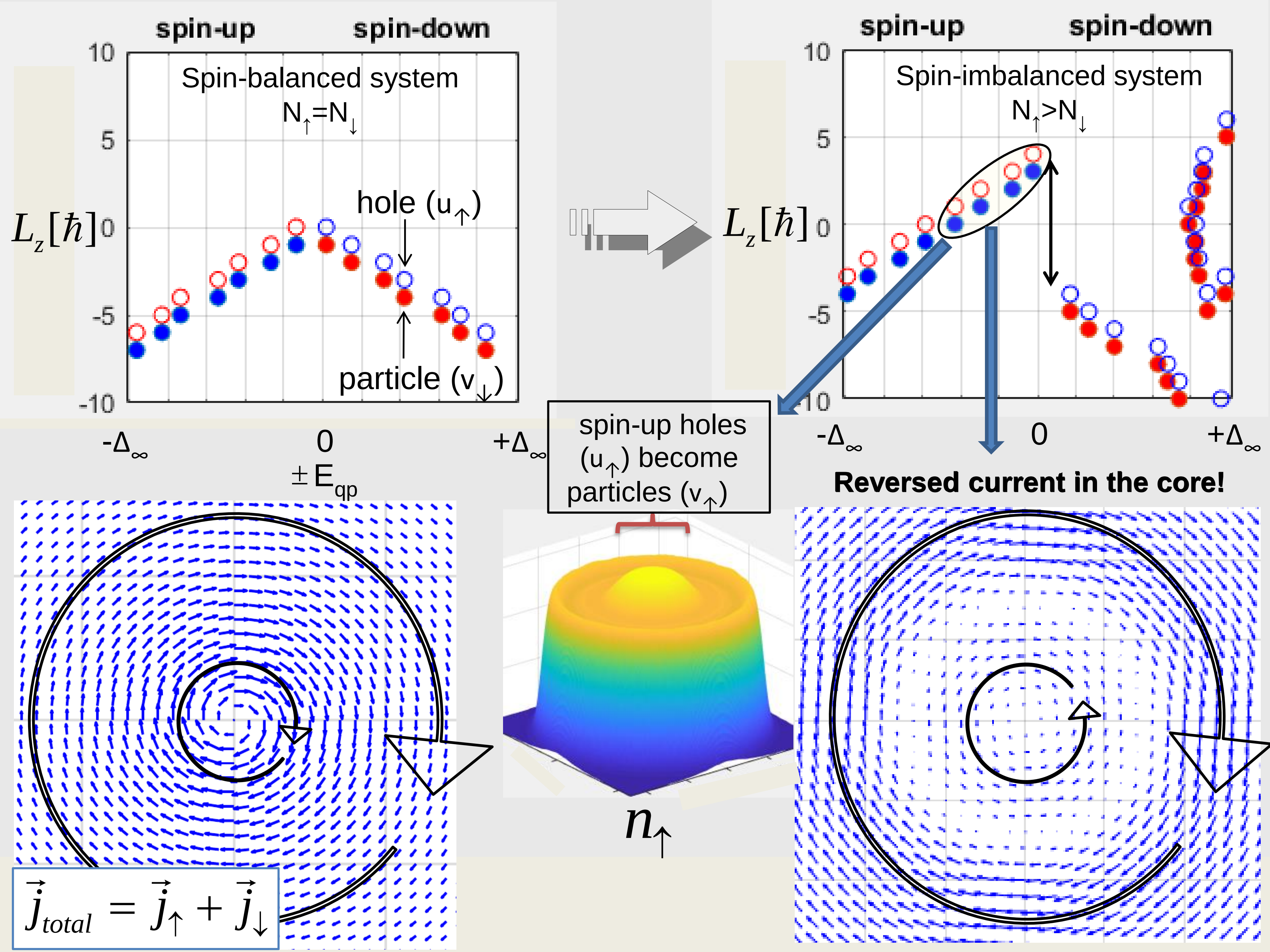
$$\kappa = \oint d\boldsymbol{l}\cdot\boldsymbol{v}_s = \frac{h}{M}$$

Order parameter: not related directly to density

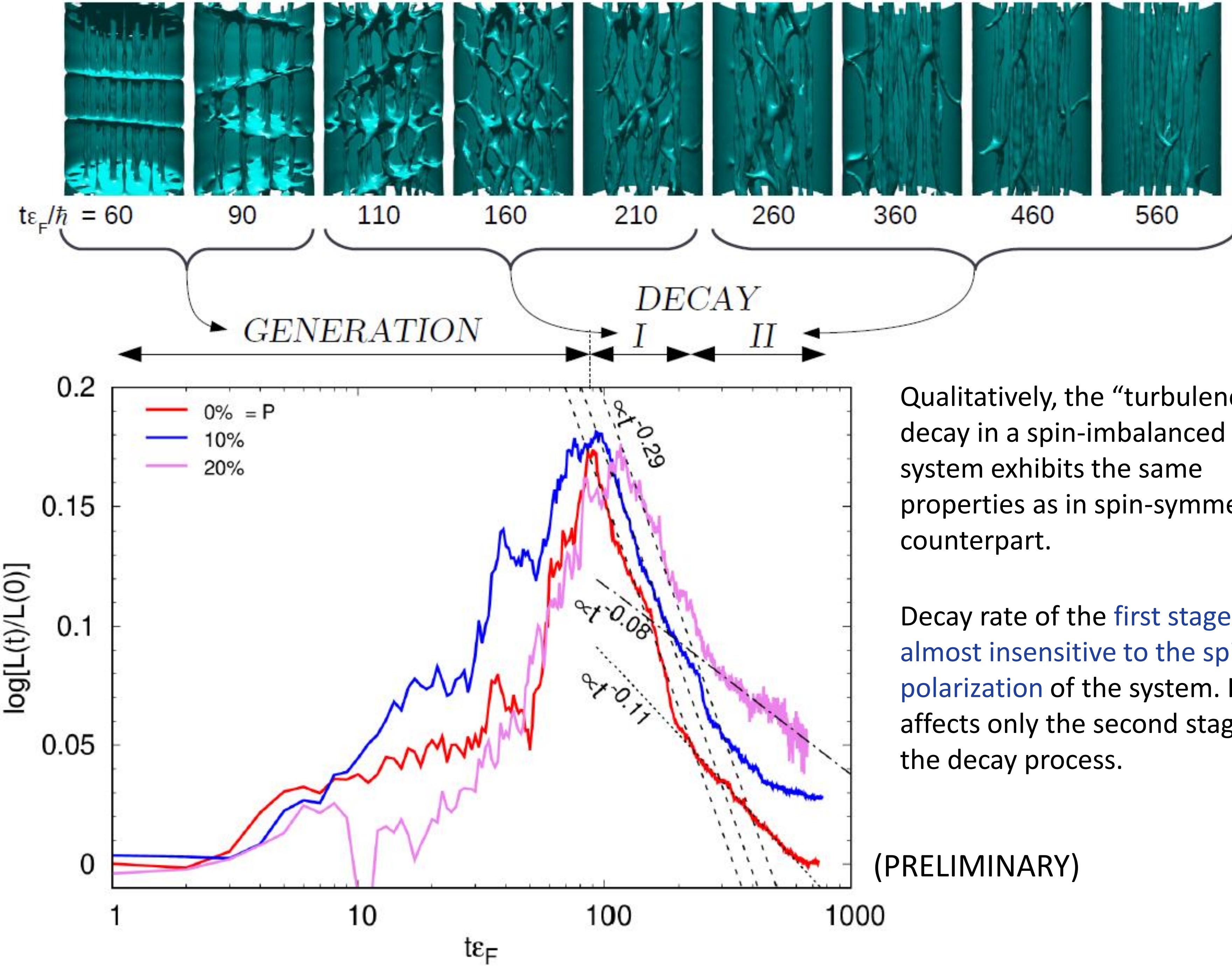
Expectations:

- Long range interaction in the system of vortices is the same for bosons and fermions, as it is governed by the superfluid flow v_S
- **Short range physics** (e.g. reconnection rate) is **different** due to the population of Andreev states in the core. It significantly modifies **the decay of the turbulent state** (Wlazłowski, Kobuszewski, Sekizawa, Magierski, in preparation)
- Note that Andreev states define the energy scale:

$\delta E \approx \frac{4}{3}\frac{|\Delta|^2}{\varepsilon_F} < |\Delta|$ - **minigap**, which affects thermal and dissipative properties of the system of vortices.



spin-up
spin-down
Spin-balanced system
$N_\uparrow = N_\downarrow$
hole ($u_\uparrow$)
particle ($v_\downarrow$)
$L_z[\hbar]$
10
5
0
-5
-10
$-\Delta_\infty$
0
$+\Delta_\infty$
$\pm E_{qp}$
spin-up
spin-down
Spin-imbalanced system
$N_\uparrow > N_\downarrow$
$L_z[\hbar]$
10
5
0
-5
-10
$-\Delta_\infty$
0
$+\Delta_\infty$
spin-up holes ($u_\uparrow$) become particles ($v_\uparrow$)
Reversed current in the core!
$n_\uparrow$
$\vec{j}_{total} = \vec{j}_\uparrow + \vec{j}_\downarrow$



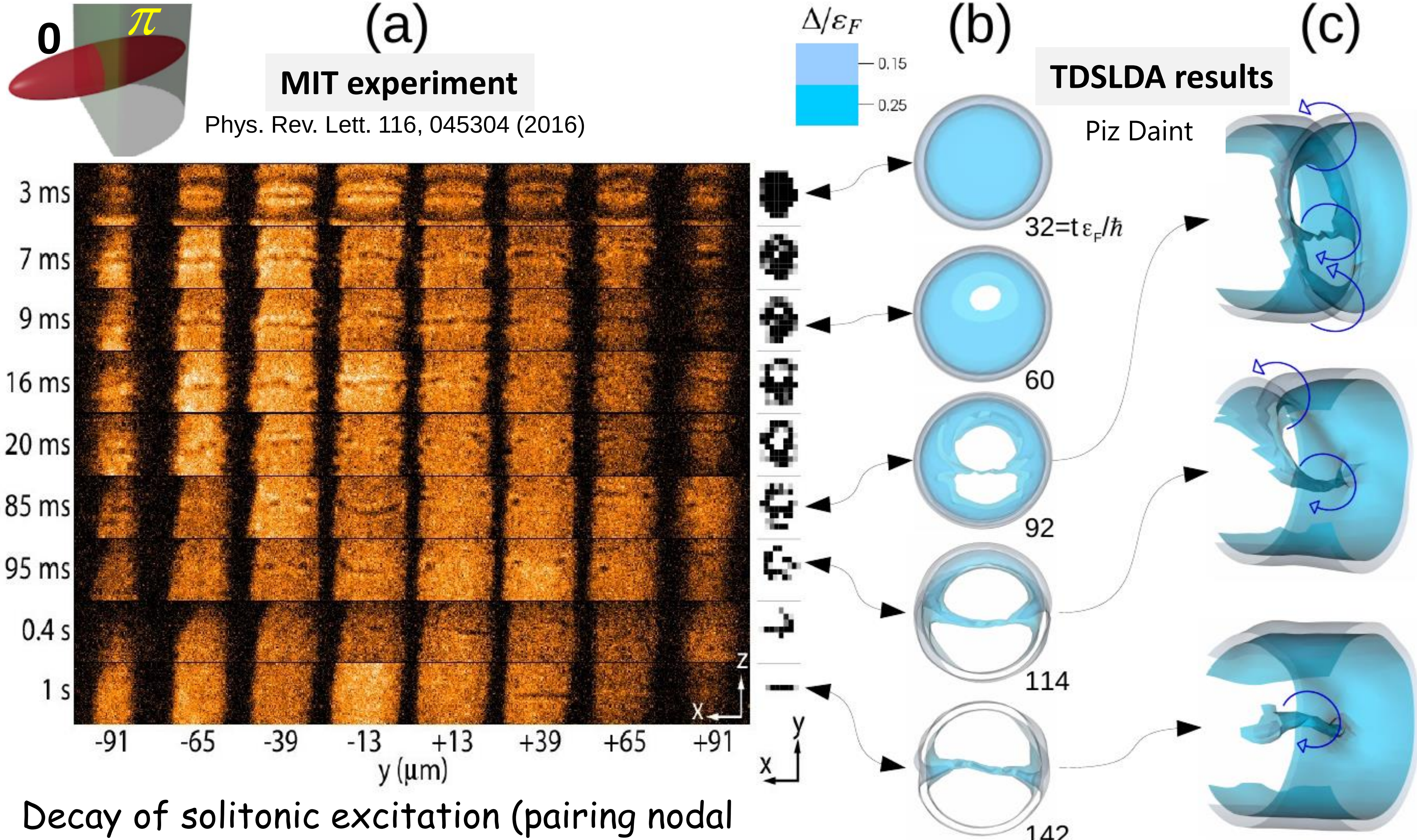
Qualitatively, the “turbulence” decay in a spin-imbalanced system exhibits the same properties as in spin-symmetric counterpart.

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

Example 3: dynamics of solitonic excitations



Decay of solitonic excitation (pairing nodal structure) generates a sequence of topological excitations involving: "Phi"-soliton and vortex line.

G. Wlazłowski, K. Sekizawa, M. Marchwiany, P. Magierski, Phys. Rev. Lett. **120**, 253002 (2018)

Nuclear collisions

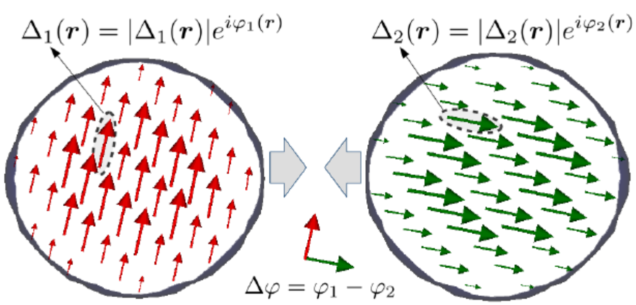
Collisions of superfluid nuclei having <u>different phases</u> of the <u>pairing fields</u>

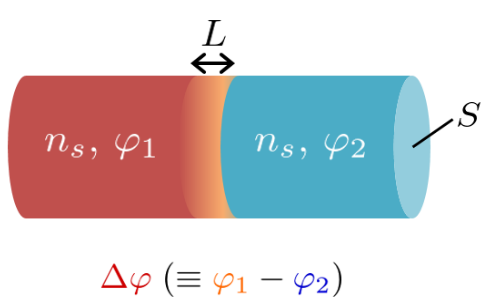
<u>The main questions are:</u>

-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.

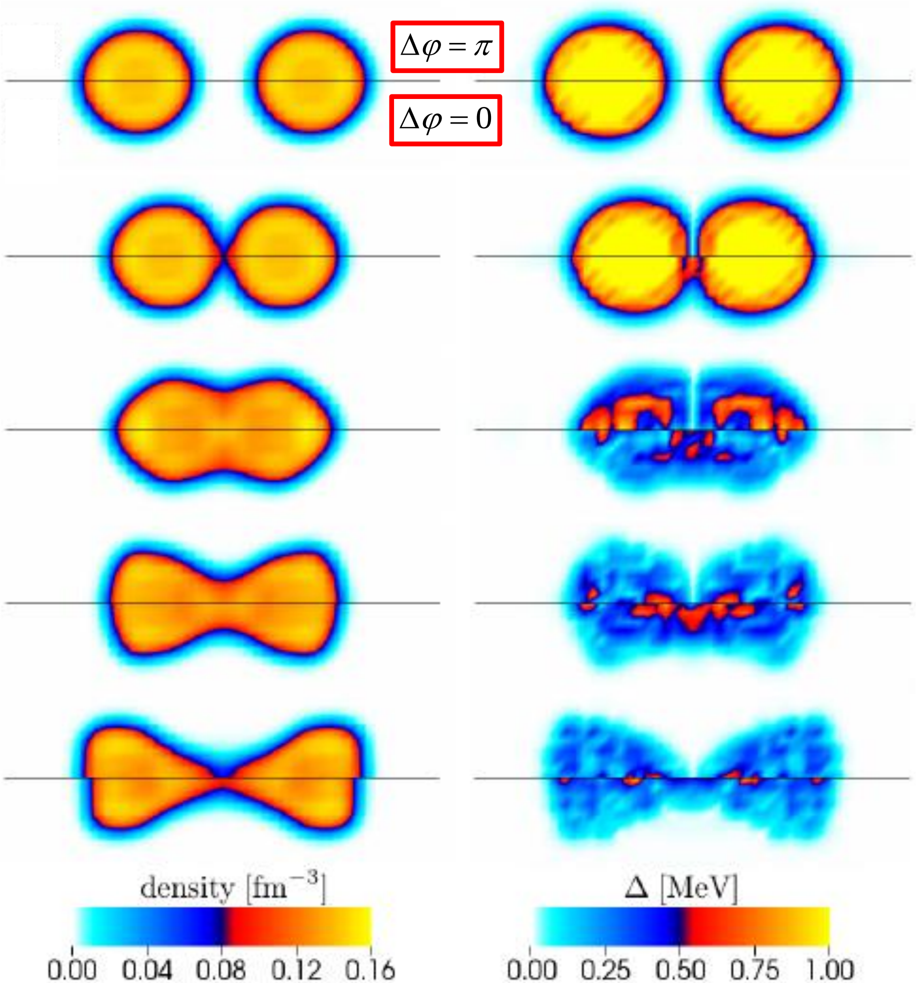




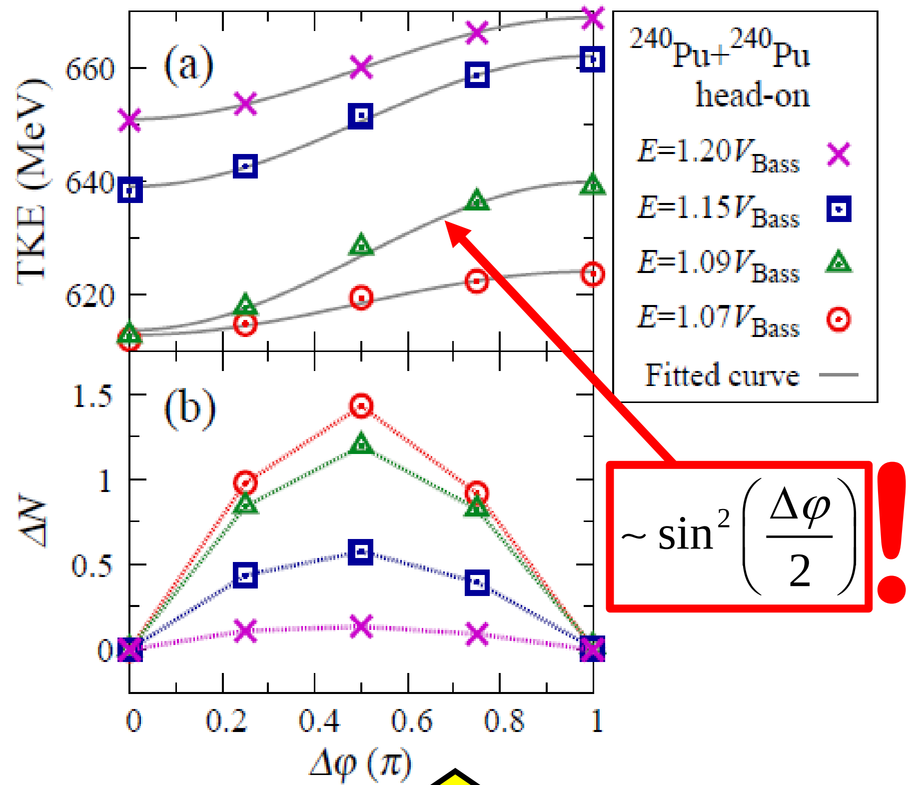
From Ginzburg-Landau (G-L) approach:

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

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



Total kinetic energy of the fragments (TKE)

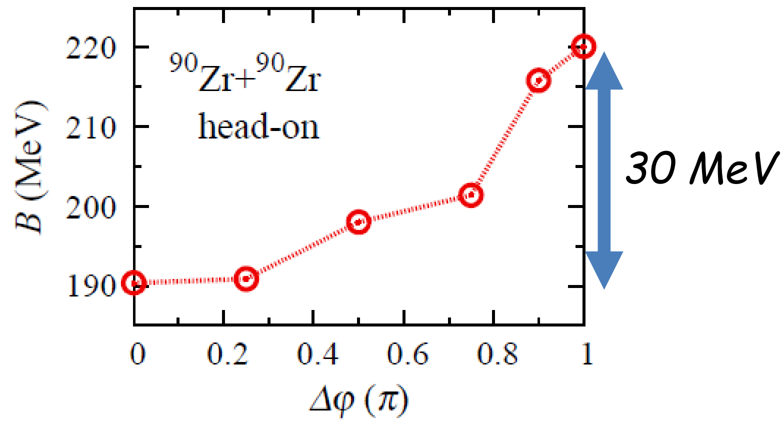


Average particle transfer between fragments.

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!

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 effect is found (within TDDFT) to be of the order of 30MeV for medium 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)

It raises (again) an interesting (and well known) question:
to what extent systems of hundreds of particles can be described using the concept of pairing field?

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

Summary

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

Open problems

1) There are easy and difficult observables in DFT.
   In general: easy observables are one-body observables. They are easily extracted and reliable.

2) But there are also important observables which are difficult to extract.
   For example:
   - S matrix
   - momentum distributions
   - transitional densities (defined in linear response regime)
   - various conditional probabilities
   - mass distributions

   Stochastic extensions of TDDFT are under investigation:
   D. Lacroix, A. Ayik, Ph. Chomaz, Prog.Part.Nucl.Phys.52(2004)497
   S. Ayik, Phys.Lett. B658 (2008) 174
   A. Bulgac, S.Jin, I. Stetcu, arxiv:1806.00694

3) Dissipation: transition between one-body dissipation regime and two-body dissipation regime.