Towards general-purpose simulation platform for superfluid fermions

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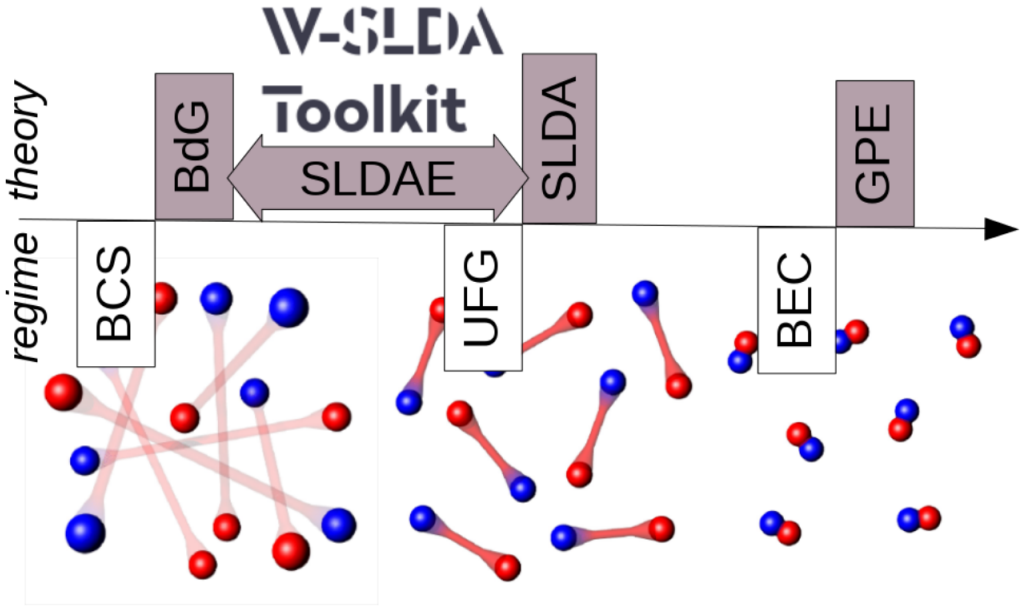

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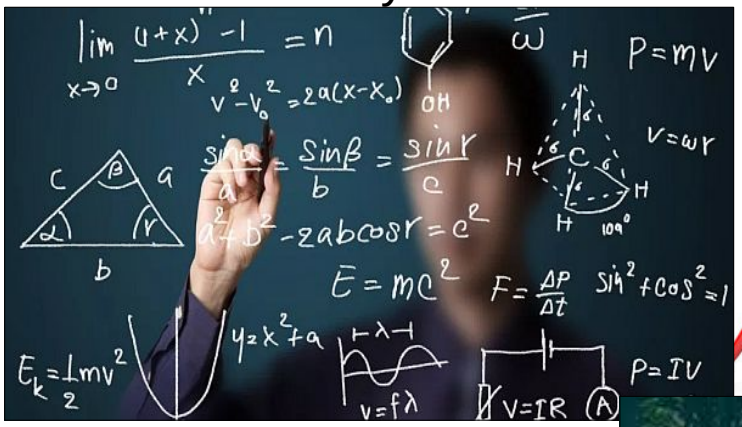
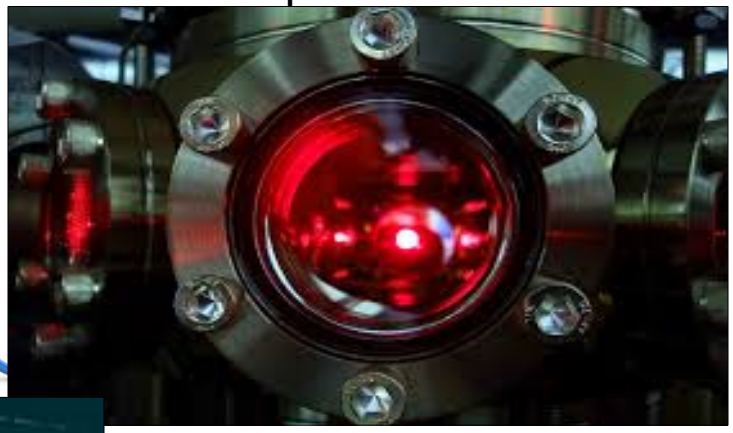
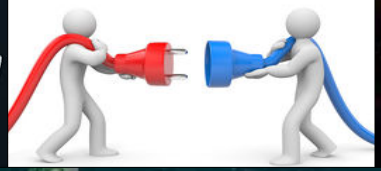
Theory



Experiment





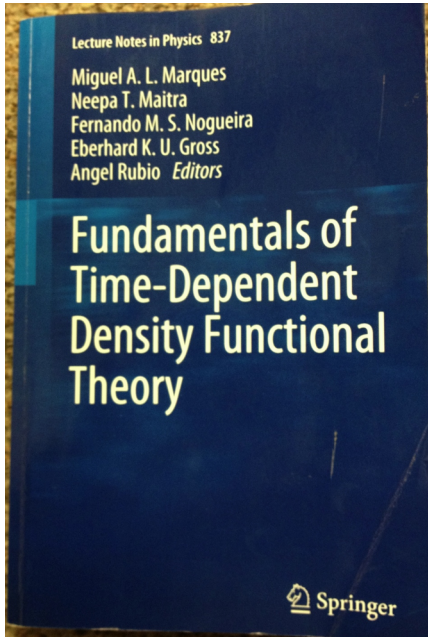
Computational physics

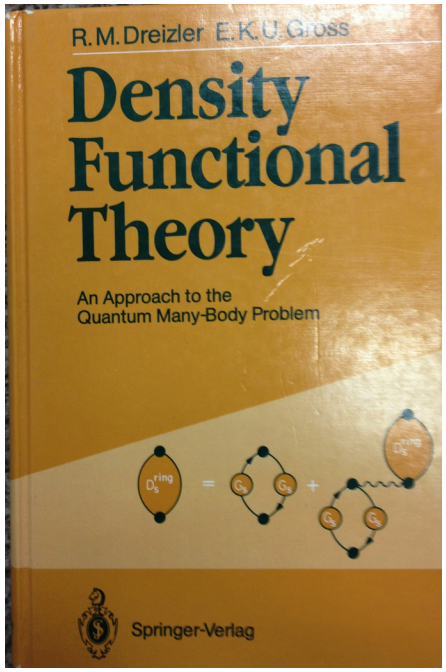
Overview:
1. *Method → DFT**
2. *Implementation*
3. *Applications*

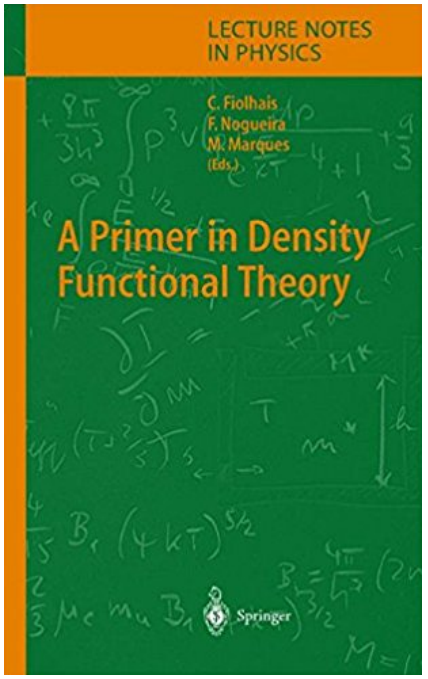
(*) Note: Many formal aspects of the theory will be presented superficially. Only general formulas...

- *General purpose method* → wide range of applicability
  → typically it has numerical complexity at most as a mean-field method
  (example for BECs: Gross-Pitaevskii equation)

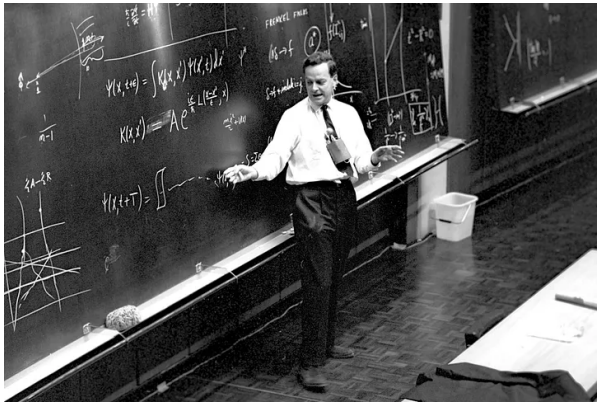
- *Specialized methods* → devoted to specific problems / quantities
  → typically *ab initio* methods like QMC, ...







- DFT is in principle exact theory
  Hohenberg-Kohn theorem (1964) implies that $\langle O \rangle = \langle \Psi[\rho] | O | \Psi[\rho] \rangle = O[\rho]$
- ... solving Schrödinger equation ↔ minimization of the energy density E[ρ]...
- ... however no mathematical recipe how to construct E[ρ].
- In practice we postulate the functional form
  dimensional arguments, renormalizability, Galilean invariance, and symmetries
- DFT allows to include "beyond mean-field" effects, while keeping the numerical cost similar to mean-field method (here mean-field=BdG or HFB)



Richard Feynman
... physics is not mathematics and mathematics is not physics ...

The fact that we postulate the functional may be regarded as a weakness of the method...
... however it turns out that the DFT is among the most popular and versatile methods available in physics.

Nature 514, 550 (2014)

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

- DFT is in principle exact theory
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Alternative frameworks

Schrödinger

$$\left(\hat{H}_{\text{int}} + \hat{U}_{\text{ext}}\right)\Psi_0 = E_0\Psi_0$$

$$\hat{H}_{\text{int}} = \hat{T} + \hat{V}$$

- Derivation of H_{int} - "*easy*"
- Solving many body Schrödinger equation - "hard"

DFT

$$E[n] = E_{\text{int}}[n] + \int n(\boldsymbol{r},t)U_{\text{ext}}(\boldsymbol{r},t)\,d\boldsymbol{r}$$

$$E_{\text{int}}[n] = T[n] + V[n] + \ldots$$

- Derivation of E_{int} - "hard"
- Solving emerging equations of motion equation - "*easy*"

Classes of Energy Functionals

Increasing quality and computing cost

Local Density Approximation (LDA)

$$E = \int d\boldsymbol{r}\, \mathcal{H}(n(\boldsymbol{r}))$$

Generalized Gradient Approximation (GGA)

$$E = \int d\boldsymbol{r}\, \mathcal{H}(n(\boldsymbol{r}), \boldsymbol{\nabla} n(\boldsymbol{r}))$$

Solving problem:

$$\frac{\delta E}{\delta n} = 0$$

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Meta – GGA
(Kohn-Sham method)

$$E = \int d\boldsymbol{r}\, \mathcal{H}(n(\boldsymbol{r}), \boldsymbol{\nabla} n(\boldsymbol{r}), \tau(r), \dots)$$

where: $n(\boldsymbol{r}) = \sum_i |\phi_i(\boldsymbol{r})|^2 \quad \tau(\boldsymbol{r}) = \sum_i |\nabla \phi_i(\boldsymbol{r})|^2$

...

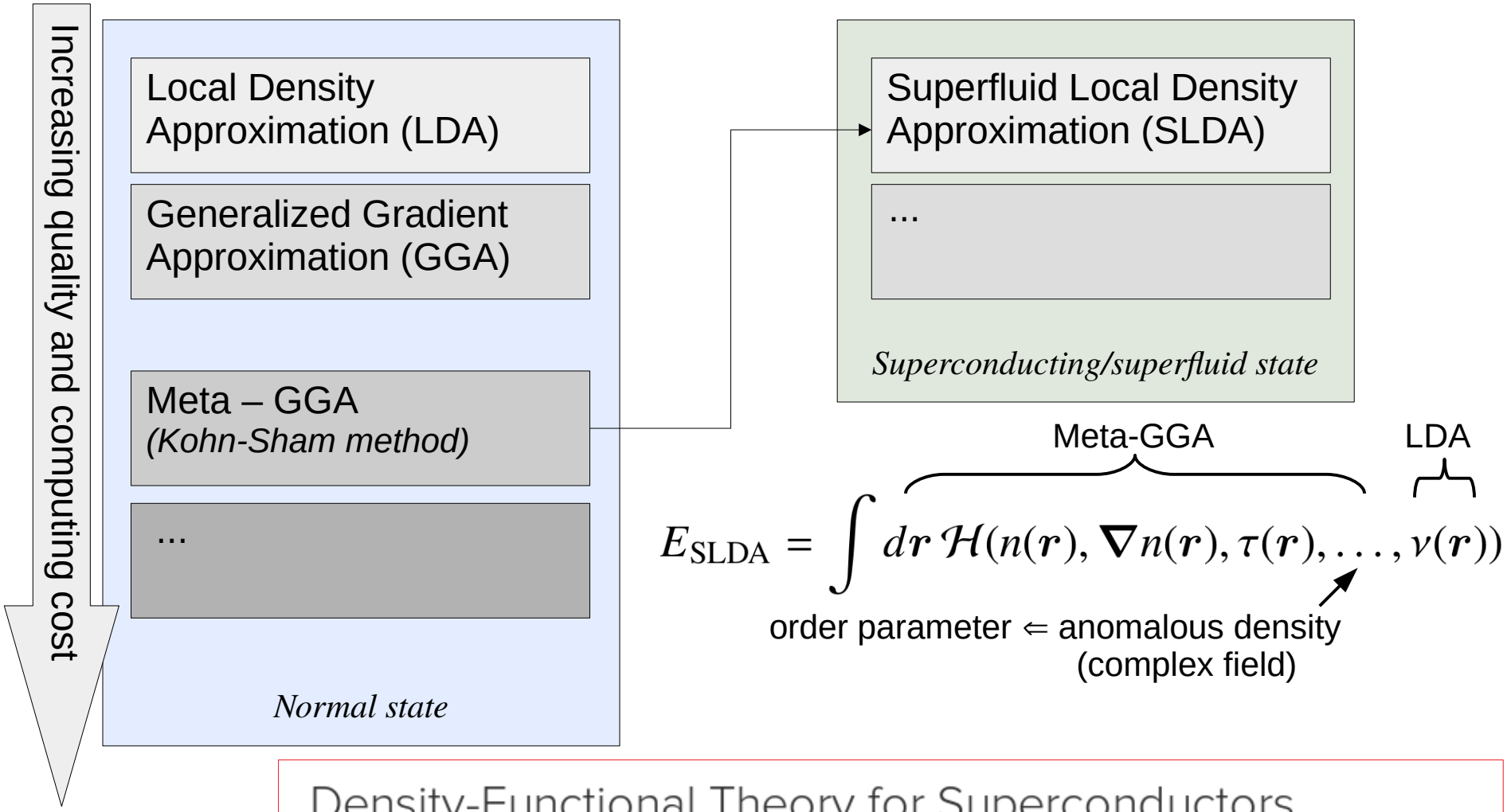
Solving problem:

$$\frac{\delta E}{\delta \phi_i} = 0$$

Formally they have the same structure as HF equations

$$\hat{h}(\{\phi_i\})\, \phi_i(\boldsymbol{r}) = \varepsilon_i \phi_i(\boldsymbol{r})$$

Classes of Energy Functionals



Density-Functional Theory for Superconductors

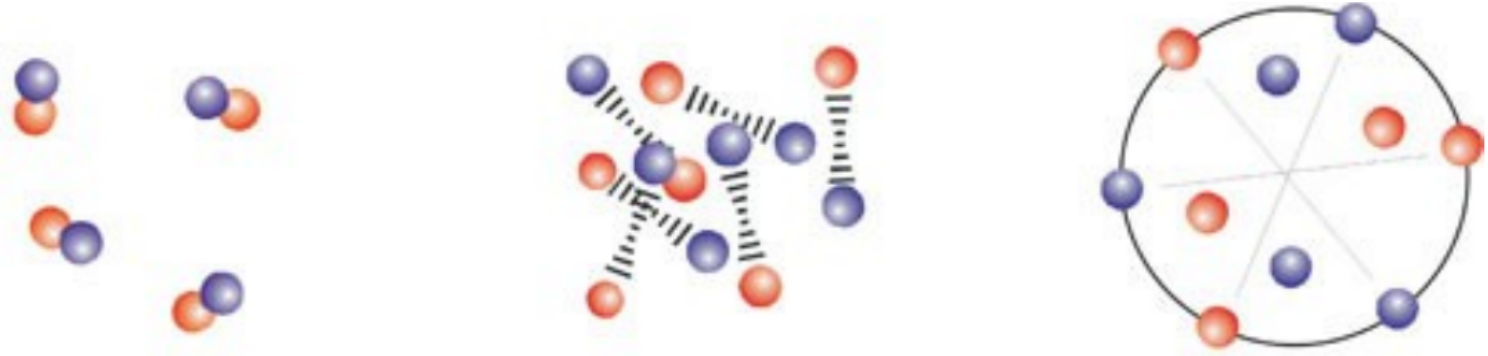
L. N. Oliveira, E. K. U. Gross, and W. Kohn
Phys. Rev. Lett. **60**, 2430 – Published 6 June 1988

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

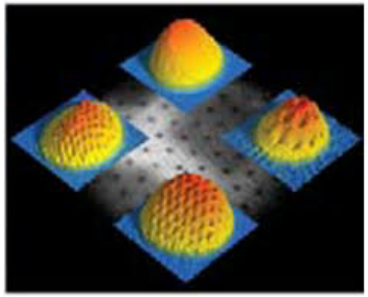
Photo from: http://www.lkb.upmc.fr/ultracoldfermigases/

BEC ← CROSSOVER → BCS

$ak_F \to 0^+$ $ak_F \to \pm\infty$ $ak_F \to 0^-$



diatomic molecules strongly interacting pairs Cooper pairs



SLDA-type functional for ultracold atoms

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

The Fermi-Dirac distribution function

normal density

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

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

kinetic density

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

+ orthonormality condition

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

current density

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

$$\int \varphi^\dagger_\eta(\boldsymbol{r}, t) \varphi_{\eta'}(\boldsymbol{r}, t)\, d^3\boldsymbol{r} = \delta_{\eta,\eta'}$$

anomalous density

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

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

Energy cut-off scale (need for regularization)

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minimization

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

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

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

Note that similar strategy is present in BEC community, but does not invoke DFT techniques.

Example: quantum droplets
GPE → GPE + LHY correction

For example, BdG is equivalent to

$$E_0 = \int \left(\frac{\tau_\uparrow(\boldsymbol{r}) + \tau_\downarrow(\boldsymbol{r})}{2} + 4\pi a |\nu(\boldsymbol{r})|^2 \right) d\boldsymbol{r}$$

$$h_\sigma = -\frac{1}{2}\boldsymbol{\nabla}^2, \quad \Delta = -4\pi a \nu,$$

SLDA-type functional

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

Dimensionless functional parameters

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

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

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

dimensional analysis + symmetries

Kinetic term

Potential term

Pairing term

Center of mass motion

Units:
$\hbar = m = 1$

SLDA-type functional

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Center of mass motion

A. Bulgac, M.M. Forbes
Phys. Rev. A 75, 031605(R) (2007)

A. Boulet, G. Wlazłowski, P. Magierski
Phys. Rev. A 106, 013306 (2022)

BdG $\lvert ak_F\rvert \ll 1$	ASLDA Asymmetric SLDA, $a\to\infty$	SLDAE SLDA Extended, p=0
$A_\lambda \to 1$	$A_\lambda \to A[p(\boldsymbol{r})]$	$A_\lambda \to A[ak_F(\boldsymbol{r})]$
$B_\lambda \to 0$	$B_\lambda \to B[p(\boldsymbol{r})]$	$B_\lambda \to B[ak_F(\boldsymbol{r})]$
$C_\lambda \to \frac{4\pi\hbar^2}{(3\pi^2)^{1/3}m}ak_F$	$C_\lambda \to C[p(\boldsymbol{r})]$	$C_\lambda \to C[ak_F(\boldsymbol{r})]$

$$p(\boldsymbol{r}) = \frac{n_\uparrow(\boldsymbol{r}) - n_\downarrow(\boldsymbol{r})}{n_\uparrow(\boldsymbol{r}) + n_\downarrow(\boldsymbol{r})}$$

$$k_F(\boldsymbol{r}) = [3\pi^2 n(\boldsymbol{r})]^{1/3}$$

SLDA-type functional

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

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dimensional analysis + symmetries

Kinetic term $+\infty$

Pairing term $-\infty$

The functional is useless without the regularization procedure!

$$\tau_\sigma \to \tau_\sigma(E_c) \quad \nu \to \nu(E_c)$$

$$C_\lambda \to C_\lambda^{\text{reg.}}(E_c)$$

→ there is no unique method of regularizing the functional...
→ there are prescriptions for BdG...
→ prescription that is numerically applicable for general case was for many years a bottleneck

Rapid Communication

Access b

Local density approximation for systems with pairing correlations

Aurel Bulgac
Phys. Rev. C **65**, 051305(R) – Published 25 April 2002

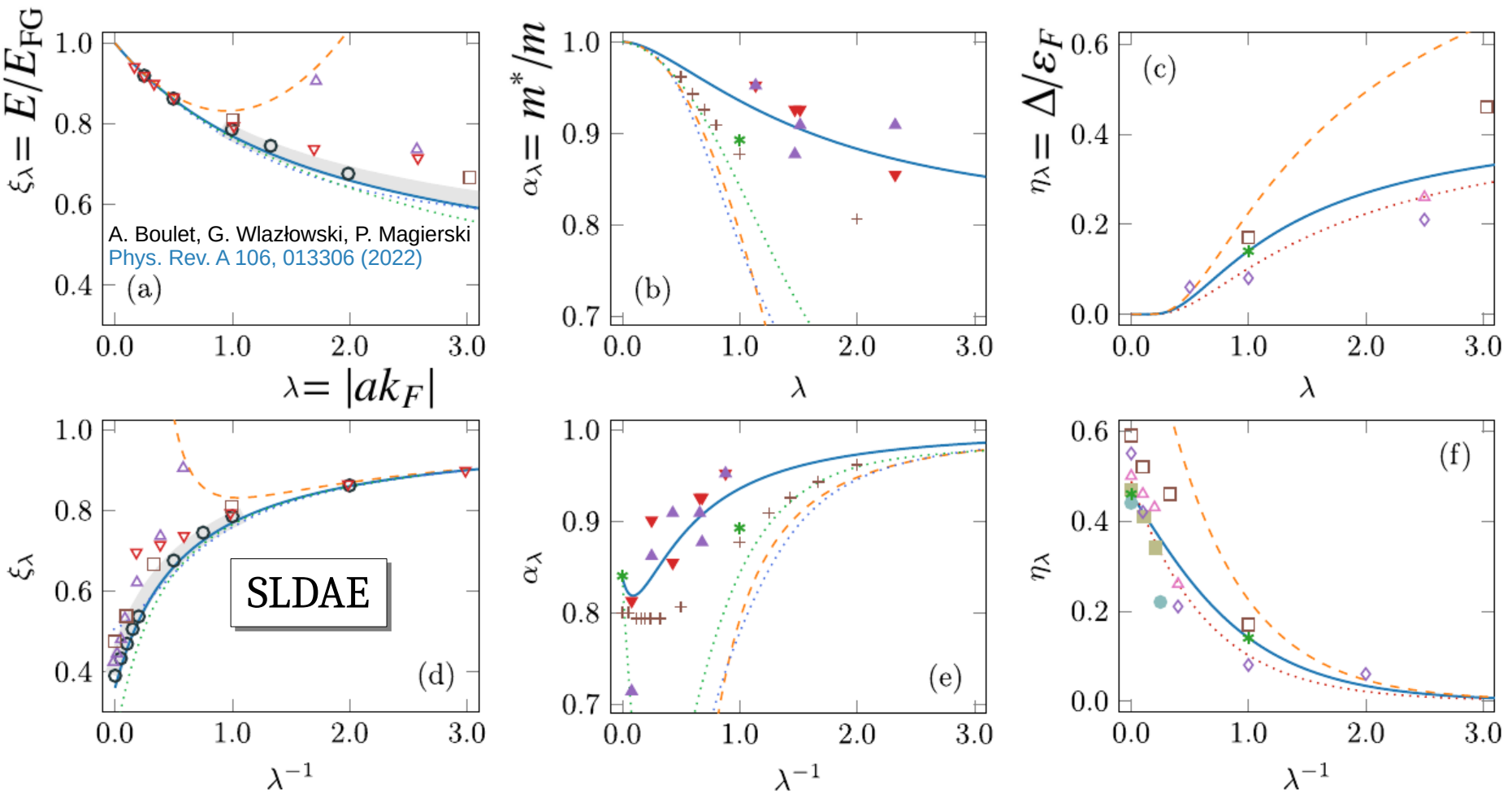
→ *ab initio* cals for E/E_{FG}, Δ/ε_F, m^*/m

→ limiting cases (EFT, scale invariance, ...)

INDUCE

Functional parameters

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



Lee – Yang formula [74–76]
exp. (Navon *et al.*, 2010) [57]
QMC (Carlson *et al.*, 2012) [86]
QMC (Astrakharchik *et al.*, 2004) [87, JS]
QMC (Astrakharchik *et al.*, 2004) [87, BCS]
QMC (Chang *et al.*, 2004) [84]
pp + hh ladder [67, 70]
pp ladder [67, 70]

Galitskii formula [77]
exp. (Sagi *et al.*, 2015) [80]
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GSCGF (Hausmann *et al.*, 2009) [72]
Brueckner – Hartree – Fock (Doggen and Kinnunen, 2015) [88]
pp + hh ladder [67, 70]
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BCS formula [62]
exp. (Schirotzek *et al.*, 2008) [82]
exp. (Hoinka et al., 2017) [81]
GSCGF (Haussmann *et al.*, 2009) [72]
QMC (Bulgac *et al.*, 2008) [83]
QMC (Chang *et al.*, 2004) [84]
QMC (Gezerlis and Carlson, 2008) [85]
ph ring [78, 79]

Towards time-dependent problems

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

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

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

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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 exits 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...

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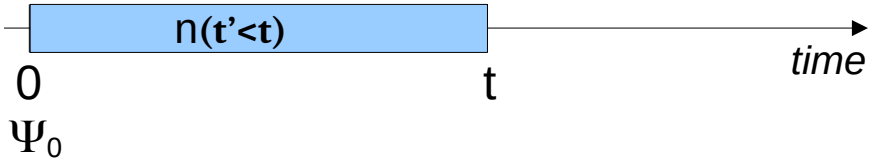
$$E(t) = E[\Psi(t=0), n(\boldsymbol{r}, t' \leqslant t), \ldots]$$



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

Adiabatic approximation

In general integro-differential equations ←

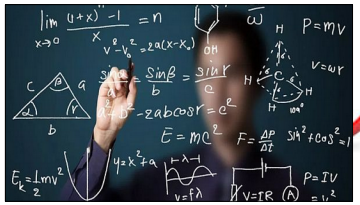
$$E(t) = \int_0^t dt' \int_V d\boldsymbol{r}\, \mathcal{E}[\Psi_0, n(\boldsymbol{r},t'), \ldots]$$

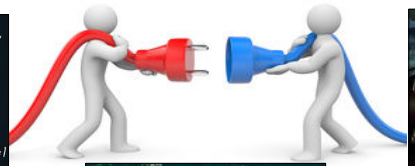
There exits analog of Hohenberg-Kohn theorem for time-dependent problems...

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

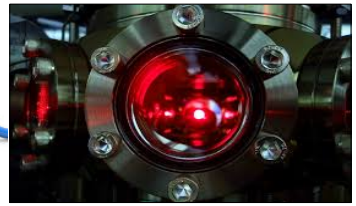
...if the evolution is slow (adiabatic), then the system follows instantaneous ground state
→ use the functional taken from static considerations.

Theoretical method





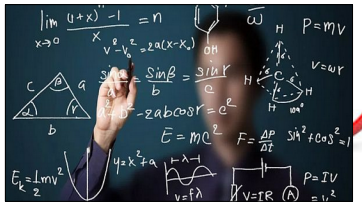
Experiment

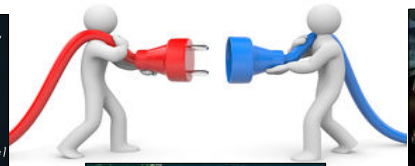


Computer code

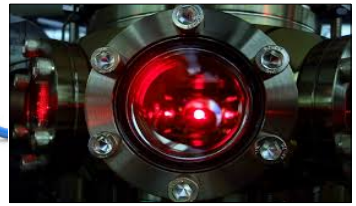
PHYSICS.WUT

Theoretical method





Experiment



Computer code

$$h_a(\boldsymbol{r},t),\ h_b(\boldsymbol{r},t),\ \Delta(\boldsymbol{r},t)$$

can be arbitrary function of densities

Predefined: BdG, ASLDA, SLDAE

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

http://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

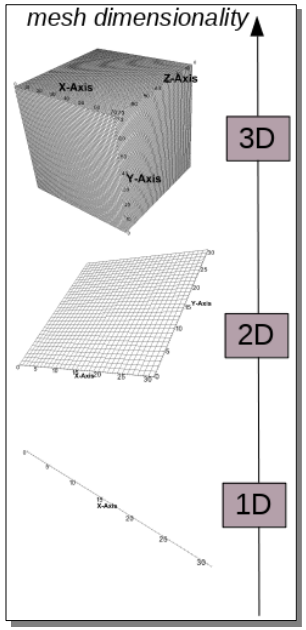
$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} u_n(\boldsymbol{r},t) \\ v_n(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} h_a(\boldsymbol{r},t) - \mu_a & \Delta(\boldsymbol{r},t) \\ \Delta^*(\boldsymbol{r},t) & -h_b^*(\boldsymbol{r},t) + \mu_b \end{pmatrix} \begin{pmatrix} u_n(\boldsymbol{r},t)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

High Performance Computing

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

NVIDIA CUDA | AMD ROCm | open source

PHYSICS.WUT



→ BCS-BEC crossover
→ spin-imbalanced systems
→ mass-imbalanced systems
→ finite temperature formalism


Marek Tylutki


Daniel Pęcak

Ongoing extensions:
→ Bose-Fermi mixtures
→ Fermi-Fermi mixtures (like nuclear systems: protons+neutrons)

Warsaw University of Technology | W-SLDA Toolkit

http://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

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



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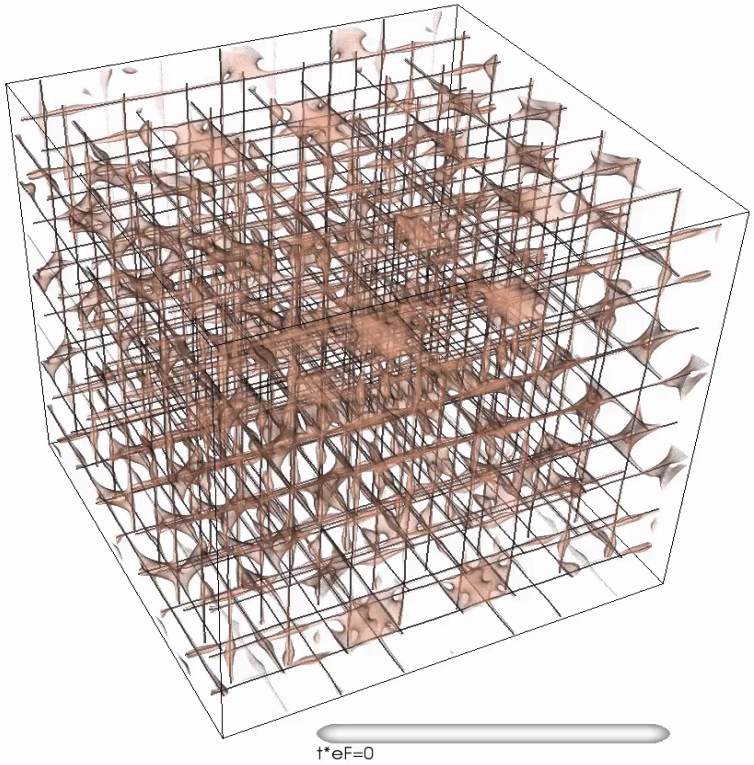


System: *unitary Fermi gas*
3D simulation on lattice 100^3

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

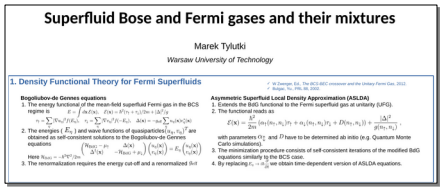
PRELIMINARY:
quantum turbulence
in the unitary Fermi gas

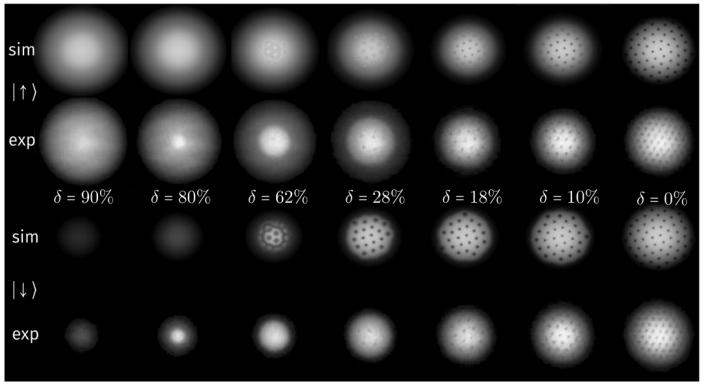
(the largest system in 3D we considered had 108,532 atoms)

Examples of applications of SLDA in recent years

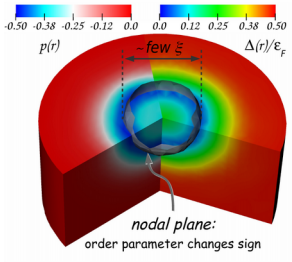
Quantum vortices

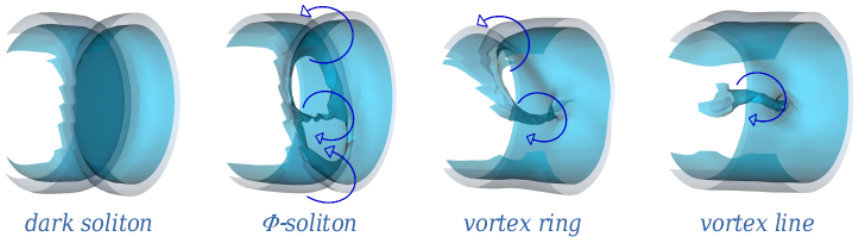
Phys. Rev. Lett. 130, 043001 (2023)
Phys. Rev. A 106, 033322 (2022)
Phys. Rev. A 104, 053322 (2021)
Phys. Rev. A 103, L051302 (2021)
[see poster by Marek Tylutki] →





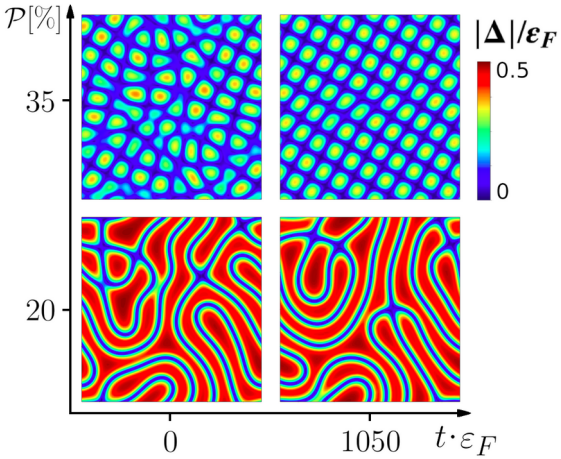
- **Quantum turbulence**
  Phys. Rev. A 105, 013304 (2022)

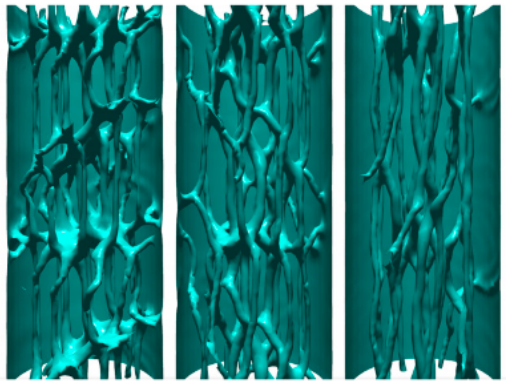




- **Spin-polarized impurities**
  Phys. Rev. A 100, 033613 (2019)
  Phys. Rev. A 104, 033304 (2021)

- **Solitonic cascades**
  Phys. Rev. Lett. 120, 253002 (2018)

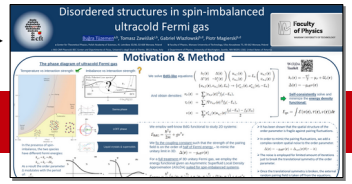


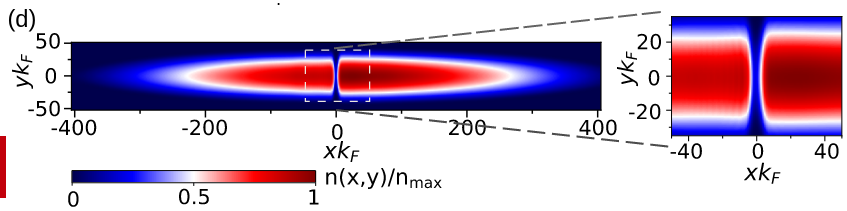


- **Higgs/amplitude mode**
  arXiv:2303.13394 (2023)

- **Josephson junction**
  Phys. Rev. Lett. 130, 023003 (2023)

- **Phase diagram of spin-imbalanced systems**
  New J. Phys. 25, 033013 (2023)
  [see poster by Buğra Tüzemen] →

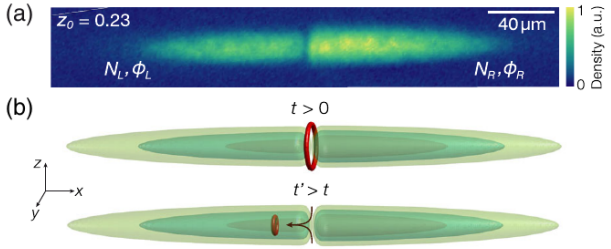




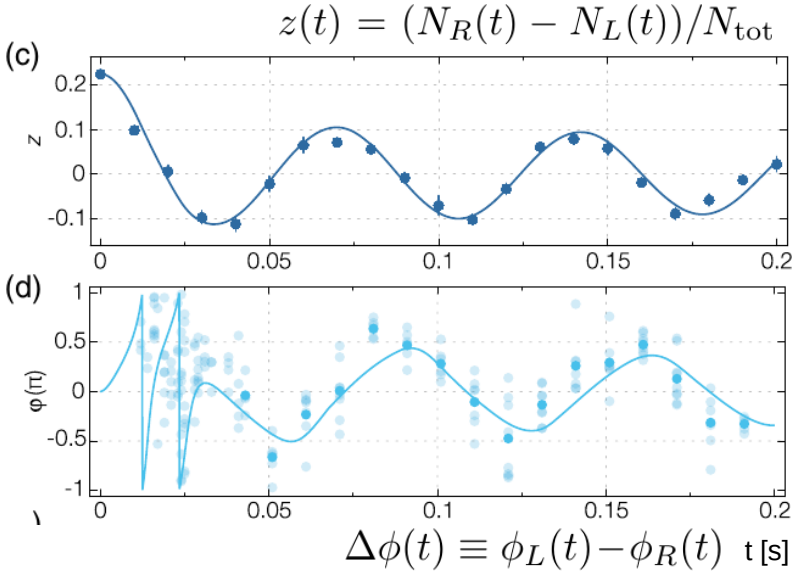
- **...**

Example: Fermionic Josephson Junction

Inspired by LENS ^{6}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: Fermionic Josephson Junction

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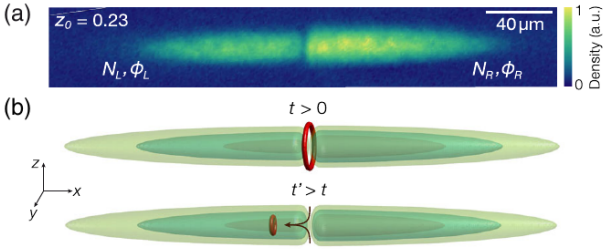
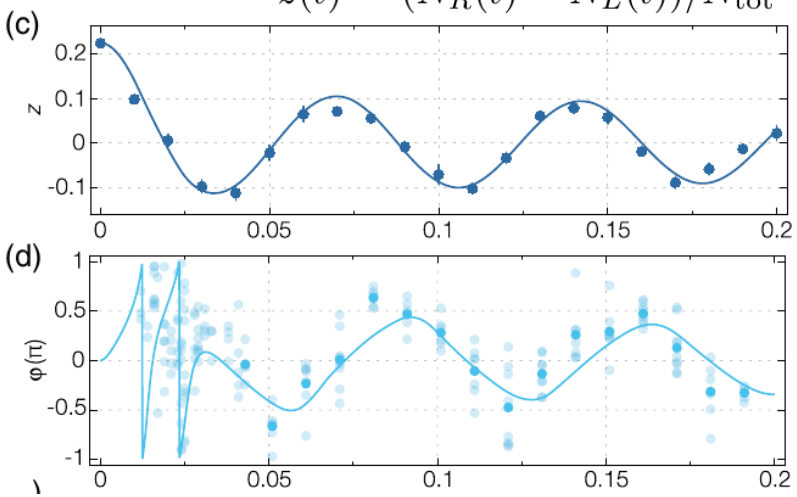


Figs from [2]

$z(t) = (N_R(t) - N_L(t))/N_{\rm tot}$



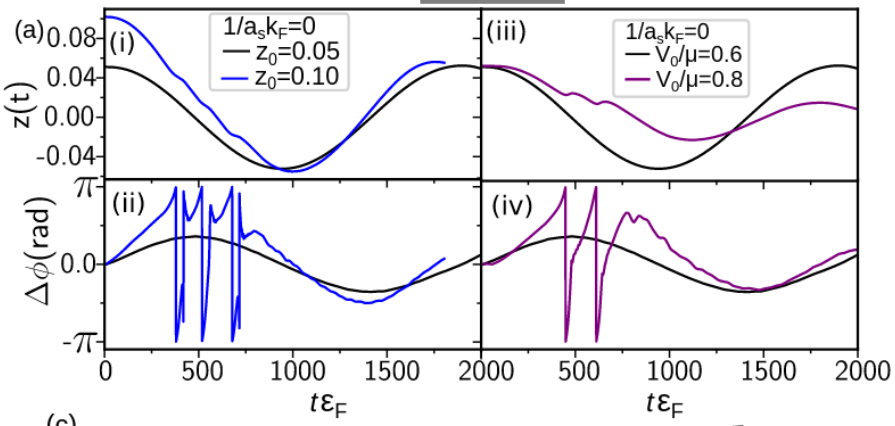
$\Delta\phi(t) \equiv \phi_L(t) - \phi_R(t)$

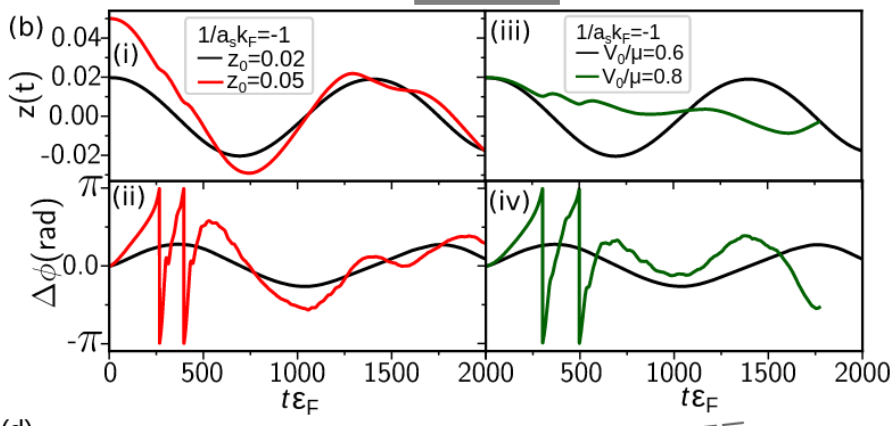
Experiment

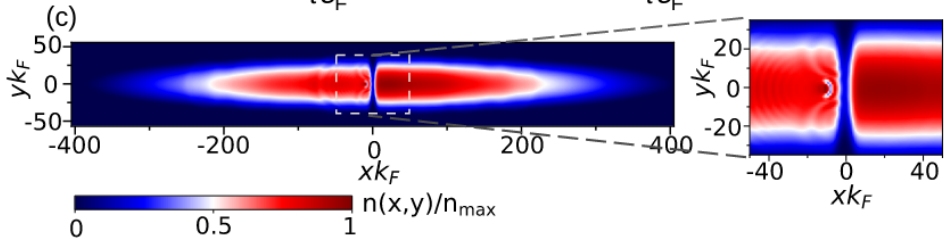
G. Wlazłowski, et.al.,
Phys. Rev. Lett. 130, 023003 (2023)

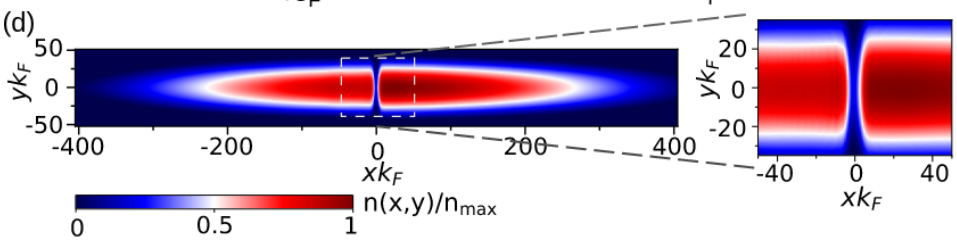
UFG

BCS





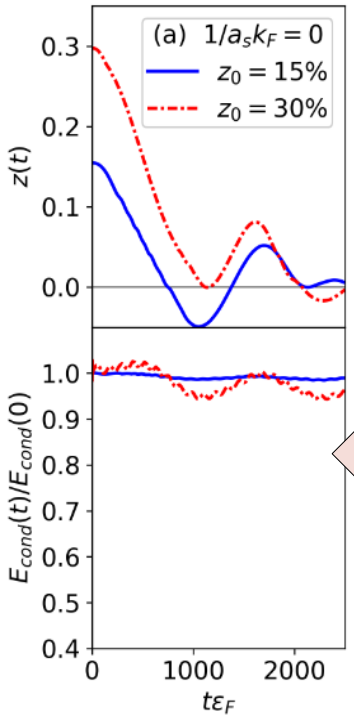




Simulation

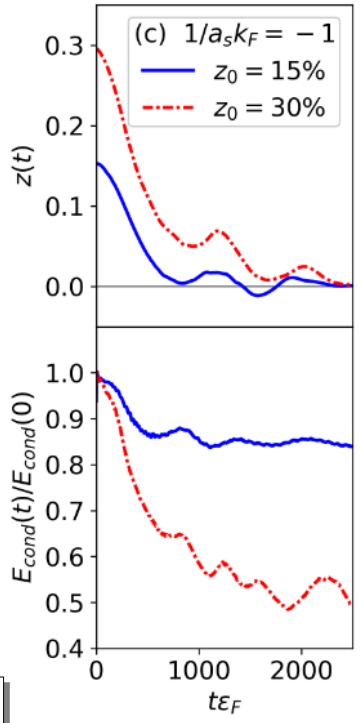
$$E_{\mathrm{BCS}} = E_{\mathrm{FG}} - \frac{3|\Delta|^2}{8\varepsilon_F} N$$

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



pair breaking is negligible

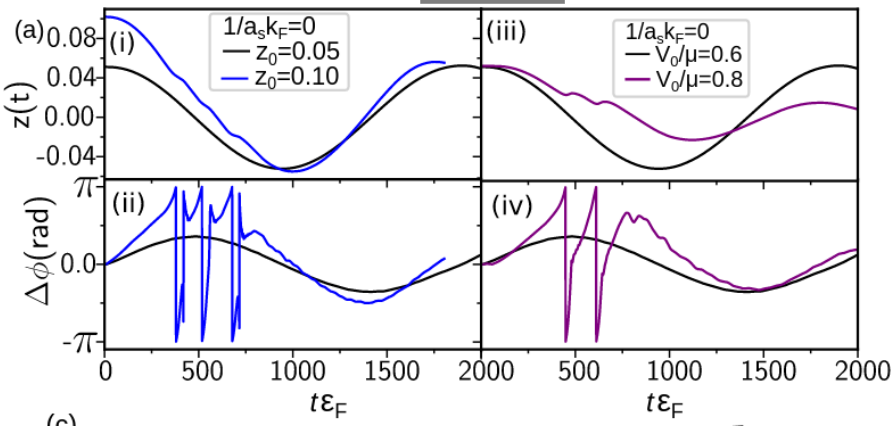
pair breaking!

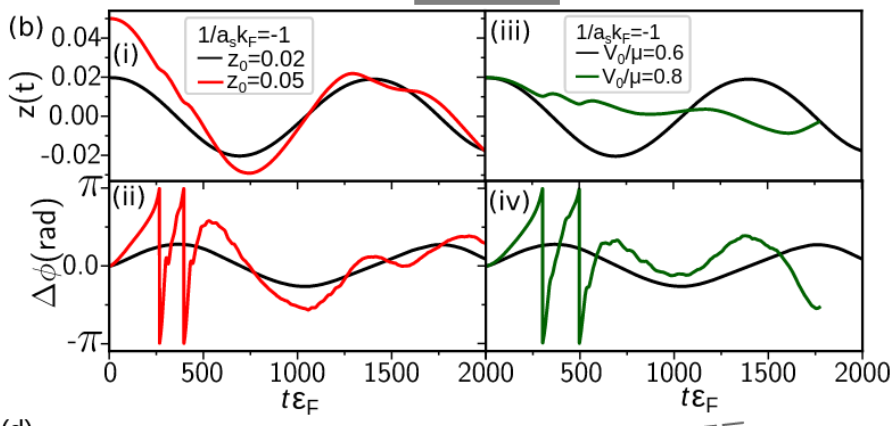


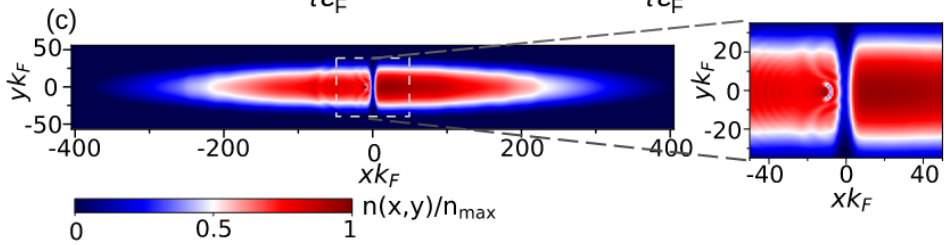
G. Wlazłowski, K. Xhani, M. Tylutki, N. Proukakis, M. Magierski, Phys. Rev. Lett. 130, 023003 (2023)

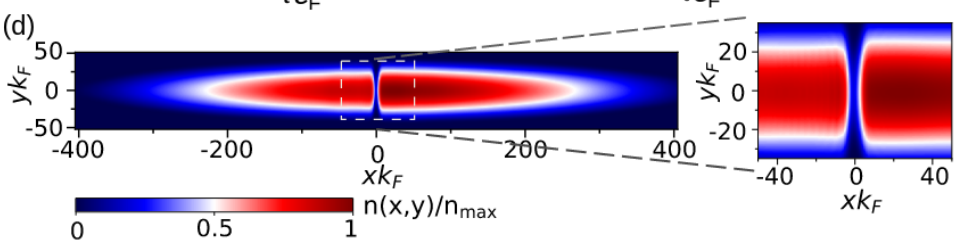
UFG

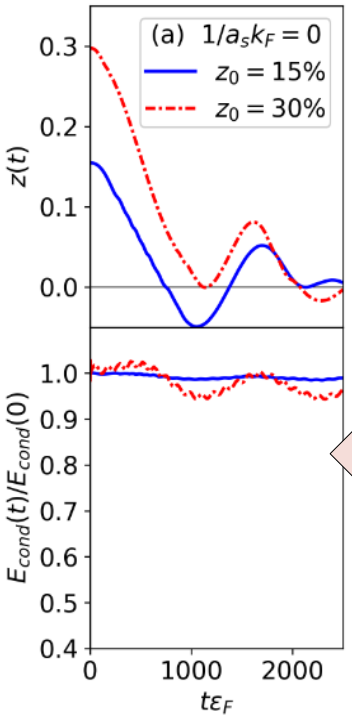
BCS











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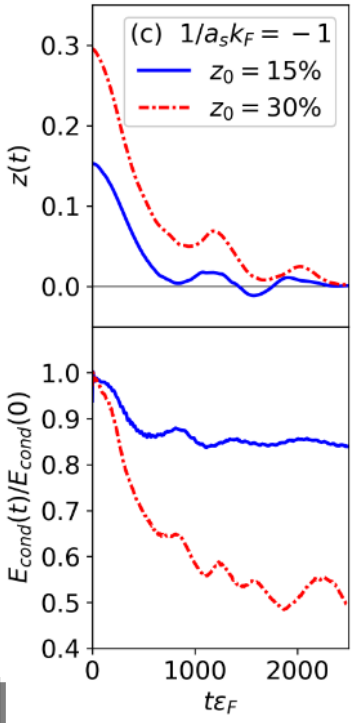
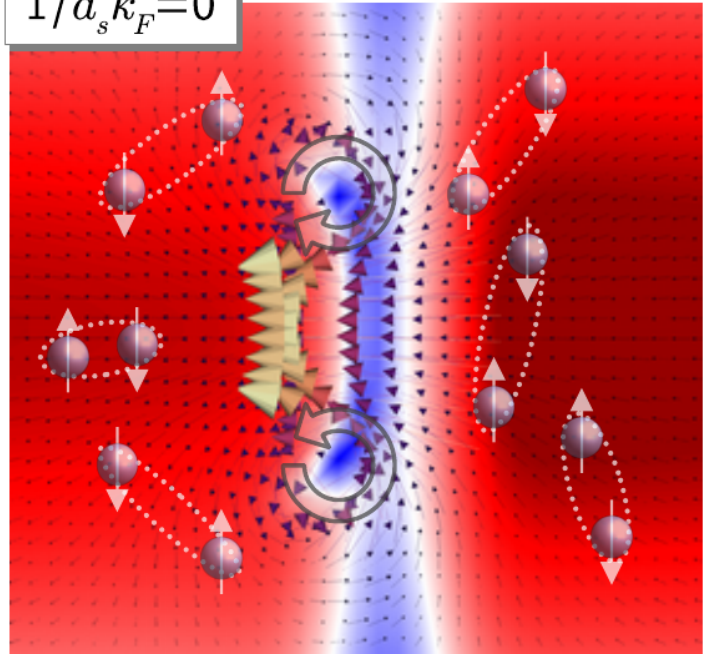


G. Wlazłowski, K. Xhani, M. Tylutki, N. Proukakis, M. Magierski, Phys. Rev. Lett. 130, 023003 (2023)

UFG

$1/a_sk_F$=0

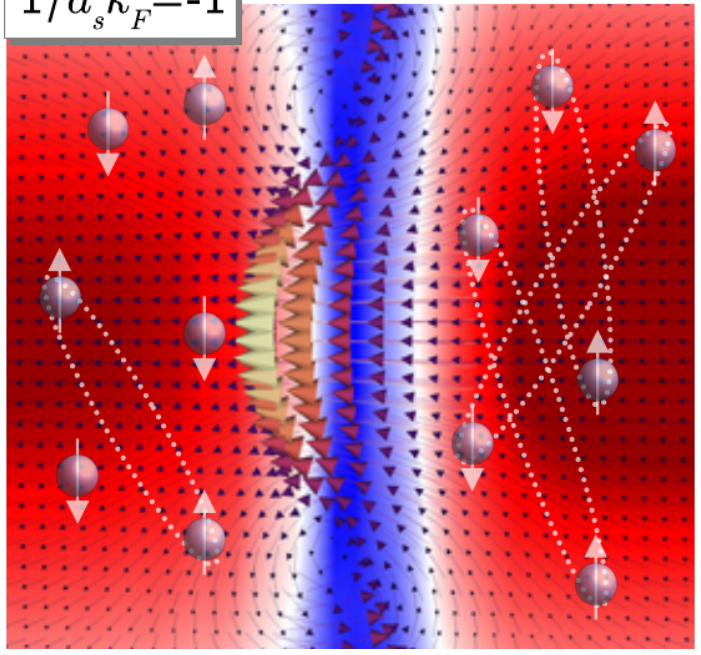


quantum vortex

Cooper pair

BCS

$1/a_sk_F$=-1



SUMMARY

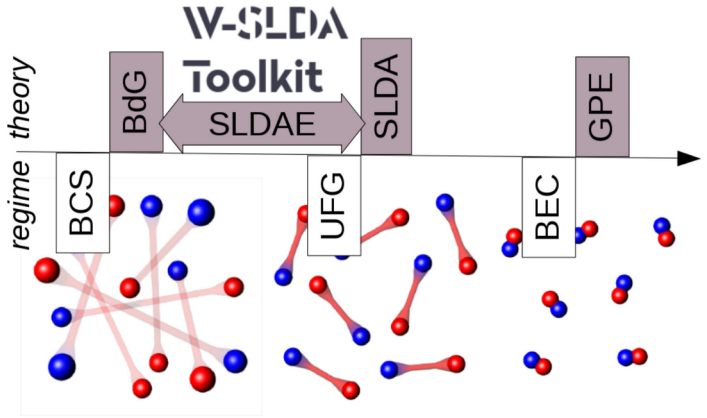
- Microscopic simulations for ultracold atoms are presently feasible for all interaction regimes:

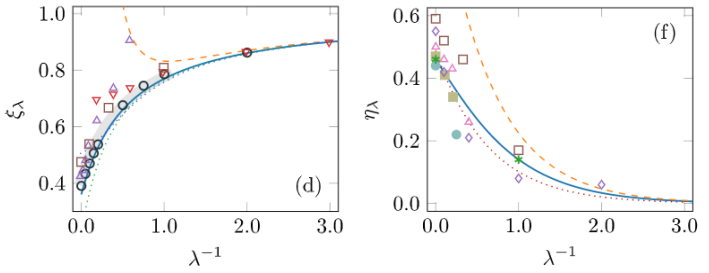
  DFT SLDA → BCS regime; strong interaction;
  GPE → BEC regime

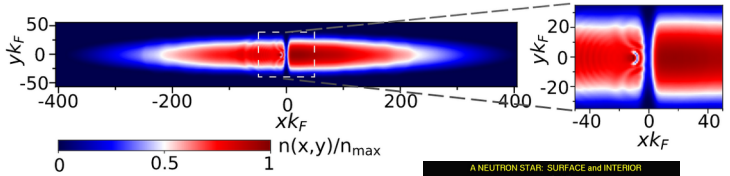
- DFT is general purpose method: it overcomes limitations of mean-field approch, while keeping numerical cost at the same level as BdG calculations.

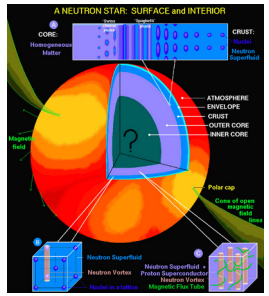
- Recent progress in High Performance Computing allows for tracking dynamics of systems consisting of thousands of fermions.

- DFT can benchmark experiments… and provide insight into problems that are not directly accessible, like neutron stars.









We have open call for post-doc position!

Collaborators: P. Magierski, M. Tylutki, D. Pęcak, A. Barresi, A. Boulet, A. Zdanowicz (WUT); M. Forbes (WSU); A. Bulgac (UW); K. Xhani (LENS); N. Proukakis (Newcastle U.); N. Chamel (U. Bruxelles)

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physics wut