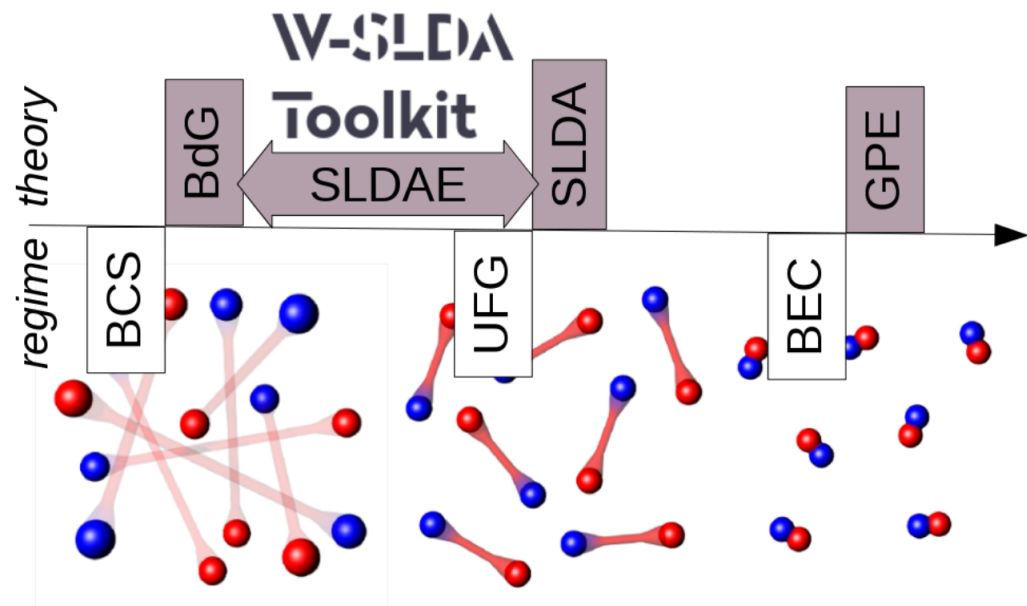




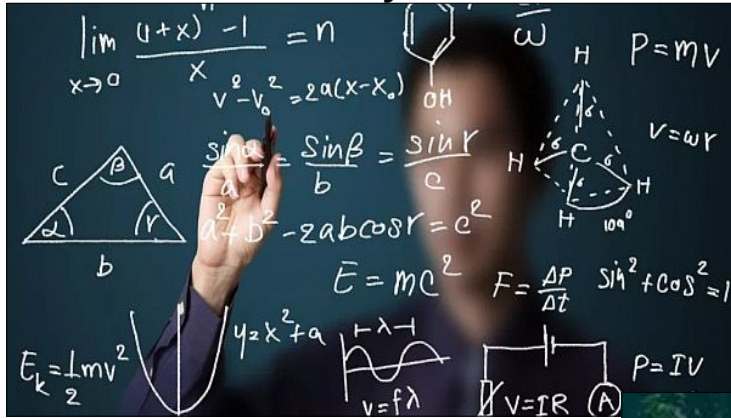
Ultracold atomic gases, neutron stars, and nuclei from the perspective of density functional theory

Gabriel Wlazłowski

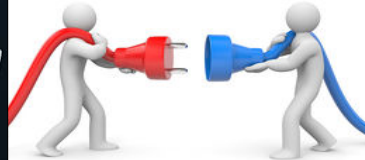
Warsaw University of Technology
University of Washington



Theory



Experiment



Overview:

1. Method \rightarrow DFT*
2. Implementation
3. Applications
4. Extensions to other systems



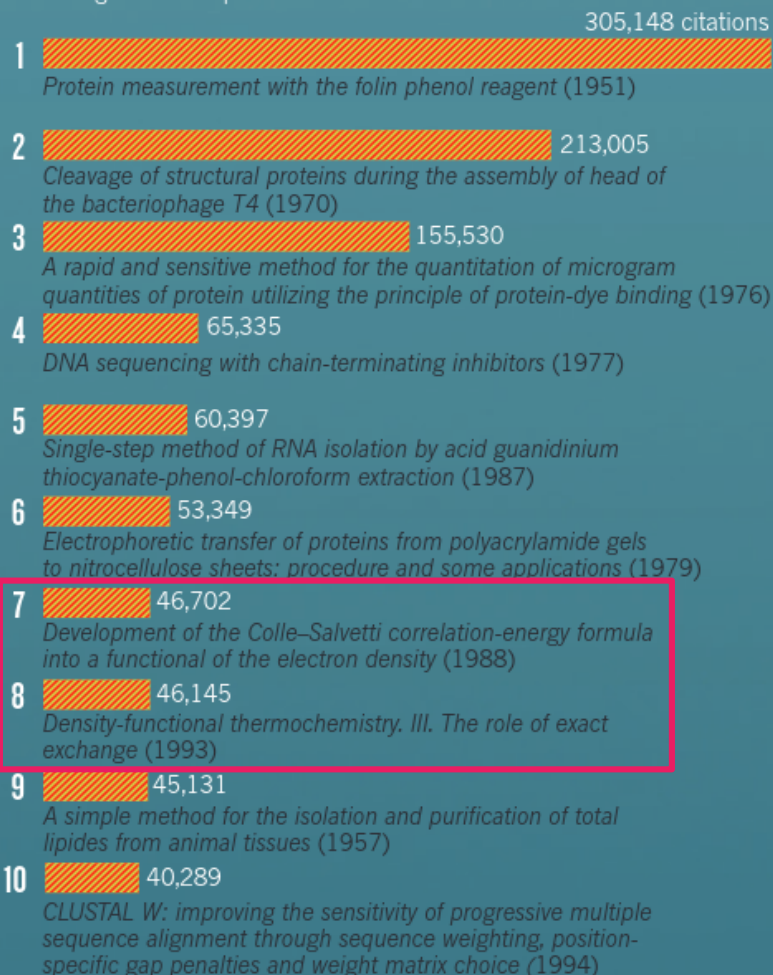
Computational physics

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

- *General purpose method* \rightarrow wide range of applicability
 \rightarrow typically it has numerical complexity at most as a mean-field method
(example for BECs: Gross-Pitaevskii equation)
- *Specialized methods* \rightarrow devoted to specific problems / quantities
 \rightarrow typically *ab initio* methods like QMC, ...

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.



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

Workhorse for ...

Solid-state physics

Quantum chemistry

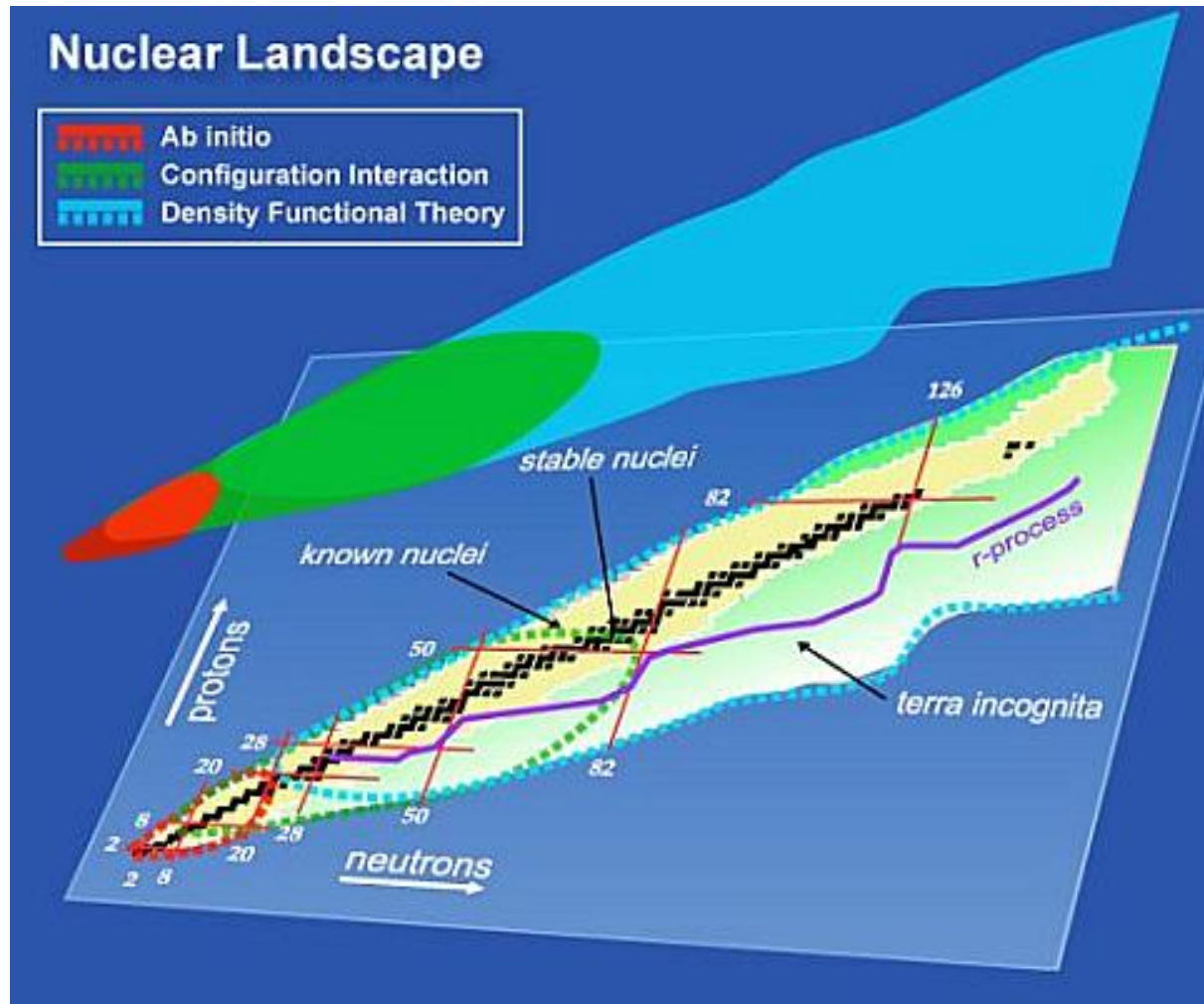
Condensed-matter physics

... also important tool for

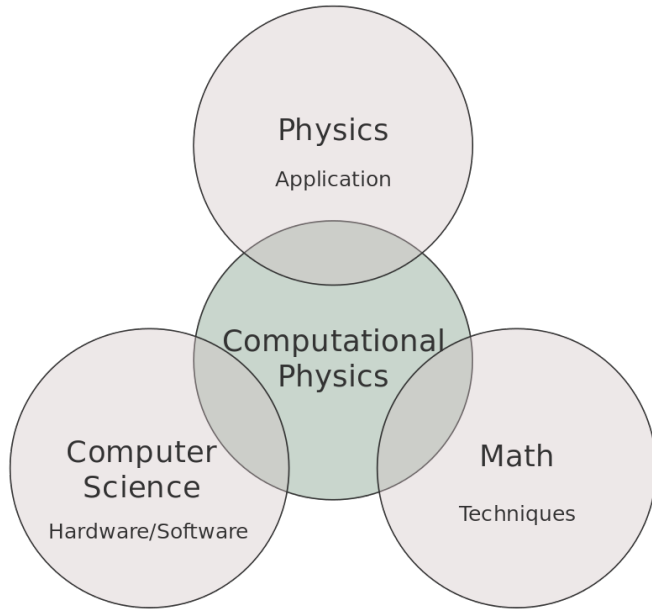
Nuclear physics

(Nuclear) astrophysics

...



DFT today is one of main tools of *computational physics*



From wiki pages:

https://en.wikipedia.org/wiki/Computational_physics

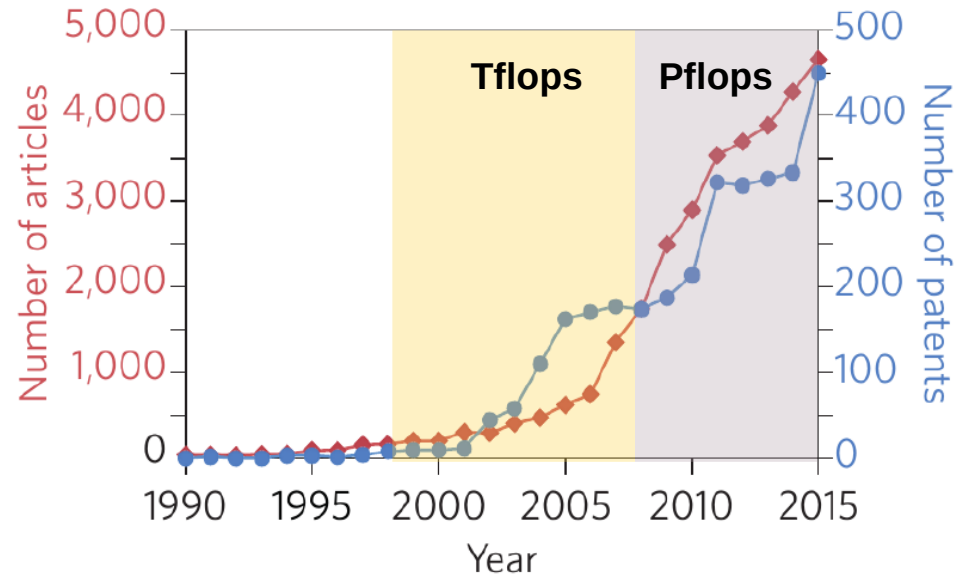



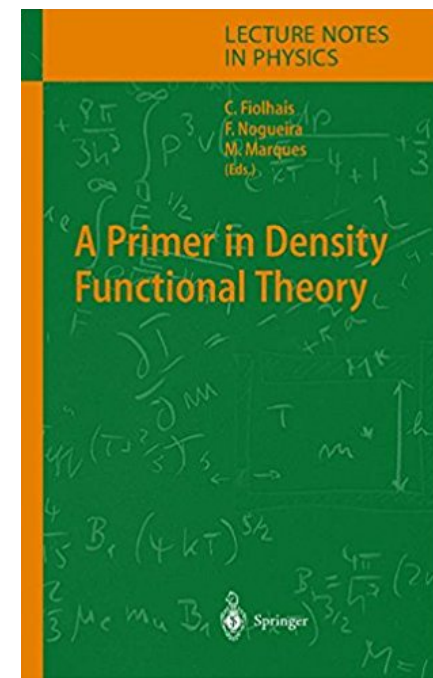
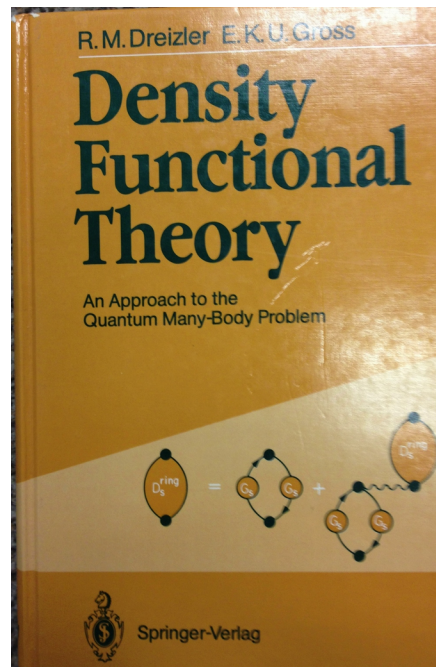
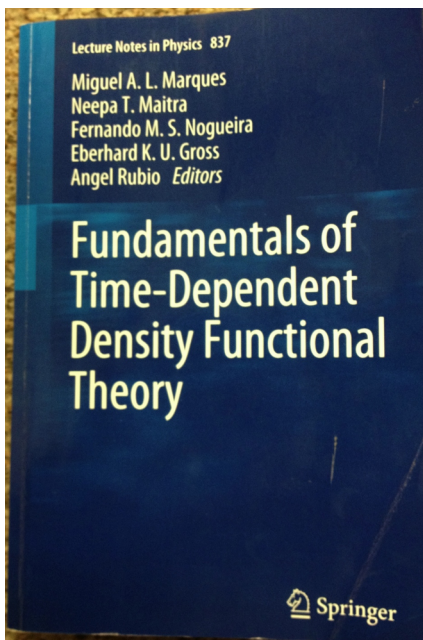
Figure 1: Number of articles and patents in materials science including the term “density functional theory” published per year during the past 25 years. Figure taken from *Boosting materials modelling*, Editorial article, *Nature Materials* **15**, 365 (2016).

Strong correlation with High Performance Computing (HPC) developments

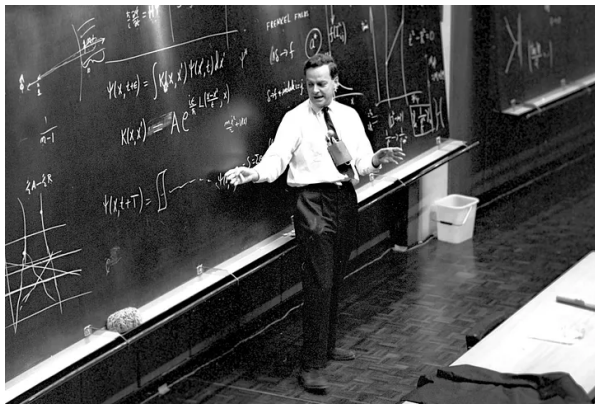


The Nobel Prize in Chemistry 1998 was divided equally between Walter Kohn "for his development of the density-functional theory" and John A. Pople "for his development of computational methods in quantum chemistry."

Credit: <https://www.nobelprize.org/>



- ◆ 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)



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 $\langle O \rangle = \langle \Psi[\rho] | O | \Psi[\rho] \rangle = O[\rho]$
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dimensional arguments, renormalizability, Galilean invariance, and symmetries
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numerical cost similar to mean-field method (here mean-field=BdG or HFB)

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

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

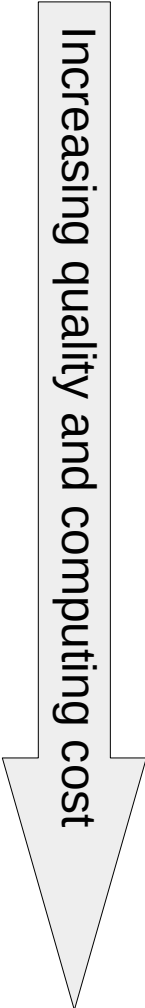
$$E_{\text{int}}[n] = T[n] + V[n] + \dots$$

- 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)

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

Generalized Gradient
Approximation (GGA)

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

Solving problem:

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

Classes of Energy Functionals

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Generalized Gradient Approximation (GGA)

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

Meta – GGA
(Kohn-Sham method)

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

...

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

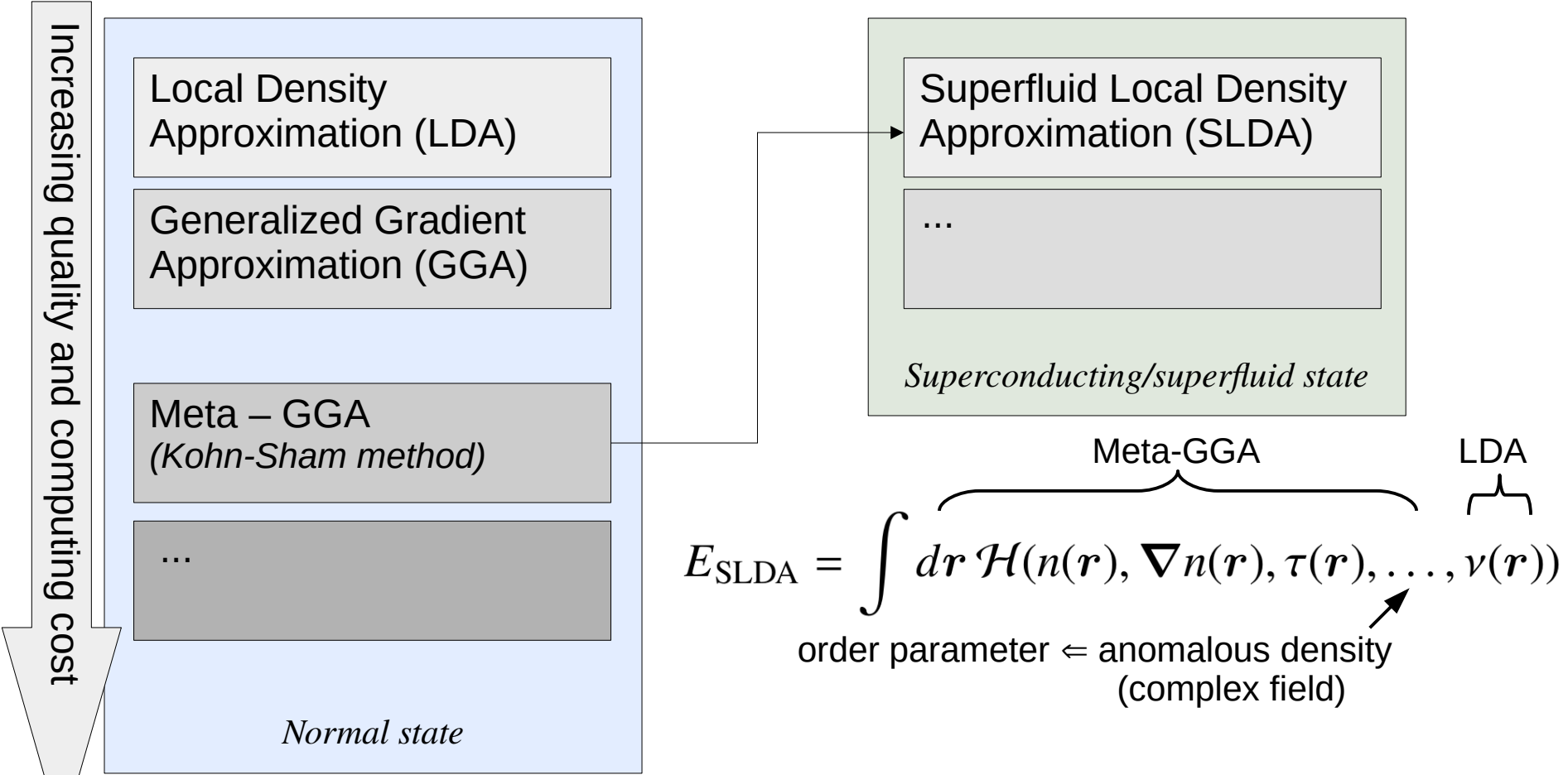
Solving problem:

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

Formally they have the same structure as HF equations

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

Classes of Energy Functionals



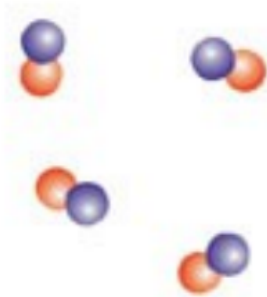
Density-Functional Theory for Superconductors

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

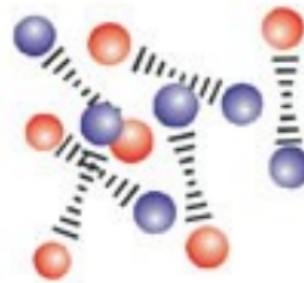
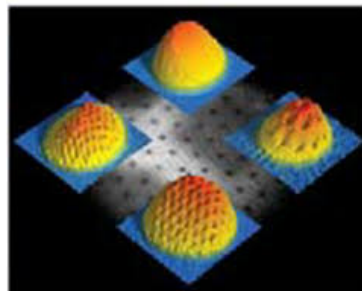


- ◆ **Ultracold atomic** systems offer possibility to test predictive power of TDDFT.
- ◆ The (bare) interaction is simple $V(\mathbf{r}-\mathbf{r}')=g\delta(\mathbf{r}-\mathbf{r}')\dots$
- ◆ ... but the interaction strength g can be tuned at will!

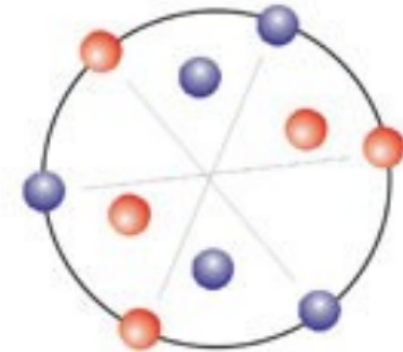
BEC ← **CROSSOVER** → **BCS**



diatomic molecules



strongly interacting pairs



Cooper pairs



SLDA-type functional for ultracold atoms

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

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

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

+ orthonormality condition

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

current density

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

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

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
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SLDA-type functional for ultracold atoms

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

minimization

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

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

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

Jargon:

BCS → for uniform systems

Bogoliubov-de-Gennes (BdG) →

generalization of BCS to non-uniform systems, coordinate basis

Hartree-Fock-Bogoliubov (HFB) →

generalization to arbitrary basis

For example, BdG is equivalent to

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

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

SLDA-type functional

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

Dimensionless
functional parameters

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

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

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

*dimensional analysis +
symmetries*

Kinetic
term

Potential
term

Pairing
term

Center of
mass motion

SLDA-type functional

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dimensional analysis + symmetries

Kinetic term

Potential term

Pairing term

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

$$A_\lambda \rightarrow 1$$

$$B_\lambda \rightarrow 0$$

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

ASLDA

Asymmetric SLDA, $a \rightarrow \infty$

$$A_\lambda \rightarrow A[p(\mathbf{r})]$$

$$B_\lambda \rightarrow B[p(\mathbf{r})]$$

$$C_\lambda \rightarrow C[p(\mathbf{r})]$$

SLDAE

SLDA Extended, $p=0$

$$A_\lambda \rightarrow A[ak_F(\mathbf{r})]$$

$$B_\lambda \rightarrow B[ak_F(\mathbf{r})]$$

$$C_\lambda \rightarrow C[ak_F(\mathbf{r})]$$

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

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

SLDA-type functional

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

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*dimensional analysis +
symmetries*

Kinetic term

$+\infty$

Pairing term

$-\infty$

*The functional is useless without
the regularization procedure!*

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

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

- 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 by

Local density approximation for systems with pairing correlations

Aurel Bulgac

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

→ *ab initio* calcs for $E/E_{\text{FG}}, \Delta/\varepsilon_F, m^*/m$
→ limiting cases (EFT, scale invariance, ...)

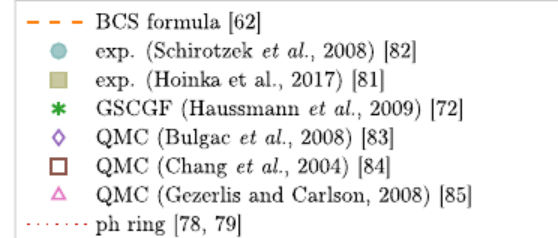
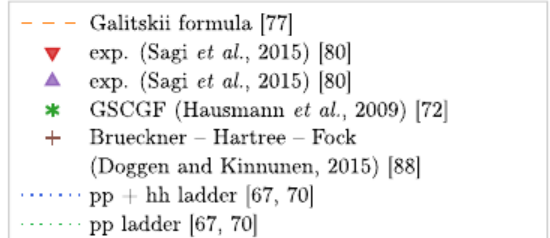
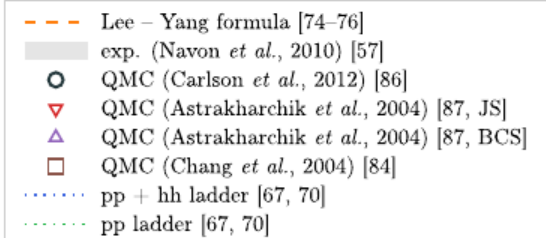
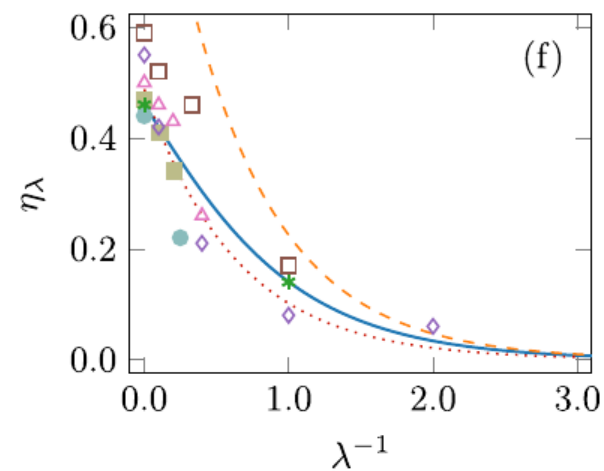
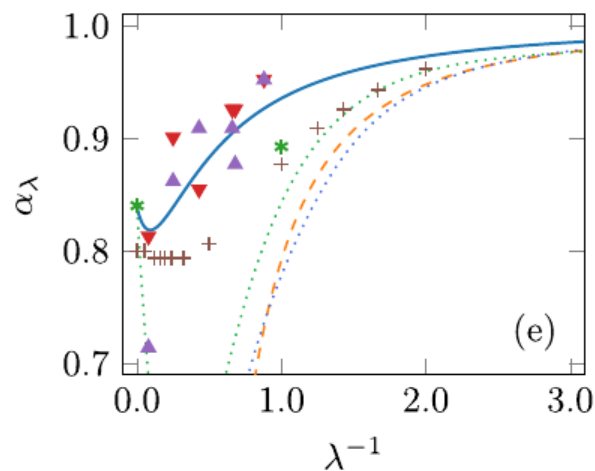
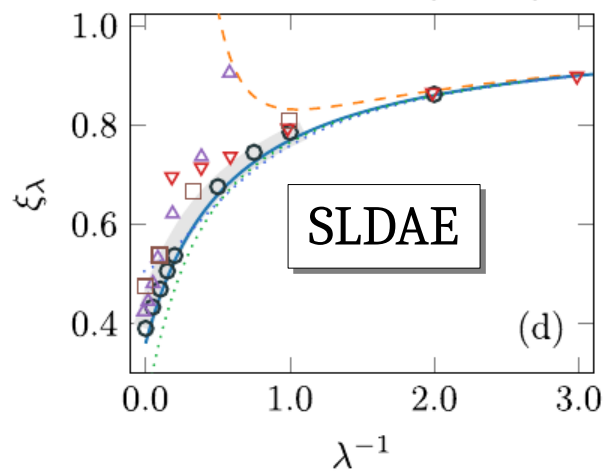
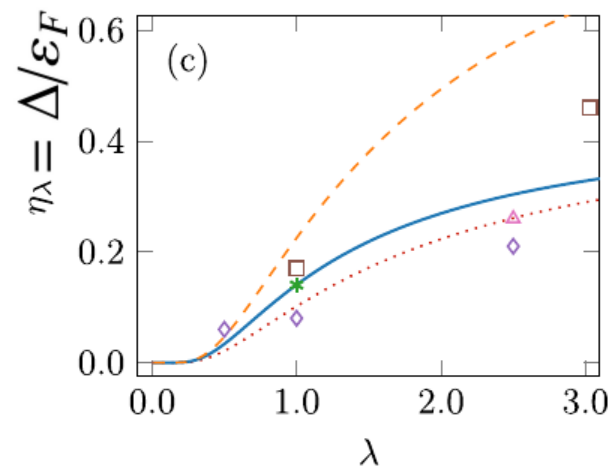
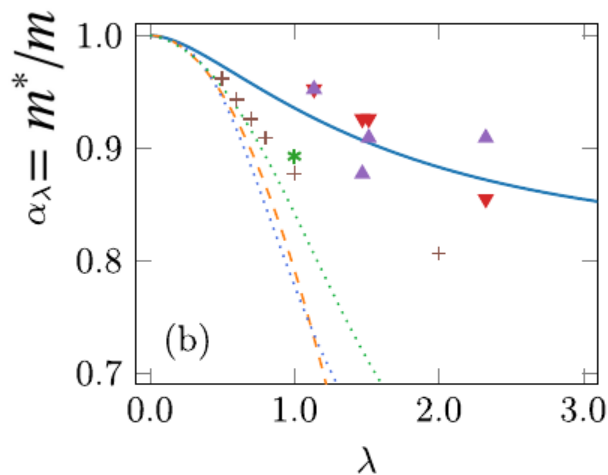
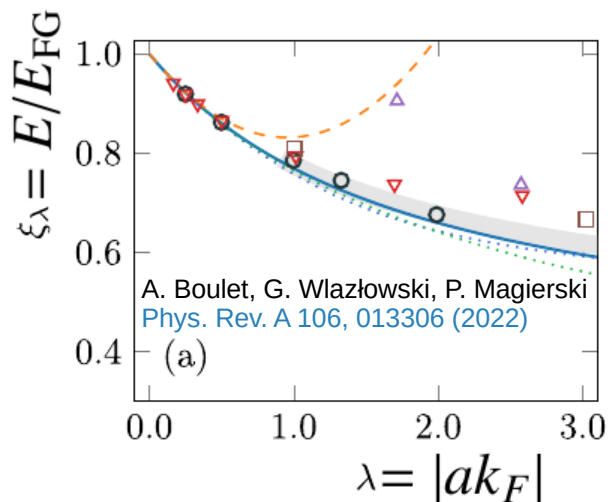
INDUCE

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

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

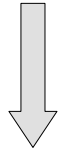
INDUCE

Functional parameters
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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

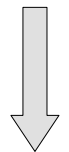
Phys. Rev. Lett. **73**, 2915 – Published 21 November 1994

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

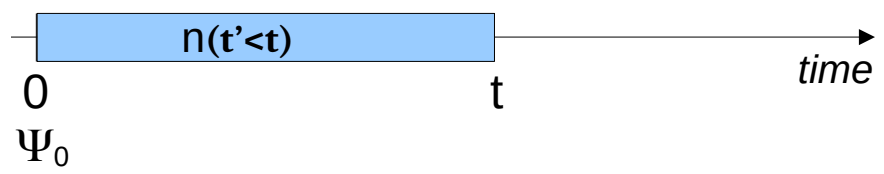
$$\begin{pmatrix} h_{\uparrow}(\mathbf{r}) - \mu_{\uparrow} & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -h_{\downarrow}^*(\mathbf{r}) + \mu_{\downarrow} \end{pmatrix} \begin{pmatrix} u_{n,\uparrow}(\mathbf{r}) \\ v_{n,\downarrow}(\mathbf{r}) \end{pmatrix} = E_n \begin{pmatrix} u_{n,\uparrow}(\mathbf{r})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



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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

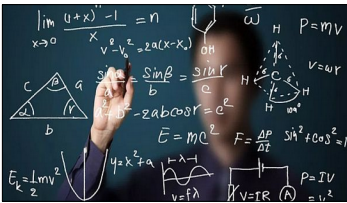
$$E(t) = \int_0^t dt' \int_V d\mathbf{r} \mathcal{E}[\Psi_0, n(\mathbf{r}, t'), \dots]$$

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

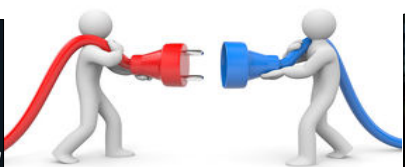
... but for time-dependent case the “exact” functional is in general different from the one that is used in static calculations...

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

Theoretical method

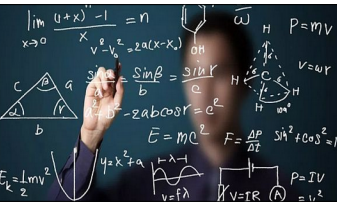


Experiment



Computer code

Theoretical method



Experiment



Computer code

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

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

time-dependent problems: td-wslda

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

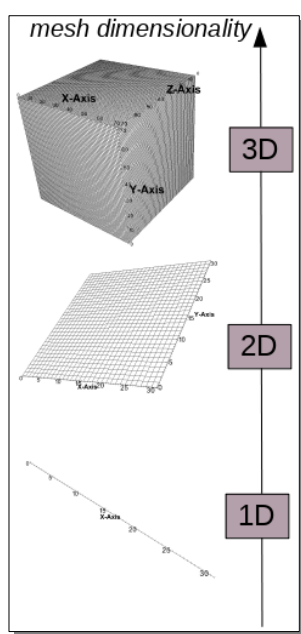


can run on "small" computing clusters as well as leadership supercomputers
 (depending on the problem size)



High Performance Computing





- 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

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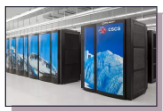
$$\begin{pmatrix} h_a(\mathbf{r}) - \mu_a & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -h_b^*(\mathbf{r}) + \mu_b \end{pmatrix} \begin{pmatrix} u_n(\mathbf{r}) \\ v_n(\mathbf{r}) \end{pmatrix} = E_n \begin{pmatrix} u_n(\mathbf{r}) \\ v_n(\mathbf{r}) \end{pmatrix}$$

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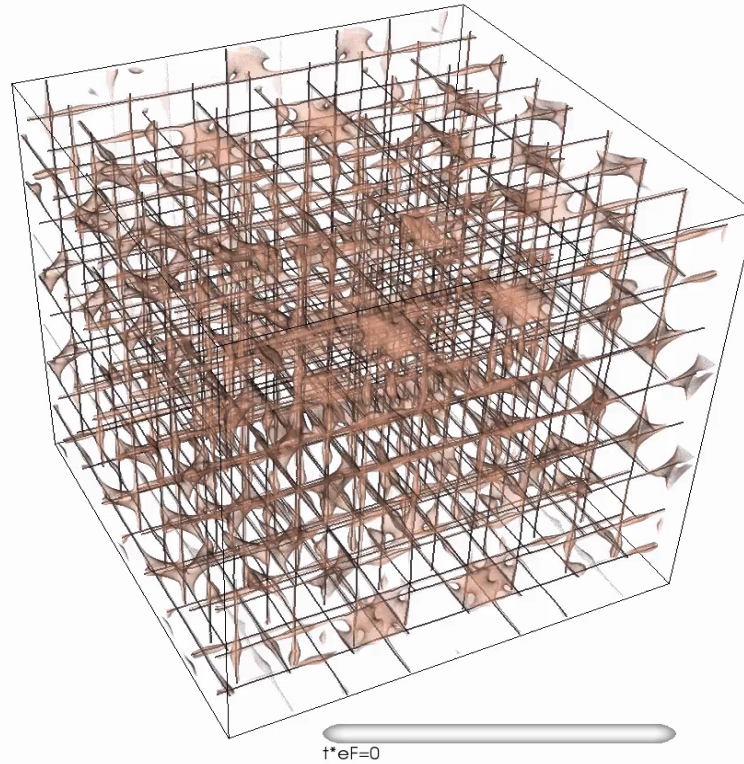
High
Performance
Computing



AMD
ROCm



PHYSICS.WUT



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

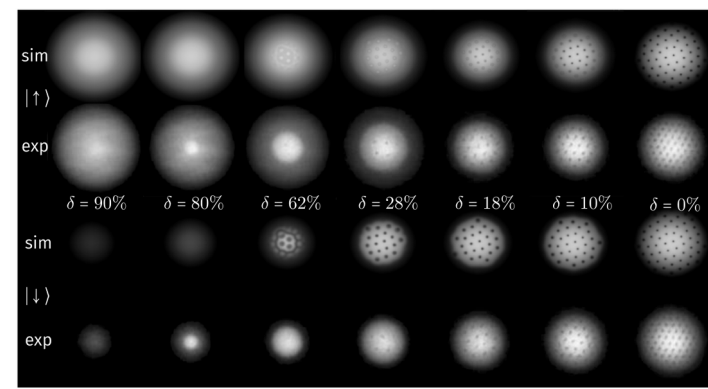
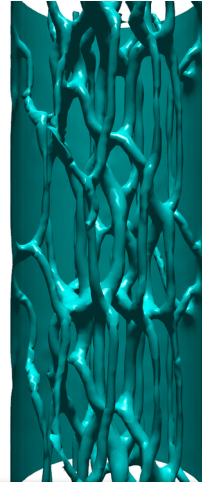
PRELIMINARY:
quantum turbulence
in the unitary Fermi gas



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)

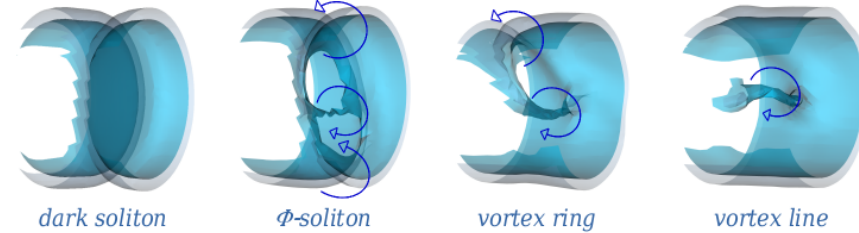


- Quantum turbulence

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

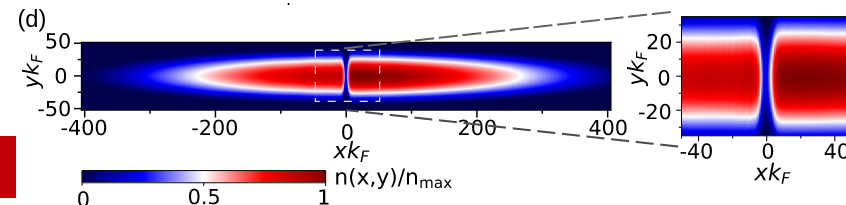
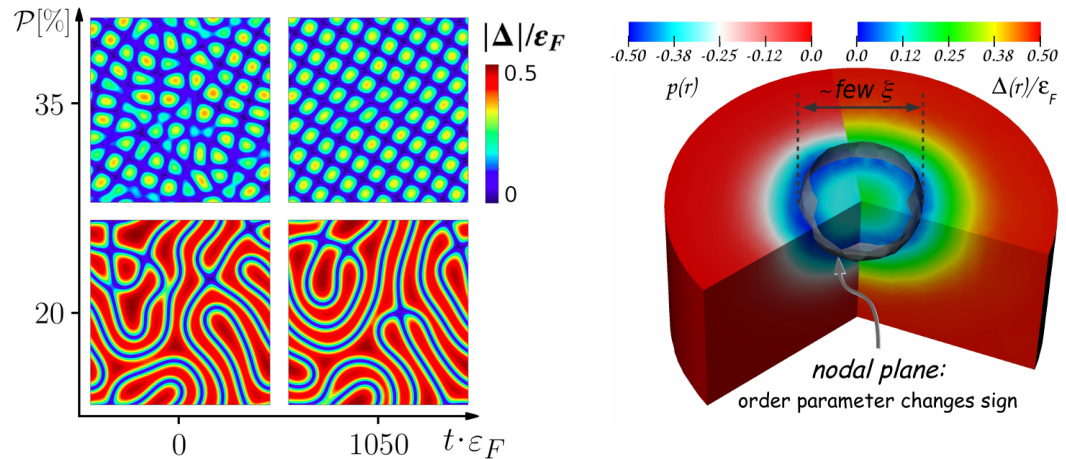
arXiv:2303.13394 (2023)

- Josephson junction

Phys. Rev. Lett. 130, 023003 (2023)

- Phase diagram of spin-imbalanced systems

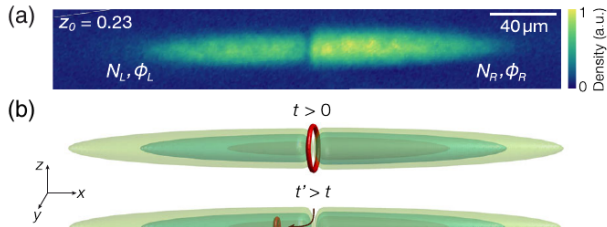
New J. Phys. 25, 033013 (2023)



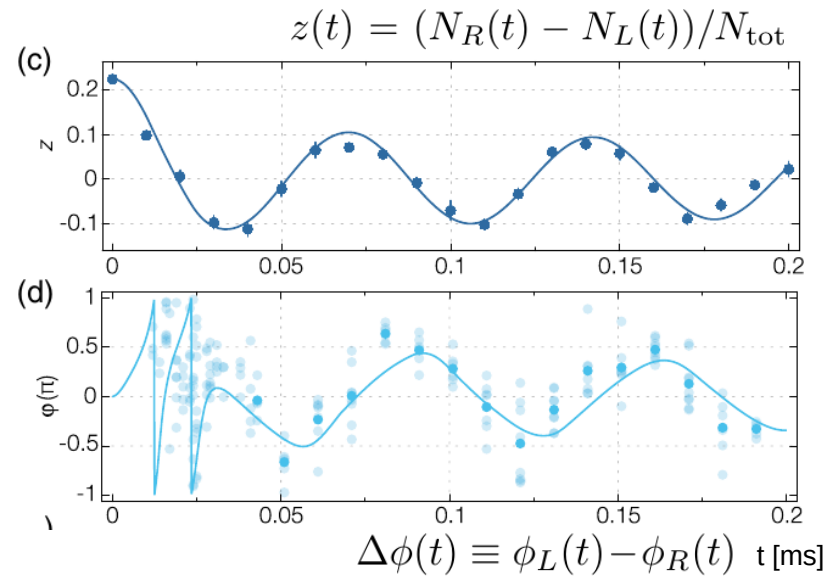
Example: Fermionic Josephson Junction

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]



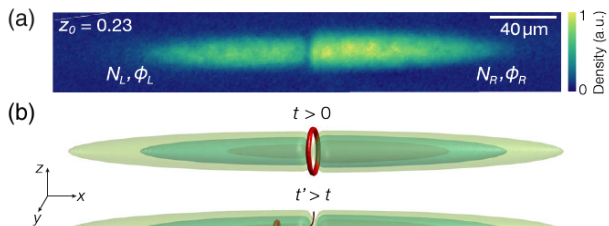
Experiment

Simulation

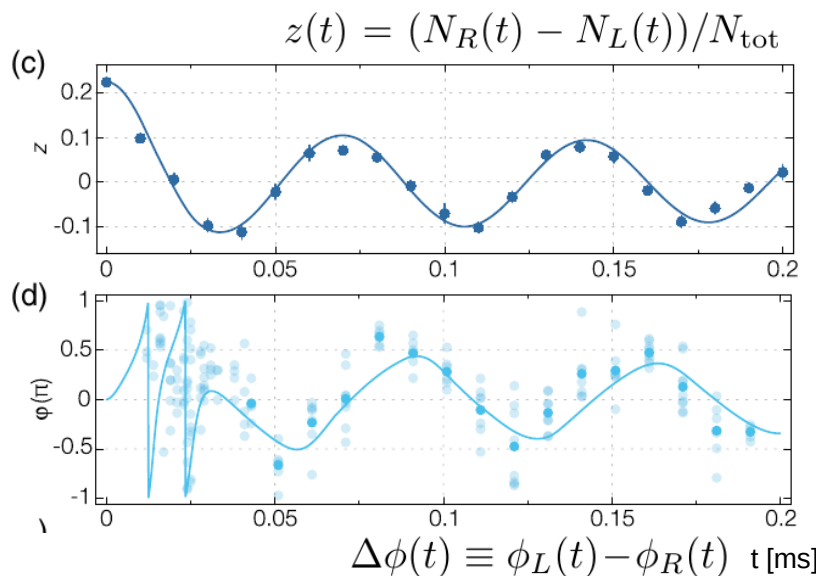
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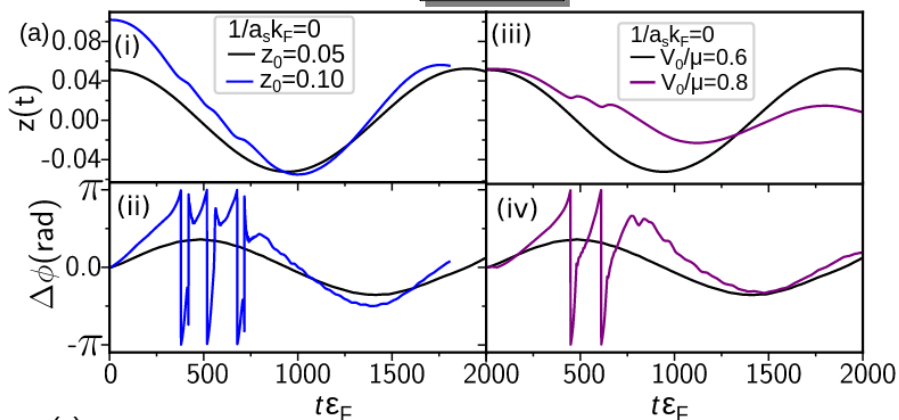
Figs from [2]



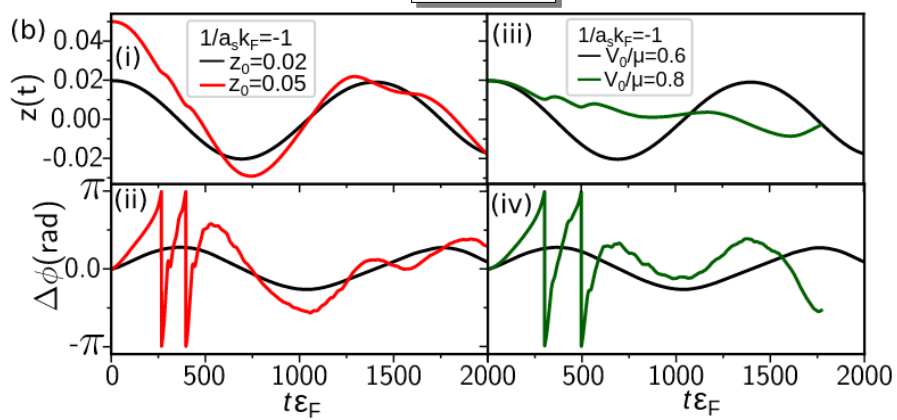
Experiment

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

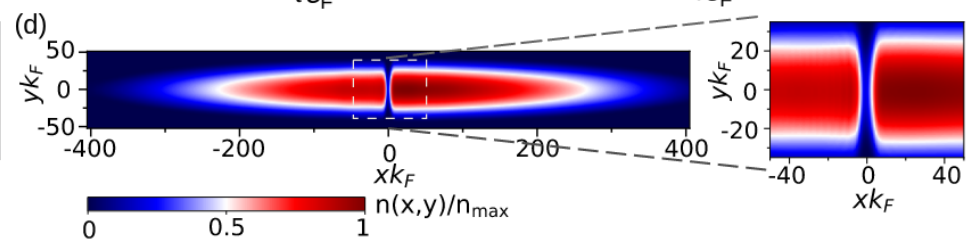
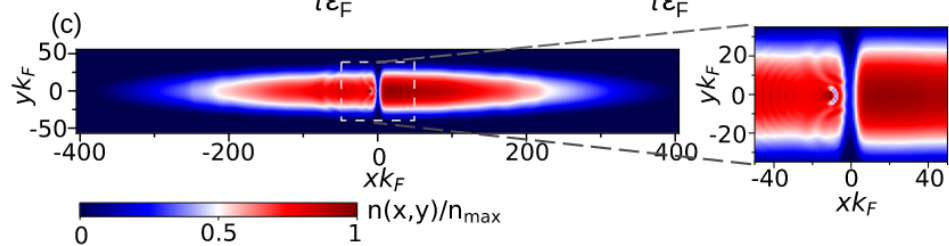
UFG



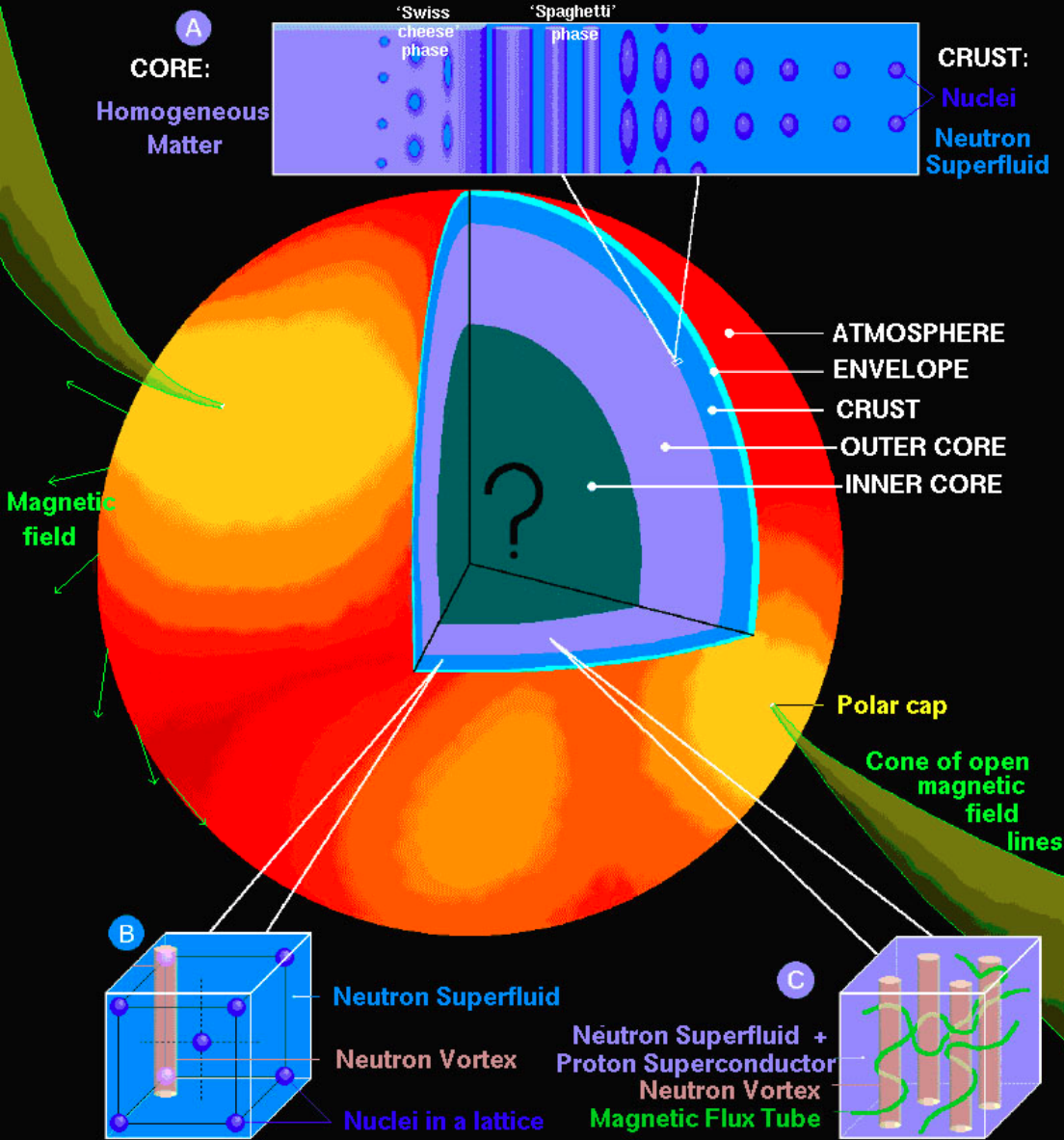
BCS



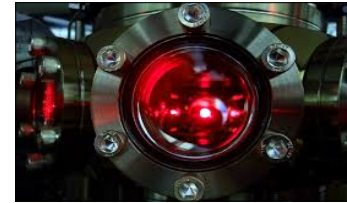
Simulation



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

Brussels-Montreal Skyrme functionals (BSk)

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

Experimental data:

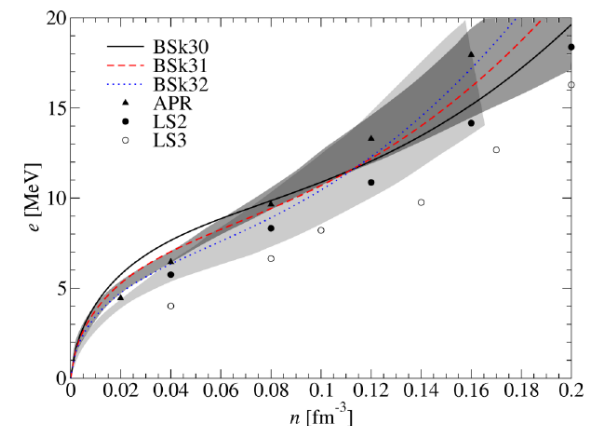
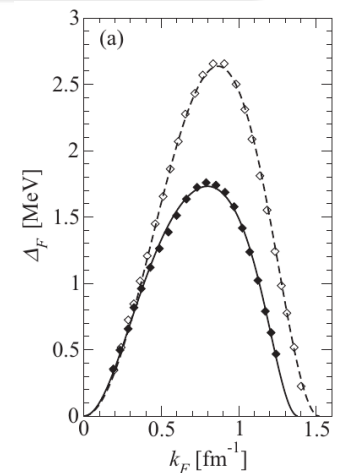
- all atomic masses with $Z, N \geq 8$ from the Atomic Mass Evaluation (root-mean square deviation: 0.5-0.6 MeV)

<http://www.astro.ulb.ac.be/bruslib/>

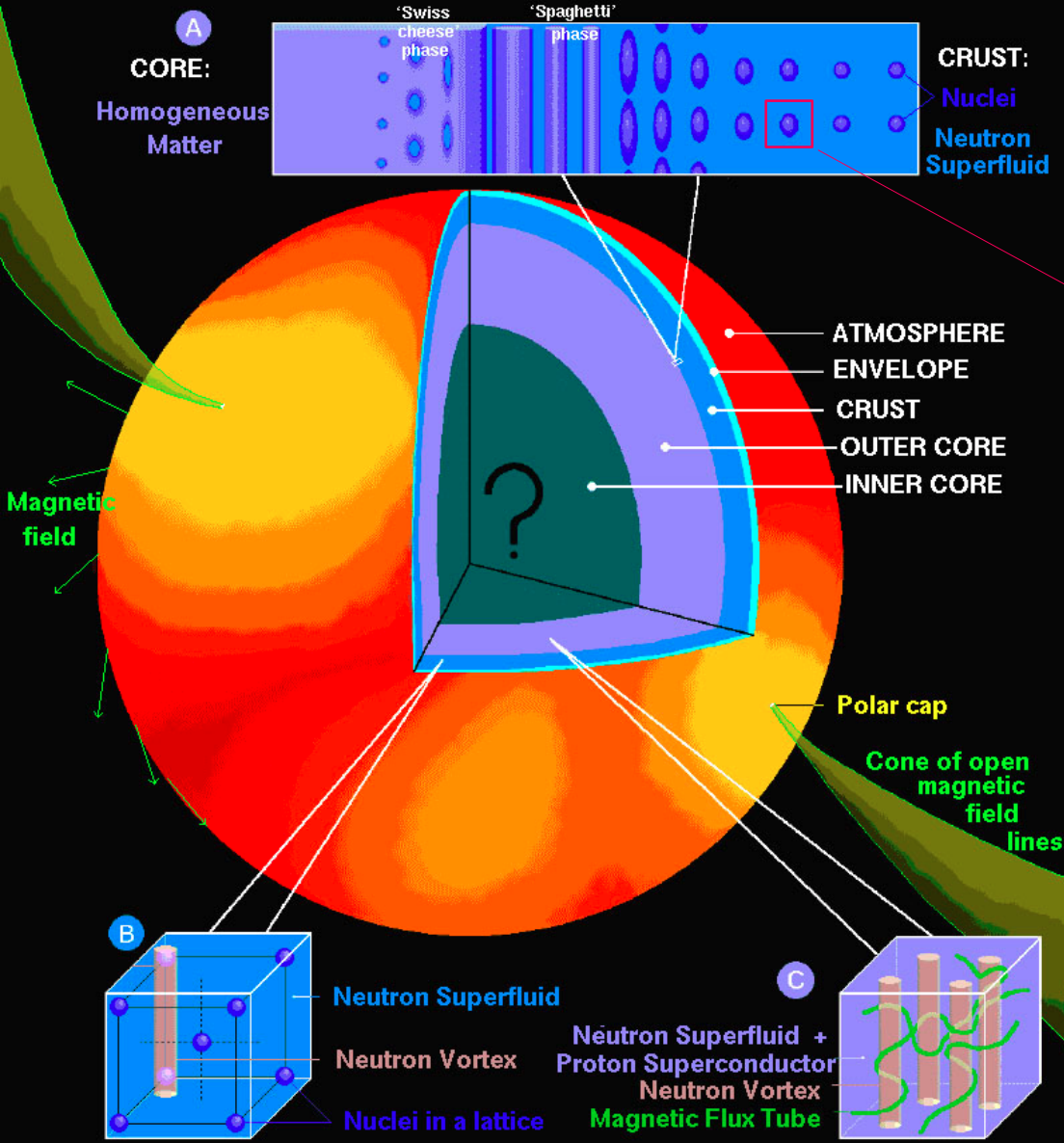
- charge radii
- incompressibility $K_V = 240 \pm 10$ MeV (ISGMR)
Colò et al., Phys.Rev.C70, 024307 (2004).

N-body calculations using realistic forces:

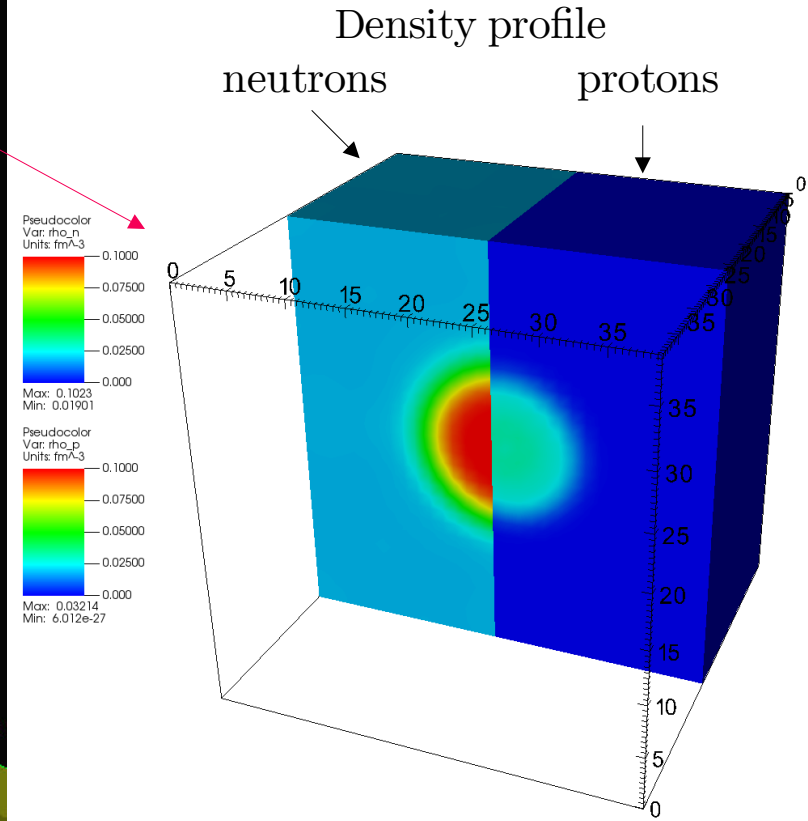
- equation of state of pure neutron matter
- 1S_0 pairing gaps in nuclear matter
- effective masses in nuclear matter



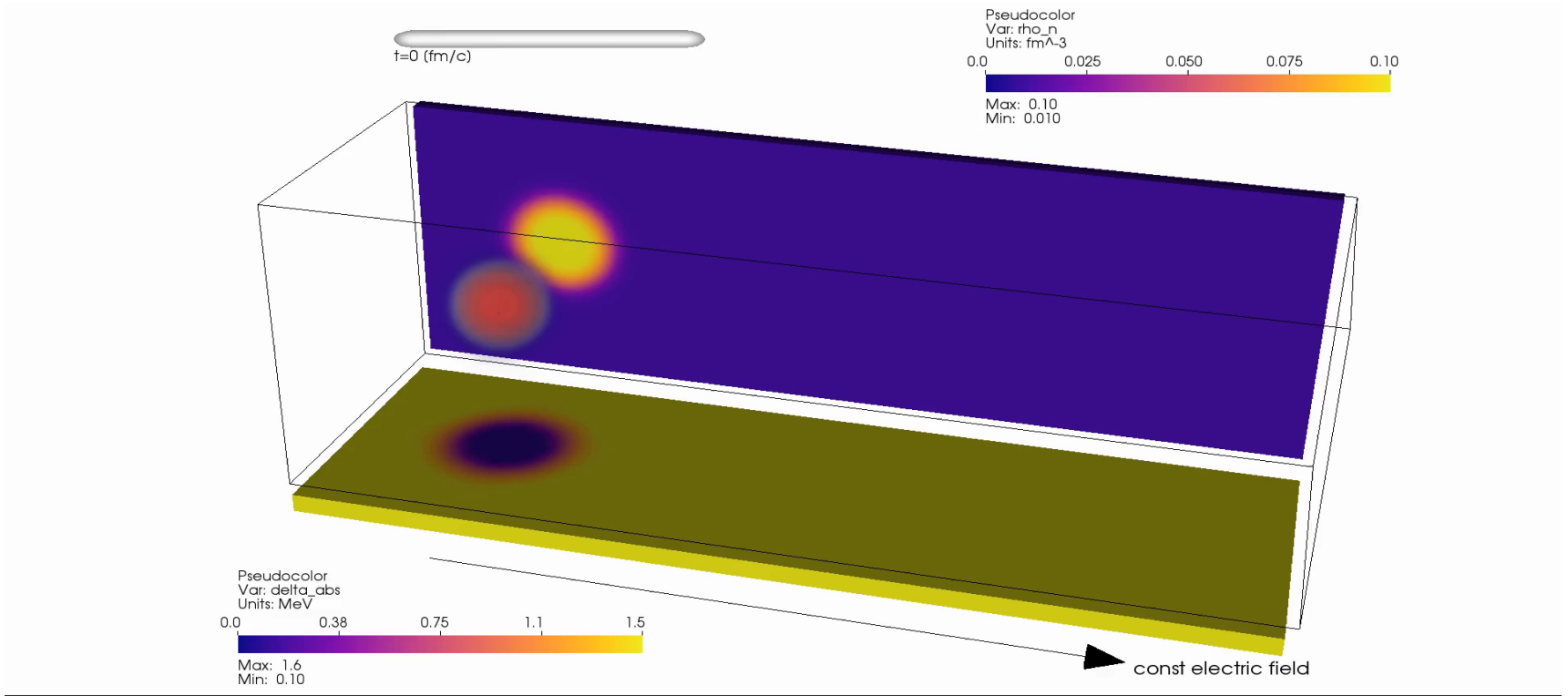
A NEUTRON STAR: SURFACE and INTERIOR



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



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



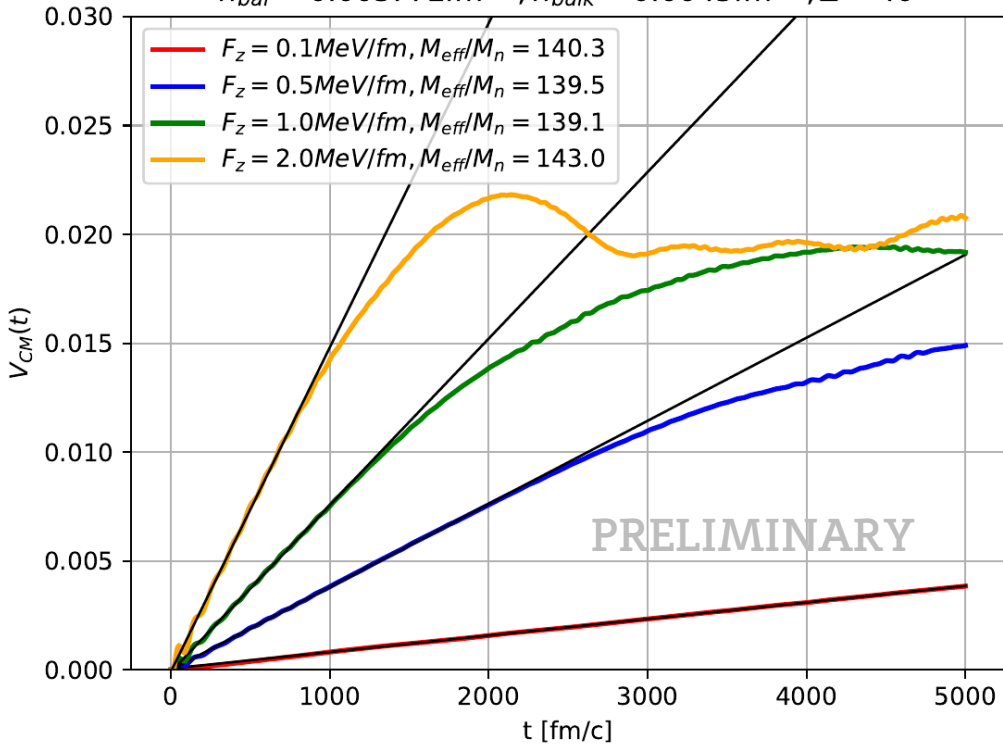
System: *nuclear matter*
 3D simulation 40 x 40 x 120 [fm]

number of neutrons: 2,104
 number of protons: 40

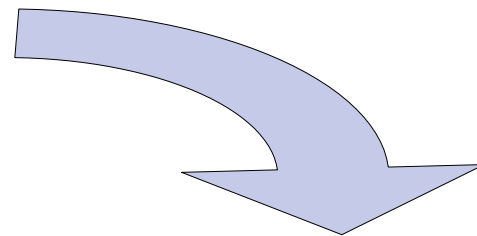
W-BSK

PRELIMINARY:
 response of nuclear impurity to
 uniform electric field

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

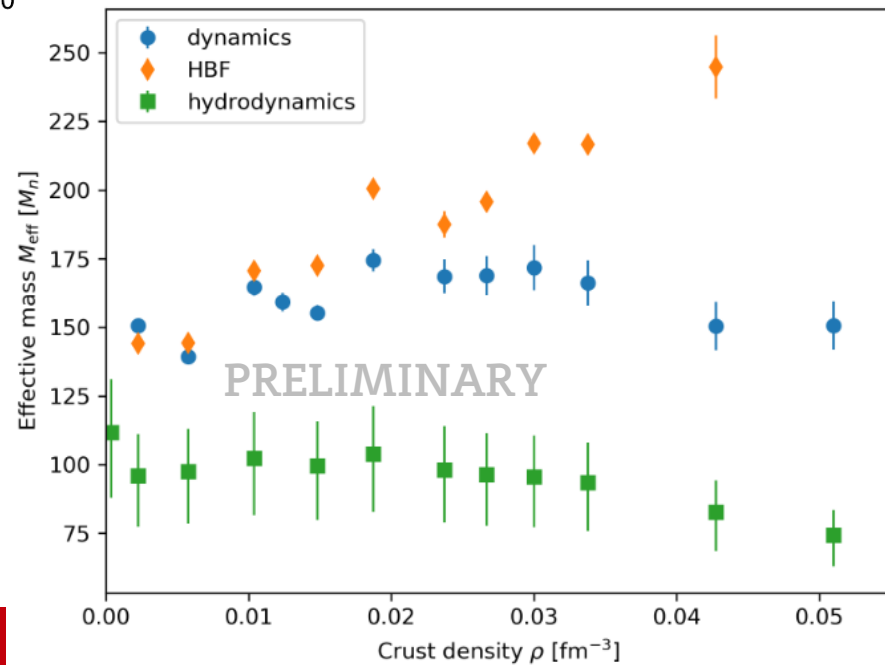


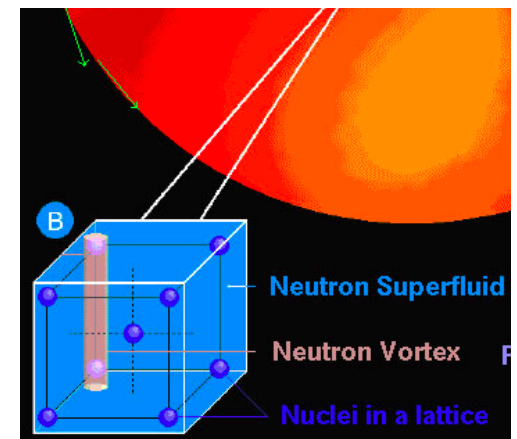
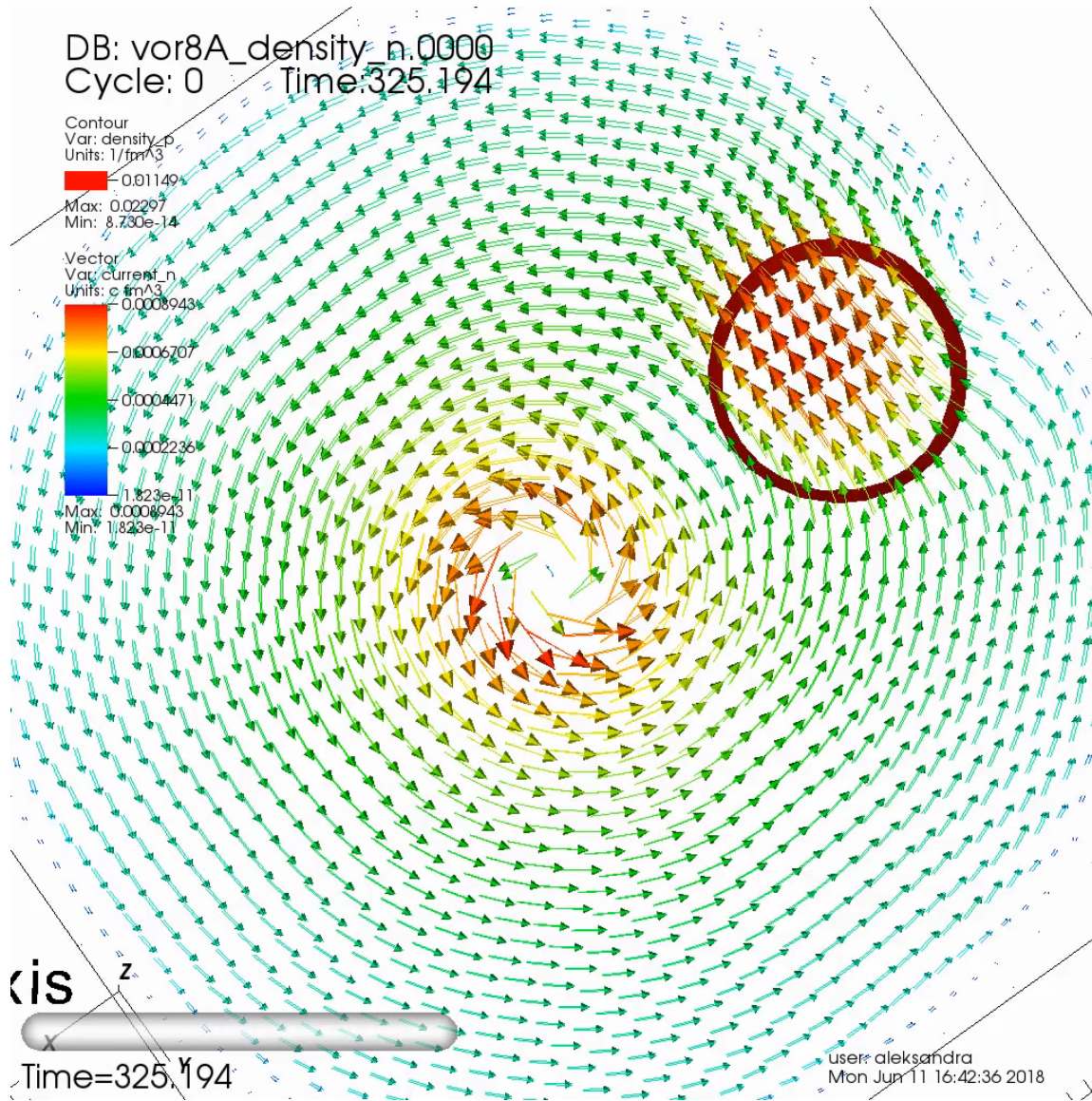
Example of application:
 → extraction of parameters
 for effective theories of
 neutron star crust.



$Z e E = F = M a$

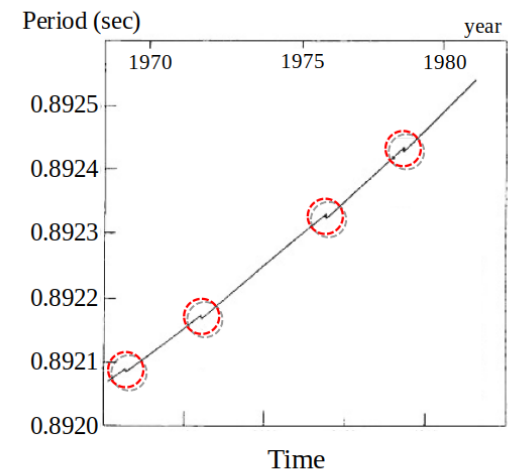
control parameter

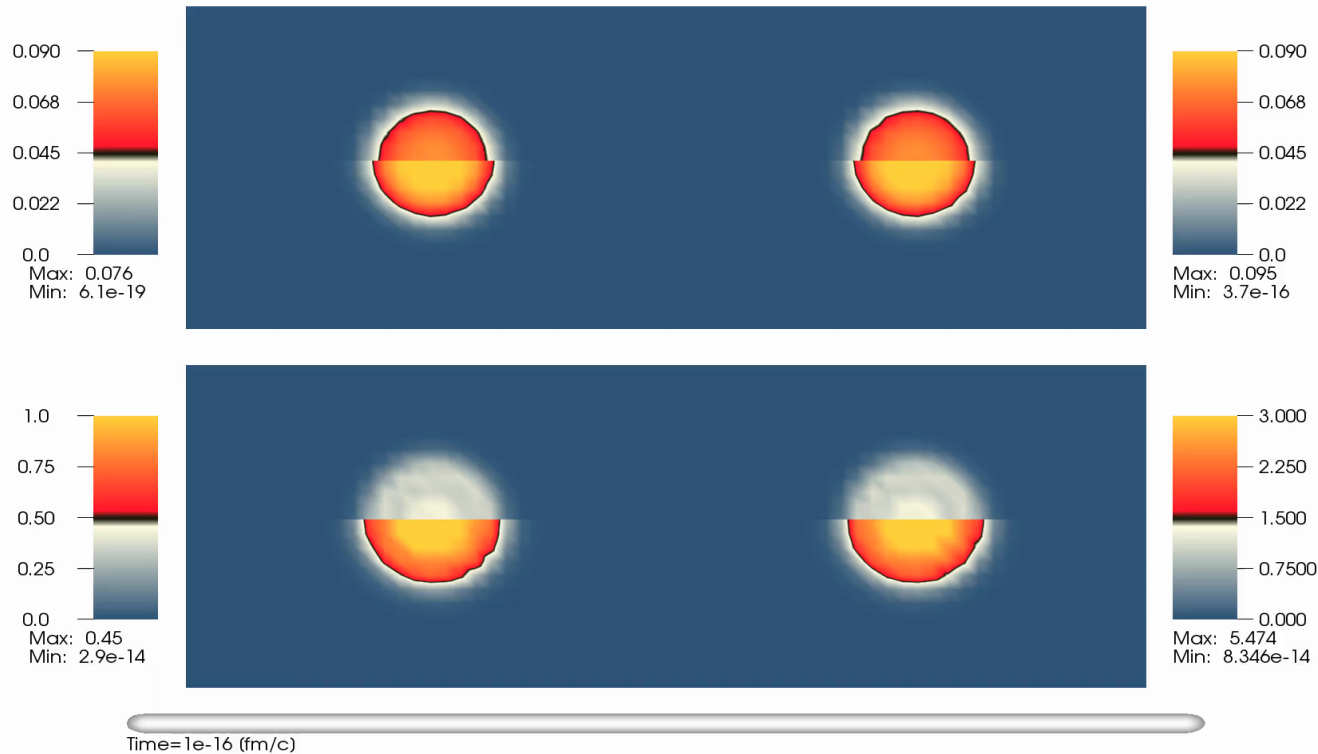




System: nuclear in presence of quantum vortex

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





Reaction: $^{96}\text{Zr}+^{96}\text{Zr}$, SkM^* , $E_{cm}=178\text{MeV}$, head-on collision

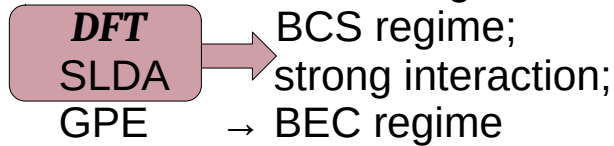
P. Magierski, A. Makowski, M.C. Barton,
K. Sekizawa, and G. Wlazłowski
Phys. Rev. C 105, 064602 (2022)

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

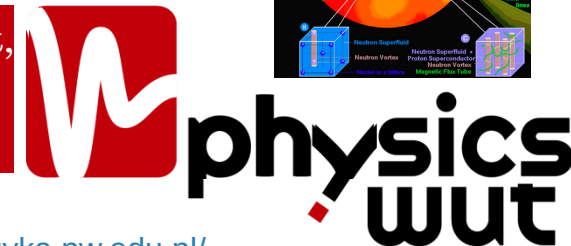
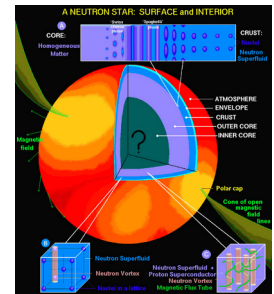
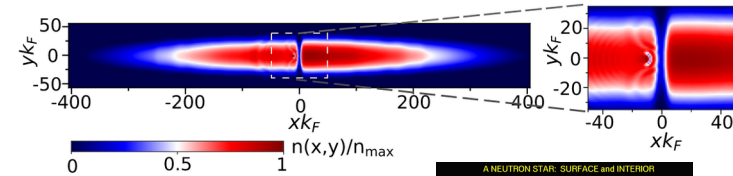
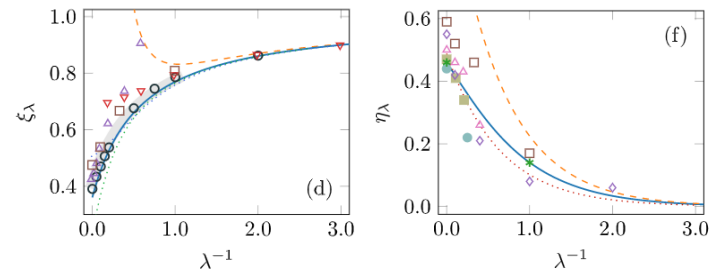
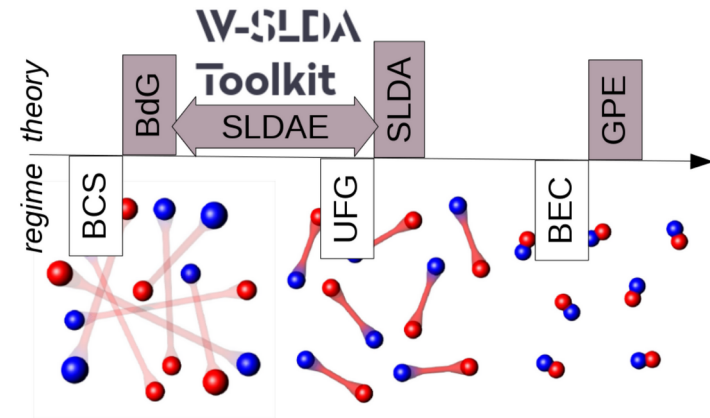
→ ... however various complications arise
(as compared to ultracold atoms or nuclear matter)

SUMMARY

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



- DFT is general purpose method: it overcomes limitations of mean-field approach, 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 ...



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

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