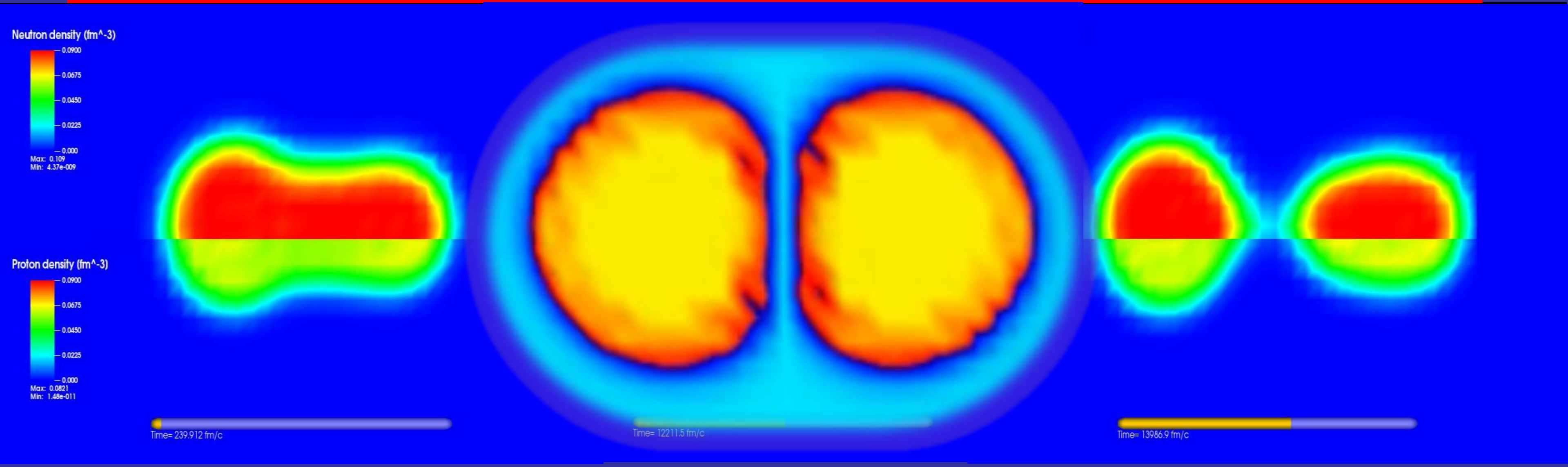
Density Functional Theory for Nuclear Reactions



Piotr Magierski

Warsaw University of Technology

<u>Collaborators (nuclear reactions only):</u>

Matthew Barton

Andrzej Makowski (Ph.D. Student)

Kazuyuki Sekizawa (Tokyo Inst. of Tech.)

Gabriel Wlazłowski

Happy Birthday Jan!

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.

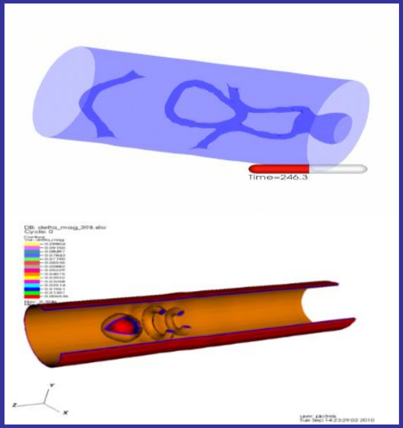
Within current computational capabilities TDDFT allows to describe real time dynamics of strongly interacting, superfluid systems of hundred of thousands fermions.

Superconducting systems of interest

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

Ultracold atomic (fermionic) gases. Unitary regime.

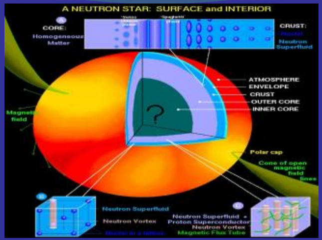
Dynamics of quantum vortices, solitonic excitations, quantum turbulence



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

Astrophysical applications.

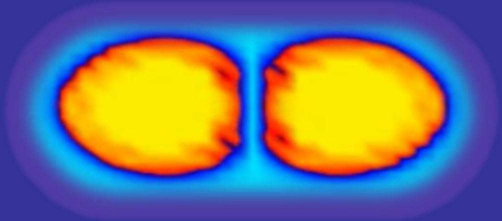
Modelling of neutron star interior (glitches): vortex dynamics, dynamics of inhomogeneous nuclear matter.

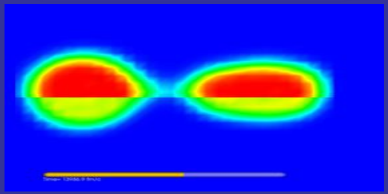


$\frac{\Delta}{\varepsilon_F} \leq 0.03$

Nuclear physics.

Induced nuclear fission, fusion, collisions.





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

Pairing correlations in time-dependent DFT (with local pairing field)

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

Stationarity requirement produces the set of equations (TDHFB eq.):

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

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

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.

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

Selected supercomputers (CPU+GPU) currently in use:

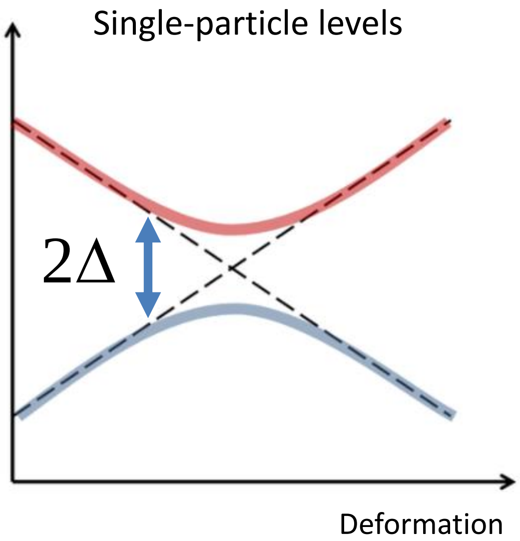
Summit (USA):
200 PFlops

LUMI (Finland):
550 PFlops

Tsubame (Japan): 12.2 PFlops

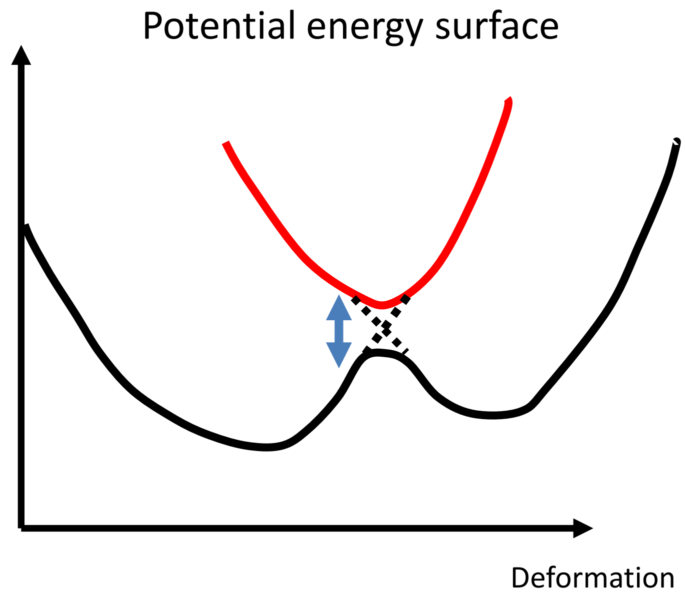
Piz Daint (Switzerland): 25.326 PFlops

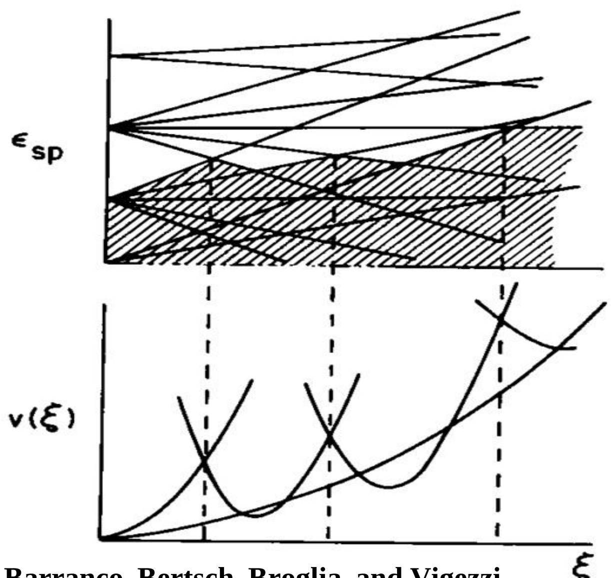
Pairing as an energy gap



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)

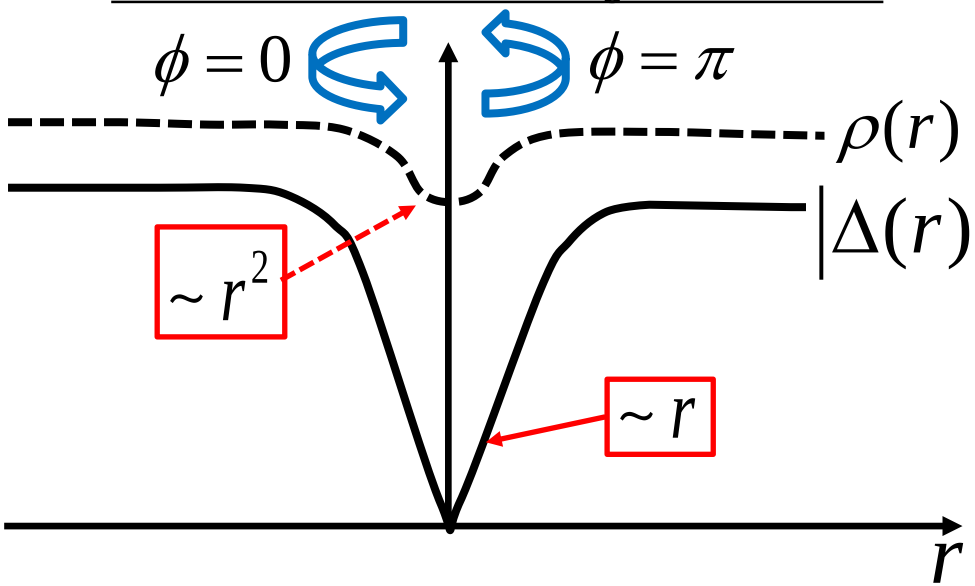
Pairing as a field

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

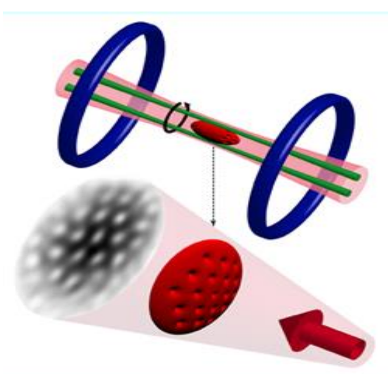
Both magnitude and phase may have a nontrivial spatial and time dependence.

Example of a nontrivial spatial dependence: *quantum vortex*

Vortex structure – section through the vortex core



Example of a topological excitation: magnitude of the pairing gap vanishes in the vortex core.



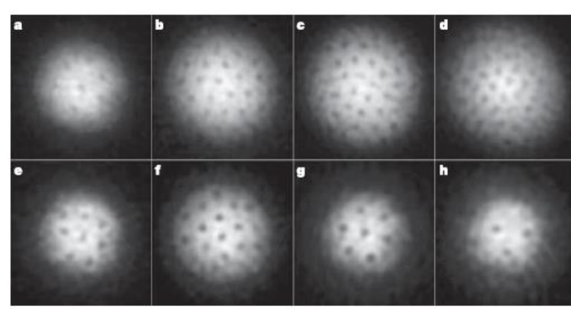


Figure 2 | Vortices in a strongly interacting gas of fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (**a**) or 500 ms (**b**–**h**) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, 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.

Experiments with ultracold Li-6 atoms: pictures of the vortex lattice.

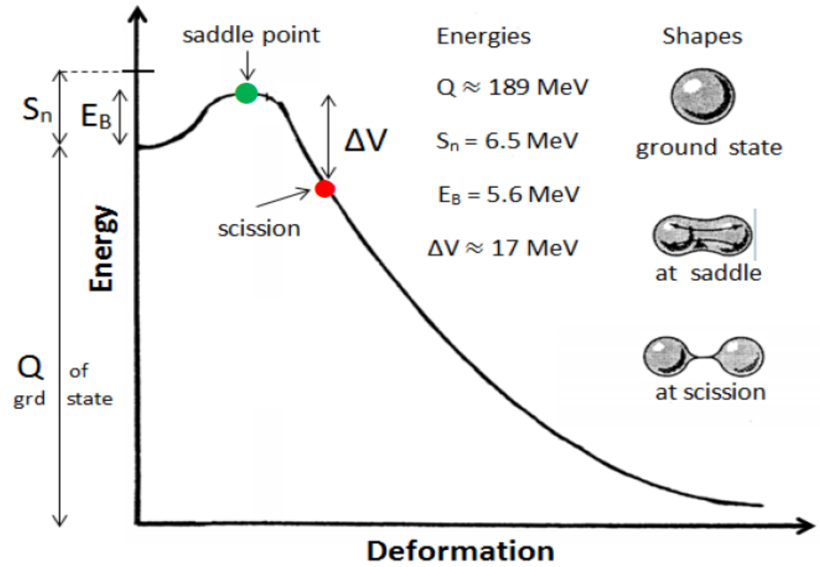
M.W. Zwierlein *et al.*, Nature, 435, 1047 (2005)

Nuclear fission dynamics

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

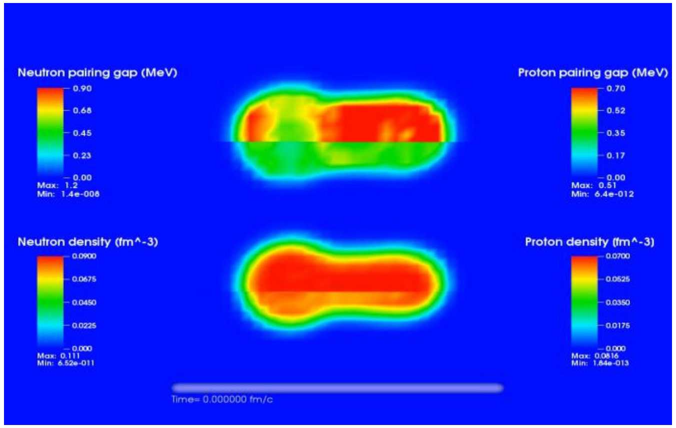
Ground state to saddle	**-**	**1 000 000 zs**
Saddle to scission	**-**	**10-100 zs**
Acceleration of fission fragments to 90% of their final velocity	**-**	**10 zs**
Neutron evaporation	**-**	**1 000 zs**

Potential energy versus deformation



From F. Gonnenwein FIESTA2014

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



Total kinetic energy of the fragments

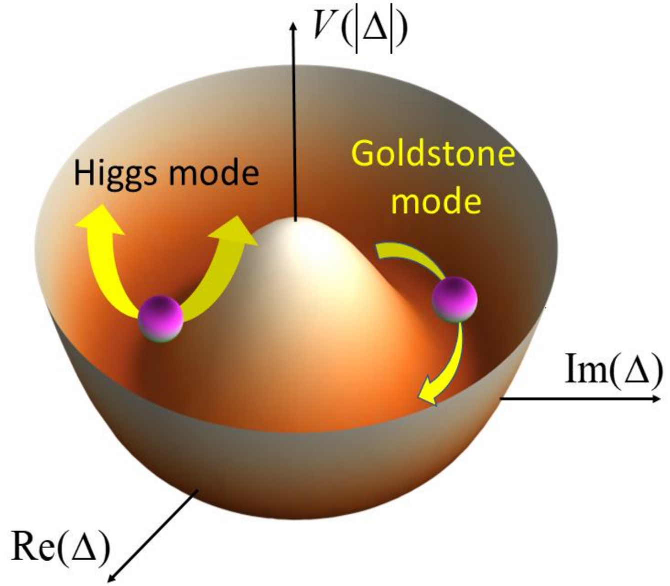
E^* (MeV)	E_n (MeV)	TKE_{TDSLDA} (MeV)	TKE_{syst} (MeV)	err (%)	Z_L	N_L
8.08	1.542	173	177.26	1.95	40.825	62.246
9.60	3.063	174	176.73	1.13	40.500	61.536
10.10	3.560	179	176.56	1.43	41.625	62.783
10.57	4.032	173	176.39	1.55	40.092	61.256
10.58	4.043	173	176.39	1.70	40.146	61.388
10.58	4.047	175	176.39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

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

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



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

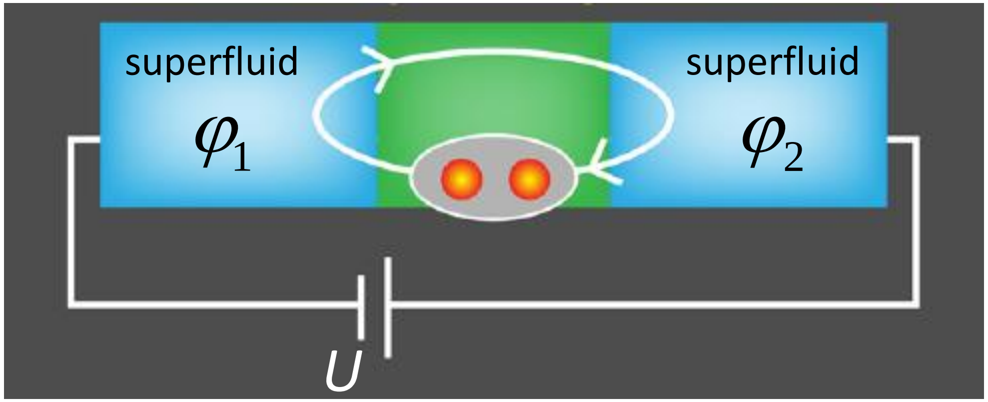
1) **Nambu-Goldstone mode** explores the degree of freedom associated with the phase: $\phi(\vec{r},t)$

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

Probing phase degree of freedom of pairing field

The well known example is Josephson junction:

- DC Josephson junction: $U = 0$
- AC Josephson junction: $U \neq 0$



$$\Delta\varphi = \varphi_1 - \varphi_2$$

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

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

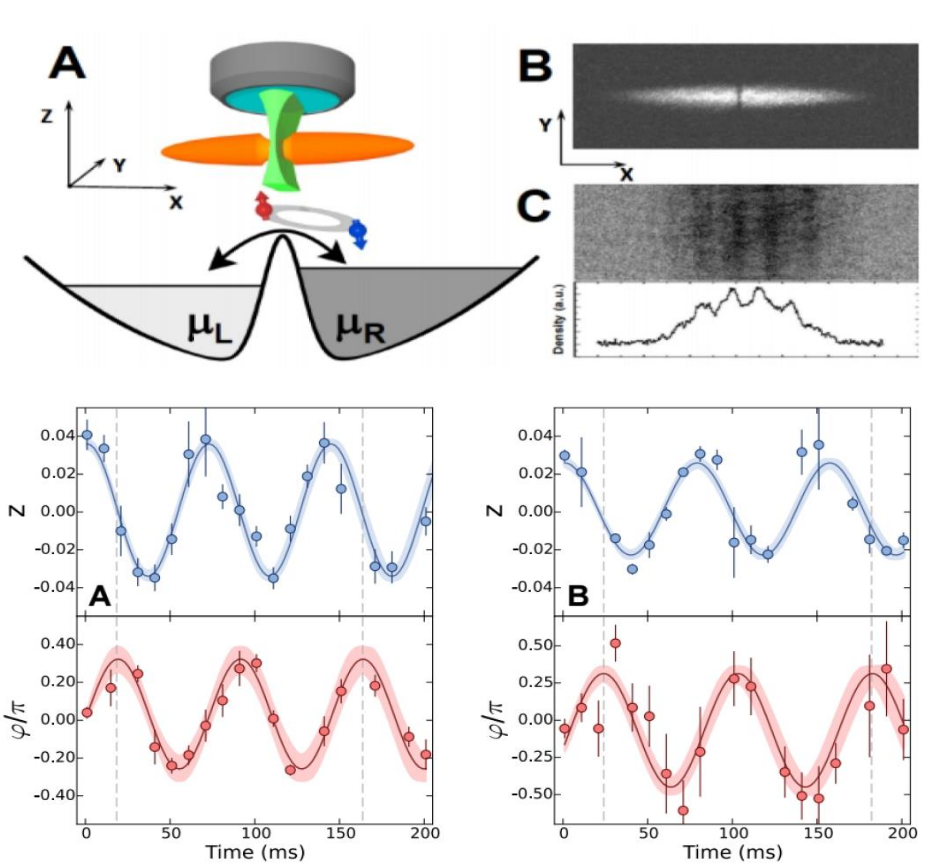
Relation between Josephson current and phase differences Between pairing fields.

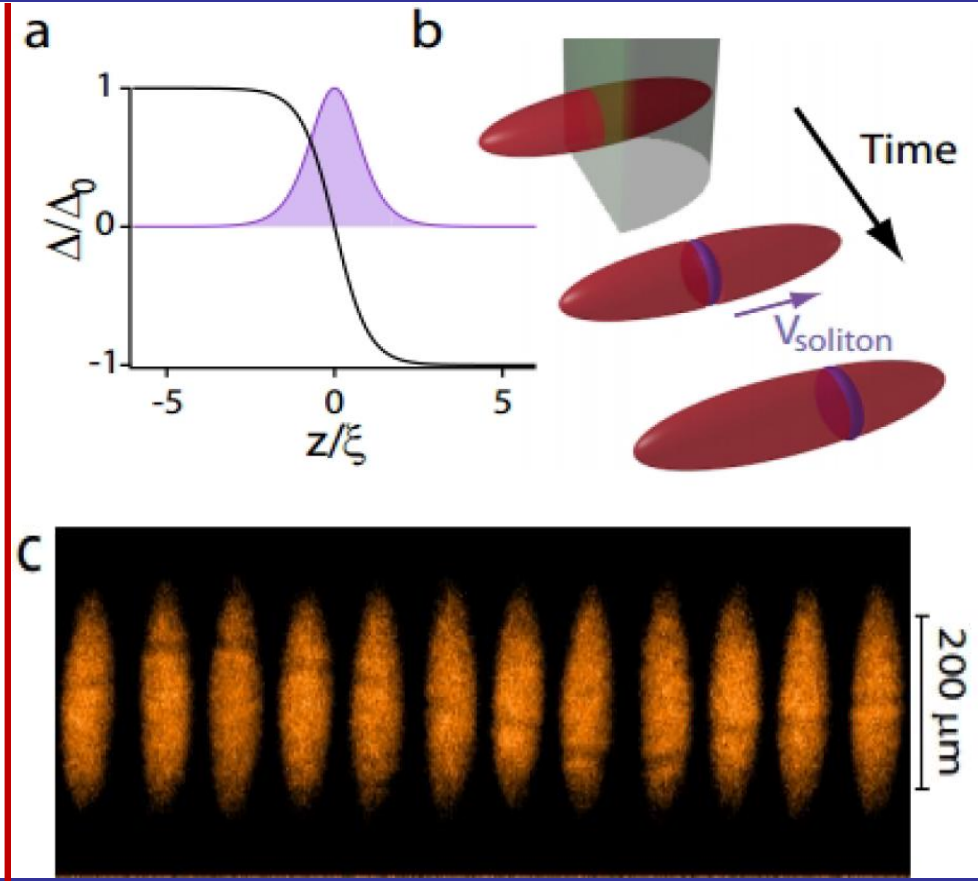
Important: Josephson junction means usually so-called ***weak link.***
Pairing condensates on both sides are assumed to remain unperturbed by the Josephson current.

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

Weak coupling (weak link)

Strong coupling





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

It need not to be accompanied by creation of a topological excitation.

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

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

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

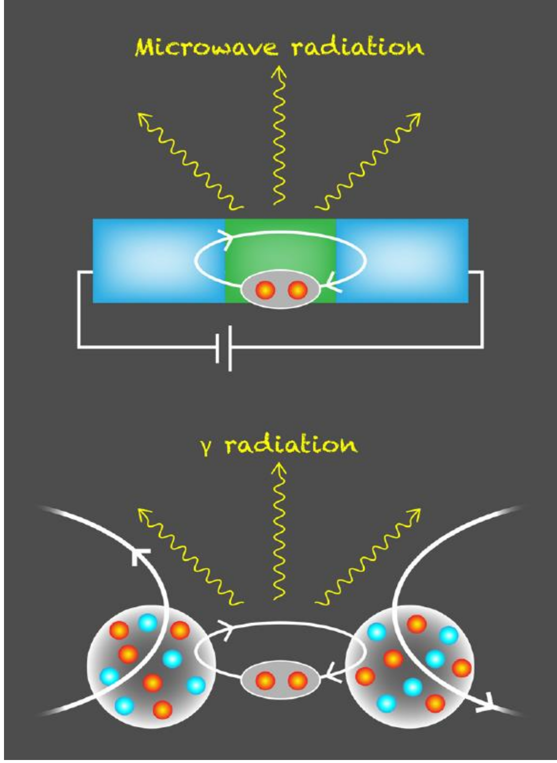
^{116}Sn+ ^{60}Ni (140.6 < Ecm < 167.95 MeV) has been analyzed by:

C.Potel, F.Barranco, E.Vigezzi, R.A. Broglia, *"Quantum entanglement in nuclear Cooper-pair tunneling with gamma rays,"* Phys.Rev. C103, L021601 (2021)
R. Broglia, F. Barranco, G. Potel, E. Vigezzi
„Transient Weak Links between Superconducting Nuclei: Coherence Length"
Nuclear Physics News 31, 25 (2021)

They realized that due to the fact that energy of a neutron pair is different in each nucleus it should create an effective „voltage" between nuclei and consequently to **AC Josephson junction**.

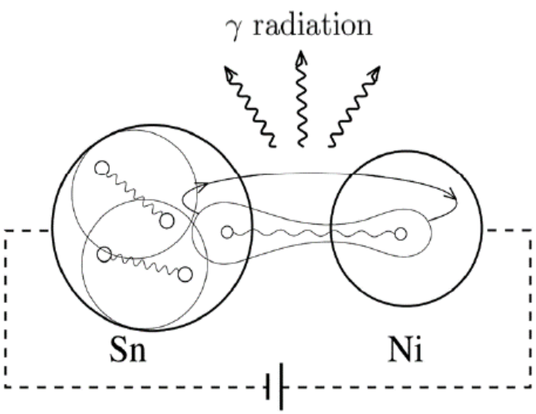
As a result one should witness **oscillatory motion of neutron Cooper pairs** between nuclei (only about 3 oscillations can occur).

This in turn would induce **proton charge oscillations** and give rise **gamma emission.**

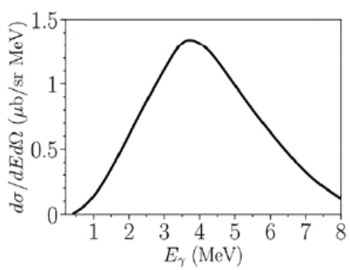


From P. Magierski, *Physics* 14 (2021) 27.

$$^{116}\mathrm{Sn} + {}^{60}\mathrm{Ni} \rightarrow \begin{cases} {}^{115}\mathrm{Sn} + {}^{61}\mathrm{Ni} & (Q_{1n} = -1.74 \ \mathrm{MeV}), \\ {}^{114}\mathrm{Sn} + {}^{62}\mathrm{Ni} & (Q_{2n} = 1.307 \ \mathrm{MeV}), \end{cases}$$



$$V^N = Q_{2n}/2e_{eff}$$



The authors state:
„...theory predicts the reduced gamma-strength [...] corresponding to an observable gamma-strength function [...] peaked at ≈ 4MeV.
It can be concluded that a nuclear analogue to the (ac) Josephson junction has been identified."
Phys.Rev. C103, L021601(2021)

„Josephson junction" above the barrier for capture

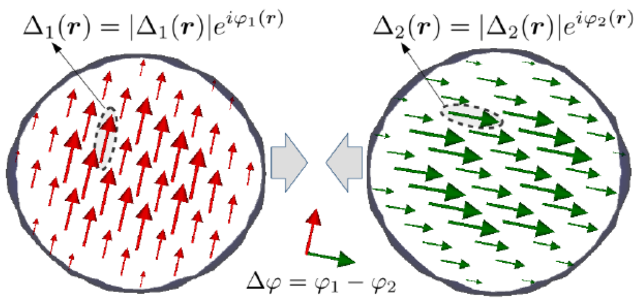
Collisions of superfluid nuclei having <u>different phases</u> of the <u>pairing fields</u>

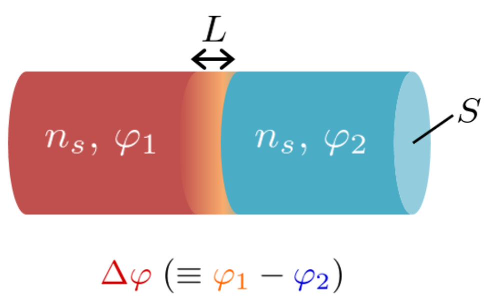
<u>The main questions are:</u>

-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.





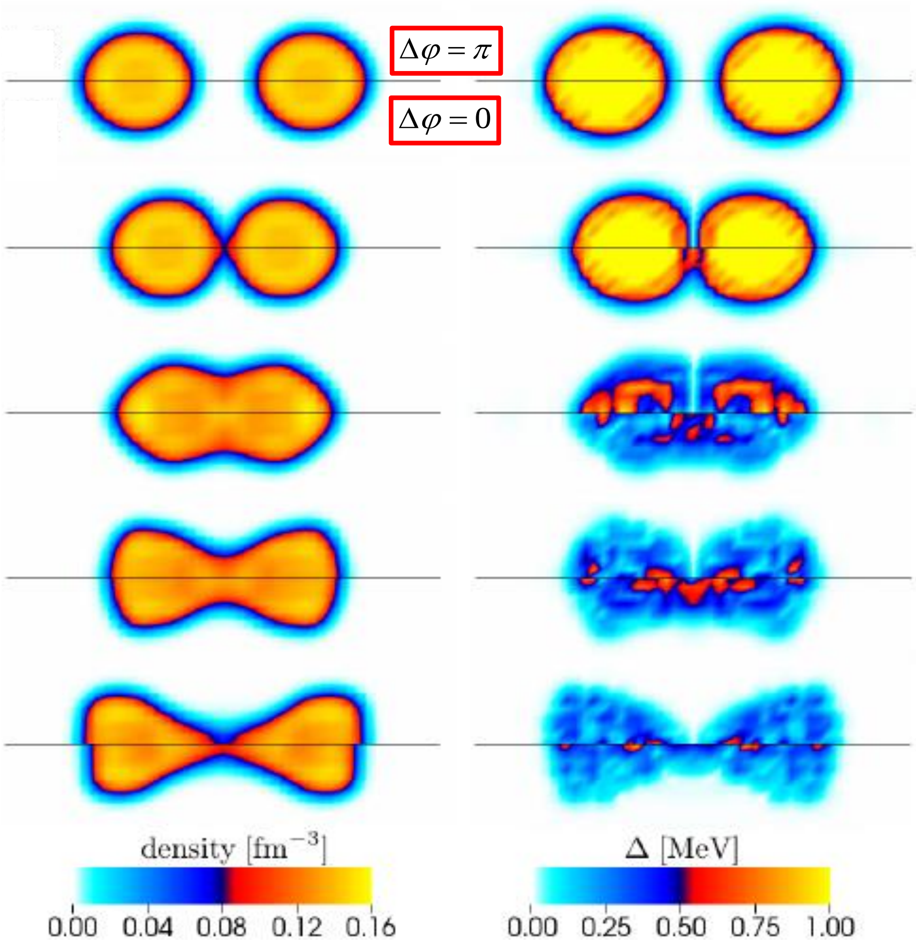
From Ginzburg-Landau (G-L) approach:

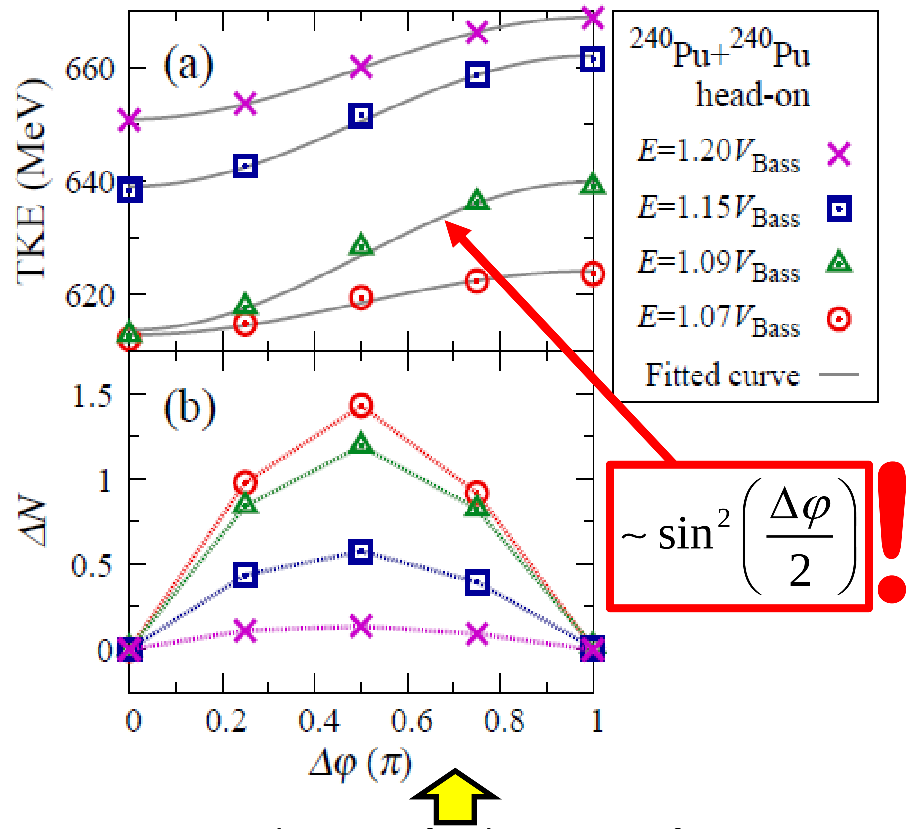
$$E_j = \frac{S}{L}\frac{\hbar^2}{2m} n_s \sin^2 \frac{\Delta\varphi}{2}$$

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

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

Total kinetic energy of the fragments (TKE)



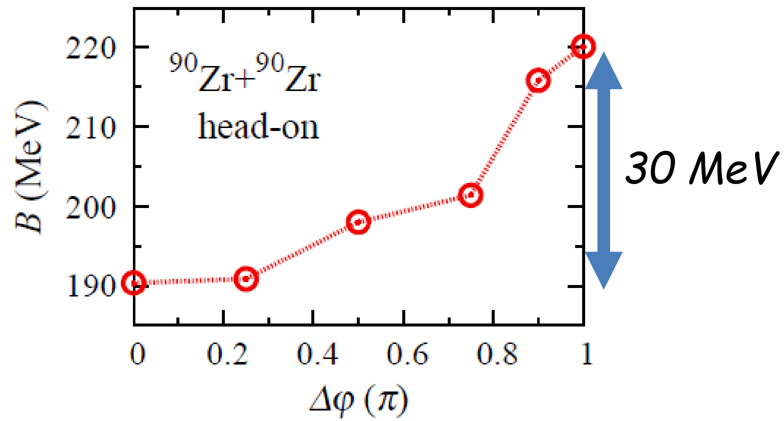


Average particle transfer between fragments.

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

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



Results with Fayans functional (no spin-orbit term)

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>.

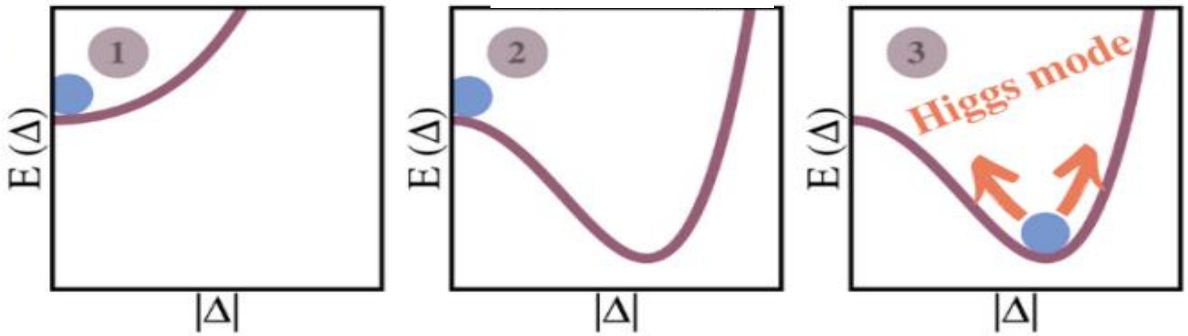
P. M., K. Sekizawa, G. Wlazłowski, Phys. Rev. Lett. 119 042501 (2017)

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 calculations with Skyrme SkM* (with spin-orbit term) functional confirmed the previous results with smaller effective barrier: **6-9 MeV**.

P.M., A. Makowski, M. Barton, K. Sekizawa, G. Wlazłowski, Phys. Rev. C (in press) arxiv:2111.05135

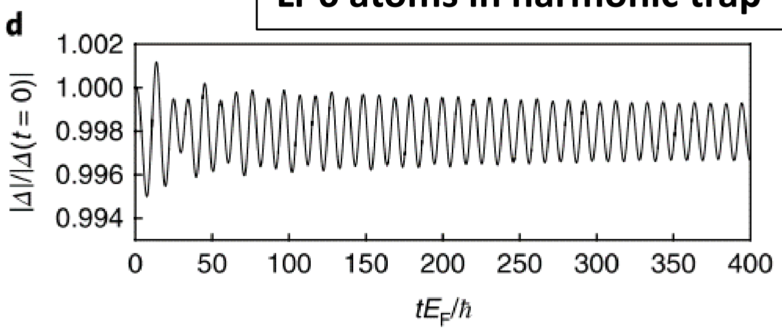
Pairing Higgs mode



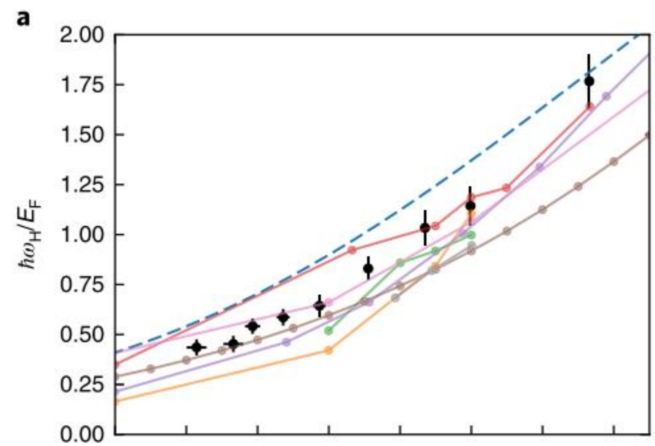
How to move from the regime 1 to regime 3 in nuclear systems?

In the ultracold atomic gas one can induce Higgs mode by varying coupling constant.

A. Behrle et al.
Higgs mode in a strongly interacting fermionic Superfluid, Nature Physics **14**, 781 (2018).
Li-6 atoms in harmonic trap



Uniform oscillation of pairing field with frequency: $2\Delta/\hbar$ (numerical simulations)



Measured peak position of the energy absorption spectra (black dots) and theory predictions for Higgs mode.

Contrary to low-energy Goldstone modes Higgs modes are in principle unstable and decay.
Precursors of Higgs modes exists even in few-body systems (J. Bjerlin et al. Phys. Rev. Lett. 116, 155302 (2016))

Nuclear pairing Higgs mode

$$\Delta = \frac{8}{e^2}\varepsilon_F \exp\left(\frac{-2}{gN(\varepsilon_F)}\right)$$

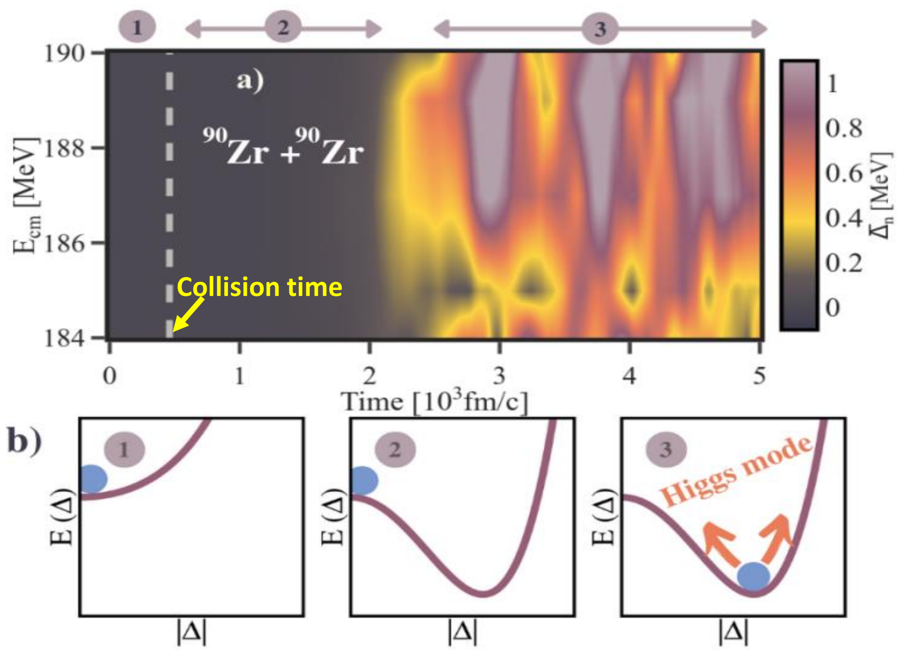
- BCS formula – weak coupling limit

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 Higgs mode.***



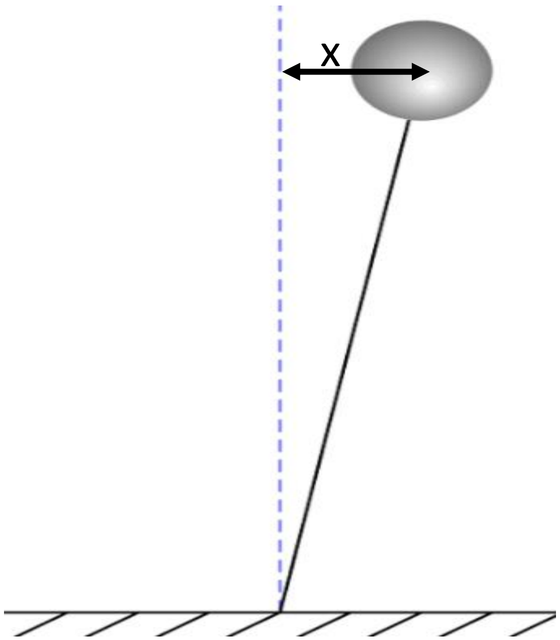
Collision of two neutron magic systems creates an elongated di-nuclear system.

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

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

P.M., A. Makowski, M. Barton, K. Sekizawa, G. Wlazłowski, Phys. Rev. C (in press) arxiv:2111.05135

Dynamics of pairing instability



After collision **the pairing configuration** corresponding to initial magic system **becomes unstable**.

It is an analogue to pendulum which suddenly become inverted.

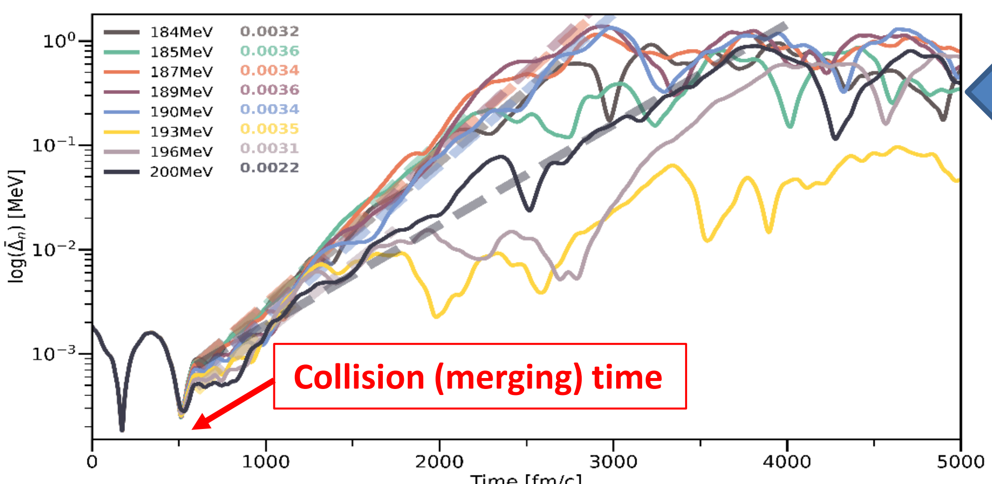
inverted pendulum eq. for small displacements i.e. close to unstable point of equilibrium:

$$\frac{d^2x}{dt^2} \approx \alpha^2 x \quad \Rightarrow \quad x(t) \approx \frac{x_0}{2}\exp(\alpha t)$$

Similarly: pairing gap behavior around the point of instability:

$$\frac{d^2\Delta}{dt^2} \approx \alpha^2 \Delta \quad \Rightarrow \quad \Delta(t) \approx \frac{\Delta_0}{2}\exp(\alpha t)$$

$^{90}Zr + {}^{90}Zr$ head-on collision above the threshold for capture



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

Excited **Higgs mode** (uniform pairing) **becomes fragmented (decays)** already **during the first period of oscillation**.

P.M., A. Makowski, M. Barton, K. Sekizawa, G. Wlazłowski, Phys. Rev. C (in press) arxiv:2111.05135

Summary and open questions

- It seems we have some experimental evidence for degree of freedom related to **the pairing phase:**
  AC Josephson junction (pair transfer) and solitonic excitations (barrier modification)

- It is likely that the **solitonic excitation** will contribute to Świątecki's ***extra-push energy***
  (W.J.Świątecki, Phys. Scr. 24 (1981) 113; Nucl.Phys. A376 (1982) 275, ...)

- The **enhancement of pairing correlations** after collision and merging as a signature for **Higgs mode** is a qualitatively new startling effect.
  It is surprising as to date it was expected that TDHF approach is sufficient, in particular for collisions involving magic nuclei.

- **Pairing enhancement** in collision of magic nuclei is **a generic feature**:
  according to the theory (TDHFB) it appears in other 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.

Systematic investigations of medium and heavy nuclei collisions close to Coulomb barrier within **TDDFT theory with inclusion of pairing correlations** <u>are needed</u>!