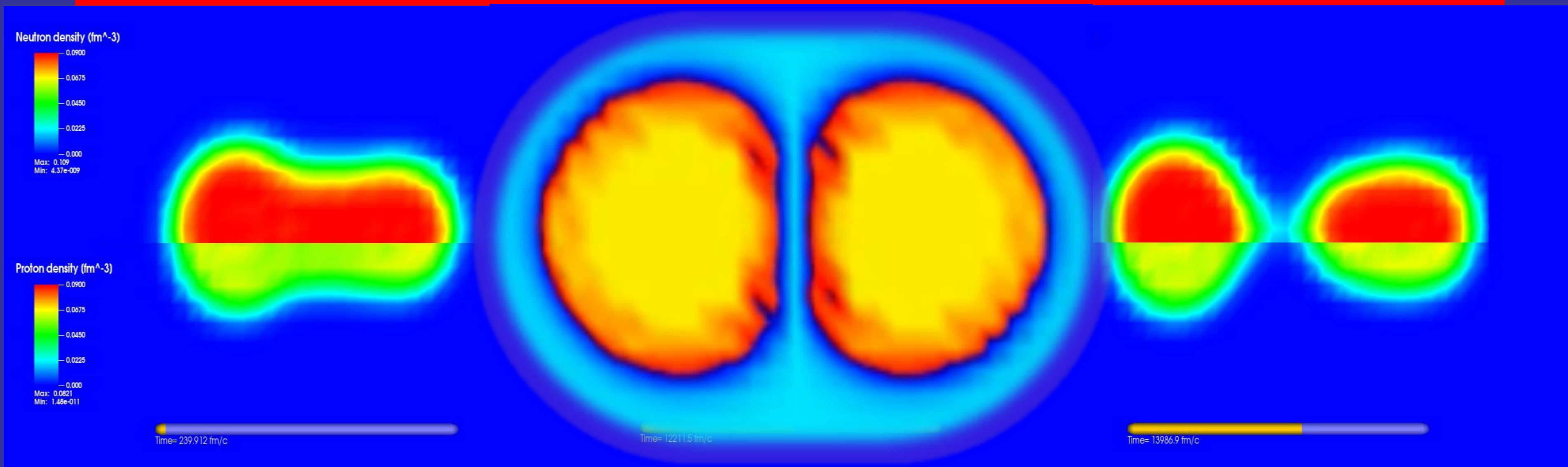
Nuclear reactions in the framework of time-dependent density functional theory with pairing correlations.



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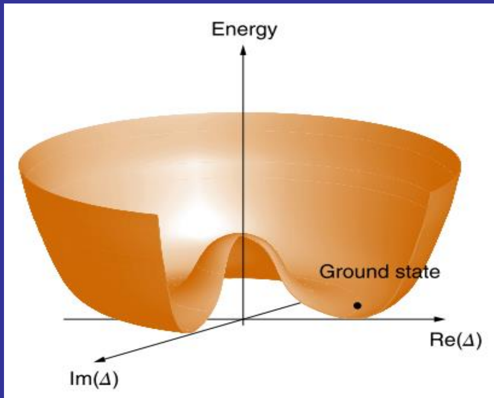

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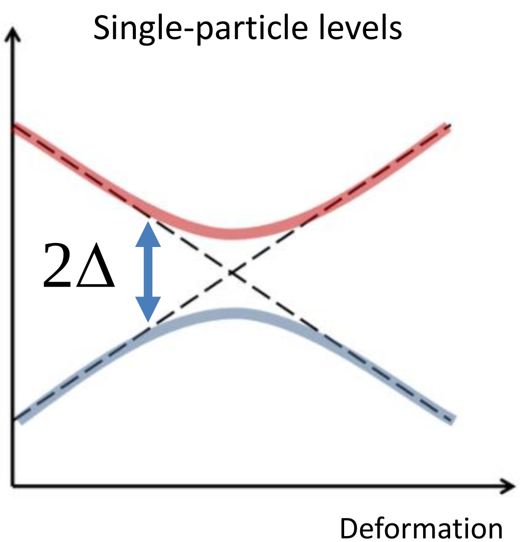
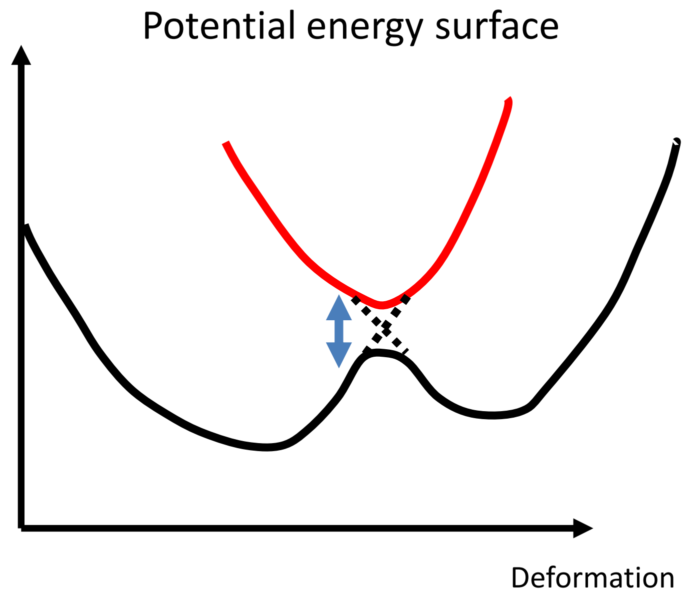
V International Conference on
Nuclear Structure & Dynamics
Valencia, 27-31 May 2024

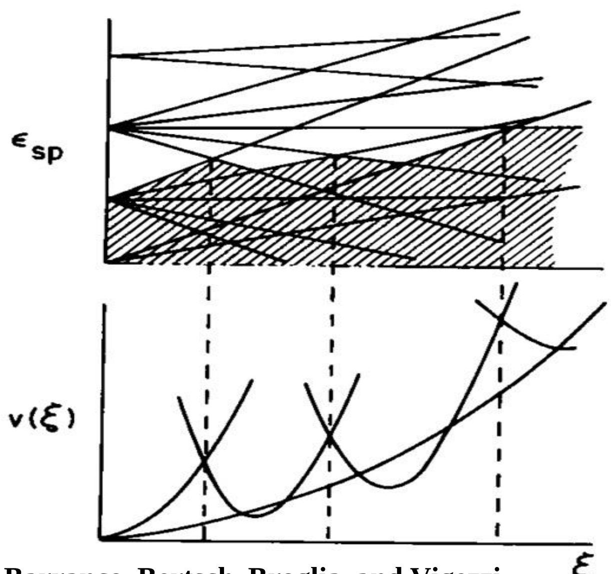
Pairing as an energy gap

Quasiparticle energy:

$$E_{qp} = \sqrt{(\varepsilon - \mu)^2 + |\Delta|^2}$$







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

As a consequence of pairing correlations large amplitude nuclear motion becomes more adiabatic.

While a nucleus elongates its Fermi surface becomes oblate and its sphericity must be restored

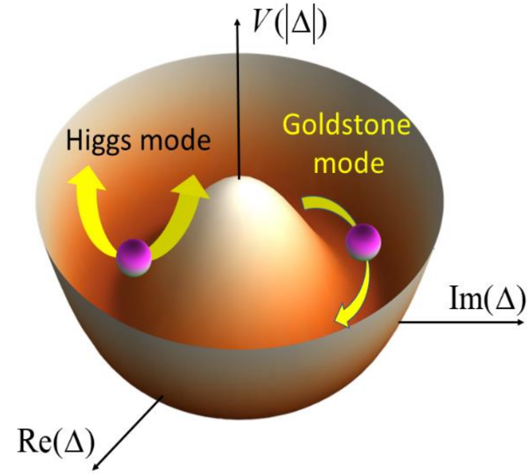
Hill and Wheeler, PRC, 89, 1102 (1953)

Bertsch, PLB, 95, 157 (1980)

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

Appearance of pairing field in Fermi systems is associated with U(1) symmetry breaking.

There are two characteristic modes associated with the field $\Delta(\vec{r},t)$



1) **Nambu-Goldstone mode** explores the degree of freedom associated with the phase: $\phi(\vec{r},t)$

2) **Higgs mode** explores the degree of freedom associated with the magnitude: $\left|\Delta(\vec{r},t)\right|$

<u>What's the difference between pairing correlations and existence of superfluid phase?</u>

- Superfluid phase exists if the *off-diagonal long range order* is present:

$$\lim_{|r-r'|\to\infty} \langle \psi_\uparrow^+(r)\psi_\downarrow^+(r')\psi_\downarrow(r')\psi_\uparrow(r)\rangle \neq 0$$

C.N. Yang, Rev. Mod. Phys. 34, 694 (1962)

- This limit is unreachable in atomic nuclei due to their finite size. Therefore it is more convenient to look, instead, for the manifestations of the phase $\Delta(\vec{r},t) = \left|\Delta(\vec{r},t)\right| e^{i\phi(\vec{r},t)}$

Note: whenever I mean theory I mean: <u>time dependent HFB (TDHFB)</u> or <u>time dependent Density Functional Theory (TDDFT)</u> with <u>local pairing field</u>.

The well known effects in superconductors where the simplified BCS approach fails

1) Quantum vortices, solitonic excitations related to pairing field (e.g. domain walls)

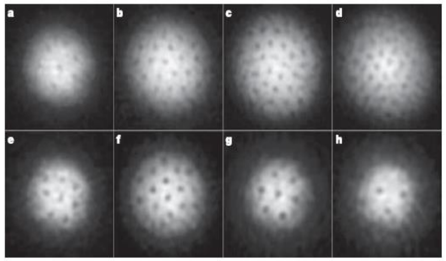
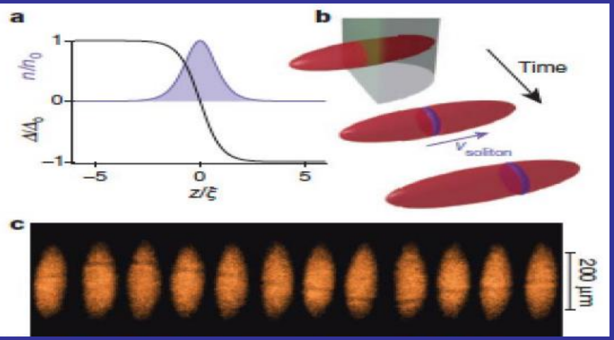
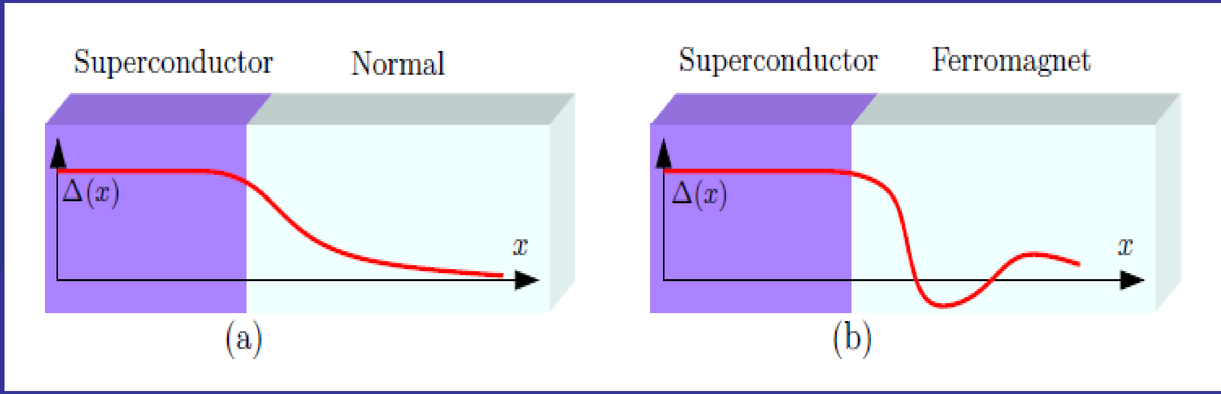


Figure 2 | Vortices in a strongly interacting gas of fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (**a**) or 500 ms (**b–h**) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, the magnetic field was ramped to 735 G for imaging (see text for details). The magnetic fields were 740 G (**a**), 766 G (**b**), 792 G (**c**), 812 G (**d**), 833 G (**e**), 843 G (**f**), 853 G (**g**) and 863 G (**h**). The field of view of each image is 880 μm × 880 μm.

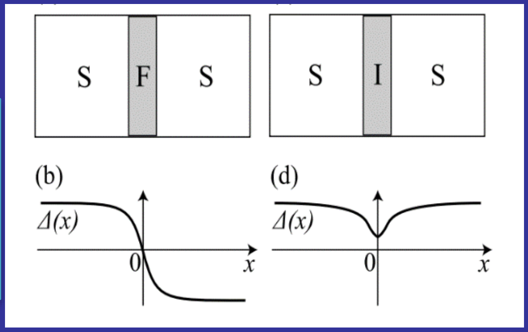


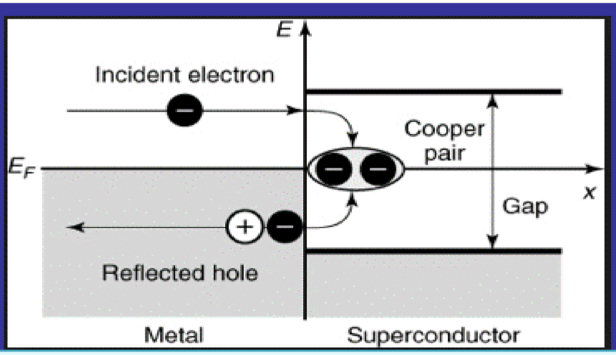
2) Bogoliubov – Anderson phonons

3) proximity effects: variations of the pairing field on the length scale of the coherence length.



4) physics of Josephson junction (superfluid - normal metal), pi-Josephson junction (superfluid - ferromagnet)





5) Andreev reflection (particle-into-hole and hole-into-particle scattering) Andreev states cannot be obtained within BCS

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 <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)

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":

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

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

$$\Delta(\mathbf{r}) = g_{eff}(\mathbf{r})\chi_c(\mathbf{r})$$

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

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)

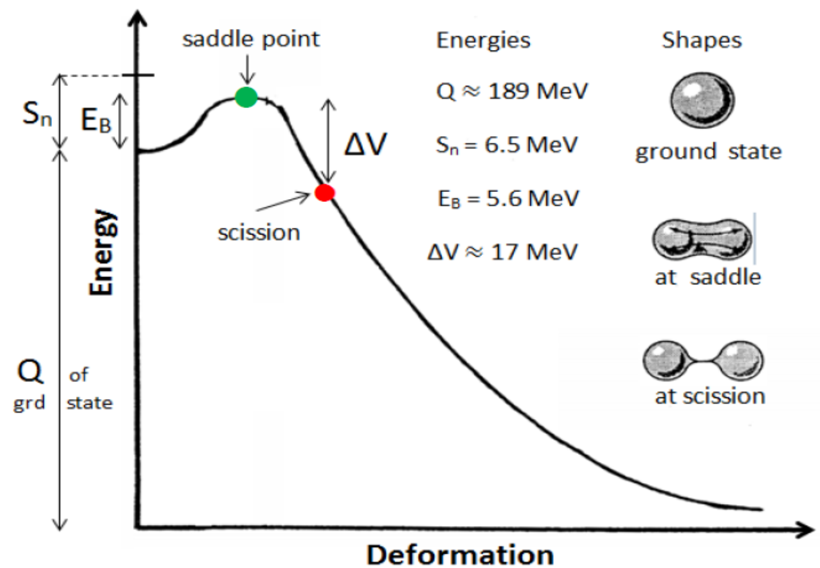
Present computing capabilities:

- 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)

Nuclear fission dynamics

Potential energy versus deformation

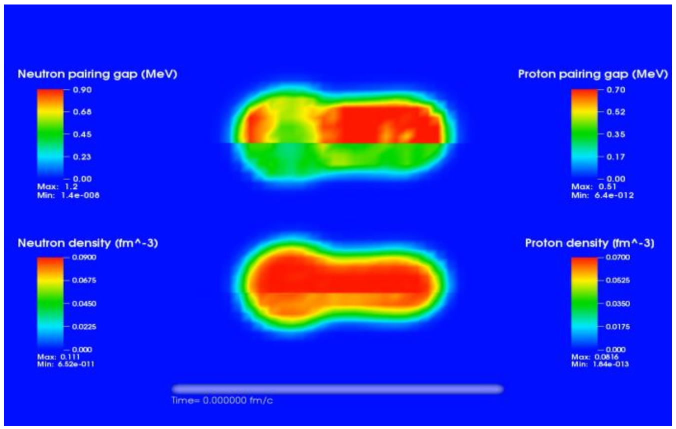


From F. Gonnenwein FIESTA2014

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

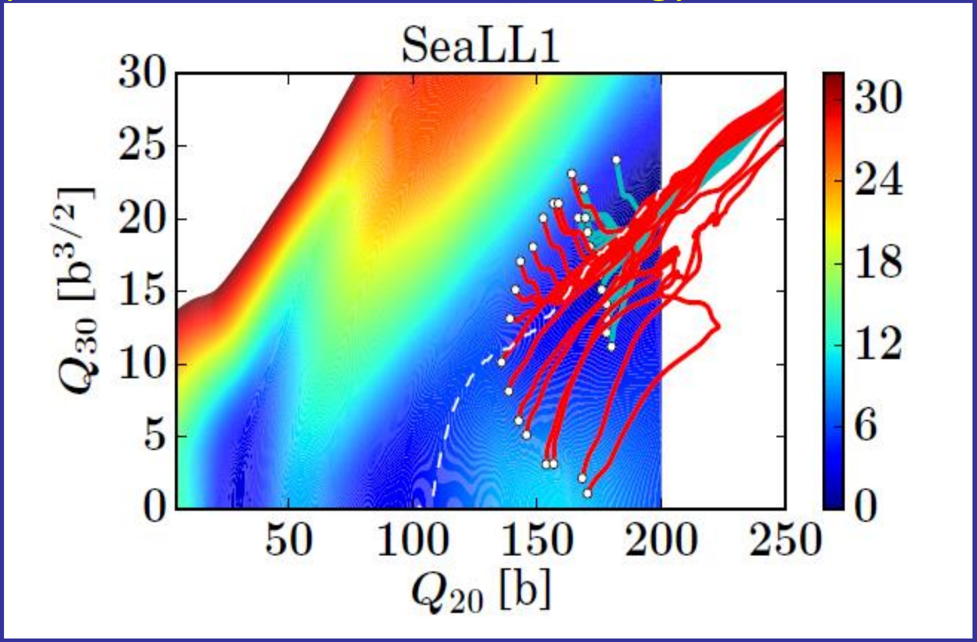
E^* (MeV)	E_n (MeV)	TKE_{TDSLDA} (MeV)	TKE_{syst} (MeV)	err (%)	Z_L	N_L
8.08	1.542	173	177.26	1.95	40.825	62.246
9.60	3.063	174	176.73	1.13	40.500	61.536
10.10	3.560	179	176.56	1.43	41.625	62.783
10.57	4.032	173	176.39	1.55	40.092	61.256
10.58	4.043	173	176.39	1.70	40.146	61.388
10.58	4.047	175	176.39	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)

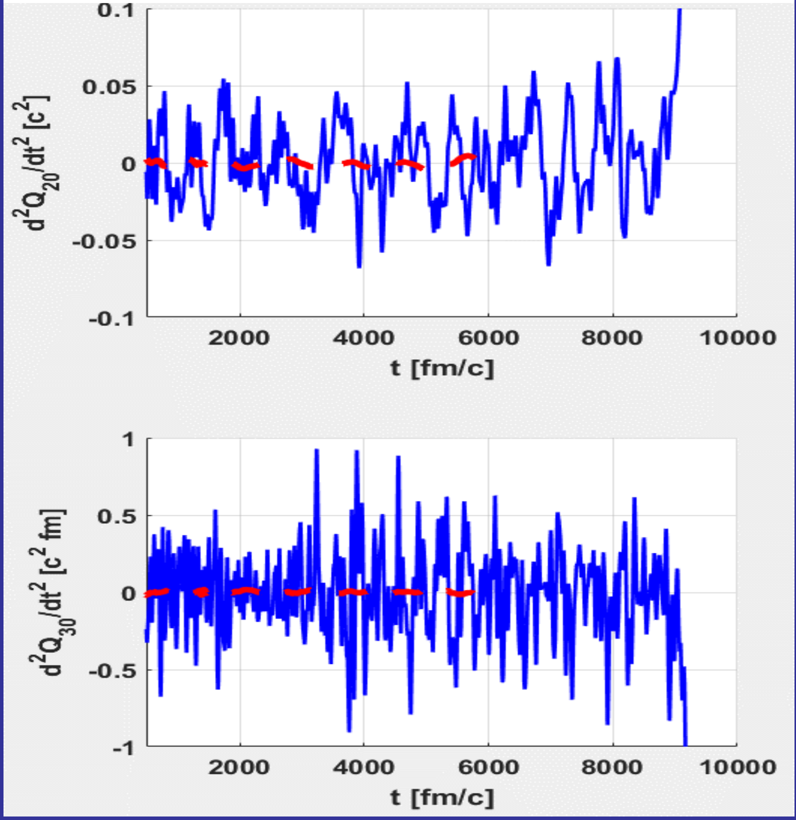
Fission dynamics of ^{240}Pu

Trajectories of fissioning ^{240}Pu in the collective space at excitation excitation energy of *E=8-9 MeV*:



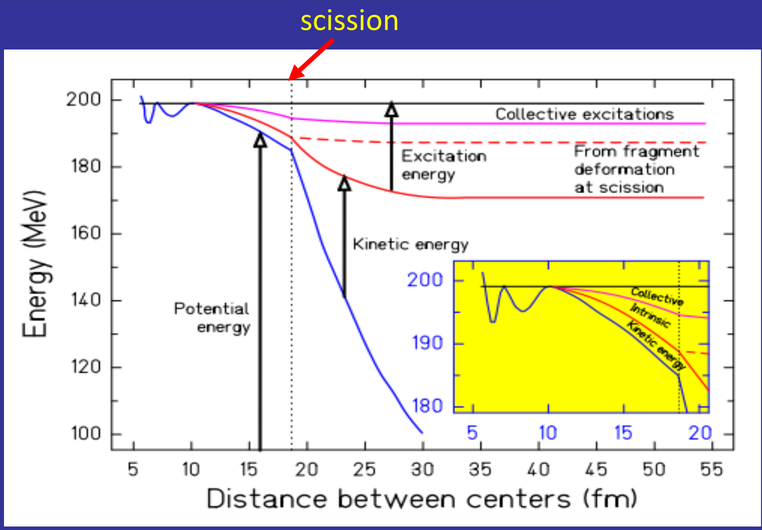
A. Bulgac, et al. Phys. Rev. C 100, 034615 (2019)

Accelerations in quadrupole and octupole moments along the fission path



Note that despite the fact that nucleus is already beyond the saddle point the collective motion on the time scale of 1000 fm/c and larger is characterized by the constant velocity (*see red dashed line for an average acceleration*) till the very last moment before splitting. On times scales, of the order of 300 fm/c and shorter, the collective motion is a subject to random-like kicks indicating strong coupling to internal d.o.f

Remarks on the fragment kinetic and excitation energy sharing within the TDDFT

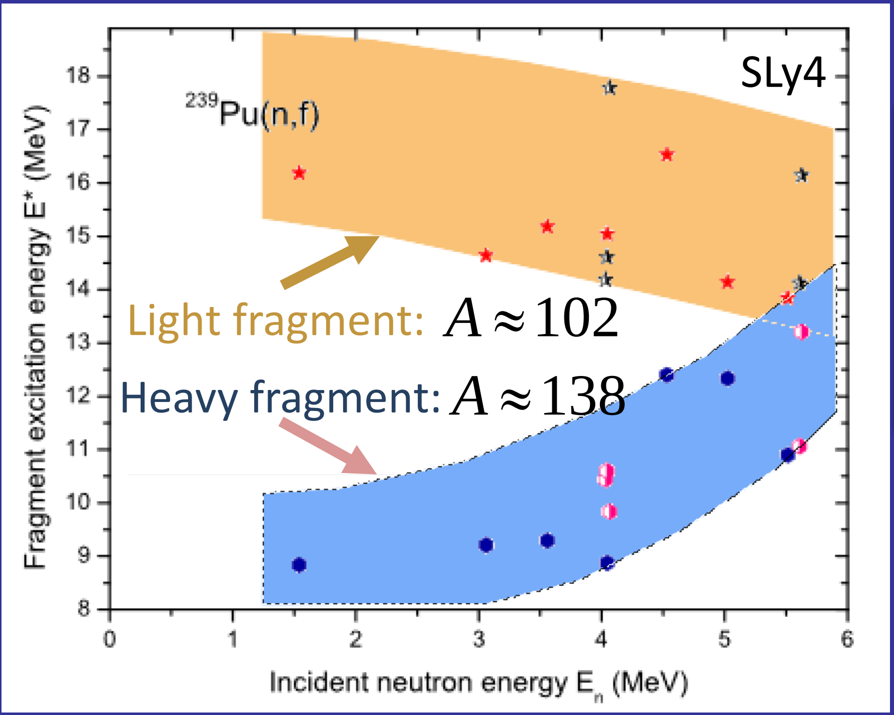


Schmidt&Jurado:Phys.Rev.C83:061601,2011

In the to-date approaches it is usually assumed that the excitation energy has 3 components (Schmidt&Jurado:Phys.Rev.C83:061601,2011 Phys.Rev.C83:014607,2011):

- deformation energy
- collective energy (energy stored in collective modes)
- intrinsic energy (specified by the temperature)

It is also assumed that the intrinsic part of the energy is sorted according to the total entropy maximization of two nascent fragments (i.e. according to temperatures, level densities) and the fission dynamics does not matter.



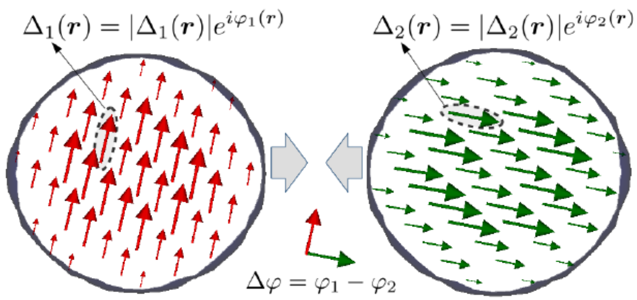
In TDDFT such a decomposition can be performed as well.
The intrinsic energy in TDDFT will be partitioned dynamically (no sufficient time for equilibration).

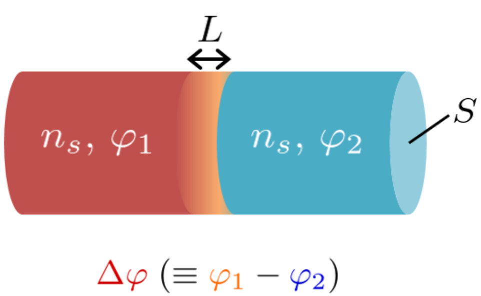
„Heavy soliton” creation in nuclear collision

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.





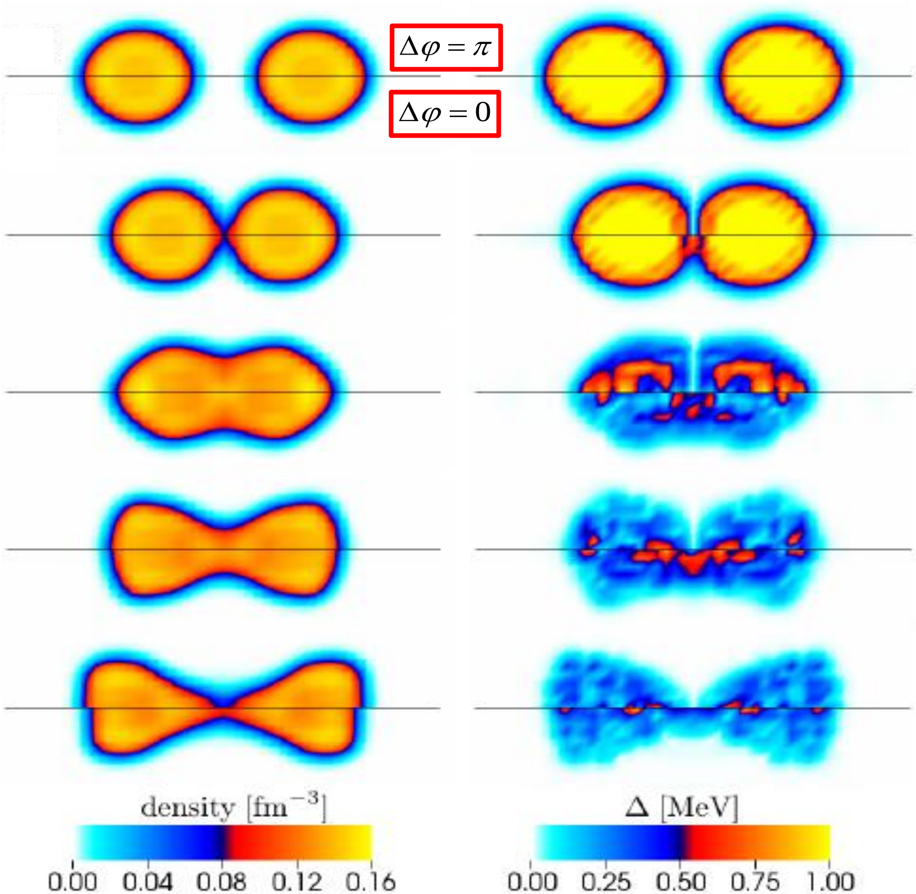
From Ginzburg-Landau (G-L) approach:

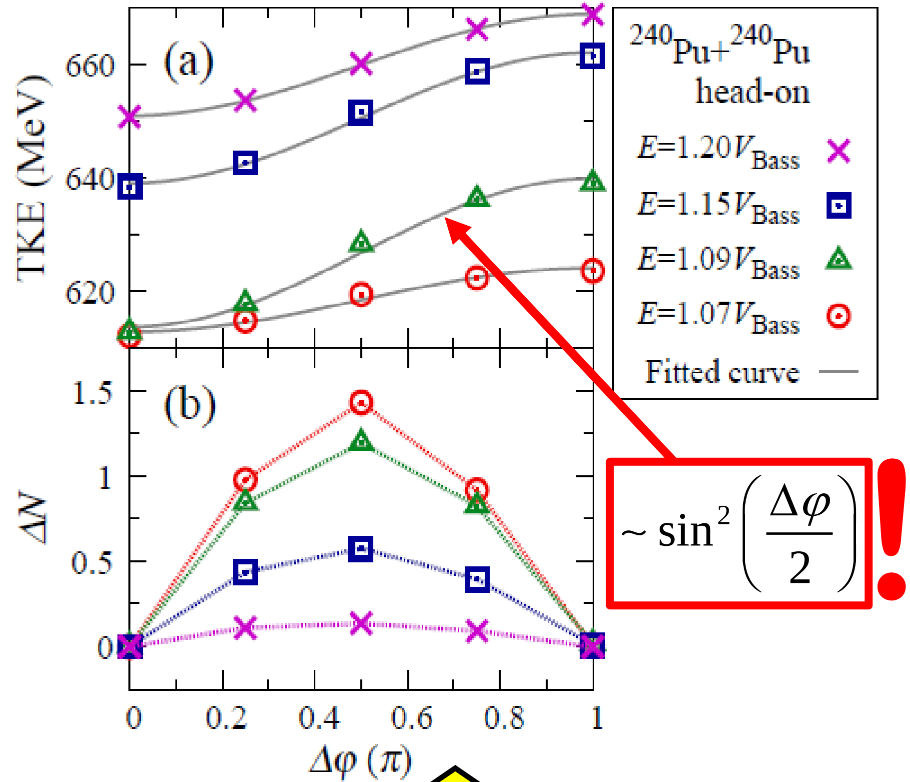
$$E_j = \frac{S}{L}\frac{\hbar^2}{2m} n_s \sin^2\frac{\Delta\varphi}{2}$$

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

$^{240}Pu + ^{240}Pu$

Total kinetic energy of the fragments (TKE)

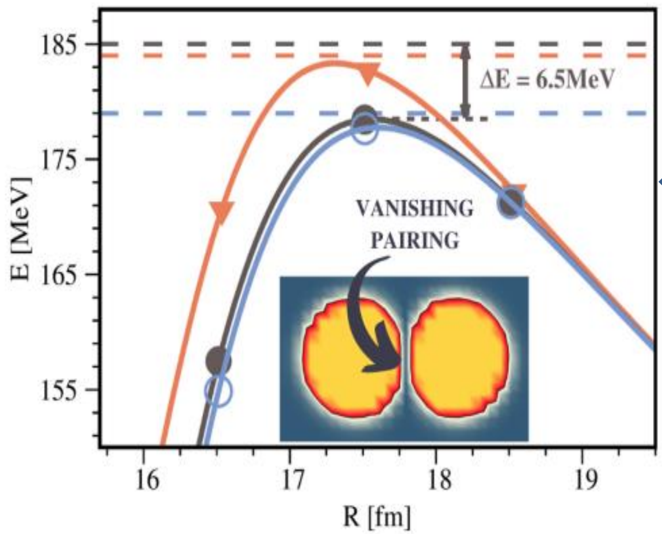




Average particle transfer between fragments.

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!

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



Dynamic nature of the effect:

Solid lines: static barrier between two nuclei (with pairing included):
90Zr+90Zr - brown
96Zr+96Zr - black (0-phase diff.) and
blue (Pi-phase diff.)
Static barriers are practically insensitive to the phase difference of pairing fields.

Dashed lines: Actual threshold for capture obtained in dynamic calculations.
Hence ΔE measures the additional energy which has to be added to the system to merge nuclei.

TABLE I: The minimum energies needed for capture in ^{90}Zr+^{90}Zr and ^{96}Zr+^{96}Zr for the case of $\Delta\phi = 0$ [$E_{\text{thresh}}(0)$] and $\Delta\phi = \pi$ [$E_{\text{thresh}}(\pi)$]. The energy difference between the two cases is shown in the last column. The average pairing gap $\overline{\Delta}_i$ is defined by Eq. (4).

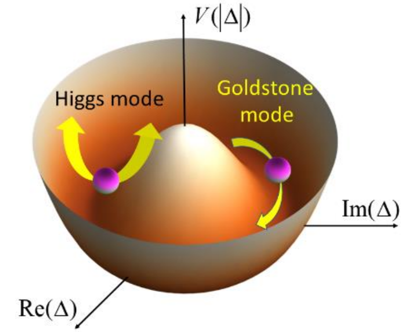
	$\overline{\Delta}_q$ (MeV)	$E_{\text{thresh}}(0)$ (MeV)	$E_{\text{thresh}}(\pi)$ (MeV)	ΔE_s
^{90}Zr	$\overline{\Delta}_n = 0.00$ $\overline{\Delta}_p = 0.09$	184	184	0
^{96}Zr	$\overline{\Delta}_n = 1.98$ $\overline{\Delta}_p = 0.32$	179	185	6
	$\overline{\Delta}_n = 2.44$ $\overline{\Delta}_p = 0.33$	178	187	9
	$\overline{\Delta}_n = 2.94$ $\overline{\Delta}_p = 0.34$	178	187	9

Dependence of the additional energy on pairing gap in colliding nuclei

P. Magierski, A. Makowski, M. Barton, K. Sekizawa, G. Wlazłowski, Phys. Rev. C 105, 064602, (2022)

G. Scamps, Phys. Rev. C 97, 044611 (2018): ***barrier fluctuations extracted from experimental data provide evidence that the effect exists.***

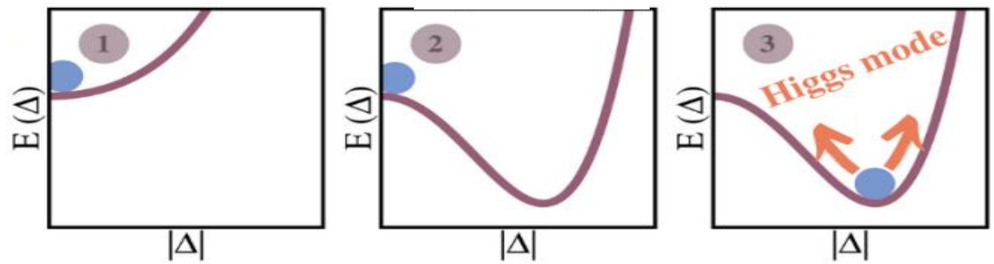
Pairing Higgs mode



Let's consider Fermi gas with schematic pairing interaction and coupling constant depending on time:

$$\hat{H} = \sum_k \varepsilon_k \hat{\psi}_k^+ \hat{\psi}_k - g(t) \sum_{k,l>0} \hat{\psi}_k^+ \hat{\psi}_{\bar{k}}^+ \hat{\psi}_{\bar{l}} \hat{\psi}_l$$

$g(t) = g_0 \theta(t)$ coupling constant is switched on withing time scale much shorter than $\hbar/\varepsilon_F$



As a result pairing becomes unstable and increases exponentially $\Delta(t) \propto e^{-i\zeta t} = e^{-i\omega t} e^{\gamma t}$

$$\frac{1}{g_0} = \sum_{k>0,\varepsilon_k>\mu} \frac{\tanh\left(\frac{\beta|\varepsilon_k-\mu|}{2}\right)}{2|\varepsilon_k - \mu| + \zeta} + \sum_{k>0,\varepsilon_k<\mu} \frac{\tanh\left(\frac{\beta|\varepsilon_k-\mu|}{2}\right)}{2|\varepsilon_k - \mu| - \zeta}$$

Time scale of growth and the period of subsequent oscillation is related to static value of pairing Δ_0 :

$$\tau = \frac{1}{\gamma} \approx \frac{\hbar}{\Delta_0}$$

Pairing instability in nuclear reaction

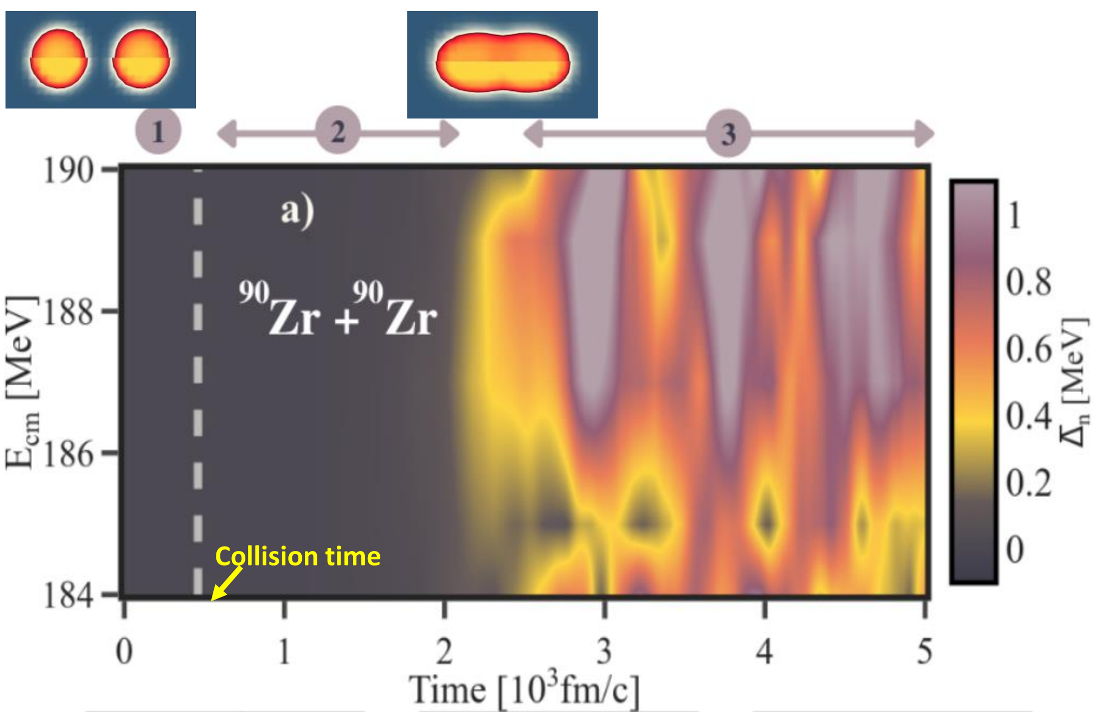
$$\Delta = \frac{8}{e^2}\varepsilon_F \exp\left(\frac{-2}{gN(\varepsilon_F)}\right)$$ - BCS formula – weak coupling limit

ε_F - Fermi energy

g - Pairing coupling constant

$N(\varepsilon_F)$ - Density of states at the Fermi level

Although one cannot change coupling constant in atomic nuclei one may affect ***density of states at the Fermi surface and consequently trigger pairing instability.***



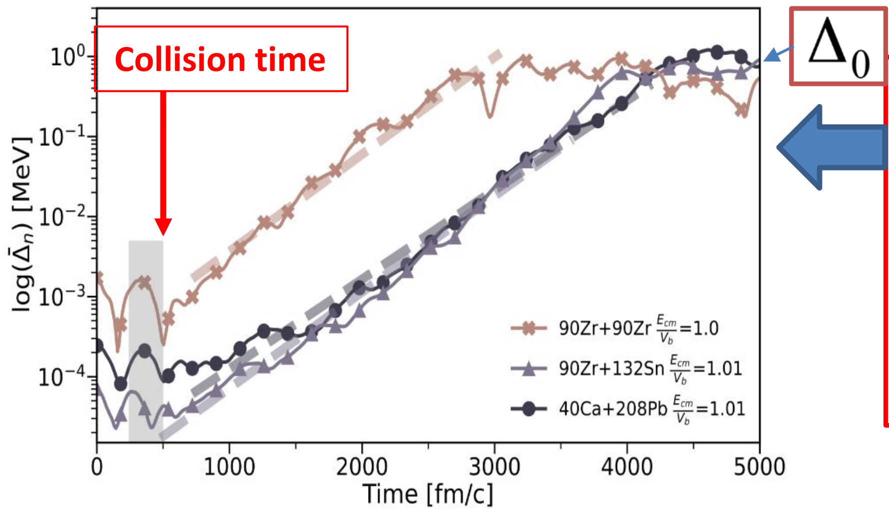
Collision of two neutron magic systems creates an elongated di-nuclear system.

Within 1500 fm/c pairing is enhanced in the system and reveals oscillations with frequency:

$$\Delta < \hbar\omega < 2\Delta$$

P.Magierski, A. Makowski, M. Barton, K. Sekizawa, G. Wlazłowski, Phys. Rev. C 105, 064602, (2022)

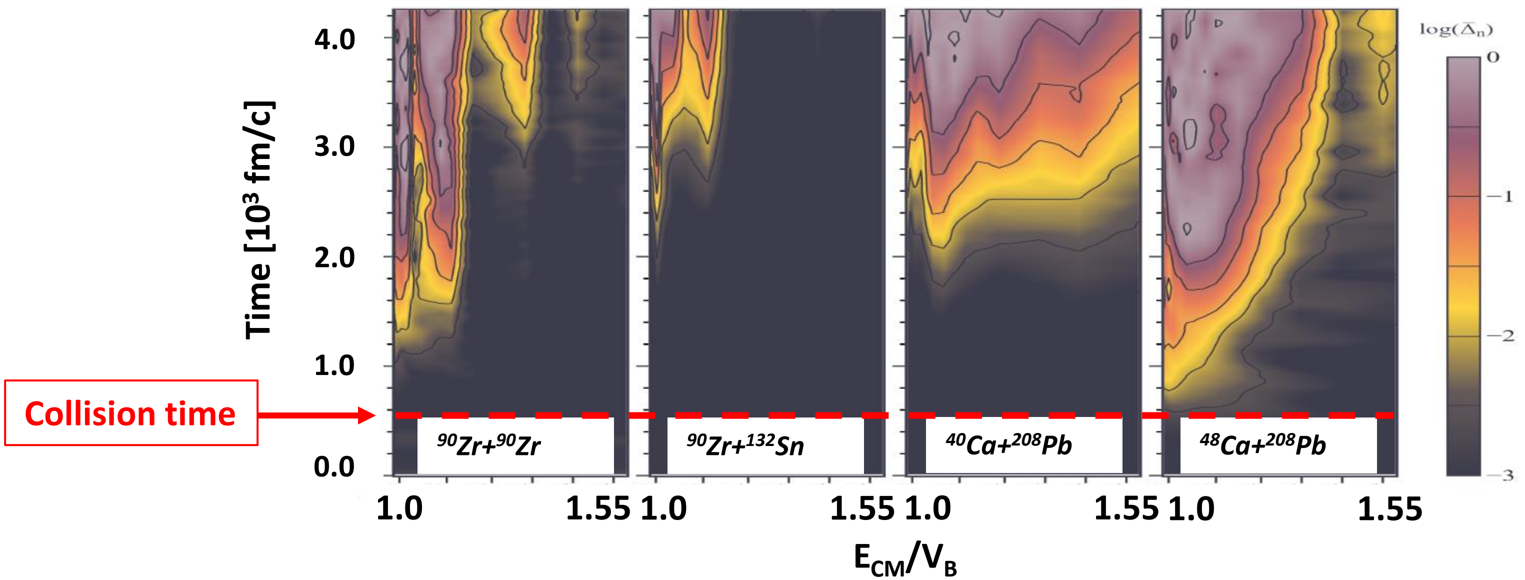
Interestingly the effect is generic and occurs for various collisions of magic nuclei.



Exponential increase of pairing gap after collision indicating **pairing instability** in di-nuclear system.
Time scale of pairing enhancement:

$$\tau \gg \frac{\hbar}{\Delta_0}$$

It occurs up to relatively high collision energies



The excitation energy of a compound system after merging exceeds **20-30 MeV**.
It corresponds to temperatures **close to critical temperature for superfluid-to-normal transition.**
Therefore it is unlikely that the system develops superfluid phase and it is rather nonequilibrium enhancement of pairing correlations.

Summary and open questions

- Induced fission: the nuclear motion from sadle to scission is not adiabatic, although it is slow.
- Excitation energy sharing: depending on dynamics and density of states at scission - very severe test for TDDFT.
- TDHFB provides evidence for nontrivial behavior of pairing correlations in highly nonequilibrium conditions which includes solitonic excitations (dynamic barrier modification for capture) and pairing enhancement as a result of collision.
- There is certain experimental evidence for solitonic excitations, although not easy to extract (G. Scamps, Phys. Rev. C C 97, 044611 (2018)).
- Pairing enhancement in collision of magic nuclei is a generic feature of TDHFB appearing in collisions of magic nuclei at energies close to the Coulomb barrier.
- Impact of pairing enhancement on dynamics is unknown and requires more theoretical effort: investigation of noncentral collisions, considerations of pairing correlations during subsequent stages of compound nucleus formation.