# Density functional theory for superfluid Fermi systems: an overview of recent developments

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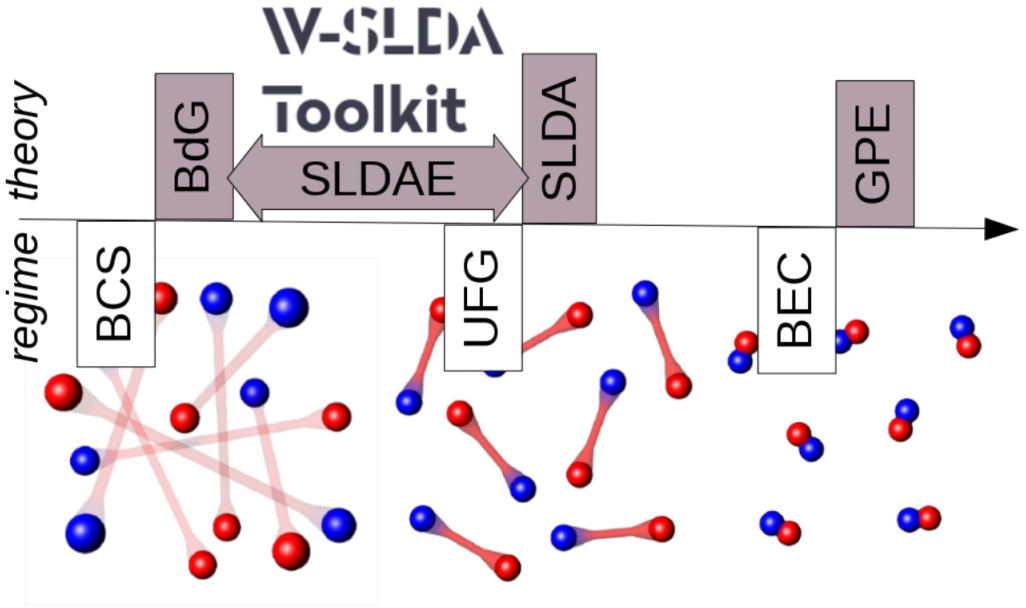
University of Washington

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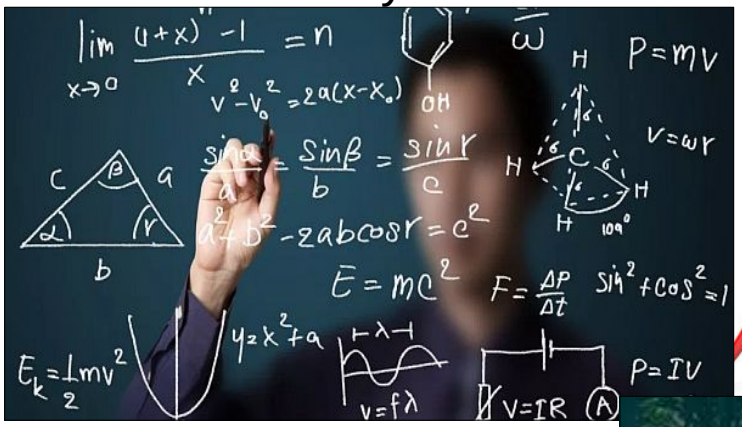
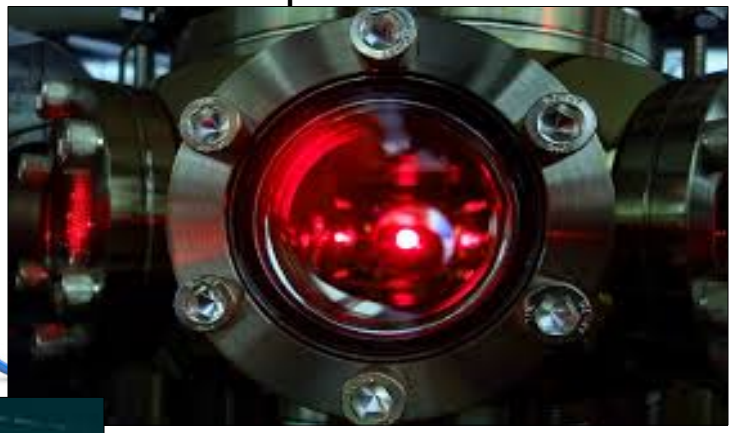
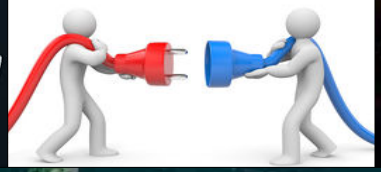
Theory




Experiment





Computational physics

*Overview:*
1. *Method → DFT**
2. *Implementation*
3. *Applications*
4. *Extensions to other systems*

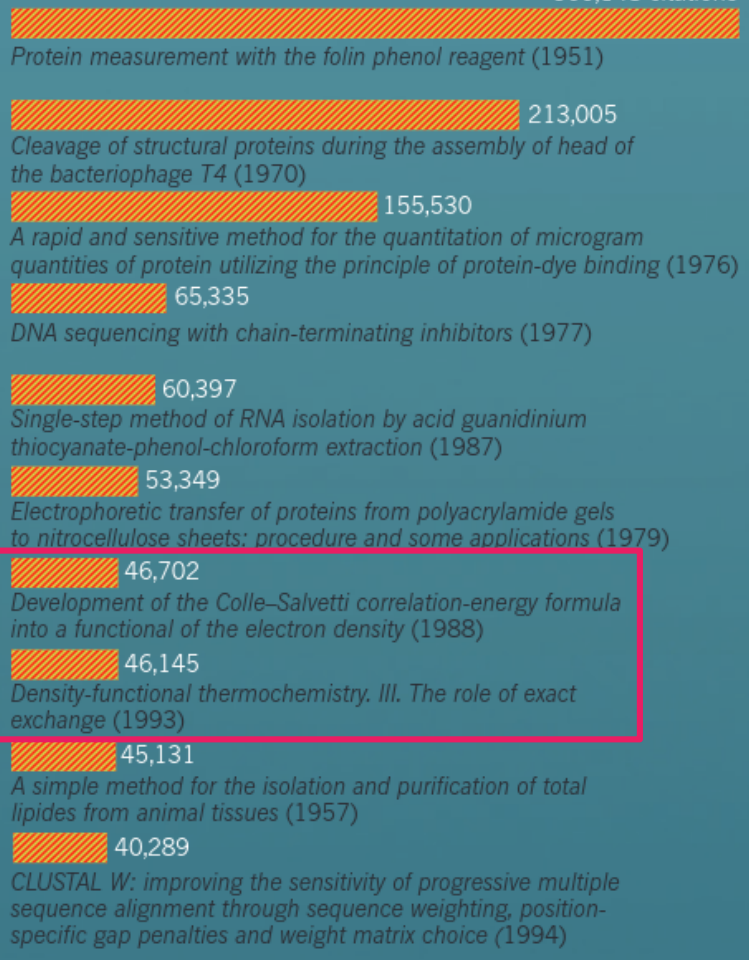
*(*) Note: Many formal aspects of the theory will be presented superficially. Only general formulas...*

- *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, ...

## 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.




NEWS FEATURE

# 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.

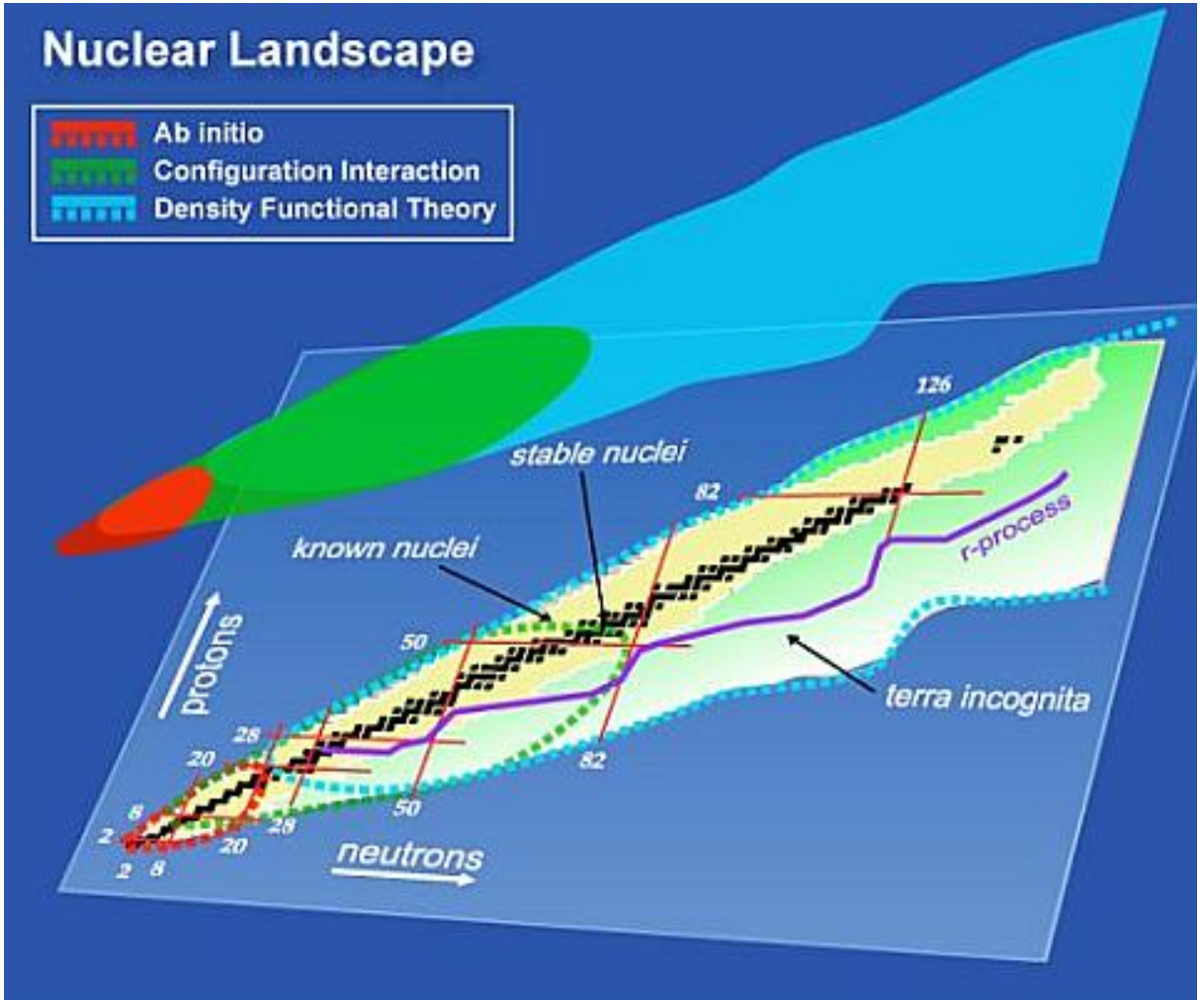
Most of this software is built on density functional theory (DFT), easily the most heavily cited concept in the physical sciences. Twelve papers on the top-100 list relate to it, including 2 of the top 10. At its heart, DFT

**Workhorse for ...**

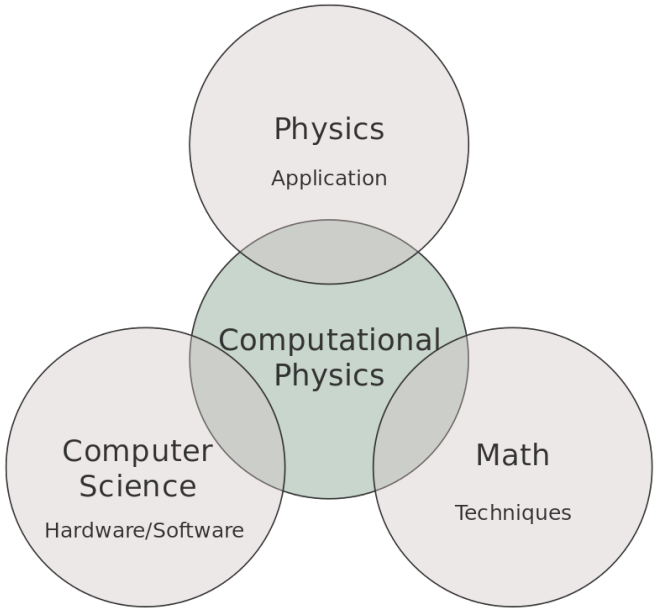
- Solid-state physics
- Quantum chemistry
- Condensed-matter physics

**… 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

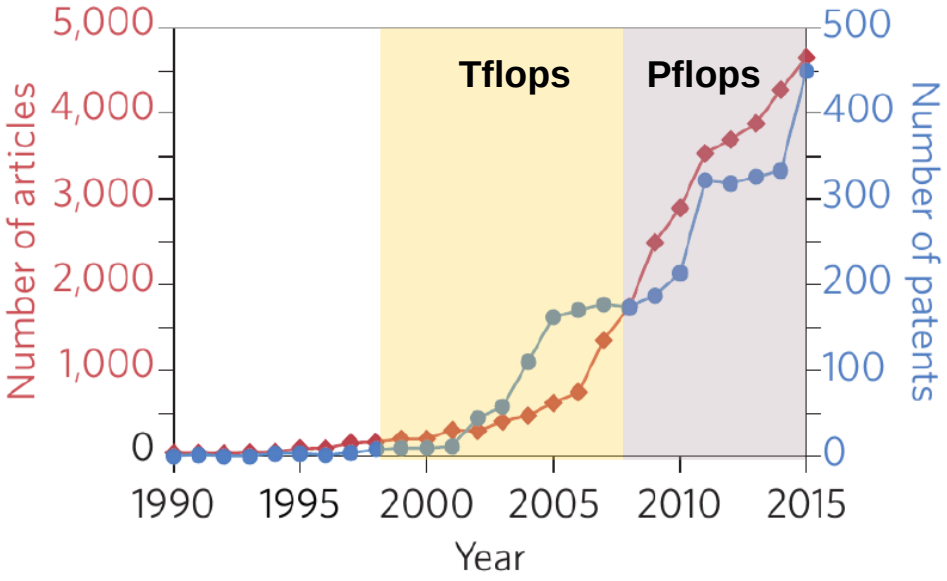


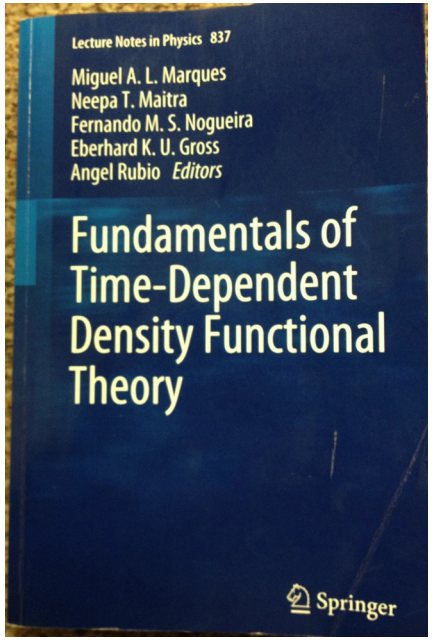

Figure 1: Number of articles and patents in materials science including the term "density functional theory" published per year during the past 25 years. Figure taken from

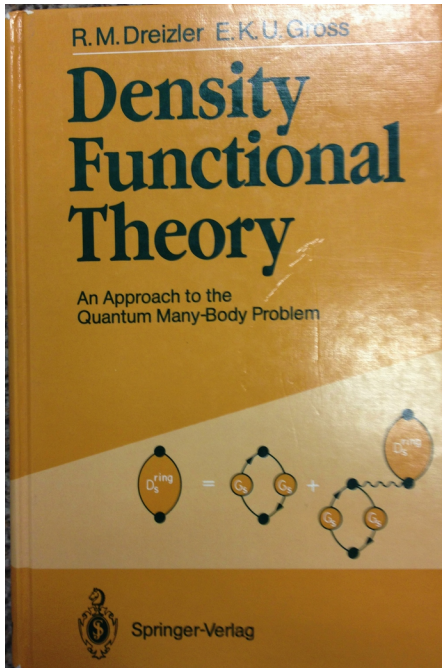
*Boosting materials modelling*,
Editorial article, Nature Materials **15**, 365 (2016).

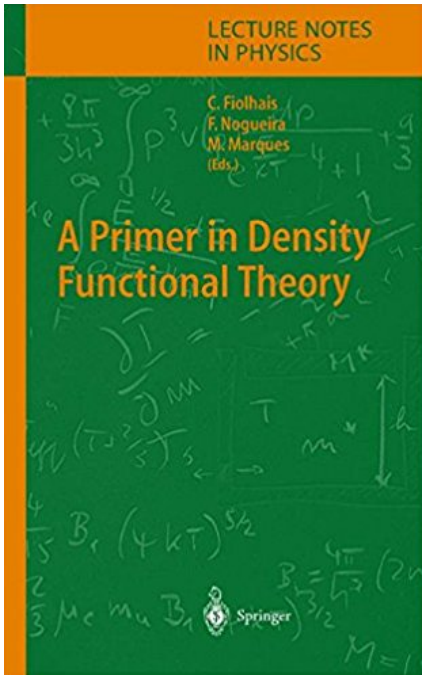
The Nobel Prize in Chemistry 1998 was divided equally between Walter Kohn "for his development of the density-functional theory" and John A. Pople "for his development of computational methods in quantum chemistry."

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 ↔ 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)

# Density Functional Theory – Idea

It can be shown that **instead of *wave function*** one may use a **density** distribution:

*contains vastly more information than the one needs*

$$\rho_1(\mathbf{x}_1, \mathbf{x}_1') = N \int \Psi(\mathbf{x}_1, \ldots, \mathbf{x}_N)\Psi(\mathbf{x}_1', \ldots, \mathbf{x}_N)^* d\mathbf{x}_2 \cdots d\mathbf{x}_N$$

*reduced object - sufficient to extract one body observables*

**Theorem (Hohenberg & Kohn):**
**The energy of the nondegenerate ground state of the Fermi system is uniquely determined by its density distribution.**

$$\Psi \overset{1\text{–}1}{\longleftrightarrow} \rho \quad \Rightarrow \quad E[\rho] = \left\langle \Psi[\rho] \middle| \hat{H} \middle| \Psi[\rho] \right\rangle$$

In general:

$$\langle O \rangle = \langle \Psi[\rho] | O | \Psi[\rho] \rangle = \mathcal{O}[\rho]$$

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In general:

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for a given system!

$$\hat{H} = \hat{H}_{\text{system}} + \hat{V}_{\text{external}} \qquad \hat{H}_{\text{system}} = \sum_{i=1} \frac{-\hbar^2 \nabla_i^2}{2m_e} + \frac{1}{2} \sum_{i \neq j} \frac{1}{4\pi\varepsilon_0} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$$

for electrons

$$\hat{H}_{\text{system}} = \sum_{i=1} \frac{-\hbar^2 \nabla_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} g\delta(\boldsymbol{r}_i - \boldsymbol{r}_j)$$

for cold atoms

# 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

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

"Universal" part that defines the system

External field

$$E[\rho] = F[\rho] + \int d\mathbf{x}\, v_{\text{ext}}(\mathbf{x})\rho(\mathbf{x})$$

Formally rigorous way of approaching any **interacting problem** by **mapping** it exactly to a much easier-to-solve **noninteracting system**.

easy, if Energy Density Functional (EDF) is known...

## *Kohn-Sham method:*

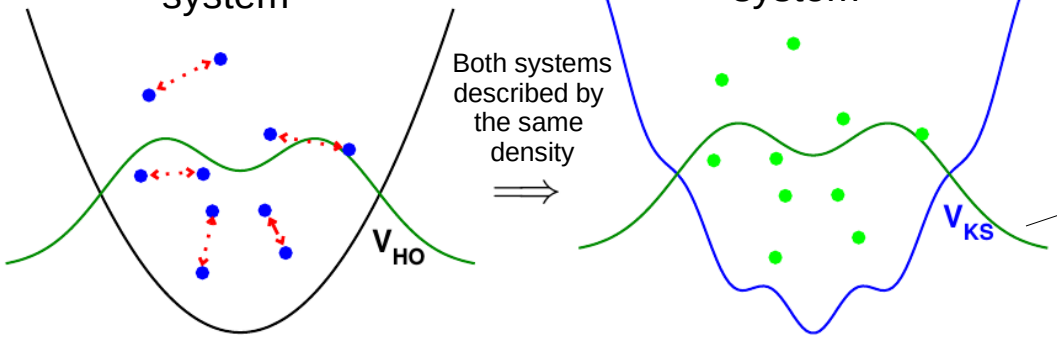



Fig. from: Prog.Part.Nucl.Phys.64:120-168,2010

$$v_{KS} = \frac{\delta F}{\delta \rho} + v_{ext}$$

$$[-\boldsymbol{\nabla}^2/2m + v_{\text{KS}}(\mathbf{x})]\phi_i(\mathbf{x}) = \varepsilon_i \phi_i(\mathbf{x})$$

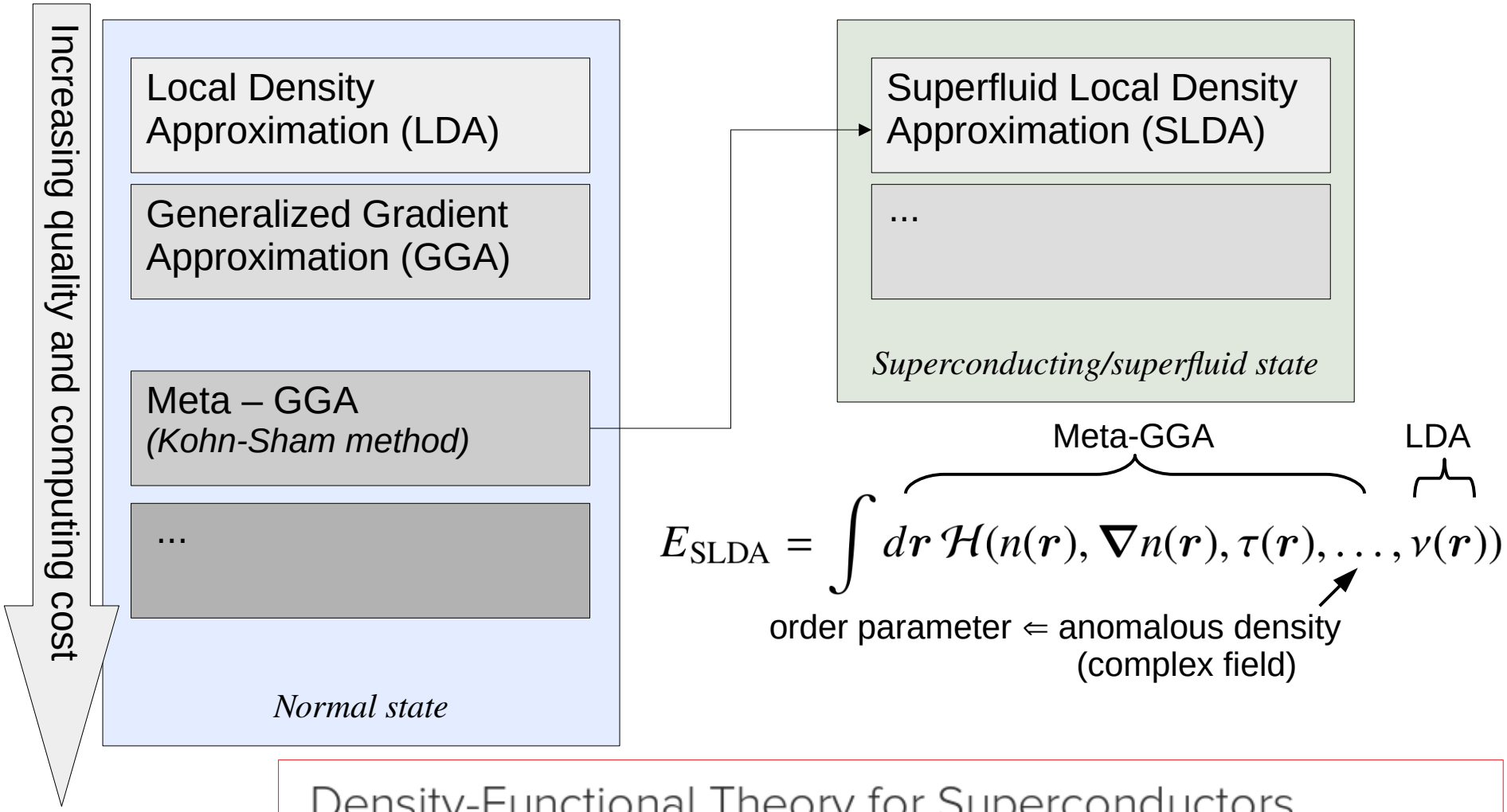
$$\rho(\mathbf{x}) = \sum_i n_i |\phi_i(\mathbf{x})|^2 \quad n_i = \theta(\varepsilon_{\text{F}} - \varepsilon_i)$$

More general:

Interacting System ⇨ System of non-interacting quasiparticles

*Note*: There are easy and difficult observables in DFT. In general: **easy** observables are **one-body** observables. They are easily extracted and reliable.

# 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

# 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

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

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

**Ultracold atoms are superfluid!**

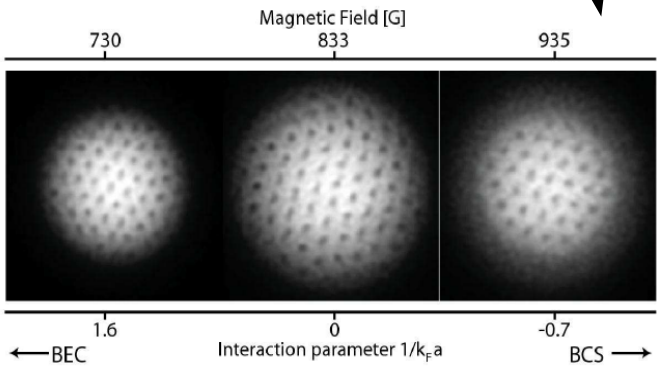


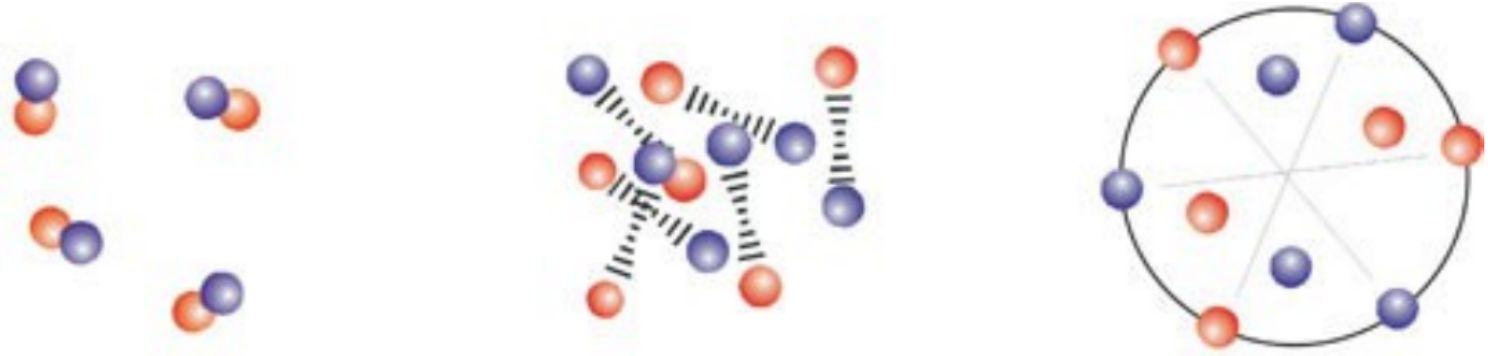

FIG. 36 Vortex lattice in a rotating gas of $^6$Li precisely at the Feshbach resonance and on the BEC and BCS side. Reprinted with permission from Zwierlein *et al.* (2005).

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

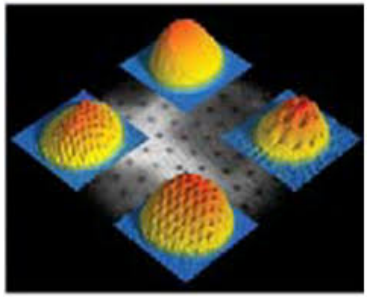
Photo from: http://www.lkb.upmc.fr/ultracoldfermigases/

BEC ⟵ CROSSOVER ⟶ BCS

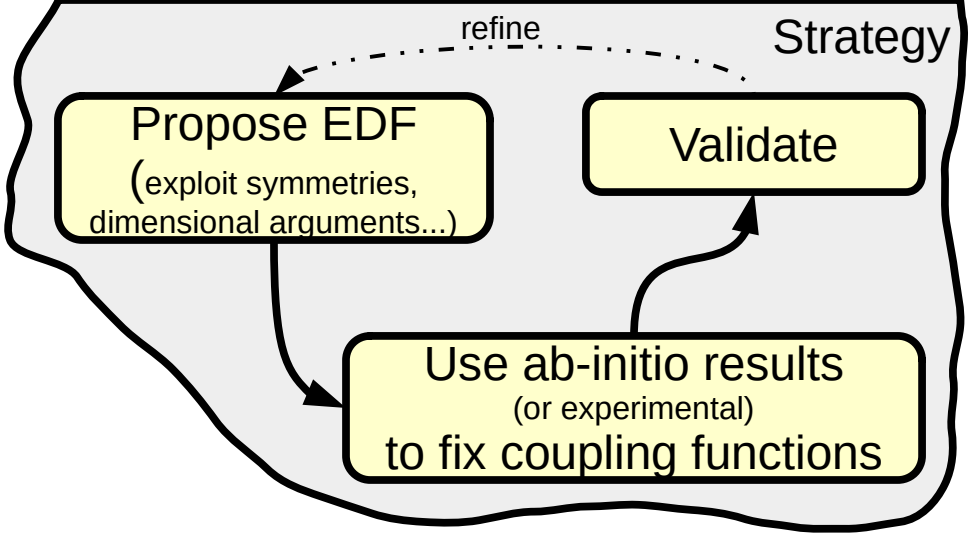
$ak_F \to 0^+$ $\quad ak_F \to \pm\infty$ $\quad ak_F \to 0^-$



diatomic molecules | strongly interacting pairs | Cooper pairs



# SLDA-type functional...



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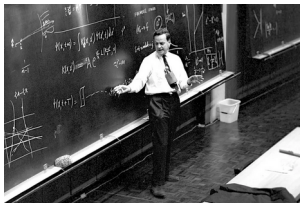
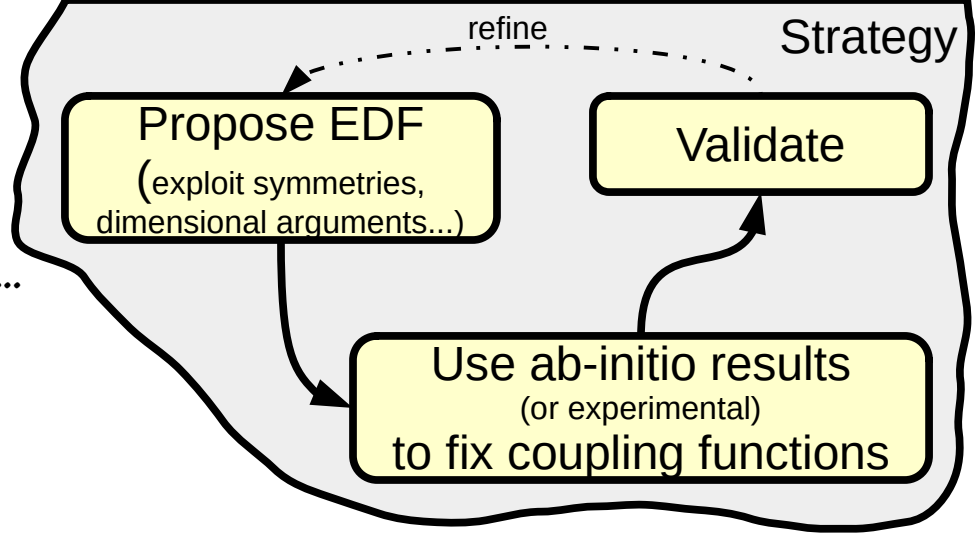


**Richard Feynman**
***... physics is not mathematics and mathematics is not physics ...***

*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.*



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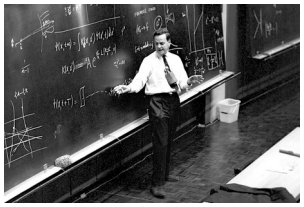

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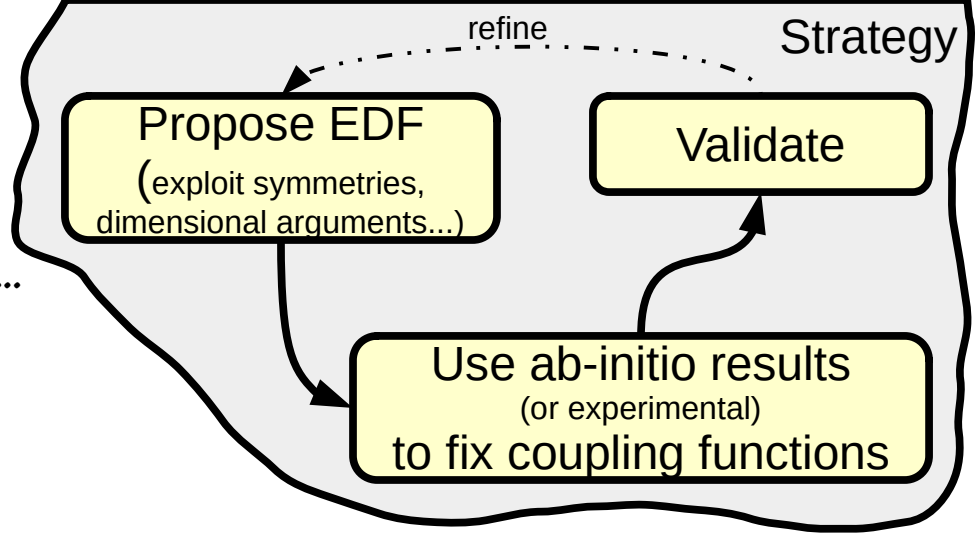



## ... for cold atoms

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

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

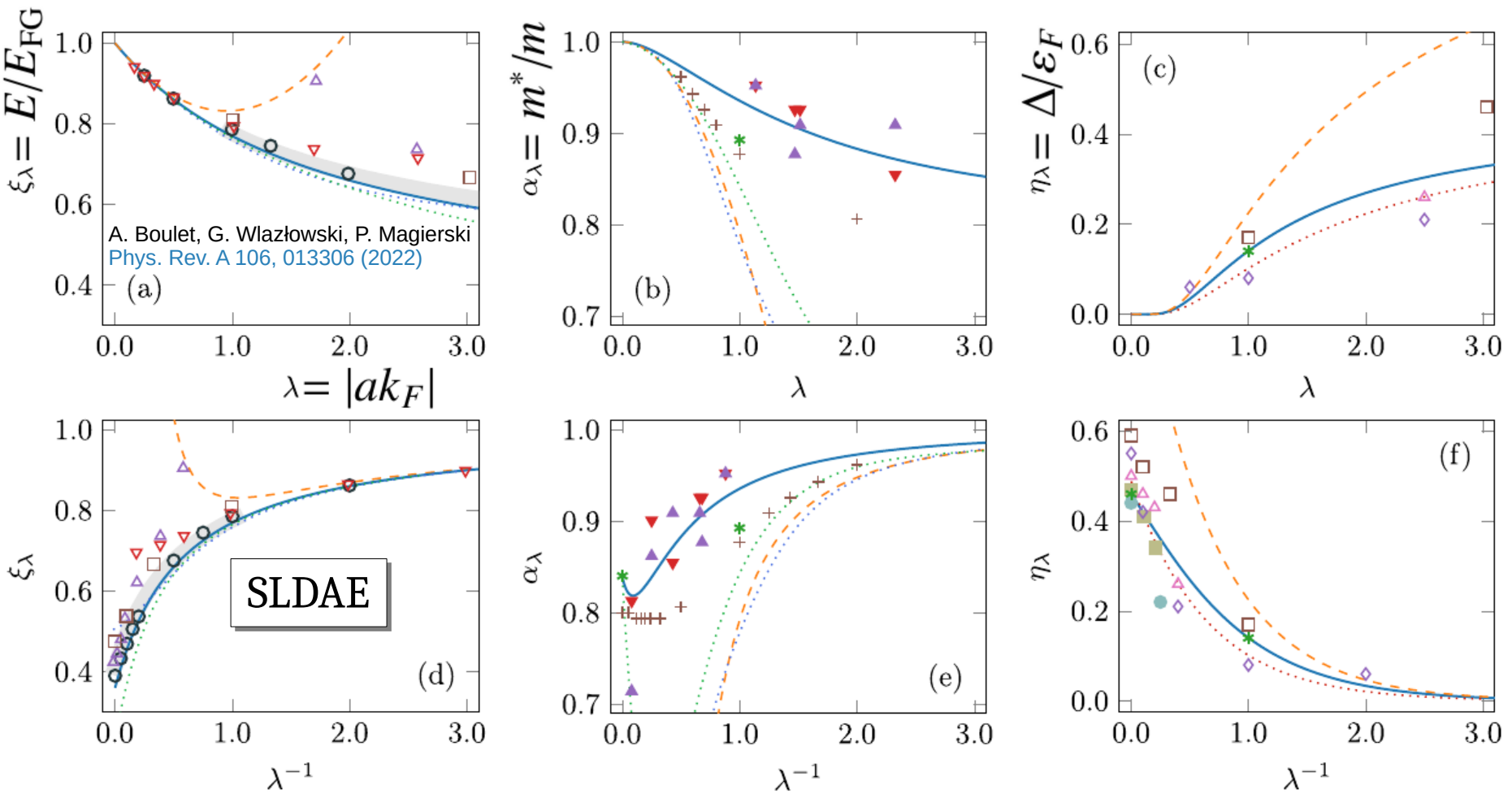
→ *ab initio* cals for $E/E_{\mathrm{FG}}$, $\Delta/\varepsilon_F$, $m^*/m$

→ 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]
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]

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*

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

# Towards time-dependent problems

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Runge & Gross theorem

$$\left.\begin{matrix} \rho(\vec{r},t) \\ \psi(...,t_0) \end{matrix}\right\} \leftrightarrow e^{i\alpha(t)}\psi(...,t)$$

up to arbitrary function α(t)

## 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...

# Towards time-dependent problems

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

… however adiabatic approximation turns out to be very successful!

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

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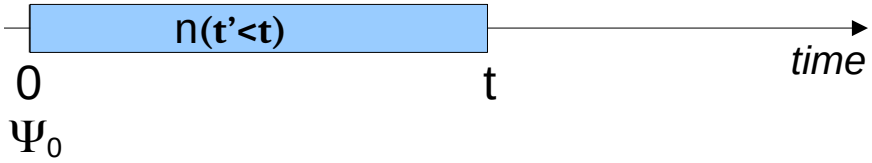
$$E(t) = E[\Psi(t=0), n(\boldsymbol{r}, t' \leqslant t), \ldots]$$




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

Adiabatic approximation

*In general integro-differential equations* ←

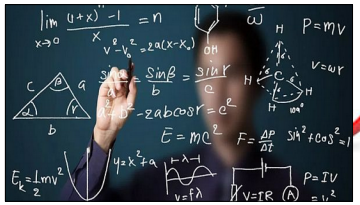
$$E(t) = \int_0^t dt' \int_V d\boldsymbol{r}\, \mathcal{E}[\Psi_0, n(\boldsymbol{r},t'), \ldots]$$

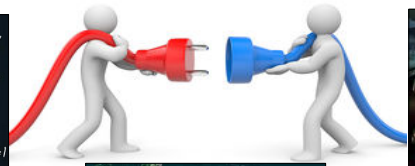
There exits analog of Hohenberg-Kohn theorem for time-dependent problems...

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

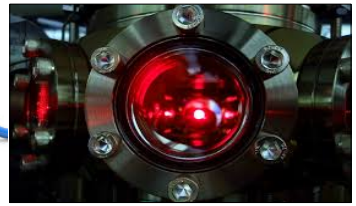
...if the evolution is slow (adiabatic), then the system follows instantaneous ground state
→ use the functional taken from static considerations.

Theoretical method





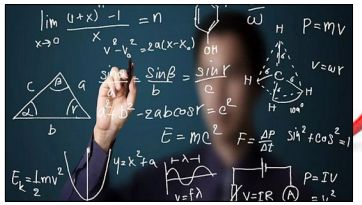
Experiment

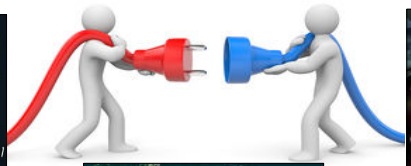


Computer code

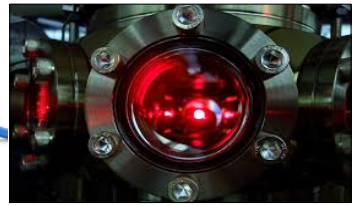
PHYSICS.WUT

Theoretical method





Experiment



Computer code

**DFT method is typically delivered to community in form of a code**


Piz Daint @ Swiss National Supercomputing Centre (Switzerland) - Access is granted thanks to PRACE.

Tsubame3.0 @ Global Scientific Information and Computing Center, Tokyo Institute of Technology (Japan)


*(2019-2020)* Prometheus @ Academic Computer Centre CYFRONET of the University of Science and Technology in Cracow (Poland). Access grated thanks to PL-Grid infrastructure.

Okeanos @ Interdisciplinary Centre for Mathematical and Computational Modelling (Poland)

ABINIT

JuKKR

VASP

QUANTUMESPRESSO

siesta

WIEN2k

...and many others, see here:
https://en.wikipedia.org/wiki/List_of_quantum_chemistry_and_solid-state_physics_software

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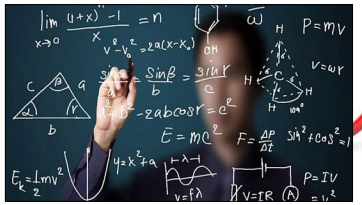
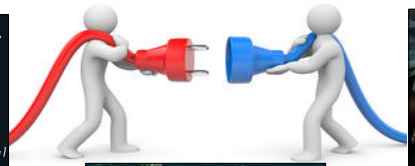
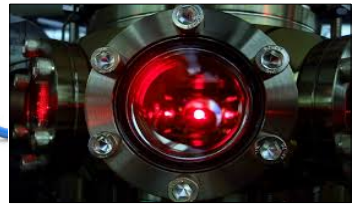
Theoretical method





Computer code

Experiment



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

Ongoing extensions:
→ Bose-Fermi mixtures
→ Fermi-Fermi mixtures

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

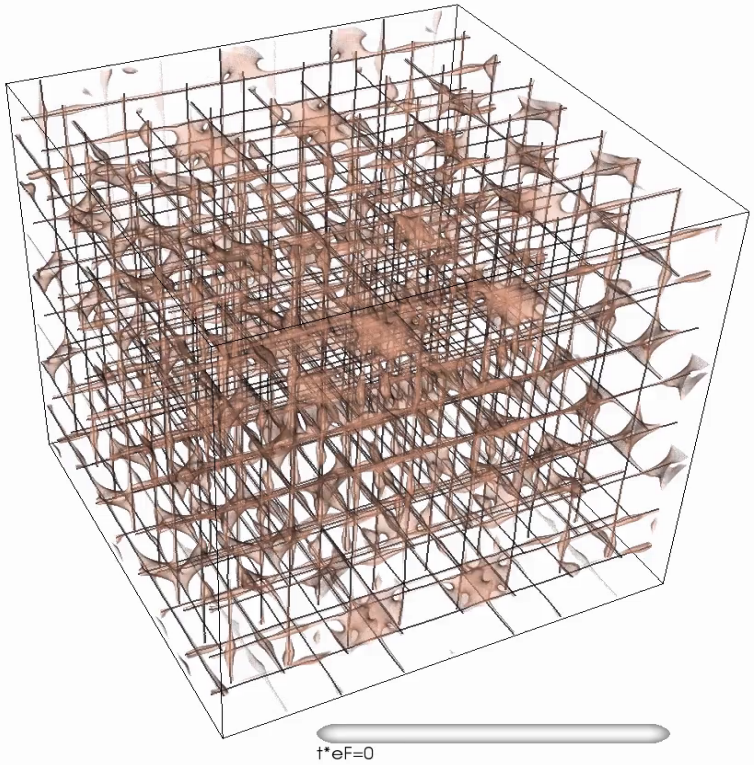
$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} u_n(\boldsymbol{r},t) \\ v_n(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} h_a(\boldsymbol{r},t) - \mu_a & \Delta(\boldsymbol{r},t) \\ \Delta^*(\boldsymbol{r},t) & -h_b^*(\boldsymbol{r},t) + \mu_b \end{pmatrix} \begin{pmatrix} u_n(\boldsymbol{r},t)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

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




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

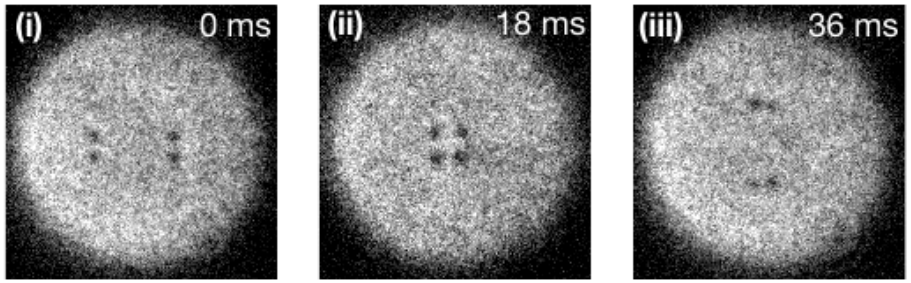
number of atoms = 26,790
number of quasi-particle states = 582,898
number of PDEs = 1,165,796

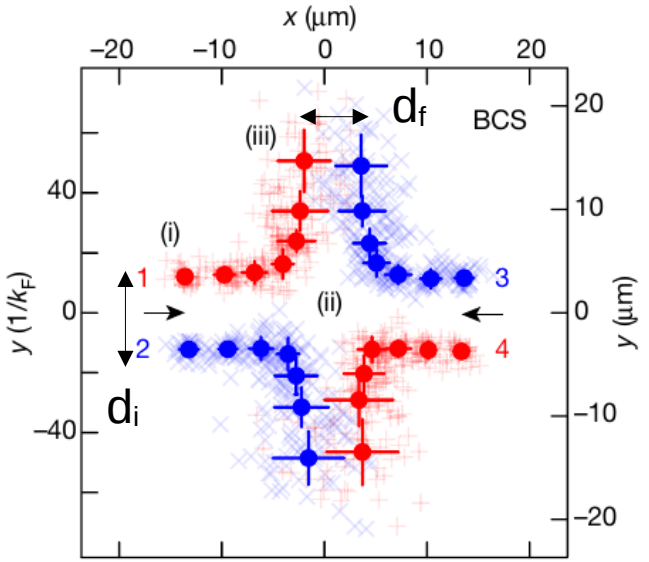
PRELIMINARY:
quantum turbulence
in the unitary Fermi gas

# Application example: Vortex collisions

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

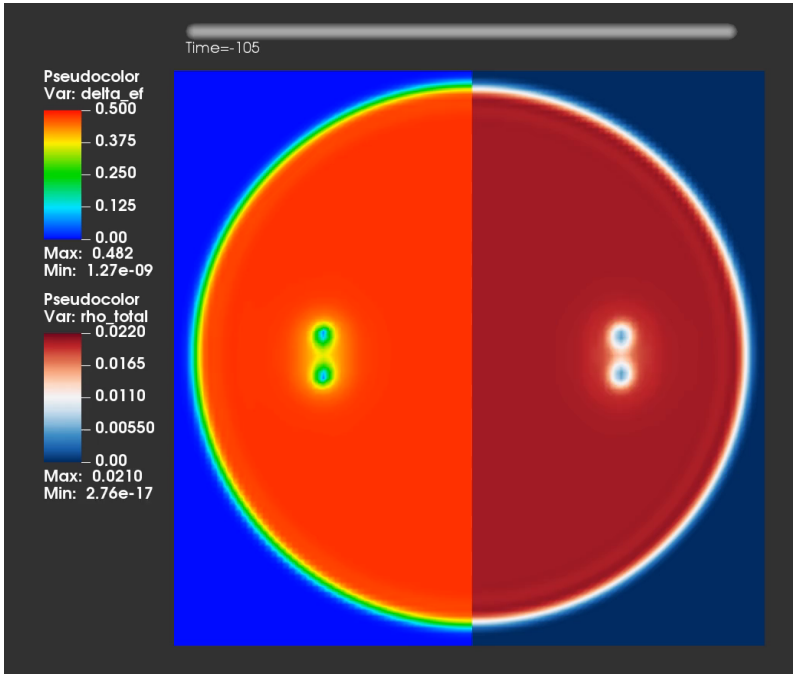
Figs from [1]

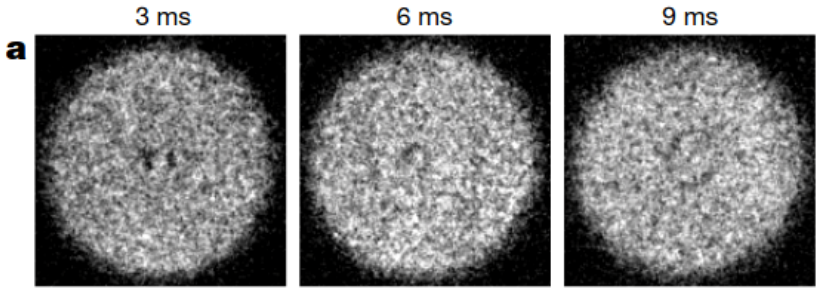



Experiment

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




Vortex annihilation seen in the experiment.

← Simulation

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

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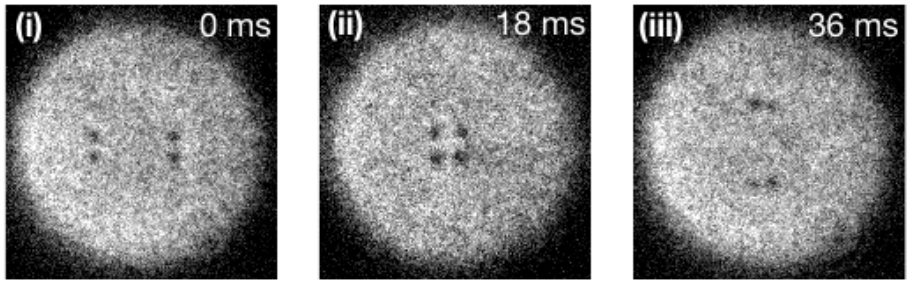


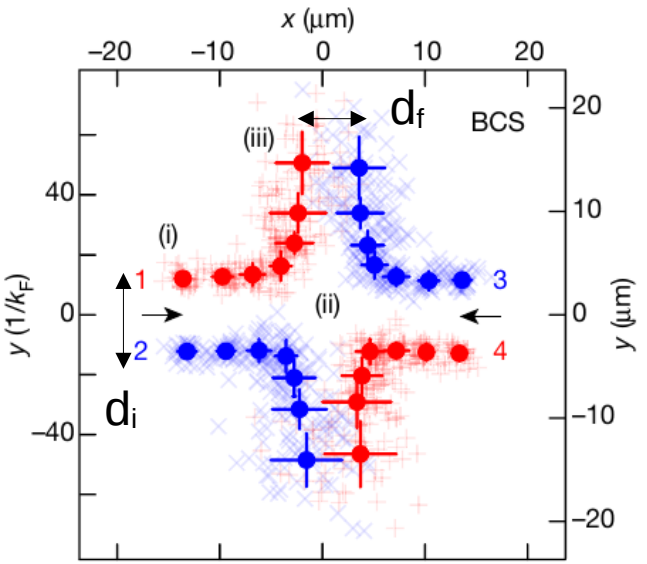


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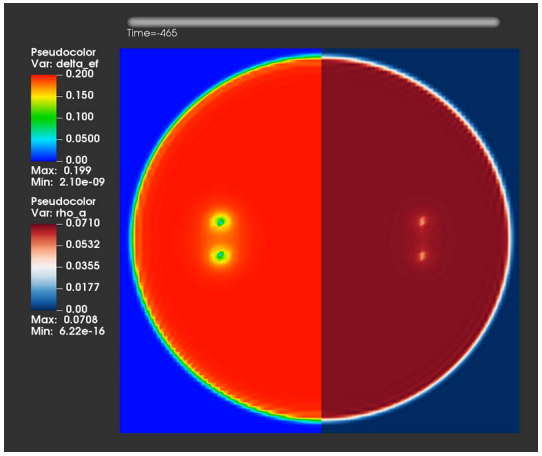
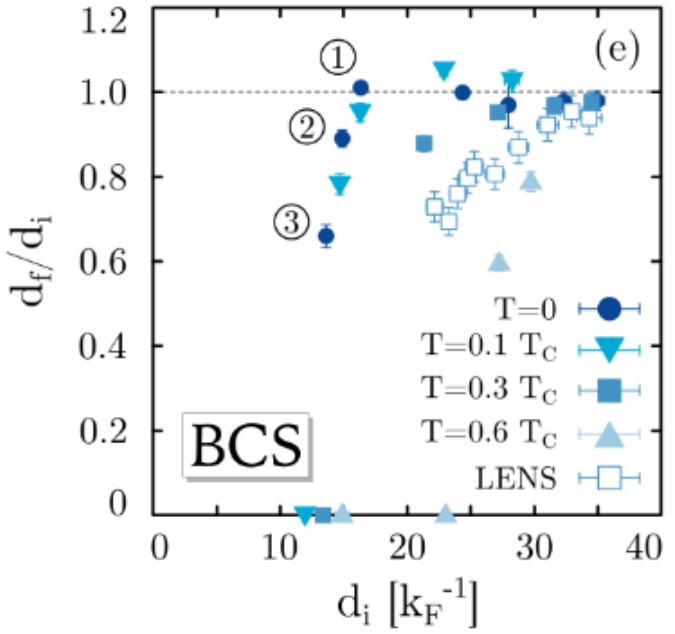
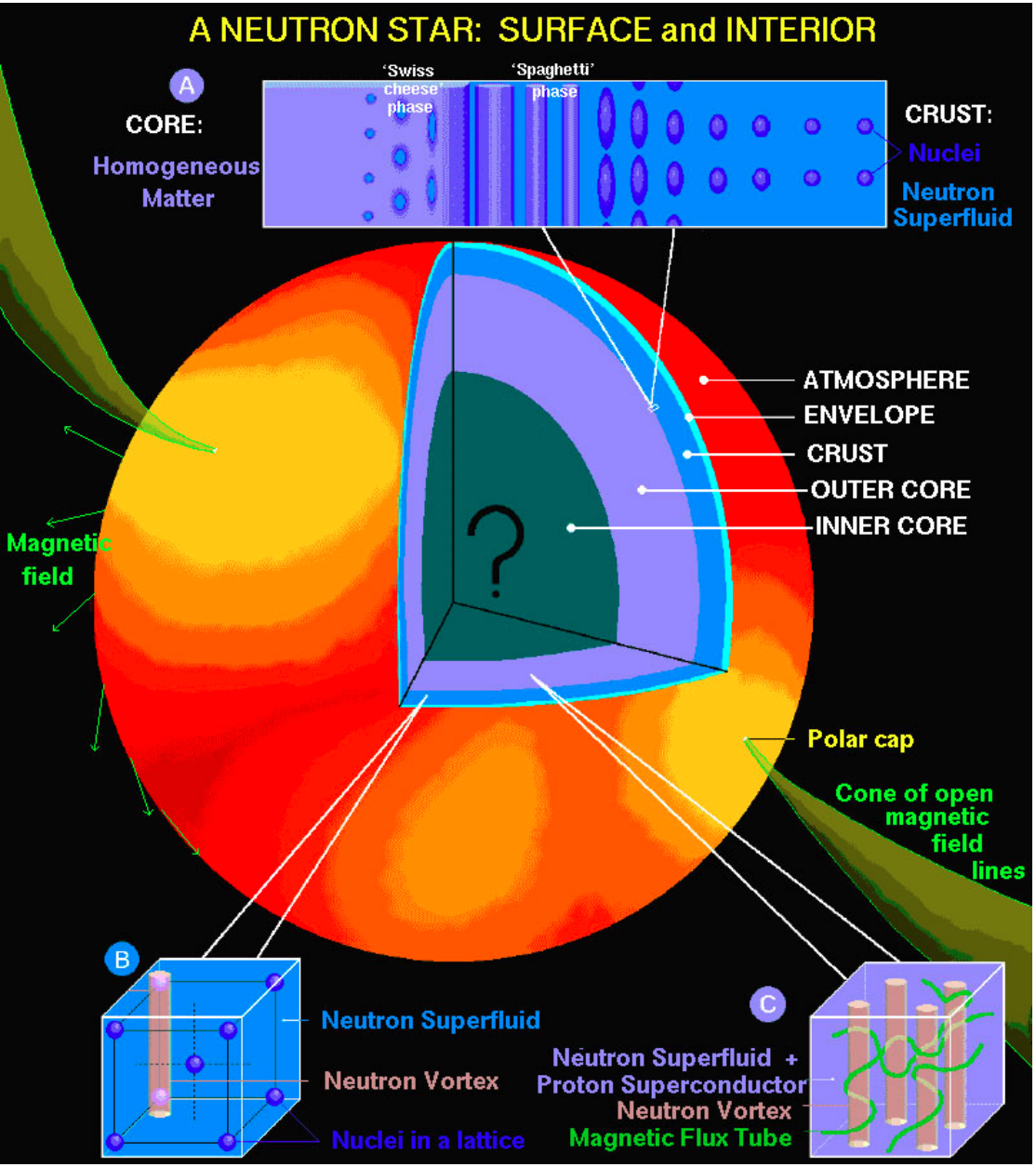


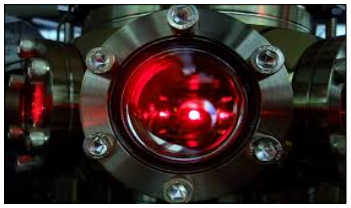

A. Barresi, A. Boulet, P. Magierski, G. Wlazłowski, Phys. Rev. Lett. 130, 043001 (2023)




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




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.

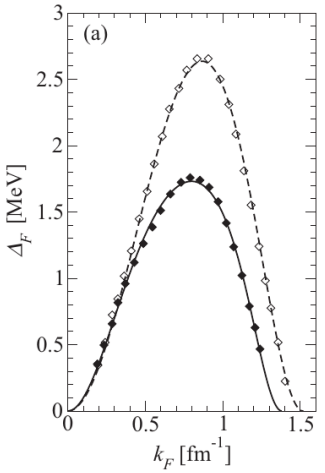
→ … for example, nuclear codes that we use are based on software that we constructed for ultracold atoms

# Brussels-Montreal Skyrme functionals (BSk)

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

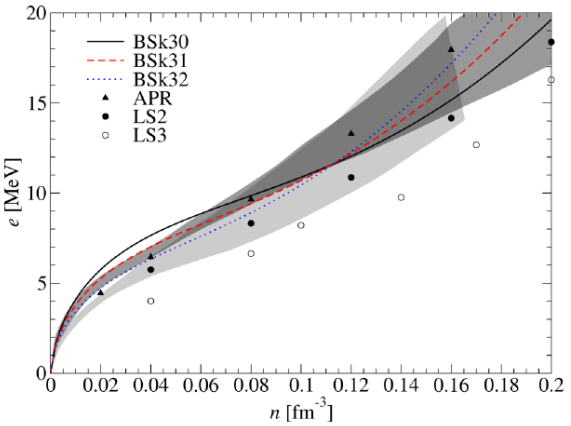
**Experimental data**:

- 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).*



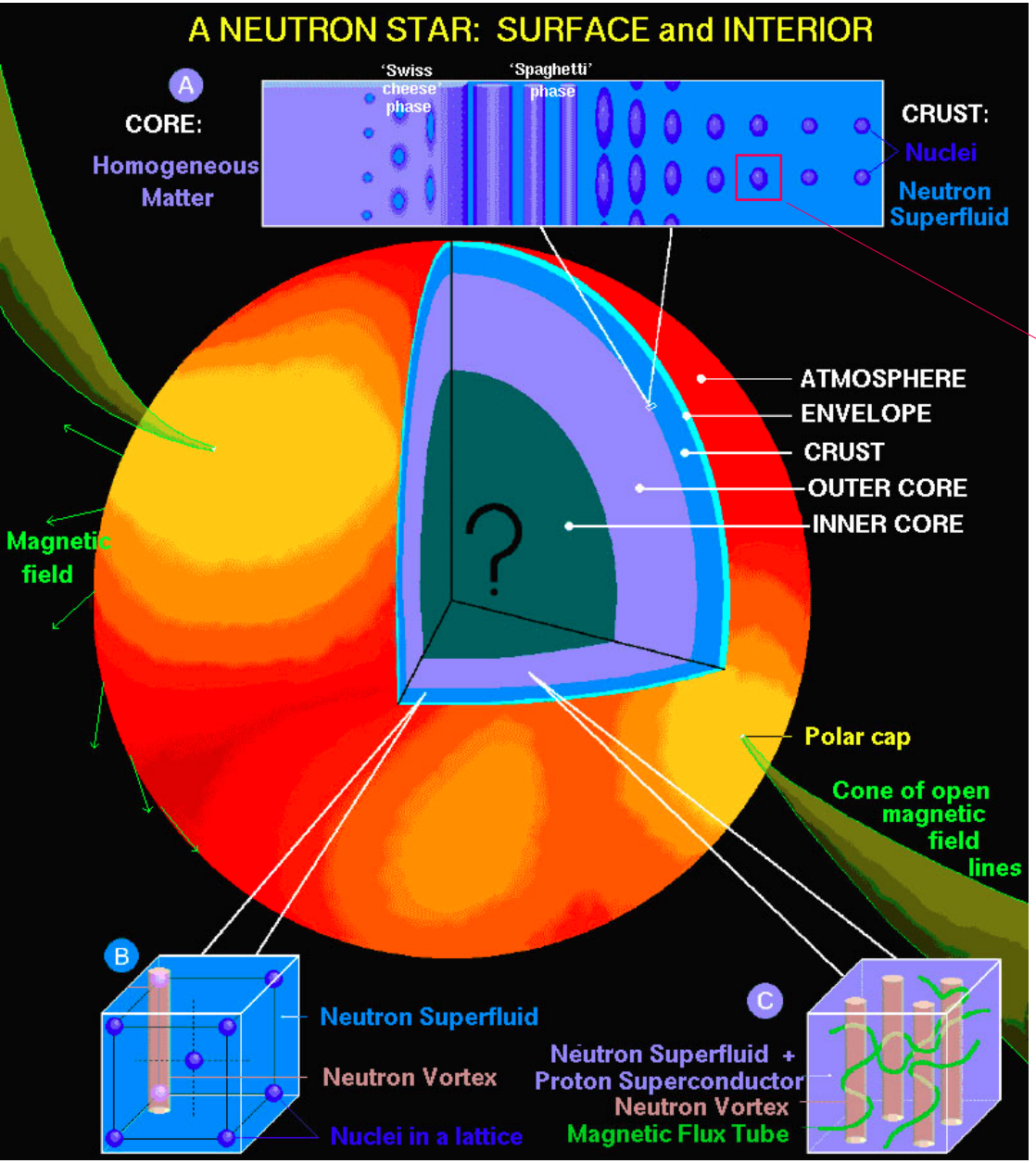

**N-body calculations using realistic forces**:

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

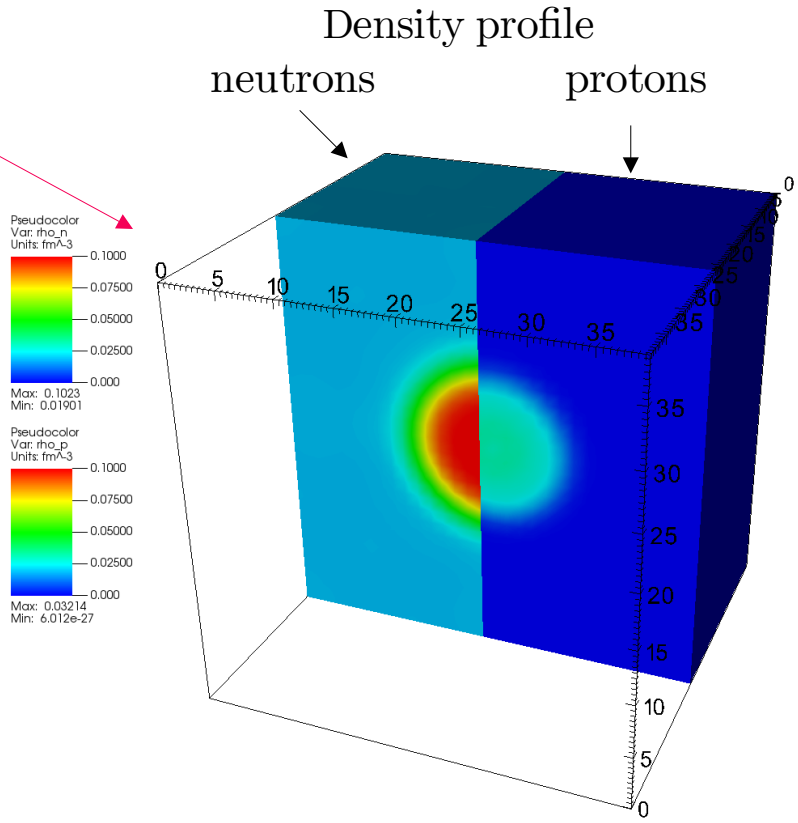



PRC 93, 034337 (2016)

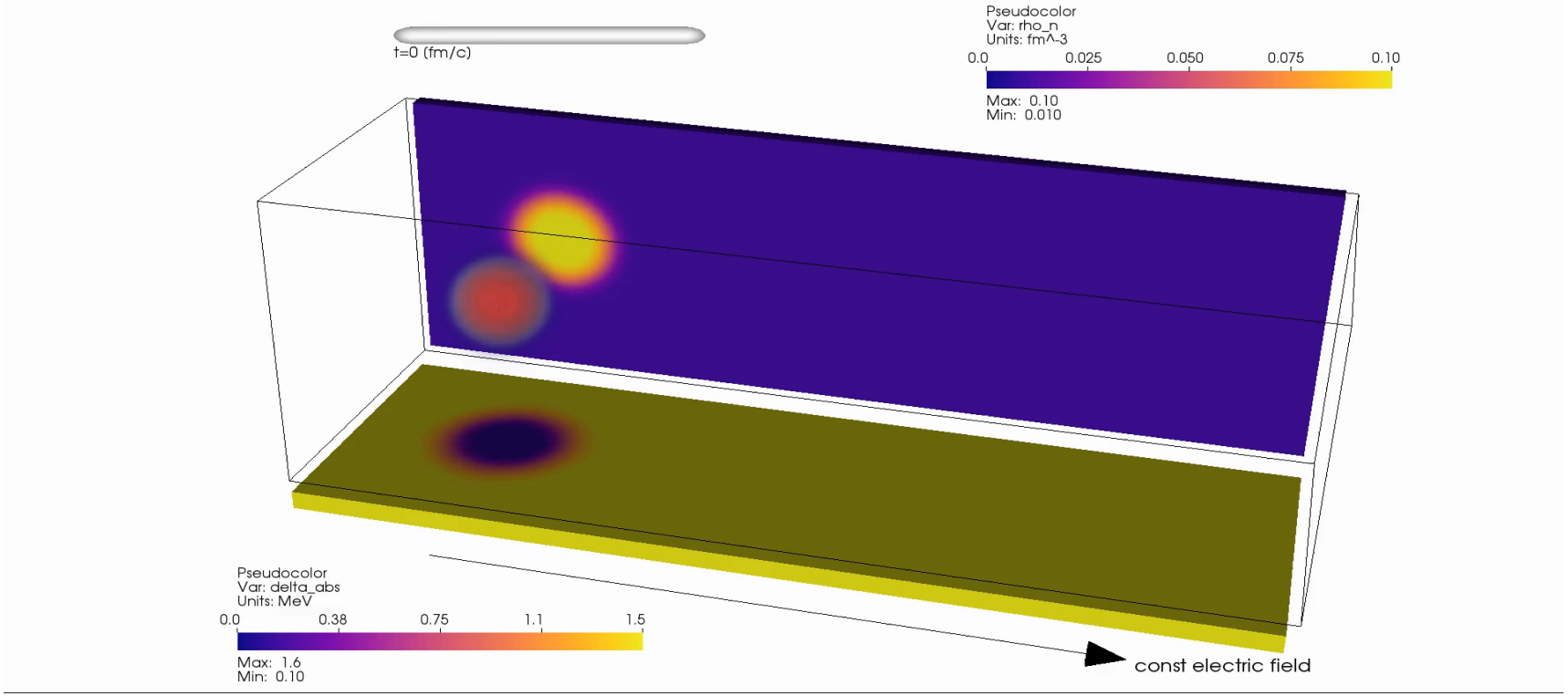
From: Nicolas Chamel talk, Buffalo, March 2016




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



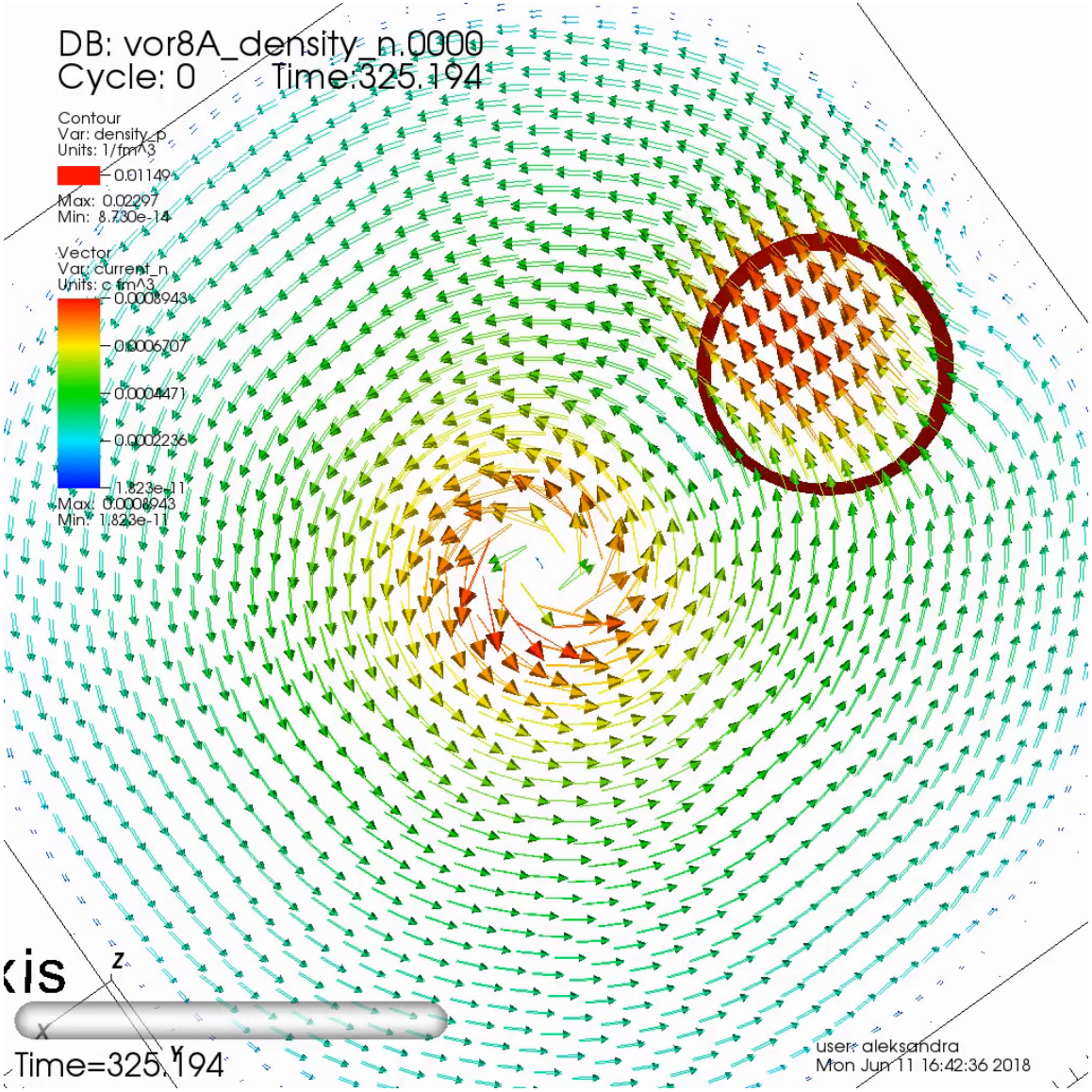

In the simulation box $(40\ \text{fm})^3$ we have 1382 neutrons and 40 protons.

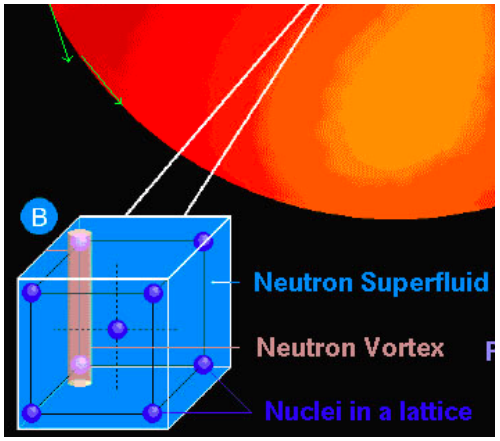



System: *nuclear matter*
3D simulation 40 x 40 x 120 [fm]

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

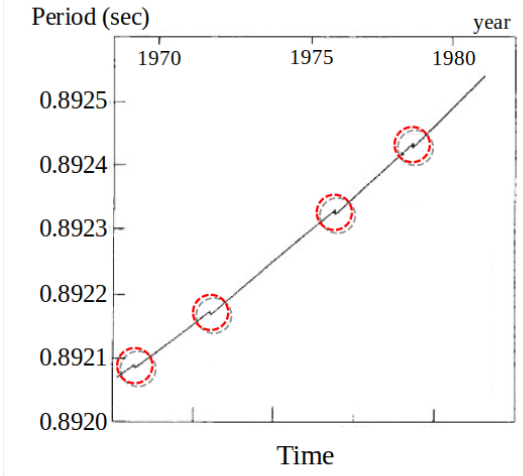
PRELIMINARY:
response of nuclear impurity to uniform electric field



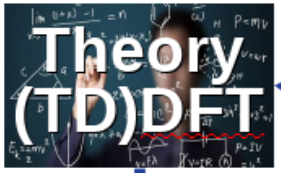

System: *nuclear in presence of quantum vortex*

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

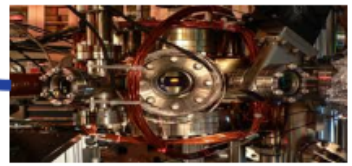



V.B. Bhatia, A Textbook of Astronomy and Astrophysics with Elements of Cosmology, Alpha Science, 2001.

# Towards effective model of neutron star...

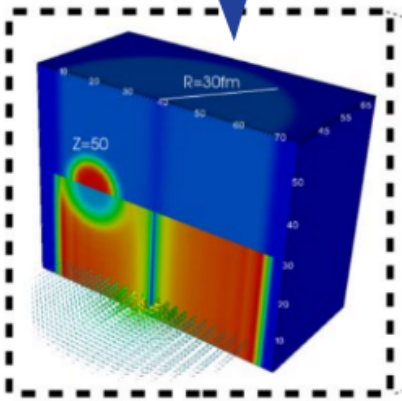



Low energy nuclear physics

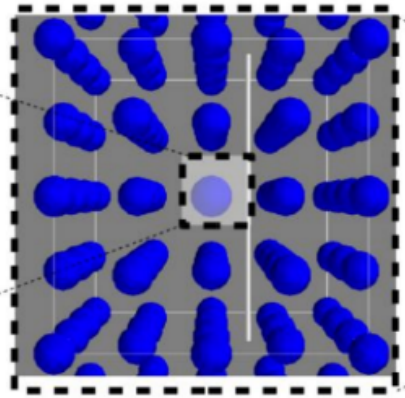


Ultra-cold atomic gases

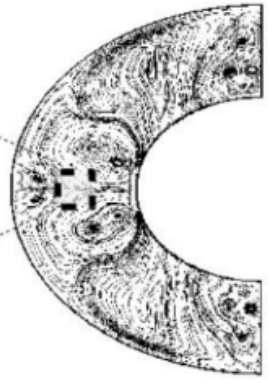
Comparison with observations




feed



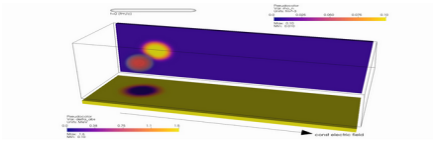
feed

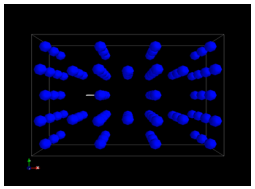


Method: TDDFT
DoF: neutrons and protons.
Scale: ~$10^{-13}$m

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

Method: Hydrodynamics
DoF: fluid elements
Scale: ~size of star





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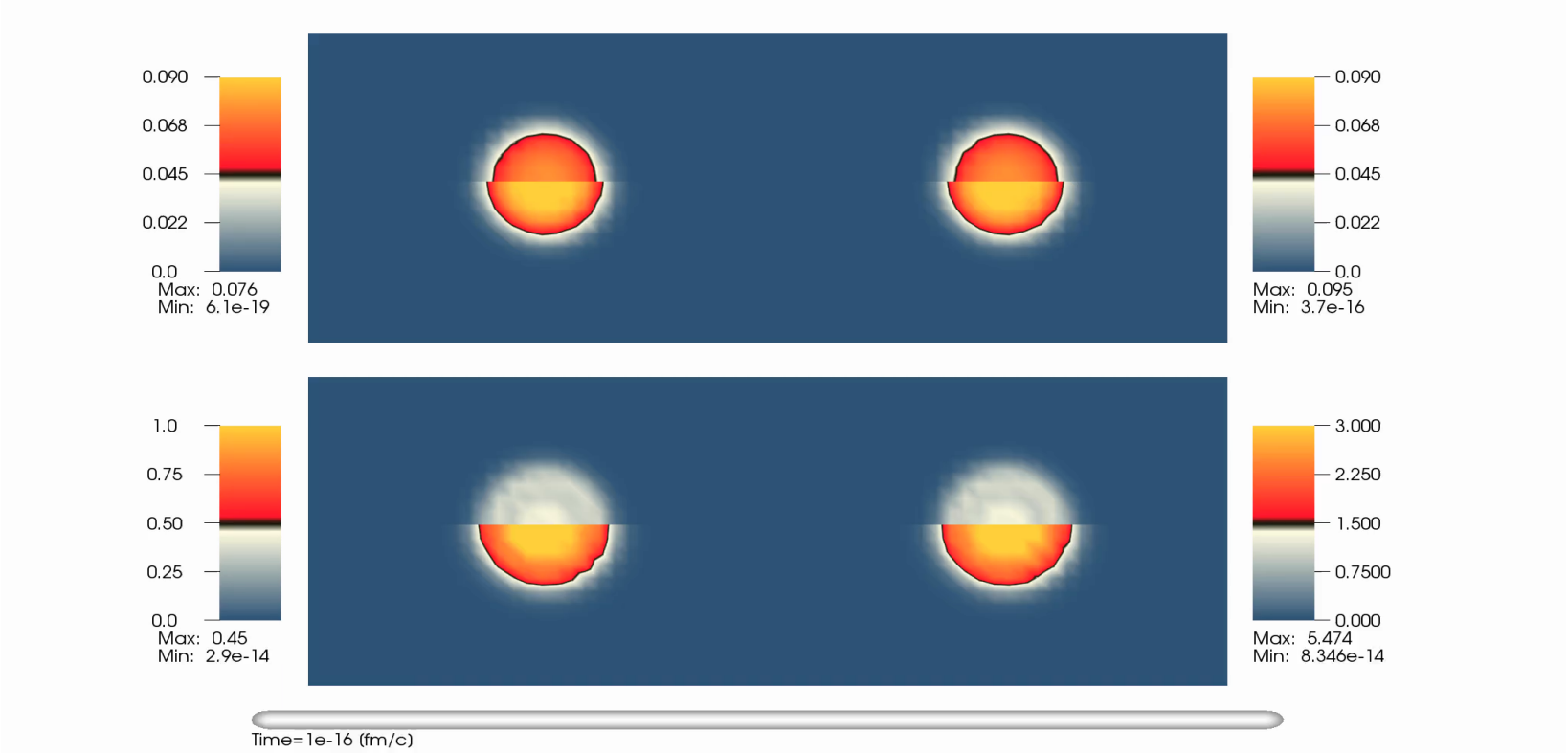


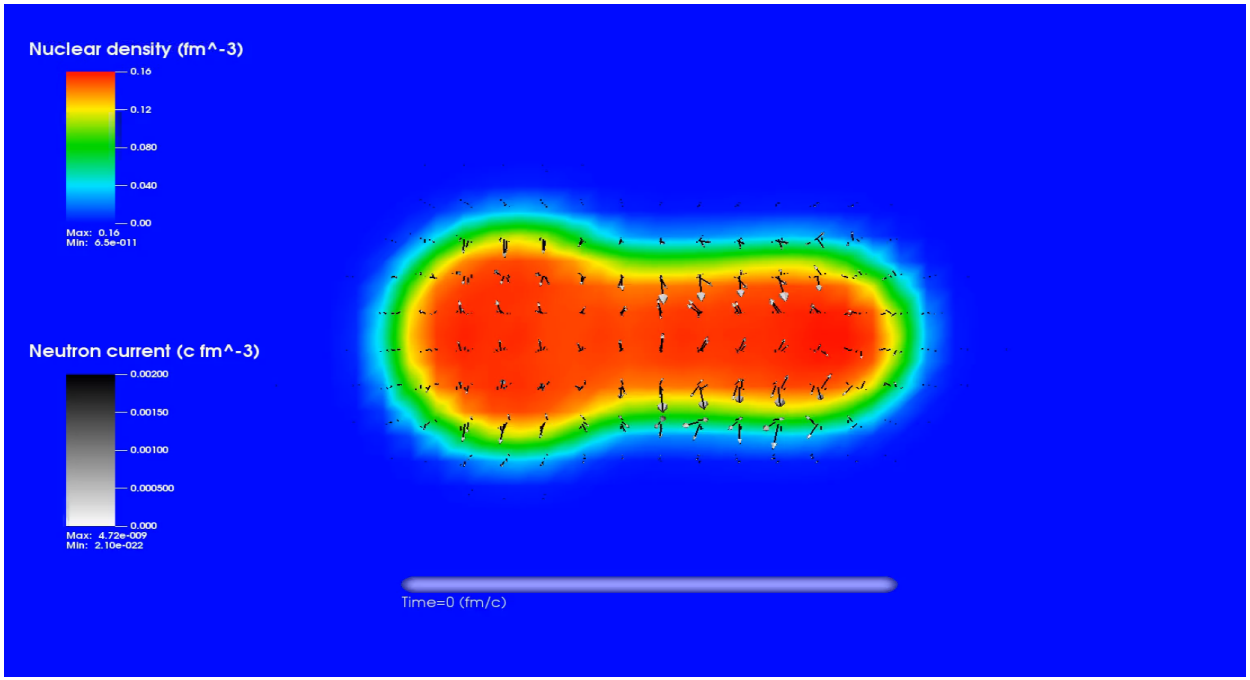

*Reaction: $^{96}Zr+^{96}Zr$, SkM*, $E_{cm}$=178MeV, head-on collision*

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

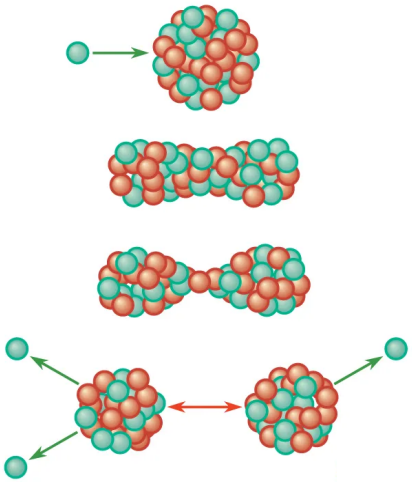
Phenomena related to nuclei (like nuclear reactions) can be also investigated by means of TDDFT.

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

# Fission of $^{240}$Pu




*...to see this process within microscopic simulations was a challenge for many years...*



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

→ *superfluidity/superconductivity works as a lubricant in the fission process*
→ *microscopic approaches that neglect superfluidity (like Hartree-Fock) typically fail to produce the fission event*

# SUMMARY

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

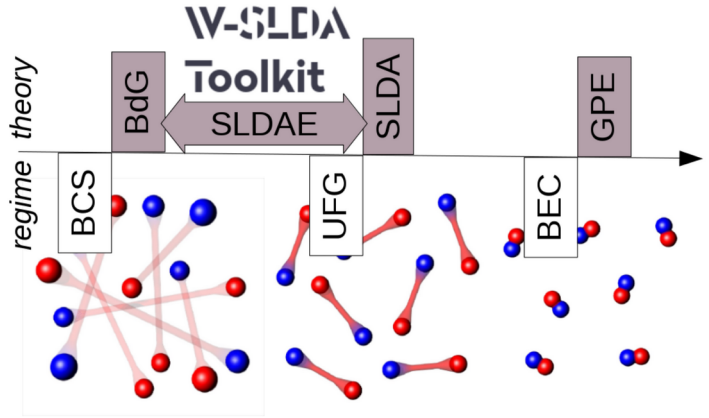
  **DFT** SLDA → BCS regime; strong interaction;
  GPE → BEC regime

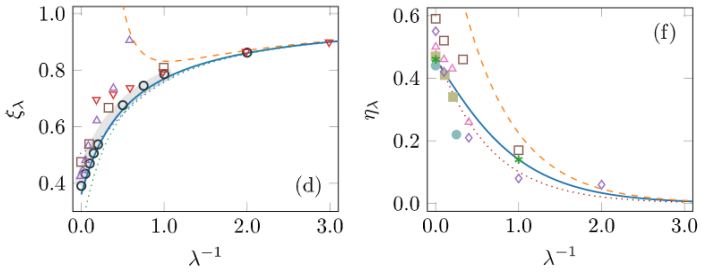
- DFT is general purpose method: it overcomes limitations of mean-field approch, while keeping numerical cost at the same level as BdG calculations.

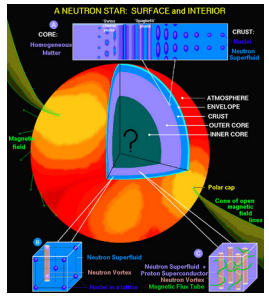
- Recent progress in High Performance Computing allows for tracking dynamics of systems consisting of thousands of fermions.

- 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 ...





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