Nuclear dynamics in the framework of timedependent density functional theory with pairing correlations.





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- 1. Introduction
- 2. Theoretical framework (Superfluid local density approximation)
- 3. Induced fission
- 4. Nucleus-nucleus collisions
- 5. Nucleus in a superfluid environment (neutron star crust)

Pairing as an energy gap







Deformation



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



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

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

$$\lim_{\boldsymbol{r}_{1}-\boldsymbol{r}_{2}|\to\infty} \langle \hat{\psi}^{\dagger}_{\uparrow}\left(\boldsymbol{r}_{1}\right) \hat{\psi}^{\dagger}_{\downarrow}\left(\boldsymbol{r}_{1}\right) \hat{\psi}_{\downarrow}\left(\boldsymbol{r}_{2}\right) \hat{\psi}_{\uparrow}\left(\boldsymbol{r}_{2}\right) \rangle \neq 0$$

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

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 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

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)

(see talk by Gregory Potel on Wednesday)



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

GOAL:

<u>Unified description</u> of nuclear dynamics involving medium and heavy nuclei based on microscopic theoretical framework including pairing correlations.

Microscopic framework = explicit treatment of fermionic degrees of freedom.

In most cases we are interested in extracting <u>one-body observables</u>.

This leads to considering Energy Density Functional (EDF) expressed in terms of <u>local densities</u>.

Kohn-Sham prescription in Time Dependent Density Functional Theory (TDDFT): replacing the interacting many-body system with the selfconsistent eqs. representing the <u>equivalent</u> noninteracting system.

Equivalence: one-body densities representing both systems are the same.

RUNGE E. and GROSS E. K. U., Phys. Rev. Lett., 52 (1984) 997.

For normal (nonsuperfluid) systems:

$$\begin{pmatrix} -\frac{\hbar^2}{2m} \nabla^2 + V_0(\boldsymbol{r}, t) \end{pmatrix} \phi_i(\boldsymbol{r}, t) = h(\boldsymbol{r}, t) \phi_i(\boldsymbol{r}, t) = i\hbar \frac{\partial}{\partial t} \phi_i \boldsymbol{r}, t),$$

$$\rho(\boldsymbol{r}, t) = \sum_{i=1}^N |\phi_i(\boldsymbol{r}, t)|^2,$$

$$h(\boldsymbol{r}, t) = \frac{\delta E[\rho]}{\delta \rho}(\boldsymbol{r}, t) + V_{ext}(\boldsymbol{r}, t).$$

TDHF eqs.

See eg. talks of C. Simenel and R. Gumbel

For superfluid systems:

$$\begin{pmatrix} h(\boldsymbol{r},t) & \Delta_0(\boldsymbol{r},t) \\ \Delta_0^*(\boldsymbol{r},t) & -h^*(\boldsymbol{r},t) \end{pmatrix} \begin{pmatrix} u_n(\boldsymbol{r},t) \\ v_n(\boldsymbol{r},t) \end{pmatrix} = i\hbar \frac{\partial}{\partial t} \begin{pmatrix} u_n(\boldsymbol{r},t) \\ v_n(\boldsymbol{r},t) \end{pmatrix}$$

$$\rho(\boldsymbol{r},t) = \sum_n |v_n(\boldsymbol{r},t)|^2,$$

$$\chi(\boldsymbol{r},t) = \sum_n v_n^*(\boldsymbol{r},t)u_n(\boldsymbol{r},t),$$

$$h(\boldsymbol{r},t) = \frac{\delta E[\rho,\chi,t]}{\delta\rho} + V_{ext}(\boldsymbol{r},t),$$

$$\Delta_0(\boldsymbol{r},t) = -\frac{\delta E[\rho,\chi,t]}{\delta\chi^*} + \Delta_{ext}(\boldsymbol{r},t)$$

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).

Kohn, W., Gross, E.K.U., Oliveira, L.N. (1989): J. de Physique (Paris) 50, 2601

S. Kurth, M. Marques, M. Lüders, E.K.U. Gross, Phys. Rev. Lett. 83 2628 (1999).

J.F. Dobson, M.J. Brunner, E.K.U. Gross, Phys. Rev. Lett. 79 1905 (1997).

G. Vignale, C. A. Ullrich, S. Conti, Phys. Rev. Lett. 79 4878 (1997).

Note that now:

 $\lim_{|\boldsymbol{r}_1 - \boldsymbol{r}_2| \to \infty} \langle \hat{\psi}^{\dagger}_{\uparrow}(\boldsymbol{r}_1) \, \hat{\psi}^{\dagger}_{\downarrow}(\boldsymbol{r}_1) \, \hat{\psi}_{\downarrow}(\boldsymbol{r}_2) \, \hat{\psi}_{\uparrow}(\boldsymbol{r}_2) \rangle = \chi^*_{\uparrow\downarrow}(\boldsymbol{r}_1) \chi_{\uparrow\downarrow}(\boldsymbol{r}_2)$

TDHFB eqs. (TDSLDA)

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

$$h \sim f_{1}(n,\nu,...)\nabla^{2} + f_{2}(n,\nu,...) \cdot \nabla + f_{3}(n,\nu,...)$$

$$h \sim f_{1}(n,\nu,...)\nabla^{2} + f_{2}(n,\nu,...) \cdot \nabla + f_{3}(n,\nu,...)$$

$$\frac{1}{2} \left(\begin{array}{ccc} u_{n,a}(\mathbf{r},t) \\ u_{n,b}(\mathbf{r},t) \\ v_{n,a}(\mathbf{r},t) \\ v_{n,b}(\mathbf{r},t) \end{array} \right) = \left(\begin{array}{ccc} h_{a}(\mathbf{r},t) & 0 & 0 & \Delta(\mathbf{r},t) \\ 0 & h_{b}(\mathbf{r},t) & -\Delta(\mathbf{r},t) & 0 \\ 0 & -\Delta^{*}(\mathbf{r},t) & -h_{a}^{*}(\mathbf{r},t) & 0 \\ \Delta^{*}(\mathbf{r},t) & 0 & 0 & -h_{b}^{*}(\mathbf{r},t) \end{array} \right) \left(\begin{array}{c} u_{n,a}(\mathbf{r},t) \\ u_{n,b}(\mathbf{r},t) \\ v_{n,a}(\mathbf{r},t) \\ v_{n,b}(\mathbf{r},t) \end{array} \right)$$

where h and Δ depends on "densities":

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

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

huge number of nonlinear coupled 3D Partial Differential Equations (in practice n=1,2,..., 10⁵ - 10⁶)

- 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)

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

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

Present computing capabilities:

- full 3D (unconstrained) superfluid dynamics
- spatial mesh up to 100³
- max. number of particles of the order of 10⁴
- up to 10⁶ time steps

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

Nuclear fission dynamics

Potential energy versus deformation



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



$$1 \text{ zs} = 10^{-21} \text{ sec.} = 300 \text{ fm/c}$$

Fission dynamics of ²⁴⁰Pu



Note that despite the fact that nucleus is already <u>beyond the saddle point</u> the collective motion on the time scale of 1000 fm/c and larger is characterized by <u>the constant velocity</u> (*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

",Heavy soliton" creation in nuclear collision

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

The main questions are:

-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.





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

²⁴⁰Pu+²⁴⁰Pu





Creation of <u>the solitonic structure</u> between colliding nuclei prevents energy transfer to internal degrees of freedom and consequently <u>enhances</u> the kinetic energy of outgoing fragments. Surprisingly, the <u>gauge angle dependence</u> from the G-L approach is perfectly well reproduced in <u>the kinetic energies of outgoing fragments</u>!

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



TABLE I: The minimum energies needed for capture in ${}^{90}\text{Zr}+{}^{90}\text{Zr}$ and ${}^{96}\text{Zr}+{}^{96}\text{Zr}$ 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).

	$\overline{\Delta}_q \ (\text{MeV})$	$E_{\rm thresh}(0) ({\rm MeV})$	$E_{\rm thresh}(\pi)$ (MeV)	ΔE_s
⁹⁰ Zr	$\overline{\Delta}_n = 0.00$	184	184	0
	$\overline{\Delta}_p = 0.09$	101		
	$\overline{\Delta}_n = 1.98$	179	185	6
	$\overline{\Delta}_p = 0.32$			
⁹⁶ Zr	$\overline{\Delta}_n = 2.44$	178	187	9
	$\Delta_p = 0.33$			
	$\Delta_n = 2.94$	178	187	9
	$\Delta_p = 0.34$			

Dynamic nature of the effect:

<u>Solid lines</u>: 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.

<u>Dashed lines</u>: 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.

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 / ε_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 :

$$\tau = \frac{1}{\mathcal{Y}} \approx \frac{\overline{h}}{\overline{\Delta_0}}$$



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

- \mathcal{E}_F Fermi energy
- g Pairing coupling constant

 $N(\mathcal{E}_{_F})$ - 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:

 $\Lambda < \hbar \omega < 2\Lambda$

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.



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.

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 correlations appearing at relatively high excitation energy provide a nonnegligible modification of the density evolution.



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. Nuclear physics. Induced nuclear fission, fusion, collisions.

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

 \mathcal{E}_F

Collisions of ultracold atomic clouds offer an insight into pairing-related effects relevant to nuclear collisions.



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

Polar cap Nutron Torrest Nut

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:

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

In general it is a complicated task as the first and the second term may not be unambiguously separated.

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.

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



D. Pecak, A.Zdanowicz, N. Chamel, P. Magierski, G. Wlazłowski, arXiv:2403.17499

Summary and open questions

- Induced fission: the nuclear motion from sadle to scission is not adiabatic, although it is slow.
- <u>Excitation energy sharing</u>: 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 <u>solitonic excitations</u> (dynamic barrier modification for capture) and <u>pairing</u> <u>enhancement</u> 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)).
- <u>Pairing enhancement</u> in collision of magic nuclei is a <u>generic feature of TDHFB</u> 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: impact on quasifission process, interplay between pairing and shell effects in nuclear collisions, ...