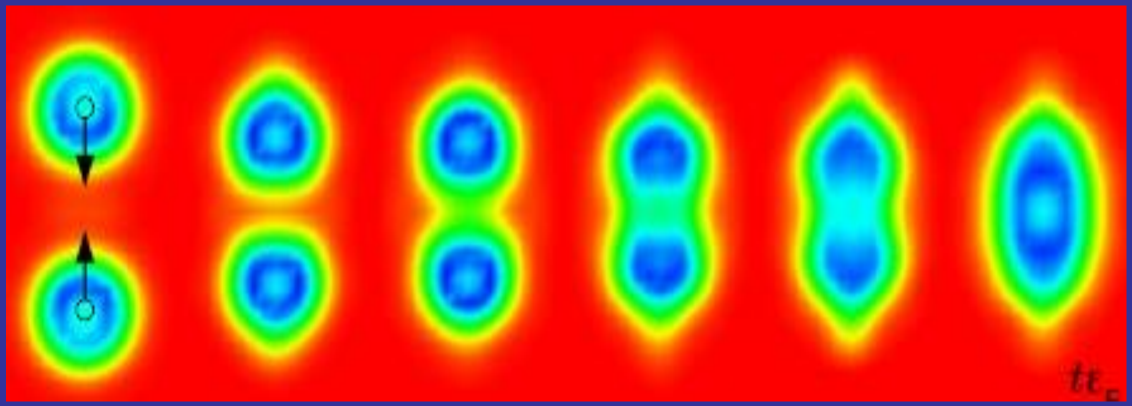
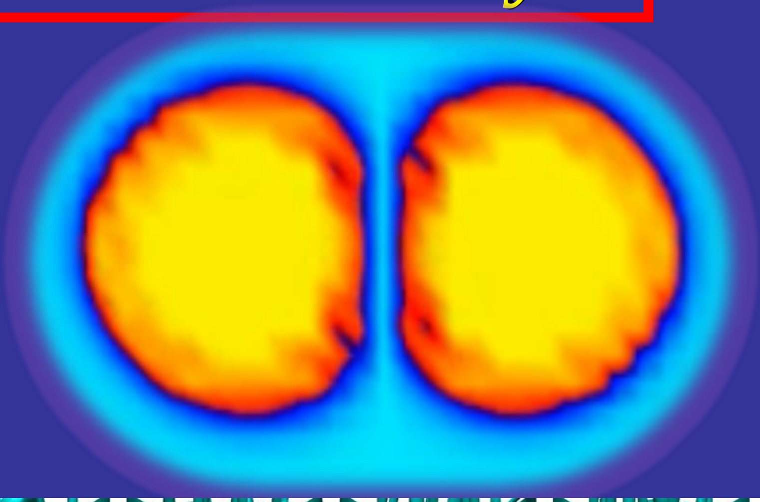
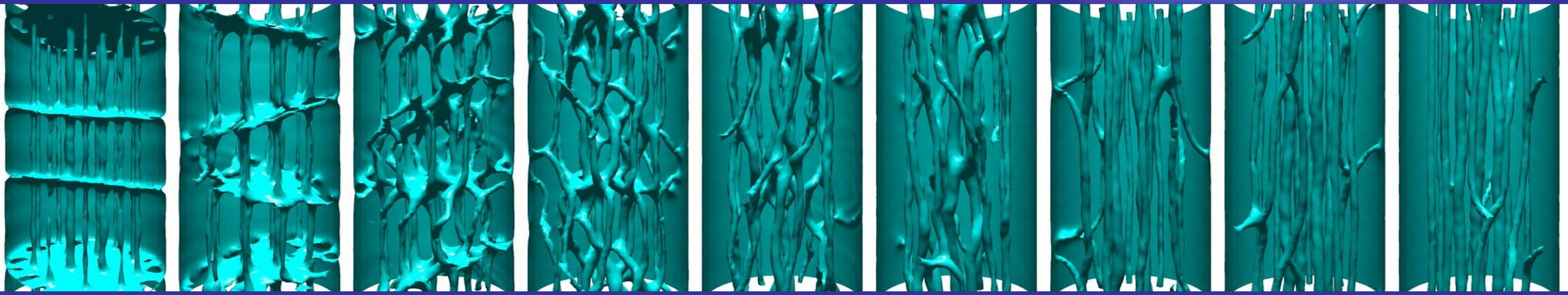
Superfluidity far from equilibrium in the light of time dependent density functional theory







Piotr Magierski
Warsaw University of Technology (WUT)

Robert B. Laughlin, Nobel Lecture, December 8, 1998:

One of my favorite times in the academic year occurs [..] when I give my class of extremely bright graduate students [..] a take home exam in which they are asked <u>TO DEDUCE SUPERFLUIDITY FROM FIRST PRINCIPLES.</u>

There is no doubt a special place in hell being reserved for me at this very moment for this mean trick, for the task is <u>IMPOSSIBLE</u>. Superfluidity [..] is an EMERGENT phenomenon – a low energy collective effect of huge number of particles that <u>CANNOT</u> be deduced from the microscopic equations of motion in a <u>RIGOROUS WAY</u> and that <u>DISAPPEARS</u> completely when the system is taken apart.

[..]students who stay in physics long enough [..] eventually come to understand that the <u>REDUCTIONIST IDEA IS WRONG</u> a great deal of the time and perhaps <u>ALWAYS.</u>

GOAL:
Unified description of superfluid dynamics of fermionic systems far from equilibrium based on microscopic theoretical framework.

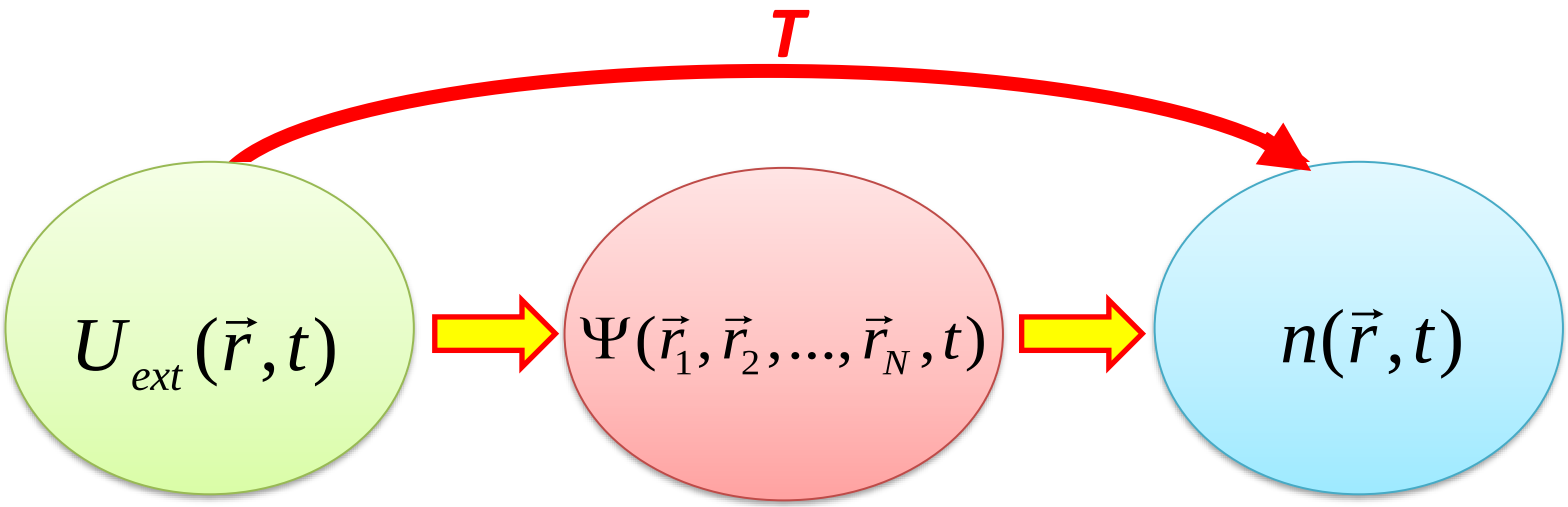
Microscopic framework = explicit treatment of fermionic degrees of freedom.

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.

Time Dependent DFT Basics



Runge-Gross mapping(1984):

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

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

$$n(\vec{r}) \leftrightarrow e^{i\alpha(t)}\Psi[n](\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)$$

TDDFT variational principle also exists but it is more tricky:

$$F[\psi_0,n] = \int_{t_0}^{t_1}\langle\psi[n]|\left(i\hbar\frac{\partial}{\partial t} - \hat{H}\right)|\psi[n]\rangle\, dt$$

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)

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:

$$\begin{aligned} \Delta(\mathbf{r}) &= g_{eff}(\mathbf{r})\chi_c(\mathbf{r}) \\ \frac{1}{g_{eff}(\mathbf{r})} &= \frac{1}{g(\mathbf{r})} - \frac{m k_c(\mathbf{r})}{2\pi^2\hbar^2}\left(1 - \frac{k_F(\mathbf{r})}{2k_c(\mathbf{r})}\ln\frac{k_c(\mathbf{r}) + k_F(\mathbf{r})}{k_c(\mathbf{r}) - k_F(\mathbf{r})}\right) \end{aligned}$$

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 <u>to reduce the size of the problem for static calculations</u> by introducing the energy cutoff

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

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

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 completeness 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)

$$\phi_n \longrightarrow (u_{n,\uparrow}, u_{n,\downarrow}, v_{n,\uparrow}, v_{n,\downarrow})$$

Densities:

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

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

EDF:

$$\mathcal{H} = \alpha_\uparrow(p)\frac{\hbar^2\tau_\uparrow}{2m_\uparrow} + \alpha_\downarrow(p)\frac{\hbar^2\tau_\downarrow}{2m_\downarrow}$$

$$+ D(n_\uparrow, n_\downarrow)$$

$$+ g(n_\uparrow, n_\downarrow)\nu^\dagger\nu$$

$$+ [1-\alpha_\uparrow(p)]\frac{j_\uparrow^2}{2n_\uparrow} + [1-\alpha_\downarrow(p)]\frac{j_\downarrow^2}{2n_\downarrow}$$

Kinetic term:
Effective mass α_σ of the particle depends on local polarization

$$p(\boldsymbol{r}) = \frac{n_\uparrow(\boldsymbol{r}) - n_\downarrow(\boldsymbol{r})}{n_\uparrow(\boldsymbol{r}) + n_\downarrow(\boldsymbol{r})}$$

and guarantees that correct limit is attained for $n_\uparrow >> n_\downarrow$, where the problem reduces to the *polaron* problem

A. Bulgac, M.M. Forbes, P. Magierski,
Lecture Notes in Physics, Vol. 836, Chap. 9, p.305-373 (2012)

$$\phi_n \longrightarrow (u_{n,\uparrow}, u_{n,\downarrow}, v_{n,\uparrow}, v_{n,\downarrow})$$

Densities:

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

EDF:

$$\mathcal{H} = \alpha_\uparrow(p)\frac{\hbar^2\tau_\uparrow}{2m_\uparrow} + \alpha_\downarrow(p)\frac{\hbar^2\tau_\downarrow}{2m_\downarrow}$$

$$+D(n_\uparrow, n_\downarrow)$$

$$+g(n_\uparrow, n_\downarrow)\nu^\dagger\nu$$

$$+[1-\alpha_\uparrow(p)]\frac{j_\uparrow^2}{2n_\uparrow} + [1-\alpha_\downarrow(p)]\frac{j_\downarrow^2}{2n_\downarrow}$$

Normal interaction energy:

$$D(n_\uparrow, n_\downarrow) \sim (n_\uparrow + n_\downarrow)^{5/3}\beta(p)$$

in order to get the proper scaling:

$$E = \xi E_{FFG}$$

A. Bulgac, M.M. Forbes, P. Magierski,
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EDF:

$$\mathcal{H} = \alpha_\uparrow(p)\frac{\hbar^2\tau_\uparrow}{2m_\uparrow} + \alpha_\downarrow(p)\frac{\hbar^2\tau_\downarrow}{2m_\downarrow}$$

$$+ D(n_\uparrow, n_\downarrow)$$

$$+ g(n_\uparrow, n_\downarrow)\nu^\dagger\nu$$

$$+ [1-\alpha_\uparrow(p)]\frac{j_\uparrow^2}{2n_\uparrow} + [1-\alpha_\downarrow(p)]\frac{j_\downarrow^2}{2n_\downarrow}$$

Pairing energy:

$$g(n_\uparrow, n_\downarrow) = \frac{\gamma(p)}{(n_\uparrow + n_\downarrow)^{1/3}}$$

in order to get proper scaling:

$$\Delta/\varepsilon_F = \text{const} \approx 0.5$$

A. Bulgac, M.M. Forbes, P. Magierski,
Lecture Notes in Physics, Vol. 836, Chap. 9, p.305-373 (2012)

$$\phi_n \longrightarrow (u_{n,\uparrow}, u_{n,\downarrow}, v_{n,\uparrow}, v_{n,\downarrow})$$

Densities:

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

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EDF:

$$\mathcal{H} = \alpha_\uparrow(p)\frac{\hbar^2\tau_\uparrow}{2m_\uparrow} + \alpha_\downarrow(p)\frac{\hbar^2\tau_\downarrow}{2m_\downarrow}$$

$$+ D(n_\uparrow, n_\downarrow)$$

$$+ g(n_\uparrow, n_\downarrow)\nu^\dagger\nu$$

$$+ [1-\alpha_\uparrow(p)]\frac{j_\uparrow^2}{2n_\uparrow} + [1-\alpha_\downarrow(p)]\frac{j_\downarrow^2}{2n_\downarrow}$$

In order to restore Galilean invariance of the functional

More details:
A. Bulgac, M.M. Forbes, P. Magierski,
The Unitary Fermi Gas: From Monte Carlo to Density Functionals,
Lecture Notes in Physics 836
ed. W. Zwerger, Springer (2011).

Superfluid Local Density Approximation (SLDA)

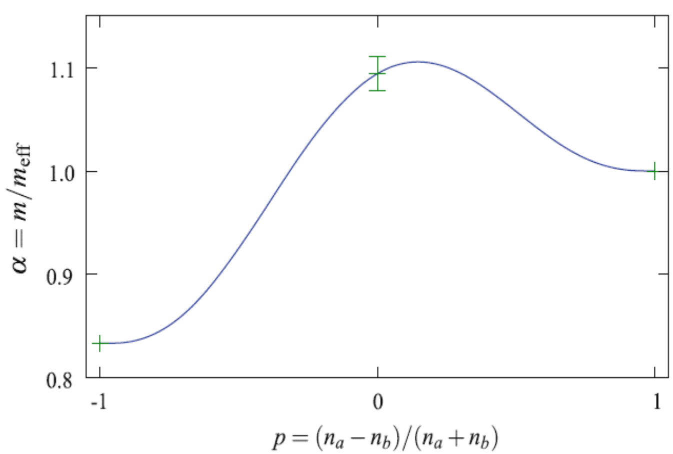
$$E_{SLDA} = \frac{\hbar^2}{m}\left(\frac{\alpha}{2}\left(\tau_\uparrow + \tau_\downarrow\right) + \beta\frac{3}{10}\left(3\pi^2\right)^{2/3}\left(n_\uparrow + n_\downarrow\right)^{5/3}\right) + g\nu^\dagger\nu + \left(1-\alpha\right)\frac{j^2}{2n}$$

Restoring Galilean invariance

Asymmetric Superfluid Local Density Approximation (ASLDA)

$$E_{ASLDA} = \frac{\hbar^2}{m}\left(\left(\frac{\alpha_\uparrow}{2}\tau_\uparrow + \frac{\alpha_\downarrow}{2}\tau_\downarrow\right) + D\left(n_\uparrow, n_\downarrow\right)\right) + g\nu^\dagger\nu + \left(1-\alpha_\uparrow\right)\frac{j_\uparrow^2}{2n_\uparrow} + \left(1-\alpha_\downarrow\right)\frac{j_\downarrow^2}{2n_\uparrow}$$

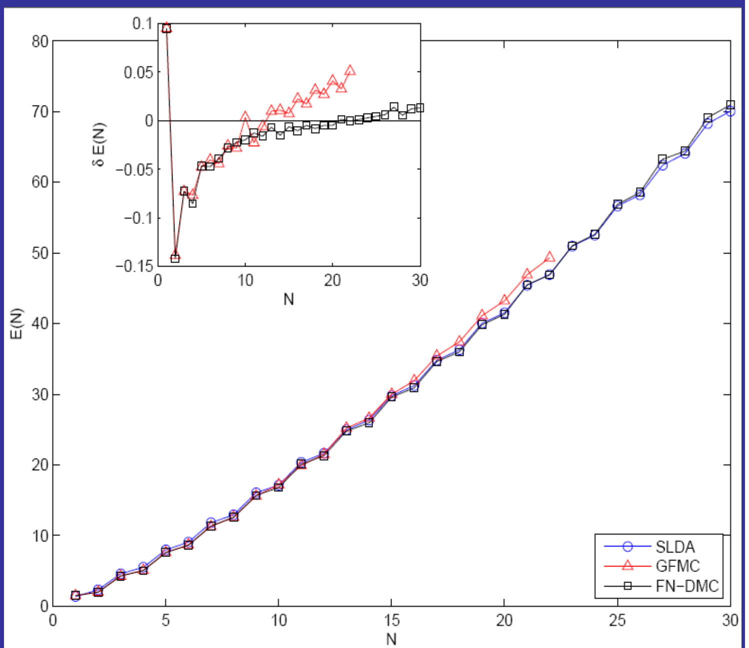
Restoring Galilean invariance



$$D\left(n_\uparrow, n_\downarrow\right) \sim \left(n_\uparrow + n_\downarrow\right)^{5/3}\beta(p)$$

$$D(n_a, n_b) = \frac{\left(6\pi^2(n_a+n_b)\right)^{5/3}}{20\pi^2}\left[G(p) - \alpha(p)\left(\frac{1+p}{2}\right)^{5/3} - \alpha(-p)\left(\frac{1-p}{2}\right)^{5/3}\right]$$

$$\alpha(p) = 1.094 + 0.156p\left(1 - \frac{2p^2}{3} + \frac{p^4}{5}\right) - 0.532p^2\left(1 - p^2 + \frac{p^4}{3}\right)$$



Normal State				Superfluid State			
(N_a, N_b)	E_{FNDMC}	E_{ASLDA}	(error)	(N_a, N_b)	E_{FNDMC}	E_{ASLDA}	(error)
(3,1)	6.6 ± 0.01	6.687	1.3%	(1,1)	2.002 ± 0	2.302	15%
(4,1)	8.93 ± 0.01	8.962	0.36%	(2,2)	5.051 ± 0.009	5.405	7%
(5,1)	12.1 ± 0.1	12.22	0.97%	(3,3)	8.639 ± 0.03	8.939	3.5%
(5,2)	13.3 ± 0.1	13.54	1.8%	(4,4)	12.573 ± 0.03	12.63	0.48%
(6,1)	15.8 ± 0.1	15.65	0.93%	(5,5)	16.806 ± 0.04	16.19	3.7%
(7,2)	19.9 ± 0.1	20.11	1.1%	(6,6)	21.278 ± 0.05	21.13	0.69%
(7,3)	20.8 ± 0.1	21.23	2.1%	(7,7)	25.923 ± 0.05	25.31	2.4%
(7,4)	21.9 ± 0.1	22.42	2.4%	(8,8)	30.876 ± 0.06	30.49	1.2%
(8,1)	22.5 ± 0.1	22.53	0.14%	(9,9)	35.971 ± 0.07	34.87	3.1%
(9,1)	25.9 ± 0.1	25.97	0.27%	(10,10)	41.302 ± 0.08	40.54	1.8%
(9,2)	26.6 ± 0.1	26.73	0.5%	(11,11)	46.889 ± 0.09	45	4%
(9,3)	27.2 ± 0.1	27.55	1.3%	(12,12)	52.624 ± 0.2	51.23	2.7%
(9,5)	30 ± 0.1	30.77	2.6%	(13,13)	58.545 ± 0.18	56.25	3.9%
(10,1)	29.4 ± 0.1	29.41	0.034%	(14,14)	64.388 ± 0.31	62.52	2.9%
(10,2)	29.9 ± 0.1	30.05	0.52%	(15,15)	70.927 ± 0.3	68.72	3.1%
(10,6)	35 ± 0.1	35.93	2.7%	(1,0)	1.5 ± 0.0	1.5	0%
(20,1)	73.78 ± 0.01	73.83	0.061%	(2,1)	4.281 ± 0.004	4.417	3.2%
(20,4)	73.79 ± 0.01	74.01	0.3%	(3,2)	7.61 ± 0.01	7.602	0.1%
(20,10)	81.7 ± 0.1	82.57	1.1%	(4,3)	11.362 ± 0.02	11.31	0.49%
(20,20)	109.7 ± 0.1	113.8	3.7%	(7,6)	24.787 ± 0.09	24.04	3%
(35,4)	154 ± 0.1	154.1	0.078%	(11,10)	45.474 ± 0.15	43.98	3.3%
(35,10)	158.2 ± 0.1	158.6	0.27%	(15,14)	69.126 ± 0.31	62.55	9.5%
(35,20)	178.6 ± 0.1	180.4	1%				

Table 9.2 Comparison between the ASLDA density functional as described in this section and the FN-DMC calculations [136, 137] for a harmonically trapped unitary gas at zero temperature. The normal state energies are obtained by fixing $\Delta = 0$ in the functional: In the FN-DMC calculations, this is obtained by choosing a nodal ansatz without any pairing. In the case of small asymmetry, the resulting "normal states" may be a somewhat artificial construct as there is no clear way of preparing a physical system in this "normal state" when the ground state is superfluid.

GFMC - Chang and Bertsch, Phys. Rev. A 76, 021603(R) (2007)
FN-DMC - von Stecher, Greene and Blume, PRL 99, 233201 (2007)
PRA 76, 053613 (2007)

From A. Bulgac, M.M. Forbes, P. Magierski, Lecture Notes in Physics, vol. 836, p.305 (2012)

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

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

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

We explicitly track fermionic degrees of freedom!

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

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

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

$$\begin{aligned} \Delta(\mathbf{r}) &= g_{eff}(\mathbf{r})\chi_c(\mathbf{r}) \\ \frac{1}{g_{eff}(\mathbf{r})} &= \frac{1}{g(\mathbf{r})} - \frac{mk_c(\mathbf{r})}{2\pi^2\hbar^2}\left(1 - \frac{k_F(\mathbf{r})}{2k_c(\mathbf{r})}\ln\frac{k_c(\mathbf{r})+k_F(\mathbf{r})}{k_c(\mathbf{r})-k_F(\mathbf{r})}\right) \end{aligned}$$

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

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

- 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)
- A. Bulgac, M.M. Forbes, P. Magierski, Lecture Notes in Physics, Vol. 836, Chap. 9, p.305-373 (2012)

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

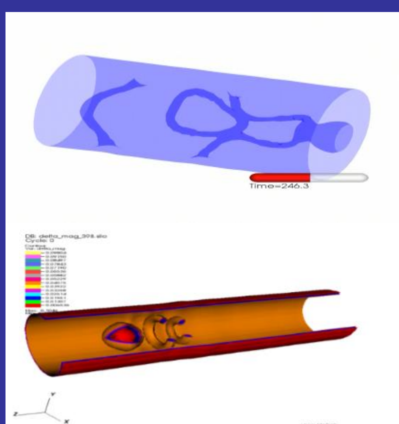
(for cold atomic systems – time scale: a few ms
for nuclei – time scale: 100 zs)

Superconducting systems of interest

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

Ultracold atomic (fermionic) gases. Unitary regime.

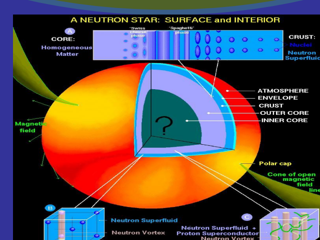
Dynamics of quantum vortices, solitonic excitations, quantum turbulence



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

Astrophysical applications.

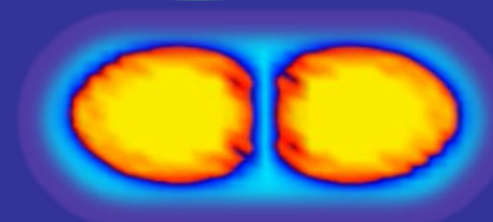
Modelling of neutron star interior (glitches): vortex dynamics, dynamics of inhomogeneous nuclear matter.

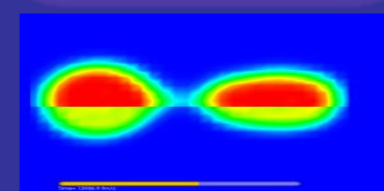


$$\frac{\Delta}{\varepsilon_F} \le 0.03$$

Nuclear physics.

Induced nuclear fission, fusion, collisions.





$\frac{\Delta}{\varepsilon_F}$ **- Pairing gap to Fermi energy ratio**

Nuclear Skyrme functional

$$E = \int d^3 r \mathcal{H}(\mathbf{r})$$

where

$$\begin{aligned}\mathcal{H}(\mathbf{r}) &= C^\rho \rho^2 + C^s \vec{s}\cdot\vec{s} + C^{\Delta\rho}\rho\nabla^2\rho + C^{\Delta s}\vec{s}\cdot\nabla^2\vec{s} + C^\tau(\rho\tau - \vec{j}\cdot\vec{j}) + \\ &+ C^{sT}(\vec{s}\cdot\vec{T} - \mathbf{J}^2) + C^{\nabla J}(\rho\vec{\nabla}\cdot\vec{J} + \vec{s}\cdot(\vec{\nabla}\times\vec{j})) + C^{\nabla s}(\vec{\nabla}\cdot\vec{s})^2 + C^\gamma\rho^\gamma - \Delta\chi^*\end{aligned}$$

where

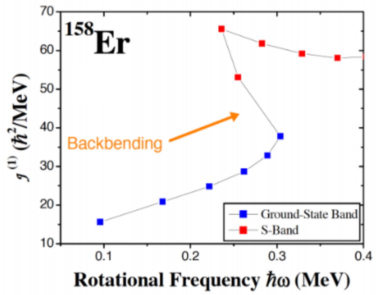
$$\begin{aligned}J_i &= \sum_{k,l}\epsilon_{ikl}\mathbf{J}_{kl}\\ \mathbf{J}^2 &= \sum_{k,l}\mathbf{J}_{kl}^2\end{aligned}$$

- density: $\rho(\mathbf{r}) = \rho(\mathbf{r},\mathbf{r}')|_{r=r'}$
- spin density: $\vec{s}(\mathbf{r}) = \vec{s}(\mathbf{r},\mathbf{r}')|_{r=r'}$
- current: $\vec{j}(\mathbf{r}) = \frac{1}{2i}(\vec{\nabla} - \vec{\nabla}')\rho(\mathbf{r},\mathbf{r}')|_{r=r'}$
- spin current (2nd rank tensor): $\mathbf{J}(\mathbf{r}) = \frac{1}{2i}(\vec{\nabla} - \vec{\nabla}')\otimes\vec{s}(\mathbf{r},\mathbf{r}')|_{r=r'}$
- kinetic energy density: $\tau(\mathbf{r}) = \vec{\nabla}\cdot\vec{\nabla}'\rho(\mathbf{r},\mathbf{r}')|_{r=r'}$
- spin kinetic energy density: $\vec{T}(\mathbf{r}) = \vec{\nabla}\cdot\vec{\nabla}'\vec{s}(\mathbf{r},\mathbf{r}')|_{r=r'}$
- anomalous (pairing) density: $\chi(\mathbf{r}) = \chi(\mathbf{r},\mathbf{r}')|_{r=r'}$

What do we know about pairing correlations in atomic nuclei?

Odd-even mass staggering gives us estimate of the pairing strength (unfortunately obscured by polarization effects)

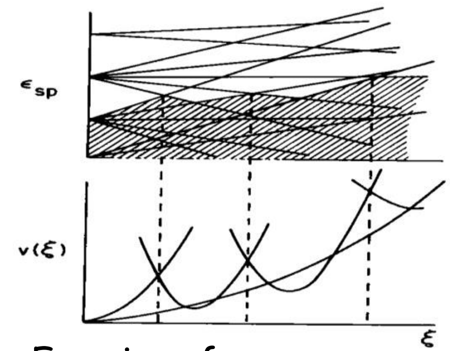
$$|\Delta| \approx \frac{12}{\sqrt{A}} \text{ MeV}$$



A. Johnson, H. Ryde, S.A. Hjorth, Nucl. Phys. A179, 753 (1972)

High spin experimental data: backbending of moments of inertia produced by the alignment of the correlated nucleon pair is a sensitive function of pairing correlations.

Theoretical description of large amplitude nuclear motion require to include pairing correlations.



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)

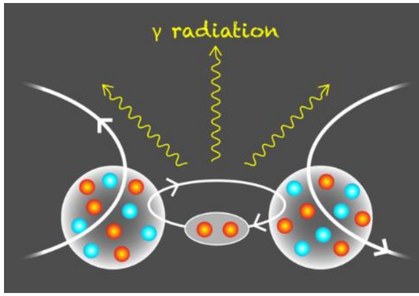
Can we probe the pairing field phase in nuclei?

Nuclear Josephson junction: enhancement of neutron pair transfer in nuclear collision

V.I. Gol'danskii, A.I. Larkin JETP 53, 1032 (1967)

K. Dietrich, Phys.Lett. B32, 428 (1970)

(Unfortunately experimental data are not conclusive)



From P.M., Physics 14,27(2021)

Recent attempt: oscillatory pair transfer (AC Josephson junction)

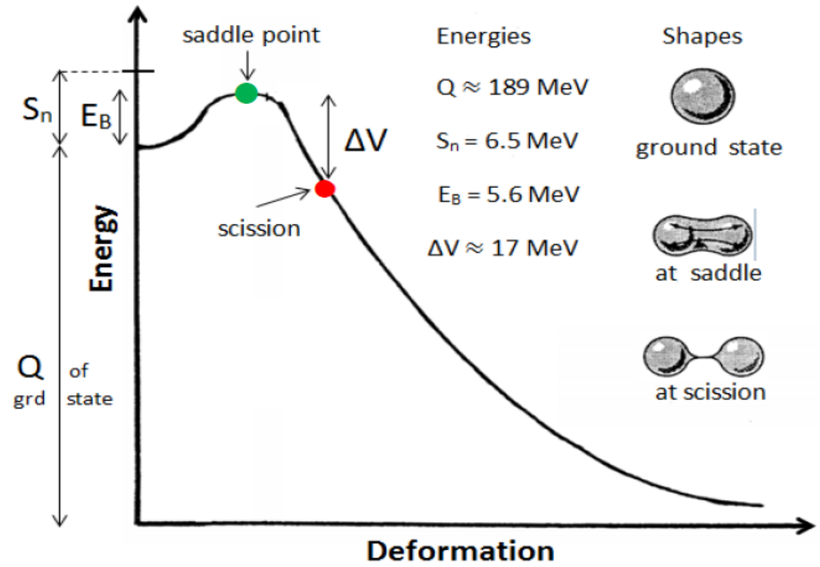
C.Potel,F.Barranco,E.Vigezzi, R.A. Broglia, Phys.Rev. C103, L021601(2021)

surprising agreement of gamma spectra with experiment!

(Although just one reaction: ^{116}Sn+ ^{60}Ni has been studied)

Nuclear fission dynamics

Potential energy versus deformation

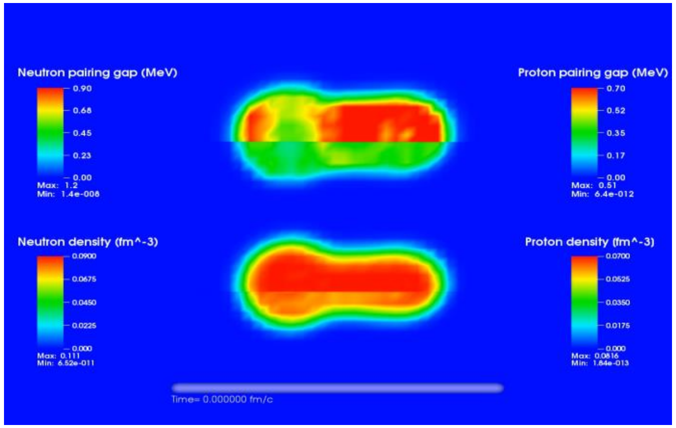


From F. Gonnenwein FIESTA2014

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
1 zs = 10^{-21} s

Fission dynamics of *^{240}Pu within TDSLDA*



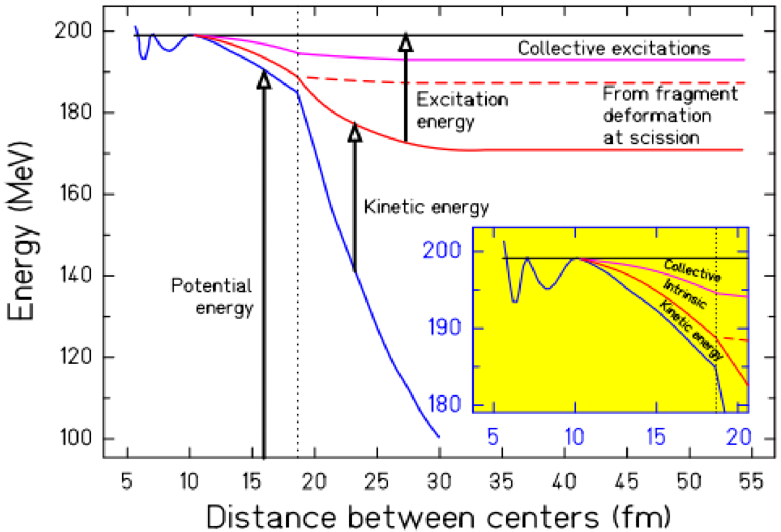
Total kinetic energy of the fragments

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)

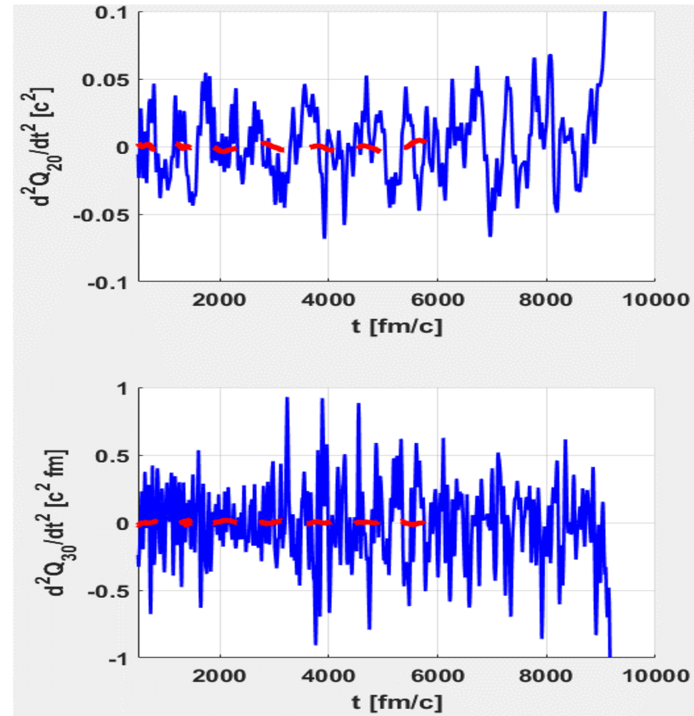
Q: Excitation energy sharing of the fragments



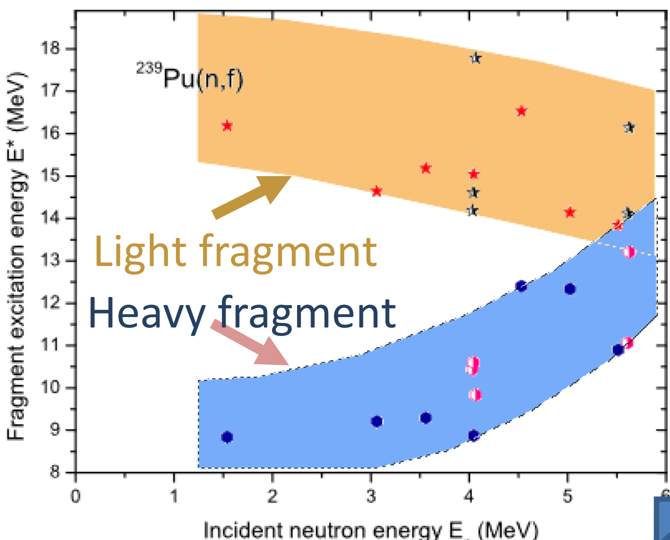
Schmidt&Jurado:Phys.Rev.C83:061601,2011

Character of nuclear motion along the fission path – from TDSLDA

Accelerations in quadrupole and octupole moments



TDSLDA energy sharing between fragments



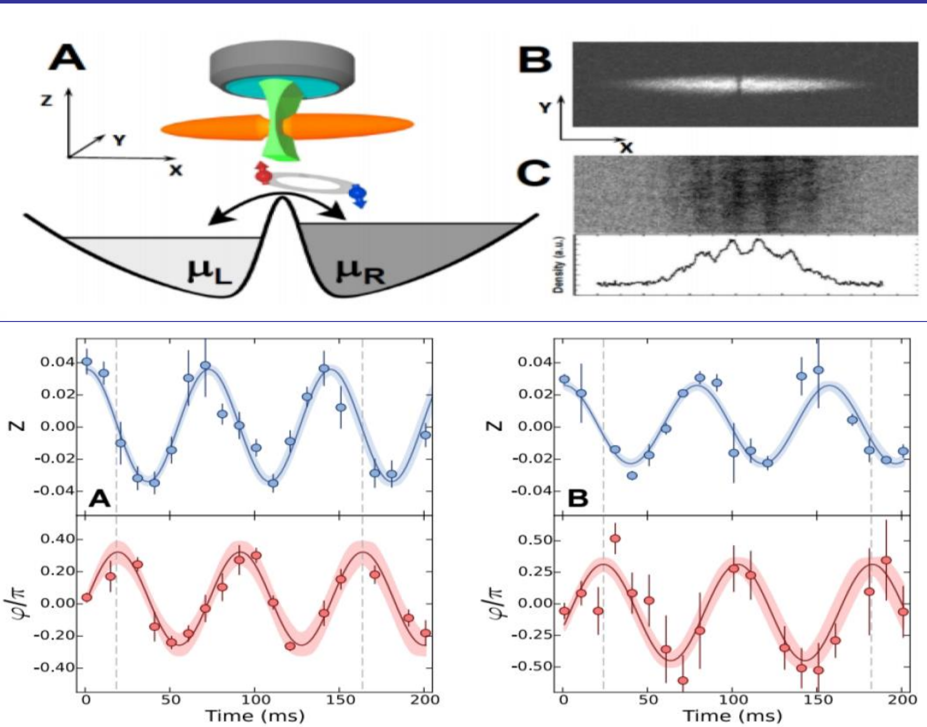
It is important to realize that these results indicate that the motion <u>is not adiabatic, although it is slow.</u>

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.

Two regimes for phase-induced effects in fermionic superfluids

Weak coupling (weak link)



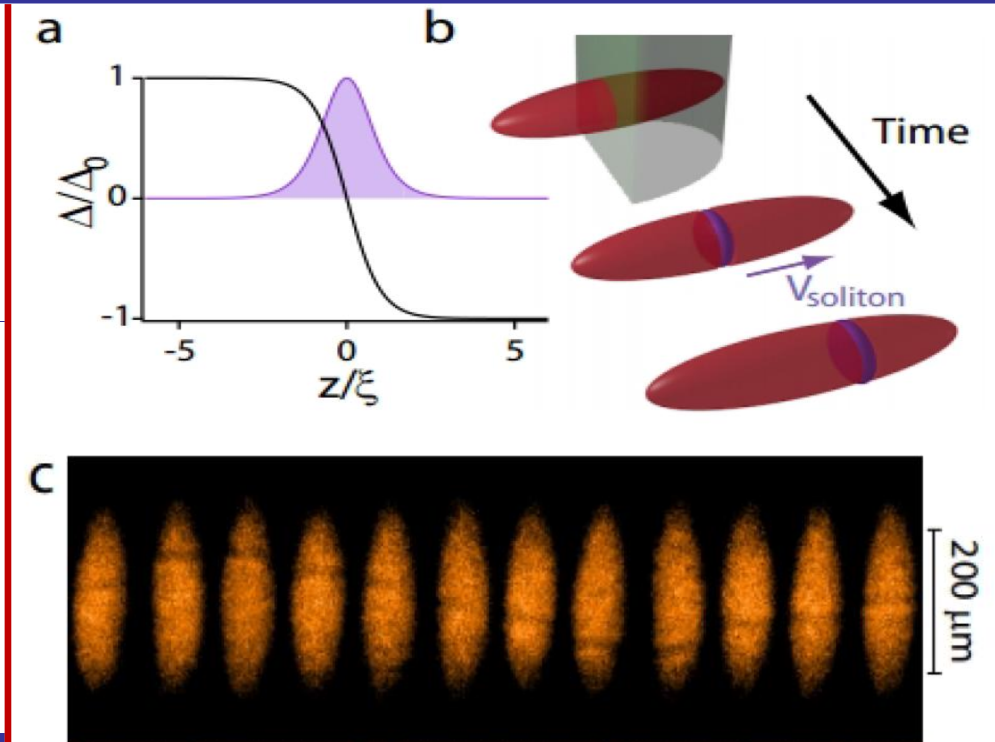
Observation of ***AC Josephson effect*** between two 6Li atomic clouds.

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

Superflow is accompanied with creation of topological excitations (vortices) leading to energy dissipation.

G. Wlazłowski, K. Xhani, M. Tylutki, N.P. Proukakis, P. Magierski, Phys. Rev. Lett. **130**, 023003 (2023)

Strong coupling



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

T. Yefsah et al., Nature 499, 426 (2013);
M.J.H. Ku et al., Phys. Rev. Lett. 116, 045304 (2016)

„Heavy soliton" decays through the unique sequence of topological excitations.

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

Nuclear collisions

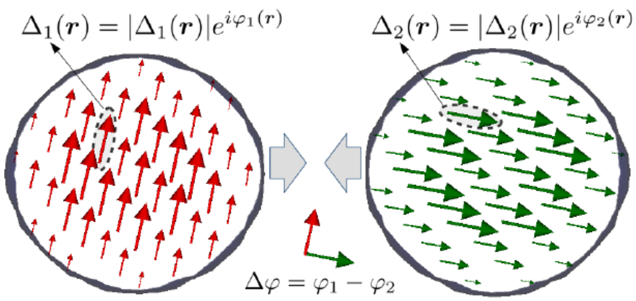
Collisions of superfluid nuclei having <u>different phases</u> of the <u>pairing fields</u>

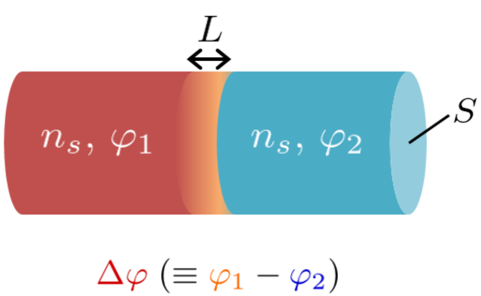
<u>The main questions are:</u>

-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.



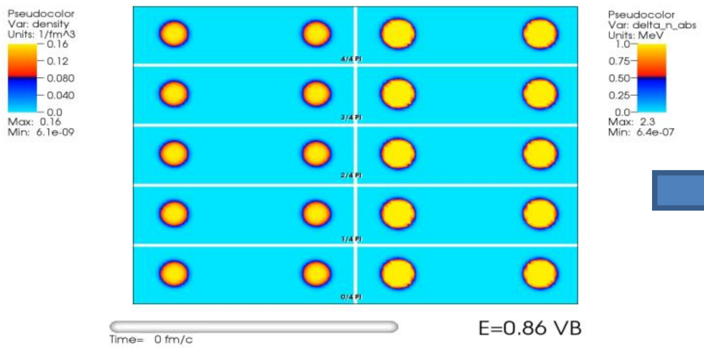


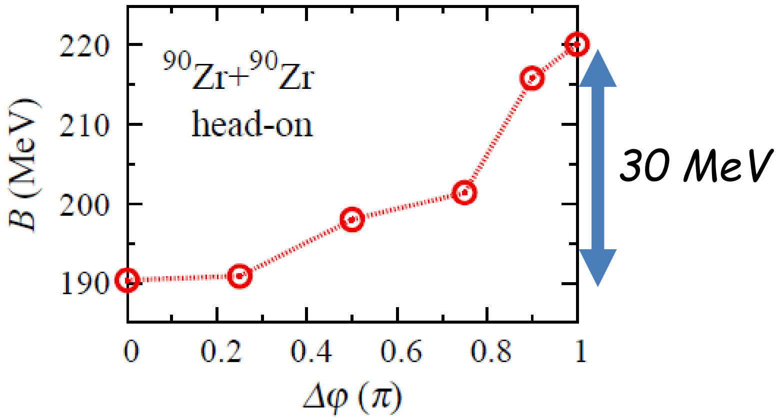
From Ginzburg-Landau (G-L) approach:

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

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

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 30MeV for medium nuclei and occur for energies up to 20-30% of the barrier height.

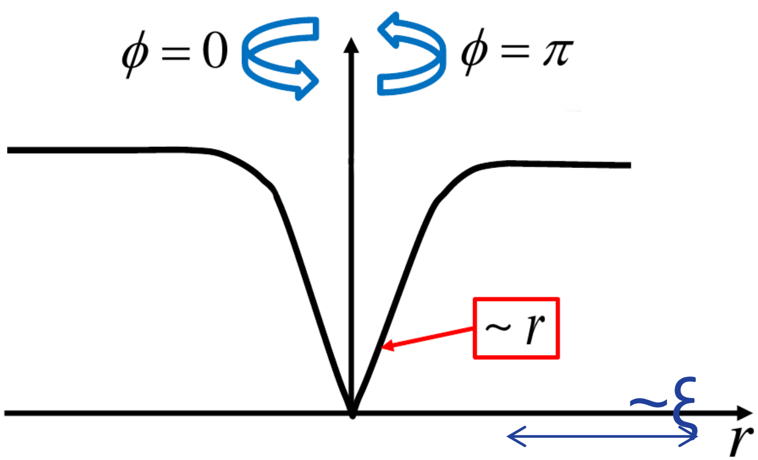
P. Magierski, K. Sekizawa, G. Wlazłowski, Phys. Rev. Lett. 119 042501 (2017)

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

Anatomy of the vortex core

BOSONS: $\Psi(\vec{r}) = \left|\Psi(\vec{r})\right| e^{i\phi(\vec{r})}$



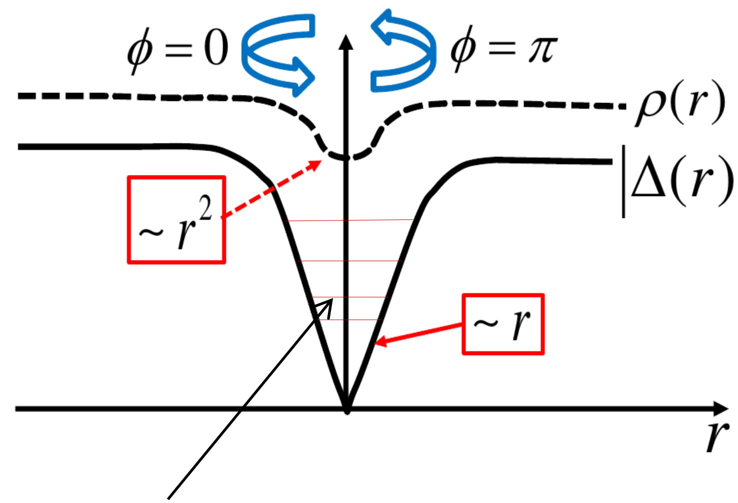
Order parameter:

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

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

At T=0 the core is empty

FERMIONS: $\Delta(\vec{r}) = \left|\Delta(\vec{r})\right| e^{i\phi(\vec{r})}$



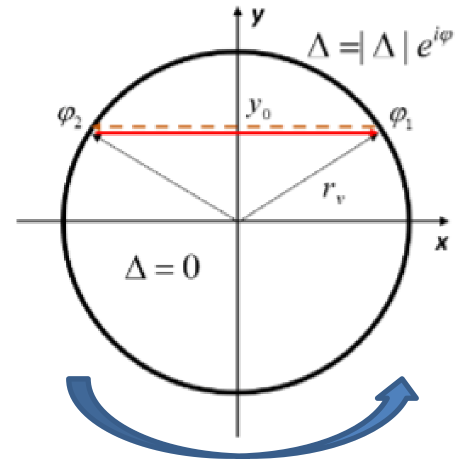
Andreev states affect the density distribution inside the core.

Order parameter: $\Delta(\vec{r},t) = \left|\Delta(\vec{r},t)\right| e^{i\phi(\vec{r},t)}$
not related directly to density

The core is not empty!

Vortex core structure in Andreev approximation:

Schematic section of the core

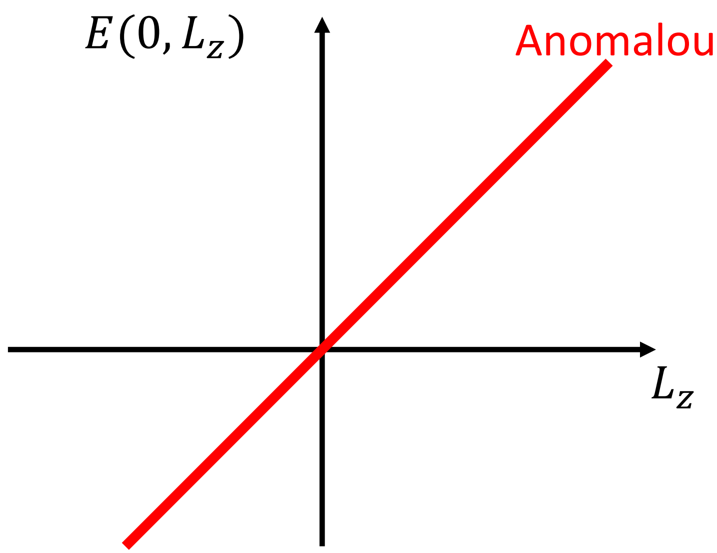


$$\frac{E(0,L_z)}{\varepsilon_F} k_F r_V \sqrt{1-\left(\frac{L_z}{k_F r_V}\right)^2} + \arccos\left(\frac{-L_z}{k_F r_V}\right) - \arccos\left(\frac{E(0,L_z)}{|\Delta_\infty|}\right) = 0$$

$$E(0,L_z) = E(0)L_z,\ E \ll |\Delta_\infty|$$

$$E(0,L_z) \approx \frac{|\Delta_\infty|^2}{\varepsilon_F \frac{r_V}{\xi}\left(\frac{r_V}{\xi}+1\right)} \frac{L_z}{\hbar}, \qquad \xi = \frac{\varepsilon_F}{k_F |\Delta_\infty|}$$

Spectrum of in-gap states

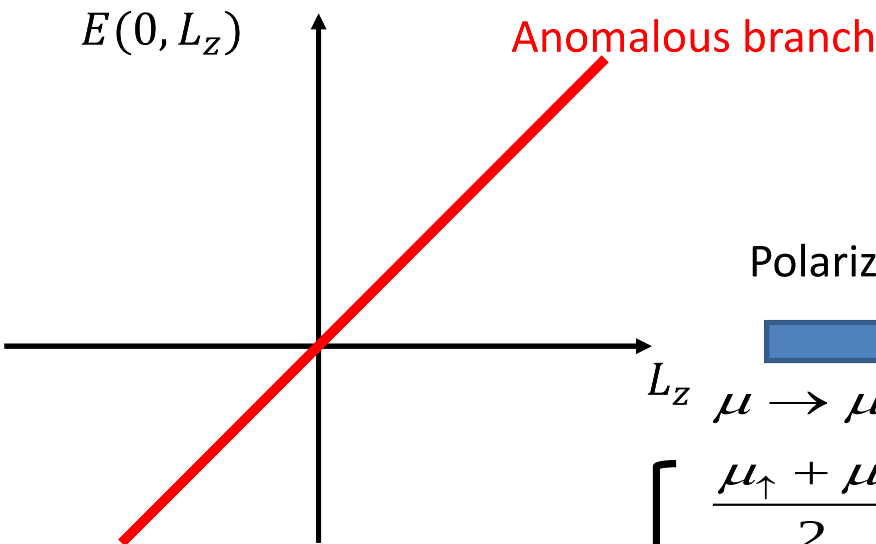


Works well in deep BCS limit: $\frac{1}{k_F a_s} \ll 0$

M. Stone, Phys. Rev. B 54, 13222 (1996)
P.M. G. Wlazłowski, A. Makowski, K. Kobuszewski, Phys. Rev. A 106, 033322 (2022)

Changes of the core structure induced by spin polarization

Unpolarized core

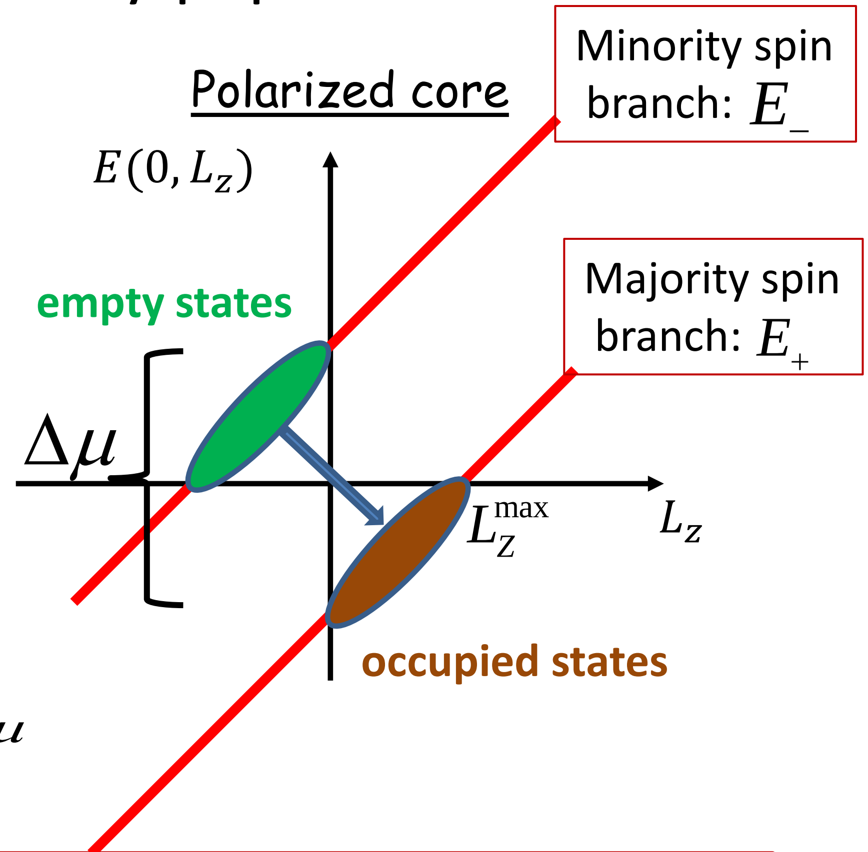


Polarization

$$\mu \rightarrow \mu_\uparrow, \mu_\downarrow$$

$$\begin{cases} \dfrac{\mu_\uparrow + \mu_\downarrow}{2} = \mu \\ \mu_\uparrow - \mu_\downarrow = \Delta\mu \end{cases}$$

Polarized core



Branches are split proportionally to polarization

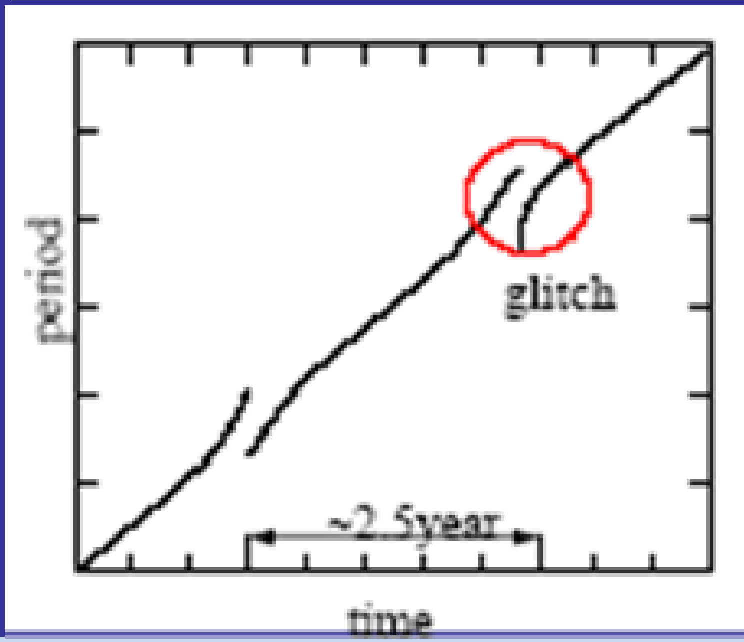
$$E_\pm(0, L_Z) \approx \frac{|\Delta_\infty|^2}{\varepsilon_F \dfrac{r_V}{\xi}\left(\dfrac{r_V}{\xi} + 1\right)} \frac{L_Z}{\hbar} \mp \frac{\Delta\mu}{2}$$

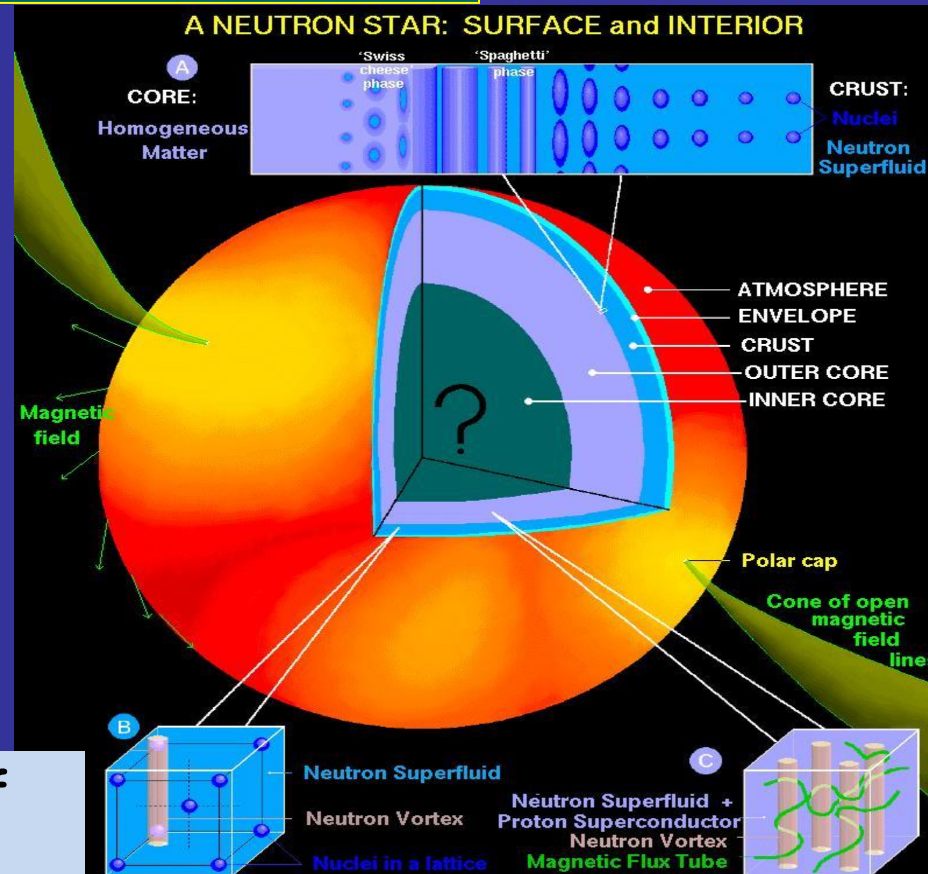
Certain fraction of majority spin particles rotate in the opposite direction!

$$L_Z^{\max} \approx \frac{1}{2} \frac{\varepsilon_F}{|\Delta_\infty|^2} \frac{r_V}{\xi}\left(\frac{r_V}{\xi} + 1\right) \hbar\Delta\mu$$

Neutron stars and quantum turbulence

Neutron star is a huge superfluid



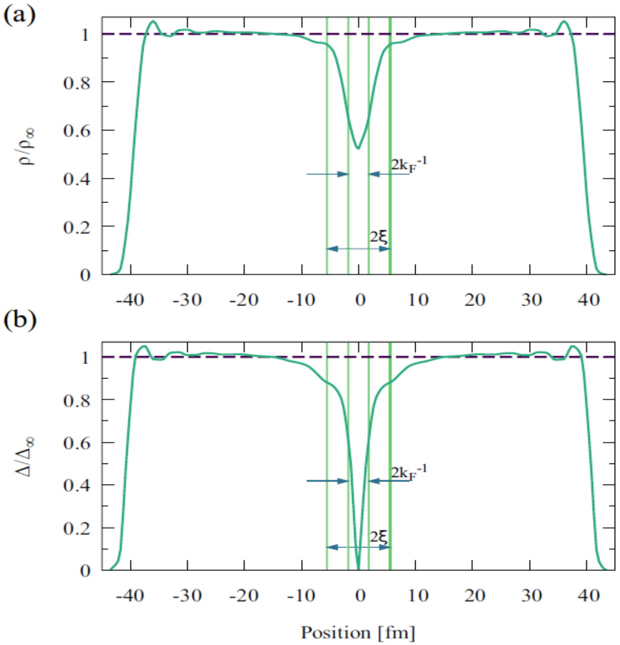


glitch phenomenon=a sudden speed up of rotation.
To date more than 300 glitches have been detected in more than 100 pulsars

Glitch phenomenon is commonly believed to be related to rearrangement of vortices in the interior of neutron stars. It would require however a correlated behavior of huge number of quantum vortices and the mechanism of such collective rearrangement is still a mystery.

Example: vortices across the neutron star crust

Section through the vortex core

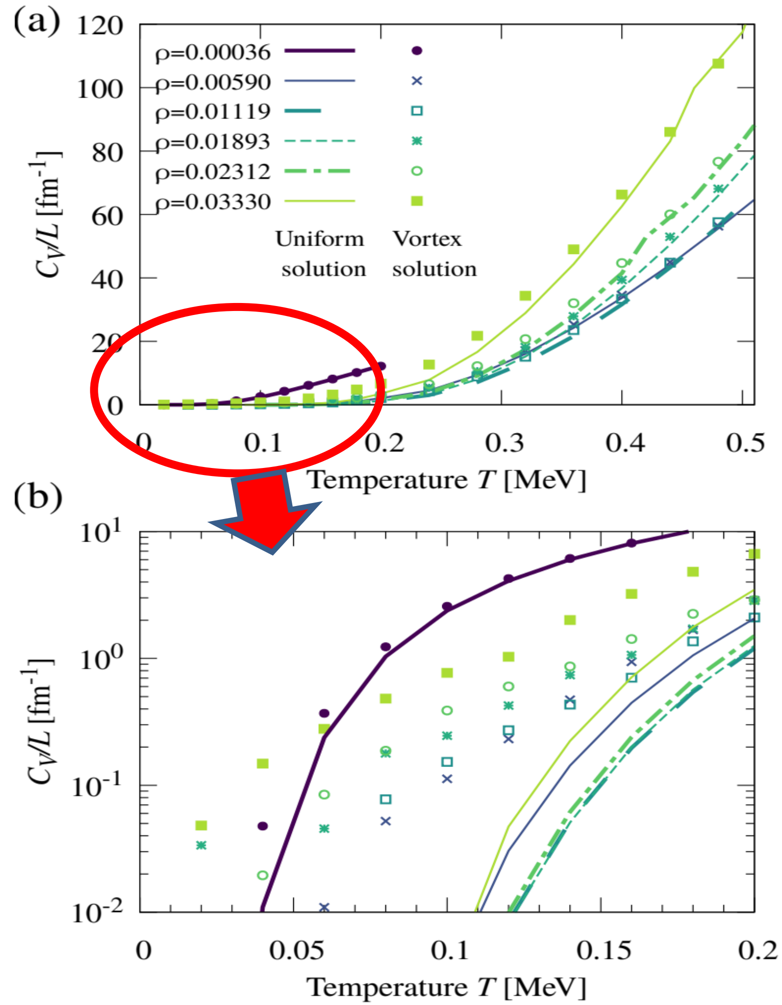


Normal density

Pairing field

Note two different length scales inside the core as explained by:
Sensarma, Randeria, Ho, Phys. Rev. Lett. 96, 090403 (2006)

Specific heat contribution vs uniform matter



ρ_∞ (fm^{-3})	0.00036	0.0059	0.0112	0.0189	0.0231	0.0333
k_F^{-1} (fm)	4.52	1.79	1.45	1.21	1.14	1.01
ξ (fm)	8.44	5.53	5.97	7.00	7.78	10.28
$R_{\rm VFM}$ (fm)	15.0	10.5	10.5	12.0	13.5	16.5
Δ_∞ (MeV)	0.35	1.33	1.53	1.55	1.50	1.28
$T_{\rm crit}$ (MeV)	0.20	0.76	0.87	0.88	0.85	0.73
$\varepsilon_{\rm F}$ (MeV)	1.01	6.48	9.93	14.09	16.10	20.53
μ (MeV)	0.80	4.21	5.80	7.30	7.91	9.09
$E_{\rm mg}$ (MeV)	0.090	0.308	0.261	0.199	0.152	0.009
$B_{\rm crit}$ (10^{15} G)	7.76	26.5	22.5	17.2	13.1	0.82

Minigap values

Magnetic field needed to polarize the core

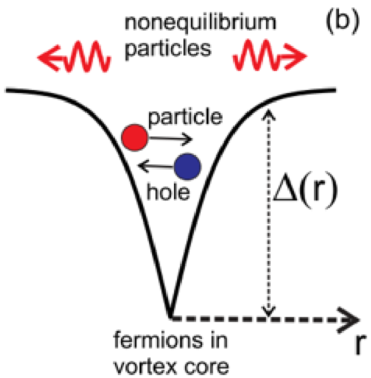
D. Pęcak, N. Chamel, P.M., G. Wlazłowski, Phys. Rev. C**104**, 055801 (2021)

How can we measure the influence of core states in ultracold gases?

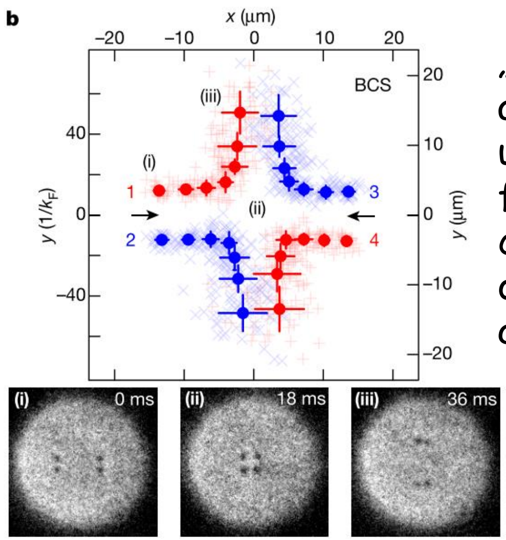
Dissipative processes involving vortex dynamics.

Silaev, Phys. Rev. Lett. 108, 045303 (2012)
Kopnin, Rep. Prog. Phys. 65, 1633 (2002)
Stone, Phys. Rev. B54, 13222 (1996)
Kopnin, Volovik, Phys. Rev. B57, 8526 (1998)
....

Classical treatment of states in the core (Boltzmann eq.).
More applicable in deep BCS limit unreachable in ultracold atoms.



Vortex-antivortex scattering in 2D



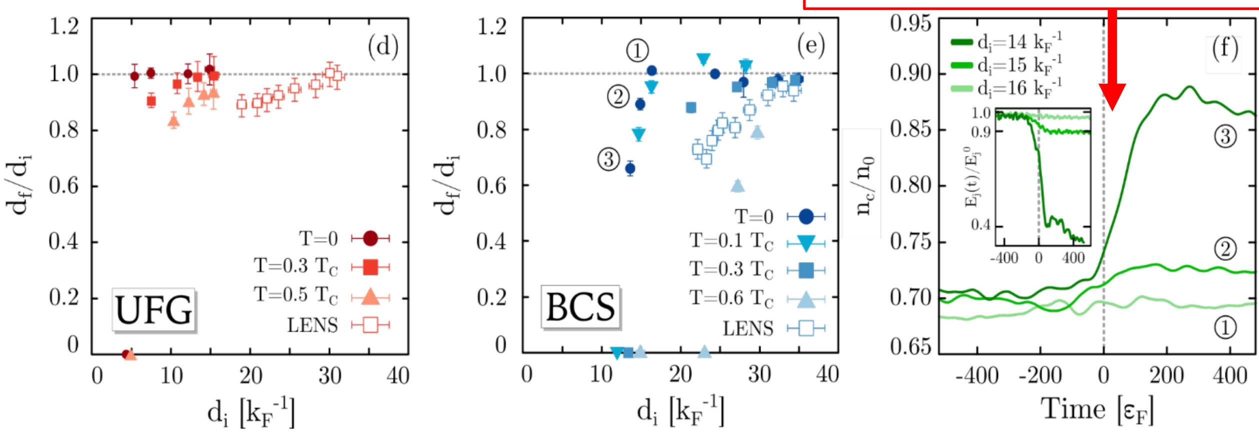
„Further, our few-vortex experiments extending across different superfluid regimes reveal non-universal dissipative dynamics, suggesting that fermionic quasiparticles localized inside the vortex core contribute significantly to dissipation, thereby opening the route to exploring new pathways for quantum turbulence decay, vortex by vortex."

W.J. Kwon et al. Nature **600**, 64 (2021)

Exciting quasiparticles in the vortex core

Indeed quasiparticles in the core are excited due to vortex acceleration but the effect is too weak to account for the total dissipation rate.

A. Barresi, A. Boulet, P.M., G. Wlazłowski, Phys. Rev. Lett. 130, 043001 (2023)



Inhomogeneous systems: Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase

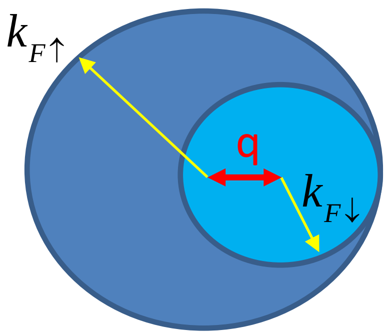
Larkin-Ovchinnikov (LO): $\Delta(r) \sim cos(\vec{q} \cdot \vec{r})$

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

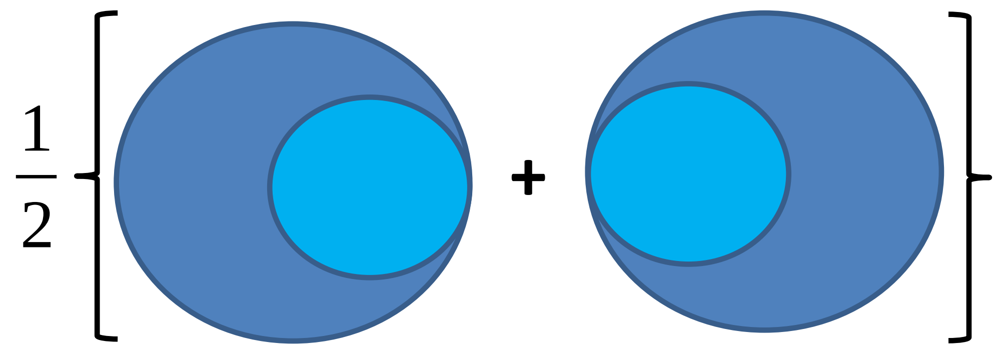
A.I. Larkin and Y. N. Ovchinnikov, Sov. Phys. JETP 20, 762 (1965)
P. Fulde and R. A. Ferrell, Phys. Rev. 135, A550 (1964)

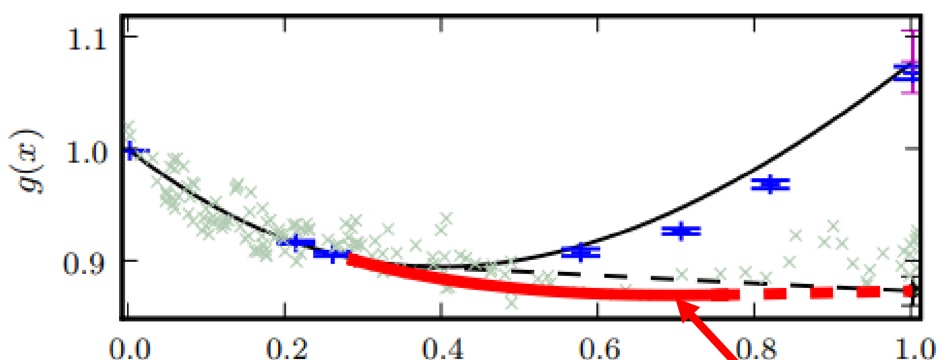
Spatial modulation of the pairing field cost energy proportional to q^2 but may be compensated by an increased pairing energy due to the mutual shift of Fermi spheres:

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)

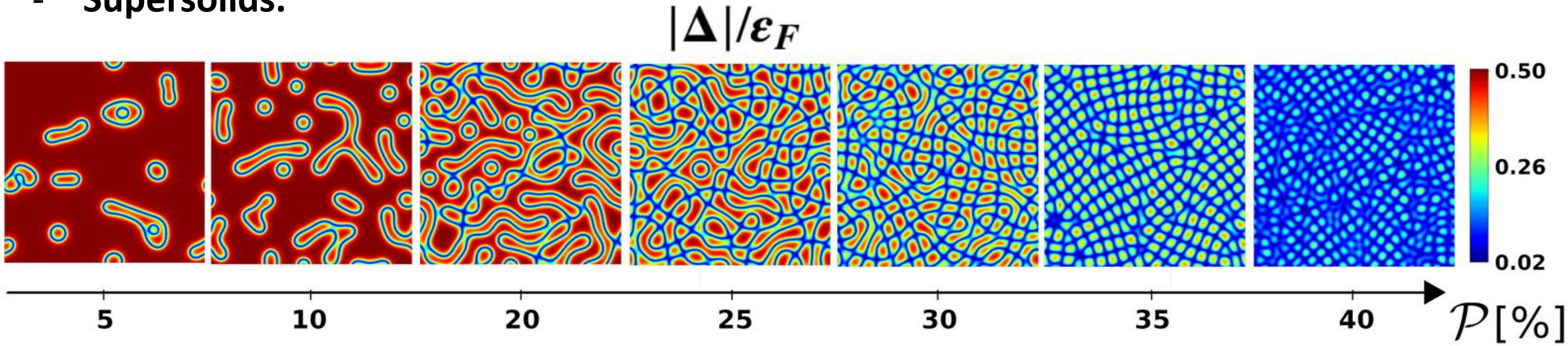
LO configuration – supersolid state

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)

What is going to happen if we keep increasing spin imbalance?

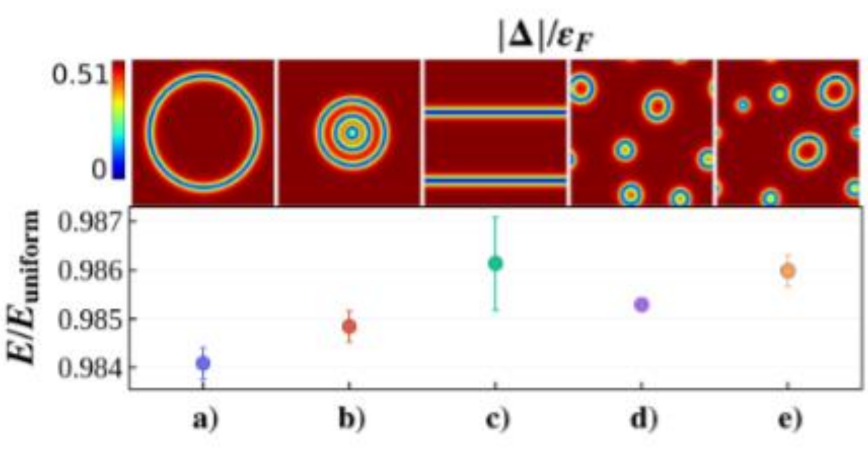
In general it will generate distortions of Fermi spheres locally and triggering the appearance of **pairing field inhomogeneity** leading to various patterns involving:

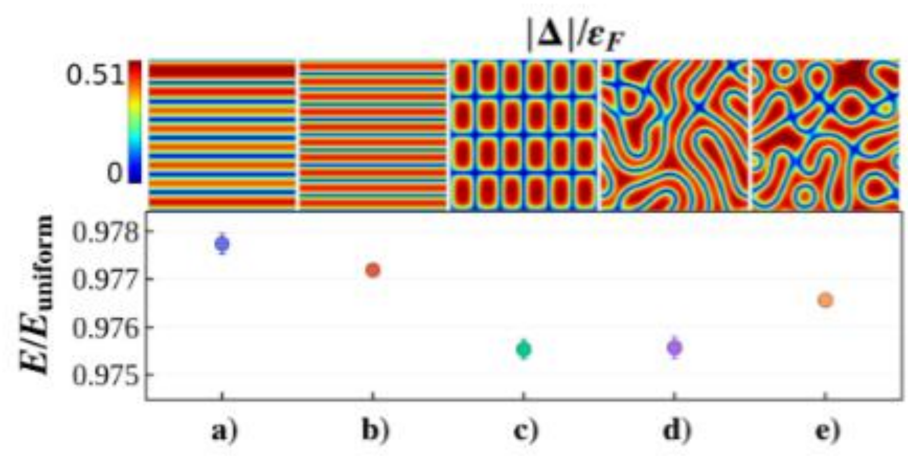
- **Separate impuritites (ferrons),**
- **Liquid crystal-like structure,**
- **Supersolids.**



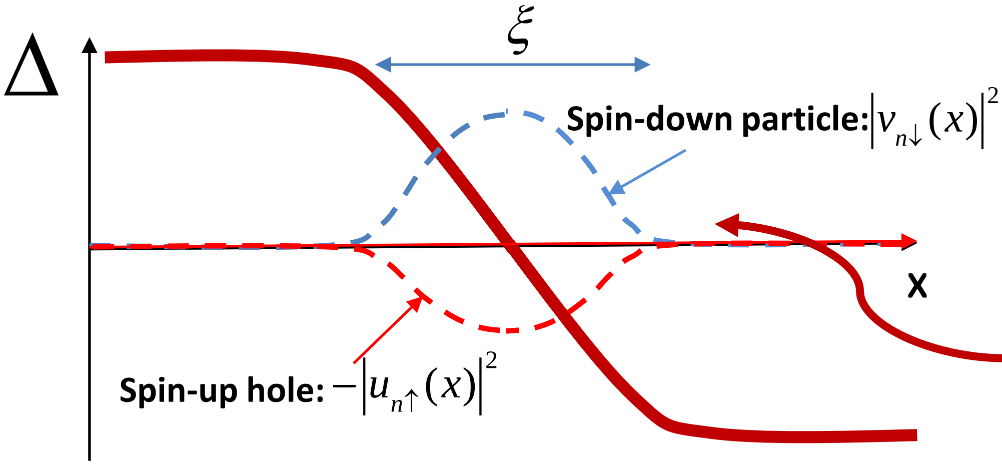
B. Tüzemen, T. Zawiślak, P.M., G. Wlazłowski, New J. Phys. 25, 033013 (2023)

$$P = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}$$





Andreev states and stability of pairing nodal points



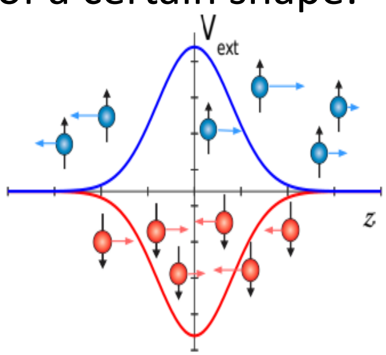
Due to quasiparticle scattering the localized Andreev states appear at the nodal point. These states induce local spin-polarization

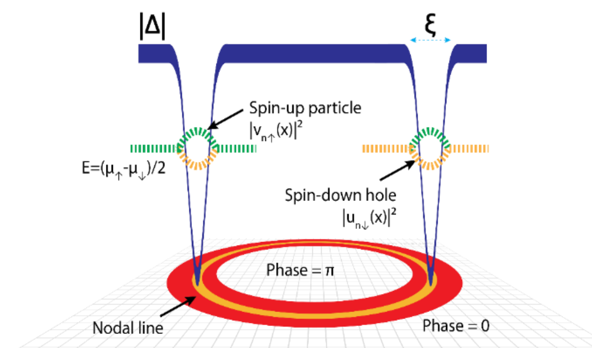
BdG in the Andreev approx. ($\Delta \ll k_F^2$)

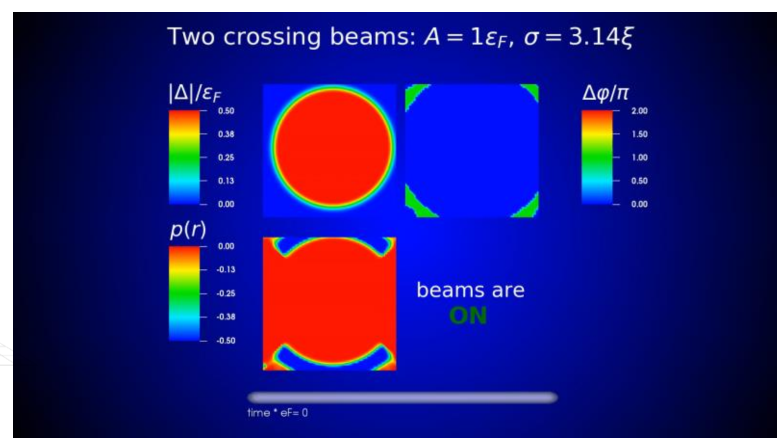
$$\begin{bmatrix} -2ik_F \dfrac{d}{dx} & \Delta(x) \\ \Delta^*(x) & 2ik_F \dfrac{d}{dx} \end{bmatrix} \begin{bmatrix} u_{n\uparrow}(x) \\ v_{n\downarrow}(x) \end{bmatrix} = E_n \begin{bmatrix} u_{n\uparrow}(x) \\ v_{n\downarrow}(x) \end{bmatrix}$$

Engineering the structure of nodal surfaces

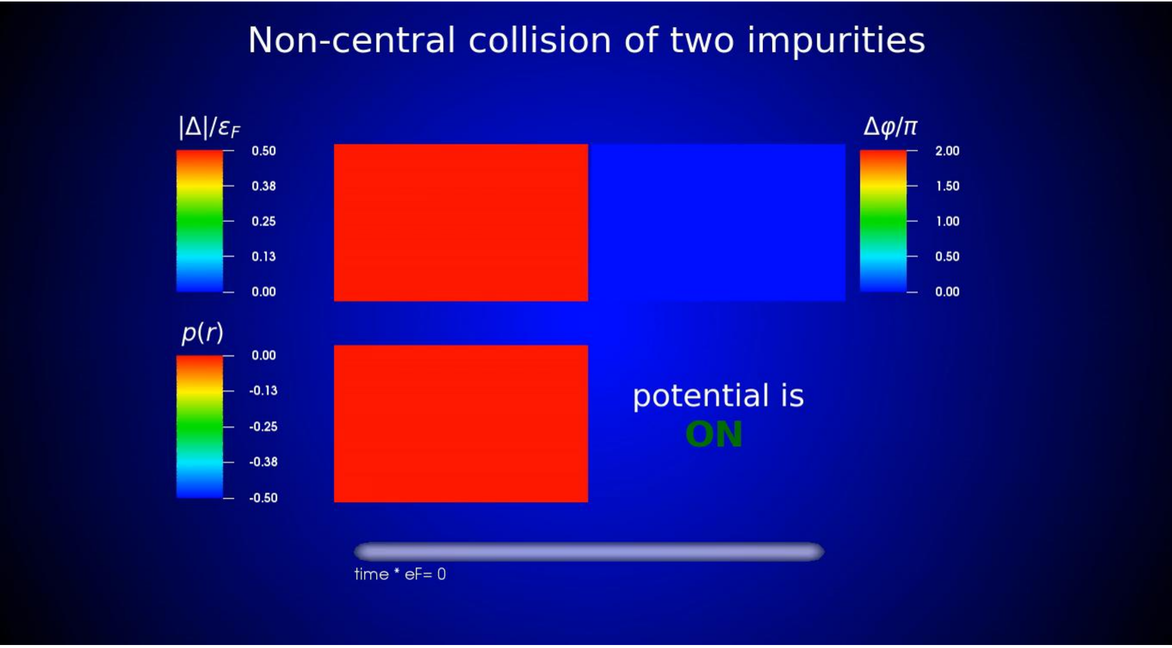
Apply the spin-selective potential of a certain shape:







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:

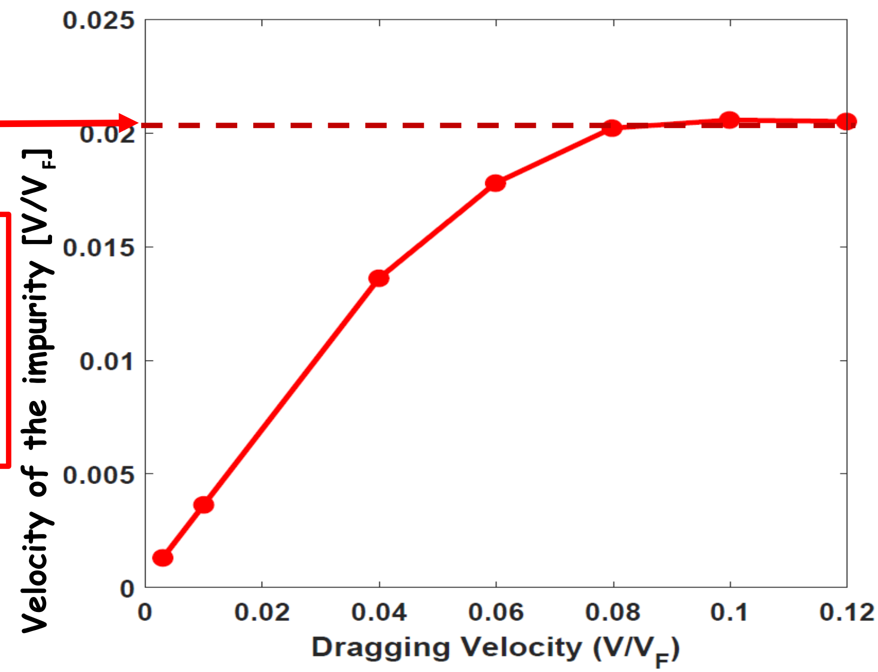
$$\Delta(r) : cos(qr) \Rightarrow \exp(iqr)$$

Surprisingly, the nodal structure remains stable even during collisions

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

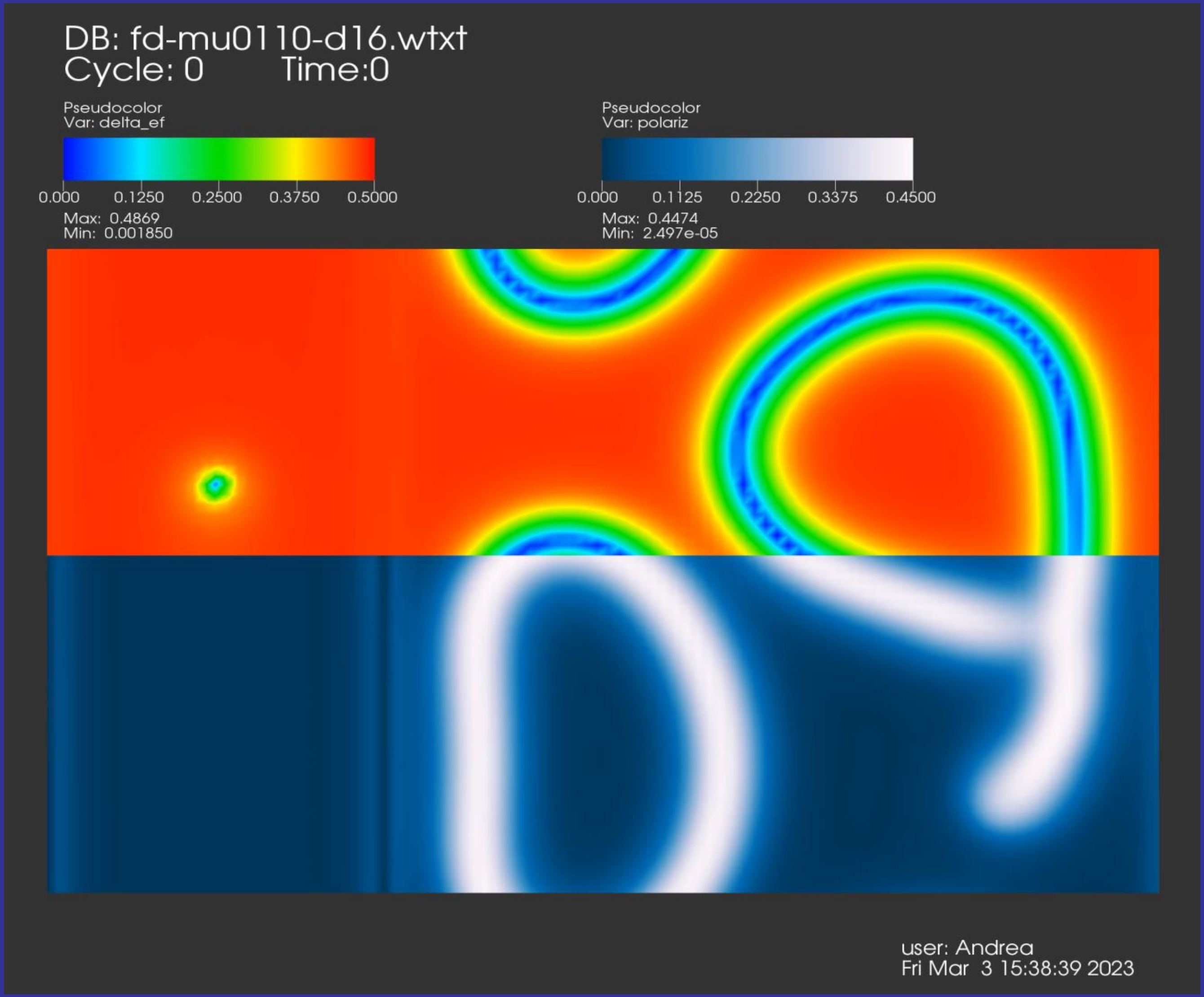
Limiting velocity with respect to superfluid background

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 100, 033613 (2019); Phys. Rev. A 104, 033304 (2021)

Complex dynamics (strongly damped) of vortices in the spin imbalanced environment



Thanks to A. Barresi *et al.*

THANK YOU

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

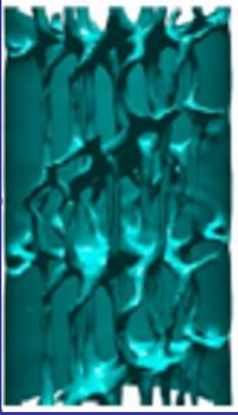
1) There are easy and difficult observables in DFT.
   In general: easy observables are one-body observables. They are easily extracted and reliable.

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

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

Nonequilibrium superfluidity in Fermi systems



Quantum turbulence

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Vortex dynamics in neutron star crust

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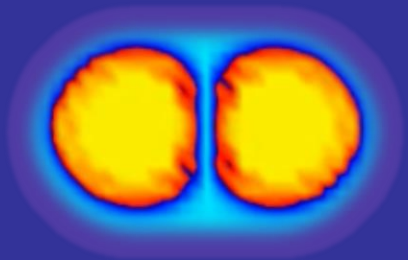

Nuclear collisions

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Josephson junction in atomic Fermi gases - dissipative effects

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Collisions of vortex-antivortex pairs

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Spin-imbalanced Fermi gases

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