Towards general-purpose simulation platform for superfluid fermions across BCS-BEC crossover

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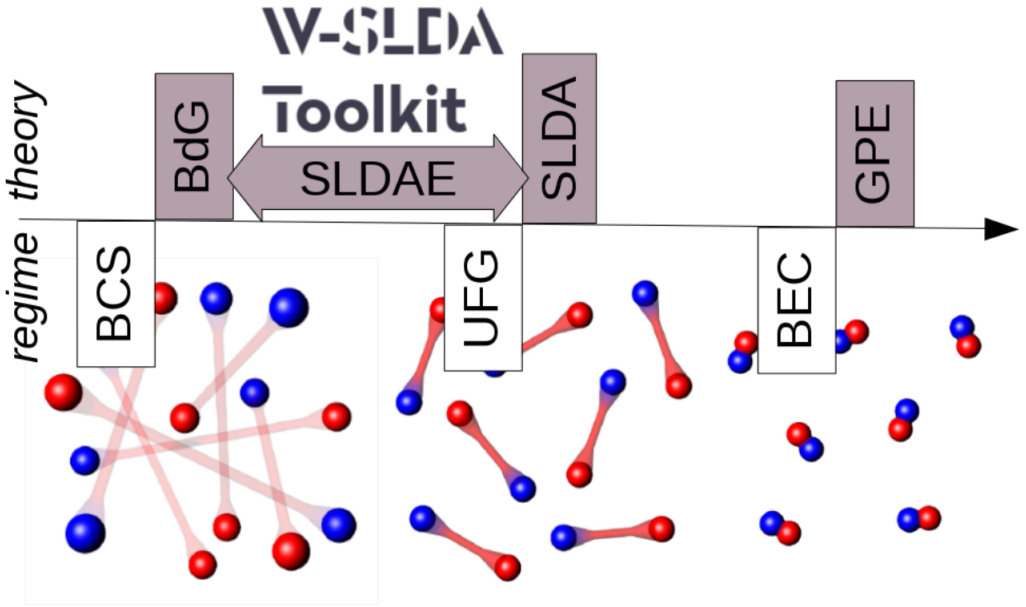

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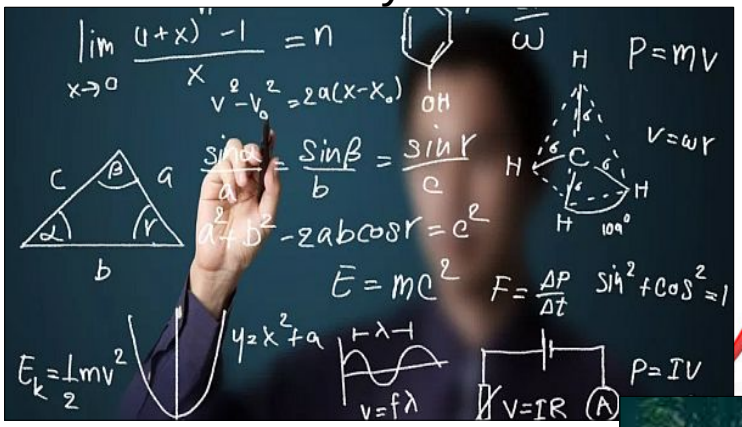
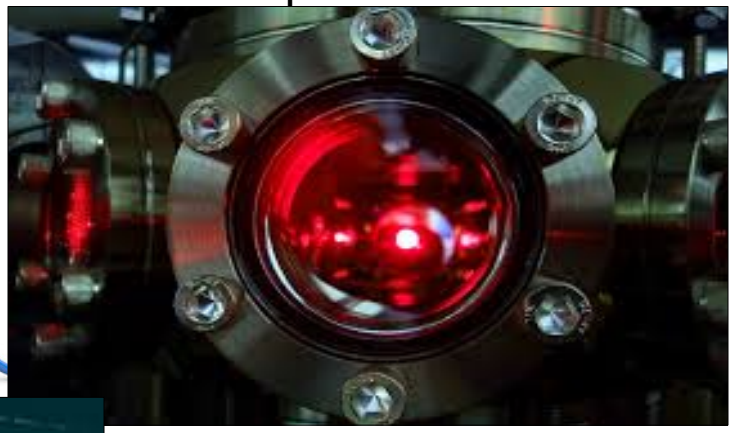
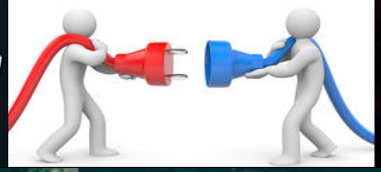
Theory



Experiment





Computational physics

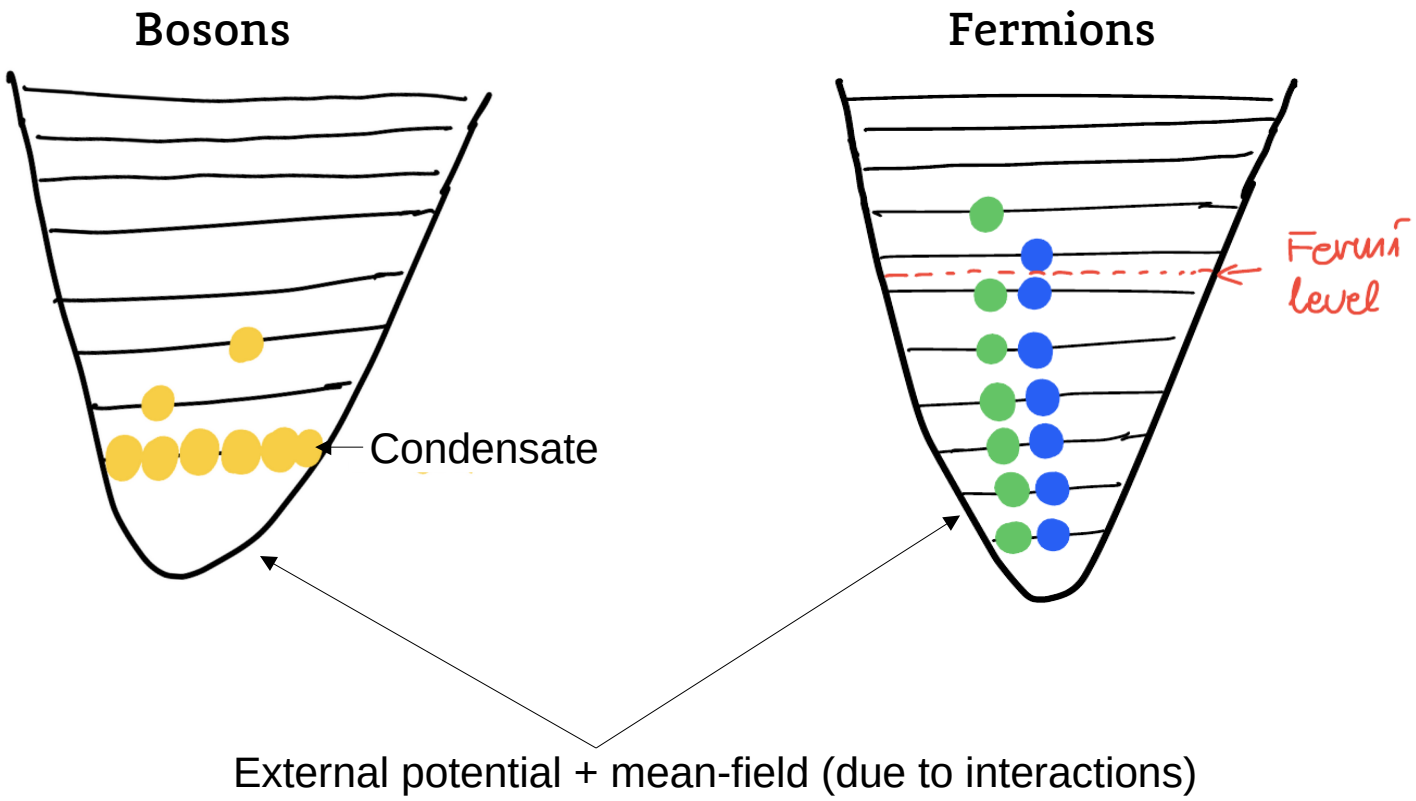
Overview:
1. *Method → DFT**
2. *Implementation*
3. *Applications*
4. *Extensions to other systems*

(*) 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, ...

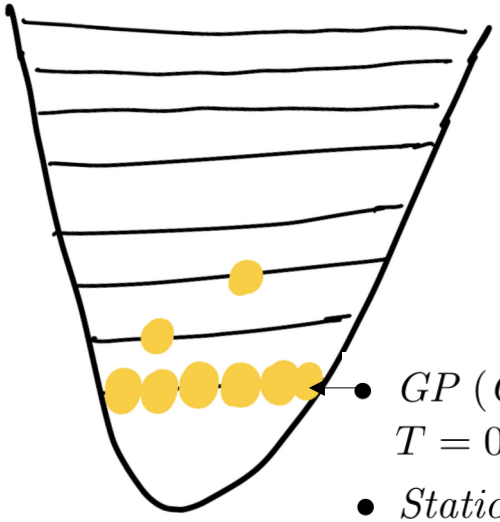
Mean-field perspective

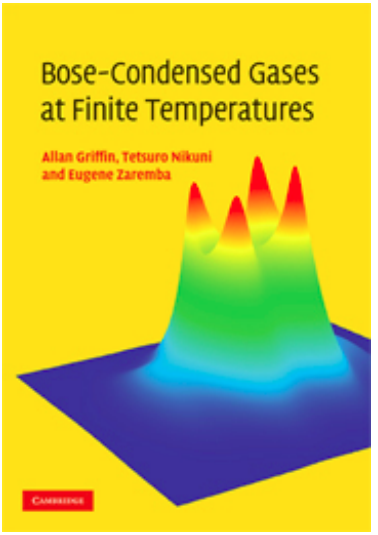


Mean-field perspective

In scientific jargon frequently:
mean-field for bosons = GP
and
beyond mean-field = BdG or HFB

Bosons

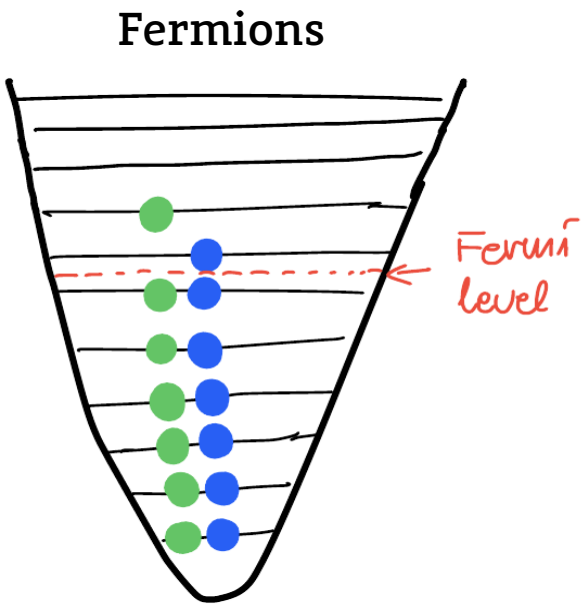




Classification taken from book by Griffin, Nikuni, Zaremba

- *GP* (*Gross–Pitaevskii*): Ignore $\tilde{n}$ and $\tilde{m}$ completely. This is only valid at $T = 0$ in a weakly interacting dilute Bose gas.
- *Static HFP* (*Hartree–Fock–Popov*): Keep $n_c(\mathbf{r}, t)$ but set $\tilde{n}(\mathbf{r}, t) = \tilde{n}_0(\mathbf{r})$ and $\tilde{m}(\mathbf{r}, t) = 0$ (Hutchinson *et al.*, 1997; Dodd *et al.*, 1998).
- *Static HFB* (*Hartree–Fock–Bogoliubov*): Keep $n_c(\mathbf{r}, t)$ but set $\tilde{n}(\mathbf{r}, t) = \tilde{n}_0(\mathbf{r})$ and $\tilde{m}(\mathbf{r}, t) = \tilde{m}_0(\mathbf{r})$ (Hohenberg and Martin, 1965; Griffin, 1996). As noted in Section 5.1, this produces an energy gap in the single-particle excitation spectrum (since $\mu_{\rm HP} \neq \mu_c$).
- *Dynamic HFB*: Treat all dynamic mean fields due to $n_c(\mathbf{r}, t)$, $\tilde{n}(\mathbf{r},t)$ and $\tilde{m}(\mathbf{r}, t)$ on an equal basis in a generalized mean-field calculation of the density response function $\chi_{nn}(1, 1')$. This will be discussed in Sections 5.3 and

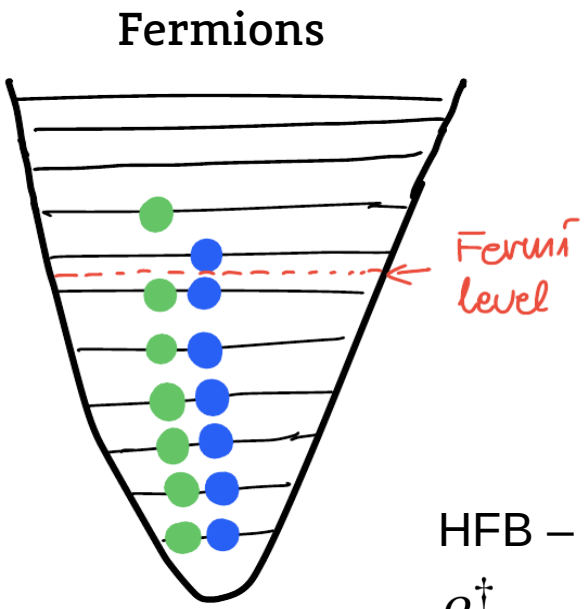
Mean-field perspective



No “GP level” – due to Pauli principle

- Static HFB (or BdG)
- Time-dependent HFB (or TDBdG)
- …

Mean-field perspective



No "GP level" – due to Pauli principle

- Static HFB (or BdG)
- Time-dependent HFB (or TDBdG)
- …

HFB – main concept

$$\beta_k^\dagger = \sum_i (u_{ik} a_i^\dagger + v_{ik} a_i)$$

Quasi-particles – mixtures of particles and holes

$$\{\beta_k, \beta_l^\dagger\} = \delta_{kl}$$

Anticommutation relations (fermions)

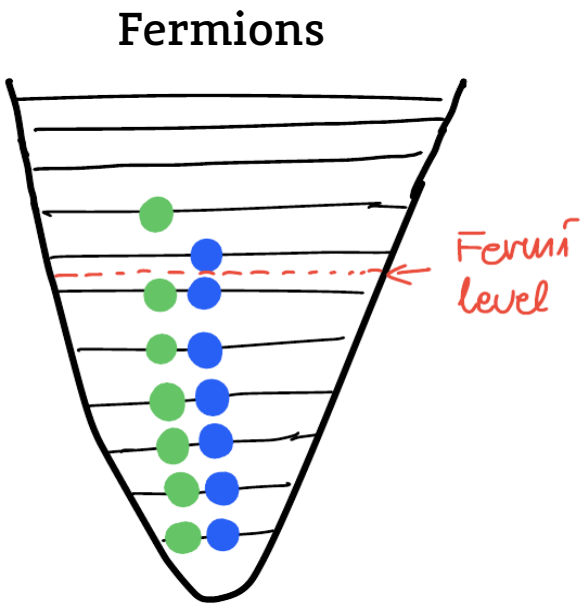
$$|\Psi\rangle = \prod_k \beta_k^\dagger |0\rangle$$

Many-body wave function is approximated by product state

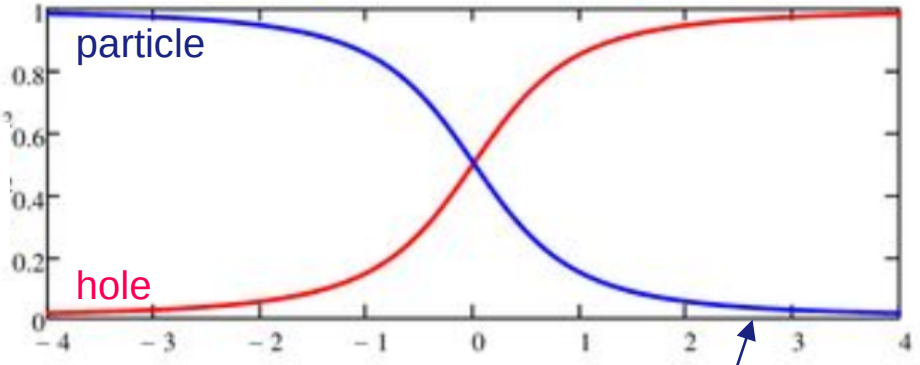
u_{ik} v_{ik} define Bogoliubov transformation
→ variational parameters

$u_{ik} \to u_n(\boldsymbol{r})$ $v_{ik} \to v_n(\boldsymbol{r})$ BdG → coordinate basis

Mean-field perspective



BCS occupation probabilities at T=0



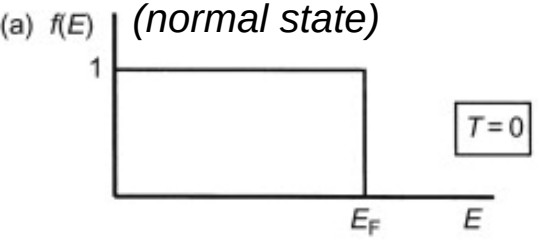
$p\text{-}p_F$

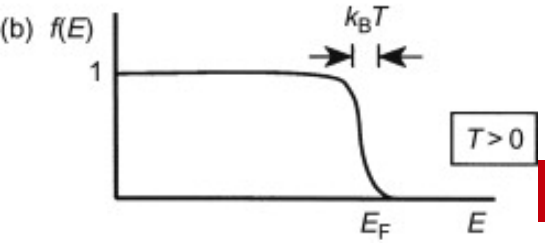
For short-range interaction

$$n(p) \to C/p^4$$

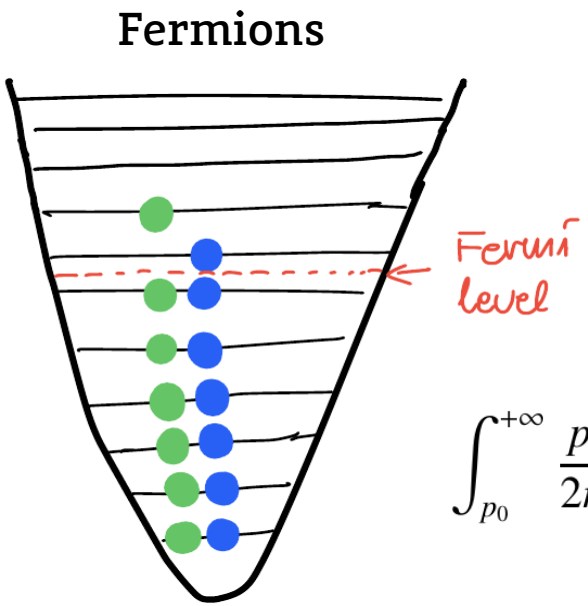
Exact result, by S. Tan, Ann. Phys. 323, 2952 (2008)

Free Fermi gas (normal state)





Mean-field perspective



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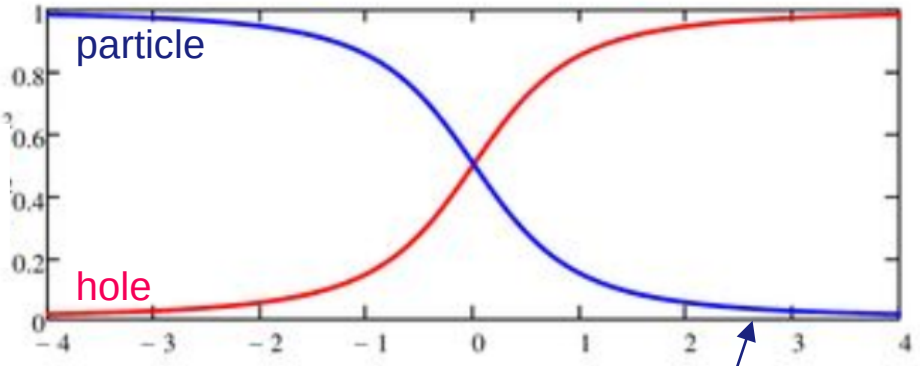

$$\int_{p_0}^{+\infty} \frac{p^2}{2m} n(p) d^d p \sim \int_{p_0}^{+\infty} \frac{p^2}{p^4} p^{d-1} dp \xrightarrow{\text{d=2,3}} \infty$$

$$n(p) \to C/p^4$$

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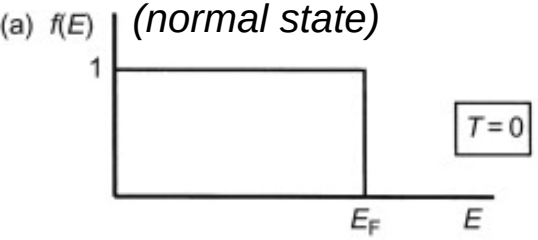
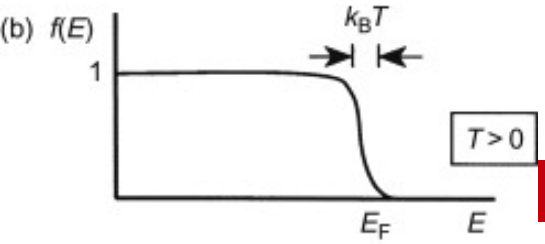


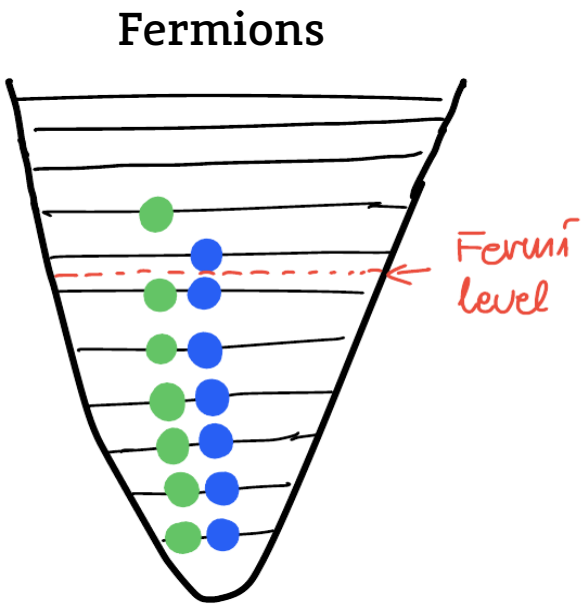


$$\hat{H} = \sum_{\boldsymbol{p},\sigma} \frac{p^2}{2m} a^\dagger_{\boldsymbol{p},\sigma} a_{\boldsymbol{p},\sigma} - g \sum_{\boldsymbol{p},\boldsymbol{k},\boldsymbol{q}} a^\dagger_{\boldsymbol{p}+\boldsymbol{q},\uparrow} a^\dagger_{\boldsymbol{k}-\boldsymbol{q},\downarrow} a_{\boldsymbol{p},\downarrow} a_{\boldsymbol{k},\uparrow}$$

$$E = \langle \hat{H} \rangle = \langle \hat{T} \rangle + \langle \hat{V} \rangle = \infty - \infty$$

Regularization is needed for attractive and short-range interaction in 2D and 3D

Mean-field perspective



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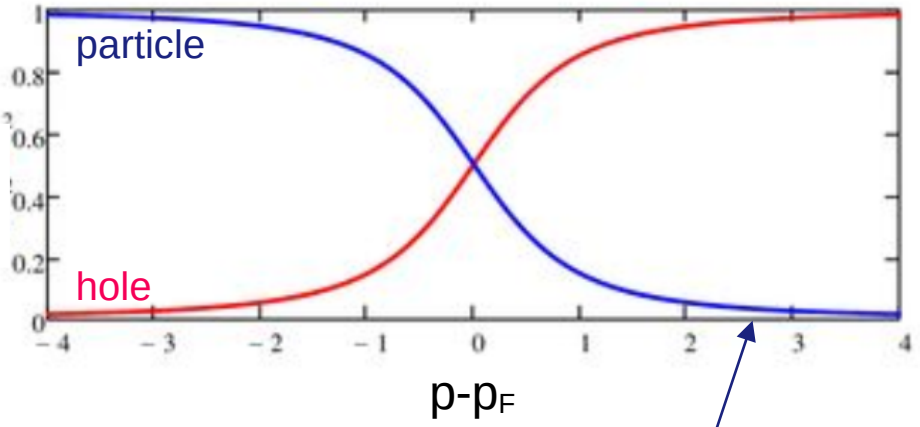

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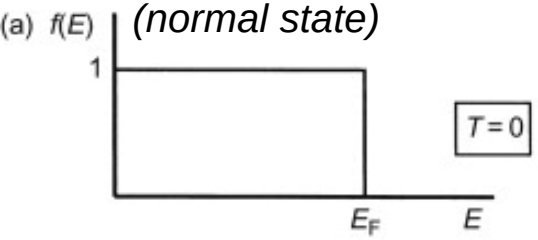
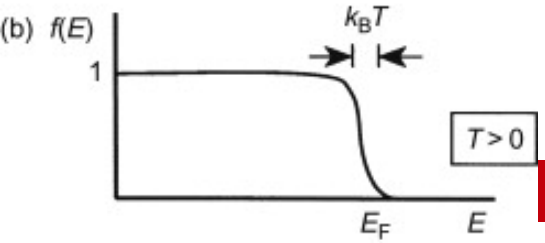
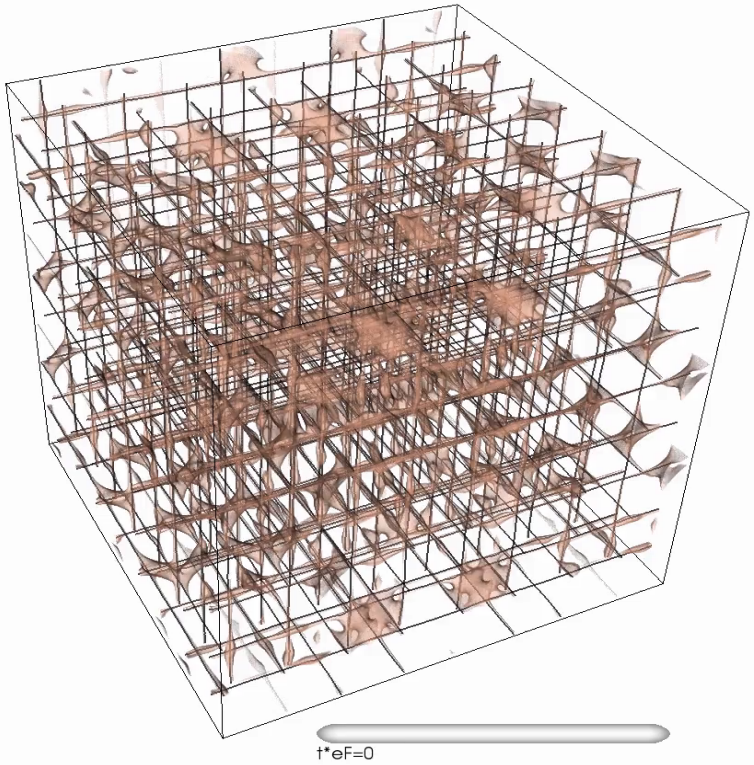




In practical applications we consider states up to some energy cut-off E_c.

Typically E_c is a few times Fermi energy ε_F.

Number of considered states is much bigger than number of particles.



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

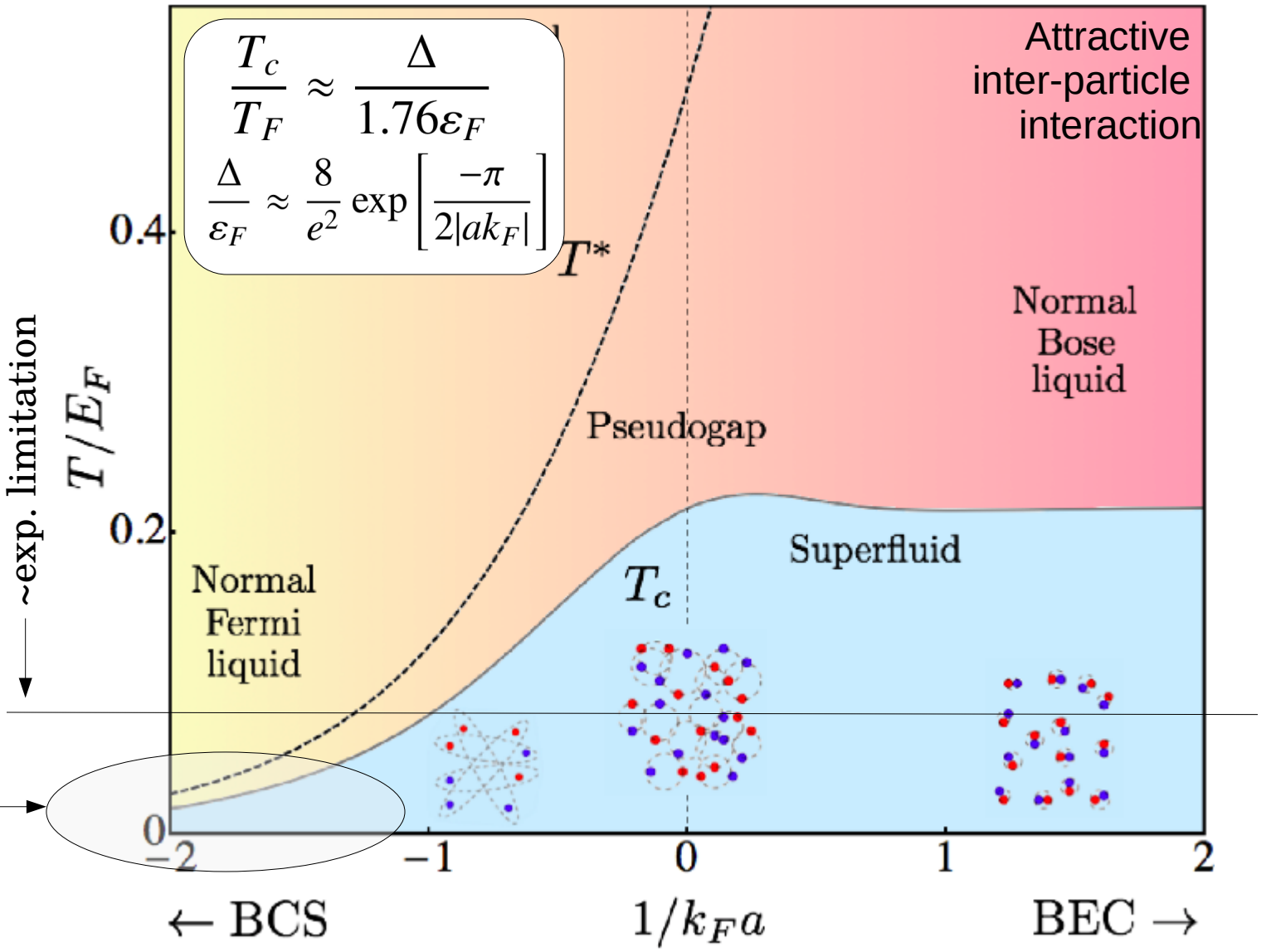
number of atoms = 26,790
number of quasi-particle states = 582,898
number of PDEs = 1,165,796

PRELIMINARY:
quantum turbulence
in the unitary Fermi gas

BCS-BEC crossover: fermions with short-range and attractive interaction

Experiments:

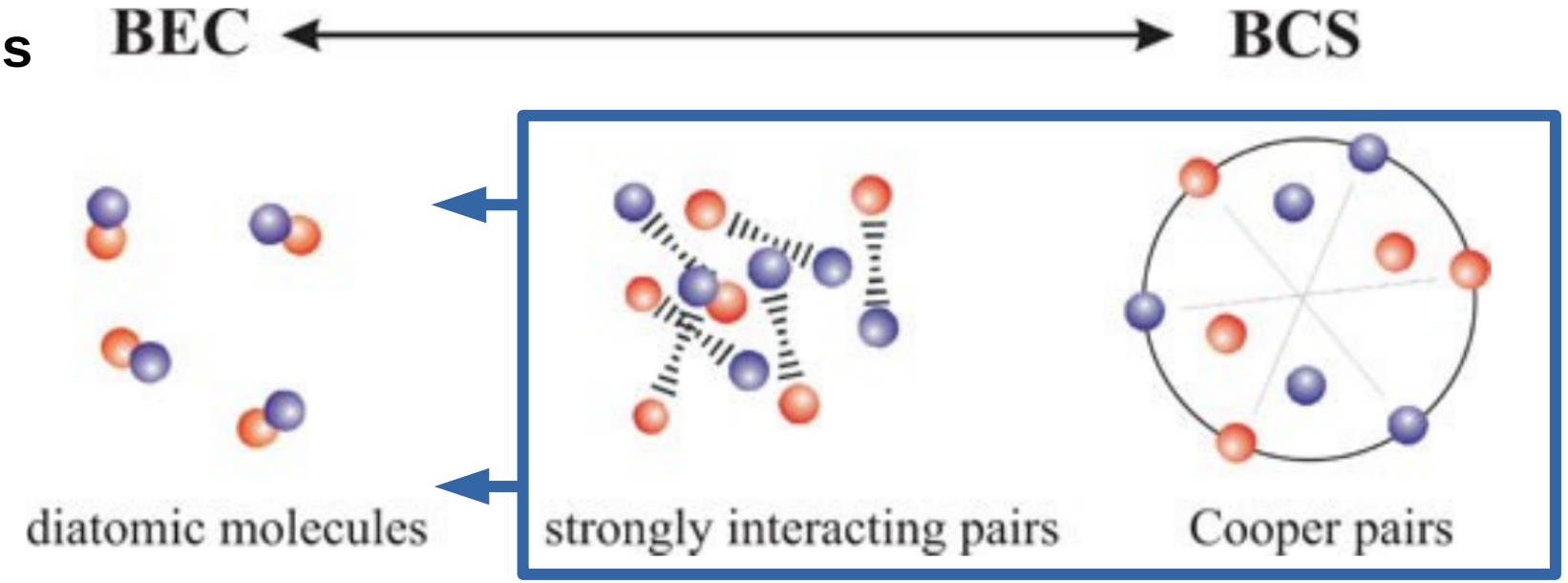
$$\frac{T}{T_F} \gtrsim 0.05 \quad \downarrow \quad |ak_F| \gtrsim 1$$



Regime of validity of BdG theory

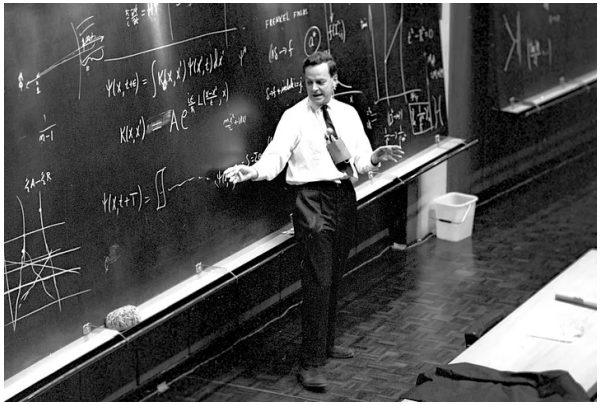
(note: BdG for uniform system = BCS theory)

Methods



Density Functional Theory:
Superfluid Local Density Approximation (SLDA)

- DFT is in principle exact theory
  Hohenberg-Kohn theorem (1964) implies that $\langle O \rangle = \langle \Psi[\rho] | \mathcal{O} | \Psi[\rho] \rangle = O[\rho]$
- ... 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)



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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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*"

Alternative frameworks

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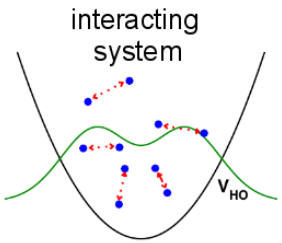
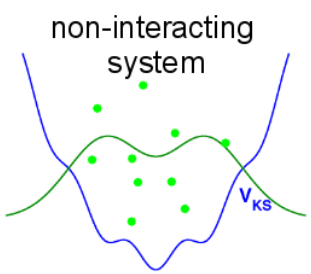
TRADE

$|\Psi\rangle$



KS mapping

$|\Phi\rangle$



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

$$\langle\Psi|\hat{O}_{1B}|\Psi\rangle = O_{1B} = \langle\Phi|\hat{O}_{1B}|\Phi\rangle$$

SLDA-type functional

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

The Fermi-Dirac distribution function

normal density

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

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

kinetic density

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

+ orthonormality condition

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

current density

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

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

anomalous density

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

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

Energy cut-off scale (need for regularization)

Density-Functional Theory for Superconductors

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

SLDA-type functional

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

minimization

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

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

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

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

Example: quantum droplets
GPE → GPE + LHY correction

For example, BdG is equivalent to

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

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

SLDA-type functional

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

Dimensionless functional parameters

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

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

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

dimensional analysis + symmetries

Kinetic term

Potential term

Pairing term

Center of mass motion

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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dimensional analysis + symmetries

Kinetic term

Potential term

Pairing term

Center of mass motion

BdG	ASLDA (A. Bulgac, M.M. Forbes, Phys. Rev. A 75, 031605(R) (2007)) Asymmetric SLDA, a→∞	SLDAE (A. Boulet, G. Wlazłowski, P. Magierski, Phys. Rev. A 106, 013306 (2022)) SLDA Extended, p=0
$A_\lambda \to 1$	$A_\lambda \to A[p(\boldsymbol{r})]$	$A_\lambda \to A[ak_F(\boldsymbol{r})]$
$B_\lambda \to 0$	$B_\lambda \to B[p(\boldsymbol{r})]$	$B_\lambda \to B[ak_F(\boldsymbol{r})]$
$C_\lambda \to \frac{4\pi\hbar^2}{(3\pi^2)^{1/3}m}ak_F$	$C_\lambda \to C[p(\boldsymbol{r})]$	$C_\lambda \to C[ak_F(\boldsymbol{r})]$

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

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

SLDA-type functional

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

Dimensionless functional parameters

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

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

dimensional analysis + symmetries

Kinetic term $+\infty$

Pairing term $-\infty$

The functional is useless without the regularization procedure!

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

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

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

Rapid Communication

Access b

Local density approximation for systems with pairing correlations

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

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

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

INDUCE

Functional parameters

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

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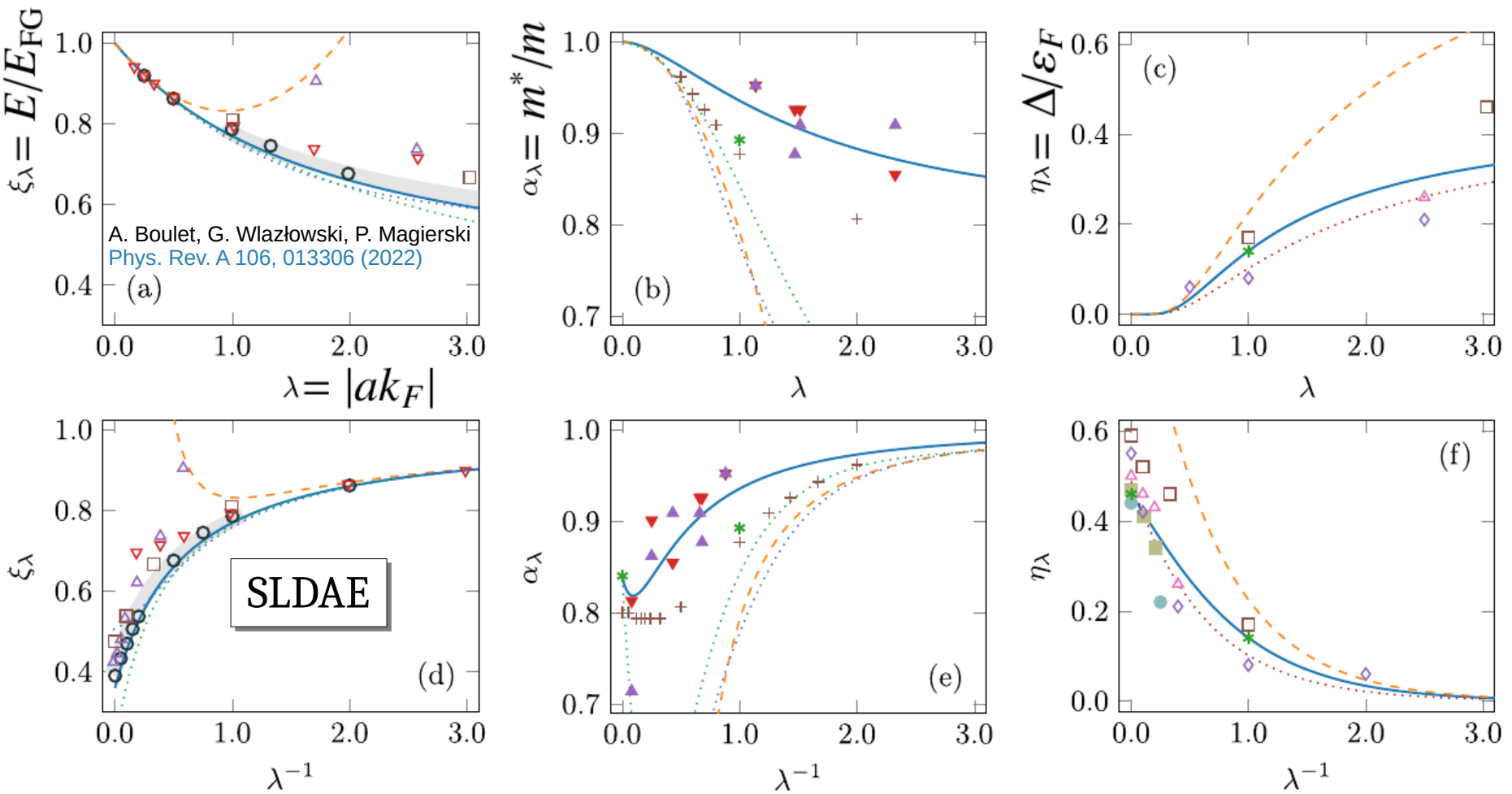

Lee – Yang formula [74–76]
exp. (Navon *et al.*, 2010) [57]
QMC (Carlson *et al.*, 2012) [86]
QMC (Astrakharchik *et al.*, 2004) [87, JS]
QMC (Astrakharchik *et al.*, 2004) [87, BCS]
QMC (Chang *et al.*, 2004) [84]
pp + hh ladder [67, 70]
pp ladder [67, 70]

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*

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

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Density-Functional Theory for Time-Dependent Systems

Erich Runge and E. K. U. Gross
Phys. Rev. Lett. **52**, 997 – Published 19 March 1984

Time-Dependent Density-Functional Theory for Superconductors

O. -J. Wacker, R. Kümmel, and E. K. U. Gross
Phys. Rev. Lett. **73**, 2915 – Published 21 November 1994

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

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

Towards time-dependent problems

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

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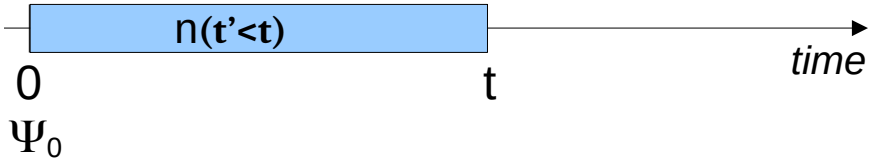
$$E(t) = E[\Psi(t=0), n(\boldsymbol{r}, t' \leqslant t), \ldots]$$



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

Adiabatic approximation

In general integro-differential equations ←

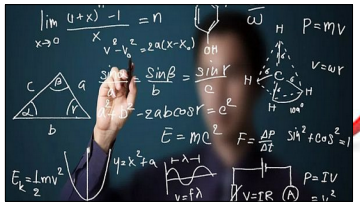
$$E(t) = \int_0^t dt' \int_V d\boldsymbol{r}\, \mathcal{E}[\Psi_0, n(\boldsymbol{r},t'), \ldots]$$

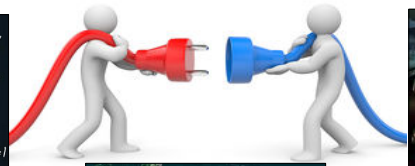
There exits analog of Hohenberg-Kohn theorem for time-dependent problems...

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

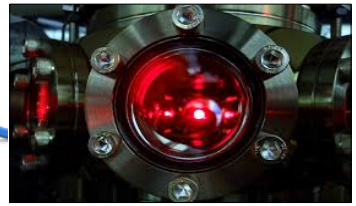
...if the evolution is slow (adiabatic), then the system follows instantaneous ground state
→ use the functional taken from static considerations.

Theoretical method





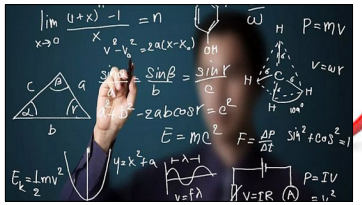
Experiment

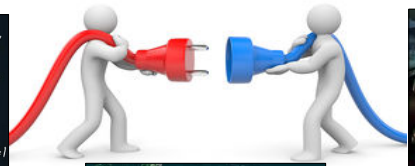


Computer code

PHYSICS.WUT

Theoretical method





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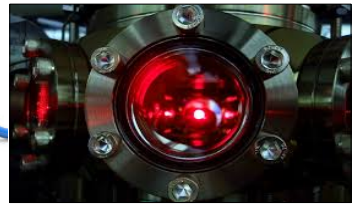

Computer code

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

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

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

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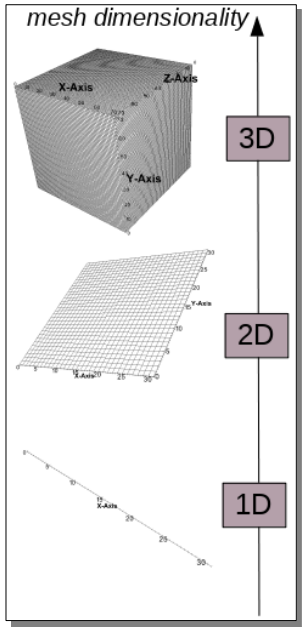
High Performance Computing

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

NVIDIA CUDA | AMD ROCm | open source

PHYSICS.WUT



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

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

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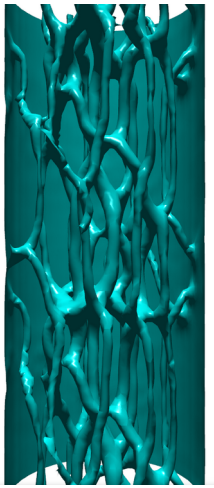
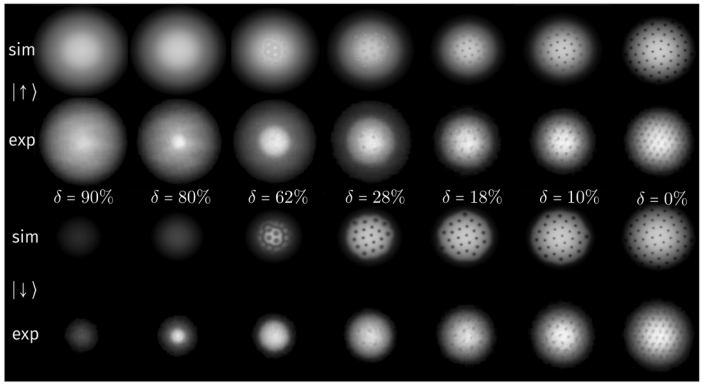
C | NVIDIA CUDA | AMD ROCm | open source

PHYSICS.WUT

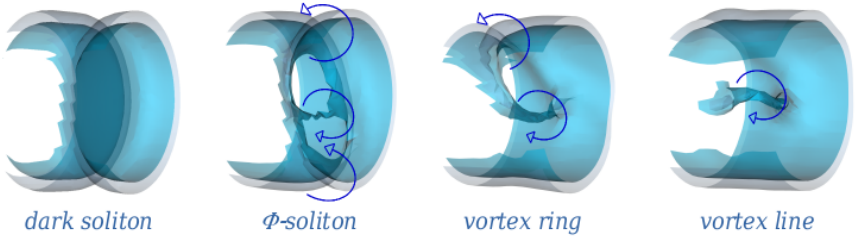
Examples of applications of SLDA in recent years

- 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)



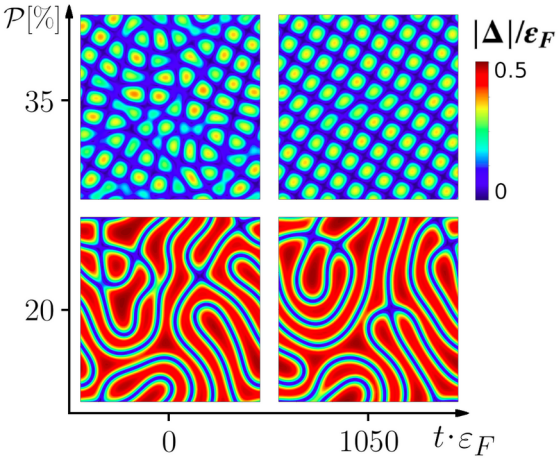


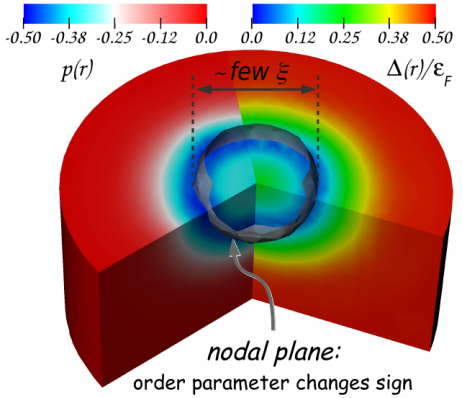
- Quantum turbulence
  - Phys. Rev. A 105, 013304 (2022)



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

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

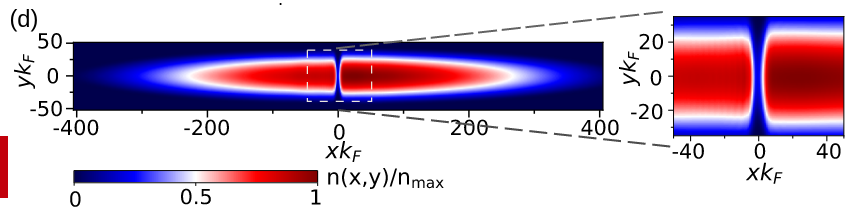




- Quantum chaos
  - Phys. Rev. C 105, 044601 (2022)

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

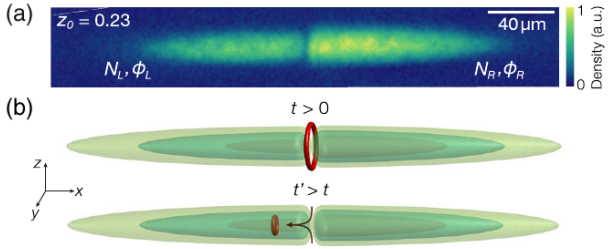
- Phase diagram of spin-imbalanced systems
  - arXiv:2211.01055



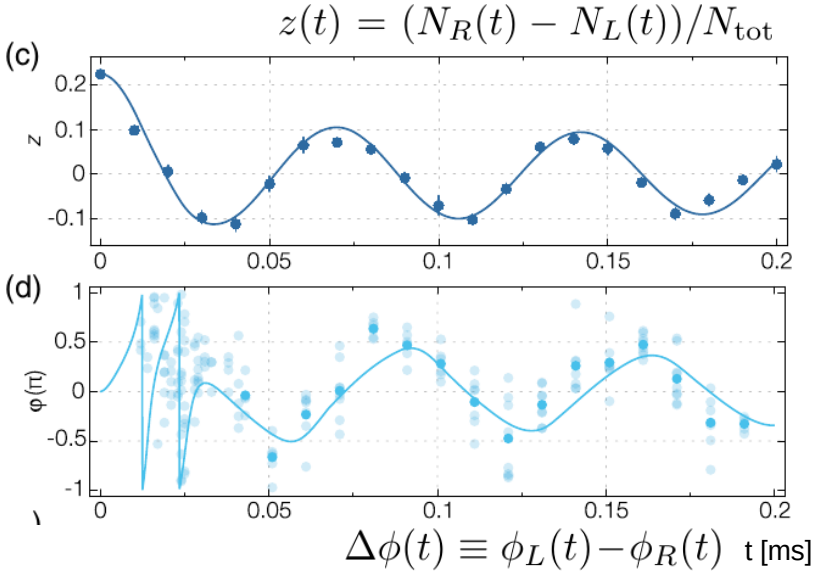
- …

Example: Fermionic Josephson Junction

Inspired by LENS ^{6}Li setup (G. Roati's group):
[1] G. Valtolina, et.al., Science **350**, 1505, (2015);
[2] A. Burchianti, et.al., Phys. Rev. Lett. **120**, 025302 (2018)
[3] K. Xhani, et.al., Phys. Rev. Lett. **124**, 045301 (2020)



Figs from [2]



Experiment

Simulation

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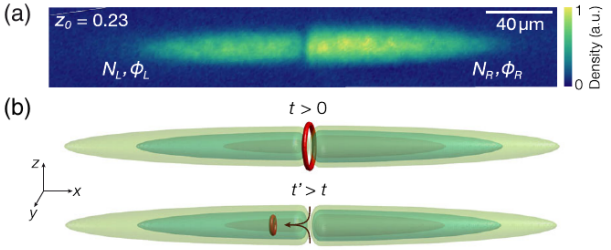
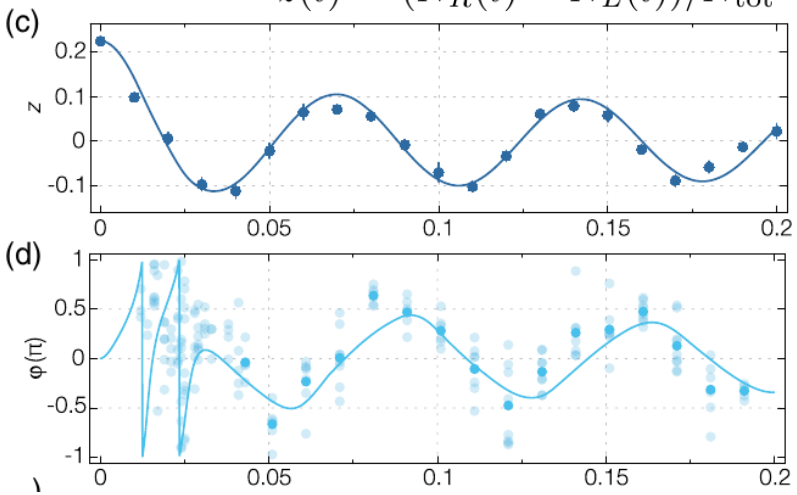


Figs from [2]

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



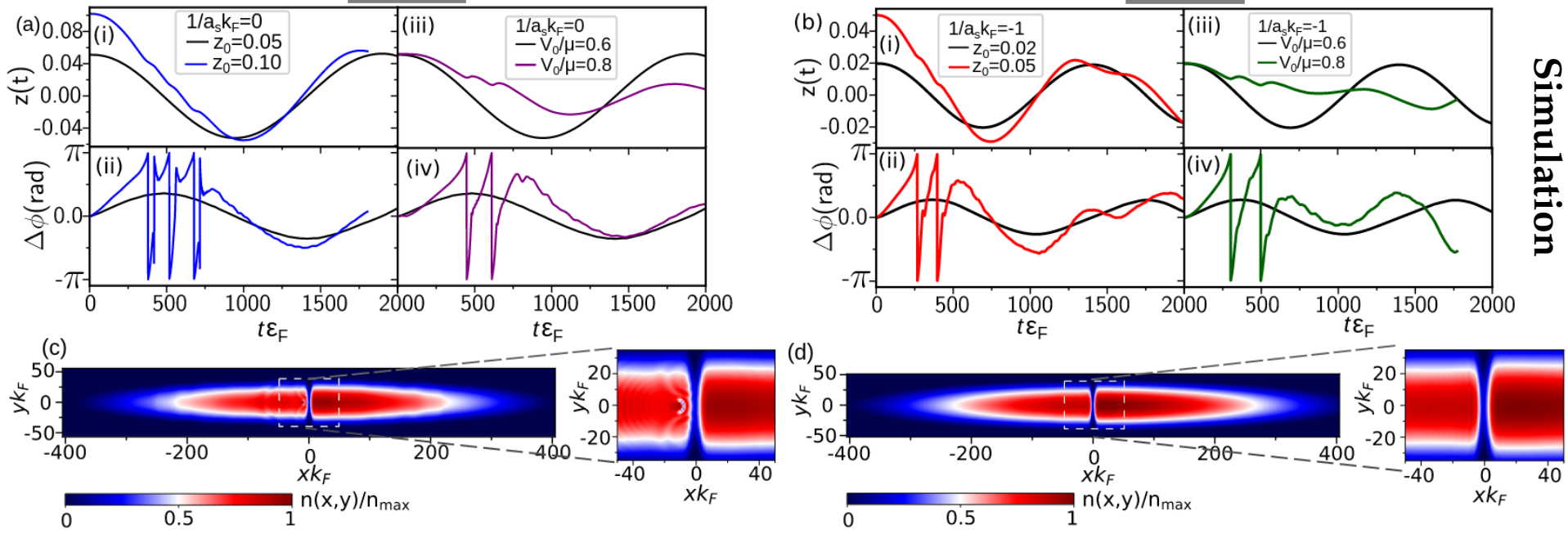
$\Delta\phi(t) \equiv \phi_L(t) - \phi_R(t)$

Experiment

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

UFG

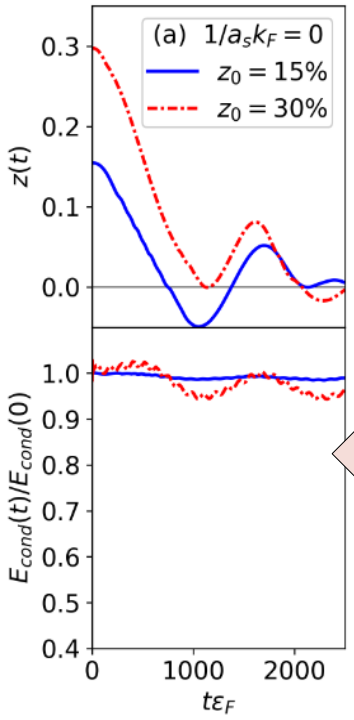
BCS



Simulation

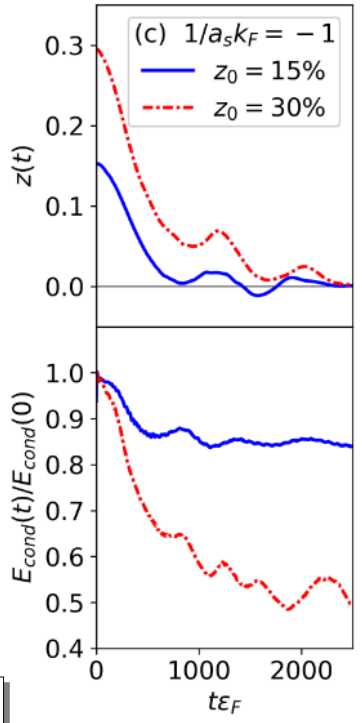
$$E_{\mathrm{BCS}} = E_{\mathrm{FG}} - \frac{3|\Delta|^2}{8\varepsilon_F} N$$

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



pair breaking is negligible

pair breaking!



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

UFG

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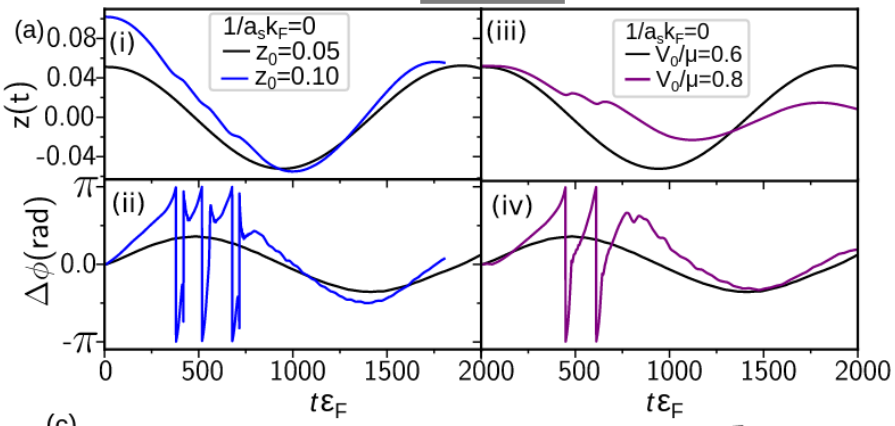

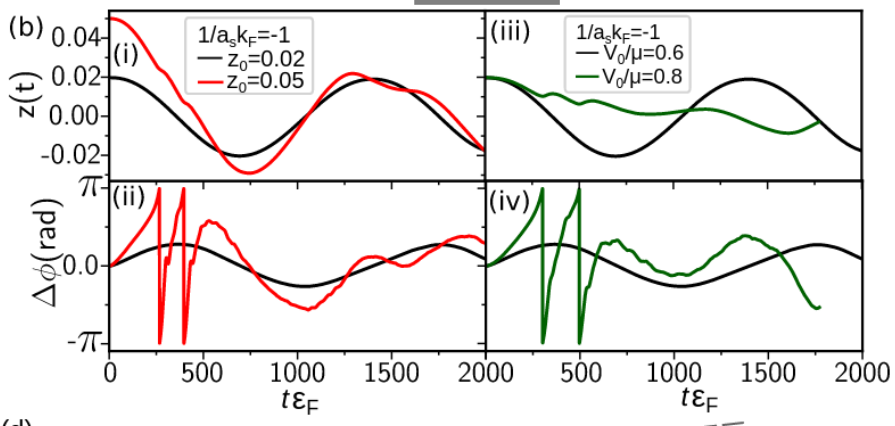

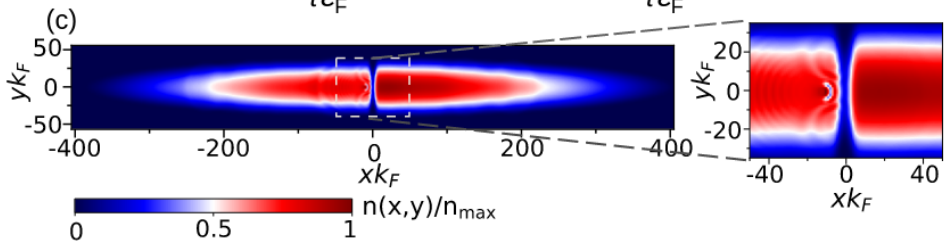

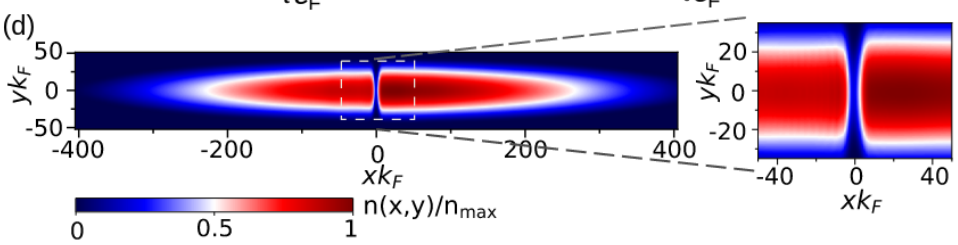

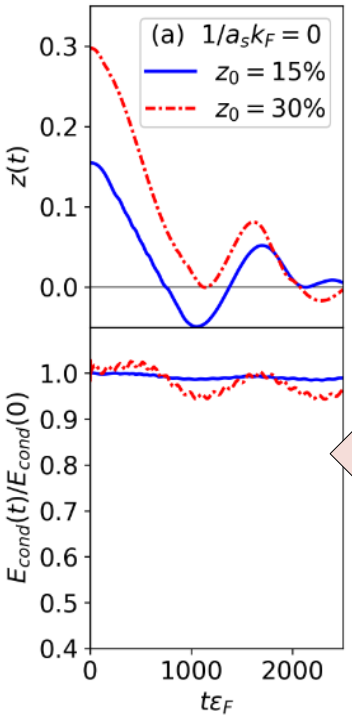

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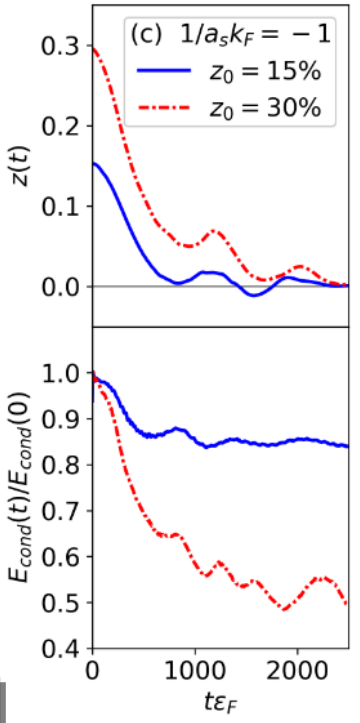
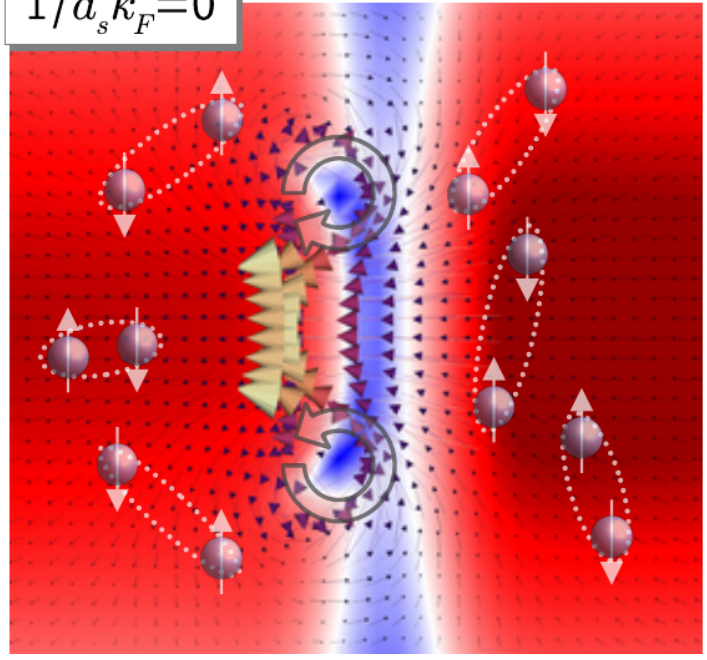
pair breaking!



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

UFG

$1/a_sk_F$=0

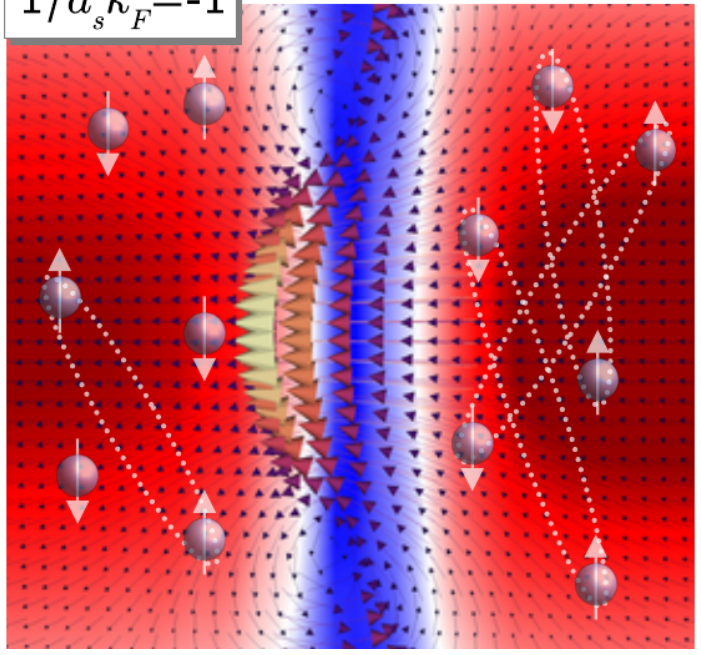


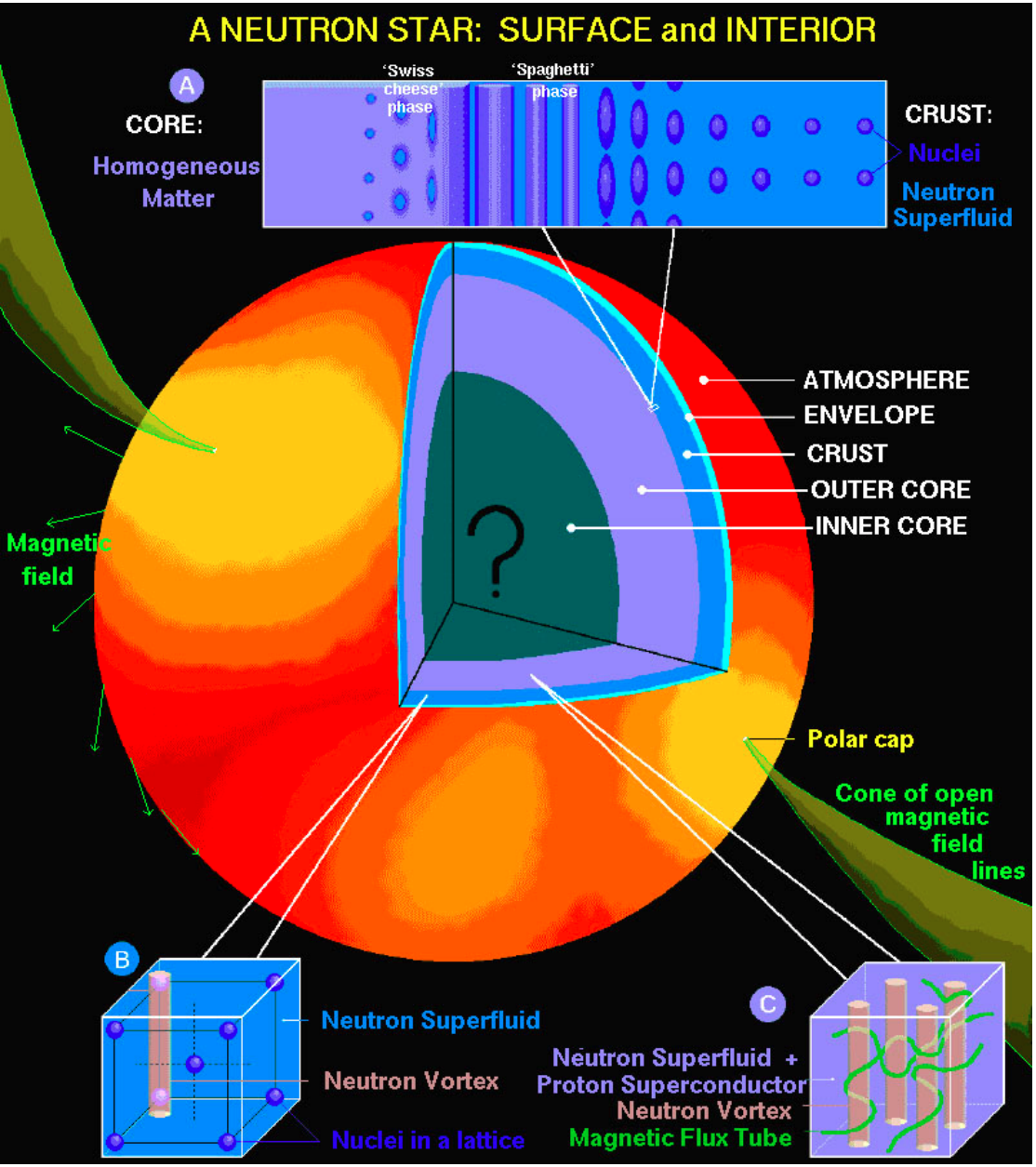
quantum vortex

Cooper pair

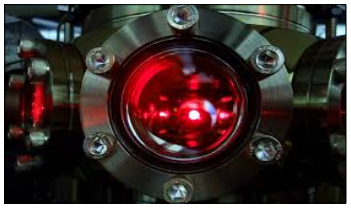
BCS

$1/a_sk_F$=-1





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.

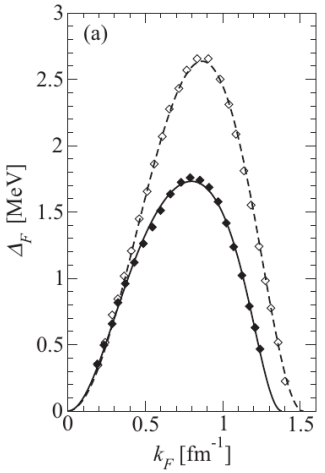
→ … for example, the codes that we use
are based on software
that we constructed for ultracold atoms

Brussels-Montreal Skyrme functionals (BSk)

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

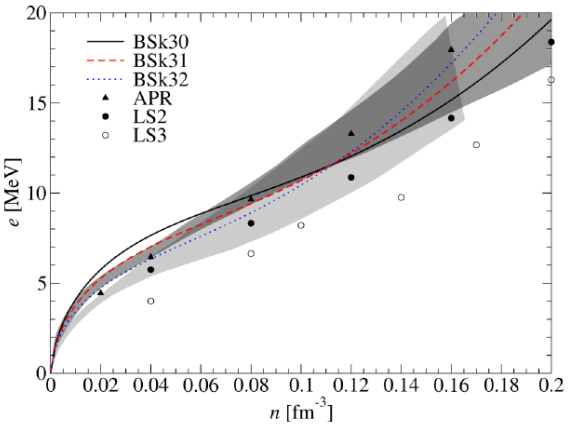
Experimental data:

- 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).



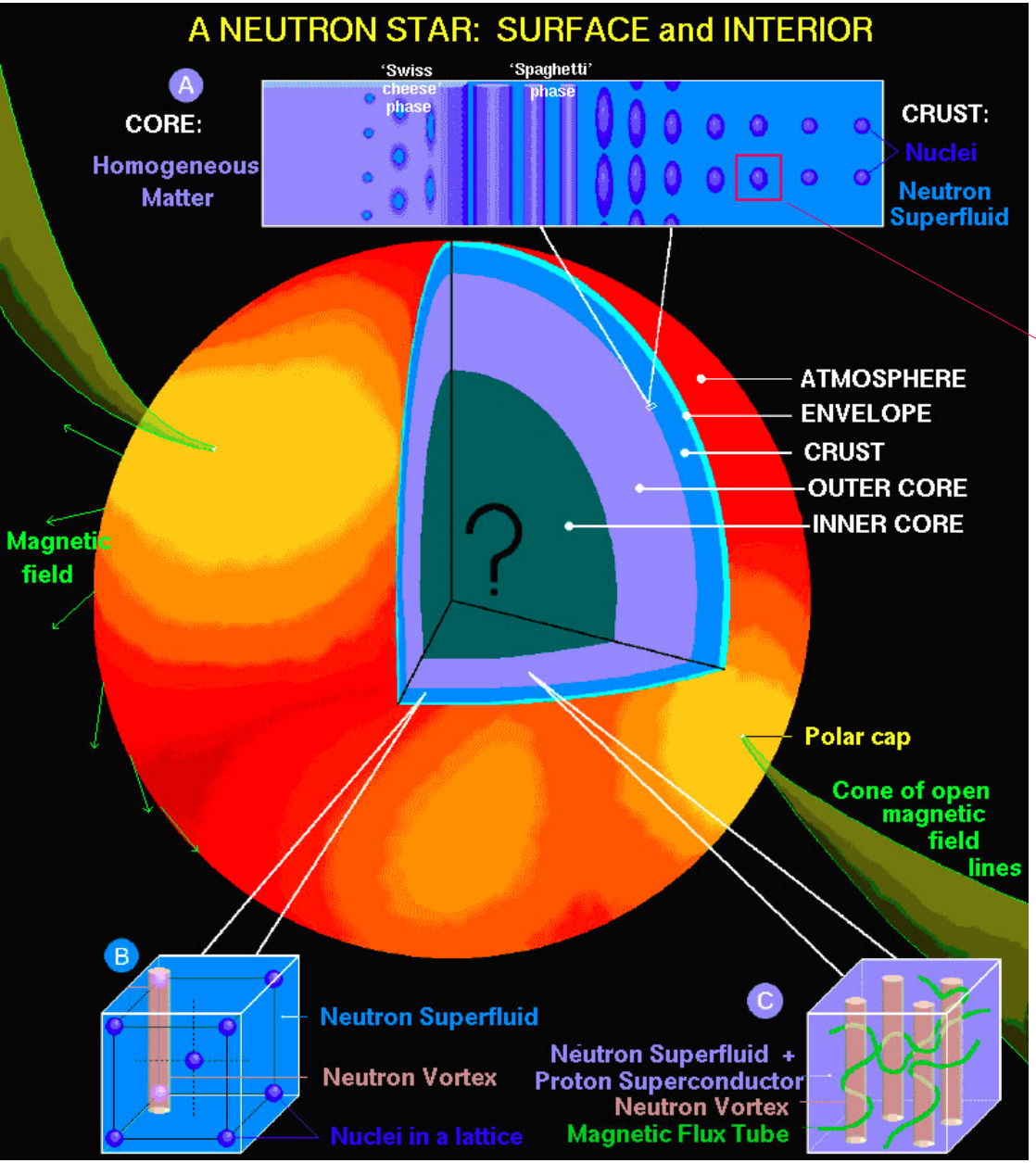
N-body calculations using realistic forces:

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

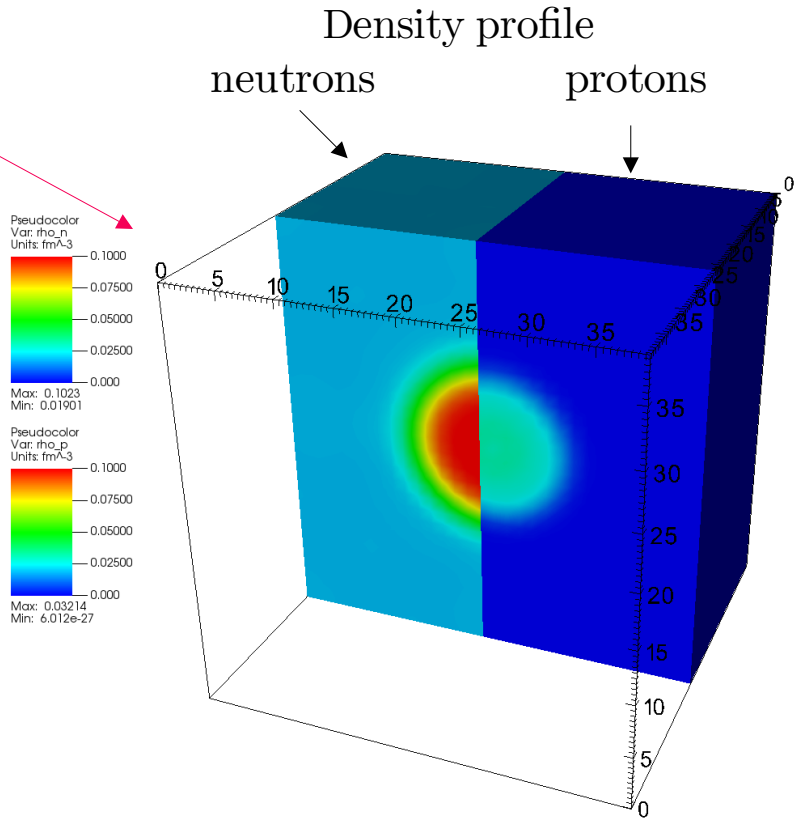


From: Nicolas Chamel talk, Buffalo, March 2016

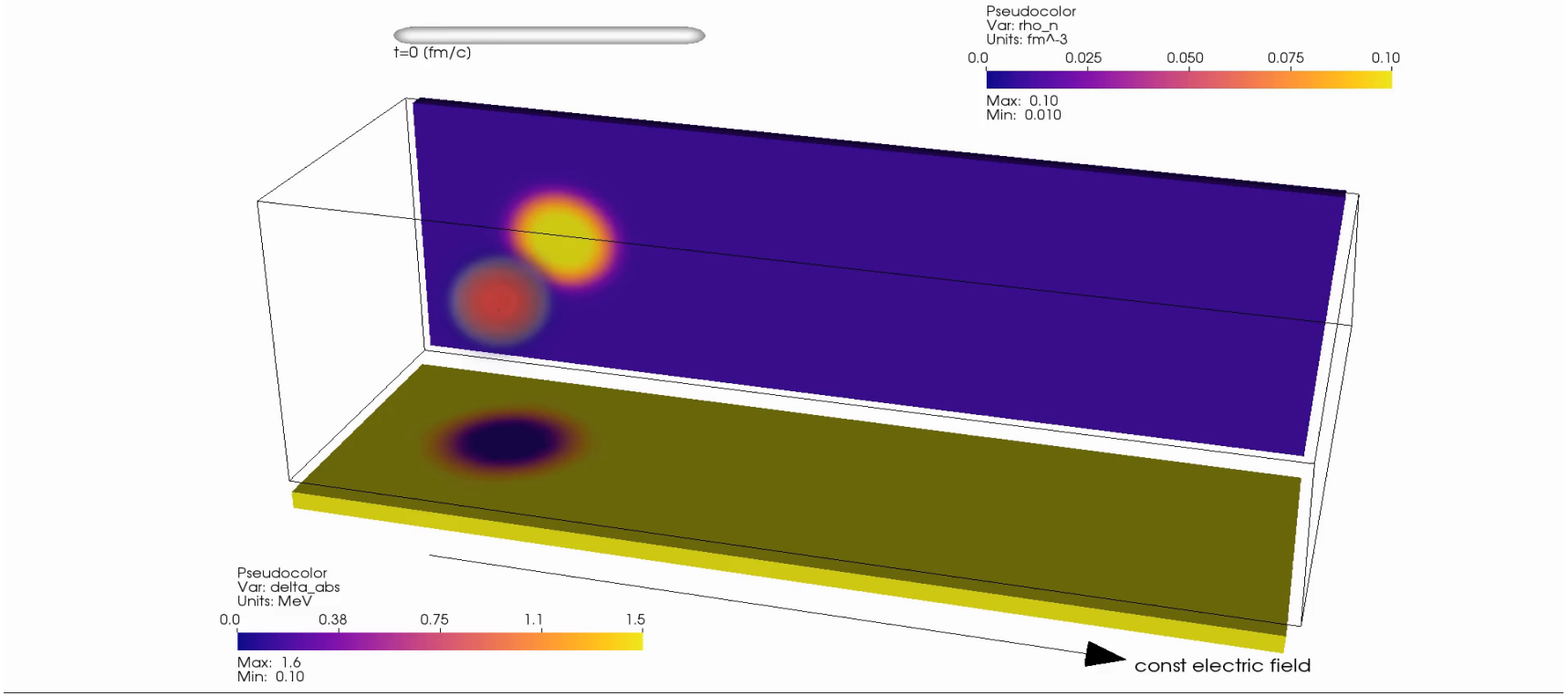
PRC 93, 034337 (2016)



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



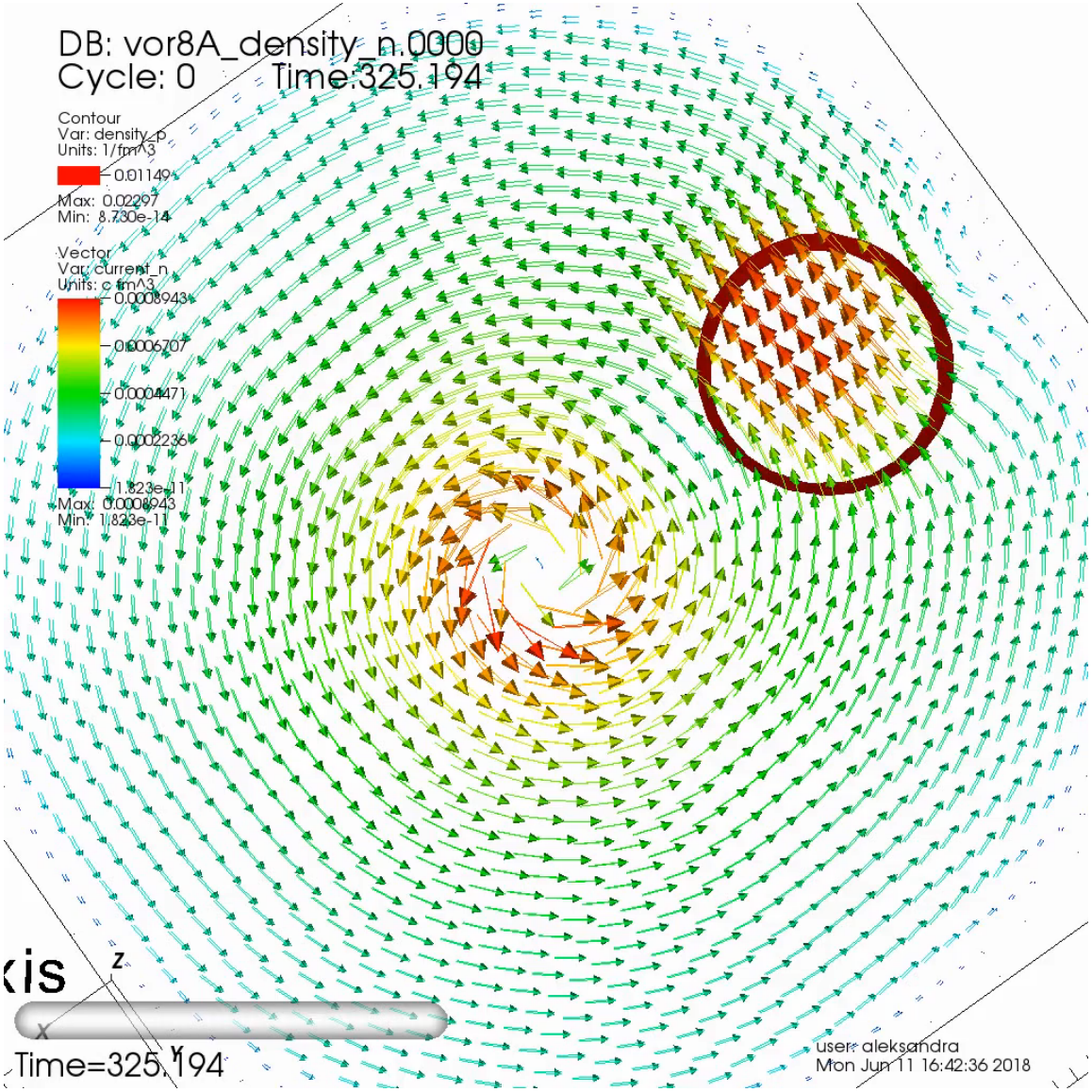
In the simulation box $(40\ \text{fm})^3$ we have 1382 neutrons and 40 protons.

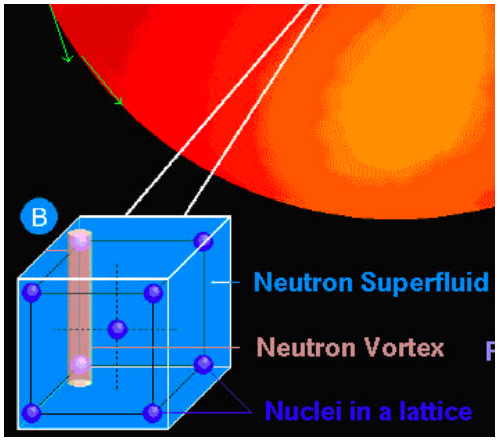


System: *nuclear matter*
3D simulation 40 x 40 x 120 [fm]

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

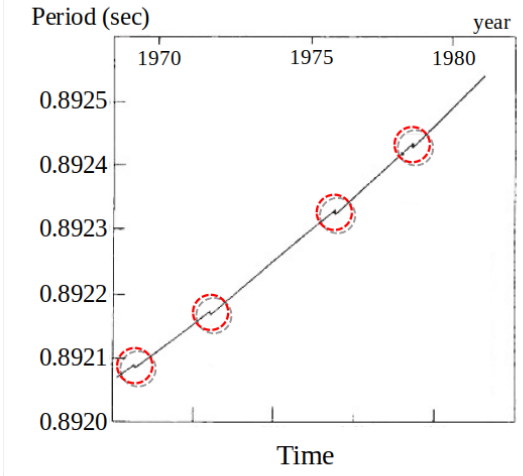
PRELIMINARY:
response of nuclear impurity to uniform electric field





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.

SUMMARY

- Microscopic simulations across whole BCS-BEC crossover are presently feasible:

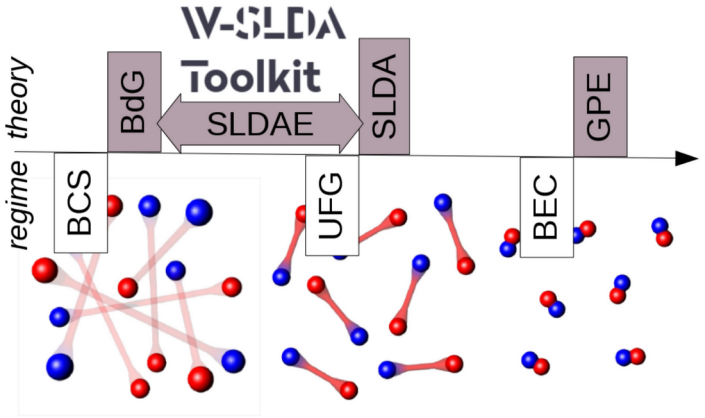
  DFT SLDA → BCS regime; strong interaction;
  GPE → BEC regime

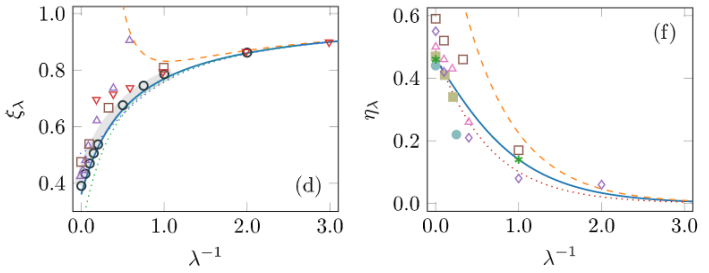
- DFT is general purpose method: it overcomes limitations of mean-field approch, while keeping numerical cost at the same level as BdG calculations.

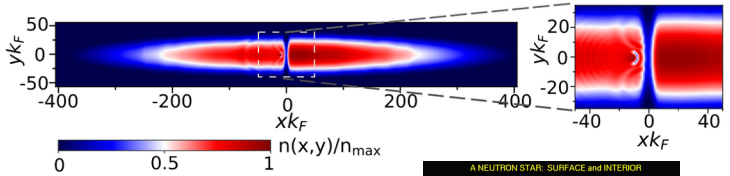
- You do not have to be an expert in DFT to use DFT. Open-source implementation is available.

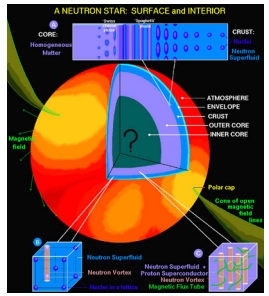
- DFT can benchmark experiments…

- … and provide insight into problems that are not directly accessible, like neutron stars









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