Towards general-purpose simulation platform for superfluid fermions

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Density functional theory for superfluid systems...

The real-time dynamics are given by equations, similar to Time-Dependent Bogolubov-de Gennes (TDBdG) equations:

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

where the single-particle Hamiltonian *h* and pairing potential *Δ* are obtained by taking the appropriate functional derivatives of the energy density functional. The TDDFT approach offers a description *beyond TDBdG* approximation!

Generic form of SLDA-type functionals

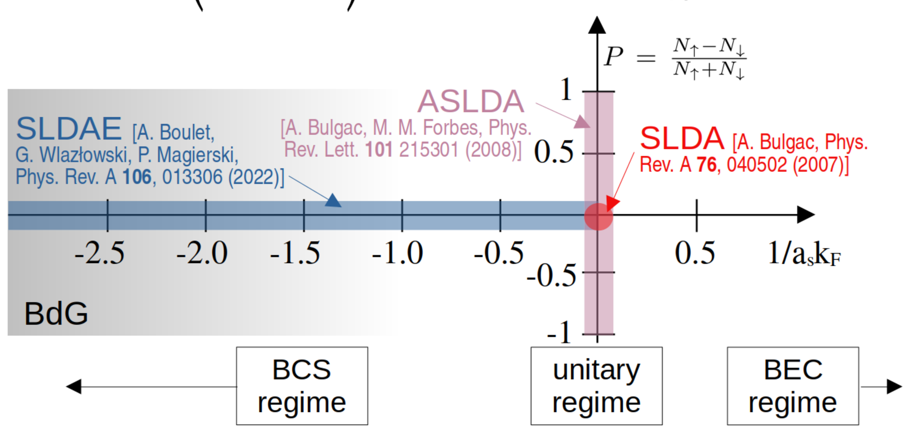
*Densities: normal n, kinetic τ, current **j** and anomalous ν are defined through quasiparticle orbitals $\varphi_n=[u_n,v_n]^T$*

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

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

$$\int\varphi_n^{\dagger}(\boldsymbol{r},t)\varphi_m(\boldsymbol{r},t)d\boldsymbol{r}=\delta_{nm}$$

(Pauli principle)



$$h_\sigma=-\nabla\frac{\delta E_0}{\delta\tau_\sigma}\nabla+\frac{\delta E_0}{\delta n_\sigma}+(V_\sigma^{(\mathrm{ext})}-\mu_\sigma)-\frac{i}{2}\left\{\frac{\delta E_0}{\delta\boldsymbol{j}_\sigma}-\boldsymbol{v}_\sigma^{(\mathrm{ext})},\nabla\right\}$$

$$\Delta=-\frac{\delta E_0}{\delta\nu^{*}}+\Delta^{(\mathrm{ext})}$$

... and High-Performance Computing

Static equations: $\hat{H}\Psi_n=E_n\Psi_n$

Time-dependent equations: $i\hbar\frac{\partial\Psi}{\partial t}=\hat{H}\Psi$

- *3D, 2D and 1D modes*
- *Weak and strong interaction regimes*
- *Spin symmetric and spin imbalanced systems*
- *Zero temperature and finite temperature modes*
- *Mass imbalanced systems (BdG only)*

W-SLDA Toolkit

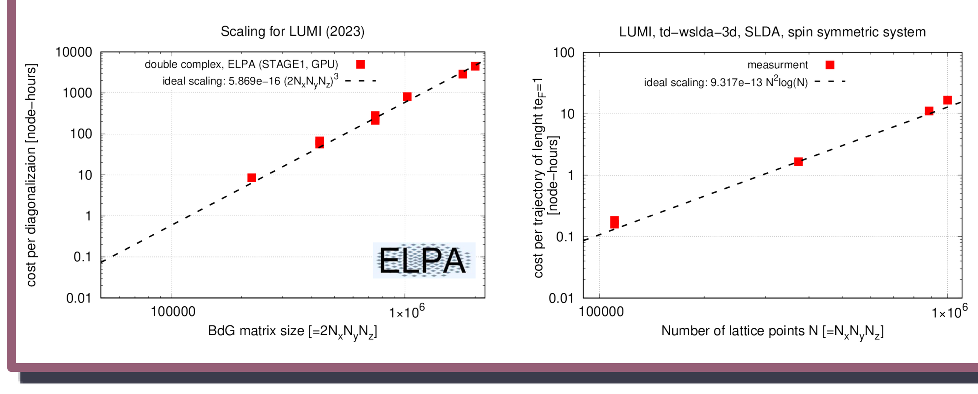
Self-consistent solver of mathematical problems which have structure formally equivalent to Bogoliubov-de Gennes equations.

Solving the problem:

- *We use lattice formulation*
  - *3D without any symmetry restrictions: Ψ=φ(x,y,z)*
  - *2D with translational invariance along z direction: Ψ=φ(x,y)exp(ik_z z)*
  - *1D with translational invariance along y and z directions: Ψ=φ(x)exp(ik_y y)exp(ik_z z)*
- *Number of evolved quasiparticle orbitals from range 10^5-10^6*
- *Derivatives are computed with spectral methods - insures very high accuracy*
- *Time integration with multi-step ABM 5th order integrator*

Present (super)computing capabilities:

- *Spatial lattice size: up to 100^3*
- *Number of atoms: up to 10^5*
- *Trajectory length: up to 2,000 $\hbar/\varepsilon_F$*



W-SLDA Toolkit

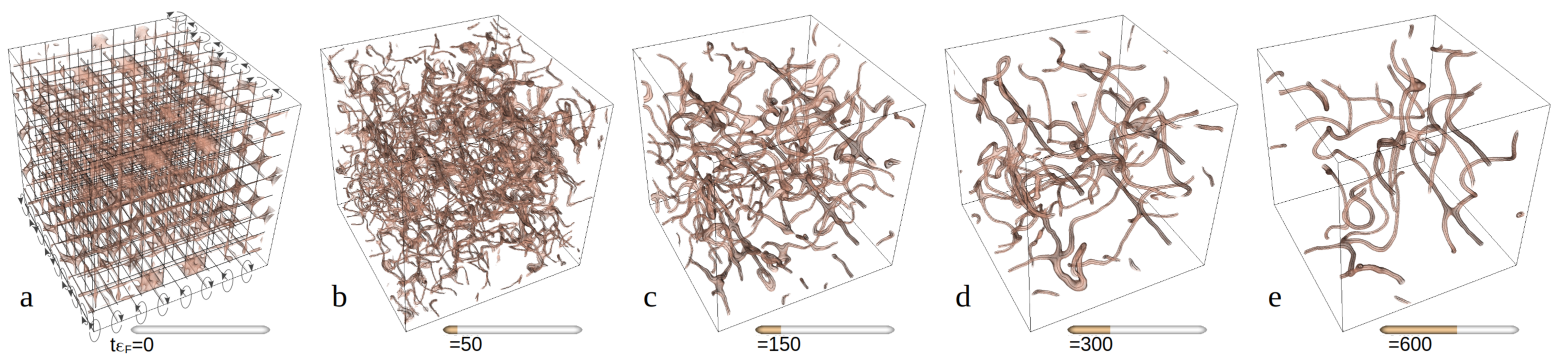
https://wslda.fizyka.pw.edu.pl/

Quantum turbulence in strongly interacting Fermi gas

G. Wlazłowski, M. M. Forbes, S. Sarkar, A. Marek, M. Szpindler, PRELIMINARY

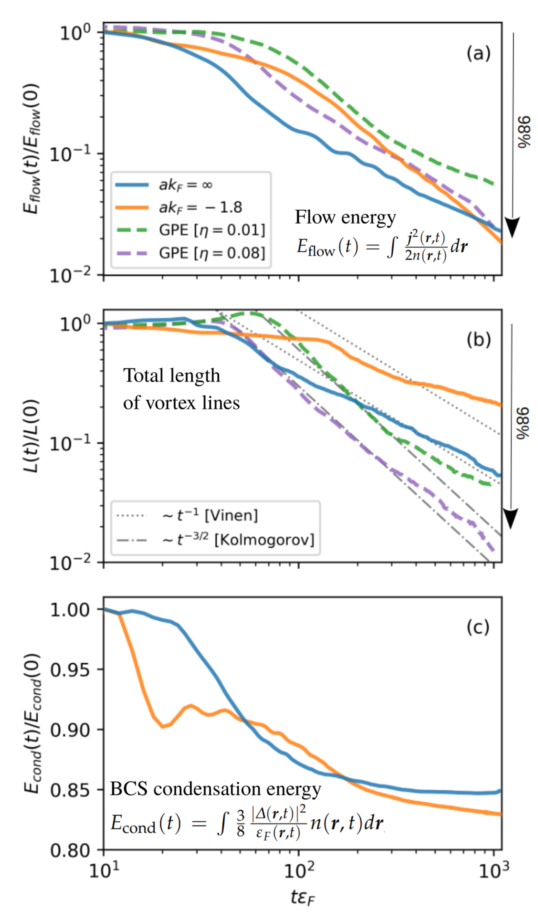
We consider the turbulent state in a ultra-cold atomic gas of fermionic type, and contrast predictions with the commonly used Gross-Pitaevskii equation. We demonstrate the importance of the energy dissipation mechanism due to the heating up of quantum vortex cores (consistent with Silaev mechanism).

Selected frames of the time evolution of the vortex tangle according to TDDFT method



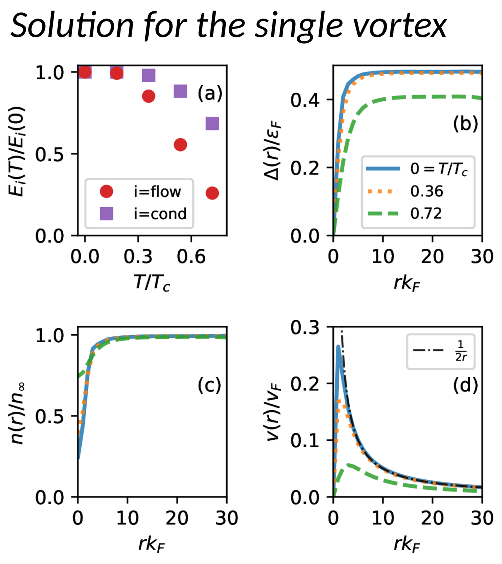
GPE equation used to contrast results with TDDFT approach (m_C – mass of Cooper pair)

$$ie^{i\eta}\frac{\partial\Psi(\boldsymbol{r},t)}{\partial t}=\left(-\frac{\hbar^2}{2m_C}\nabla^2+2\frac{\delta\mathcal{E}_{\mathrm{GPE}}}{\delta n}\right)\Psi(\boldsymbol{r},t)\quad \mathcal{E}_{\mathrm{GPE}}=\xi\tfrac{3}{5}\varepsilon_F n\quad n=2|\Psi|^2$$



In all three cases (TDDFT and GPE run with η = 0.08) the amount of dissipated flow energy is about the same, being at the end of the simulation about 98% of the initial value ... but the total vortex length does not exhibit similar trend!

Solution for the single vortex



Simulation settings:

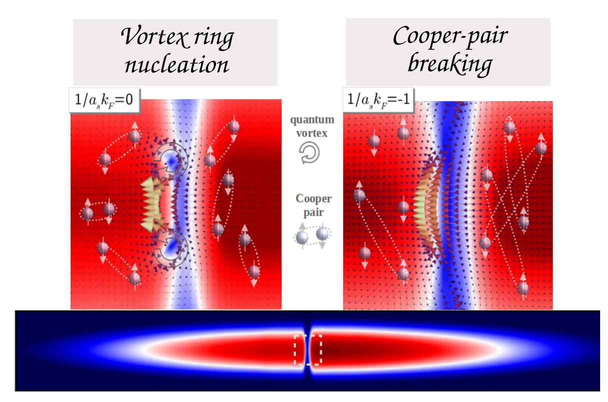
- *Systems:*
  Unitary Fermi Gas: $ak_F\to-\infty$
  BCS Fermi Gas: $ak_F\to -1.8$
- *Lattice: 100^3*
- *Number of atoms $N_\uparrow+N_\downarrow$*
  Unitary Fermi Gas: ≈27k
  BCS Fermi Gas: ≈108k
- *Number of PDEs: ≈1.1M*
- *Computer: LUMI (CSC, Finland)*

Dissipation in fermionic Josephson junction

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

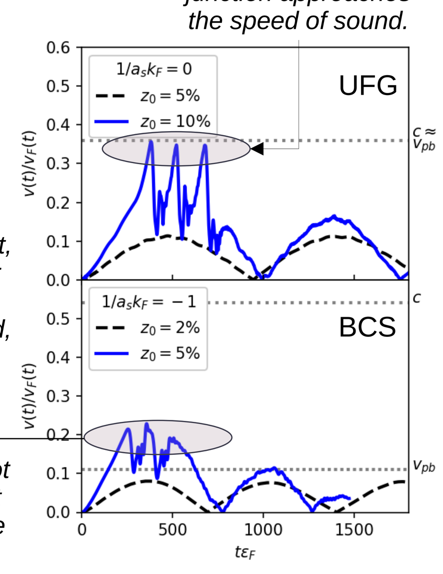
We identify the distinct microscopic origins of emerging dissipative dynamics across the weakly (BCS) and strongly (UFG) interacting limits.

A quantum vortex is nucleated whenever the flow through the junction approaches the speed of sound.



In the BCS limit, the flow never reaches the speed of sound, but it exceeds pair-breaking velocity.

Vortices are not nucleated, but oscillations are damped.

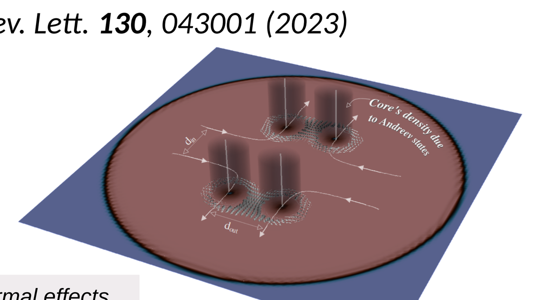


The setup is inspired by LENS (Florence) experiment: A. Burchianti et. al., Phys. Rev. Lett. **120**, 025302 (2018).

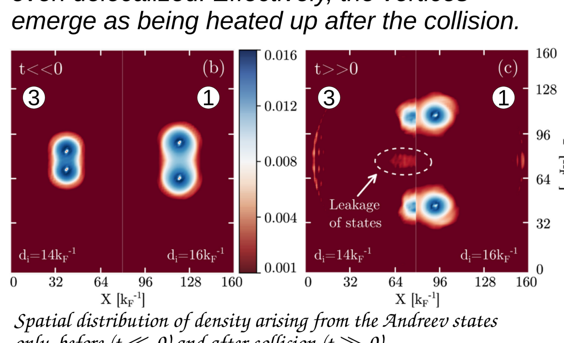
Dissipative dynamics of quantum vortices

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

We expose the impact of the vortex-bound states on dissipative dynamics in a fermionic superfluid.

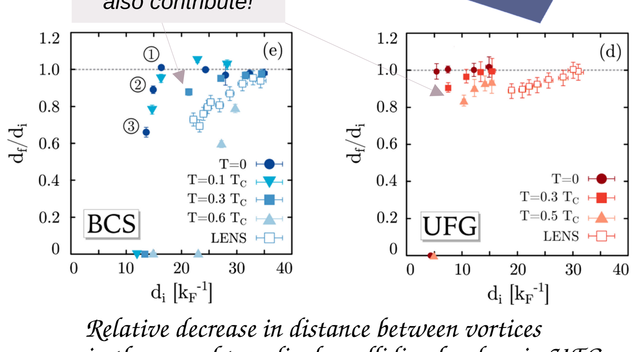


Distribution of Andreev states is affected during the collision, and some of these states become even delocalized. Effectively, the vortices emerge as being heated up after the collision.



Spatial distribution of density arising from the Andreev states only, before ($t\ll 0$) and after collision ($t\gg 0$).

Thermal effects also contribute!



Relative decrease in distance between vortices in the case of two dipoles colliding head-on in UFG and BCS regimes at various temperatures.

The setup is inspired by LENS (Florence) experiment: W. J. Kwon et. al., Nature **600**, 64 (2021).

Disordered structures in spin-imbalanced Fermi gas

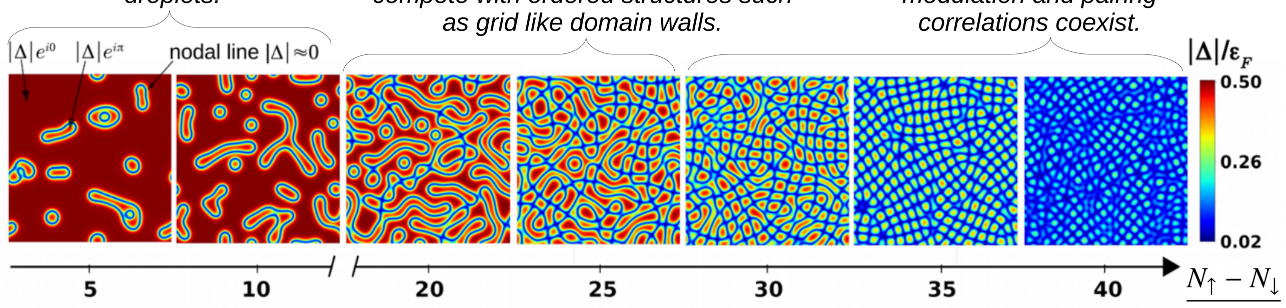
B. Tüzemen, T. Zawiślak, G. Wlazłowski, P. Magierski, New J. Phys. **25**, 033013 (2023)

We investigate properties of spin-imbalanced ultracold Fermi gas in a large range of spin imbalances.

At low polarization values we predict the structure of the system as consisting of several spin-polarized droplets.

*As the polarization increases, the system self-organizes into a **disordered structures** similar to liquid crystals, and energetically they can compete with ordered structures such as grid like domain walls.*

At higher polarizations the system starts to develop regularities that, in principle, can be called supersolid, where periodic density modulation and pairing correlations coexist.



$$E_{\mathrm{BdG}}=\int\left(\frac{\tau_\uparrow(\boldsymbol{r})}{2}+\frac{\tau_\downarrow(\boldsymbol{r})}{2}+g|\nu(\boldsymbol{r})|^2\right)d\boldsymbol{r}$$

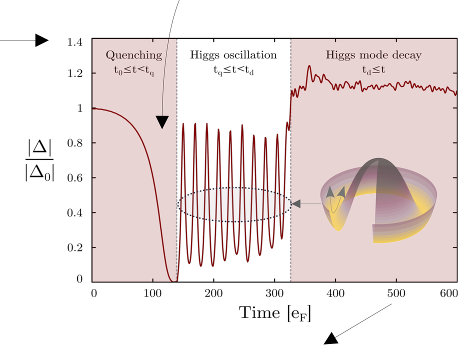
These results were obtained with BdG functional: kinetic energy for both spin components + pairing correlations

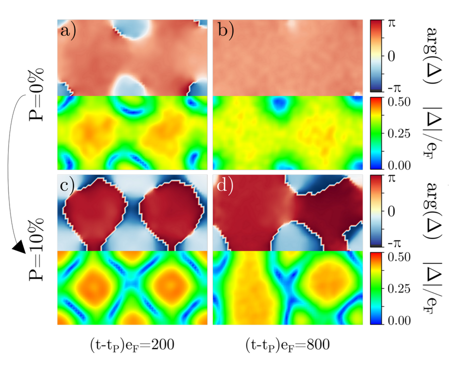
Generation and decay of Higgs mode

A. Barresi, A. Boulet, G. Wlazłowski, P. Magierski, Sci. Rep. **13**, 11285 (2023)

We study the life cycle of the large amplitude Higgs mode in strongly interacting superfluid Fermi gas.

The Higgs mode is induced by the interaction quench.

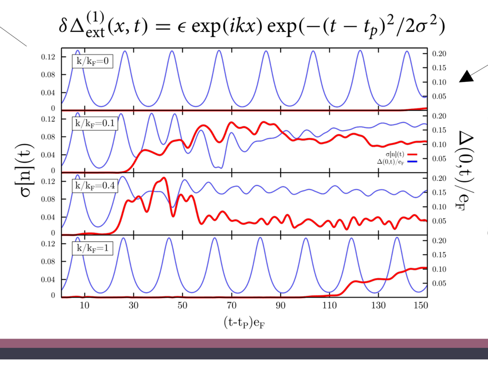




We identify similarities with FFLO states, which become more prominent at nonzero spin imbalances.

The post-decay state is characterized by spatial fluctuations of the order parameter and density at scales comparable to the superfluid coherence length scale.

$$\delta\Delta_{\mathrm{ext}}^{(1)}(x,t)=\epsilon\exp(ikx)\exp(-(t-t_p)^2/2\sigma^2)$$



*The mode is **dynamically unstable** against external perturbation.*

The appearance of inhomogeneities in the density is associated with the decay

$$\sigma[n](t)=\frac{\sqrt{\langle n^2\rangle(t)-\langle n\rangle^2(t)}}{\langle n\rangle(t=0)}$$

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