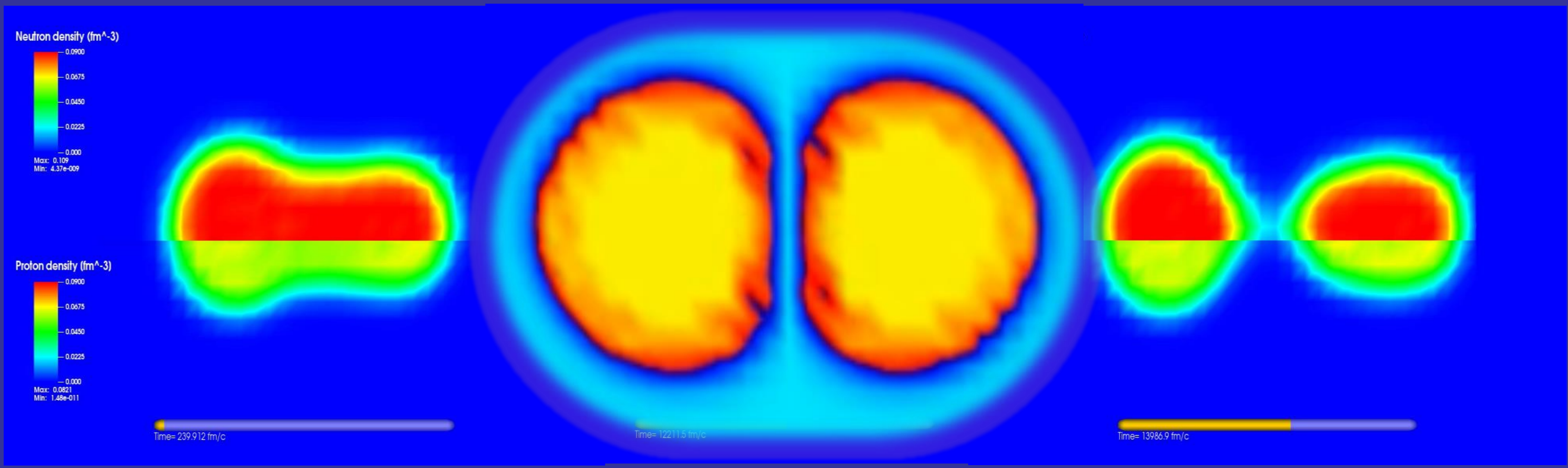
Recent achievements with the TDSLDA



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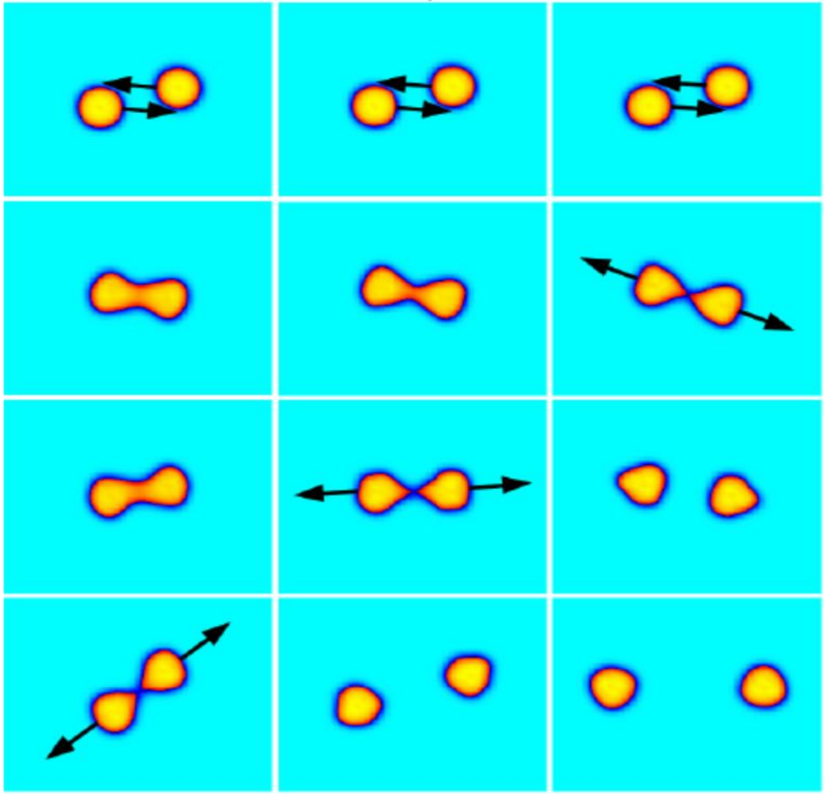
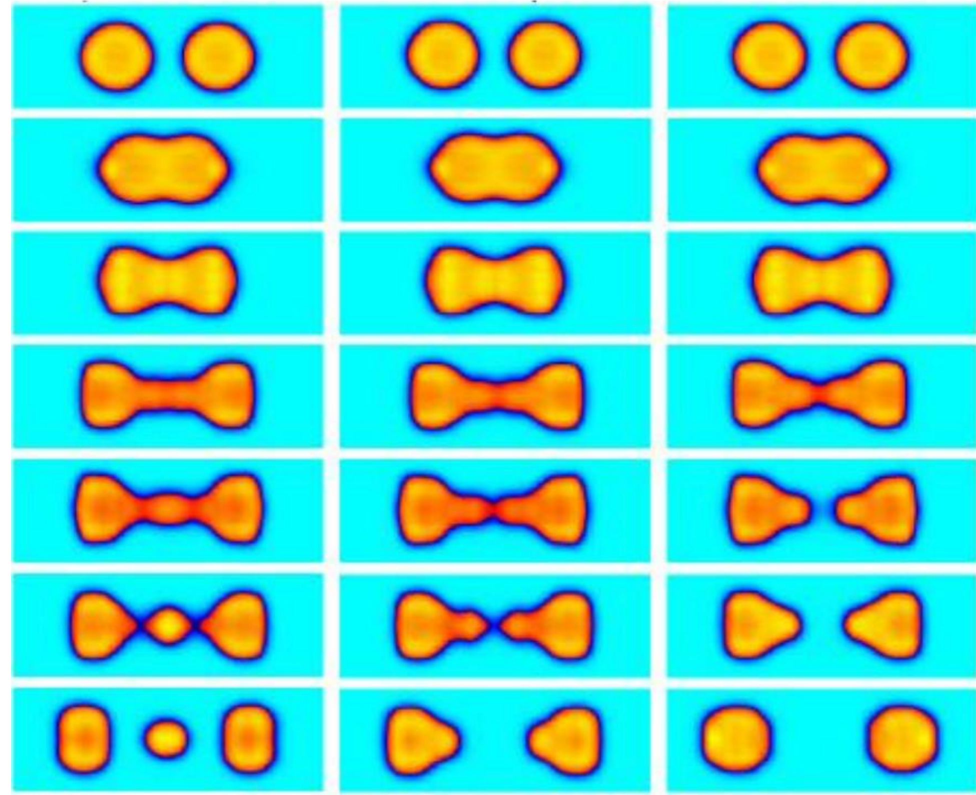
ESNT Workshop: Dynamics of Nuclear Fission





1. Introduction.
2. Theoretical framework – TDDFT.
3. Remarks on fission dynamics and pairing.
4. Dynamic pairing enhancement in nucleus-nucleus collisions .
5. Effective mass of a nucleus in a superfluid environment (neutron star crust).

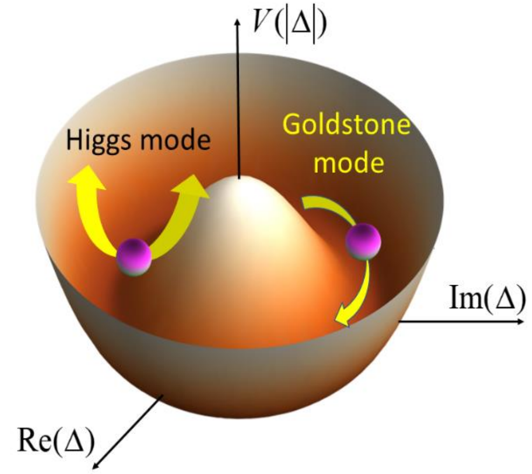
$$\Delta(\vec{r},t) = \left|\Delta(\vec{r},t)\right| e^{i\phi(\vec{r},t)}$$

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: $\left|\Delta(\vec{r},t)\right|$



What's the difference between pairing correlations and existence of superfluid phase?

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

$$\lim_{|\boldsymbol{r}_1-\boldsymbol{r}_2|\to\infty} \langle \hat{\psi}^\dagger_\uparrow(\boldsymbol{r}_1)\,\hat{\psi}^\dagger_\downarrow(\boldsymbol{r}_1)\,\hat{\psi}_\downarrow(\boldsymbol{r}_2)\,\hat{\psi}_\uparrow(\boldsymbol{r}_2)\rangle \neq 0$$

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

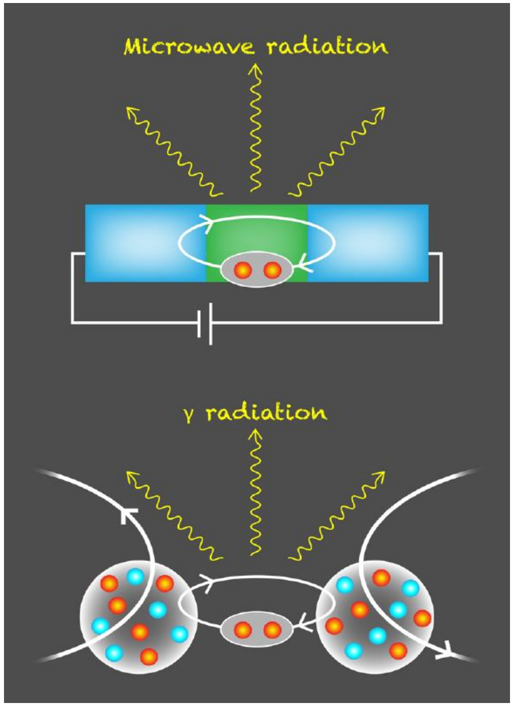
Nuclear systems

Some evidence for a nuclear **DC Josephson effect** has been gathered over the years, following ideas presented in papers:
V.I. Gol'danskii, A.I. Larkin, JETP 26, 617 (1968), K. Dietrich, Phys. Lett. 32B 428 (1970)

Experimental evidence of enhanced nucleon pair transfer reported eg. in:
M.C. Mermaz, Phys. Rev. C36 1192, (1987), M.C. Mermaz, M. Girod, Phys. Rev. C53 1819 (1996)

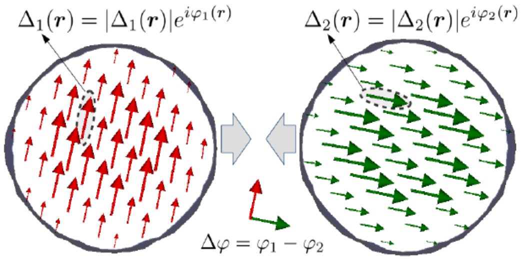
Surprisingly evidence for AC Josephson effect has also been found

G.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)



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

Solitonic excitations in nuclear collision – dynamic enhancement of the barier for capture.



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

P. Magierski, K. Sekizawa, G. Wlazłowski, Phys. Rev. Lett. 119 042501 (2017)
Y. Hashimoto, G. Scamps, Phys. Rev. 94, 014610 (2016)
G. Scamps, Phys. Rev. C 97, 044611 (2018)
P. Magierski, A. Makowski, M. Barton, K. Sekizawa, G. Wlazłowski, Phys. Rev. C 105, 064602, (2022)

Solving time-dependent problem for superfluids within TDSLDA

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

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

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

where *h* and Δ depends on “densities”:

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

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

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

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

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

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

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.

If one is interested in extracting <u>one-body observables</u> (TD)DFT is usually the most useful approach.

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

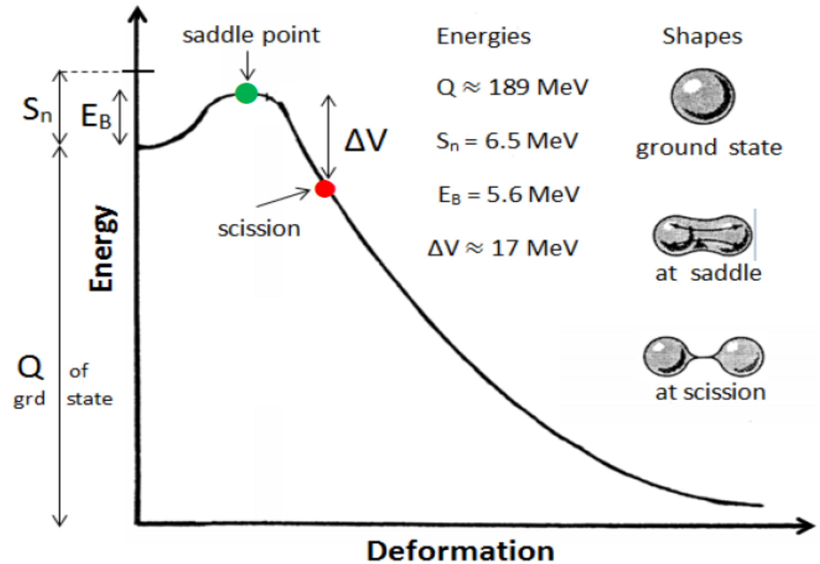
Nuclear fission dynamics

Potential energy versus deformation

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

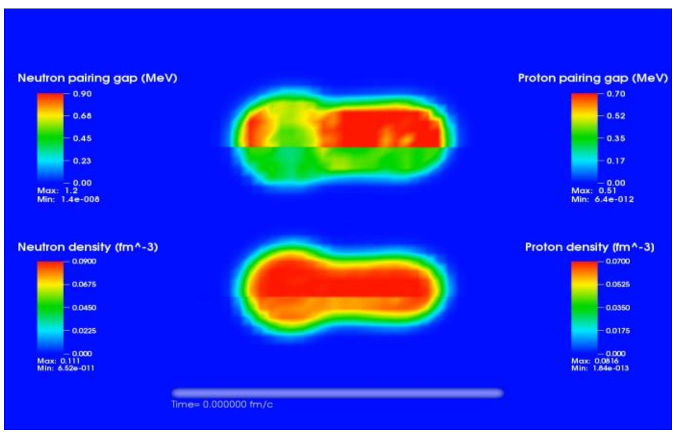
Ground state to saddle	-	1 000 000 zs
Saddle to scission	-	10-100 zs
Acceleration of fission fragments to 90% of their final velocity	-	10 zs
Neutron evaporation	-	1 000 zs

1 zs = 10^{-21} s



From F. Gonnenwein FIESTA2014

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



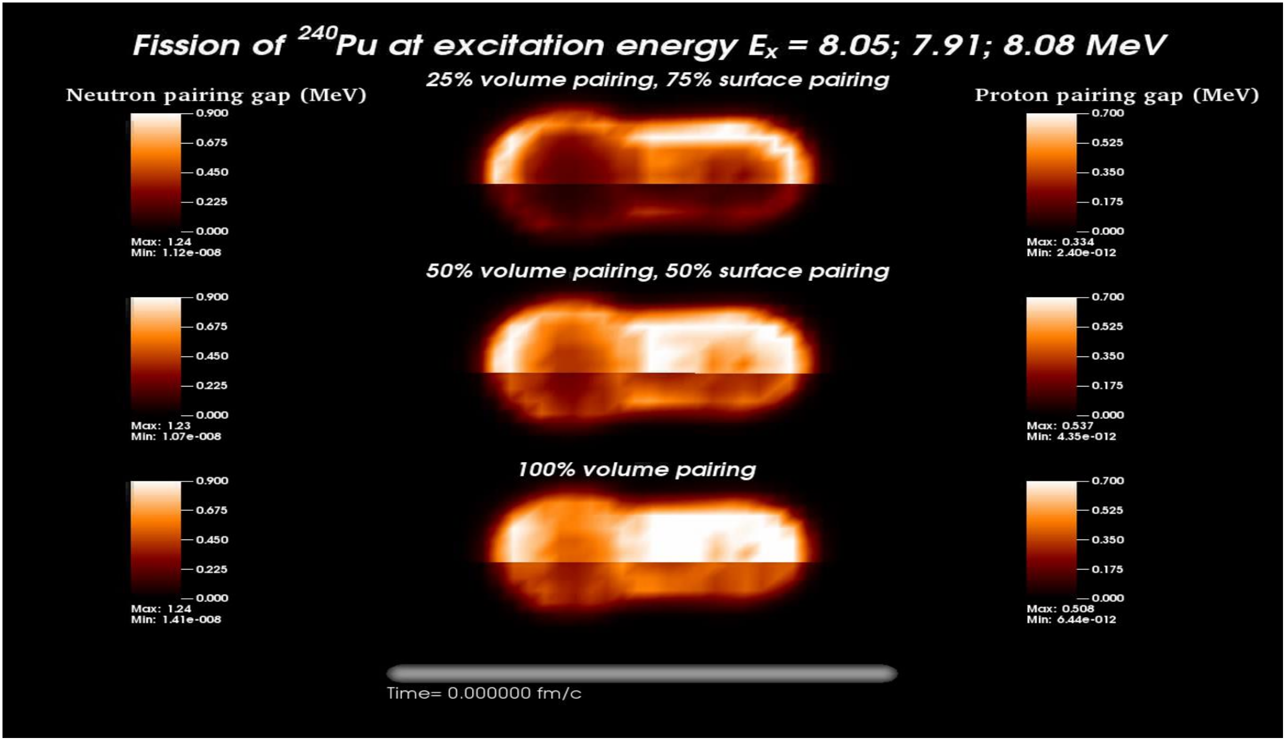
Total kinetic energy of the fragments

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

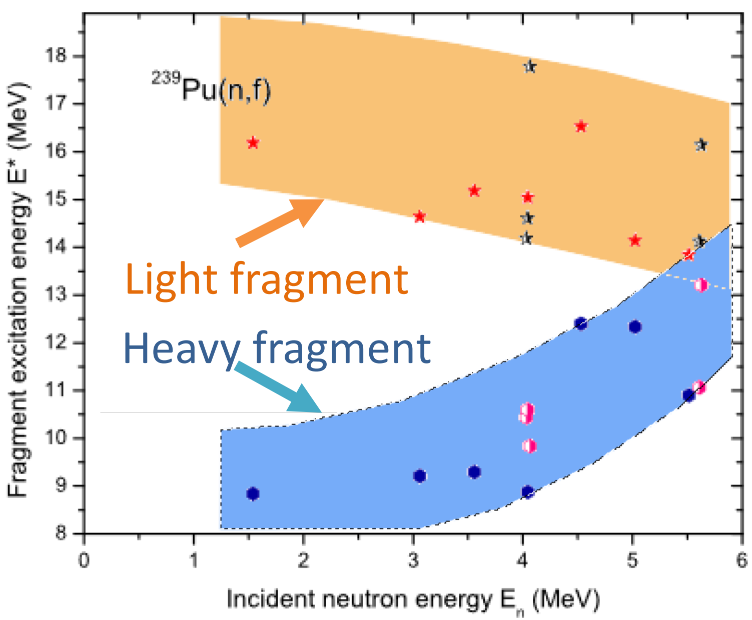
Calculated TKEs reproduce experimental data with accuracy < 2%

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

Pairing dynamics

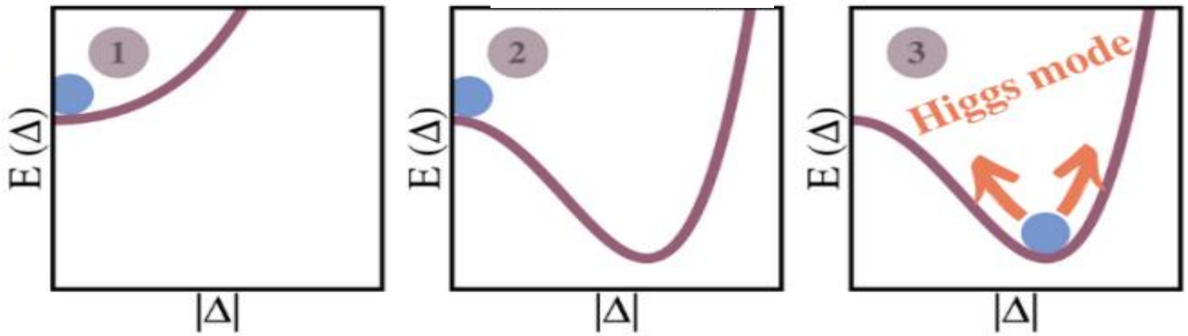


Excitation energy sharing from TDSLDA (unpublished)



E^* (MeV)	E_n (MeV)	$t_{fission}$ (fm/c)	TKE (MeV)	Z_L	N_L
8.08	1.542	8517	173.81	40.825	62.246
9.60	3.063	9215	174.73	40.500	61.536
10.10	3.560	9287	179.09	41.625	62.783
10.57	4.032	7243	173.67	40.092	61.256
10.58	4.043	7287	173.39	40.146	61.388
10.58	4.047	7134	175.11	40.313	61.475
10.60	4.065	7737	174.75	40.904	62.611
11.07	4.534	6444	176.46	41.495	63.134
11.56	5.024	6261	175.15	40.565	61.894
12.05	5.515	5898	176.75	40.412	61.809
12.15	5.610	6100	176.36	40.355	61.695
12.16	5.626	7404	176.10	41.386	62.764

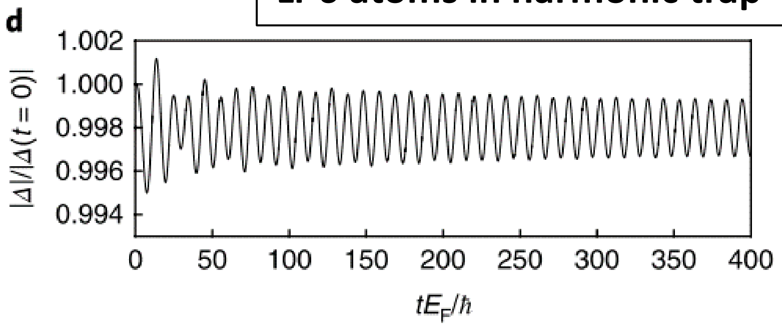
Pairing Higgs mode



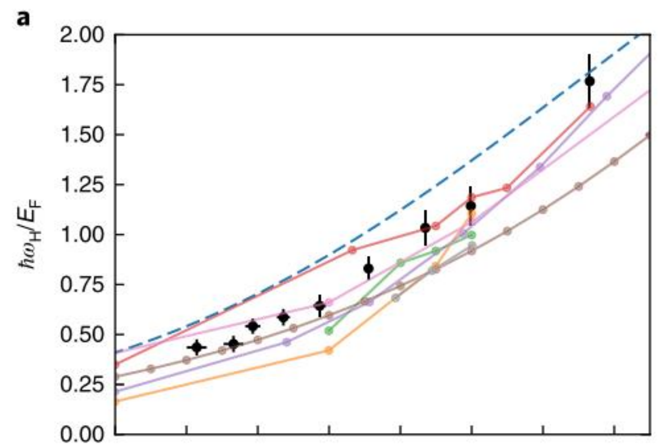
How to move from the regime 1 to regime 3 in nuclear systems?

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)

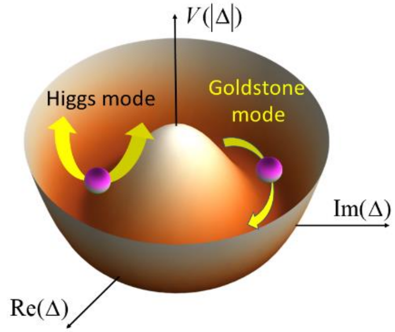


Measured peak position of the energy absorption spectra (black dots) and theory predictions for Higgs mode.

Contrary to low-energy Goldstone modes Higgs modes are in principle unstable and decay.
(A. Boulet, A. Barresi, G. Wlazłowski, P.Magierski, Sci. Rep. 13, 11285 (2023))

Precursors of Higgs modes exists even in few-body systems (J. Bjerlin et al. Phys. Rev. Lett. 116, 155302 (2016))

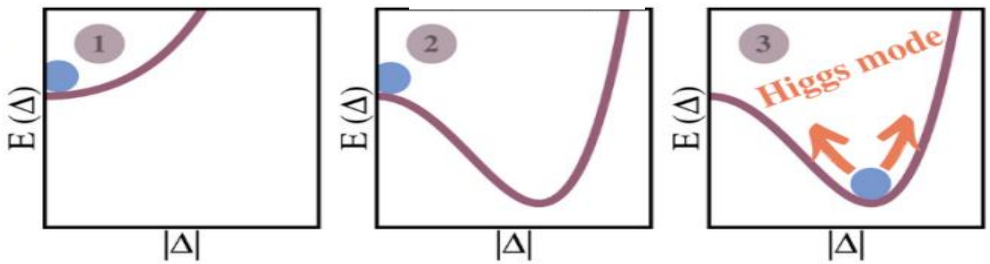
Pairing Higgs mode



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 and temperaturę. At *T=0*:

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

Pairing instability in nuclear reaction

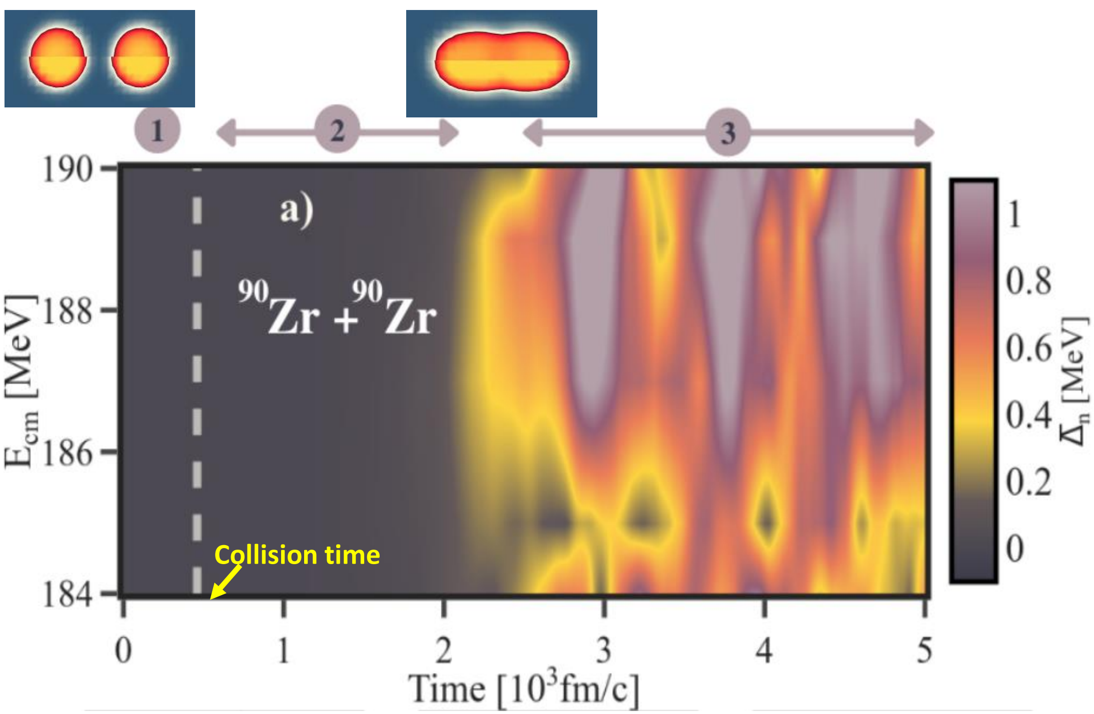
$$\Delta = \frac{8}{e^2}\varepsilon_F \exp\left(\frac{-2}{gN(\varepsilon_F)}\right)$$ - BCS formula – weak coupling limit

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.***



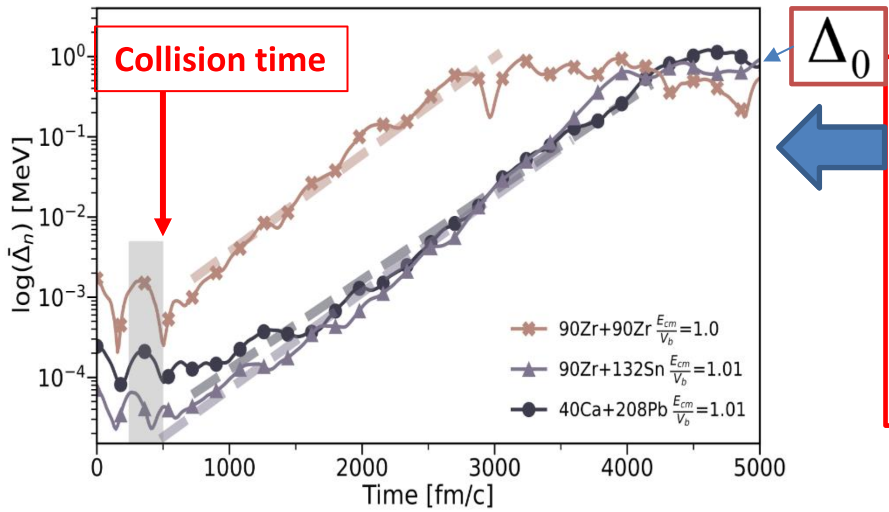
Collision of two neutron magic systems creates an elongated di-nuclear system.

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)

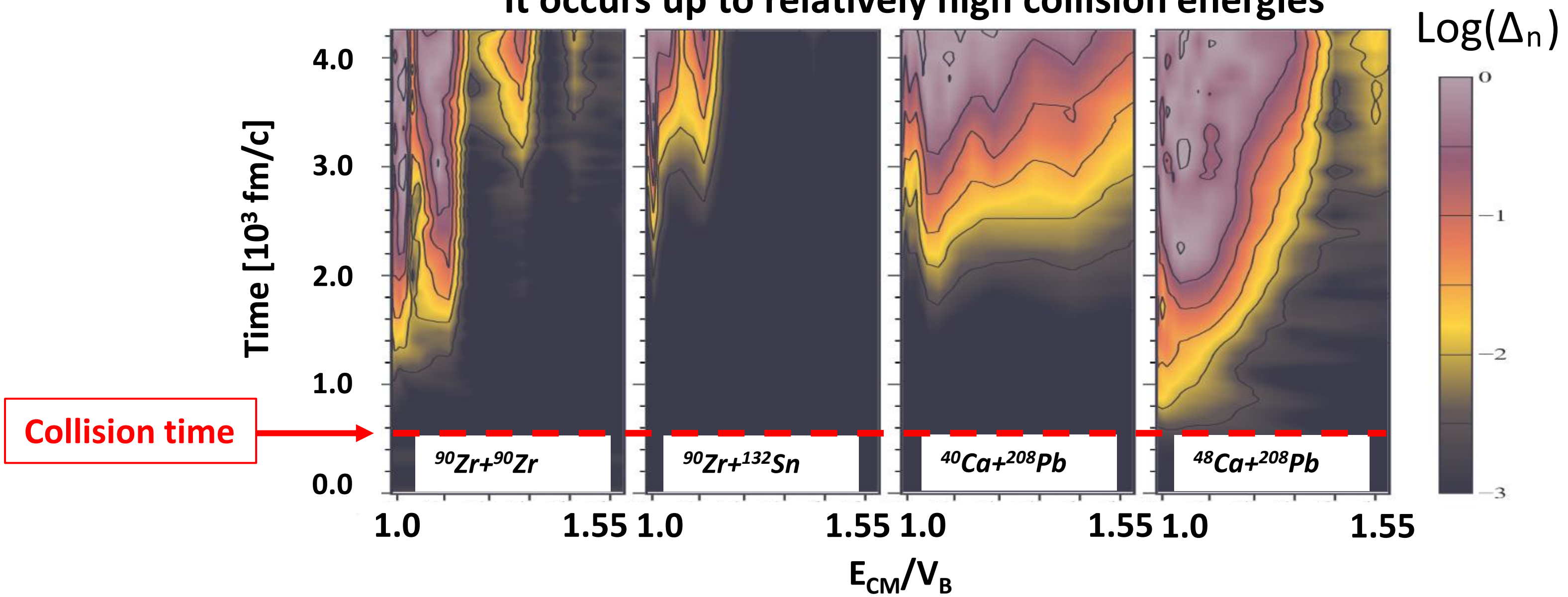
Interestingly, the effect is generic and occurs for various collisions of magic nuclei.



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

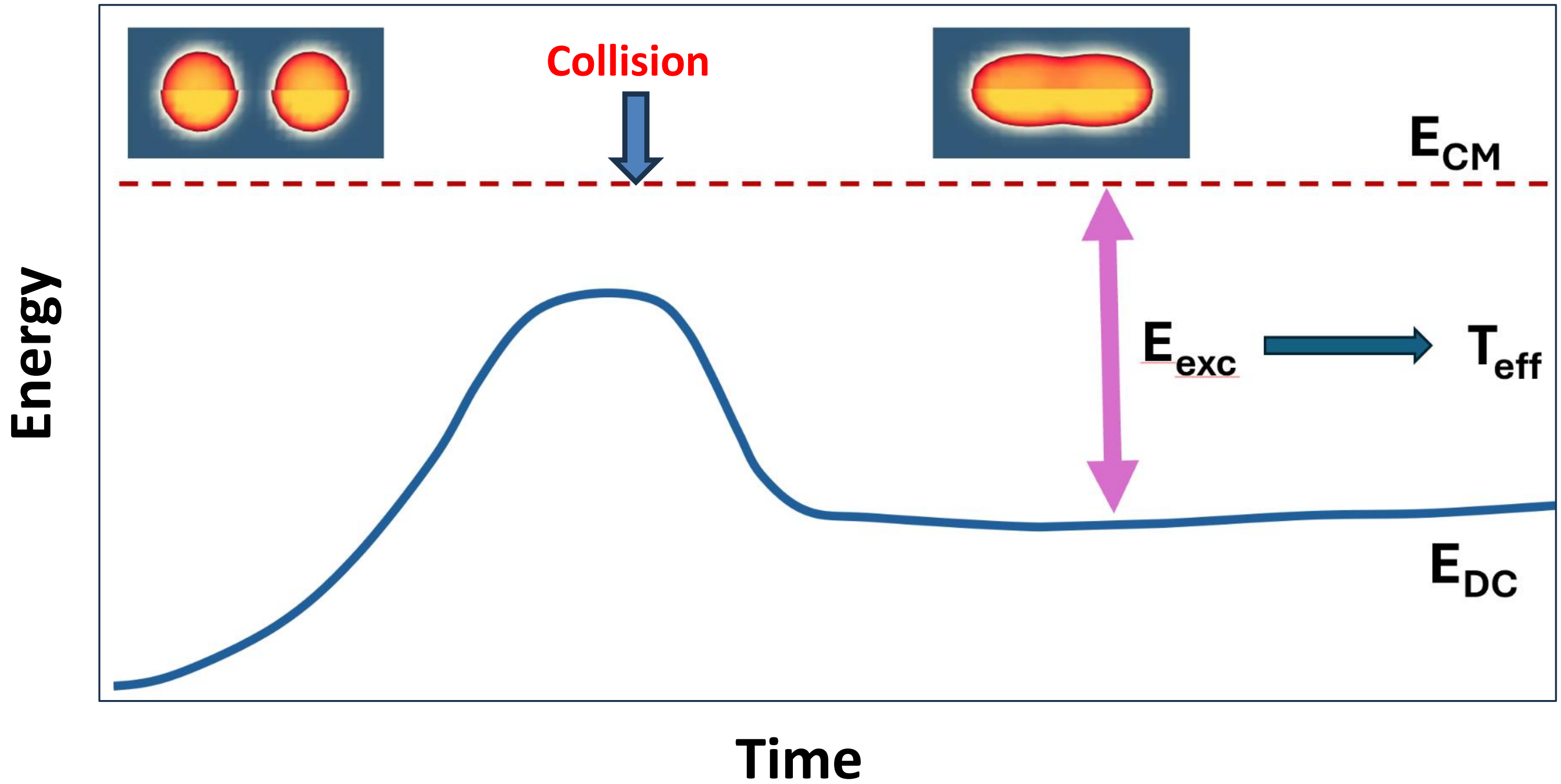
$$\tau \gg \frac{\hbar}{\Delta_0}$$

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 or even higher than the 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.

Schematic energy vs time plot for a capture process

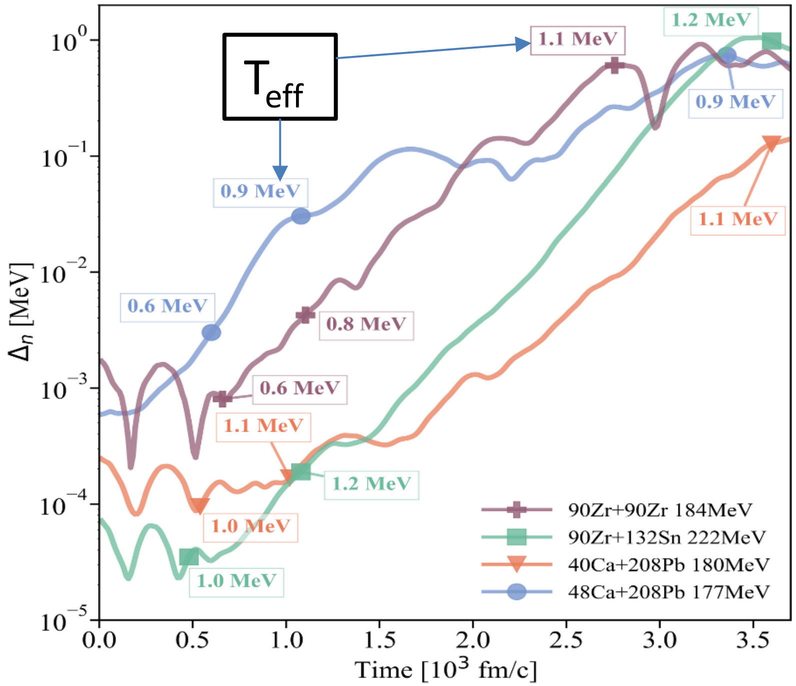


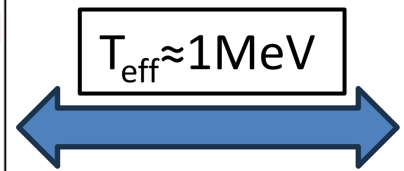
E_{DC} - Static total energy for a density distribution provided by TDDFT.

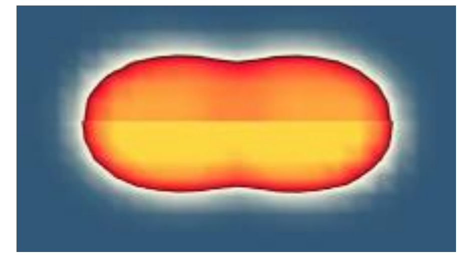
$$E_{DC}(T_{eff}) = E_{CM}$$

T_{eff} - effective temperature with respect to an instantaneous mean-field configuration.

Dynamic pairing enhancement







Temperatures, associated with excitation energies relative to the nuclear configuration after merging, are about **1 MeV .**
They **exceed** the critical temperature for **the superfluid-to-normal transition**.

$$i\hbar\frac{d\rho}{dt} = [h,\rho] + \Delta\chi^{\dagger} - \chi\Delta^{\dagger}$$

TDHF (collisionless part) Pairing („collision” term)

Pairing field mimics two-body correlations and does not indicate the presence of superfluidity.

Warsaw University of Technology | W-SLDA Toolkit W-BSk Toolkit

https://wslda.fizyka.pw.edu.pl/

W-SLDA Toolkit

Self-consistent solver of mathematical problems which have structure formally equivalent to Bogoliubov-de Gennes equations.

static problems: st-wslda

$$\begin{pmatrix} h_a(\boldsymbol{r}) - \mu_a & \Delta(\boldsymbol{r}) \\ \Delta^*(\boldsymbol{r}) & -h_b^*(\boldsymbol{r}) + \mu_b \end{pmatrix} \begin{pmatrix} u_n(\boldsymbol{r}) \\ v_n(\boldsymbol{r}) \end{pmatrix} = E_n \begin{pmatrix} u_n(\boldsymbol{r}) \\ v_n(\boldsymbol{r}) \end{pmatrix}$$

time-dependent problems: td-wslda

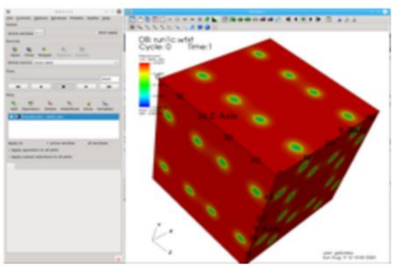
$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} u_n(\boldsymbol{r},t) \\ v_n(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} h_a(\boldsymbol{r},t) - \mu_a & \Delta(\boldsymbol{r},t) \\ \Delta^*(\boldsymbol{r},t) & -h_b^*(\boldsymbol{r},t) + \mu_b \end{pmatrix} \begin{pmatrix} u_n(\boldsymbol{r},t) \\ v_n(\boldsymbol{r},t) \end{pmatrix}$$

Extension to nuclear matter in neutron stars

Unified solvers for static and time-dependent problems

Dimensionalities of problems: 3D, 2D and 1D

Integration with VisIt: visualization, animation and analysis tool



W-SLDA is integrated with the open-source VisIt tool. It allows for:

visualizing 3D, 2D and 1D results,
data processing,
creating animations for time-dependent simulations.

ALL FUNCTIONALITIES →

Integration with VisIt: visualization, animation and analysis tool

Speed-up calculations by exploiting High Performance Computing

Functionals for studies of BCS and unitary regimes

Getting the code

DOWNLOAD

The W-SLDA & W-BSk Toolkits are free to download. It is published as open source under GNU GPL License. In order to get W-SLDA or W-BSk Toolkit click "Read more" and follow instructions.

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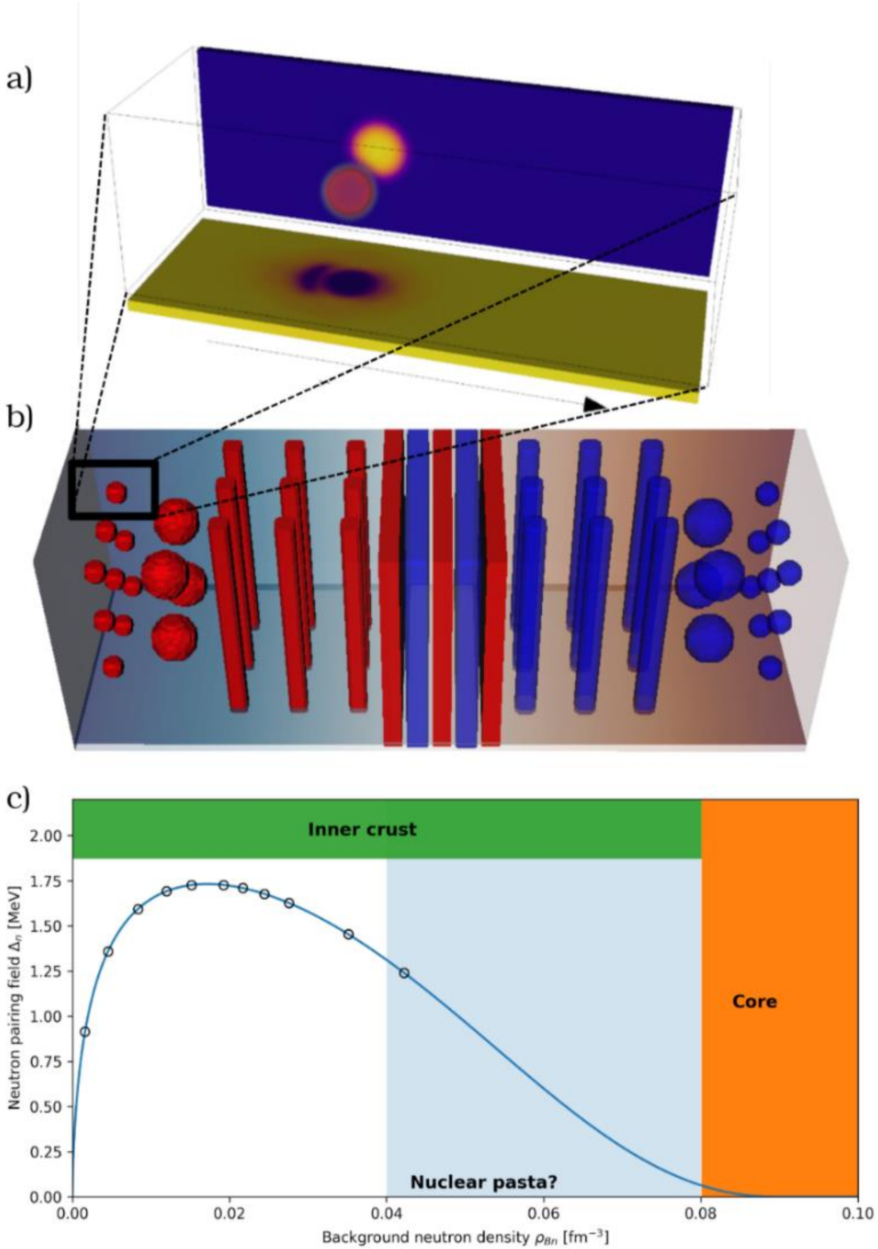
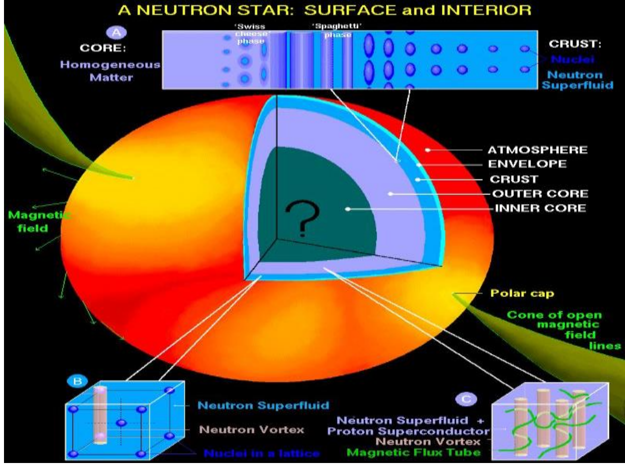
Time-Dependent Nuclear Energy-Density Functional Theory Toolkit for Neutron Star Crust: Dynamics of a Nucleus in a Neutron Superfluid

Daniel Pęcak[1,2,*], Agata Zdanowicz[1], Nicolas Chamel[3,†], Piotr Magierski[1,4,‡], and Gabriel Wlazłowski[1,4,§]

Phys. Rev. X **14**, 041054 – **Published 3 December, 2024**

Determination of the neutron star crust properties: dynamics of nuclear Coulomb crystal





Plasma frequency:

$$\omega_p = \sqrt{4\pi \rho_{ion} Z^2 e^2 / M}$$

- **Specific heat** of the Coulomb crystal (phonon spectrum).
- **Thermal and electric conductivities**. (electron-phonon scattering, eg. Umklapp processes).

Towards effective low-energy theory of the inner crust of neutron stars.

see eg. V. Cirigliano, S. Reddy, R. Sharma, Phys. Rev. C84, 045809 (2011)

Effective mass of a nucleus in superfluid neutron environment

Suppose we would like to evaluate an effective mass of a heavy particle immersed in a Fermi bath.
Can one come up with the effective (classical) equation of motion of the type:

$$M\frac{d^2q}{dt^2} - F_D\left(\frac{dq}{dt},...\right) + \frac{dE}{dq} = 0 \quad ?$$

In general it is a complicated task as the first and the second term may not be unambiguously separated.
(A. Rosch. Adv. Phys. 48, 295 (1999), R. Schmidt et al. Rep. Prog. Phys. 81, 024401 (2018).)

Moreover, if there is no gap in the system then the slight displacement (δ) of the impurity results in a huge number of particle-hole excitations, which makes the many-body wave function practically orthogonal to the initial one (if the particle number N goes to infinity):

$$\langle\Psi(0)|\Psi(\delta)\rangle \propto N^{-\delta}$$

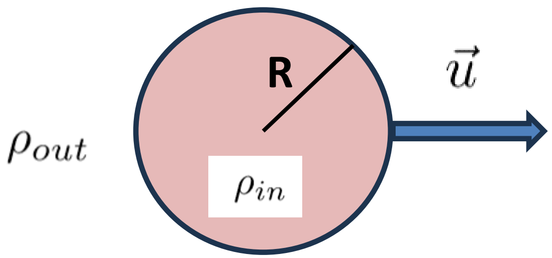
P.W. Anderson Phys. Rev. Lett. 18, 1049 (1967)

However for the superfluid system it can be done as for sufficiently slow motion (below the critical velocity) the second term may be neglected due to the presence of the pairing gap.

Two approximate methods of extracting the effective mass

Hydrodynamic description:

Impurity in irrotational fluid.



Φ – velocity field

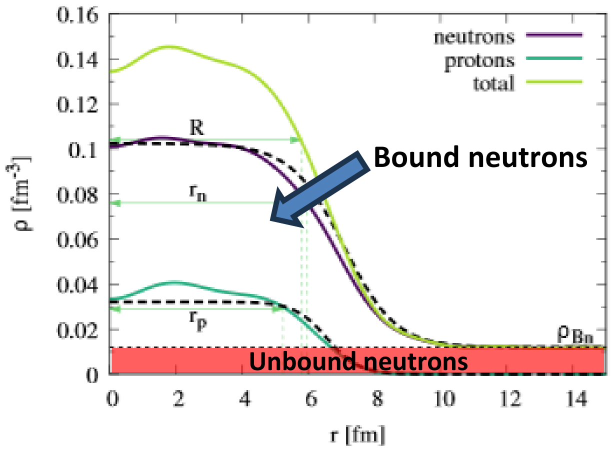
$$\Phi_{in}|_{r=R} = \Phi_{out}|_{r=R},$$
$$\rho_{in}\left(\frac{\partial}{\partial r}\Phi_{in} - \vec{n}\cdot\vec{u}\right)|_{r=R} = \rho_{out}\left(\frac{\partial}{\partial r}\Phi_{out} - \vec{n}\cdot\vec{u}\right)|_{r=R},$$
$$\Phi_{out}|_{r\to\infty} = 0,$$

$$M_{\rm eff}^{(h)} = \frac{4}{3}\pi R_h^3 m_n \frac{(\rho_{\rm in}-\rho_{\rm out})^2}{\rho_{\rm in}+2\rho_{\rm out}}.$$

P. M., Int. J. Mod. Phys. E13 (2004) 371
P. M., A. Bulgac, Acta Phys. Pol. B35, 1203 (2004)

Static description:

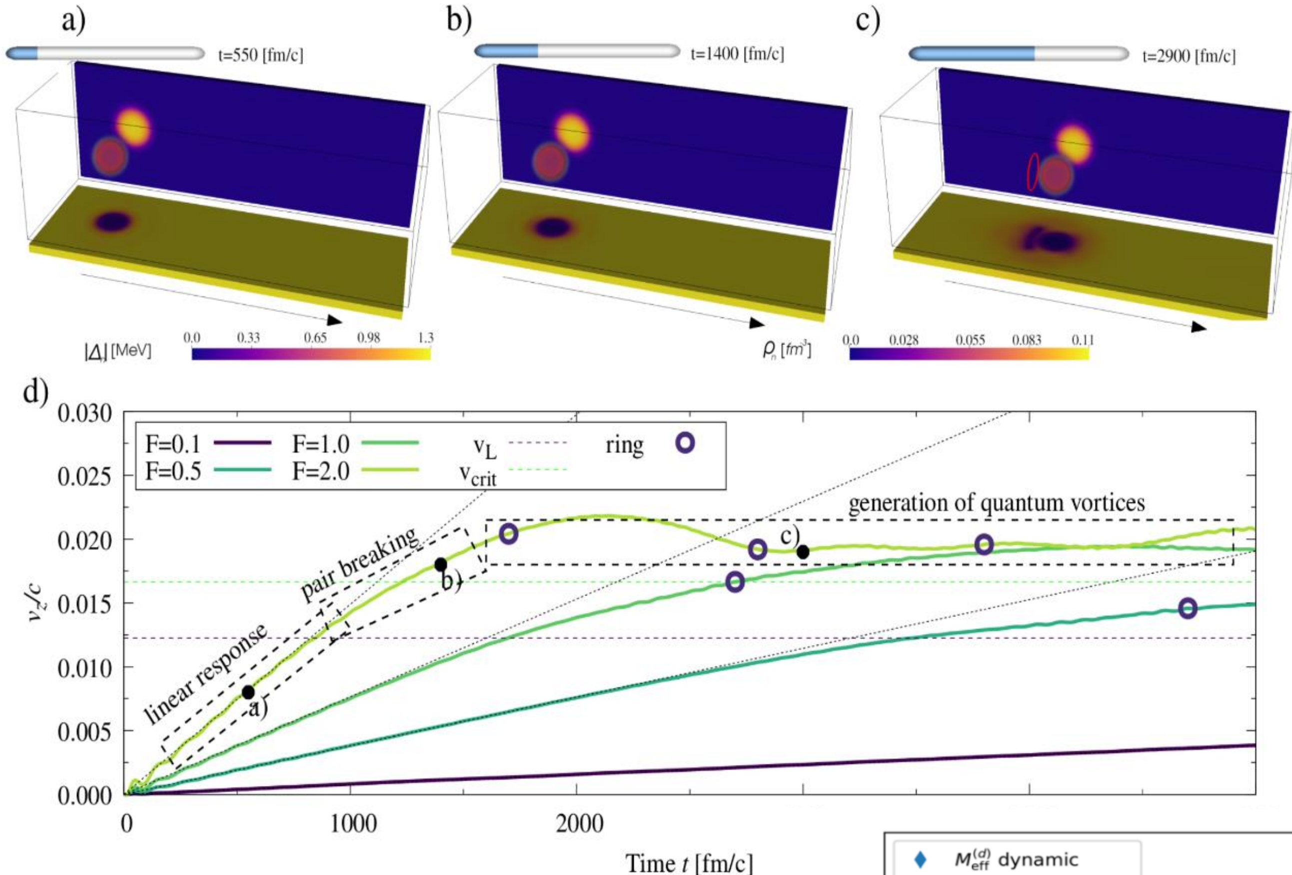
Discriminate between bound and unbound neutrons

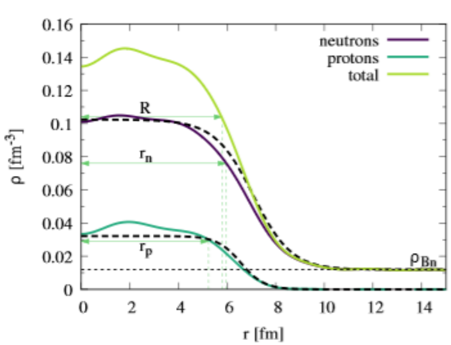


$$M_{\rm eff}^{(s)} = Zm_p + N_{\rm bound}m_n,$$

Which one offers a better approximation?

Dynamics of nuclear impurity in the neutron star crust: effective mass and energy dissipation

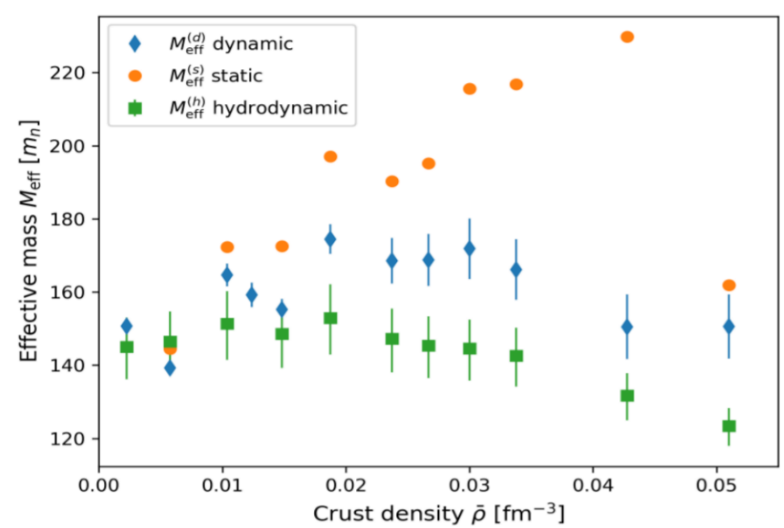




$$M_{\text{eff}}^{(d)} = a_z/F$$

$$M_{\text{eff}}^{(s)} = Zm_p + N_{\text{bound}}m_n,$$

$$M_{\text{eff}}^{(h)} = \frac{4}{3}\pi R_h^3 m_n \frac{(\rho_{\text{in}} - \rho_{\text{out}})^2}{\rho_{\text{in}} + 2\rho_{\text{out}}}.$$



D. Pęcak, A.Zdanowicz, N. Chamel, P. M., G. Wlazłowski, Phys. Rev. X14 041054 (2024)

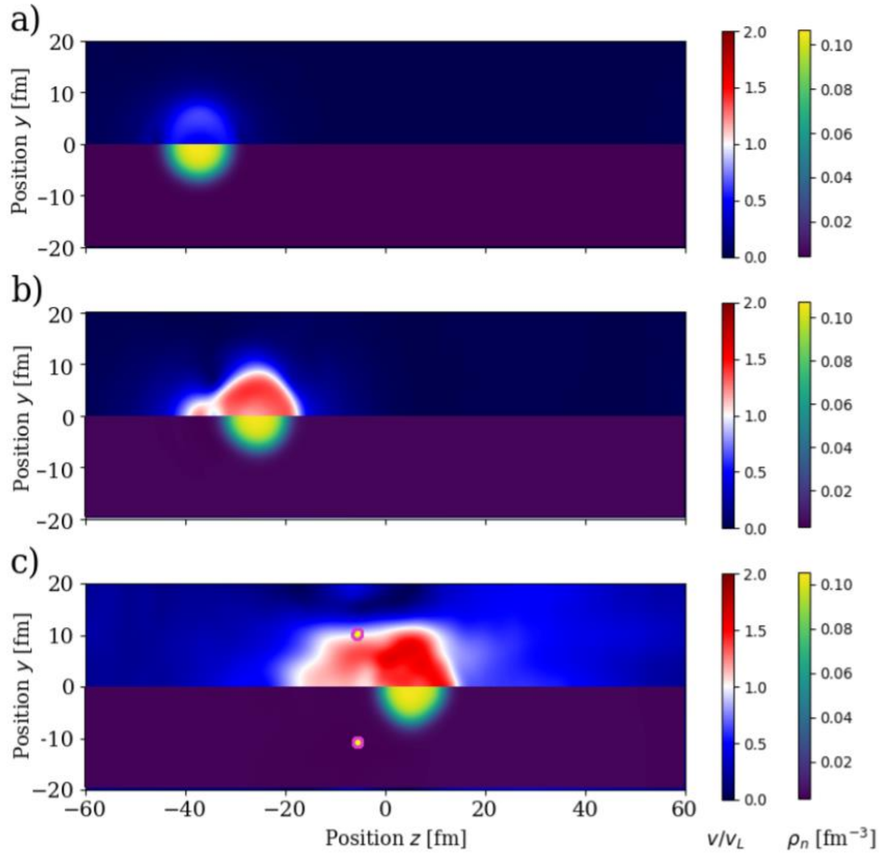
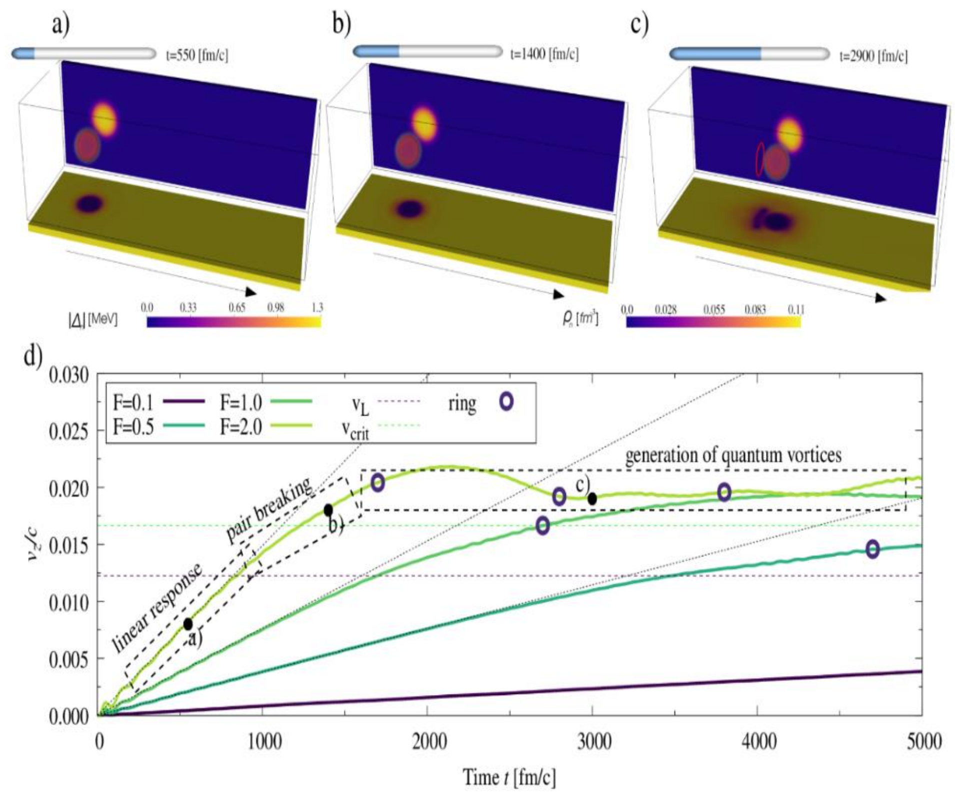


FIG. 6. Each panel presents the neutron density cross section through $x = 0$ (lower part), and local velocity in units of bulk Landau velocity (upper part). The consecutive panels are taken at times 550, 1400, and 2900 fm/c, which correspond to Fig. 3a)–c). a) in the linear response regime mainly the impurity is moving. b) in the breaking pair regime the free neutrons in the vicinity of impurity are affected. c) in the turbulent regime a large volume of neutrons is affected. Two points shown behind the impurity (at $z \approx -5\,\mathrm{fm}$) are the cross section of the vortex ring generated in this regime.



$$v_{\mathrm{L}} = \frac{\Delta_n}{\hbar k_{\mathrm{F}n}},$$ - Quasiparticle exc. energy is zero (gapless regime)

$$v_{\mathrm{crit}} = \frac{e}{2} v_{\mathrm{L}} \approx 1.4 v_{\mathrm{L}}$$ - Pairing disappears

V. Allard, N. Chamel, Phys. Rev. C108, 015801 (2023)

D. Pęcak, A.Zdanowicz, N. Chamel, P. M., G. Wlazłowski, Phys. Rev. X14 041054 (2024)

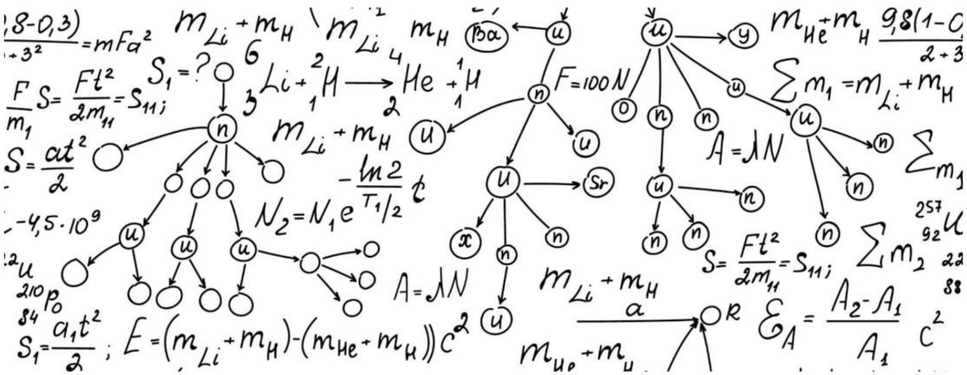
Summary

- 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.

- **Pairing enhancement** in collision of magic nuclei is a generic feature of TDHFB appearing in collisions at energies close to the Coulomb barrier.
  What is the **impact on subsequent evolution of the system and the quasifission process?**

- **TDDFT with pairing correlations** can be used to extract couplings between superfluid and solid in the neutron star crust.

NONEQUILIBRIUM PHENOMENA IN SUPERFLUID SYSTEMS: ATOMIC NUCLEI, LIQUID HELIUM, ULTRACOLD GASES, AND NEUTRON STARS



12 May 2025 — 16 May 2025

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See complete details and information

Registration

Registration available from 10/03/2025 until 18/04/2025.