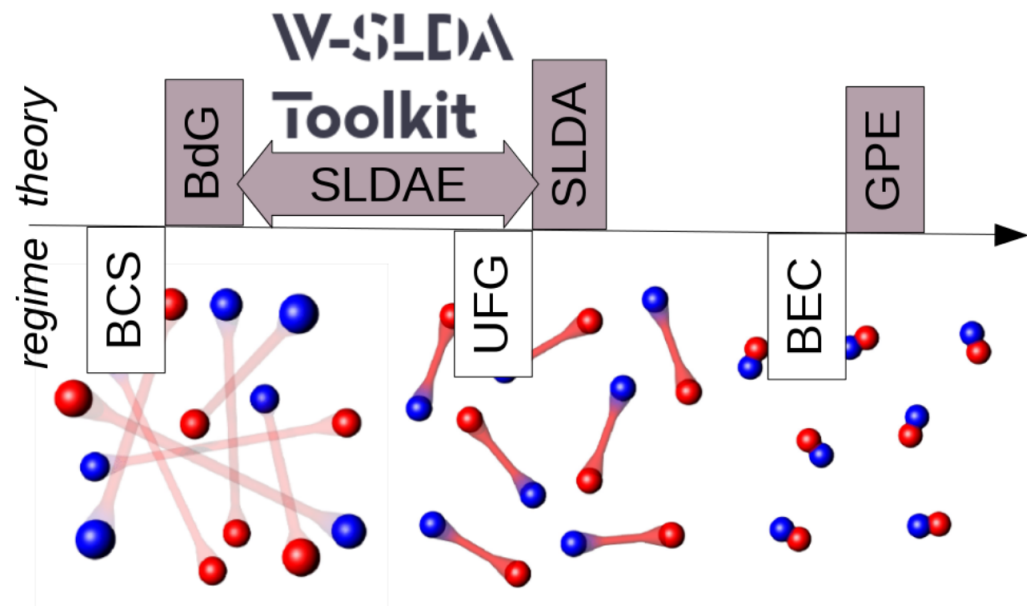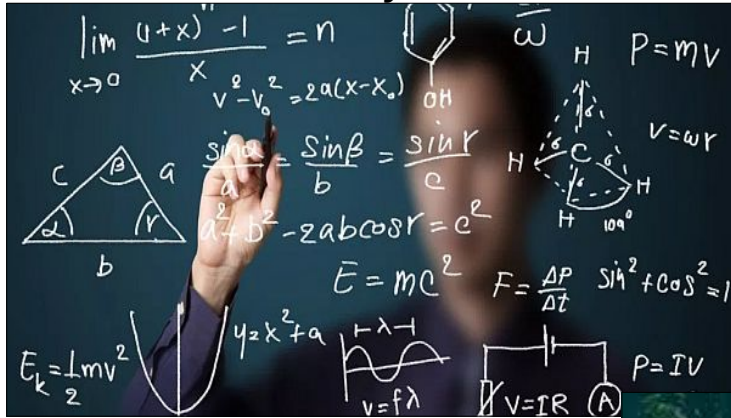# Ultracold atomic gases, neutron stars, and nuclei from the perspective of density functional theory

Gabriel Wlazłowski

Warsaw University of Technology
University of Washington

University of Wrocław, 7 June 2023

Theory

Experiment

Computational physics

Overview:
1. Method → DFT*
2. Implementation
3. Applications
4. Extensions to other systems
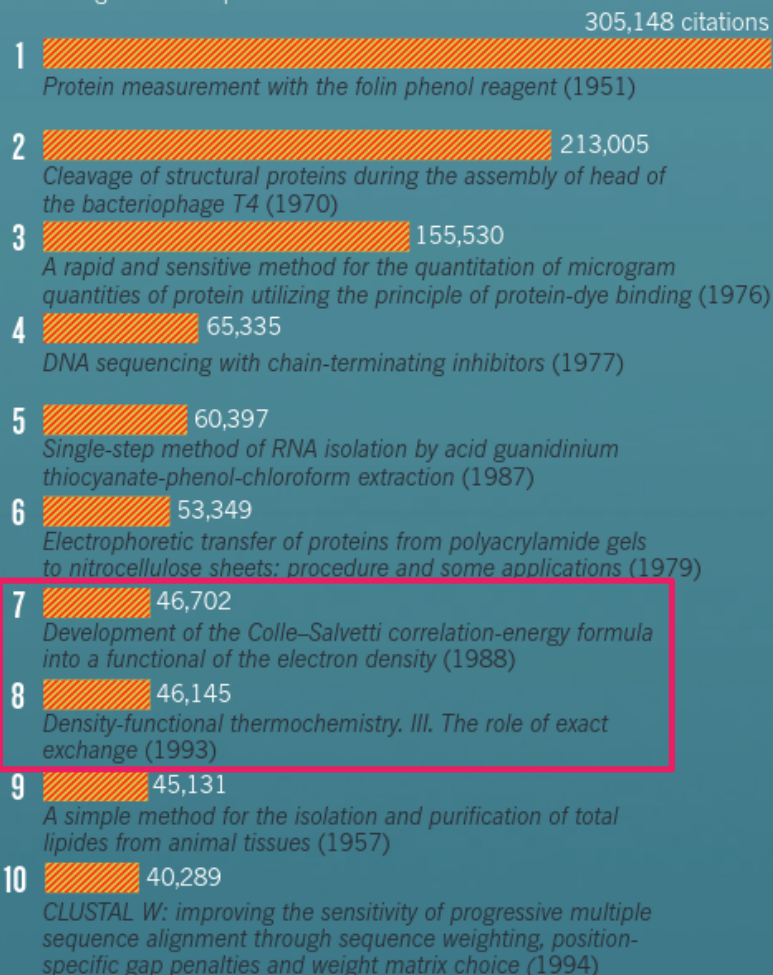
(*) Note: Many formal aspects of the theory will be presented superficially. Only general formulas...

- *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, ...

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TOP-10 PAPERS

Just 3 papers have received more than 100,000 citations, putting them well ahead of the rest. These runaway hits all cover biological lab techniques, which in general dominate the list of most-cited literature, including 7 of the top 10.

1 — 305,148 citations
Protein measurement with the folin phenol reagent (1951)

2 — 213,005
Cleavage of structural proteins during the assembly of head of the bacteriophage T4 (1970)

3 — 155,530
A rapid and sensitive method for the quantitation of microgram quantities of protein utilizing the principle of protein-dye binding (1976)

4 — 65,335
DNA sequencing with chain-terminating inhibitors (1977)

5 — 60,397
Single-step method of RNA isolation by acid guanidinium thiocyanate-phenol-chloroform extraction (1987)

6 — 53,349
Electrophoretic transfer of proteins from polyacrylamide gels to nitrocellulose sheets: procedure and some applications (1979)

7 — 46,702
Development of the Colle–Salvetti correlation-energy formula into a functional of the electron density (1988)

8 — 46,145
Density-functional thermochemistry. III. The role of exact exchange (1993)

9 — 45,131
A simple method for the isolation and purification of total lipides from animal tissues (1957)

10 — 40,289
CLUSTAL W: improving the sensitivity of progressive multiple sequence alignment through sequence weighting, position-specific gap penalties and weight matrix choice (1994)

THE TOP 100 PAPERS

Nature *explores the most-cited research of all time.*

BY RICHARD VAN NOORDEN,
BRENDAN MAHER AND REGINA NUZZO

DENSITY FUNCTIONAL THEORY

When theorists want to model a piece of matter — be it a drug molecule or a slab of metal — they often use software to calculate the behaviour of the material's electrons. From this knowledge flows an understanding of numerous other properties: a protein's reactivity, for instance, or how easily Earth's liquid iron outer core conducts heat.

Most of this software is built on density functional theory (DFT), easily the most heavily cited concept in the physical sciences. Twelve papers on the top-100 list relate to it, including 2 of the top 10. At its heart, DFT

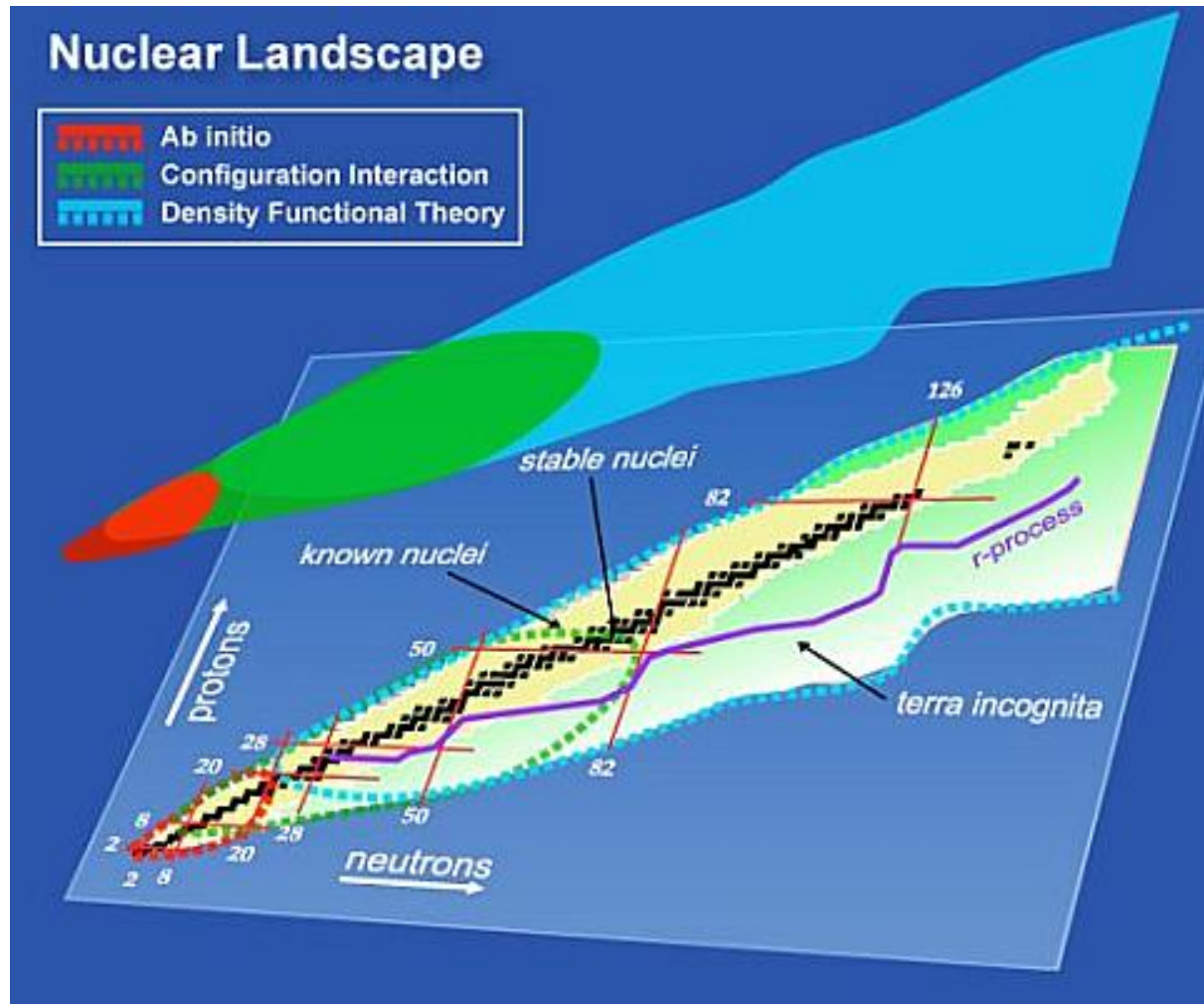**PHYSICS.WUT**

Workhorse for ...

Solid-state physics

Quantum chemistry

Condensed-matter physics

… also important tool for

Nuclear physics

(Nuclear) astrophysics

…

Nuclear Landscape

- Ab initio
- Configuration Interaction
- Density Functional Theory

126

stable nuclei

82

r-process

known nuclei

50

protons

terra incognita

28

20

82

8

50

2

8   28

2   8   20

neutrons

DFT today is one of main tools of *computational physics*
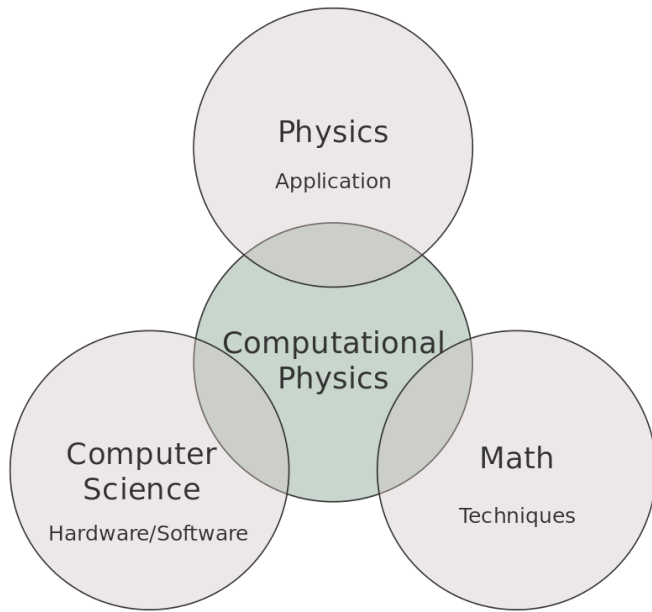
From wiki pages:
https://en.wikipedia.org/wiki/Computational_physics
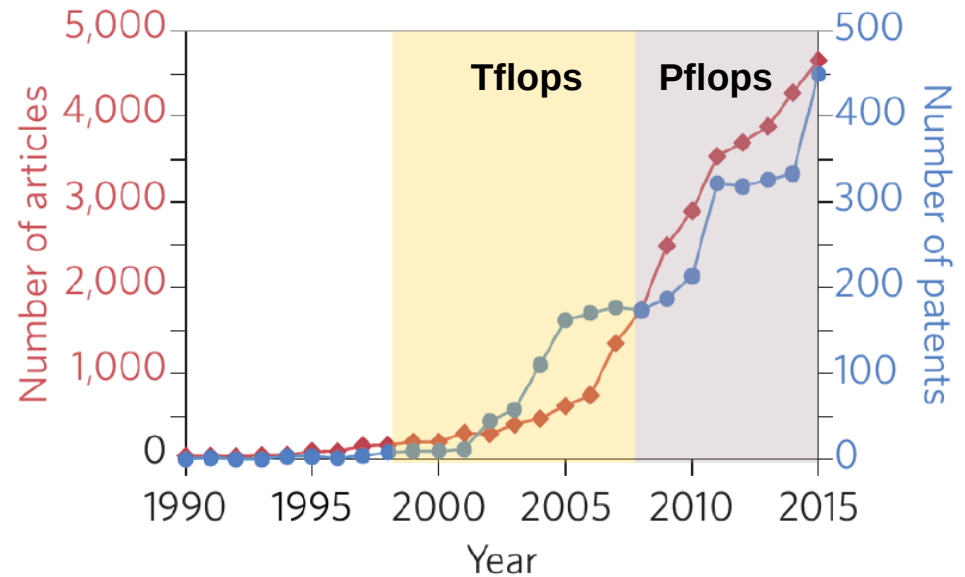
Figure 1: Number of articles and patents in materials science including the term "density functional theory" published per year during the past 25 years. Figure taken from *Boosting materials modelling*, Editorial article, Nature Materials **15**, 365 (2016).
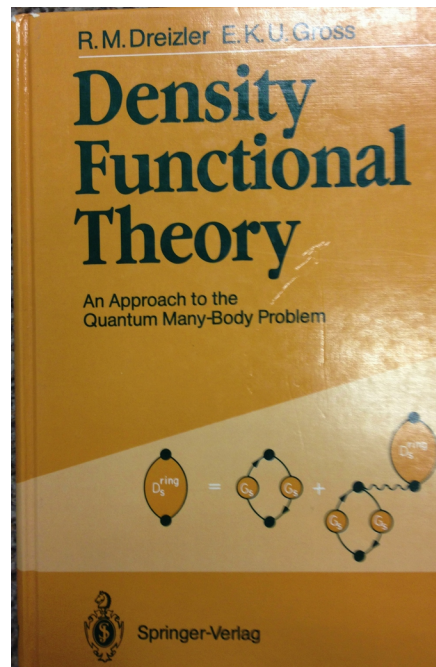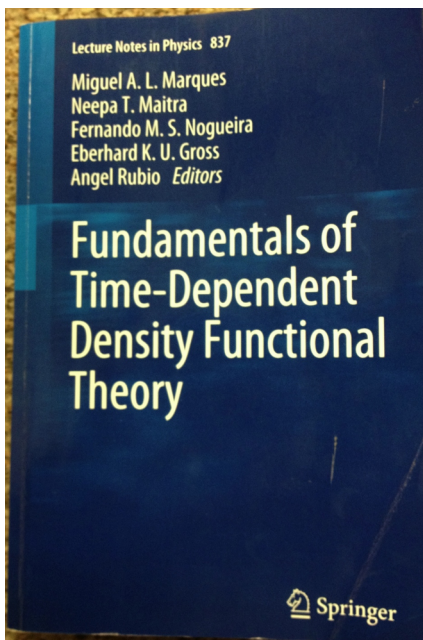
The Nobel Prize in Chemistry 1998 was divided equally between Walter Kohn "for his development of the density-functional theory" and John A. Pople "for his development of computational methods in quantum chemistry."

Credit: https://www.nobelprize.org/
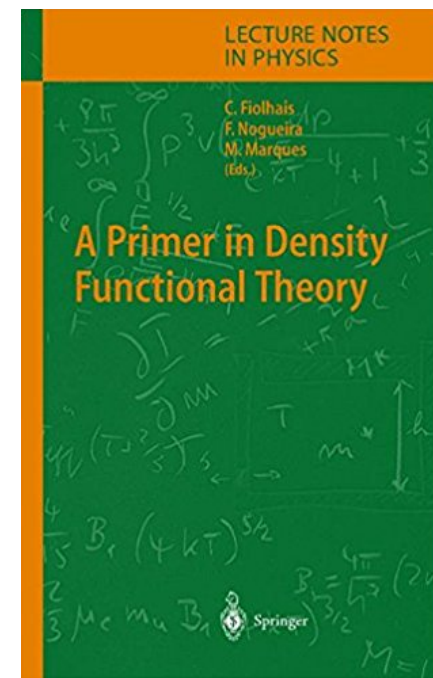
Strong correlation with High Performance Computing (HPC) developments

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- 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 $\leftrightarrow$ minimization of the energy density $E[\rho]$...

- ... however no mathematical recipe how to construct $E[\rho]$.

- 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)

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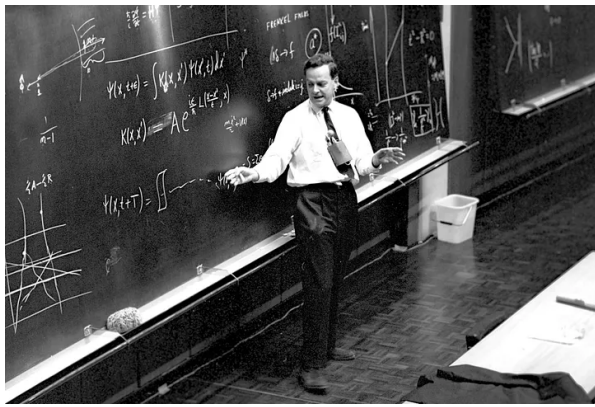
Richard Feynman
... physics is not mathematics and mathematics is not physics ...

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.

- ◆ 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 $E[\rho]$...

- ◆ ... however no mathematical recipe how to construct $E[\rho]$.

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  - dimensional arguments, renormalizability, Galilean invariance, and symmetries

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Alternative frameworks

| Schrödinger | DFT |

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

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

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

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

▱ Derivation of H_{int} - "*easy*"

▱ Solving many body Schrödinger equation - "hard"

TRADE

▱ 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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Solving problem:

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

Meta – GGA
(Kohn-Sham method)

...

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

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

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

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Classes of Energy Functionals

Increasing quality and computing cost

Normal state

- Local Density Approximation (LDA)
- Generalized Gradient Approximation (GGA)
- Meta – GGA *(Kohn-Sham method)*
- ...

Superconducting/superfluid state

- Superfluid Local Density Approximation (SLDA)
- ...

Meta-GGA   LDA

$$E_{\mathrm{SLDA}} = \int d\boldsymbol{r}\, \mathcal{H}(n(\boldsymbol{r}), \boldsymbol{\nabla} n(\boldsymbol{r}), \tau(\boldsymbol{r}), \dots, \nu(\boldsymbol{r}))$$

order parameter ⇐ anomalous density (complex field)
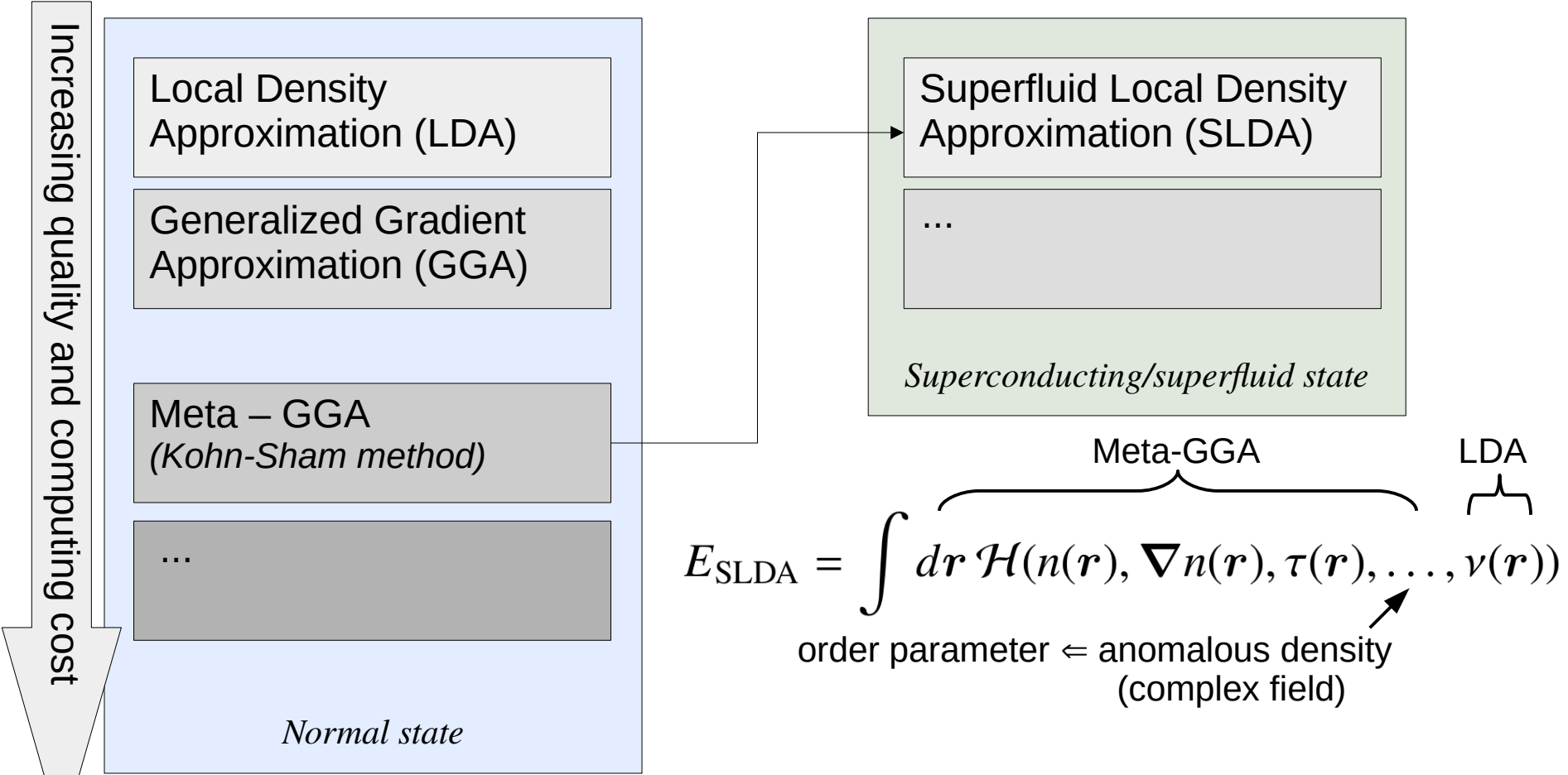
Density-Functional Theory for Superconductors

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!

CROSSOVER

BEC ⟵   ⟶ **BCS**

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

diatomic molecules   strongly interacting pairs   Cooper pairs

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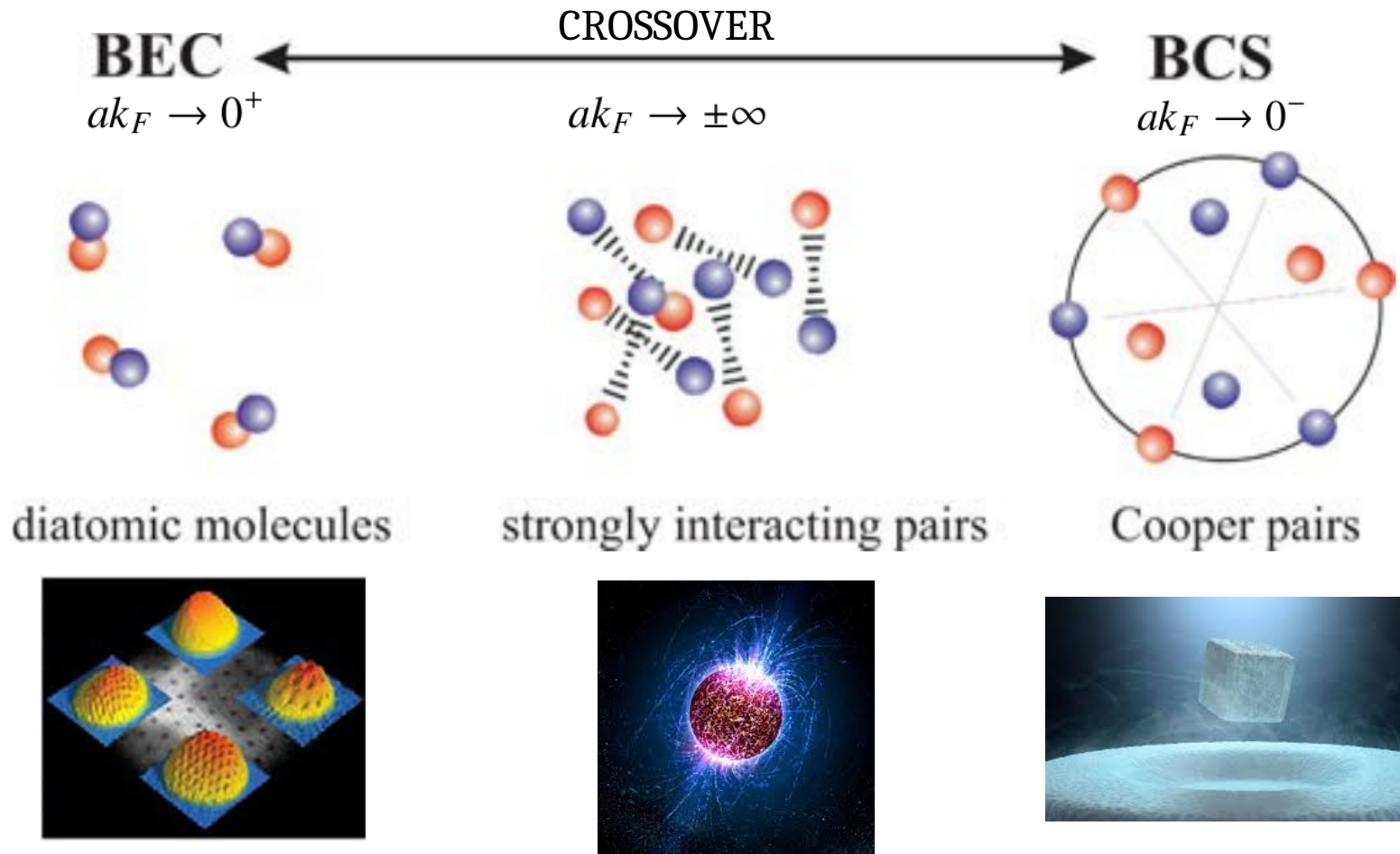
SLDA-type functional for ultracold atoms

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

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

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

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

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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SLDA-type functional for ultracold atoms

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

minimization

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

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

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

Jargon:

BCS $\rightarrow$ for uniforms systems
Bogoliubov-de-Gennes (BdG) $\rightarrow$ generalization of BCS to non-uniform systems, coordinate basis
Hartree-Fock-Bogoliubov (HFB) $\rightarrow$ generalization to arbitrary basis

For example, BdG is equivalent to

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

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

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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:
$\hbar = m = 1$

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

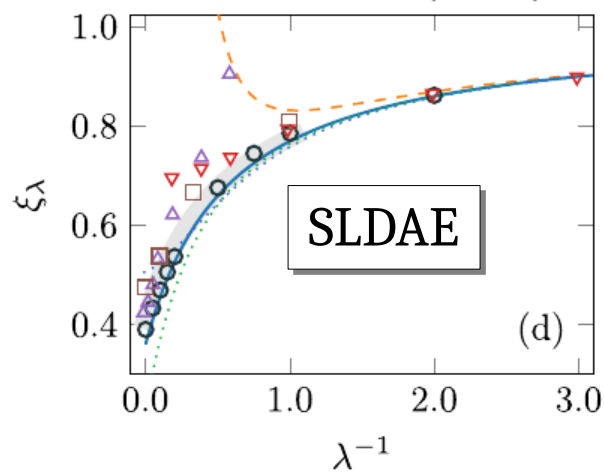$$\mathcal{E} = \frac{A_\lambda}{2}\left(\tau - \frac{\boldsymbol{j}^2}{n}\right) + \frac{3}{5} B_\lambda \, n \, \varepsilon_F + \frac{C_\lambda}{n^{1/3}}|\nu|^2 + \frac{\boldsymbol{j}^2}{2n}$$

dimensional analysis + symmetries

Kinetic term

Potential term

Pairing term

Center of mass motion

Units: $\hbar=m=1$

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

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

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

SLDA-type functional

Dimensionless functional parameters

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

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

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

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

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

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

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

INDUCE

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

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

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

INDUCE

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

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

SLDAE

Panel (a): $\xi_\lambda = E/E_{\mathrm{FG}}$ vs $\lambda = |ak_F|$

Panel (b): $\alpha_\lambda = m^*/m$ vs λ

Panel (c): $\eta_\lambda = \Delta/\varepsilon_F$ vs λ

Panel (d): ξ_λ vs λ^{-1}

Panel (e): α_λ vs λ^{-1}

Panel (f): η_λ vs λ^{-1}

Legend (left):
- 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]

Legend (middle):
- Galitskii formula [77]
- exp. (Sagi *et al.*, 2015) [80]
- exp. (Sagi *et al.*, 2015) [80]
- GSCGF (Hausmann *et al.*, 2009) [72]
- Brueckner – Hartree – Fock (Doggen and Kinnunen, 2015) [88]
- pp + hh ladder [67, 70]
- pp ladder [67, 70]

Legend (right):
- BCS formula [62]
- exp. (Schirotzek *et al.*, 2008) [82]
- exp. (Hoinka et al., 2017) [81]
- GSCGF (Hausmann *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*

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

Towards time-dependent problems

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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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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*

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

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

n(t'<t)

0
Ψ_0

t

time

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

Adiabatic approximation
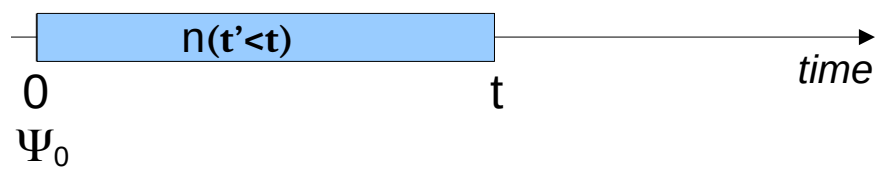
In general integro-differential equations ⟵ $$E(t) = \int_0^t dt' \int_V d\boldsymbol{r}\, \mathcal{E}[\Psi_0, n(\boldsymbol{r}, t'), \ldots]$$

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
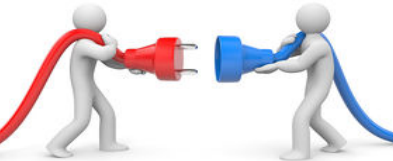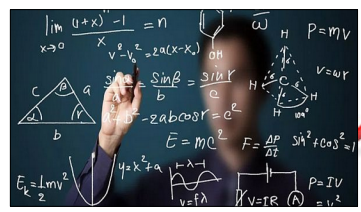
Computer code

Experiment
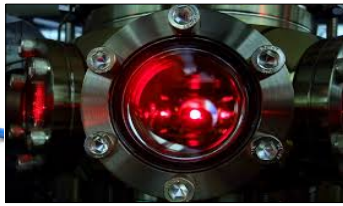
Theoretical method
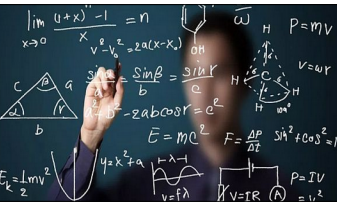
Experiment

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

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

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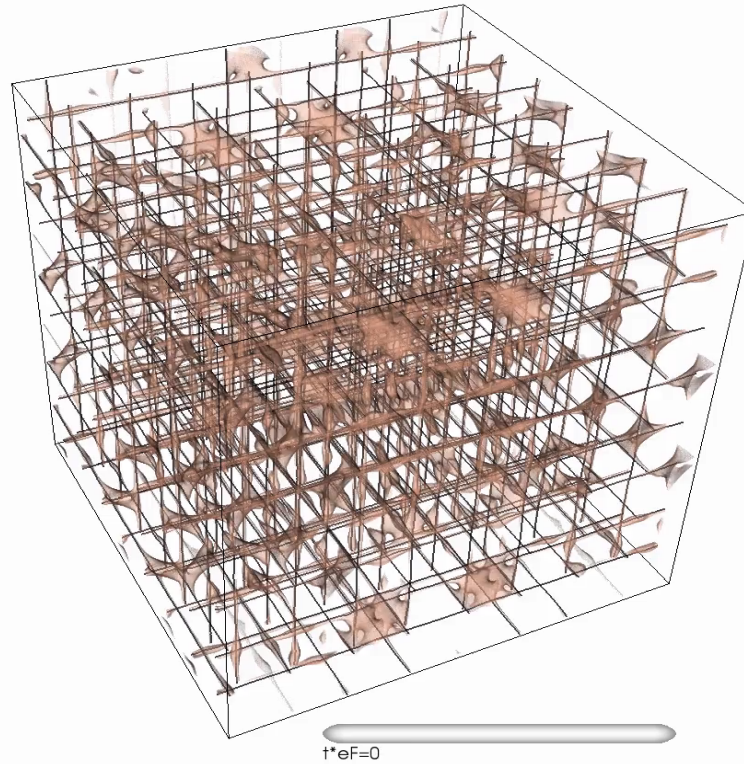(depending on the problem size)

High **P**erformance **C**omputing

NVIDIA CUDA

AMD ROCm

open source

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mesh dimensionality

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

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

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

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

High **P**erformance **C**omputing

NVIDIA CUDA   AMD ROCm   open source

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t*eF=0

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)

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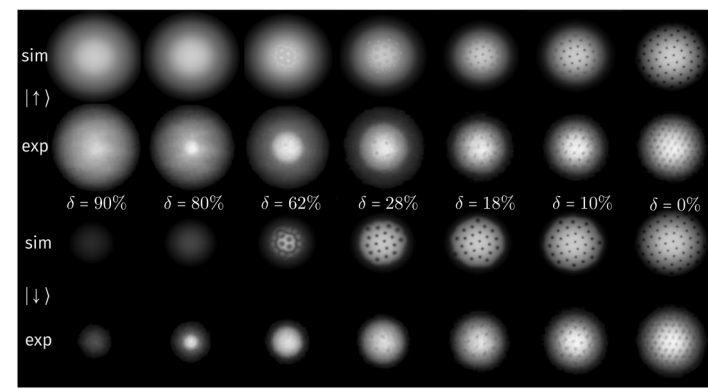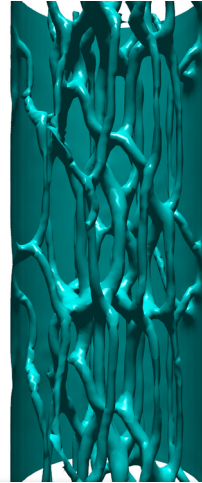
- ## Quantum turbulence
  Phys. Rev. A 105, 013304 (2022)

- ## Spin-polarized impurities
  Phys. Rev. A 100, 033613 (2019)
  Phys. Rev. A 104, 033304 (2021)
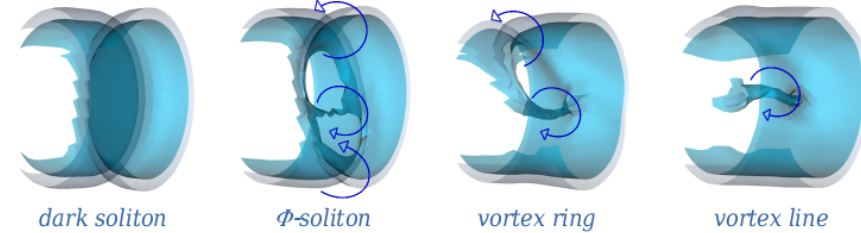
- ## Solitonic cascades
  Phys. Rev. Lett. 120, 253002 (2018)

- ## 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)
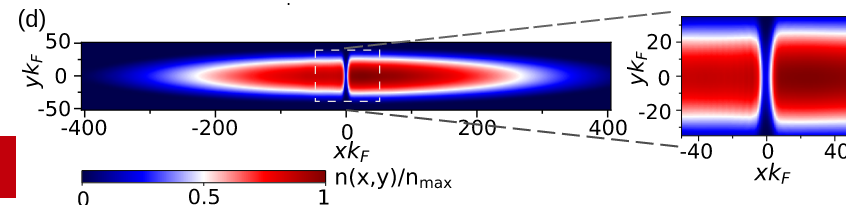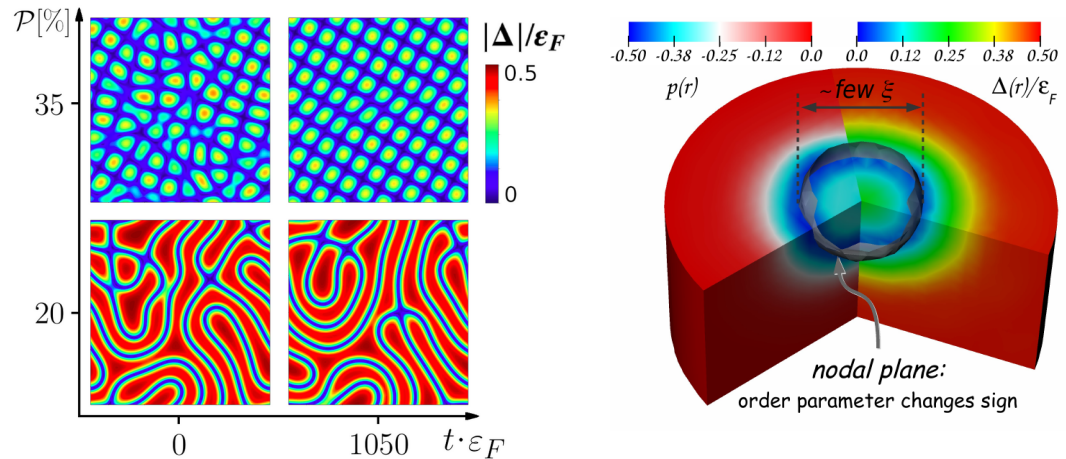
- ...

dark soliton   Φ-soliton   vortex ring   vortex line

nodal plane: order parameter changes sign

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]

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

$$\Delta\phi(t) \equiv \phi_L(t) - \phi_R(t) \quad \text{t [ms]}$$
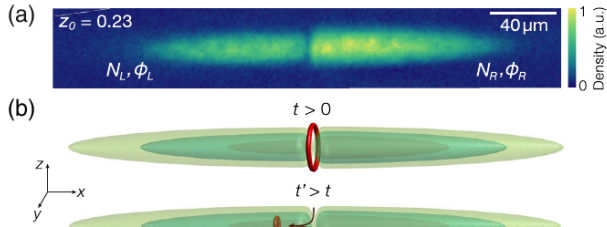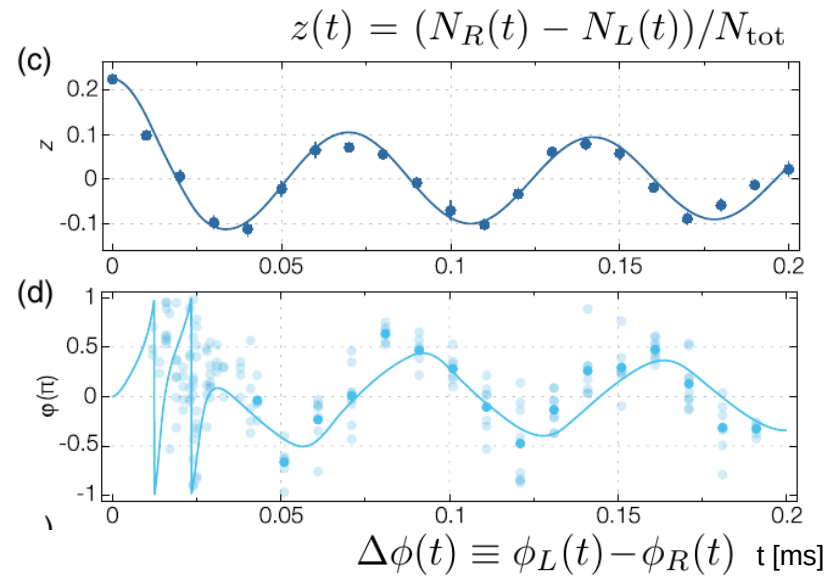
Experiment

Simulation

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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)
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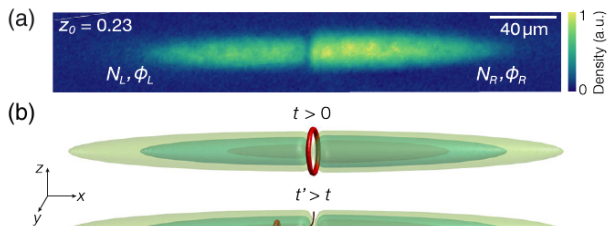
Figs from [2]
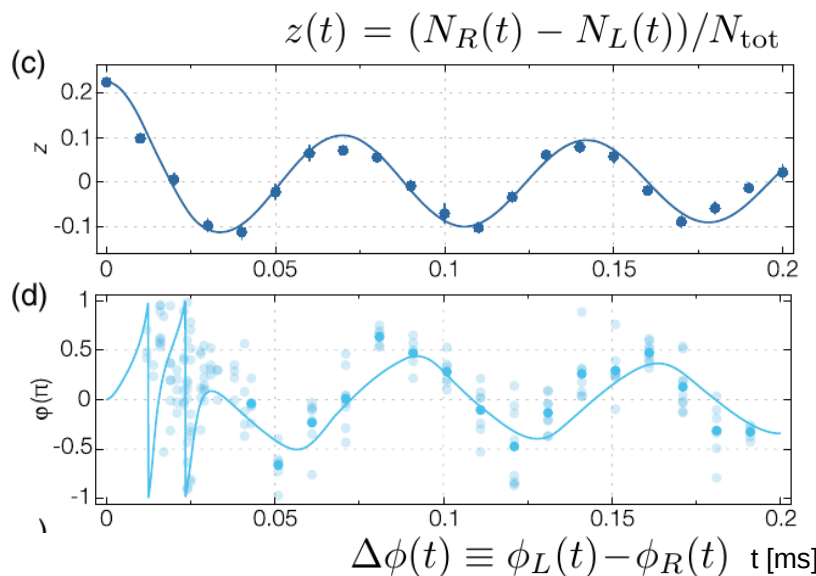
G. Wlazłowski, et.al.,
Phys. Rev. Lett. 130, 023003 (2023)

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

$$\Delta\phi(t) \equiv \phi_L(t) - \phi_R(t) \quad t\,[ms]$$

Experiment

UFG
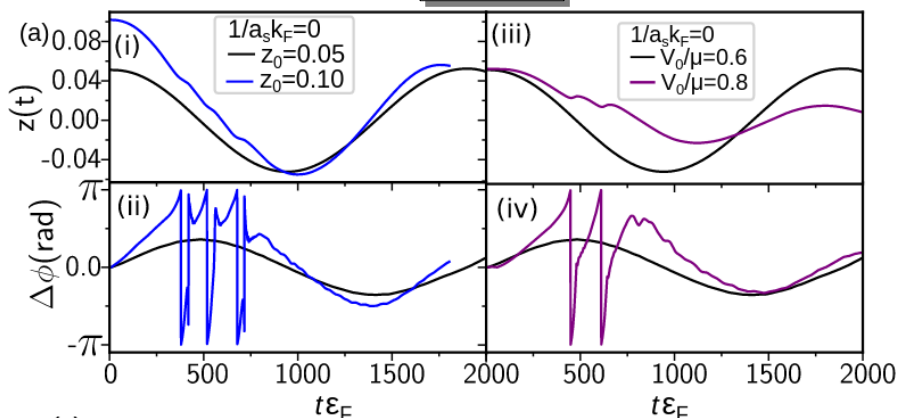
BCS
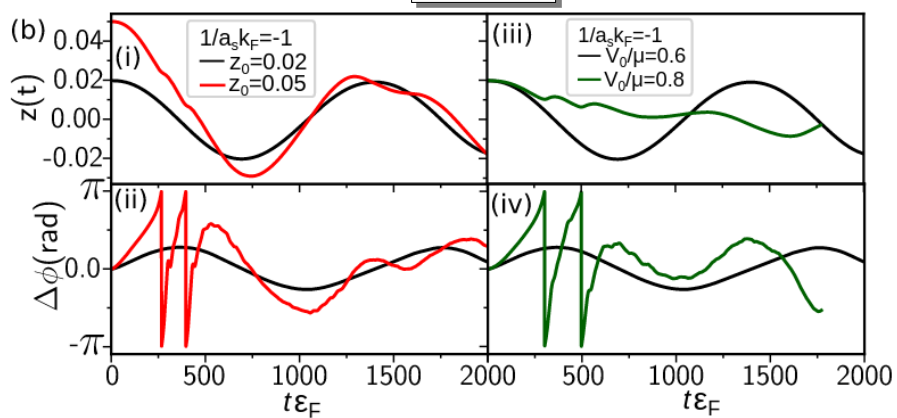
Simulation
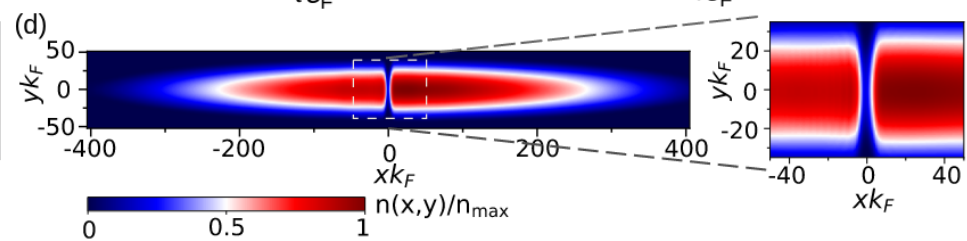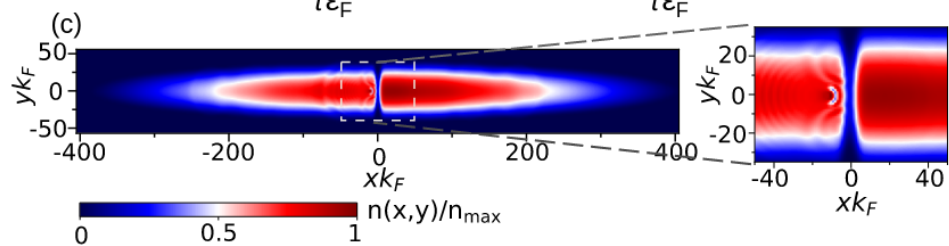
A NEUTRON STAR: SURFACE and INTERIOR
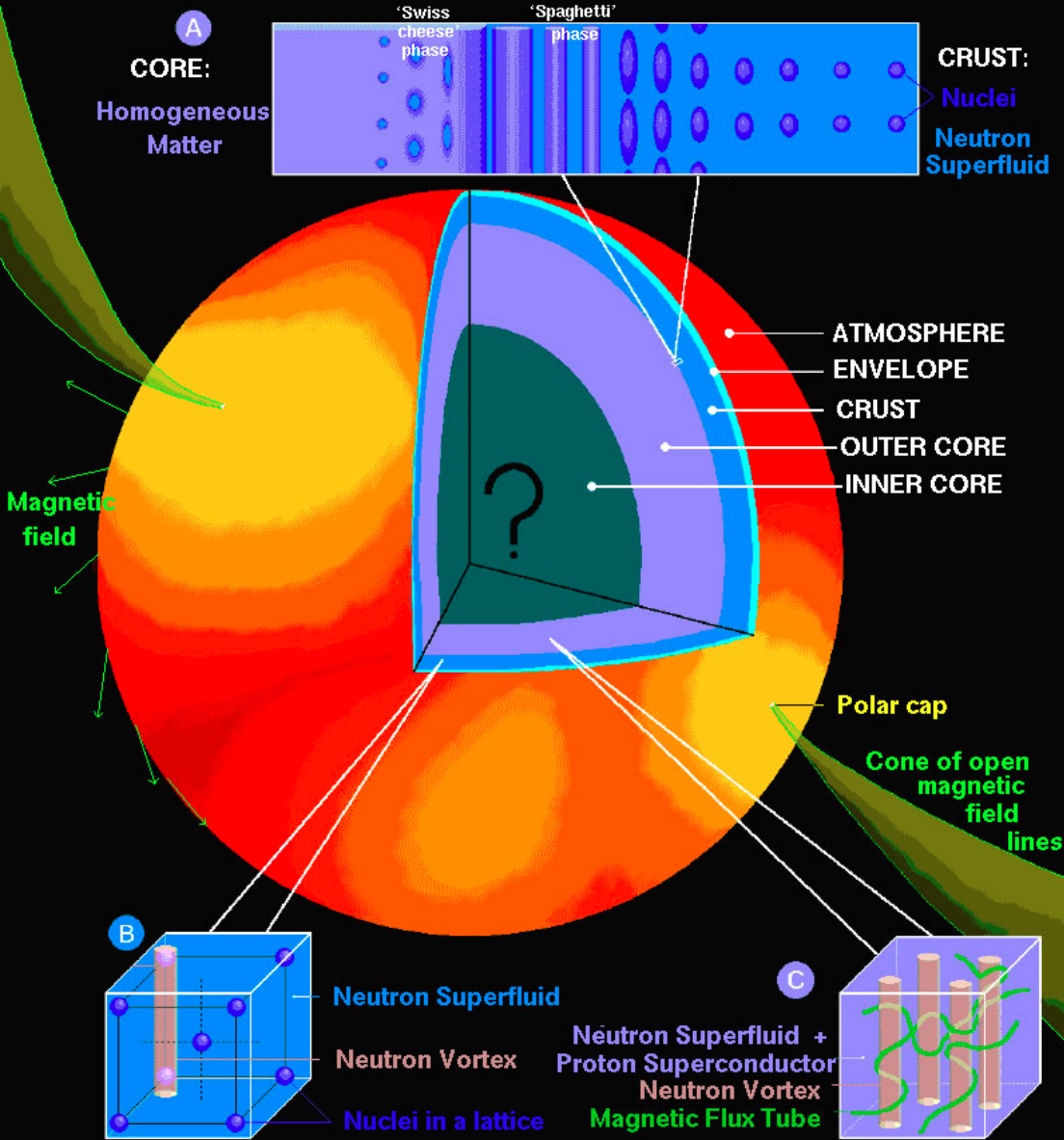
Computational physics (modeling) plays a key role in the study of objects that are not directly accessible
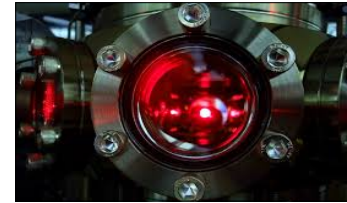
Ultracold atomic gases:

→ when designing the functional, we follow the same general strategies

→ we use ultracold atoms to learn about predictive power of the method

Next we apply the method to neutrons stars.

→ … for example, nuclear codes that we use are based on software that we constructed for ultracold atoms

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Brussels-Montreal Skyrme functionals (BSk)

These functionals were fitted to both experimental data and N-body calculations using realistic forces.

Experimental data:

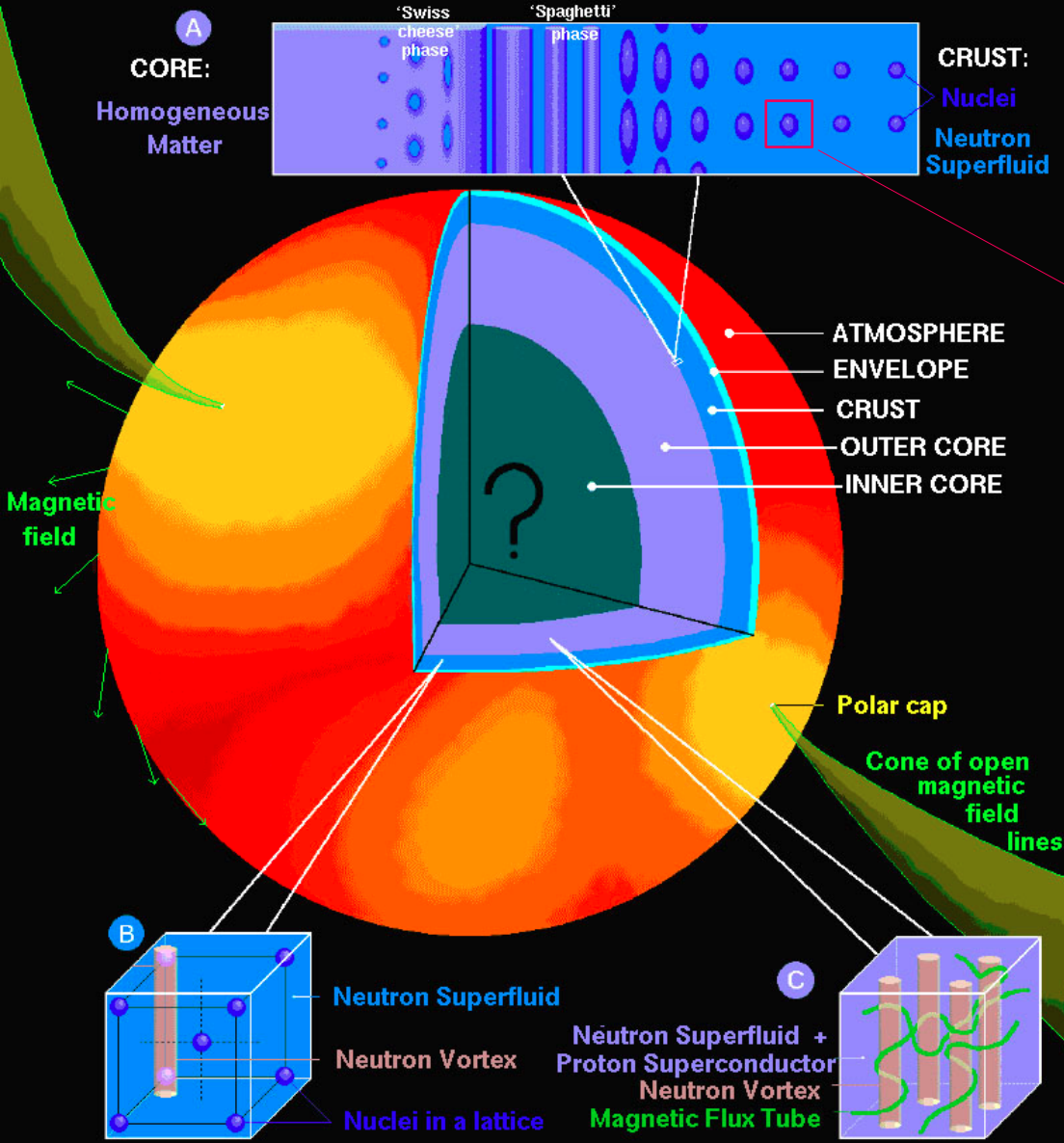- all atomic masses with $Z, N \geq 8$ from the Atomic Mass Evaluation (root-mean square deviation: 0.5-0.6 MeV)

  `http://www.astro.ulb.ac.be/bruslib/`

- charge radii

- incompressibility $K_v = 240 \pm 10$ MeV (ISGMR)
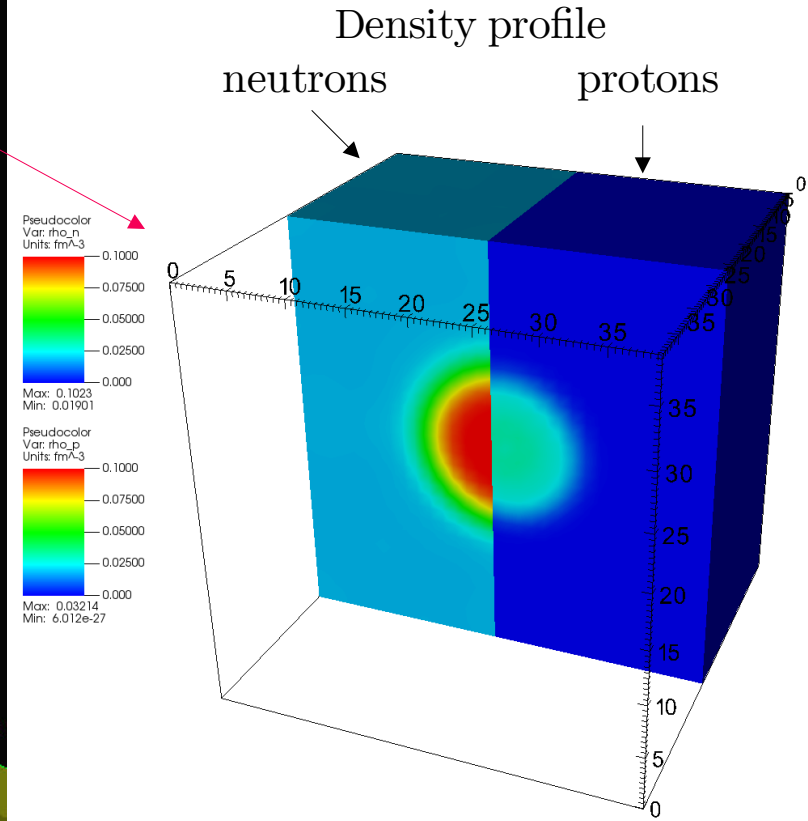 *Colò et al., Phys.Rev.C70, 024307 (2004).*

N-body calculations using realistic forces:

- equation of state of pure neutron matter
- $^1S_0$ pairing gaps in nuclear matter
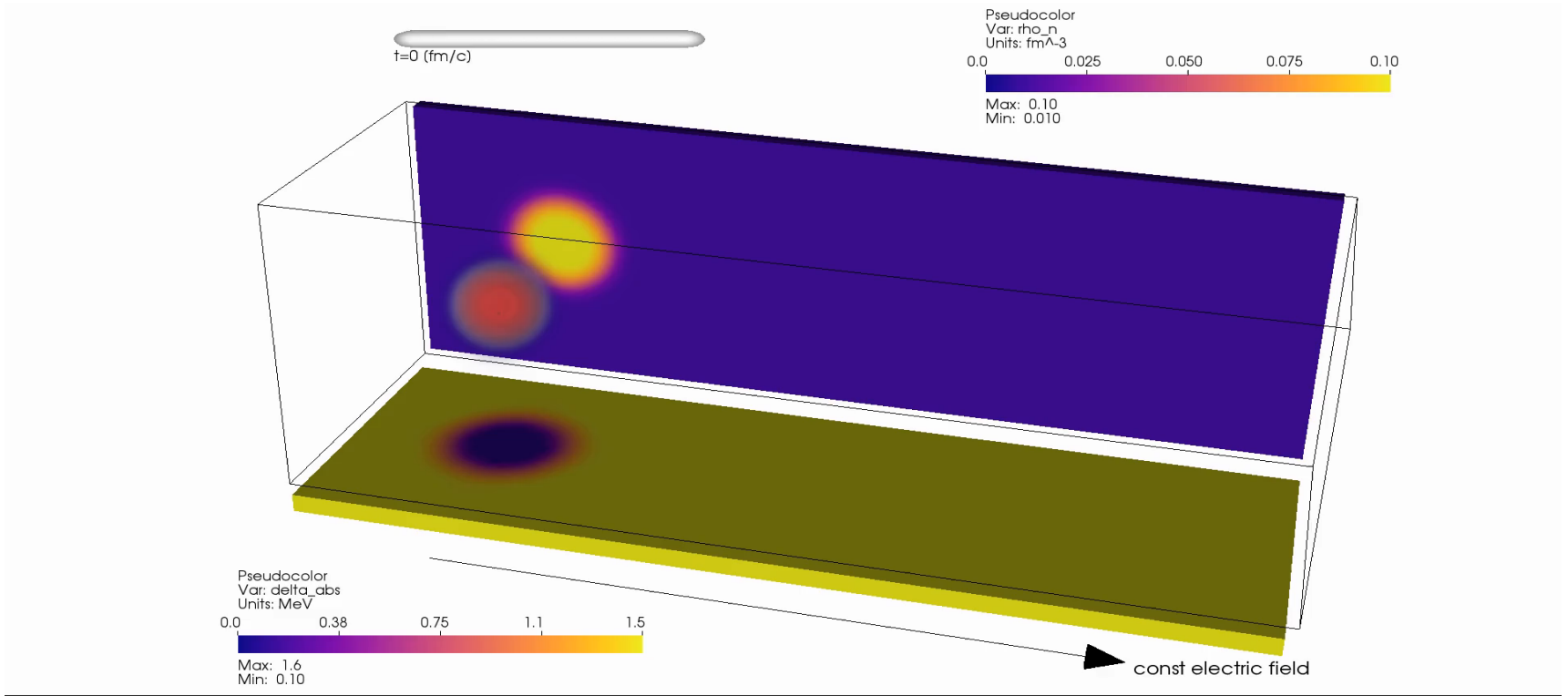- effective masses in nuclear matter

A NEUTRON STAR: SURFACE and INTERIOR

A

CORE:

Homogeneous Matter

'Swiss cheese' phase   'Spaghetti' phase

CRUST:

Nuclei

Neutron Superfluid

- ATMOSPHERE
- ENVELOPE
- CRUST
- OUTER CORE
- INNER CORE

Magnetic field

?

Polar cap

Cone of open magnetic field lines

B

Neutron Superfluid

Neutron Vortex

Nuclei in a lattice

C

Neutron Superfluid + Proton Superconductor

Neutron Vortex

Magnetic Flux Tube

Computational physics (modeling) plays a key role in the study of objects that are not directly accessible

Density profile

neutrons   protons

Pseudocolor
Var: rho_n
Units: fm^-3
0.1000
0.07500
0.05000
0.02500
0.000
Max: 0.1023
Min: 0.01901

Pseudocolor
Var: rho_p
Units: fm^-3
0.1000
0.07500
0.05000
0.02500
0.000
Max: 0.03214
Min: 6.012e-27

In the simulation box $(40 \text{ fm})^3$ we have 1382 neutrons and 40 protons.

System: *nuclear matter*
3D simulation 40 x 40 x 120 [fm]
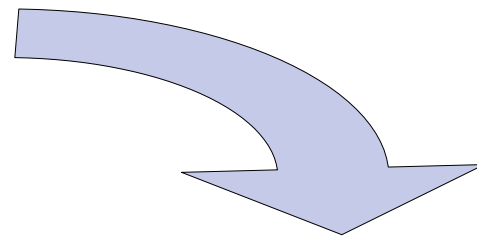
number of neutrons: 2,104
number of protons: 40

W-BSK

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$n_{bar} = 0.005772 fm^{-3}, n_{bulk} = 0.0045 fm^{-3}, Z = 40$

- $F_z = 0.1 MeV/fm, M_{eff}/M_n = 140.3$
- $F_z = 0.5 MeV/fm, M_{eff}/M_n = 139.5$
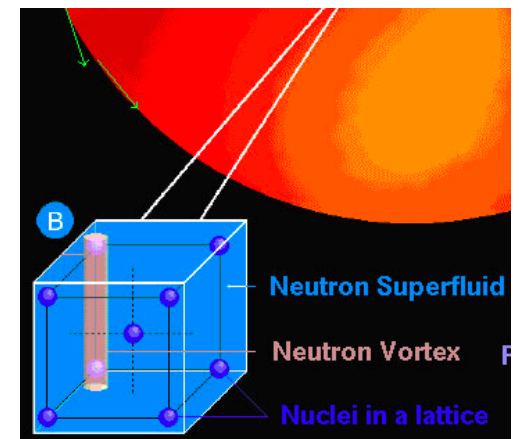- $F_z = 1.0 MeV/fm, M_{eff}/M_n = 139.1$
- $F_z = 2.0 MeV/fm, M_{eff}/M_n = 143.0$

PRELIMINARY
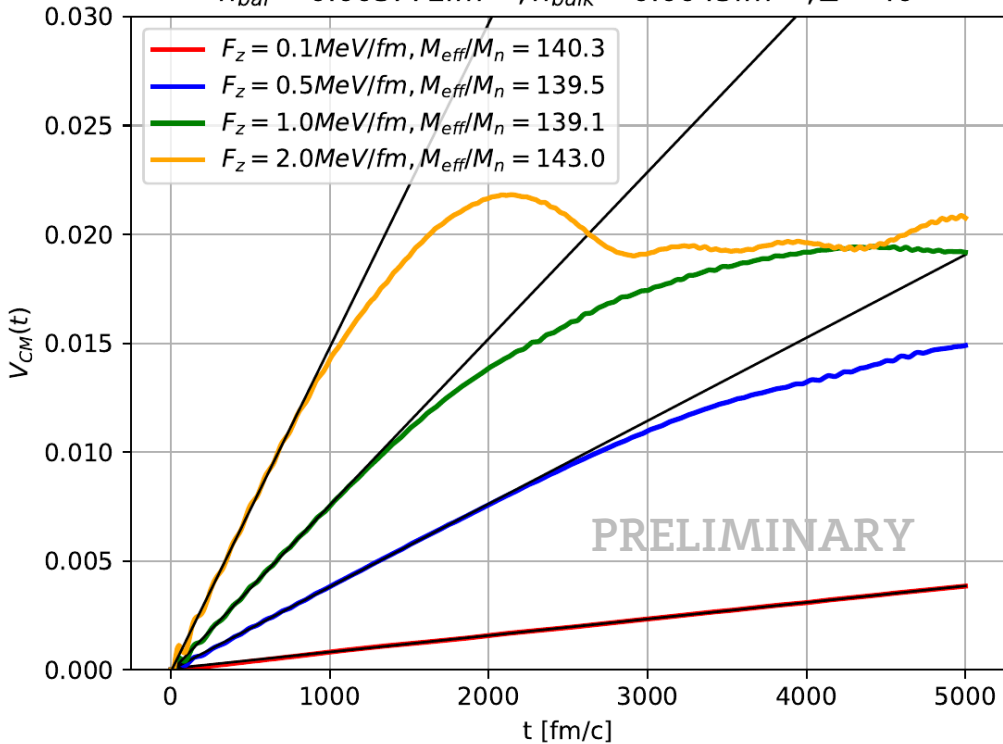
Example of application:
→ extraction of parameters
for effective theories of
neutron star crust.

$$ZeE = F = Ma$$

control
paramater

PRELIMINARY
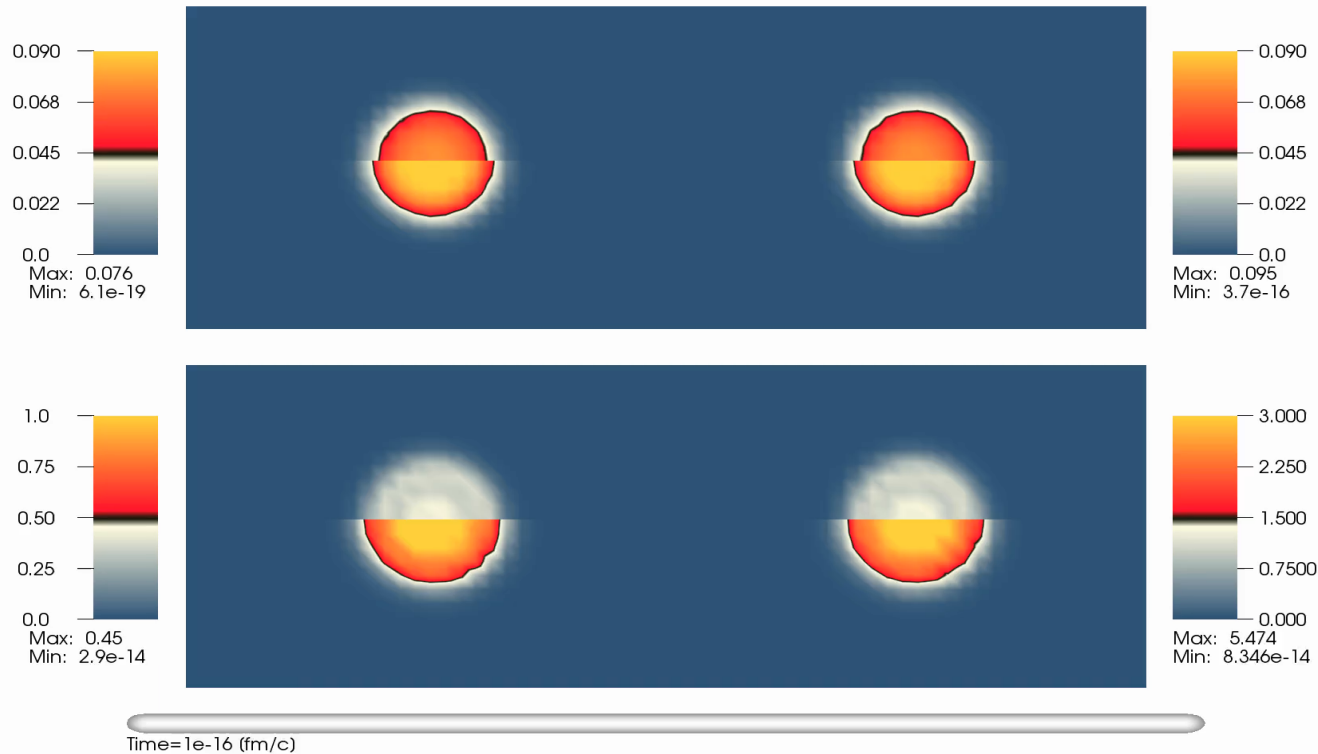
DB: vor8A_density_n.0000
Cycle: 0   Time:325.194

Contour
Var: density_p
Units: 1/fm^3

Max: 0.02297
Min: 8.730e-14

Vector
Var: current_n
Units: c fm^3

Max: 0.0008943
Min: 1.823e-11

Time=325.194

user: aleksandra
Mon Jun 11 16:42:36 2018

Neutron Superfluid

Neutron Vortex

Nuclei in a lattice
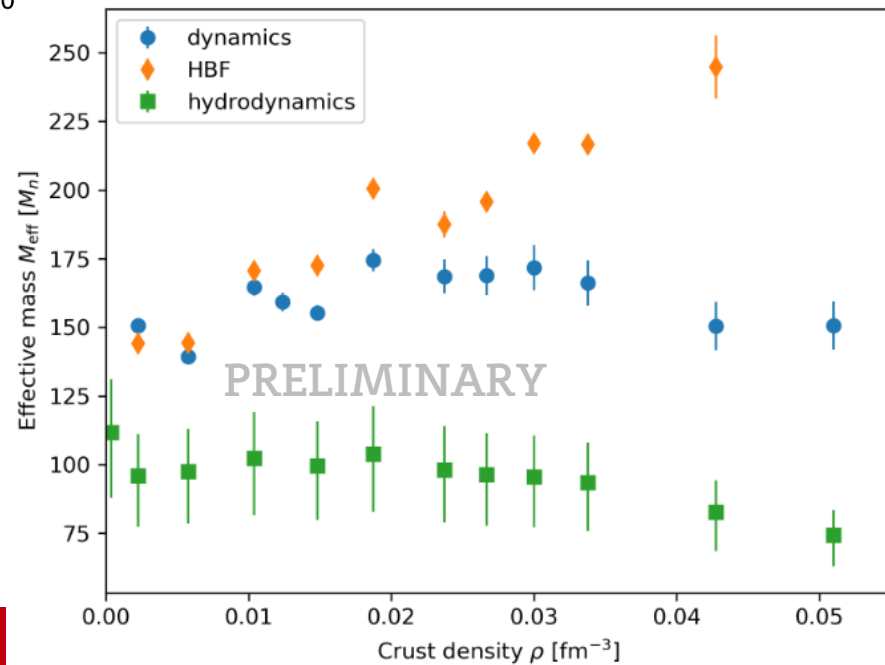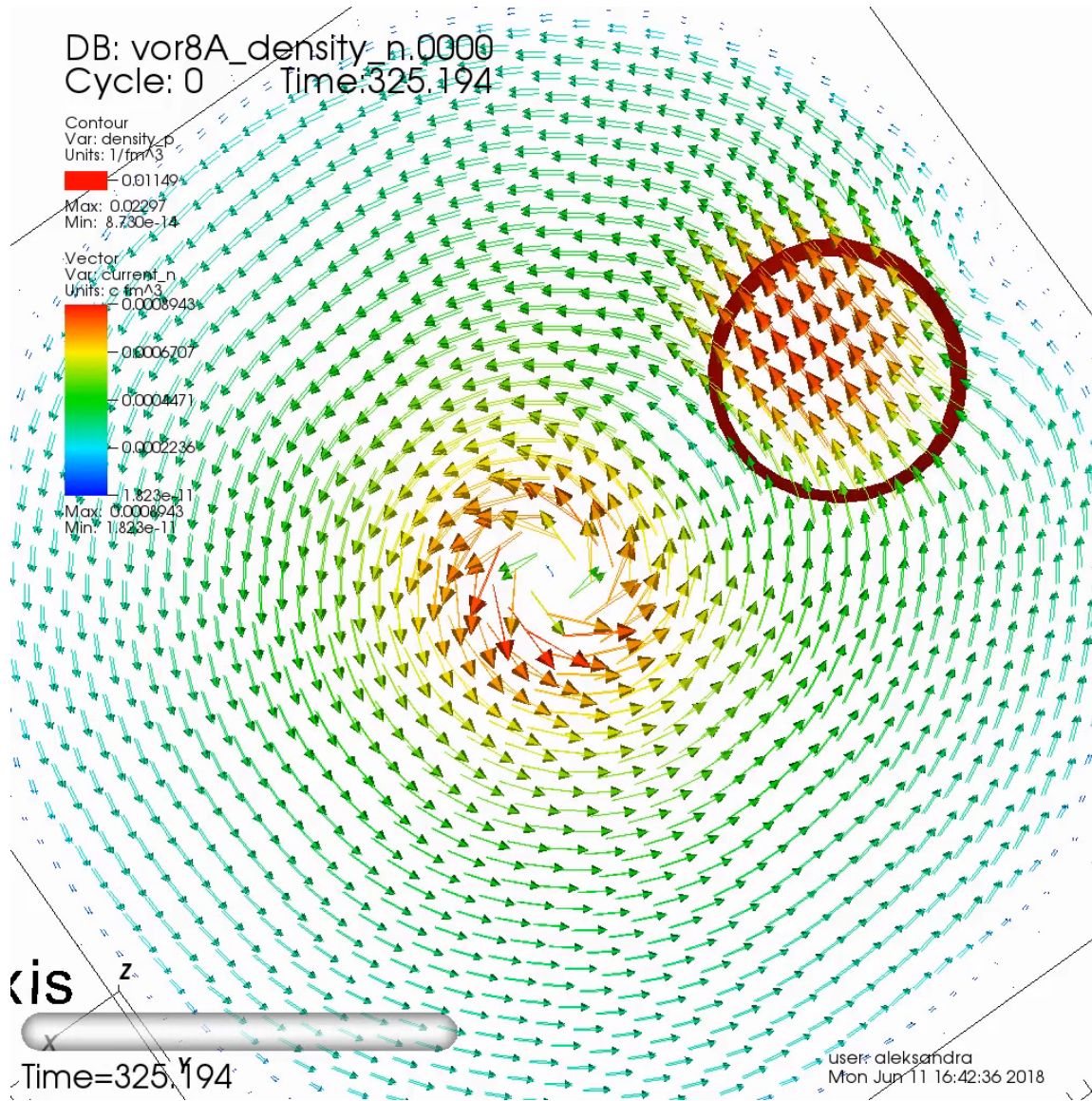
System: *nuclear in presence of quantum vortex*

Understanding of the vortex–impurity interaction is required in order or understand the phenomenon of neutron star glitches.

V.B. Bhatia, A Textbook of Astronomy and Astrophysics with Elements of Cosmology, Alpha Science, 2001.
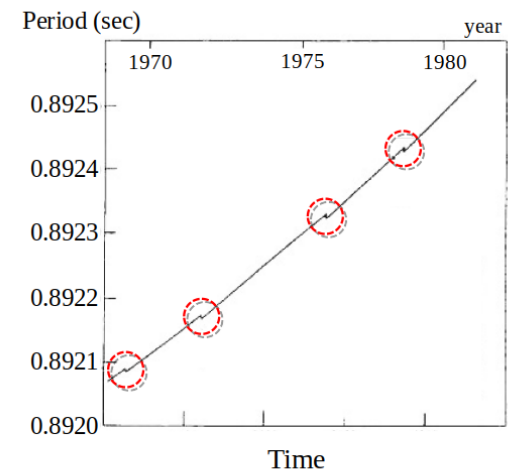
Reaction: $^{96}Zr+^{96}Zr$, SkM*, $E_{cm}=178MeV$, head-on collision

Phenomena related to nuclei (like nuclear reactions) can be also investigated by means of TDDFT.

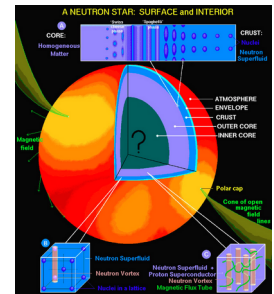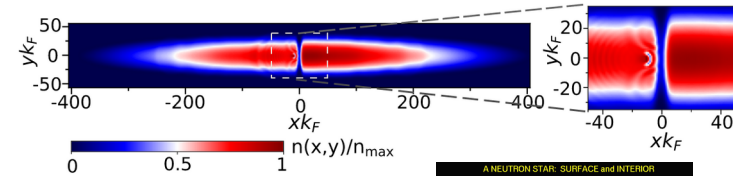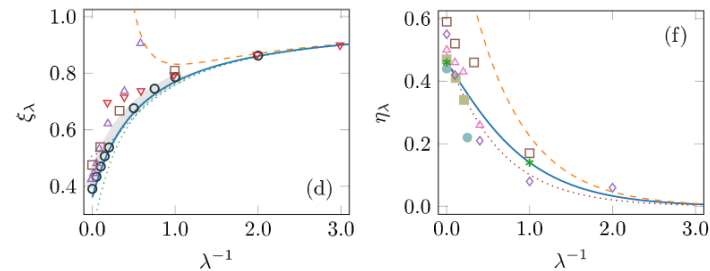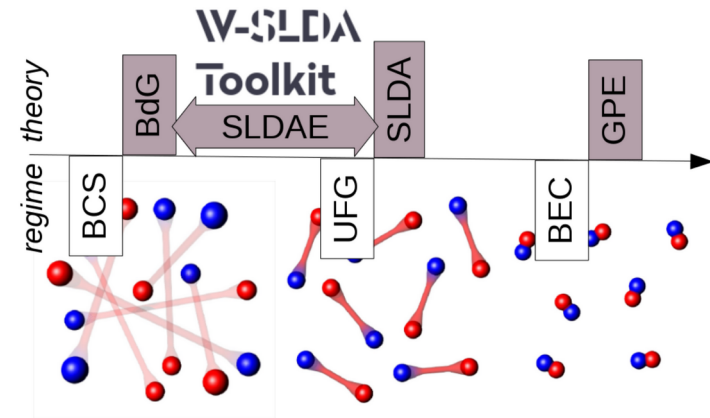→ … however various complications arise
(as compared to ultracold atoms or nuclear matter)

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SUMMARY

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

  DFT / SLDA → BCS regime; strong interaction;

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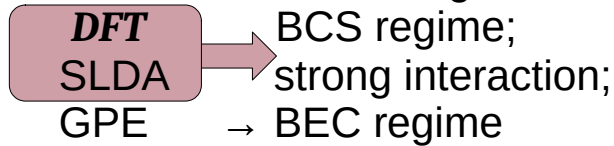
- DFT is general purpose method: it overcomes limitations of mean-field approch, while keeping numerical cost at the same level as BdG calculations.

- 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, … and contribute to better understanding of nuclear systems ...

Contact:
gabriel.wlazlowski@pw.edu.pl
http://wlazlowski.fizyka.pw.edu.pl

We have open call for post-doc position!

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

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