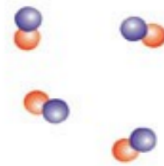




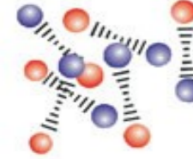
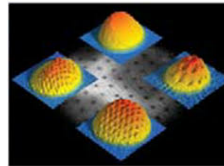
Ultracold Fermi gases as benchmark platform for neutron star studies: density functional theory approach

Gabriel Wlazłowski

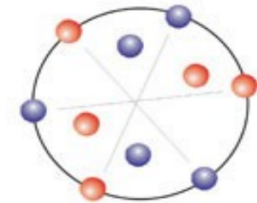
Warsaw University of Technology
University of Washington



diatomic molecules



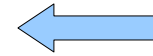
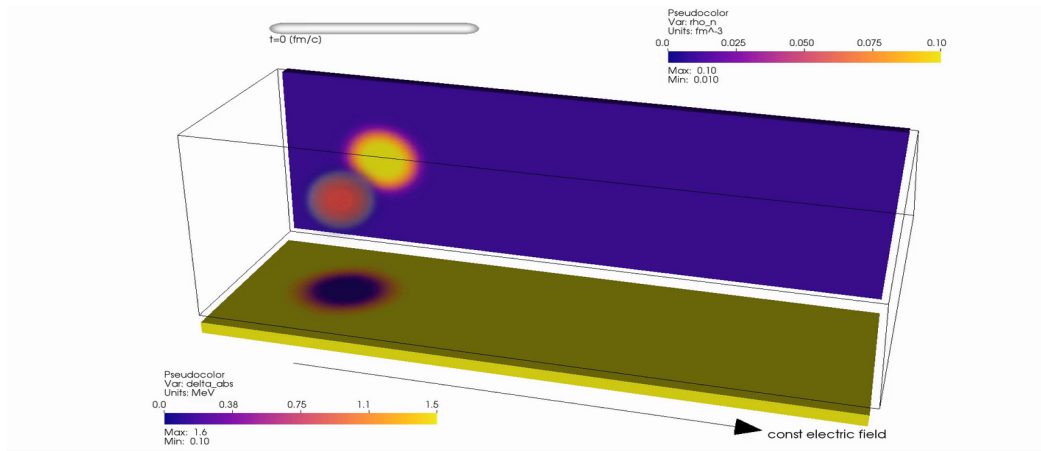
strongly interacting pairs



Cooper pairs

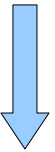


Context: superfluid dynamics in neutron stars



Nuclear impurity in superfluid neutron matter
(see talk by Daniel Peřak)

and in vicinity of quantum vortex:



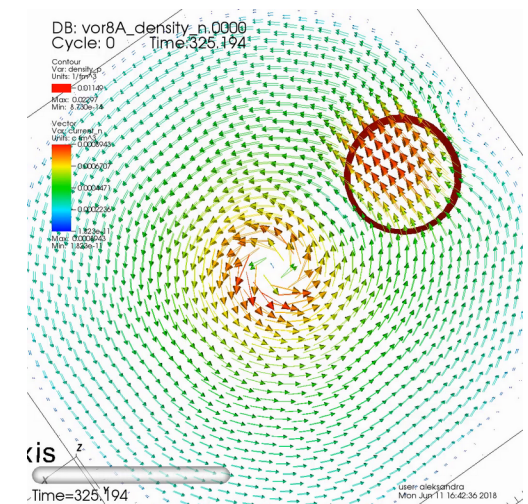
Source: D. Peřak, et. al, arXiv:2403.17499

To what extent can we trust these types of calculations?

Overview:

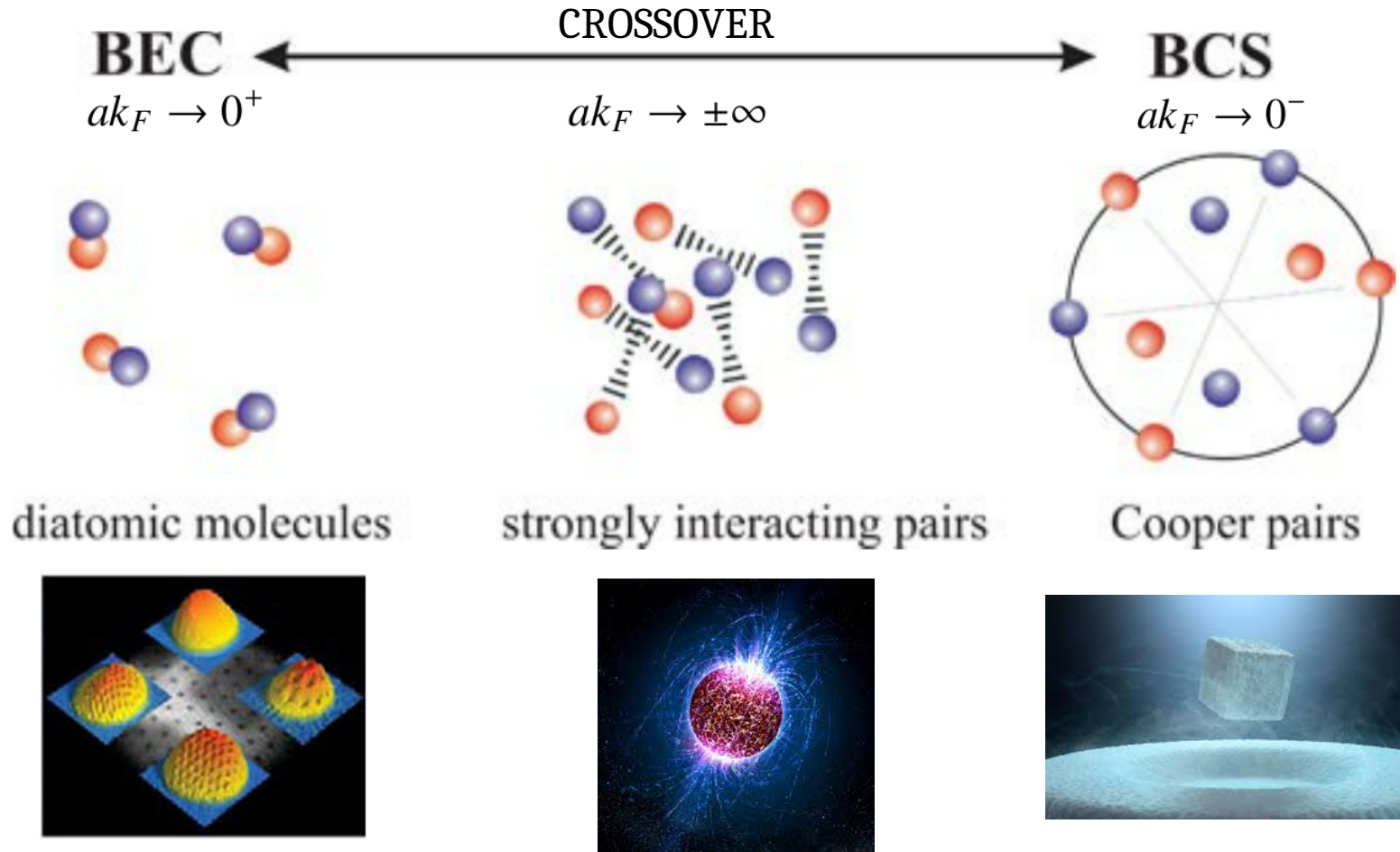
1. Method \rightarrow DFT*
2. DFT for ultracold atoms and nuclear systems
3. Testing predictive power of DFT with ultracold gases
4. Long term challenges

(* Note: Many formal aspects of the theory will be presented superficially. Only general formulas...



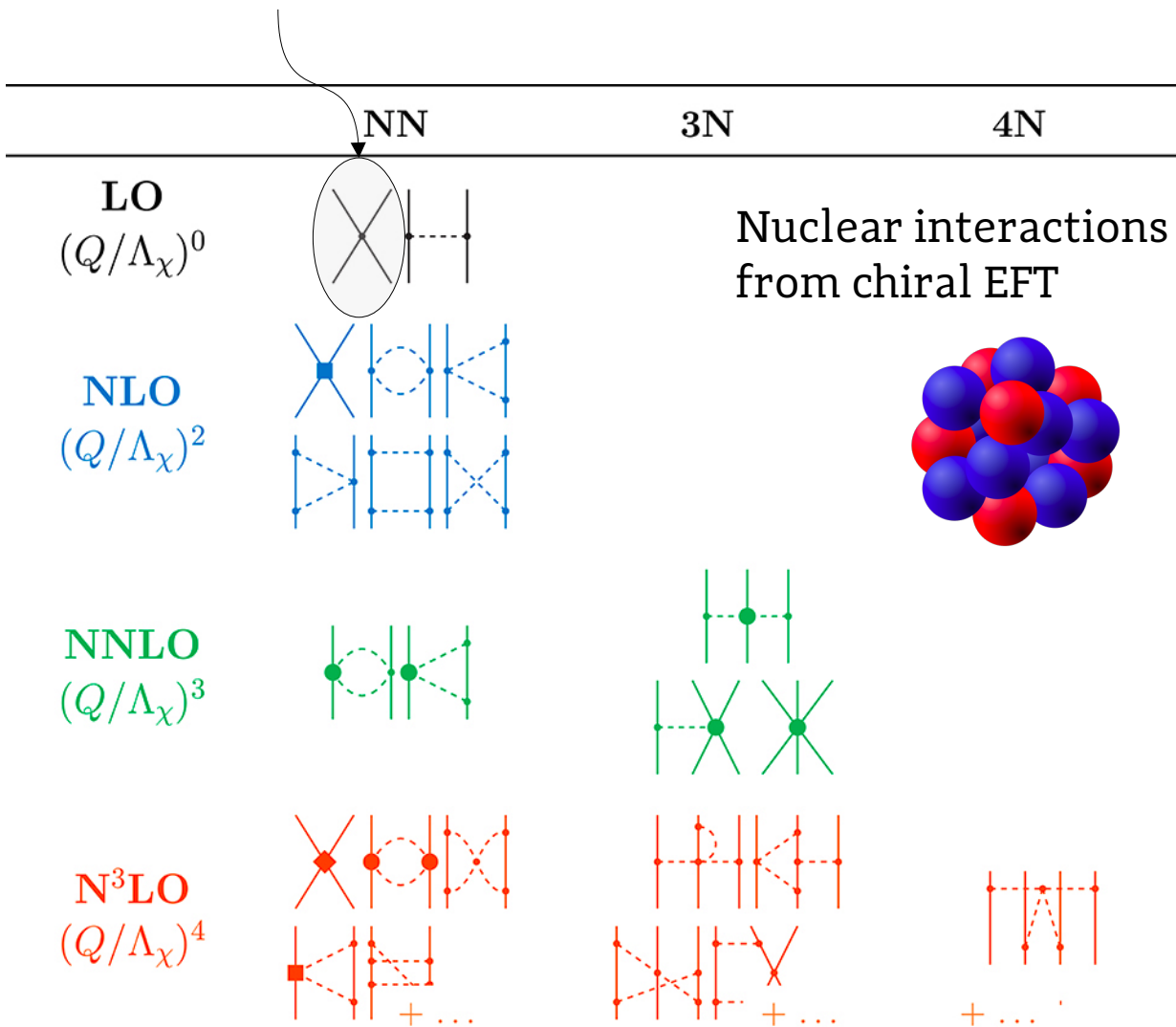


- ◆ **Ultracold atomic** systems offer possibility to test predictive power of many-body methods.
- ◆ The (bare) interaction is simple $V(\mathbf{r}-\mathbf{r}')=g\delta(\mathbf{r}-\mathbf{r}')\dots$
- ◆ ... but the interaction strength g can be tuned at will!



$$V(\mathbf{r}-\mathbf{r}') = g\delta(\mathbf{r}-\mathbf{r}')$$

contact interaction



Expectation: the method when applied to “ultra-cold” atomic system should provide higher accuracy results as compared to applications in context of “nuclear” systems...

... upper limit for predictive power of the method.

Fig from: Hergert H, Front. Phys. 8:379 (2020); doi:10.3389/fphy.2020.00379

Density Functional Theory (DFT):

Workhorse for ...

Solid-state physics

Quantum chemistry

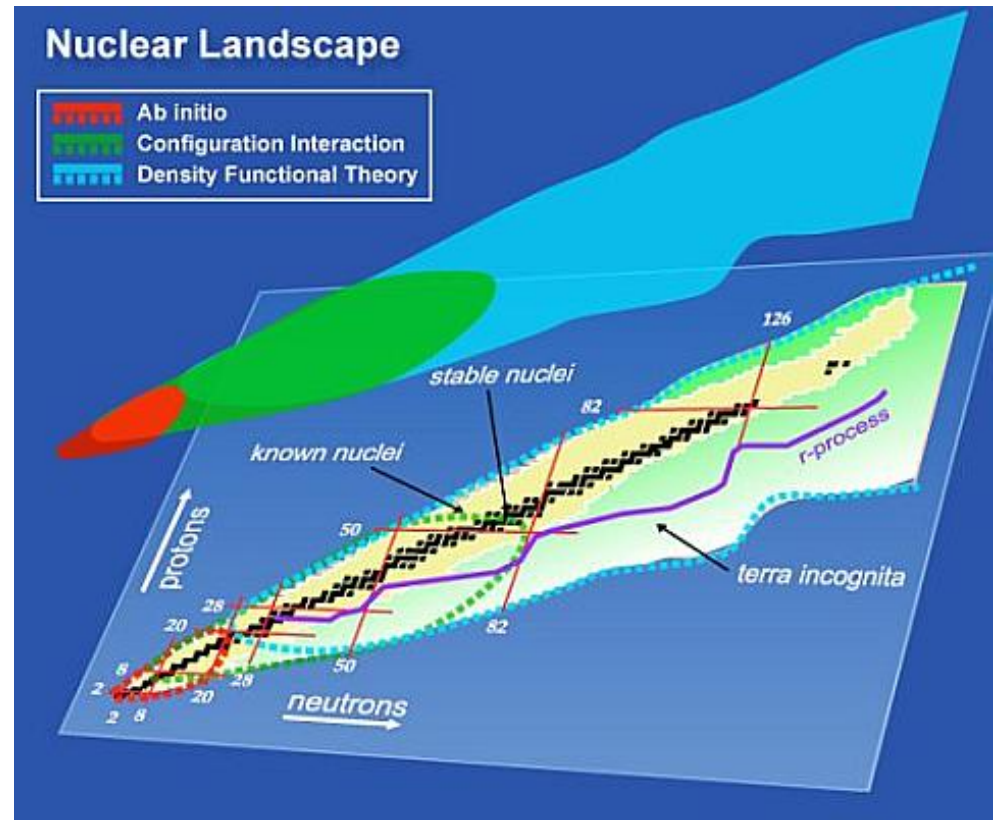
Condensed-matter physics

... also important tool for

Nuclear physics

(Nuclear) astrophysics

Plasma physics ...



DFT is, in principle, exact theory

(due to Hohenberg-Kohn theorem)...

... in practice not – we need to construct the energy functional (no mathematical recipe how to derive it)

Many extensions: time-dependent formalism, finite temperature, normal/superconducting systems, non-relativistic/relativistic, ...

General purpose framework

Nature 514, 550 (2014)

... Twelve papers on the top-100 list relate to it [DFT], including 2 of the top 10.

SLDA-type functional

$$E_0 = \int \mathcal{E}[n_\sigma(\mathbf{r}), \tau_\sigma(\mathbf{r}), \mathbf{j}_\sigma, \nu(\mathbf{r})] d\mathbf{r}$$

The Fermi-Dirac distribution function

normal density

$$n_\sigma(\mathbf{r}) = \sum_{|E_n| < E_c} |v_{n,\sigma}(\mathbf{r})|^2 f_\beta(-E_n),$$

Densities are **parametrized** via Bogoliubov quasiparticle wave functions

kinetic density

$$\tau_\sigma(\mathbf{r}) = \sum_{|E_n| < E_c} |\nabla v_{n,\sigma}(\mathbf{r})|^2 f_\beta(-E_n),$$

quasiparticle = mixture of hole particle

$$\varphi_\eta(\mathbf{r}, t) = [u_\eta(\mathbf{r}, t), v_\eta(\mathbf{r}, t)]^T$$

current density

$$\mathbf{j}_\sigma(\mathbf{r}) = \sum_{|E_n| < E_c} \text{Im}[v_{n,\sigma}(\mathbf{r}) \nabla v_{n,\sigma}^*(\mathbf{r})] f_\beta(-E_n),$$

$$\int \varphi_\eta^\dagger(\mathbf{r}, t) \varphi_{\eta'}(\mathbf{r}, t) d^3\mathbf{r} = \delta_{\eta,\eta'}$$

+ orthonormality condition (Pauli principle)

anomalous density

$$\nu(\mathbf{r}) = \frac{1}{2} \sum_{|E_n| < E_c} [u_{n,a}(\mathbf{r}) v_{n,b}^*(\mathbf{r}) - u_{n,b}(\mathbf{r}) v_{n,a}^*(\mathbf{r})] f_\beta(-E_n).$$

Additional density required by DFT theorem for systems with broken U(1) symmetry

Energy cut-off scale (need for regularization)

Density-Functional Theory for Superconductors

L. N. Oliveira, E. K. U. Gross, and W. Kohn
Phys. Rev. Lett. **60**, 2430 – Published 6 June 1988

SLDA-type functional

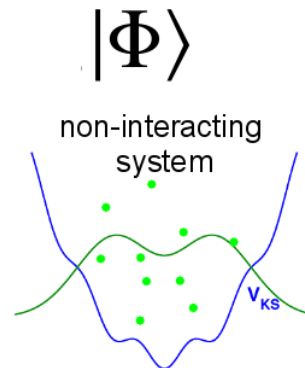
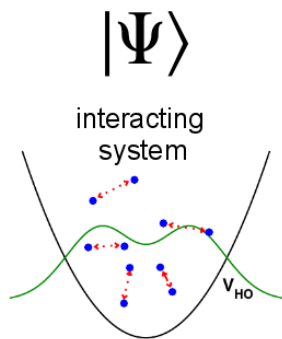
$$E_0 = \int \mathcal{E}[n_\sigma(\mathbf{r}), \tau_\sigma(\mathbf{r}), \mathbf{j}_\sigma, \nu(\mathbf{r})] d\mathbf{r}$$

minimization

By construction minimization of the SLDA-type functional leads to equations that are mathematically equivalent to BdG or HFB equations

$$\begin{pmatrix} h_\uparrow(\mathbf{r}) - \mu_\uparrow & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -h_\downarrow^*(\mathbf{r}) + \mu_\downarrow \end{pmatrix} \begin{pmatrix} u_{n,\uparrow}(\mathbf{r}) \\ v_{n,\downarrow}(\mathbf{r}) \end{pmatrix} = E_n \begin{pmatrix} u_{n,\uparrow}(\mathbf{r}) \\ v_{n,\downarrow}(\mathbf{r}) \end{pmatrix}$$

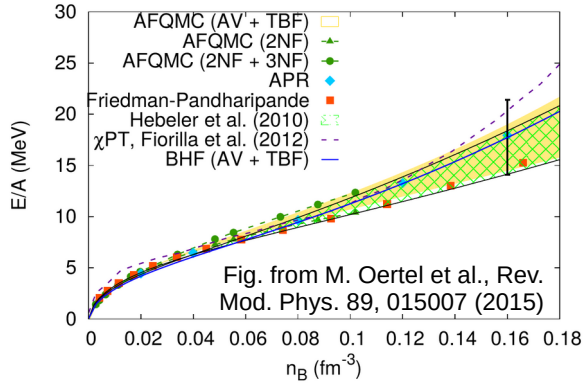
$$h_\sigma = -\nabla \frac{\delta E_0}{\delta \tau_\sigma} \nabla + \frac{\delta E_0}{\delta n_\sigma} - \frac{i}{2} \left\{ \frac{\delta E_0}{\delta \mathbf{j}_\sigma}, \nabla \right\}, \quad \Delta = -\frac{\delta E_0}{\delta \nu^*}.$$



DFT method from practical point of view:

DFT method allows for the description of many-body quantum systems with higher accuracy than the mean-field method while keeping the computational complexity at the same level as for the mean-field method.

EoS (typically from QMC)

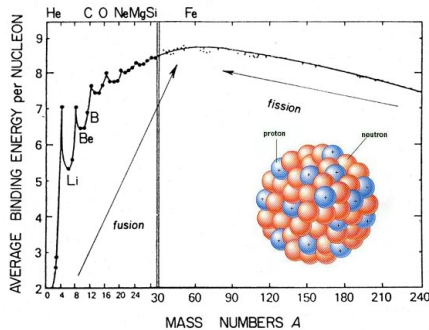


Dimensional arguments, renormalizability, Galilean invariance, and symmetries (translational, rotational, gauge, parity, ...)

Postulate

Validation against other quantities

Exp. data for nuclei (masses, radii, ...)

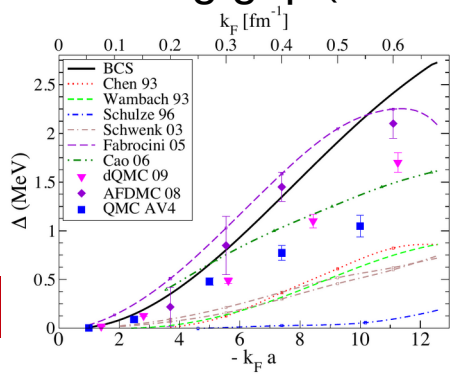


Input 2

Energy Density Functional $E[n, \dots]$

Note: EDF \rightarrow EoS but EoS \nrightarrow EDF

Pairing gap (s-wave)



Input 3

Predictions...

The quality of DFT results strongly depends on the quality of the functional, ... which in turn depends on the quality of input data.

Brussels Skyrme functionals BSk(G)

We have fitted a series of nuclear energy-density functionals with full HFB calculations using extended Skyrme functionals

Experimental data/constraints:

- ~ 2300 atomic masses (rms $\sim 0.5 - 0.6 \text{ MeV}/c^2$)
- ~ 900 nuclear charge radii (rms $\sim 0.03 \text{ fm}$)
- symmetry energy $29 \leq J \leq 32 \text{ MeV}$
- incompressibility $K_V = 240 \pm 10 \text{ MeV}$ (giant resonances in nuclei)

Many-body ab initio calculations:

- equation of state of pure neutron matter
- 1S_0 pairing gaps in nuclear matter
- effective masses in nuclear matter (+giant resonances in nuclei)
- stability against spin and spin-isospin fluctuations

SLDA-type functional

for ultra-cold atoms

$$E_0 = \int \mathcal{E}[n(\mathbf{r}), \tau(\mathbf{r}), \mathbf{j}(\mathbf{r}), \nu(\mathbf{r})] d\mathbf{r}$$

Dimensionless
functional parameters

$$\{A_\lambda, B_\lambda, C_\lambda\}$$

Densities
 $n(\mathbf{r}), \tau(\mathbf{r}), \nu(\mathbf{r})$
are defined via
 $[u_\eta(\mathbf{r}, t), v_\eta(\mathbf{r}, t)]^T$

$$\lambda = ak_F$$

$$\mathcal{E} = \frac{A_\lambda}{2} \left(\tau - \frac{\mathbf{j}^2}{n} \right) + \frac{3}{5} B_\lambda n \varepsilon_F + \frac{C_\lambda}{n^{1/3}} |\nu|^2 + \frac{\mathbf{j}^2}{2n}$$

*dimensional analysis +
symmetries*

Kinetic
term

Potential
term

Pairing
term

Center of
mass motion

Units:
 $\hbar=m=1$

SLDA-type functional

for ultra-cold atoms

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Densities $n(\mathbf{r}), \tau(\mathbf{r}), \nu(\mathbf{r})$ are defined via $[u_n(\mathbf{r}, t), v_n(\mathbf{r}, t)]^T$

$$\lambda = ak_F$$

$$\mathcal{E} = \frac{A_\lambda}{2} \left(\tau - \frac{\mathbf{j}^2}{n} \right) + \frac{3}{5} B_\lambda n \varepsilon_F + \frac{C_\lambda}{n^{1/3}} |\nu|^2 + \frac{\mathbf{j}^2}{2n}$$

dimensional analysis + symmetries

Kinetic term

Potential term

Pairing term

Center of mass motion

Units:
 $\hbar = m = 1$

Example: The simplest choice

BdG (mean-field)

$$A_\lambda \rightarrow 1$$

$$B_\lambda \rightarrow 0$$

$$C_\lambda \rightarrow \frac{4\pi\hbar^2}{(3\pi^2)^{1/3}m} \lambda ak_F$$

$$\mathcal{E}_{\text{BdG}} = \frac{\tau}{2} + 4\pi a |\nu(\mathbf{r})|^2$$

minimization

$$\begin{pmatrix} -\frac{\hbar^2}{2} \nabla^2 - \mu & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & \frac{\hbar^2}{2} \nabla^2 + \mu \end{pmatrix} \begin{pmatrix} u_n(\mathbf{r}) \\ v_n(\mathbf{r}) \end{pmatrix} = E_n \begin{pmatrix} u_n(\mathbf{r}) \\ v_n(\mathbf{r}) \end{pmatrix}$$

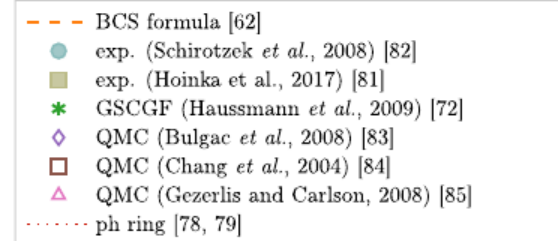
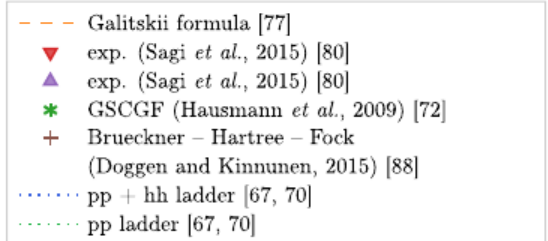
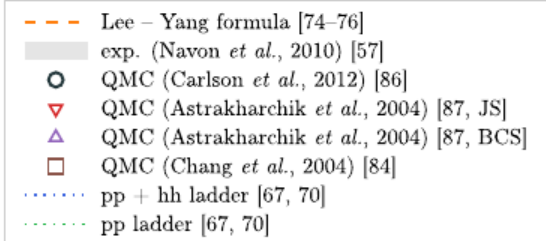
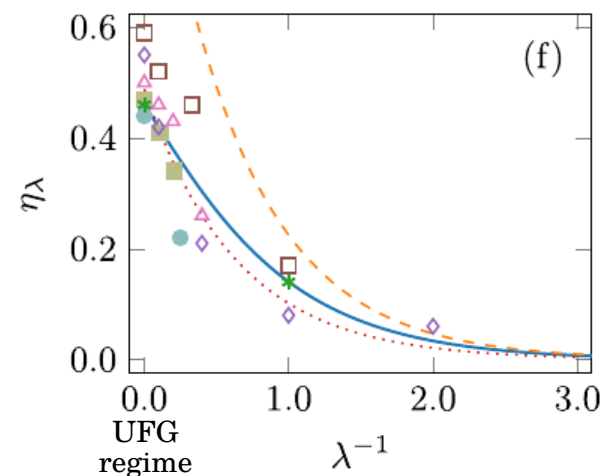
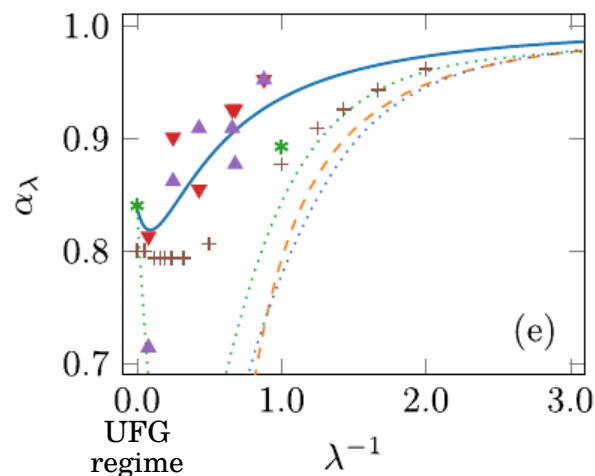
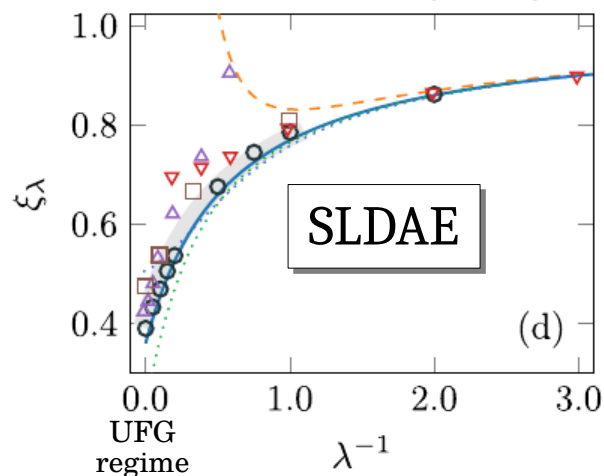
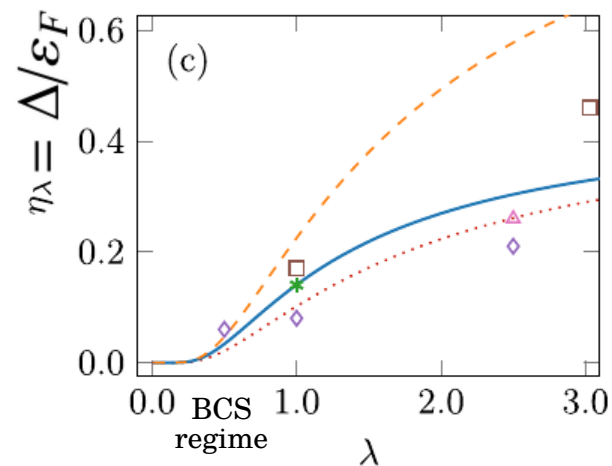
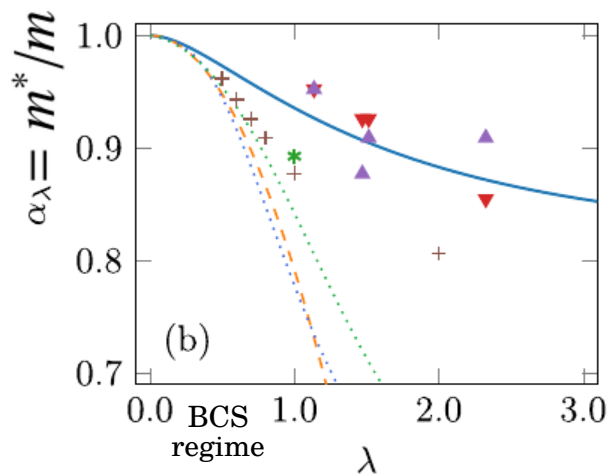
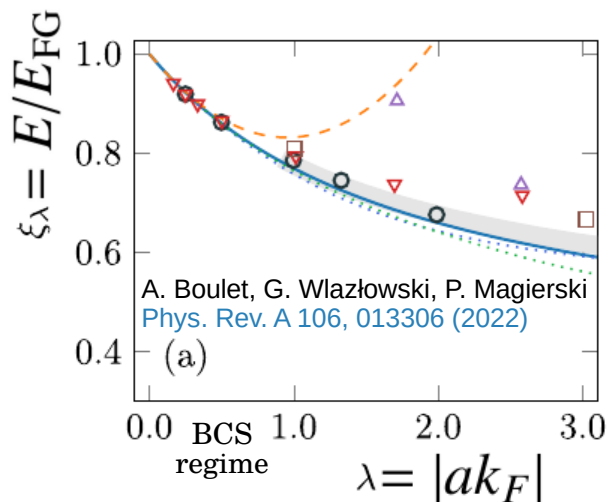
$$\Delta = -4\pi a \sum_{|E_n| < E_c} u_n(\mathbf{r}) v_n^*(\mathbf{r}) \frac{f_\beta(-E_n) - f_\beta(E_n)}{2}$$

There always exists a functional that after minimization provides equations identical to the mean-field equations (zeroth order).

→ *ab initio* calcs for E/E_{FG} , Δ/ε_F , m^*/m
 → limiting cases (EFT, scale invariance, ...)

INDUCE

Functional parameters
 $\{A_\lambda, B_\lambda, C_\lambda\}$



Towards time-dependent problems

$$\begin{pmatrix} h_{\uparrow}(\mathbf{r}) - \mu_{\uparrow} & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -h_{\downarrow}^*(\mathbf{r}) + \mu_{\downarrow} \end{pmatrix} \begin{pmatrix} u_{n,\uparrow}(\mathbf{r}) \\ v_{n,\downarrow}(\mathbf{r}) \end{pmatrix} = E_n \begin{pmatrix} u_{n,\uparrow}(\mathbf{r}) \\ v_{n,\downarrow}(\mathbf{r}) \end{pmatrix}$$



From point of view of DFT this step represents
uncontrolled approximation,
called *adiabatic approximation*

$$\begin{pmatrix} h_{\uparrow}(\mathbf{r}, t) - \mu_{\uparrow} & \Delta(\mathbf{r}, t) \\ \Delta^*(\mathbf{r}, t) & -h_{\downarrow}^*(\mathbf{r}, t) + \mu_{\downarrow} \end{pmatrix} \begin{pmatrix} u_{n,\uparrow}(\mathbf{r}, t) \\ v_{n,\downarrow}(\mathbf{r}, t) \end{pmatrix} = i\hbar \frac{\partial}{\partial t} \begin{pmatrix} u_{n,\uparrow}(\mathbf{r}, t) \\ v_{n,\downarrow}(\mathbf{r}, t) \end{pmatrix}$$

Towards time-dependent problems

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Density-Functional Theory for Time-Dependent Systems

Erich Runge and E. K. U. Gross

Phys. Rev. Lett. **52**, 997 – Published 19 March 1984

Time-Dependent Density-Functional Theory for Superconductors

O. -J. Wacker, R. Kümmel, and E. K. U. Gross

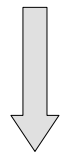
Phys. Rev. Lett. **73**, 2915 – Published 21 November 1994

There exists analog of Hohenberg-Kohn theorem for time-dependent problems...

... but for time-dependent case the “exact” functional is in general different from the one that is used in static calculations...

Towards time-dependent problems

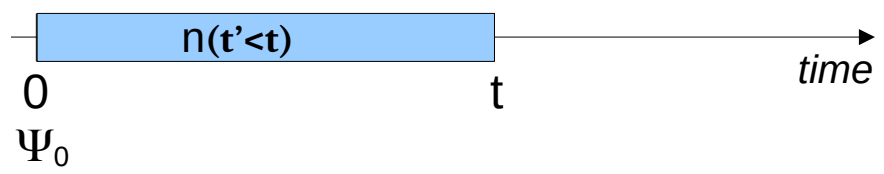
$$\begin{pmatrix} h_{\uparrow}(\mathbf{r}) - \mu_{\uparrow} & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -h_{\downarrow}^*(\mathbf{r}) + \mu_{\downarrow} \end{pmatrix} \begin{pmatrix} u_{n,\uparrow}(\mathbf{r}) \\ v_{n,\downarrow}(\mathbf{r}) \end{pmatrix} = E_n \begin{pmatrix} u_{n,\uparrow}(\mathbf{r}) \\ v_{n,\downarrow}(\mathbf{r}) \end{pmatrix}$$



From point of view of DFT this step represents uncontrolled approximation, called *adiabatic approximation*

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$$E(t) = E[\Psi(t=0), n(\mathbf{r}, t' \leq t), \dots]$$



In general integro-differential equations

$$E(t) = \int_V d\mathbf{r} \mathcal{E}[n(\mathbf{r}, t), \dots]$$

Adiabatic approximation

$$E(t) = \int_0^t dt' \int_V d\mathbf{r} \mathcal{E}[\Psi_0, n(\mathbf{r}, t'), \dots]$$

There exists analog of Hohenberg-Kohn theorem for time-dependent problems...

... but for time-dependent case the “exact” functional is in general different from the one that is used in static calculations...

...if the evolution is slow (adiabatic), then the system follows instantaneous ground state
 → use the functional taken from static considerations.

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

W-SLDA Toolkit

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

static problems: st-wslda

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

time-dependent problems: td-wslda

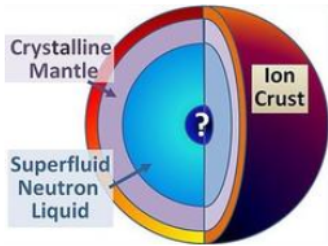
$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} u_n(\mathbf{r}, t) \\ v_n(\mathbf{r}, t) \end{pmatrix} = \begin{pmatrix} h_a(\mathbf{r}, t) - \mu_a & \Delta(\mathbf{r}, t) \\ \Delta^*(\mathbf{r}, t) & -h_b^*(\mathbf{r}, t) + \mu_b \end{pmatrix} \begin{pmatrix} u_n(\mathbf{r}, t) \\ v_n(\mathbf{r},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

Extension to nuclear matter in neutron stars

Extension to nuclear matter in neutron stars

Unified solvers for static and time-dependent problems

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



The W-SLDA Toolkit has been expanded to encompass nuclear systems, now available as the W-BSk Toolkit.

Integration with VisIt: visualization, animation and analysis tool

Speed-up calculations by exploiting High Performance Computing

Functionals for studies of BCS and unitary regimes

ALL FUNCTIONALITIES →



can run on "small" computing clusters as well as leadership supercomputers (depending on the problem size)

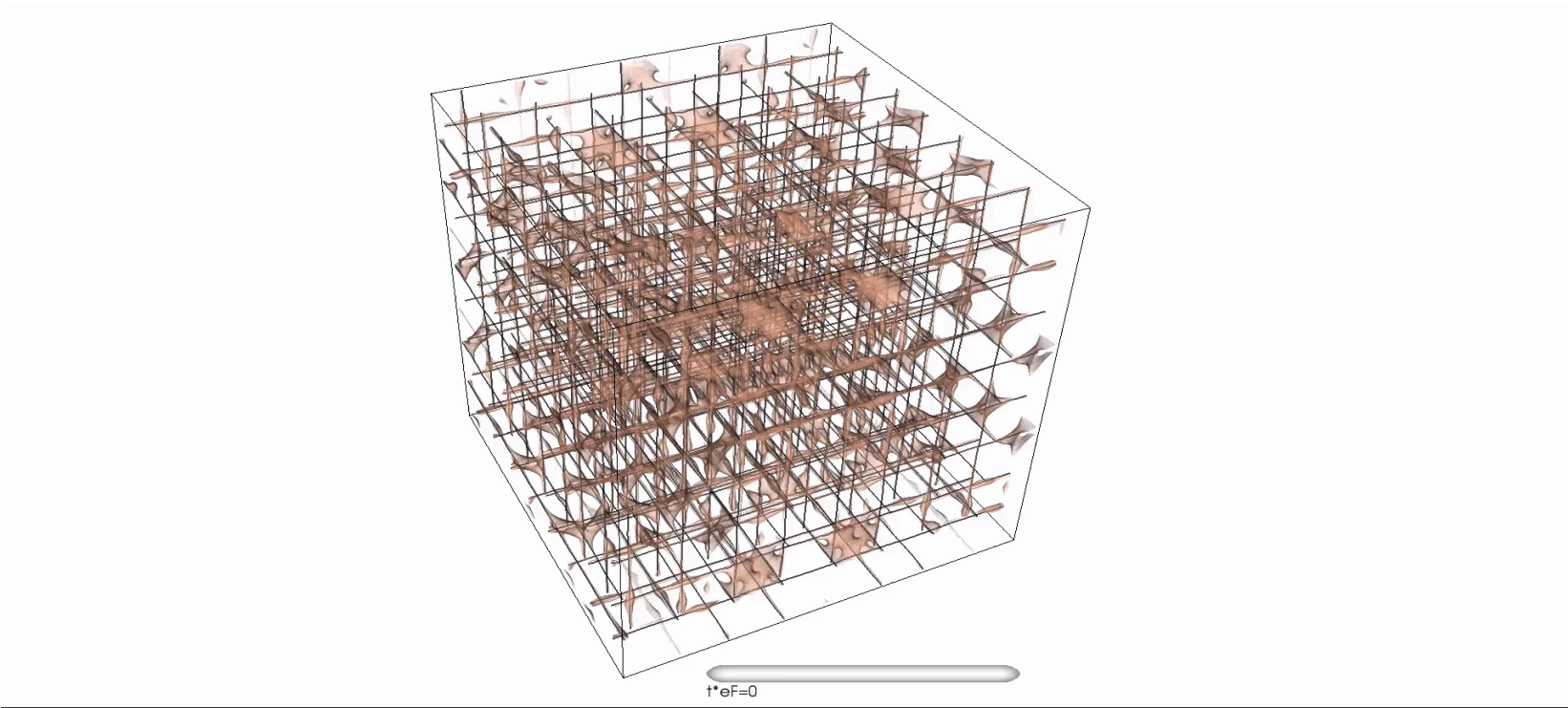


High Performance Computing



... we follow this good practice also in case of developments for cold atoms and neutron stars...



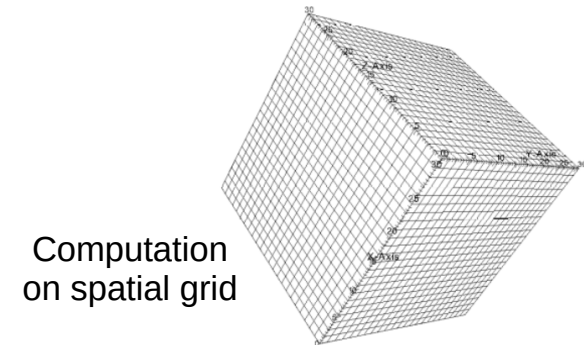


System: *unitary Fermi gas*
 3D simulation on lattice 100^3

number of atoms = 26,790
 number of quasi-particle states = 582,898
 number of PDEs = 1,165,796

Quantum turbulence in the unitary Fermi gas

PNAS Nexus, pgae160 (2024)



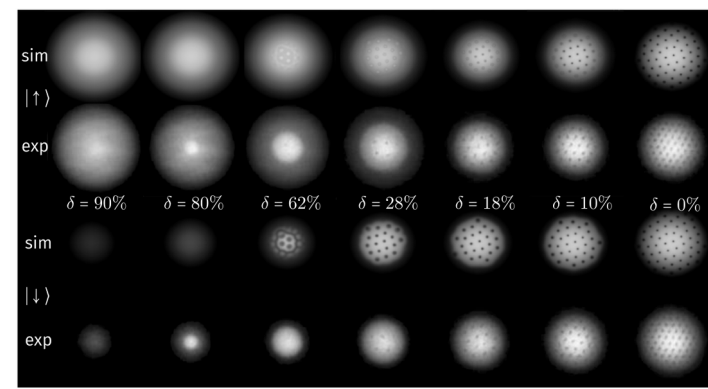
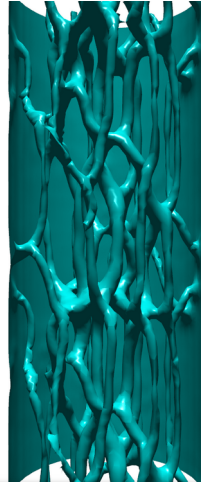
Computation
 on spatial grid

(the largest system in 3D we considered had 108,532 atoms)

Applications in a broad context: getting knowledge about predictive power.

- **Quantum vortices**

PRL 130, 043001 (2023); PRA 106, 033322 (2022); PRA 104, 053322 (2021)
PRA 103, L051302 (2021); PRL 112, 025301 (2014); Science 332, 1288 (2011)

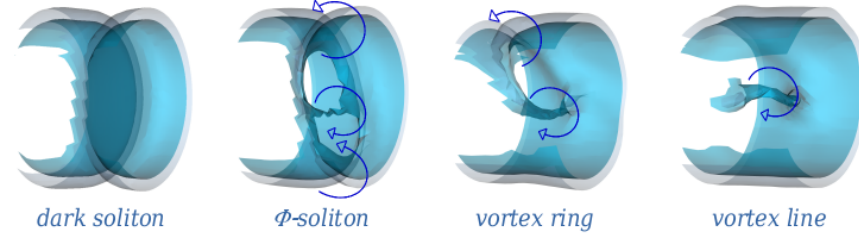


- **Quantum turbulence**

PRA 91, 031602 (2015); PRA 105, 013304 (2022); PNAS Nexus, pgae160 (2024)

- **Spin-polarized impurities**

PRA 100, 033613 (2019); PRA 104, 033304 (2021); ...



- **Solitonic cascades**

PRL 120, 253002 (2018)

- **Higgs/amplitude mode**

Sci. Rep. 13, 11285 (2023);
PRL 102, 085302 (2009)

- **Josephson junction**

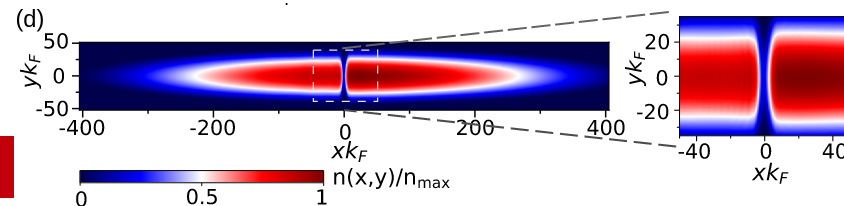
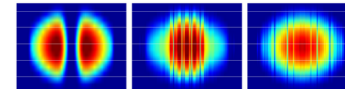
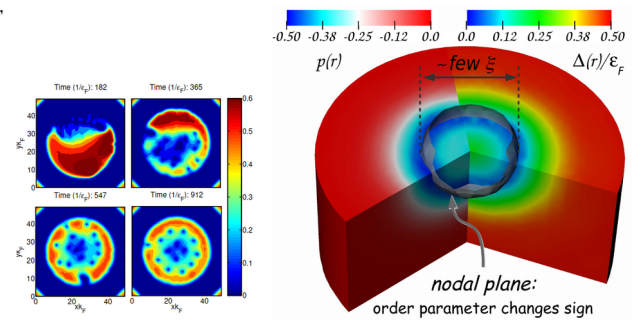
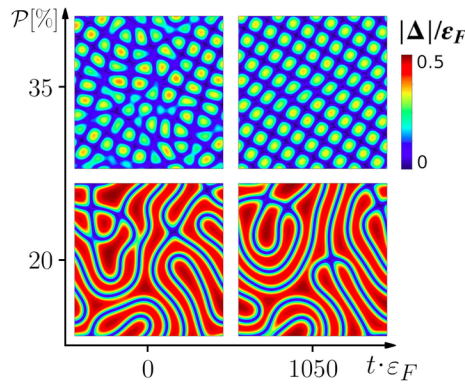
PRL, 023003 (2023)

- **Phase diagram of spin-imbalanced systems**

New J. Phys. 25, 033013 (2023); PRL, 101, 215301 (2008)

- **Shock waves**

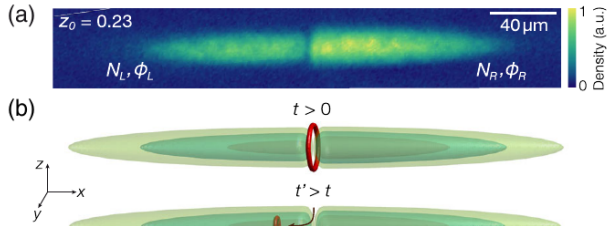
Phys. Rev. Lett. 108, 150401 (2012)



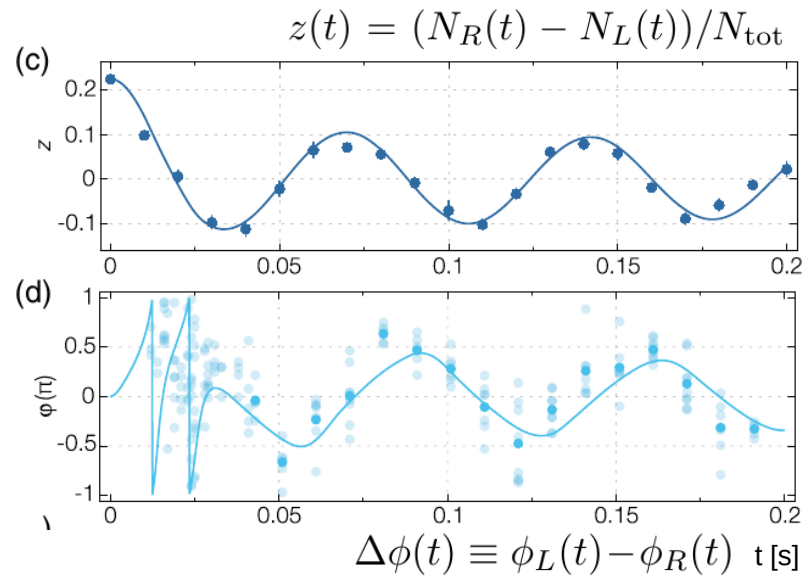
Example #1: Fermionic Josephson Junction

Inspired by LENS ${}^6\text{Li}$ setup (G. Roati's group):

- [1] G. Valtolina, et.al., Science **350**, 1505, (2015);
- [2] A. Burchianti, et.al., Phys. Rev. Lett. **120**, 025302 (2018)
- [3] K. Xhani, et.al., Phys. Rev. Lett. **124**, 045301 (2020)



Figs from [2]



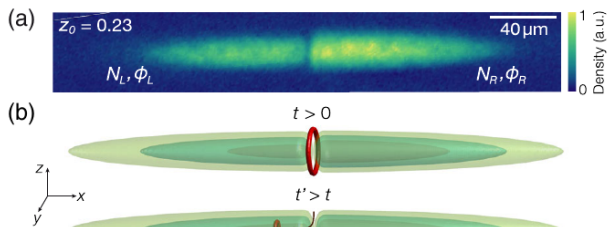
Experiment

Simulation

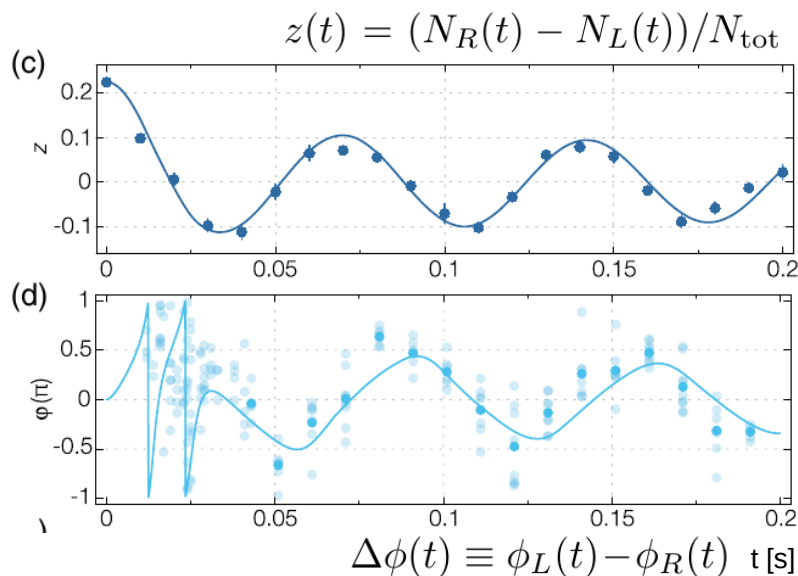
Example #1: Fermionic Josephson Junction

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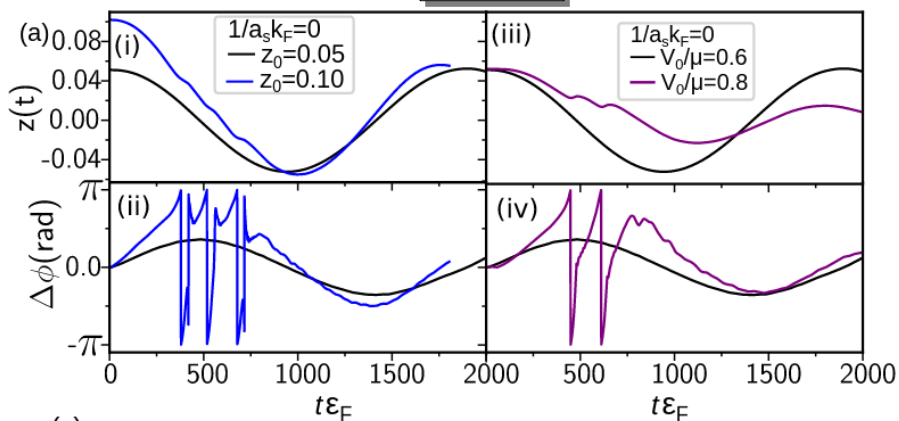
Figs from [2]



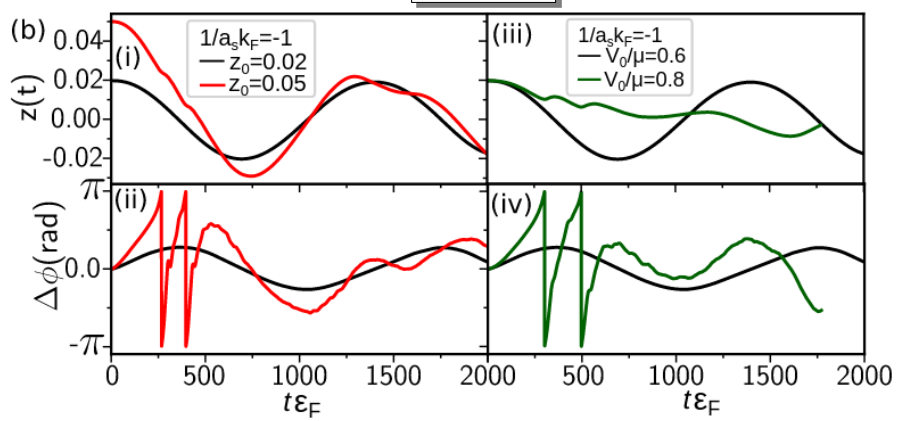
Experiment

G. Wlazłowski, et.al.,
Phys. Rev. Lett. 130, 023003 (2023)

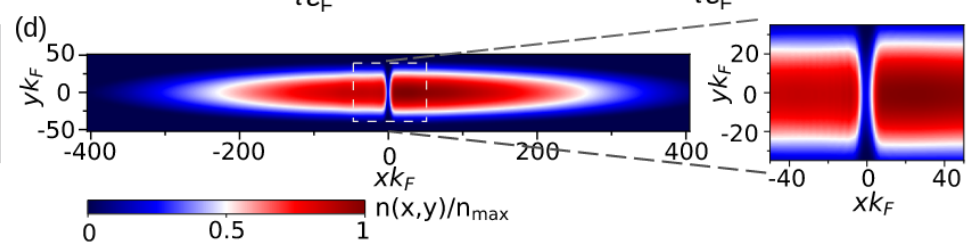
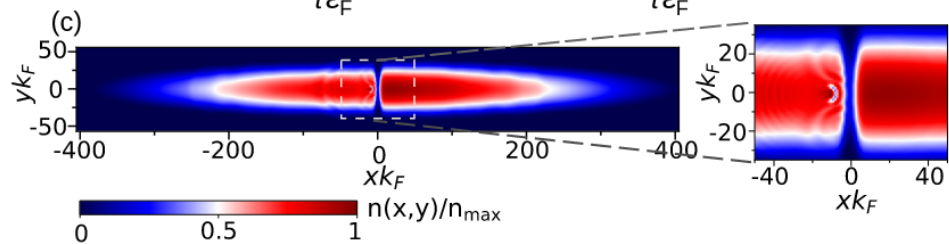
UFG



BCS



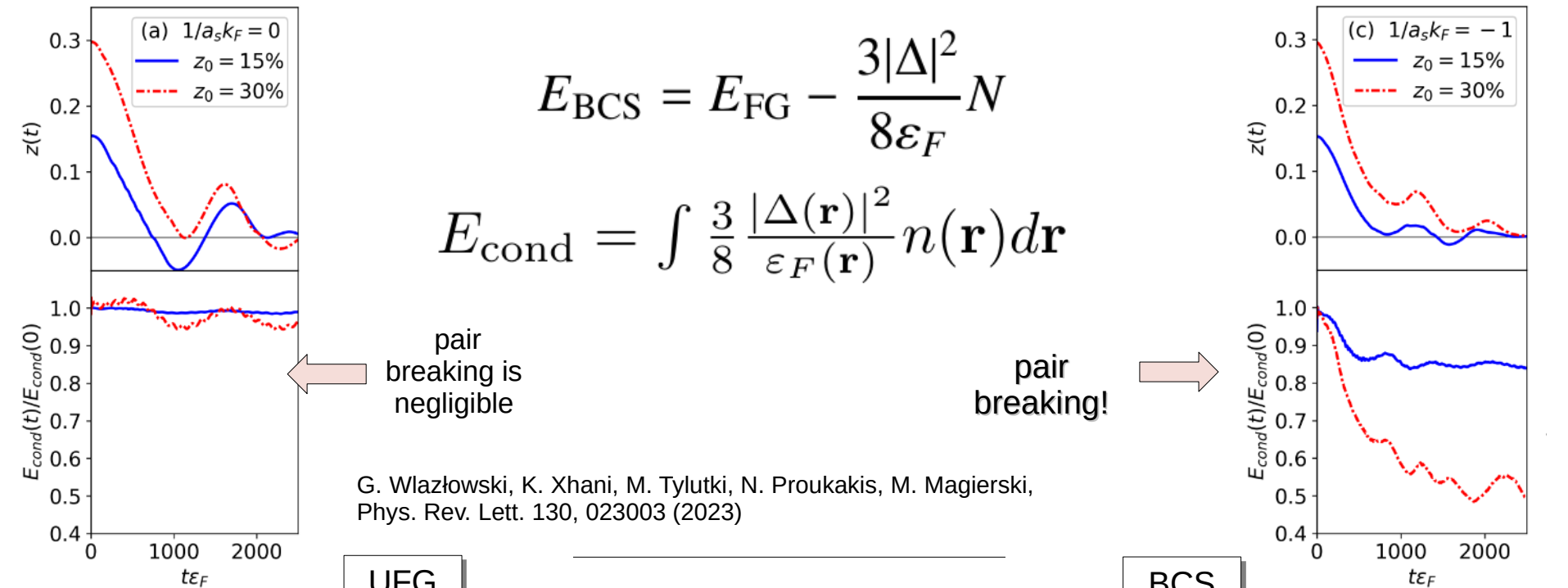
Simulation



$$E_{\text{BCS}} = E_{\text{FG}} - \frac{3|\Delta|^2}{8\varepsilon_F} N$$

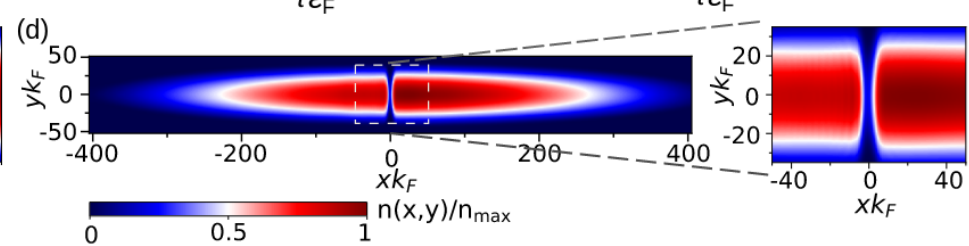
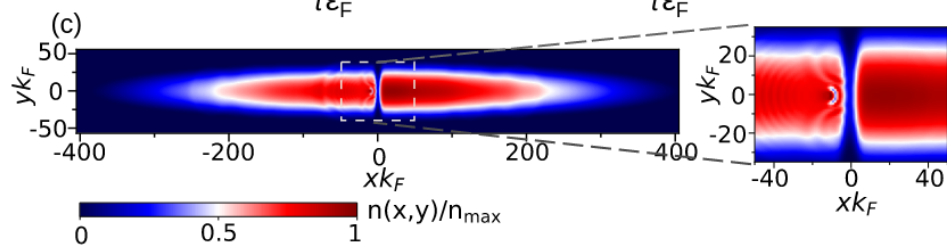
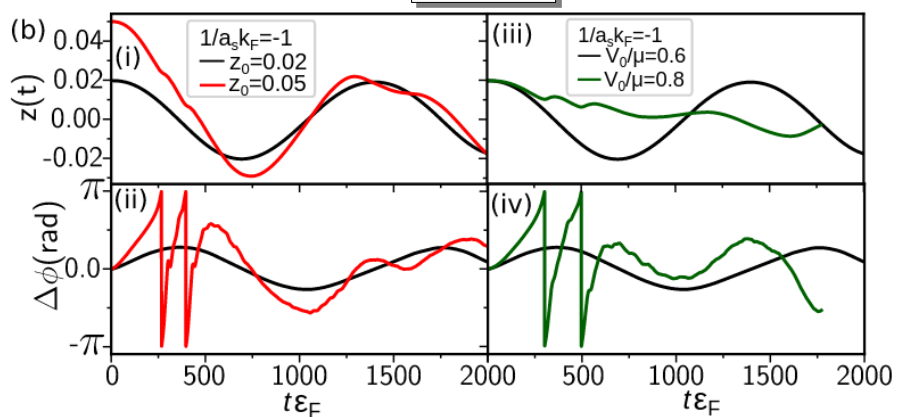
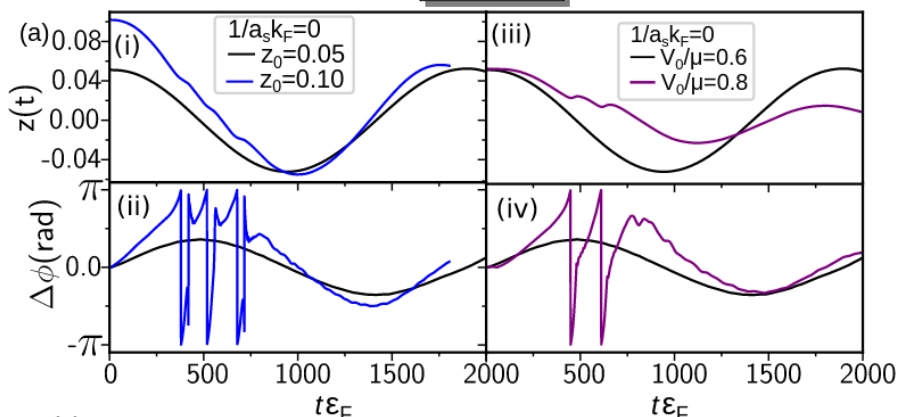
$$E_{\text{cond}} = \int \frac{3}{8} \frac{|\Delta(\mathbf{r})|^2}{\varepsilon_F(\mathbf{r})} n(\mathbf{r}) d\mathbf{r}$$

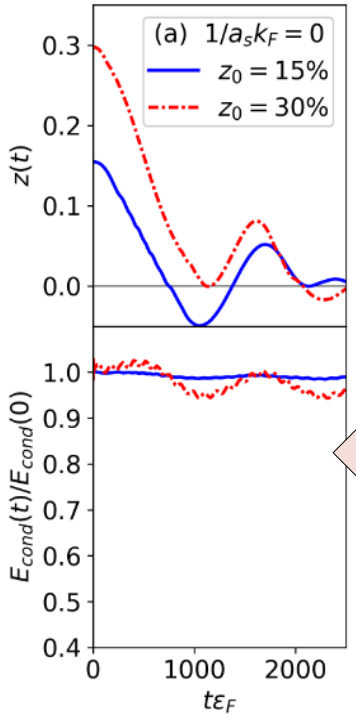
G. Wlazłowski, K. Xhani, M. Tylutki, N. Proukakis, M. Magierski,
Phys. Rev. Lett. 130, 023003 (2023)



UFG

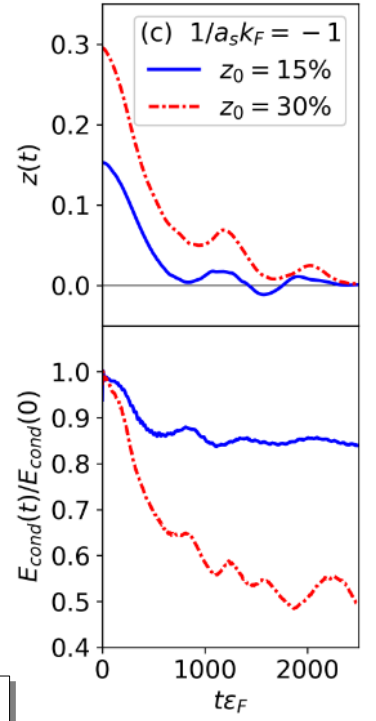
BCS





$$E_{\text{BCS}} = E_{\text{FG}} - \frac{3|\Delta|^2}{8\varepsilon_F} N$$

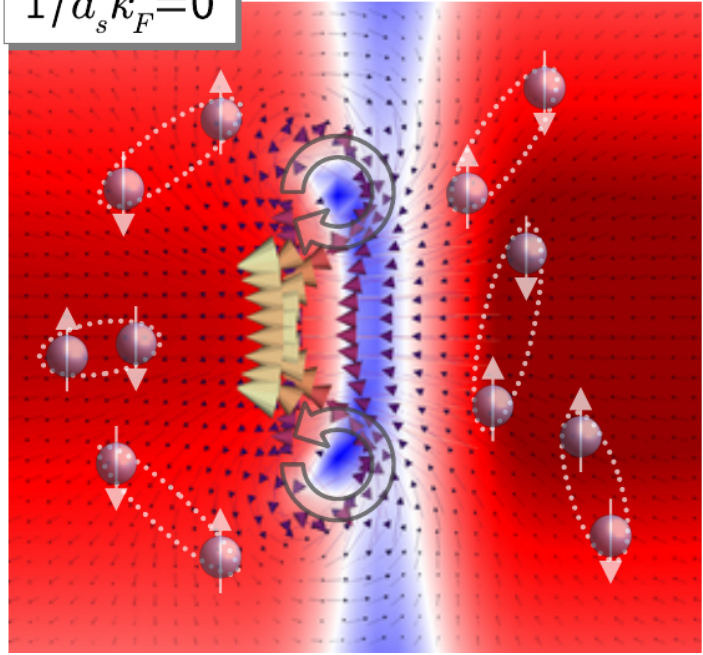
$$E_{\text{cond}} = \int \frac{3}{8} \frac{|\Delta(\mathbf{r})|^2}{\varepsilon_F(\mathbf{r})} n(\mathbf{r}) d\mathbf{r}$$



G. Wlazłowski, K. Xhani, M. Tylutki, N. Proukakis, M. Magierski, Phys. Rev. Lett. 130, 023003 (2023)

$1/a_s k_F = 0$

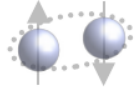
UFG



quantum vortex

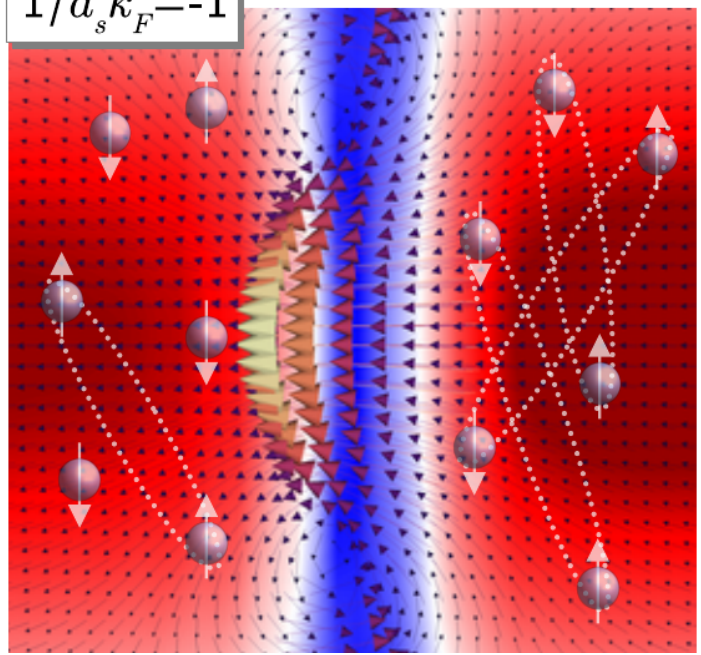


Cooper pair



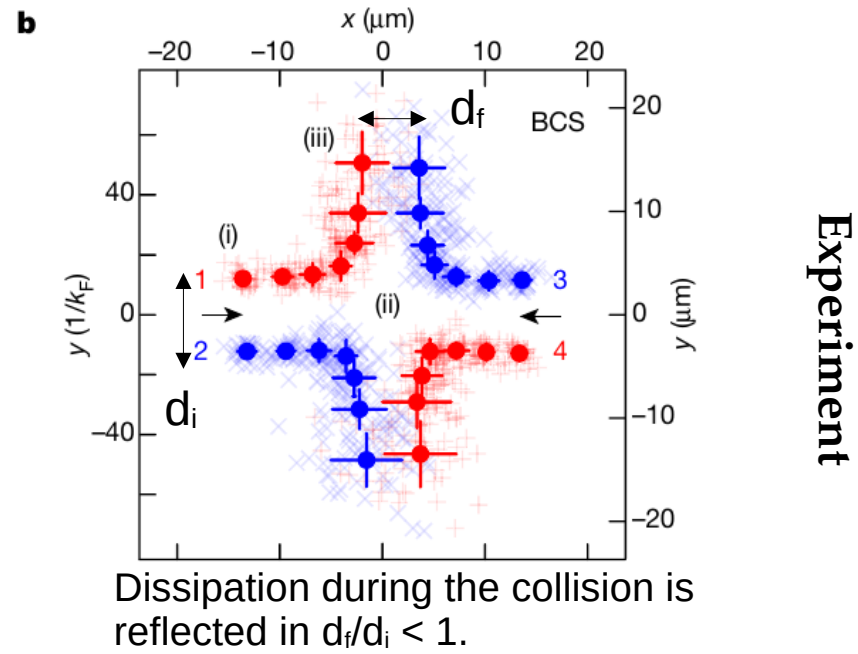
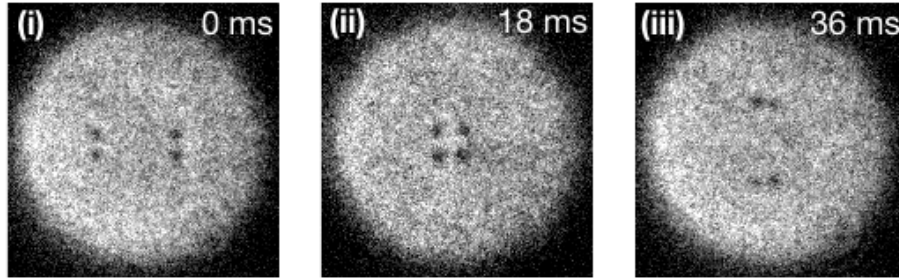
$1/a_s k_F = -1$

BCS



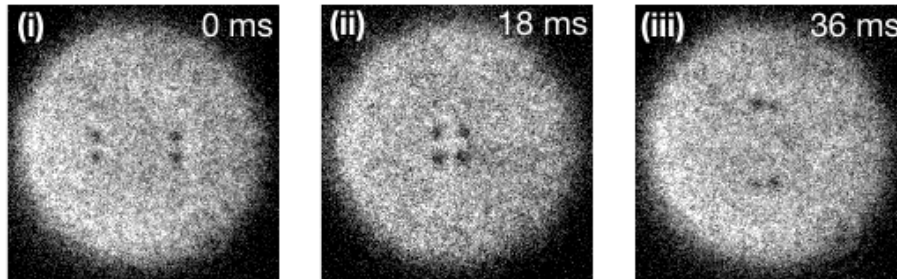
Example #2: Vortex collisions

Inspired by LENS ${}^6\text{Li}$ setup (G. Roati's group):
[1] W. J. Kwon, et.al., Nature 600, 64-69 (2021)

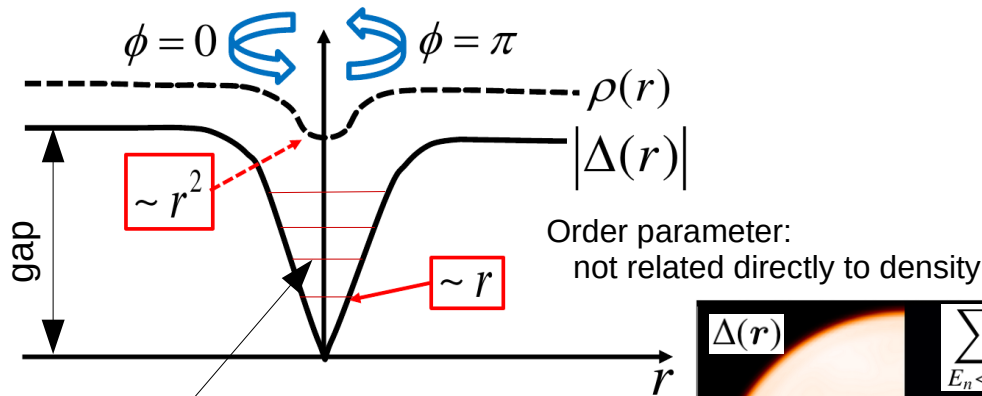


Example #2: Vortex collisions

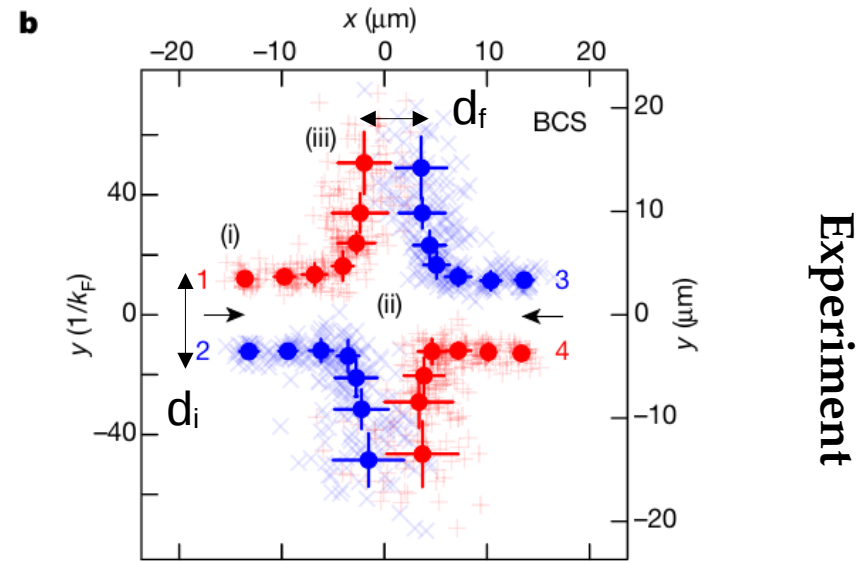
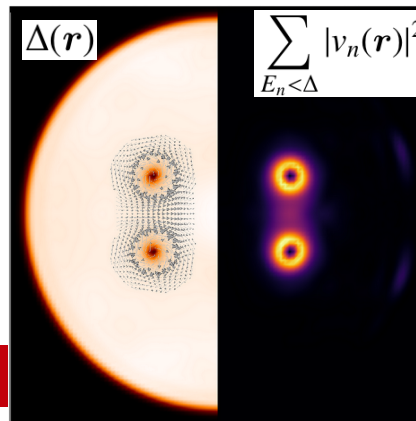
Inspired by LENS ${}^6\text{Li}$ setup (G. Roati's group):
 [1] W. J. Kwon, et.al., Nature 600, 64-69 (2021)



Vortex solution: Fermi gas \rightarrow BdG



Occupation of Andreev states give rise to significant particle density inside the core.



Dissipation during the collision is reflected in $d_f/d_i < 1$.

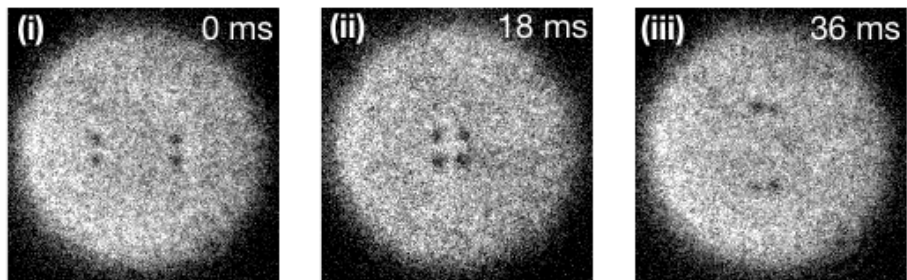
Do the internal structure of vortices contribute to the dissipation?

Prediction [M. Silaev, PRL. 108 (2012)]:

- \rightarrow Andreev quasiparticles can be excited (effective increase of the vortex core temperature), ...
- \rightarrow and eventually converted into delocalized states
- \rightarrow the impact of this process gets stronger as we move towards BCS regime

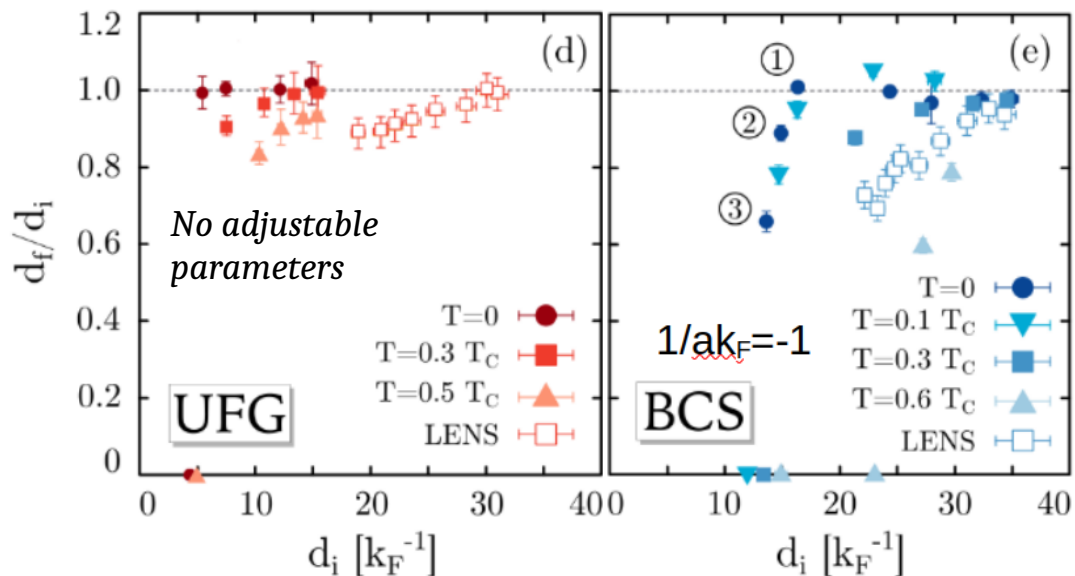
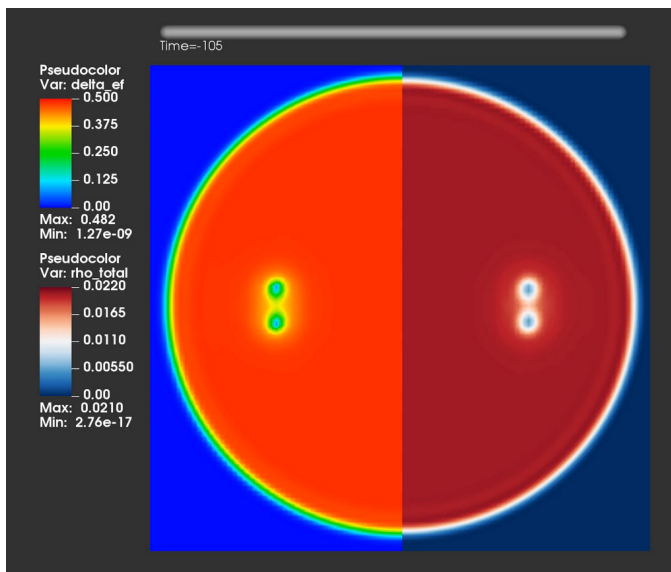
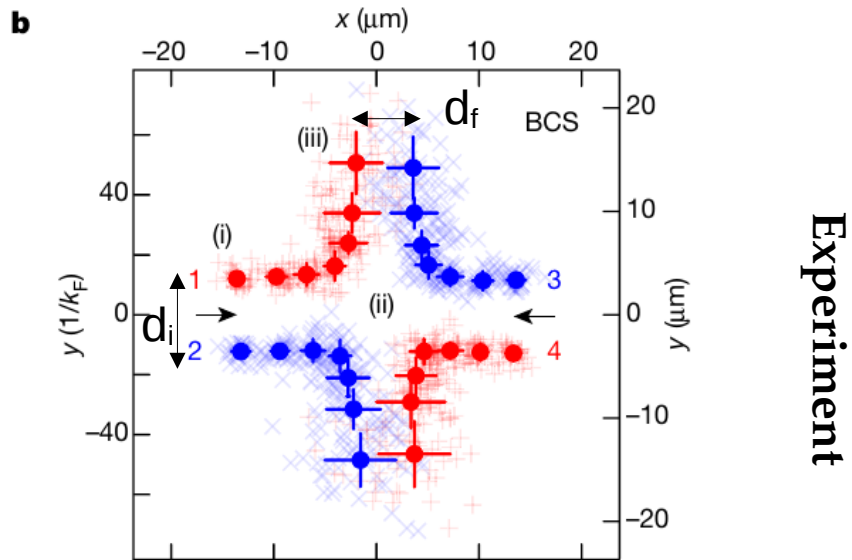
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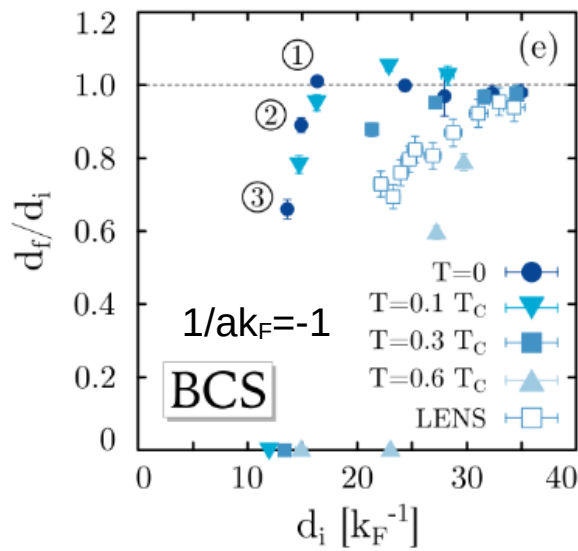
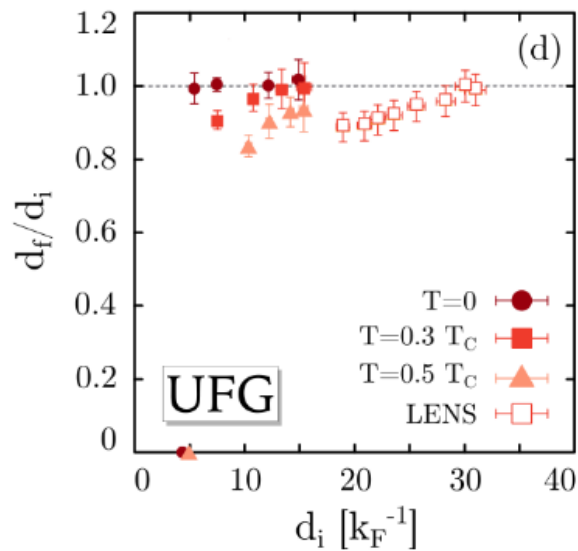
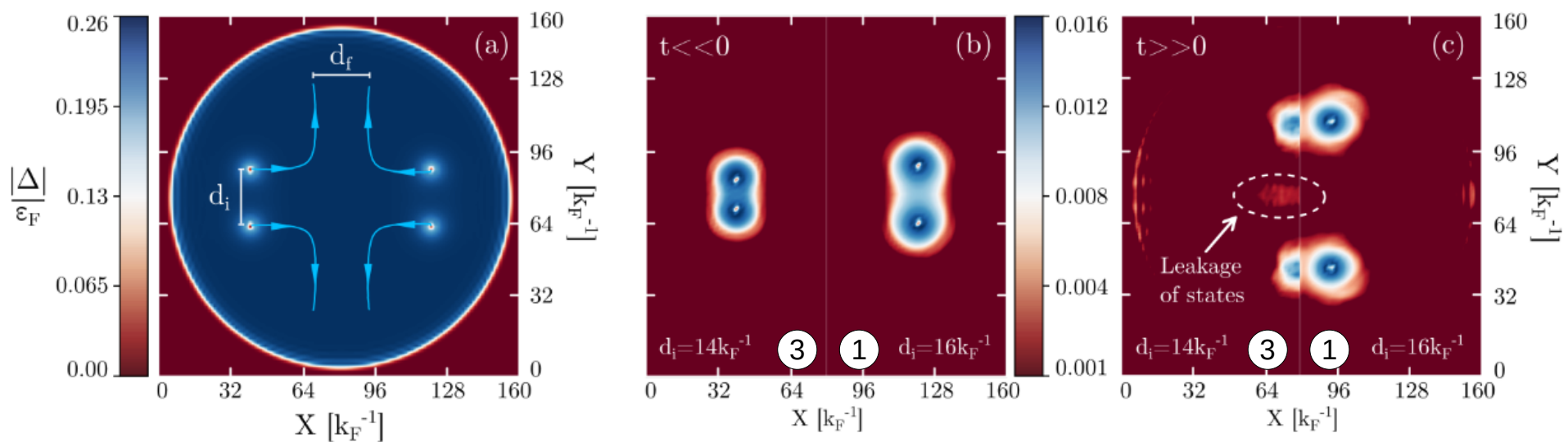
Inspired by LENS ${}^6\text{Li}$ experiment (G. Roati's group):
 [1] W. J. Kwon, et.al., Nature 600, 64-69 (2021)



Figs from [1]

$$T_{\text{exp}} = (0.3-0.4) T_c$$





A. Barresi, A. Boulet, P. Magierski, G. Wlazłowski, Phys. Rev. Lett. 130, 043001 (2023)

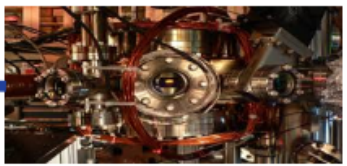
- the dissipation due to Andreev states is detected in BCS regime
(it can be interpreted as effective increase of the vortex core temperature)
- the effect is too weak to explain the experimental measurements
- significant sensitivity of the results to the temperature

Towards effective model of neutron star...

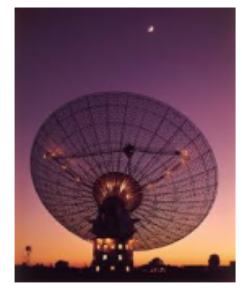
Theory (TD)DFT



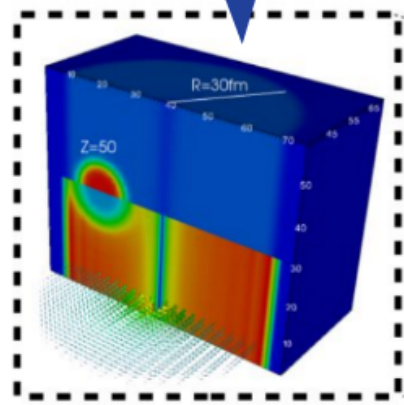
Low energy nuclear physics
← ab-initio



Ultra-cold atomic gases

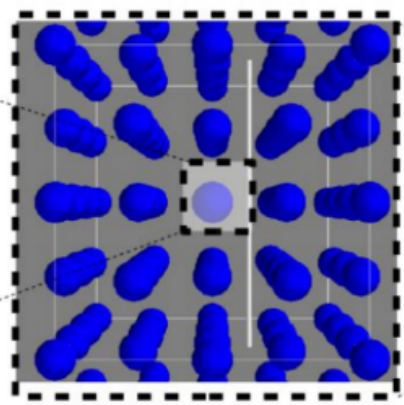


Comparison with observations



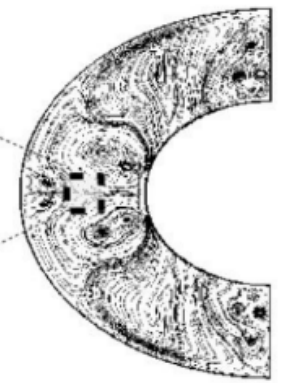
Method: TDDFT
DoF: neutrons and protons.
Scale: $\sim 10^{-13}m$

feed



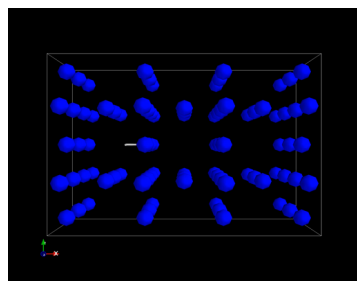
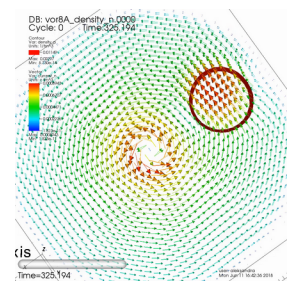
Method: Vortex Filament Model
DoF: impurities and vortices
Scale: $\sim 10^{-9}m$

feed



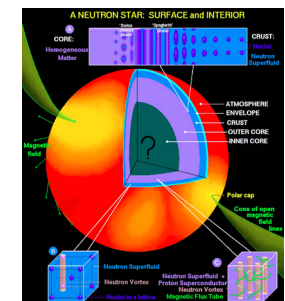
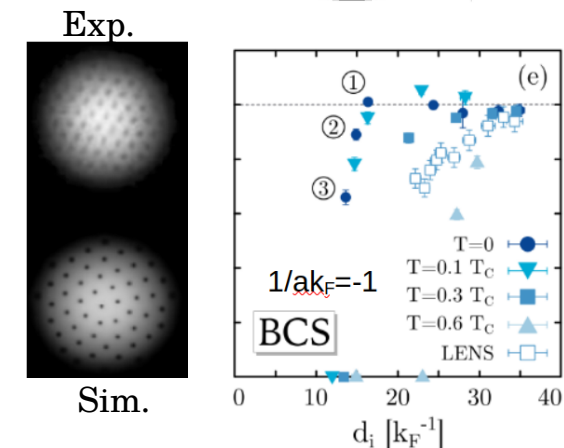
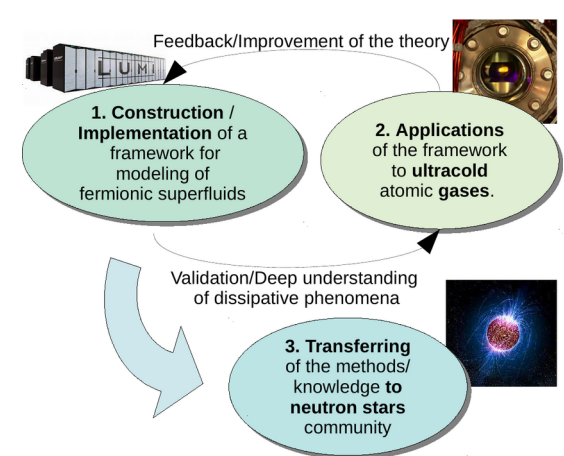
Method: Hydrodynamics
DoF: fluid elements
Scale: \sim size of star

↑



SUMMARY

- Ultracold Fermi gases and neutron matter share a lot of similarities. UFG regime can be used as a benchmark platform for testing the predictive power of many-body techniques, which are subsequently used for neutron star studies.
- (TD)DFT is general purpose framework: it overcomes limitations of mean-field approach, while keeping numerical cost at the same level as (TD)HFB calculations.
- For problems that have been (so far) contrasted with experimental measurements: *Predictions by functionals for ultracold Fermi gases (SLDA), created within similar methodology as for nuclear systems, are at least at the qualitative level in agreement with the measurements, ... in many cases, good quantitative agreement is obtained.*
- (TD)DFT and its implementations reached the level of maturity that allows for providing predictions for large and complex systems: neutron star's crust structure and its dynamics, transport coefficients, ...



Collaborators: P. Magierski, D. Pęcak, M. Tyłutki, A. Barresi, A. Boulet (WUT); N. Chamel (U. Bruxelles); M. Forbes, S. Sarkar, (WSU); A. Bulgac (UW); K. Khani (LENS); N. Proukakis (Newcastle U.); A. Marek (MPCDF), M. Szpindler (Cyfronet).