# **Exotic features of superfluidity far from** equilibrium



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Collaborators:

Matthew Barton (WUT) Aurel Bulgac (UoW) Janina Grineviciute (WUT) Konrad Kobuszewski (WUT - Ph.D. student) Kenneth Roche (PNNL) Kazuyuki Sekizawa (WUT -> Niigata U.) Ionel Stetcu (LANL) Buğra Tüzemen (WUT - Ph.D. student) Gabriel Wlazłowski (WUT) <u>Unified description</u> of <u>superfluid dynamics</u> of fermionic systems <u>far from equilibrium</u> based on microscopic theoretical framework.

GOAL:

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 <u>hundred of thousands</u> fermions.

## **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 
$$~\chi({f r}\sigma,{f r}'\sigma')=\langle\hat\psi_{\sigma'}({f r}')\hat\psi_{\sigma}({f r})
angle$$

However in the limit of the local field these quantities diverge unless one renormalizes the coupling constant:

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

which ensures that the term involving the kinetic and the pairing energy density is finite:

$$\frac{\tau_c(r)}{2m} - \Delta(r)\chi_c(r), \quad \tau_c(r) = \nabla \cdot \nabla' \rho_c(r, r')|_{r=r'}$$

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

It allows to reduce the size of the problem for static calculations by introducing the energy cutoff

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

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

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 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.

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

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

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

where h and  $\Delta$  depends on "densities":

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

We explicitly track fermionic degrees of freedom!

 $v(\mathbf{r},t) = \sum_{E_n < E_c} u_{n,\uparrow}(\mathbf{r},t) v_{n,\downarrow}^*(\mathbf{r},t), \qquad \mathbf{j}_{\sigma}(\mathbf{r},t) = \sum_{E_n < E_c} \operatorname{Im}[v_{n,\sigma}^*(\mathbf{r},t) \nabla v_{n,\sigma}(\mathbf{r},t)],$ huge number of nonlinear coupled 3D
Partial Differential Equations
(in practice n=1,2,..., 10<sup>5</sup> - 10<sup>6</sup>)
Present

Present computing capabilities:

- full 3D (unconstrained) superfluid dynamics
- spatial mesh up to 100<sup>3</sup>
- max. number of particles of the order of 10<sup>4</sup>
- ▶ up to 10<sup>6</sup> time steps

(for cold atomic systems - time scale: a few ms for nuclei - time scale: 100 zs) How reliably can we describe superfluid dynamics in various Fermi systems within TDSLDA?

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

## Areas of applications



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

Astrophysical applications. Modelling of neutron star interior (glitches): vortex dynamics, dynamics of inhomogeneous nuclear matter (in strong magnetic fields). Nuclear physics. Induced nuclear fission, fusion, collisions.

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

## **Example 1: nuclear fission dynamics**

#### Potential energy versus deformation



11.56 5.024

12.15 5.610

12.16 5.626

5.515

12.05

175

176

176

176

176.05 0.51 40.565

175.88 0.49 40.412

175.84 0.29 40.355

175.84 0.15 41.386

61.894

61.809

61.695

62.764

experimental data

with accuracy < 2%

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



#### TDSLDA energy sharing between fragments



#### J. Grineviciute et al. – in preparation

# Character of nuclear motion along the fission path – from TDSLDA

Accelerations in quadrupole and octupole moments



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

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</u> of freedom.

Severe test for the theory – unfortunately no exp. data are available yet.

## **Example 2: spin-imbalanced unitary Fermi gas**

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 costs energy proportional to  $q^2$  but may be compensated by an increased pairing energy due to the mutual shift of Fermi spheres:



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)

## 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. (
$$\Delta \ll k_F^2$$
)  

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

Engineering the structure of nodal surfaces

Apply the spin-selective potential of a certain shape: V



Wait until the proximity effects of the pairing field generate the nodal structure and remove the potential.





#### Andreev states and anatomy of the vortex core

#### FERMIONS:

Vortex structure: Fermi gas  $\rightarrow$  BdG eq.



Andreev states inside the core give rise to anomalous branch of excitations

(of chiral fermions):



#### **BOSONS:**

Vortex structure: Bose gas  $\rightarrow$  Gross-Pitaevskii eq. (GPE)



#### **Expectations**:

- Long range interaction in the system of vortices is the same for bosons and fermions, as it is governed by the superfluid flow  $v_s$
- Short range physics (e.g. reconnection rate) is different due to the population of Andreev states in the core. It
- significantly modifies the decay of the turbulent state (Wlazłowski, Kobuszewski, Sekizawa, Magierski, in preparation)
- Note that Andreev states define the energy scale:

 $\delta E \approx \frac{4}{3} \frac{|\Delta|^2}{\varepsilon_E} < |\Delta|$  - **minigap**, which affects thermal and dissipative properties of the system of vortices.





Wlazłowski, Kobuszewski, Sekizawa, Magierski, in preparation

## **Example 3: dynamics of solitonic excitations**



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

Nuclear collisions

Collisions of superfluid nuclei having different phases of the pairing fields 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:  $E_j \approx 30 MeV$ 



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>! Effective barrier height for fusion as a function of the phase difference



What is an average extra energy needed for the capture?

$$E_{extra} = \frac{1}{\pi} \int_{0}^{\pi} \left( B\left(\Delta\varphi\right) - V_{Bass} \right) d\left(\Delta\varphi\right) \approx 10 MeV$$

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. 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

## 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**

- 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
- A. Bulgac, S.Jin, I. Stetcu, arxiv:1806.00694
- 3) Dissipation: transition between one-body dissipation regime and twobody dissipation regime.