

SCIENCE

CENTRE

Quantum turbulence in superfluid Fermi gases: results of numerical modeling

Gabriel Wlazłowski

Warsaw University of Technology University of Washington



Nonequilibrium phenomena in strongly-correlated ultracold matter Erice-Sicily, 9 - 15 May 2024

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Quantum turbulence



System: *unitary Fermi gas (spin-symmetric)* number of atoms = 26,790 Method: *Time-Dependent Density Functional Theory* PNAS Nexus, pgae160 (2024)



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Computation on spatial grid

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

Quantum turbulence in Bose systems





E. A. L. Henn, J. A. Seman, G. Roati, K. M. F. Magalhães, and V. S. Bagnato, Phys. Rev. Lett. 103, 045301 (2009)

Reviews:

. . .

- L. Madeira, et al., Ann. Rev. of Cond. Mat. Phys., 11 (2020)
- M.C. Tsatsos, et al., Phys. Rep. 622, 1 (2016).
- M. Tsubota, et al., J. Low. Temp. Phys. 188, 119 (2017)

... Superfluid helium J. T. Mäkinen, et.al., Nat. Phys. 19, 898 (2023)



. . .



H. A. J. Middleton-Spencer, A. D. G. Orozco, L. Galantucci, M. Moreno, N. G. Parker, L. A. Machado, V. S. Bagnato, and C. F. Barenghi, Phys. Rev. Research 5, 043081 (2023)



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Nir Navon, Alexander L. Gaunt, Robert P. Smith & Zoran Hadzibabic Nature 539, p. 72–75 (2016)

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An active field of research!

Superfluidity across BEC-BCS crossover



Comparing Bose & Fermi superfluids



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

M. W. Zwierlein, J. R. Abo-Shaeer, A. Schirotzek, C. H. Schunck, and W. Ketterle, Nature 435, 1047 (2005).

Scientific question: What is **impact of quantum statistics** on superfluid (turbulent) dynamics?





$$\begin{split} \frac{\partial \mathbf{v}_n}{\partial t} + (\mathbf{v}_n \cdot \nabla) \mathbf{v}_n &= -\frac{1}{\rho} \nabla P - \frac{\rho_s}{\rho_n} S \nabla T + \nu_n \nabla^2 \mathbf{v}_n + \frac{\rho_s}{\rho} \mathbf{F}, \\ \frac{\partial \mathbf{v}_s}{\partial t} + (\mathbf{v}_s \cdot \nabla) \mathbf{v}_s &= -\frac{1}{\rho} \nabla P + S \nabla T + \mathbf{T} - \frac{\rho_n}{\rho} \mathbf{F}, \end{split}$$

 $\mathbf{f}_D + \mathbf{f}_M = 0,$

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C. F. Barenghi R. J. Donnelly W. F. Vinen (Eds.), QuantizedVortex Dynamics and Superfluid Turbulence, Springer

$$\mathbf{f}_D = -\alpha \rho_s \Gamma \mathbf{s}' \times [\mathbf{s}' \times (\mathbf{v}_n - \mathbf{v}_{s,tot})] - \alpha' \rho_s \Gamma \mathbf{s}' \times (\mathbf{v}_n - \mathbf{v}_{s,tot}),$$

Microscopic Gross-Pitaevskii equation (GPE)

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi - m\mathcal{E}\psi + V_0\psi|\psi|^2,$$



$$\begin{split} \frac{\partial \mathbf{v}_n}{\partial t} + (\mathbf{v}_n \cdot \nabla) \mathbf{v}_n &= -\frac{1}{\rho} \nabla P - \frac{\rho_s}{\rho_n} S \nabla T + \nu_n \nabla^2 \mathbf{v}_n + \frac{\rho_s}{\rho} \mathbf{F} \\ \frac{\partial \mathbf{v}_s}{\partial t} + (\mathbf{v}_s \cdot \nabla) \mathbf{v}_s &= -\frac{1}{\rho} \nabla P + S \nabla T + \mathbf{T} - \frac{\rho_n}{\rho} \mathbf{F}, \end{split}$$

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Microscopic (Bose) Gross-Pitaevskii equation (GPE) $i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi - m\mathcal{E}\psi + V_0\psi|\psi|^2,$

Microscopic (Fermi) Bogolubov-de Gennes equations (BdG)

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} u_{\eta}(\mathbf{r},t) \\ v_{\eta}(\mathbf{r},t) \end{pmatrix} = \mathcal{H}_{BdG} \begin{pmatrix} u_{\eta}(\mathbf{r},t) \\ v_{\eta}(\mathbf{r},t) \end{pmatrix}$$
$$\mathcal{H}_{BdG} = \begin{pmatrix} h_{\uparrow}(\mathbf{r},t) - \mu_{\uparrow} & \Delta(\mathbf{r},t) \\ \Delta^{*}(\mathbf{r},t) & -h_{\downarrow}^{*}(\mathbf{r},t) + \mu_{\downarrow} \end{pmatrix}$$

The system is described as a collection of quasiparticles (a mixture of hole
$$u_{\eta}$$
 and particle v_{η}).

In GPE formalism, only one state is considered, while in BdG, one needs to consider many of them!

- \rightarrow High-Performance Computing (HPC) \leftarrow we use this approach
- \rightarrow Construction of effective approaches like Local Phase Density Approximation [Strinati et. al.]

Synergy: theory & experiment





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Synergy: theory & experiment

including 2 of the top 10.



General purpose framework

SLDA-type functional

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

normal density

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

kinetic density

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

current density

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

anomalous density

$$\nu(\boldsymbol{r}) = \frac{1}{2} \sum_{|E_n| < E_c} \left[u_{n,a}(\boldsymbol{r}) v_{n,b}^*(\boldsymbol{r}) - u_{n,b}(\boldsymbol{r}) v_{n,a}^*(\boldsymbol{r}) \right] f_{\beta}(-E_n).$$
Energy cut-off scale (need for regularization)

Superfluid Local Density Approximation

The Fermi-Dirac distribution function

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

quasiparticle = mixture of
hole particle
$$\varphi_{\eta}(\boldsymbol{r},t) = [u_{\eta}(\boldsymbol{r},t), v_{\eta}(\boldsymbol{r},t)]^T$$

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

+ orthonormality condition (Pauli principle)

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

SLDA (and BdG) allows for solutions: $n \neq 0$ and v=0 \rightarrow Cooper pair breaking \rightarrow effectively normal component $PPHYSICS_WUT$

SLDA-type functional

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

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

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

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



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From point of view of DFT this step represents uncontrolled approximation, called *adiabatic approximation* DFT method from practical point of view:

DFT method allows for the description of many-body quantum systems with higher accuracy than the mean-field method while keeping the computational complexity at the same level as for the mean-field method.

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



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Example: The simplest choice

BdG (mean-field)
$$\mathcal{E}_{BdG} = \frac{\tau}{2} + 4\pi a |\nu(r)|^2$$
There always exists a functional that after minimization provides equations identical to the mean-field equations (zeroth order). $A_{\lambda} \rightarrow 1$ $\int minimization$ $\int minimization$ $\int minimization$ $B_{\lambda} \rightarrow 0$ λ $\int minimization$ $\int minimization$ $\int minimization$ $C_{\lambda} \rightarrow \frac{4\pi\hbar^2}{(3\pi^2)^{1/3}m} ak_F$ $\int minimization$ $\Delta(r)$ $\Delta(r)$ $\Delta(r)$ $\lambda = -4\pi a \sum_{|E_n| < E_c} u_n(\mathbf{r})v_n^*(\mathbf{r}) \frac{f_{\beta}(-E_n) - f_{\beta}(E_n)}{2}$ **PHYSICS.UUT**



Quantum turbulence in 3D



initial state:

- \rightarrow zero temperature (T = 0)
- → regular lattice of imprinted vortices in all three directions
- → the lattice consists of alternately arranged vortices and anti-vortices
- \rightarrow small long-wavelength perturbations of vortex lines

G. Wlazłowski, M.M.Forbes, S. Sarkar, A. Marek, M. Szpindler, PNAS Nexus, pgae160 (2024)





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Calculations:

 \rightarrow TDDFT for two coupling constants: $ak_{F} = \infty$ and $ak_{F} = -1.8$

 \rightarrow modified GPE (Extended Thomas Fermi) for the same initial conditions

Quantum turbulence in 3D - observables



→ flow energy
$$E_{\text{flow}}(t) = \int \frac{\dot{j}^2(\mathbf{r}, t)}{2n(\mathbf{r}, t)} d^3\mathbf{r}$$
,

 \rightarrow total vortex length L(t)

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Quantum turbulence in 3D - observables



Quantum turbulence in 3D – observables



Quantum turbulence in 3D - observables



Quantum turbulence in 3D - observables



PNAS Nexus, pgae160 (2024)



Radial dependence of the:

(a) density n(r),

(b) order parameter $\Delta(r)$,

(c) velocity v(r) = j(r)/n(r)

for a single straight vortex line

at various temperatures in the BCS regime ($k_{Fa} = -1.8$).



PNAS Nexus, pgae160 (2024) rk_F

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Radial dependence of the: (a) density n(r), (b) order parameter $\Delta(r)$, (c) velocity v(r) = j(r)/n(r)for a single straight vortex line at various temperatures in the BCS regime ($k_{Fa} = -1.8$).



PNAS Nexus, pgae160 (2024) rk_F

The thin gray lines show the profiles of selected vortices from the TDDFT calcs taken at time $t\varepsilon_F = 1,000$ → the system effectively heats up!



100

80

60

40

20

100

100

80

60

40

The temperature dependence of the vortex-core density n_{core} allows use fermionic vortices as a local thermometers.

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The temperature dependence of the vortex-core density n_{core} allows use fermionic vortices as a local thermometers.





- → the effective temperature of vortex lines is higher in regions of higher curvature (reconnections, kelvin waves)
- $\rightarrow\,$ similarity to the heating of wire, which is sharply bent back and forth...
- \rightarrow ... also to mechanism proposed by Silaev.

Fig. from: M.A. Silaev, *Universal Mechanism of Dissipation in Fermi Superfluids at Ultralow Temperatures,* Phys. Rev. Lett. 108, 045303 (2012)

SUMMARY (1)

- (TD)DFT is general purpose framework: it overcomes limitations of mean-field approach, while keeping numerical cost at the same level as (TD)BdG calculations.
- (TD)DFT, its implementations and HPC reached the level of maturity that allows for providing predictions for large and complex systems: ~10⁴-10⁵ atoms.
- Dissipation mechanisms play a key role in differentiating fermionic from bosonic turbulence:
 - → role of pair breaking mechanism (production of the "normal component") increases as we move towards BCS regime!





Superfluidity in spin-imbalanced systems $(N_{\uparrow} \neq N_{\downarrow})$



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Superfluidity in spin-imbalanced systems $(N_{\uparrow} \neq N_{\downarrow})$

Spin-up particle Spin-down particle

This so-called LOFF phase remains one of the long-sought phenomena in ultracold Fermi gases

... recent review: J.J. Kinnunen et al 2018 Rep. Prog. Phys. 81 046401

Cooper pairs ~superfluid component (?)

unpaired particles ~normal component (?)

Larkin and Ovchinnikov (LO), and Fulde and Ferrel (FF) proposed new state, with spatial modulation of the pairing field Δ (due to the mismatch between the Fermi surfaces).

 $\Delta(\mathbf{r}) \sim |\Delta| \cos(\mathbf{q} \cdot \mathbf{r})$



Superfluidity in spin-imbalanced systems from numerical modeling

Instead of postulating ansatz for the pairing field [like $\Delta(x) = |\Delta(x)|\cos(kx)$], we let a computer to search for the energy minimum:

→ B. Tüzemen et al 2023 New J. Phys. 25 033013

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Superfluidity in spin-imbalanced systems from numerical modeling

Instead of postulating ansatz for the pairing field $[like \Delta(x) = |\Delta(x)|cos(kx)]$, we let a computer to search for the energy minimum: $\rightarrow B$. Tüzemen et al 2023 New J. Phys. 25 033013 But general concept that we have non-uniformly distributed normal component still holds...



Quantum vortices as a probe of the medium

Inspired by LENS experiments with ⁶Li atoms (G. Roati's group) Figures below from: W. J. Kwon, et.al., Nature 600, 64-69 (2021)



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Quantum vortices can be created at will, manipulated and observed with high precision!

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-1

x (R)

Quantum vortices as a probe of the medium

Inspired by LENS experiments with ⁶Li atoms (G. Roati's group) Figures below from: W. J. Kwon, et.al., Nature 600, 64-69 (2021)



a



TDDFT result: Vortex dipoles can be used as robust probes if the normal component is distributed uniformly or non-uniformly.

In preparation: A. Barresi, P. Magierski, G. Wlazłowski (2024)







Warsaw University W-SLDA Toolkit of Technology W-BSk Toolkit

W-SLDA Toolkit

Self-consistent solver of mathematical problems which have structure formally equivalent to Bogoliubov-de Gennes equations.

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

time-dependent problems: td-wslda

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

Extension to nuclear matter in neutron stars

Unified solvers for static and time-dependent problems

Dimensionalities of problems: 3D, 2D and 1D



The W-SLDA Toolkit has been expanded to encompass nuclear systems, now available as the W-BSk Toolkit.

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Integration with VisIt: visualization, animation and analysis tool

static problems: st-wslda

Speed-up calculations by exploiting High Performance Computing

Functionals for studies of BCS and unitary regimes





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



Extension to nuclear matter in neutron stars



... all tools we create for Fermi gas simulations are publicly accessible as open-source...

SUMMARY (2)

- (TD)DFT is general purpose framework: it overcomes limitations of mean-field approach, while keeping numerical cost at the same level as (TD)BdG calculations.
- (TD)DFT, its implementations and HPC reached the level of maturity that allows for providing predictions for large and complex systems: ~10⁴-10⁵ atoms.
- Dissipation mechanisms play a key role in differentiating fermionic from bosonic turbulence:
 - → role of pair breaking mechanism (production of the "normal component") increases as we move towards BCS regime!
- Quantum vortices can be used as probes if the normal component is distributed uniformly or non-uniformly.
 - → indirect tests for existence of exotic phases in spin-imbalanced gases.

Thank you!

Contributors: P. Magierski, A. Barresi (WUT); A. Boulet (WUT→Le Mans); M. Forbes, S. Sarkar,(WSU); A. Bulgac (UW); B. Tüzemen (WUT→PAS); T. Zawiślak (WUT→U.Trento); A. Marek (MPCDF), M. Szpindler (Cyfronet).

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

Theoretical

method



Experiment



