Vortices in Bose and Fermi superfluids: similarities and differences

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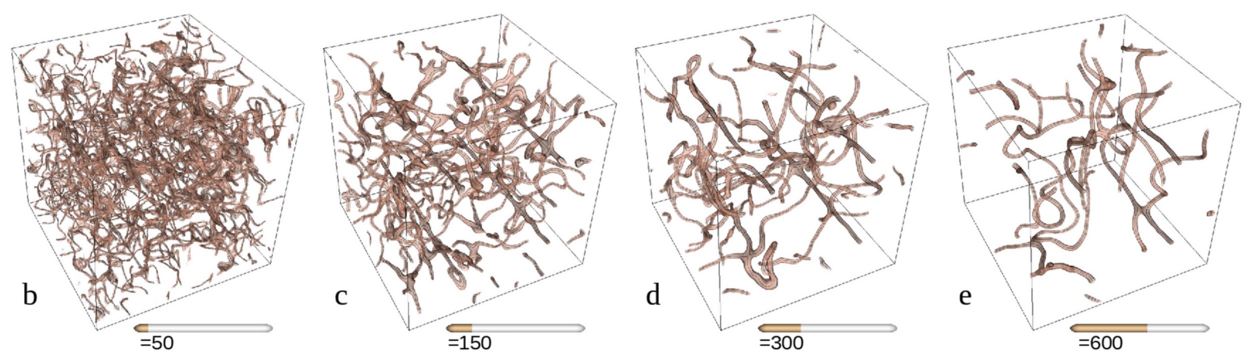
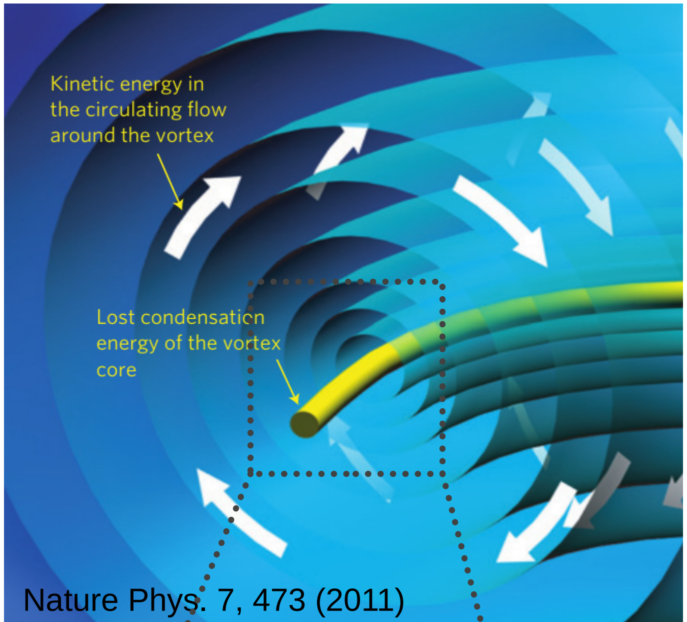
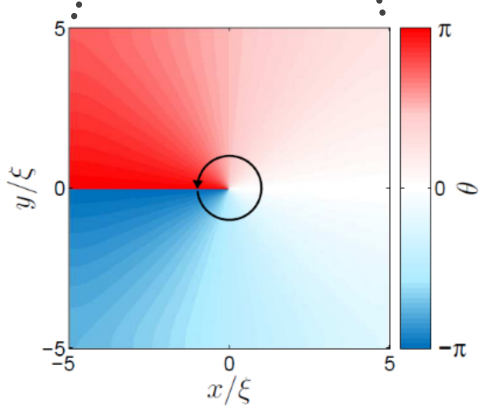


NATIONAL SCIENCE CENTRE POLAND

COST Action CA23134 webinar, 25-04-2025

Microscopic properties of quantum vortices across BCS-BEC crossover



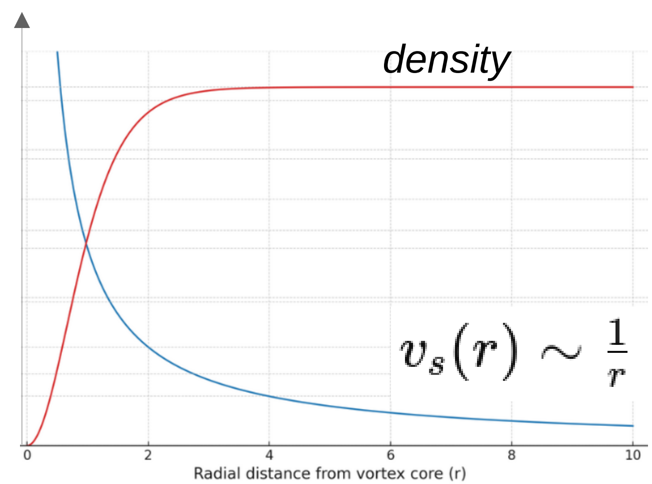


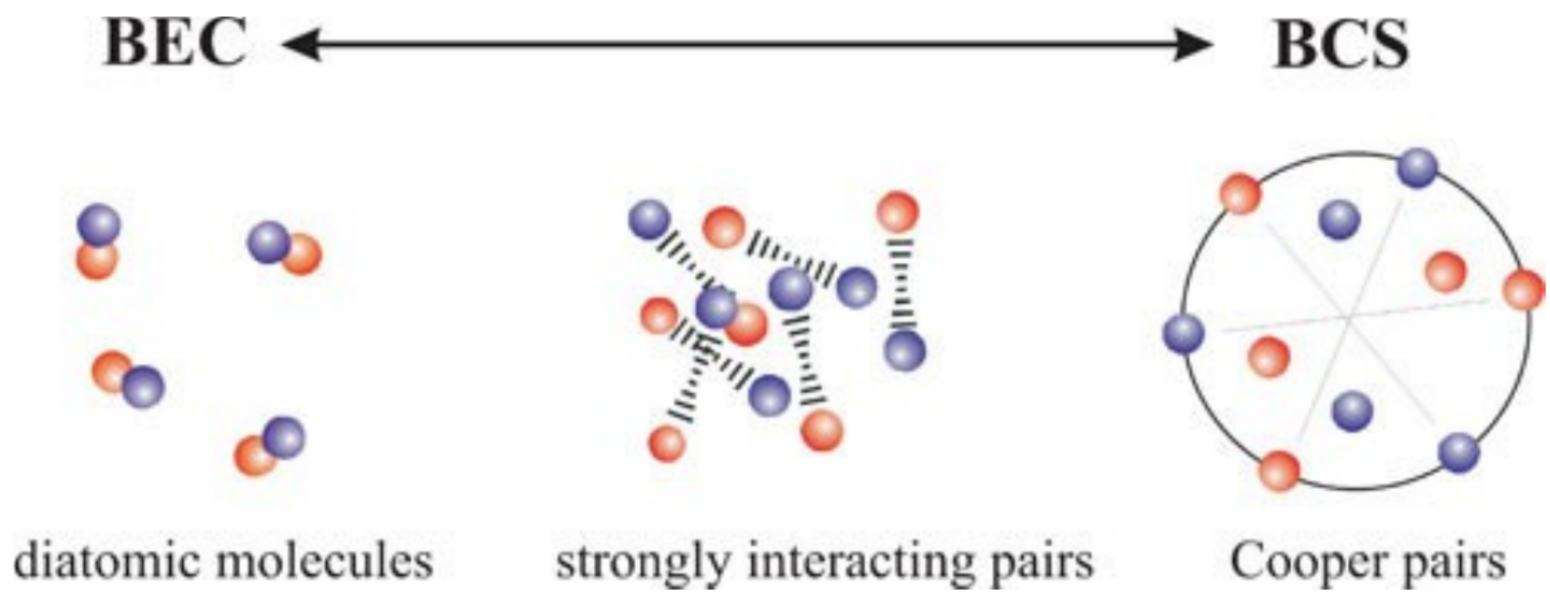
Quantization of circulation

$$\oint_C \mathbf{v}_s \cdot d\mathbf{l} = \kappa = \frac{h}{m} n$$

... for straight vortex line it implies

Many properties of quantum vortices originate from the topology of the order parameter, but not all...





Bound states are created: dimers. Effective dimer-dimer interaction is weak.

Strong attraction: Cooper pairs become comparable in size with the interparticle distance.

Weak attraction induces correlations: Cooper pairs

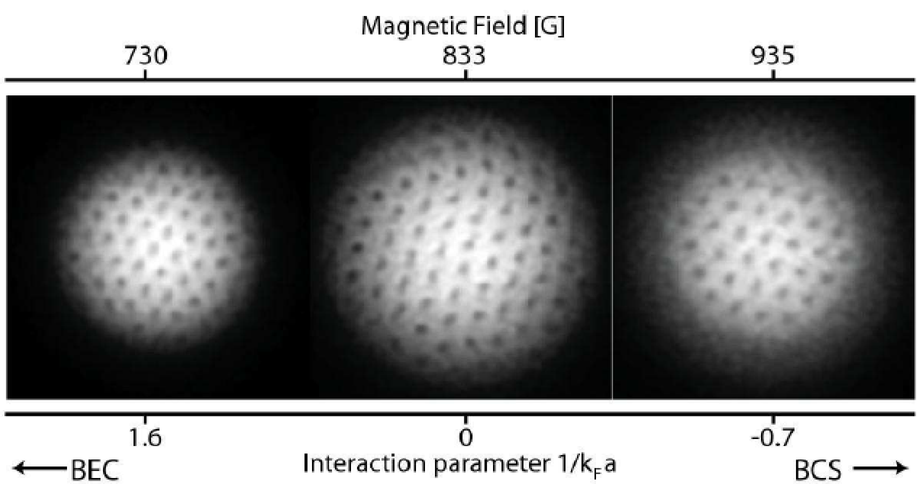
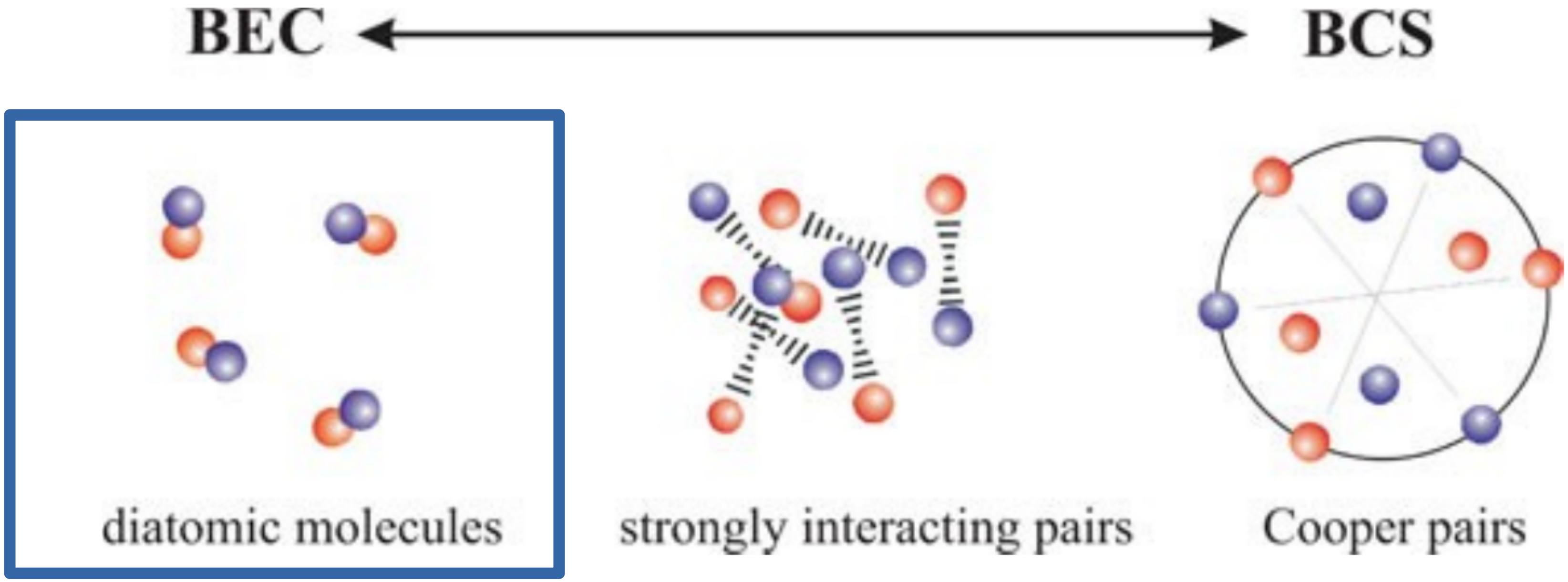


FIG. 36 Vortex lattice in a rotating gas of ^{6}Li precisely at the Feshbach resonance and on the BEC and BCS side. Reprinted with permission from Zwierlein *et al.* (2005).

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



Gross- Pitaevskii equation (GPE):

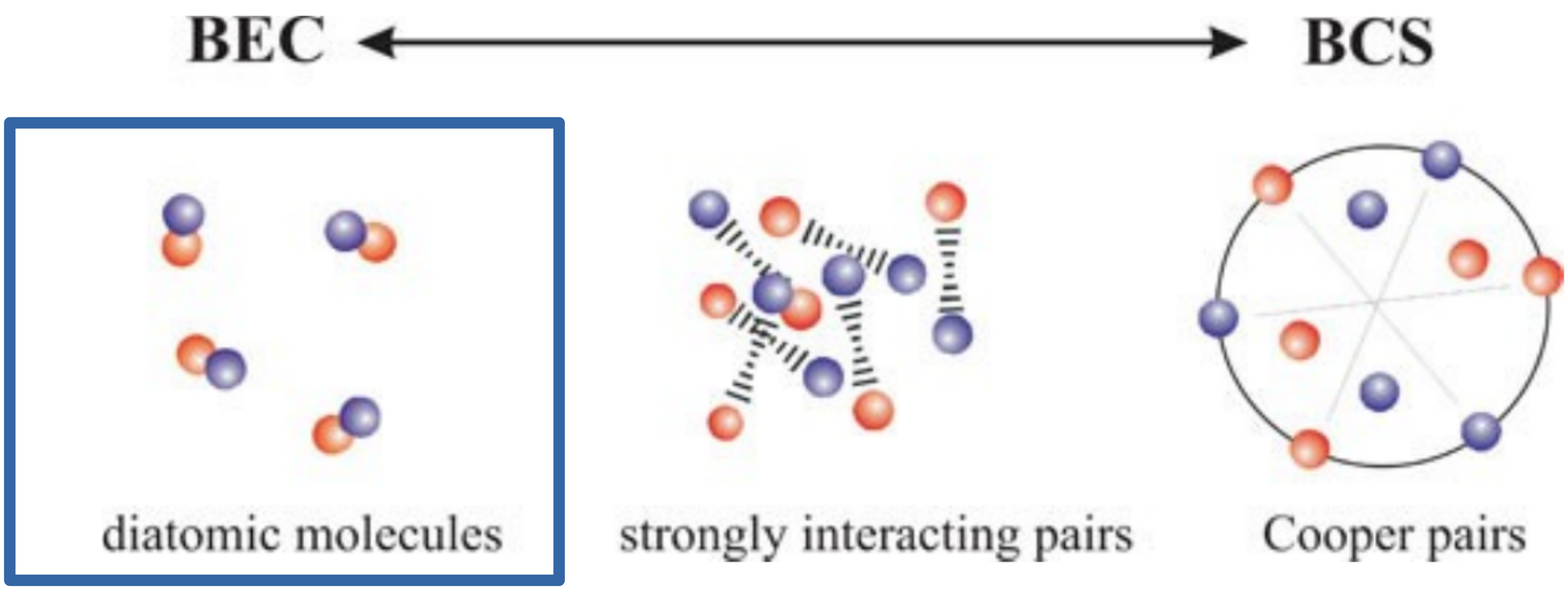
$n^{1/3}a_{dd} << 1$

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2M}\nabla^2 + V_{\text{trap}} + g|\psi(\vec{r},t)|^2\right)\psi(\vec{r},t)$$

mass of dimer = 2m

Depends on dimer-dimer scattering length a_{dd}

The nonlinear Schrodinger equation is regarded as the one that captures quantum vortex properties at the microscopic level.



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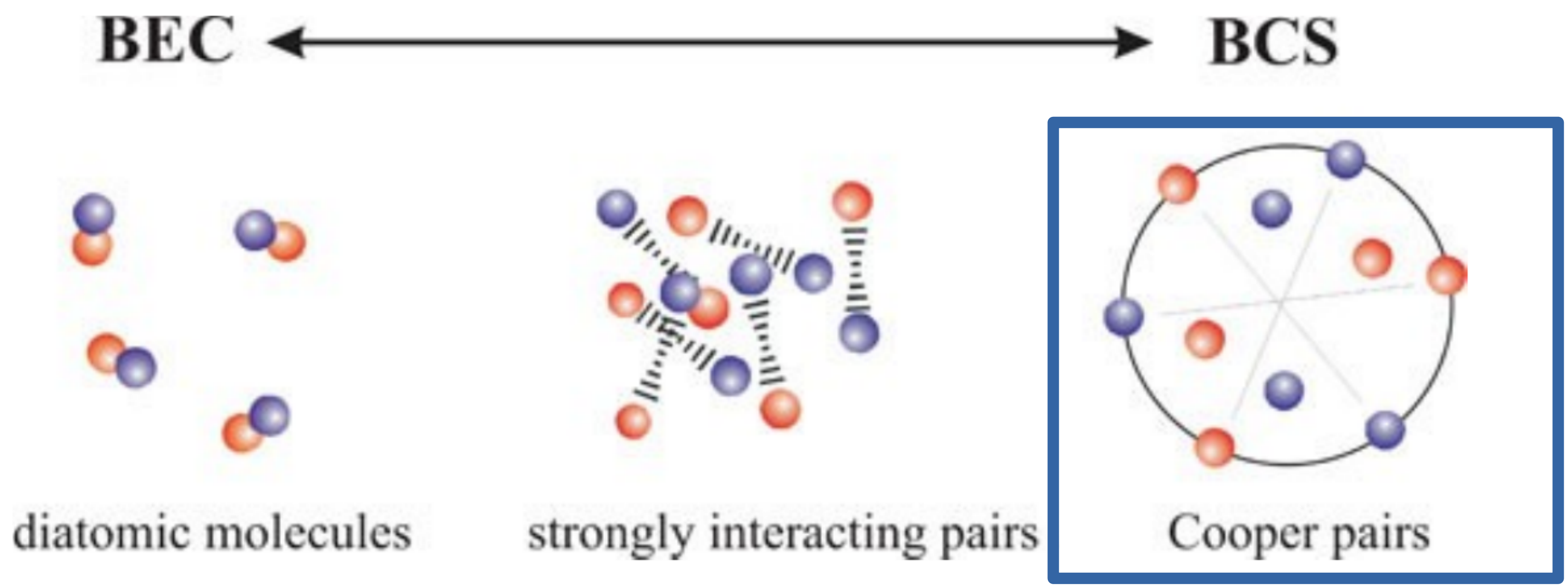
The nonlinear Schrodinger equation is regarded as the one that captures quantum vortex properties at the microscopic level.

$$n(\boldsymbol{r}) = |\psi(\boldsymbol{r})|^2 \rightarrow \psi(\boldsymbol{r}) = \sqrt{n(\boldsymbol{r})}e^{i\phi(\boldsymbol{r})}$$

$$\begin{aligned} \boldsymbol{j}(\boldsymbol{r}) &= \frac{\hbar}{2Mi}\left(\psi^*(\boldsymbol{r})\nabla\psi(\boldsymbol{r}) - \psi(\boldsymbol{r})\nabla\psi^*(\boldsymbol{r})\right) \\ &= n(\boldsymbol{r})\frac{\hbar}{M}\nabla\phi(\boldsymbol{r}) = n(\boldsymbol{r})\boldsymbol{v}_s(\boldsymbol{r}) \end{aligned}$$

Definition of
the superfluid velocity

$$\boldsymbol{v}_s(\boldsymbol{r}) = \frac{\hbar}{M}\nabla\phi(\boldsymbol{r})$$



$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_\eta(\mathbf{r},t) \\ v_\eta(\mathbf{r},t)\end{pmatrix} = \mathcal{H}_{\mathrm{BdG}}\begin{pmatrix} u_\eta(\mathbf{r},t) \\ v_\eta(\mathbf{r},t)\end{pmatrix}$$

Bogoliubov-de Gennes equations (BdG): $|k_F a| << 1$

$[a<0;\ k_F=(3\pi^2 n)^{1/3}]$

$$\mathcal{H}_{\mathrm{BdG}} = \begin{pmatrix} h_\uparrow(\mathbf{r},t)-\mu_\uparrow & \Delta(\mathbf{r},t) \\ \Delta^*(\mathbf{r},t) & -h_\downarrow^*(\mathbf{r},t)+\mu_\downarrow \end{pmatrix}$$

$$h_\sigma(\mathbf{r},t) = -\hbar^2\nabla^2/2m + V_\sigma(\mathbf{r},t)$$ Single particle hamiltonian

$$\Delta(\mathbf{r},t) = g\nu(\mathbf{r},t)$$ Pairing potential (order parameter) $g = 4\pi\hbar^2 a/m$

$$\nu(\mathbf{r},t) = \frac{1}{2}\sum_{|E_\eta|<E_c} u_{\eta,\uparrow}(\mathbf{r},t)v^*_{\eta,\downarrow}(\mathbf{r},t)\left(f_\beta(-E_\eta) - f_\beta(E_\eta)\right)$$

Anomalus density

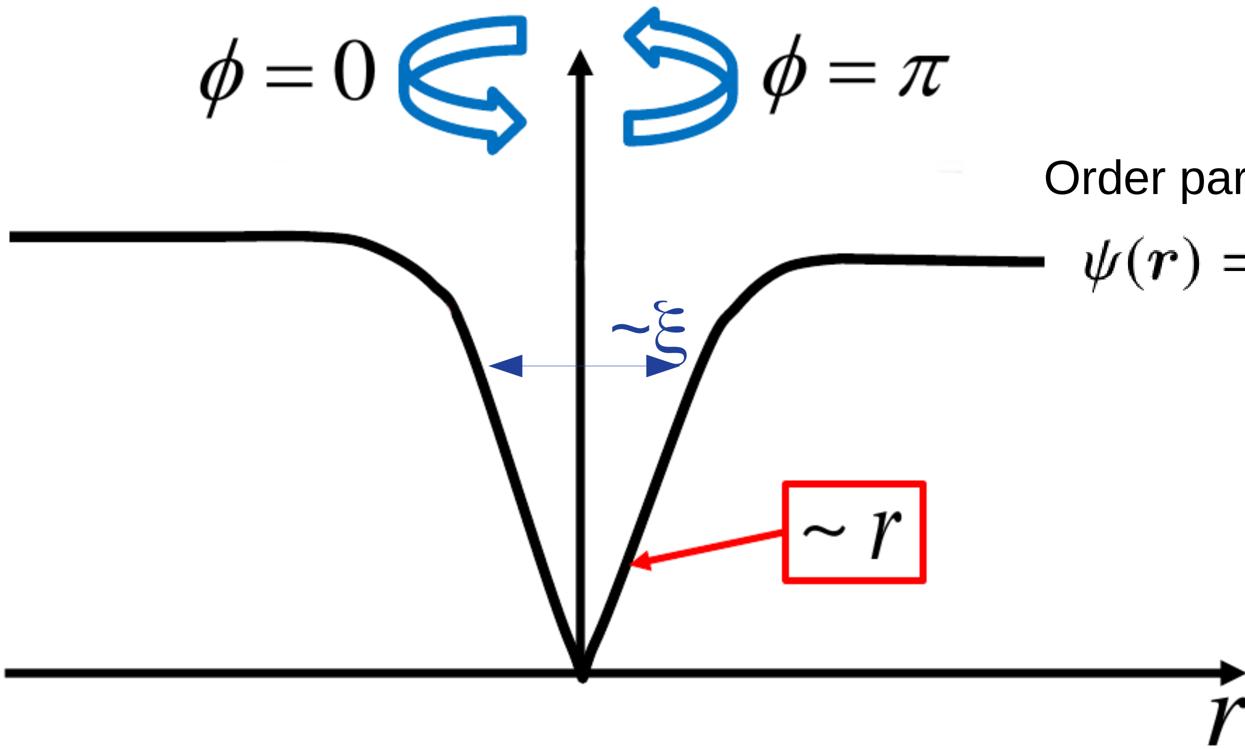
amplitude probability hole / particle

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

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

Pauli exclusion principle

Vortex solution: Bose gas → GPE



Order parameter:

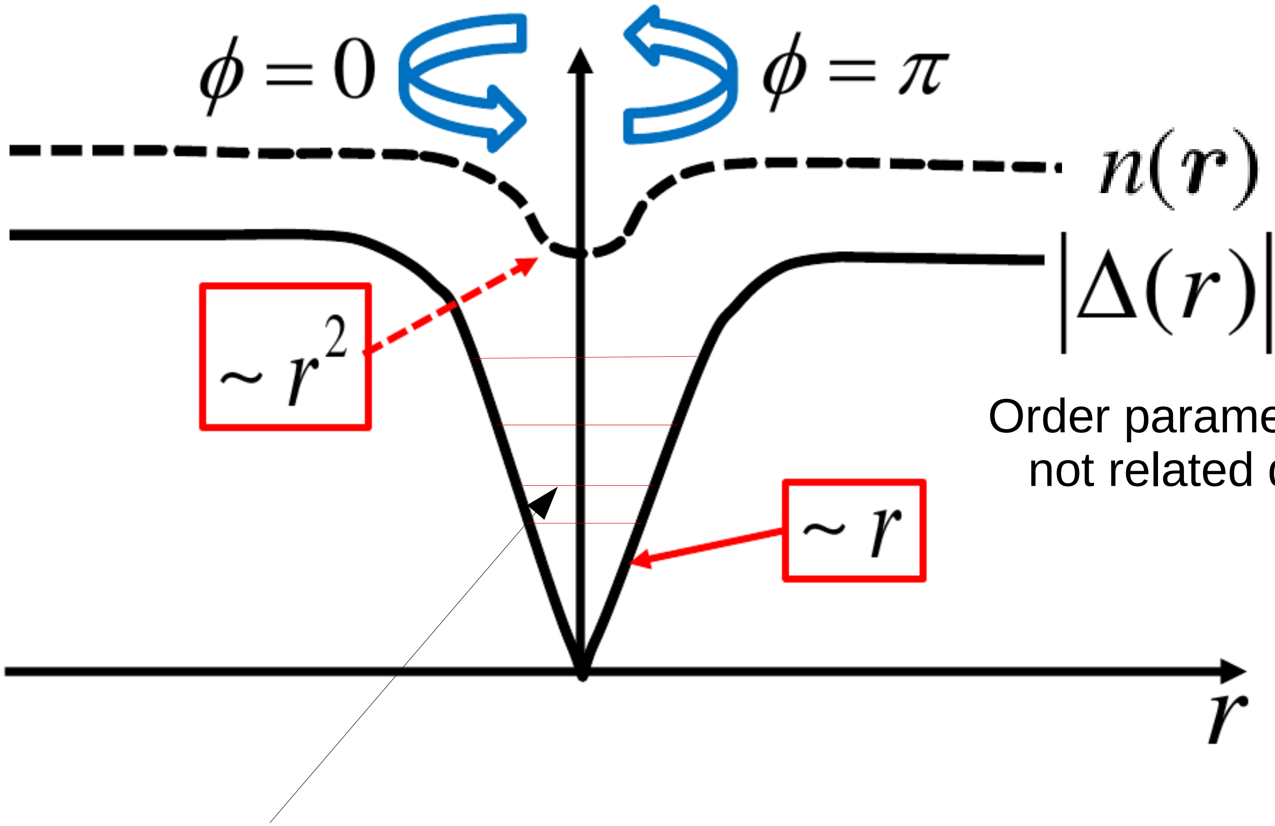
$$\psi(\boldsymbol{r}) = \sqrt{n(\boldsymbol{r})}e^{i\phi(\boldsymbol{r})}$$

$$\boldsymbol{v}_s = \frac{\hbar}{M}\boldsymbol{\nabla}\phi$$

$$\kappa = \oint d\boldsymbol{l}\cdot\boldsymbol{v}_s = \frac{h}{M}$$

Vortex solution: Fermi gas → BdG

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



Order parameter:
not related directly to density

Occupation of Caroli–de Gennes–Matricon (CdGM) states contributes particle density inside the core.

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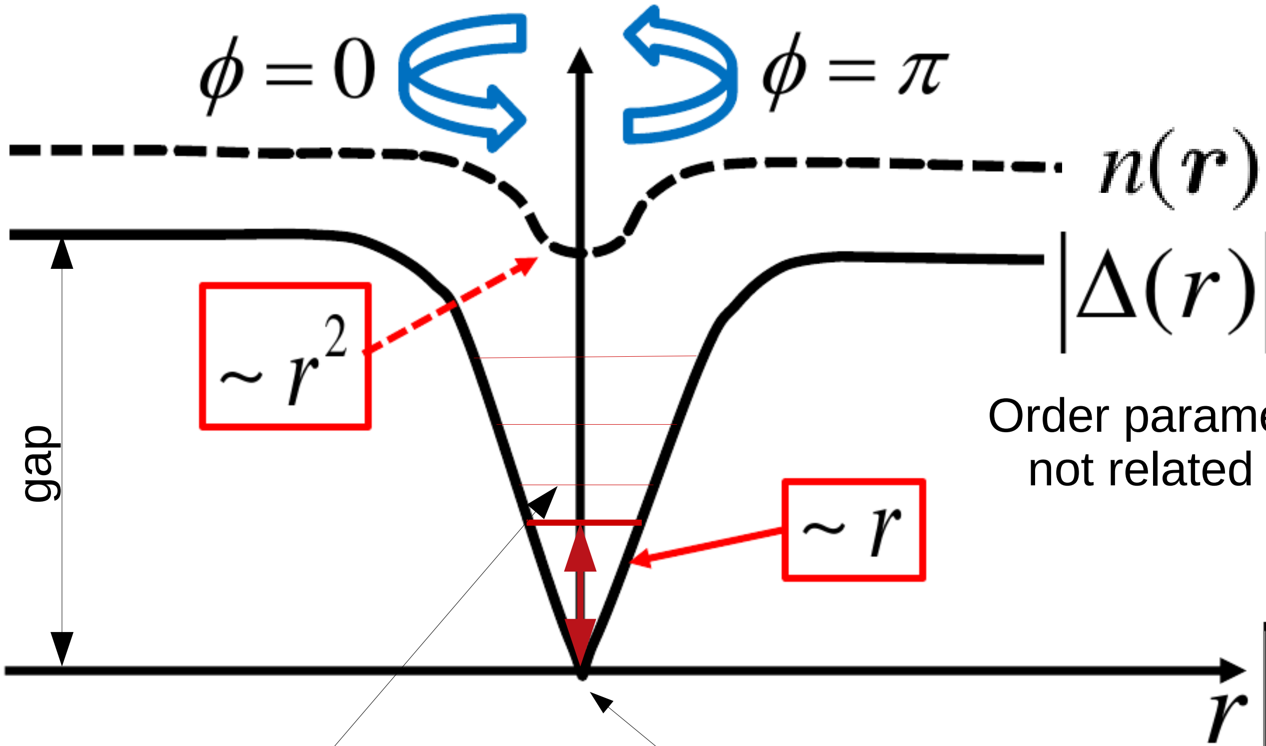

Order parameter:
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"minigap":

$$E_0 \sim \frac{|\Delta|^2}{\varepsilon_F}$$

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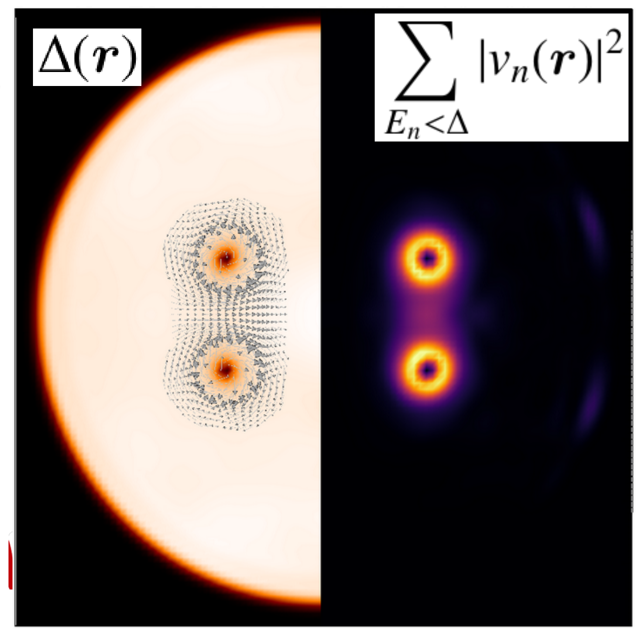
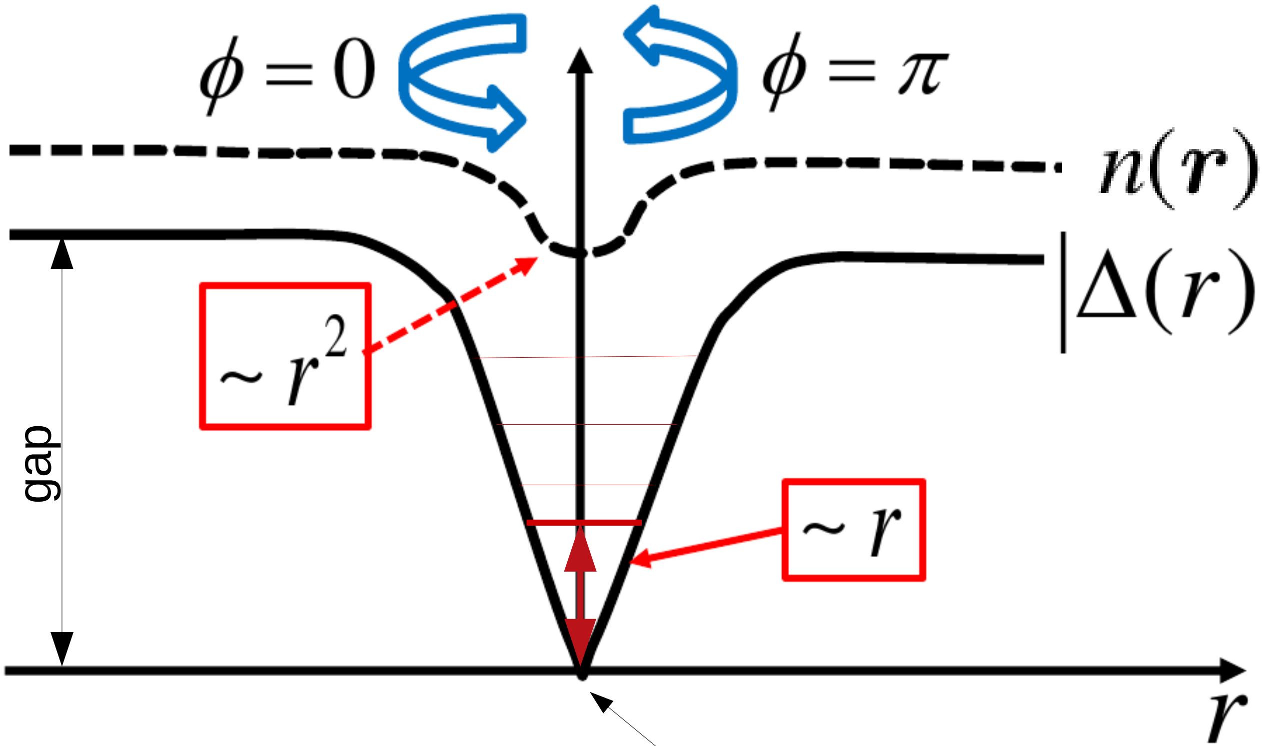
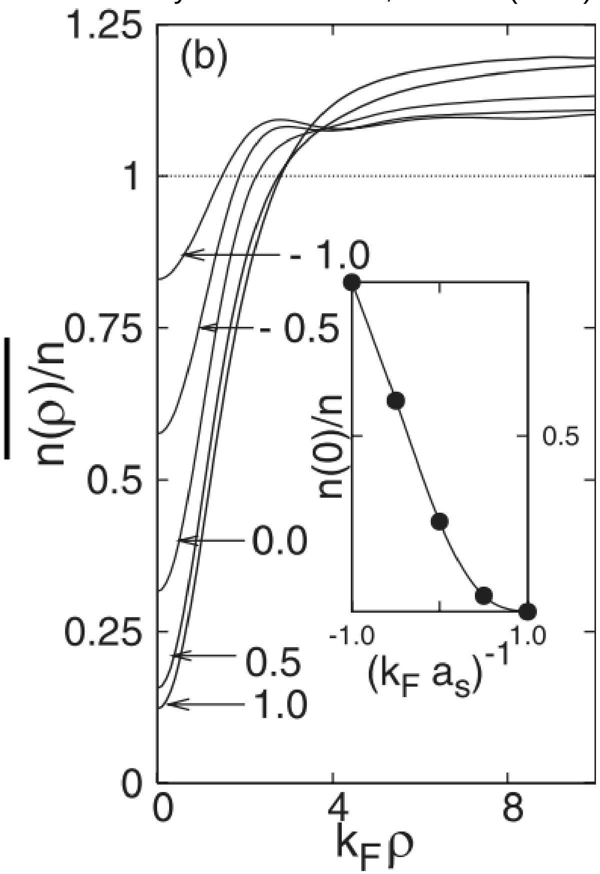


Vortex solution: Fermi gas

R. Sensarma, M. Randeria, and T.-L. Ho, Phys. Rev. Lett. 96, 090403 (2006).





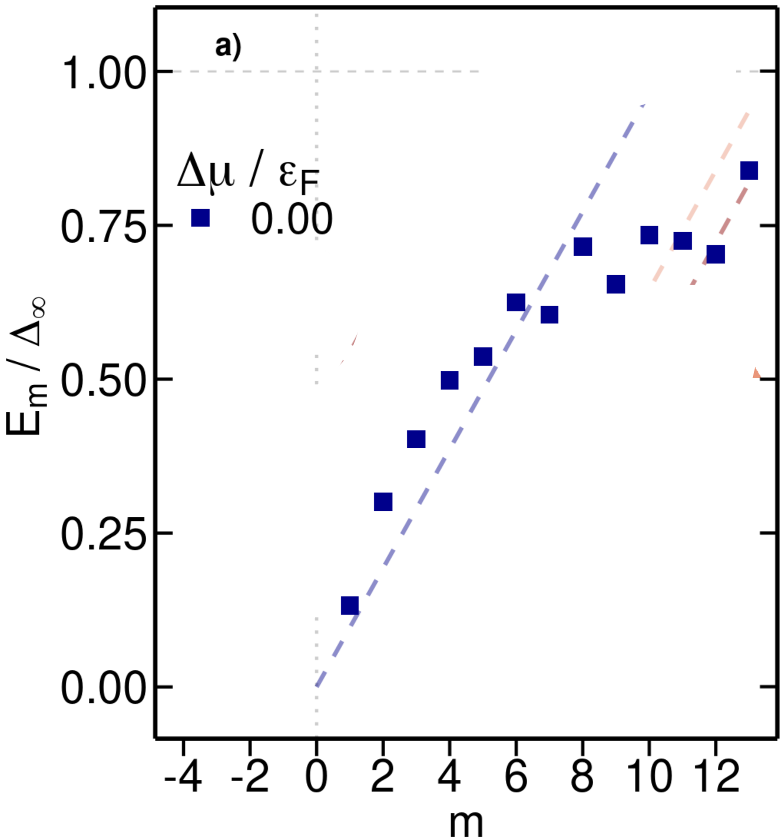
"minigap":

$$\frac{\Delta}{\varepsilon_F} \approx \frac{8}{e^2} \exp\left[\frac{-\pi}{2|ak_F|}\right]$$

$$E_0 \sim \frac{|\Delta|^2}{\varepsilon_F}$$

- BCS: many CdGM states
  → small depletion of density in the core
- UFG: a few CdGM states
  → significant depletion
- BEC: no CdGM states:
  → empty vortex core

Vortex structure within QMC:
L Madeira, A Lovato, F Pederiva, KE Schmidt, Phys. Rev. A 95, 053603 (2017);
L Madeira, S Gandolfi, KE Schmidt, VS Bagnato, Phys. Rev. C 100, 014001 (2019)



$$\mu_\uparrow = \mu$$

$$\mu_\downarrow = \mu$$

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

Generic form of solutions for straight vortex

$$u_\eta(\mathbf{r}) = u_{nmk_z}(\rho) e^{im\varphi} e^{ik_z z}$$

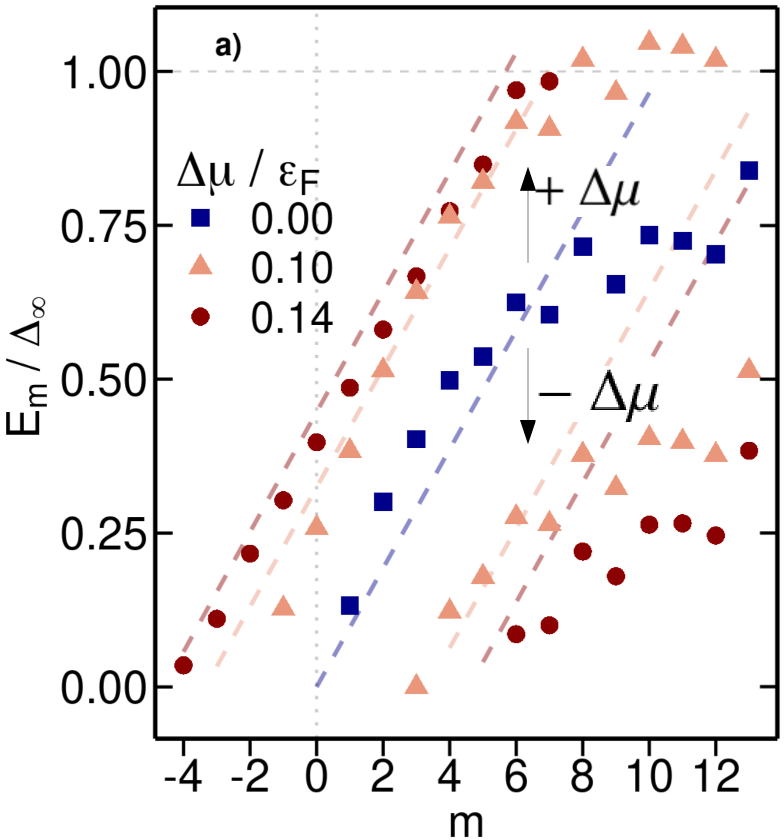
$$v_\eta(\mathbf{r}) = v_{nmk_z}(\rho) e^{i(m+1)\varphi} e^{ik_z z},$$

Individual particles have different *m* (Pauli principle) but

$$\frac{<\hat{L}_z>}{N_{\text{Copper.pairs}}} = \hbar$$

In BCS regime:

$$E_{\pm n=0,m} \approx \frac{|\Delta|^2}{\varepsilon_F \frac{r_v}{\xi}\left(\frac{r_v}{\xi}+1\right)} |m|$$



$$\boxed{\begin{aligned}\mu_\uparrow &= \mu + \Delta\mu \\ \mu_\downarrow &= \mu - \Delta\mu\end{aligned}}$$

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

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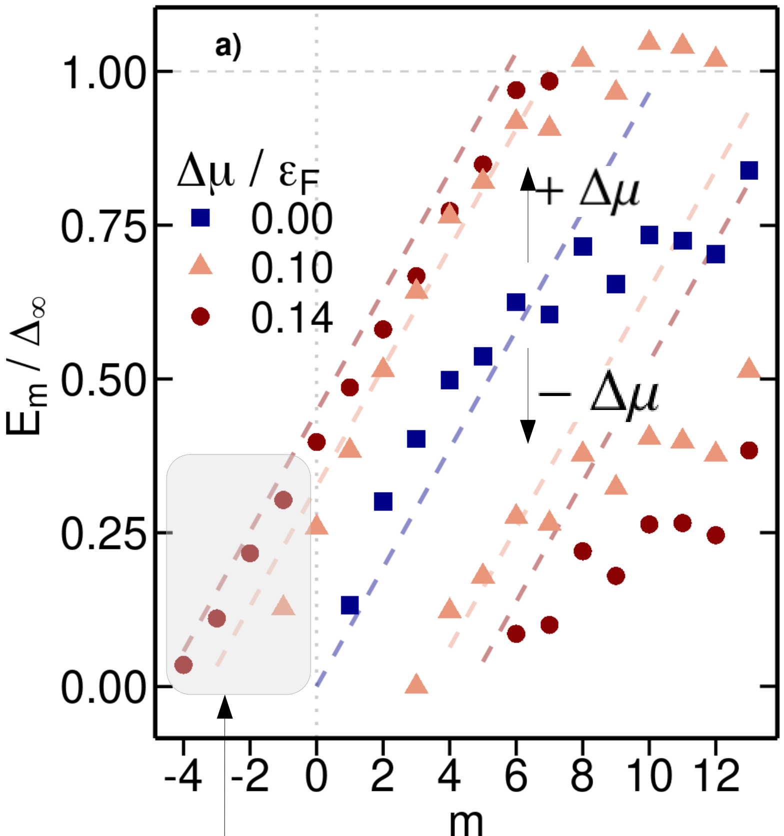
$$E_{\pm n=0,m} \approx \frac{|\Delta|^2}{\varepsilon_F \frac{r_v}{\xi}\left(\frac{r_v}{\xi} + 1\right)} |m| \mp \frac{\Delta\mu}{2}$$

Population imbalance

$$P = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}$$



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$$\mu_\uparrow = \mu + \Delta\mu$$

$$\mu_\downarrow = \mu - \Delta\mu$$

Population imbalance

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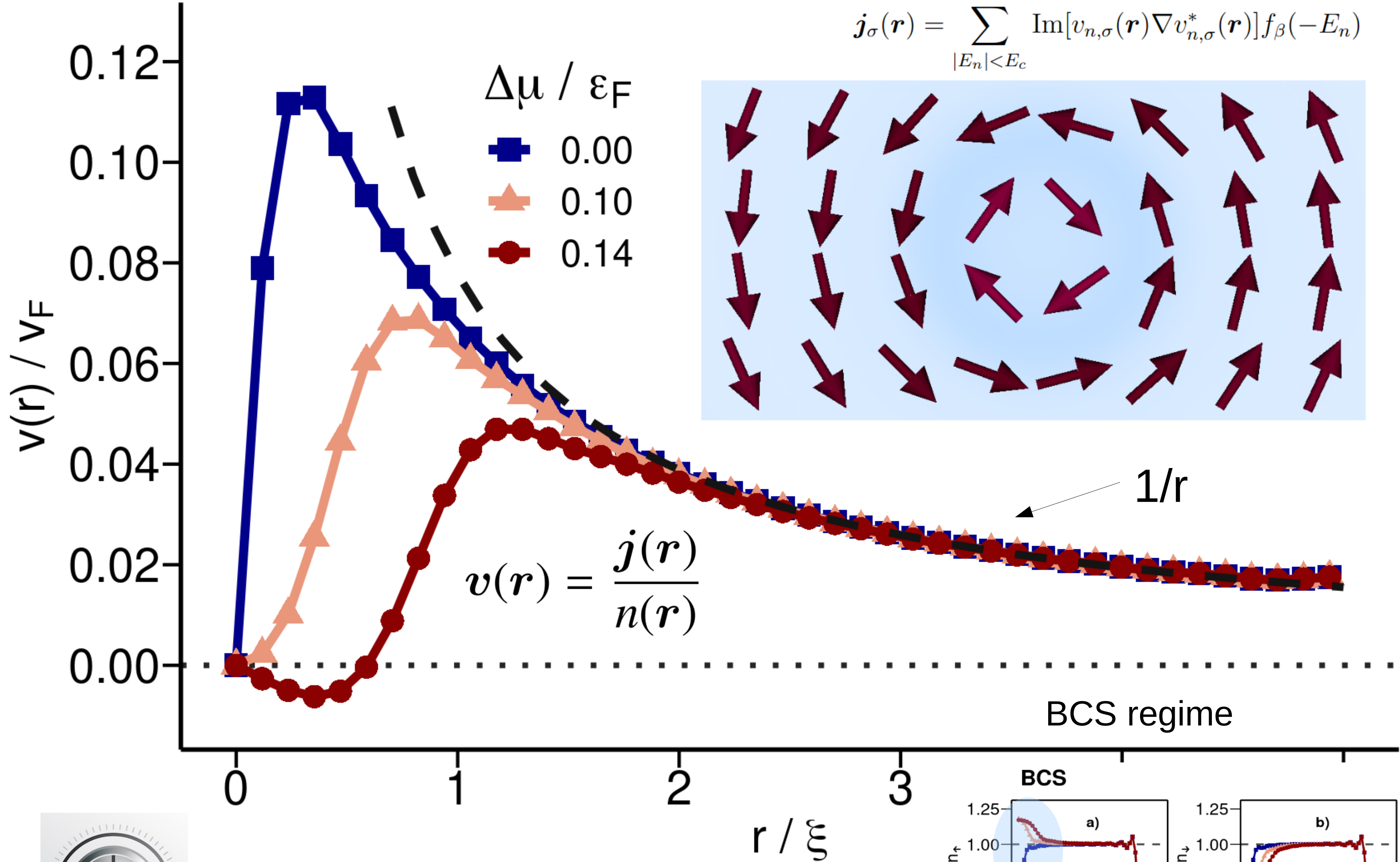
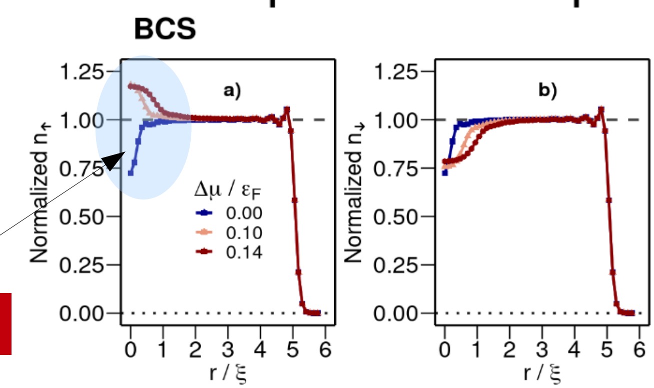
States in the vortex core with negative angular momentum m<0!



Controls circulation inside the core

Majority component accumulates in the core.



GPE: $\boldsymbol{j} = n\boldsymbol{v}_s = n\frac{\hbar}{M}\nabla\phi, \quad n = |\psi|^2,\ \phi = \arg(\psi)$

BdG: $\boldsymbol{j} \neq n\boldsymbol{v}_s = n\frac{\hbar}{M}\nabla\phi, \quad n = \sum_{E_n>0} |v_n|^2,\ \phi = \arg(\Delta),\ M = 2m$

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In general: $\boldsymbol{j} = \underbrace{n_s\boldsymbol{v}_s}_{\textit{superfluid}} + \underbrace{n_n\boldsymbol{v}_n}_{\textit{normal}}$

One should define n_s or n_n not directly via the quantum wave-function, but as the response to the external perturbation, like a "phase twist".

GPE: $\boldsymbol{j} = n\boldsymbol{v}_s = n\frac{\hbar}{M}\nabla\phi, \quad n = |\psi|^2, \ \phi = \arg(\psi)$

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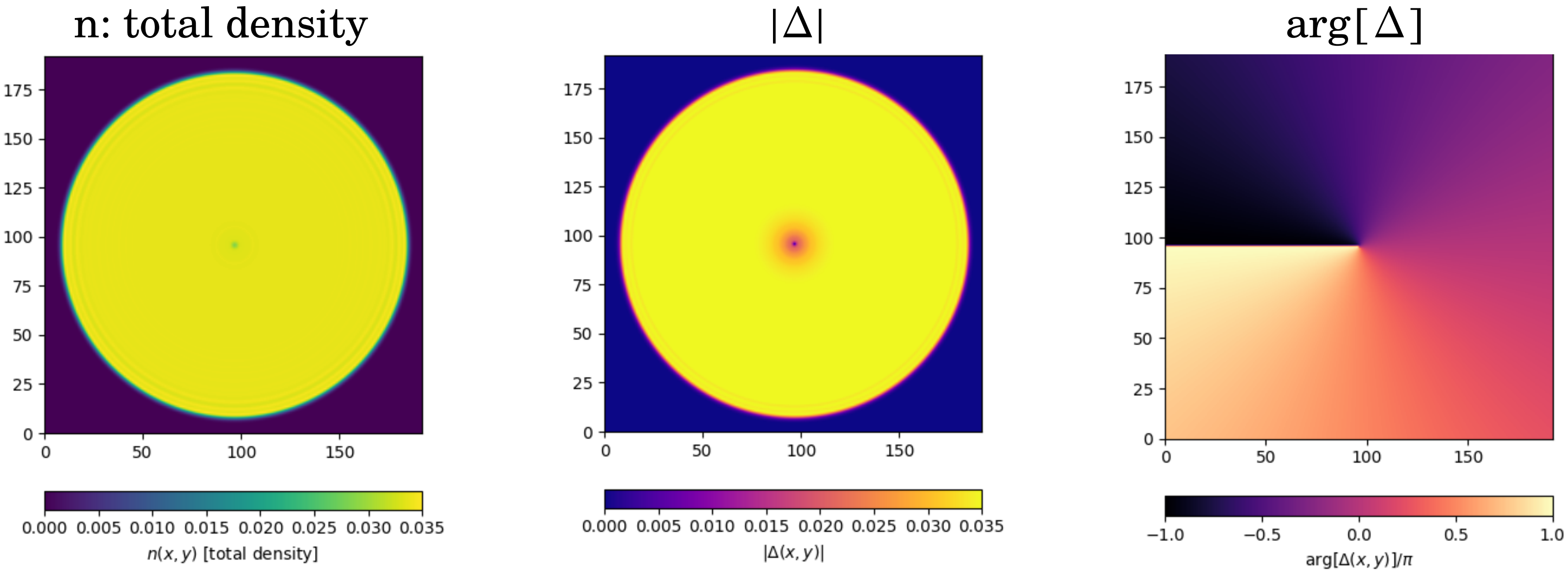
Example:

1. Start with the static solution with **j**=0,
2. Imprint the phase pattern $\phi(r) \rightarrow v_s=\hbar/M \nabla\phi$
3. Measure the current j (phase imprint should induce only superfow) $\rightarrow n_s = j/v_s$
4. Extract the normal density as $n_n = n - n_s$

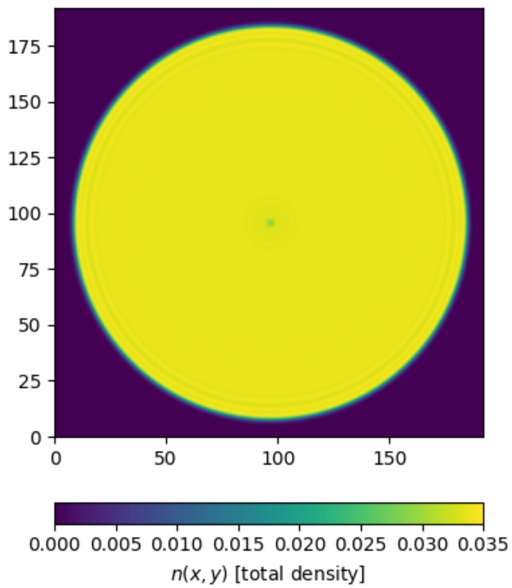
See also G. Orso & S. Stringari, Phys. Rev. A 109, 023301 (2024) for formal definition of the superfluid fraction

Numerical result from BdG [ak_F=-0.70, T=0]

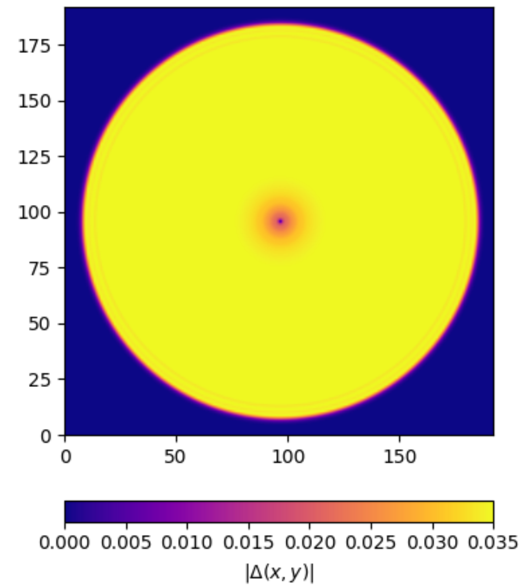


Numerical result from BdG [ak_F=-0.70, T=0]

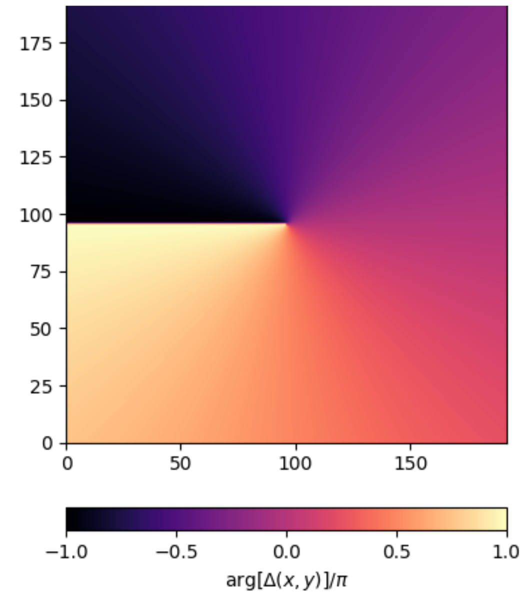
n: total density

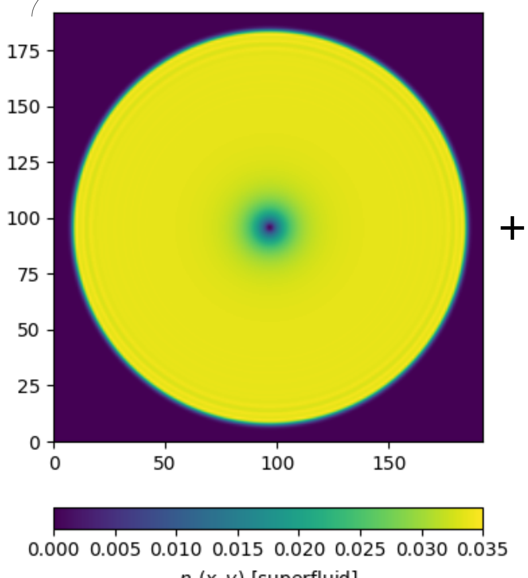


|Δ|



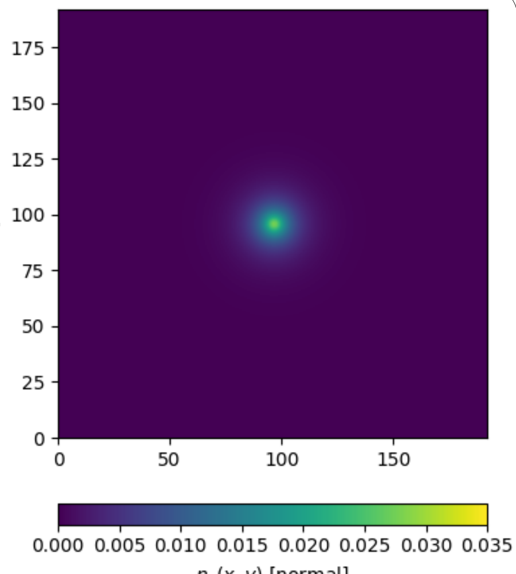
arg[Δ]





superfluid

+

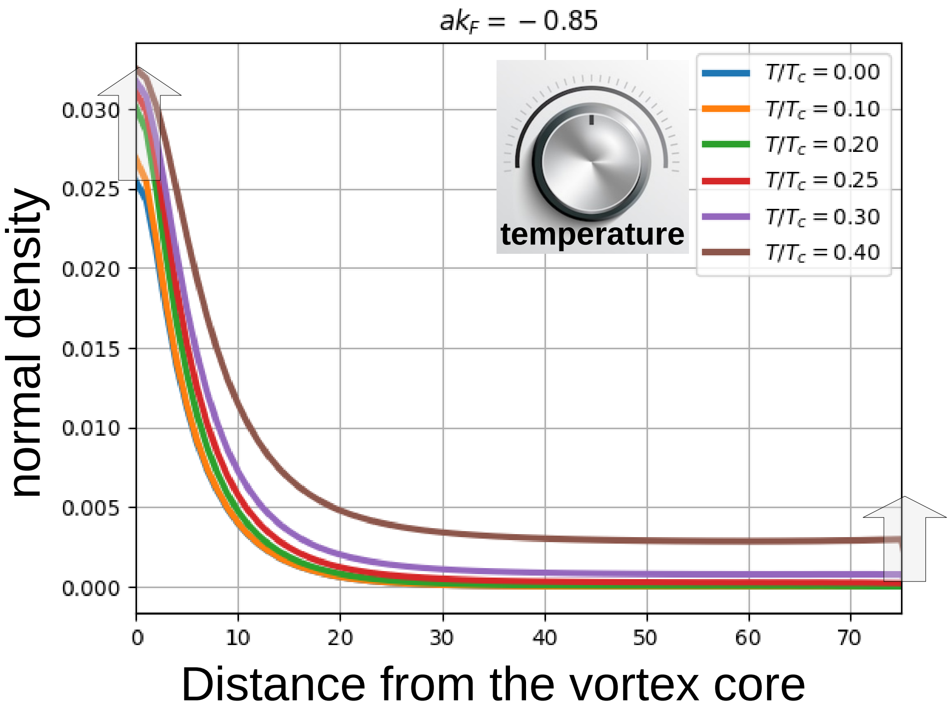


normal

The vortex cores in Fermi superfluids are filled with the normal component, even at zero temperature!

Numerical result from finite temperature BdG [ak_F=-0.85]

Temperature enhances the normal component localized at the vortex core first...



... and, for sufficiently large temperatures, also in the bulk

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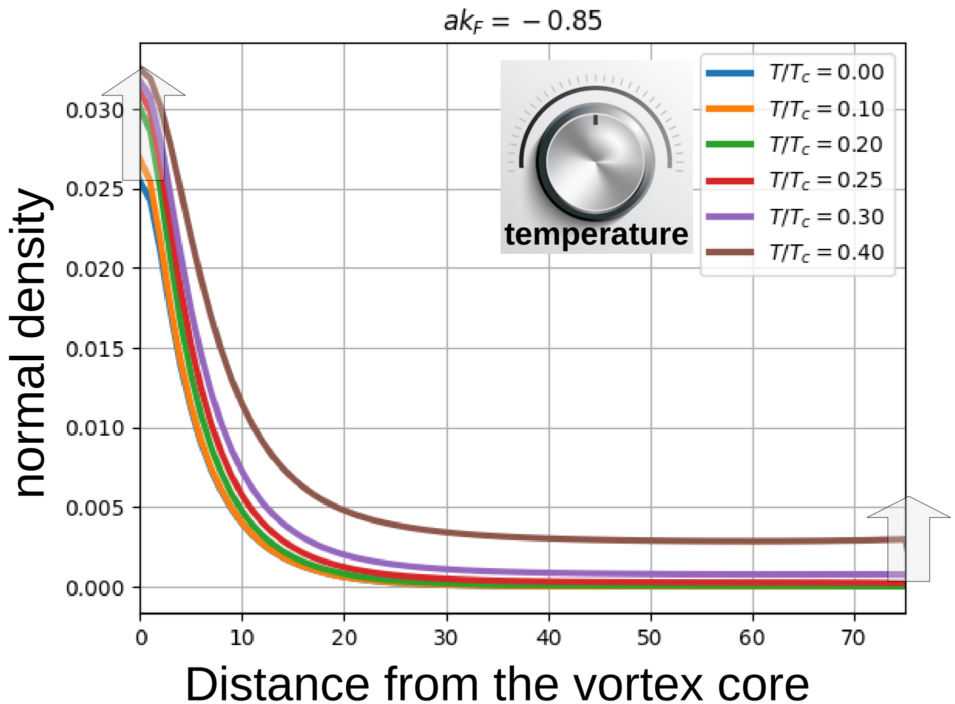

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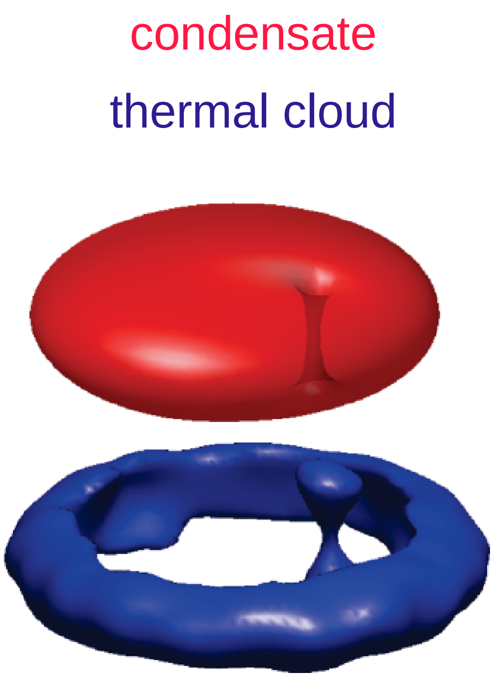
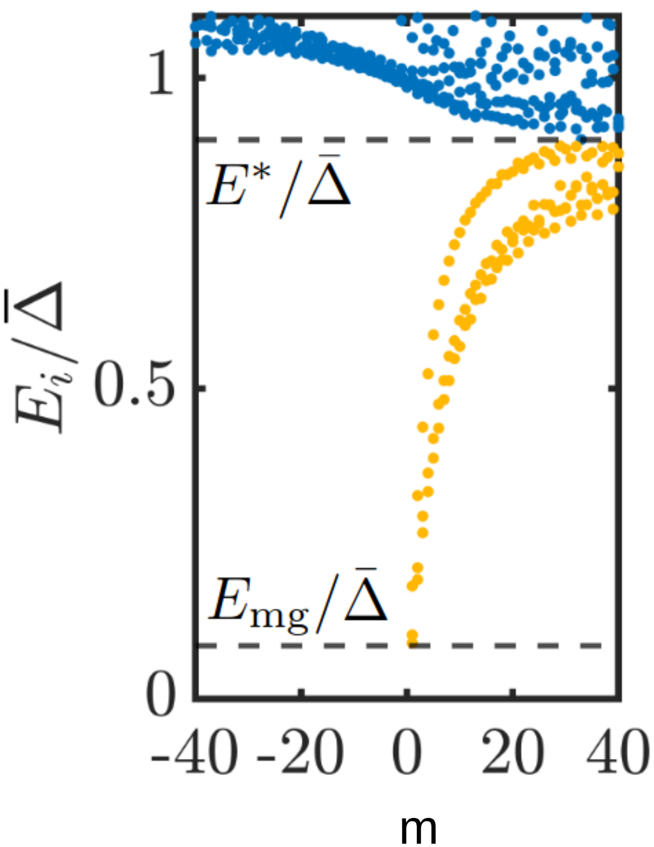
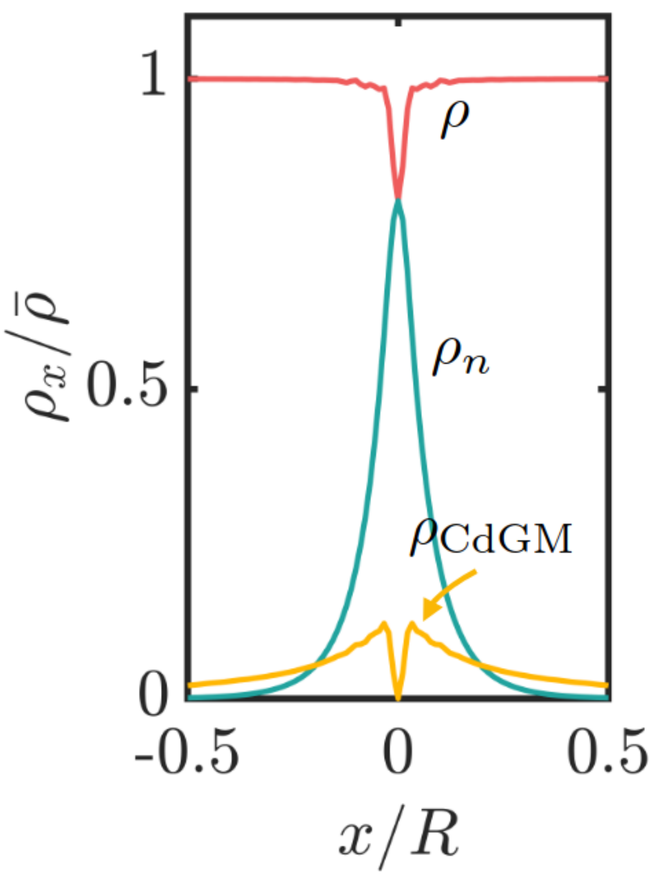


Similar effect is observed for BEC at finite T

Fig from: A. J. Allen, Phys. Rev. A 87, 013630 (2013): Zaremba, Nikuni, and Griffin (ZNG) formalism [here n (density) ↔ ρ]





A. Richaud et al, arXiv:2410.12417

$\rho_{\rm CdGM}$ significantly departs from ρ_n…

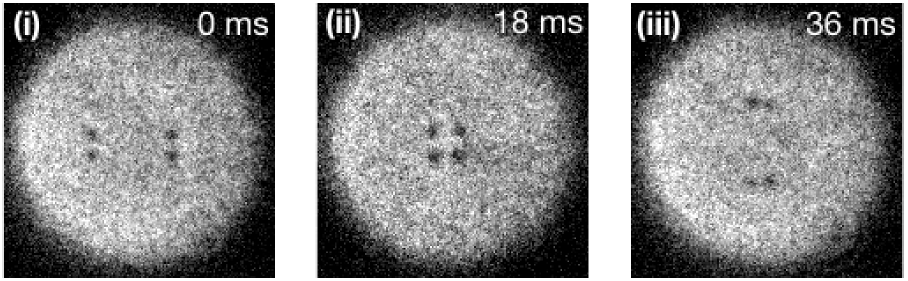
→ the need to elucidate the relationship between the macroscopic quantity ρ_n and the microscopic structure of the quasiparticle states

$$\rho_{\rm CdGM}(\boldsymbol{r}) = 2 \sum_{E_n < E^*} |v_n(\boldsymbol{r})|^2$$

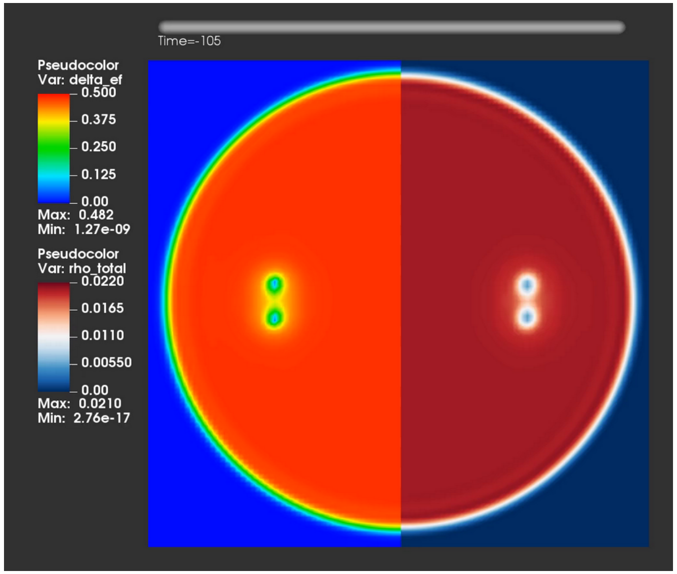
$$\rho(\boldsymbol{r}) = 2 \sum_{E_n < E_{cut}} |v_n(\boldsymbol{r})|^2$$

Internal vortex structure:
does it matter when considering dynamics?

[1] W. J. Kwon, et.al., Nature 600, 64-69 (2021)   Figs from [1]



LENS ^{6}Li experiment (G. Roati's group)
Unitary Fermi gas ($ak_F \to \infty$)
$T_{exp} = (0.3\text{-}0.4)\,T_c$



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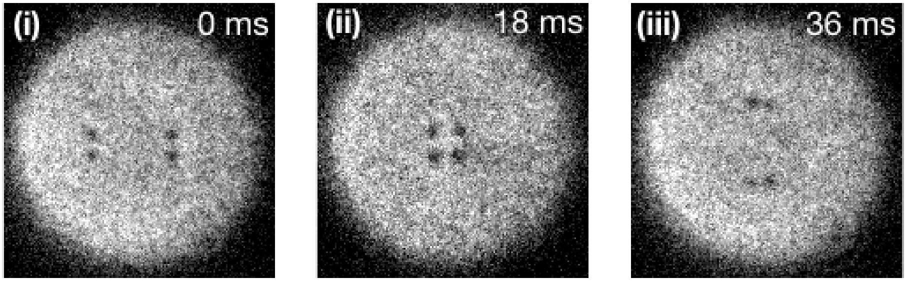

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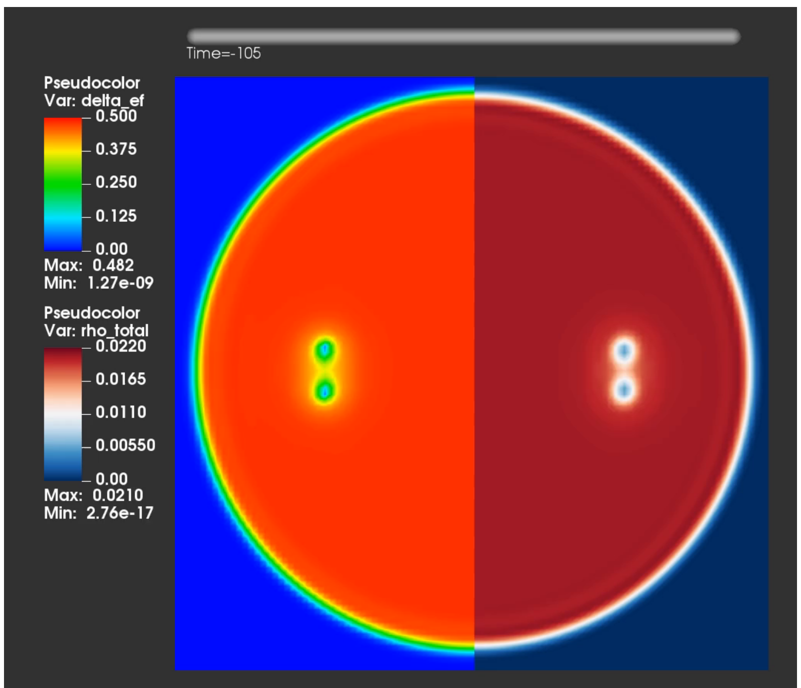


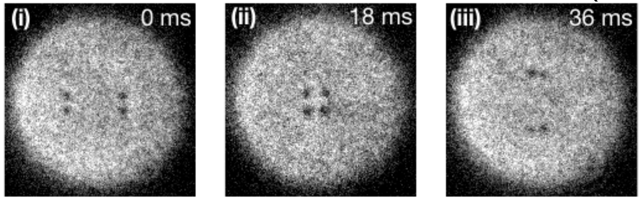
Vortex Point Model (2D) or **Vortex Filament Model** (3D):

$$m_V \frac{d^2 \boldsymbol{r}_V}{dt^2} = \boldsymbol{F}_{\text{Magnus}} + \\ + \boldsymbol{F}_{\text{boundry}} + \boldsymbol{F}_{\text{dissipative}+\ldots}$$

Movie from: Phys. Rev. Lett. 130, 043001 (2023)

Vortex Point Model

Source: W. J. Kwon, et.al., Nature 600, 64-69 (2021)



Vortex mass
in most cases the vortices are regarded as massless particles $m_V \approx 0$

$$m_V \frac{d^2 \boldsymbol{r}_V}{dt^2} = \boldsymbol{F}_{\text{Magnus}} + \boldsymbol{F}_{\text{boundry}} + \boldsymbol{F}_{\text{dissipative+...}}$$

Vortex Point Model

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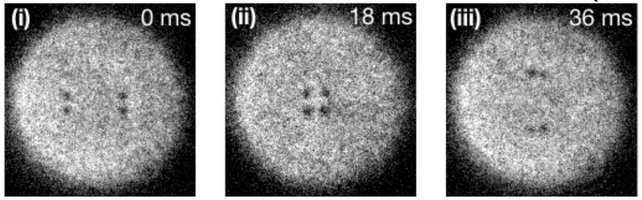

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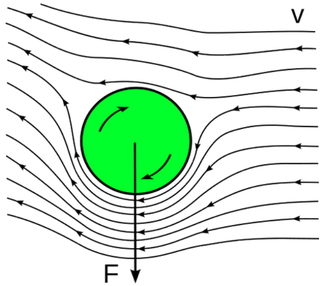
$$m_V \frac{d^2 \boldsymbol{r}_V}{dt^2} = \boldsymbol{F}_{\text{Magnus}} + \boldsymbol{F}_{\text{boundry}} + \boldsymbol{F}_{\text{dissipative}+\ldots}$$



$$\mathbf{F}_{\text{Magnus}} = n_s \kappa \, \hat{\mathbf{z}} \times (\mathbf{v}_V - \mathbf{v}_s)$$

Biot–Savart Law in 2D

Superflow is generated by all other vortices

$$\mathbf{v}_s(\mathbf{r}) = \frac{\kappa}{2\pi} \sum_{j \neq i} \frac{\hat{\mathbf{z}} \times (\mathbf{r} - \mathbf{r}_j)}{|\mathbf{r} - \mathbf{r}_j|^2}$$

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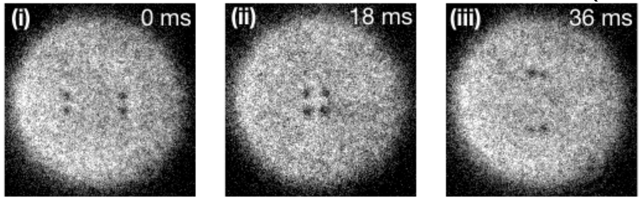
Vortex Point Model

Source: W. J. Kwon, et.al., Nature 600, 64-69 (2021)



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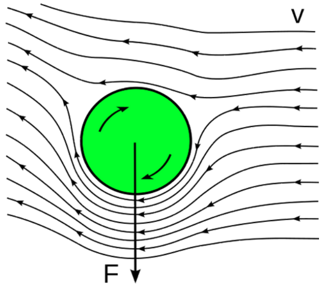

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Can be modeled by means of image vortices.

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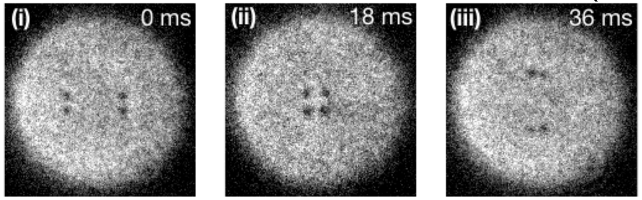

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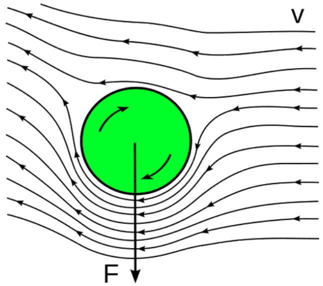

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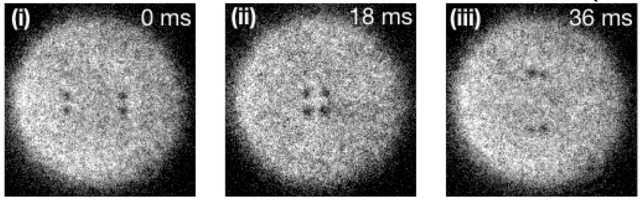

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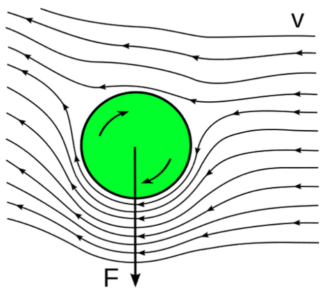

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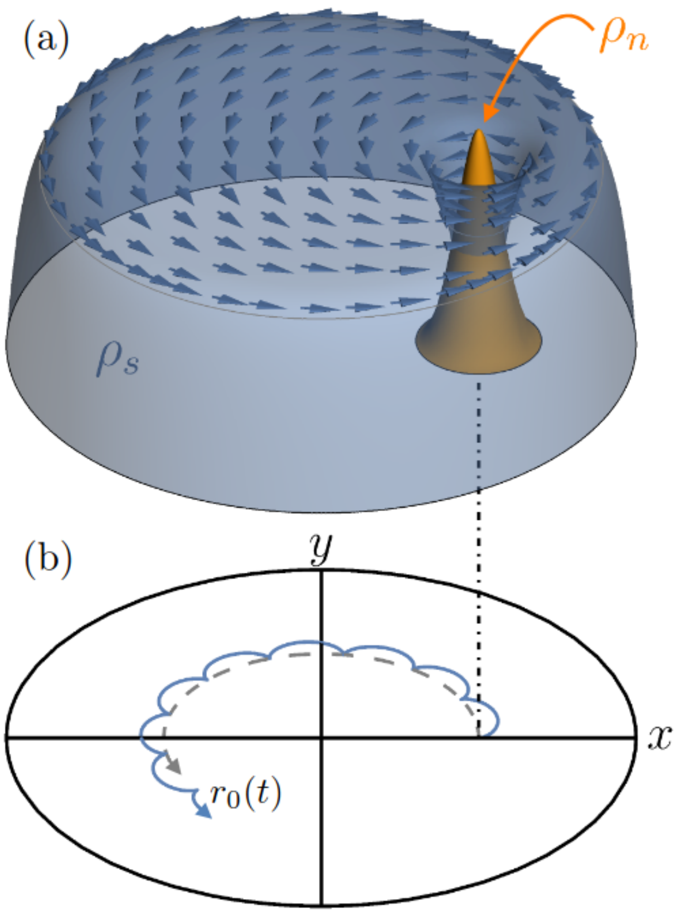
Properties affected by the internal vortex structure

Vortex mass



Consider: quantum vortex at disc of radius R, zero temperature limit (no dissipative forces)

$$m_V \frac{d^2 \boldsymbol{r}_V}{dt^2} = n_s \kappa\, \hat{\mathbf{z}} \times \left(\frac{d\boldsymbol{r}_V}{dt} - \mathbf{v}_s \right)$$

generated by an oppositely-charged image vortex located at position $\boldsymbol{r}_0' = (R/r_0)^2\, \boldsymbol{r}_0$ which ensures the no-flow condition across the boundary.

Related works:
T. Simula, Phys. Rev. A 97, 023609 (2018);
A. Richaud, V. Penna, and A. L. Fetter, Phys. Rev. A 103, 023311 (2021);
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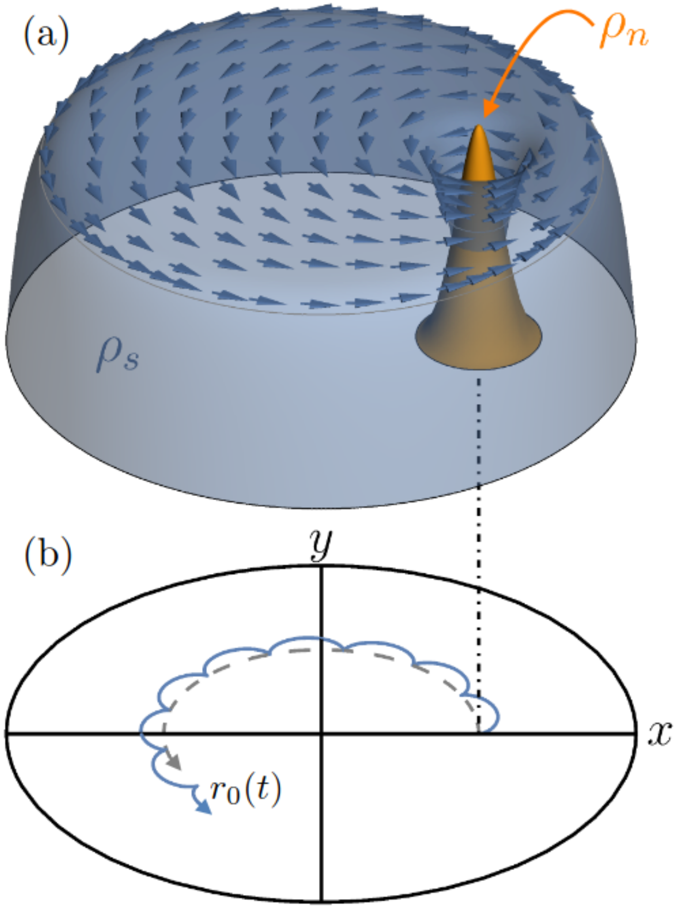

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If m_V=0: first order PDE $r(t) = r_0$ **(circular orbit)**

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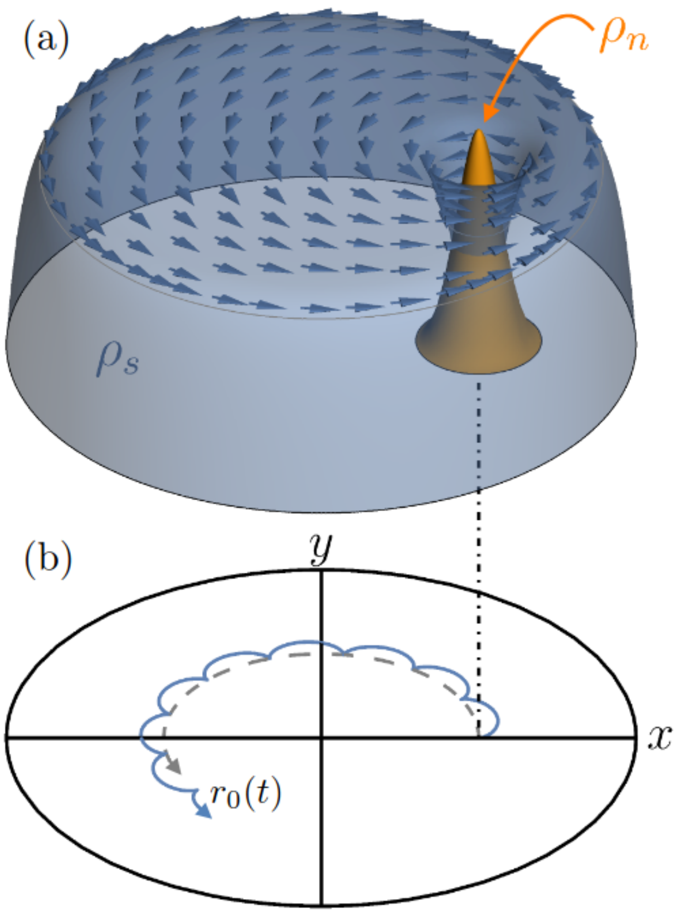

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If m_V=0: first order PDE $r(t) = r_0$ **(circular orbit)**

If m_V>0: second order PDE:

$$r(t) = r_0 + A(v_0, \mathfrak{m}) \sin(\omega(\mathfrak{m})t)$$

$$\mathfrak{m} = \frac{m_V}{M_s}, \quad M_s = \int n_s(\boldsymbol{r})\, \mathrm{d}\boldsymbol{r}$$

(+ transverse oscillations)

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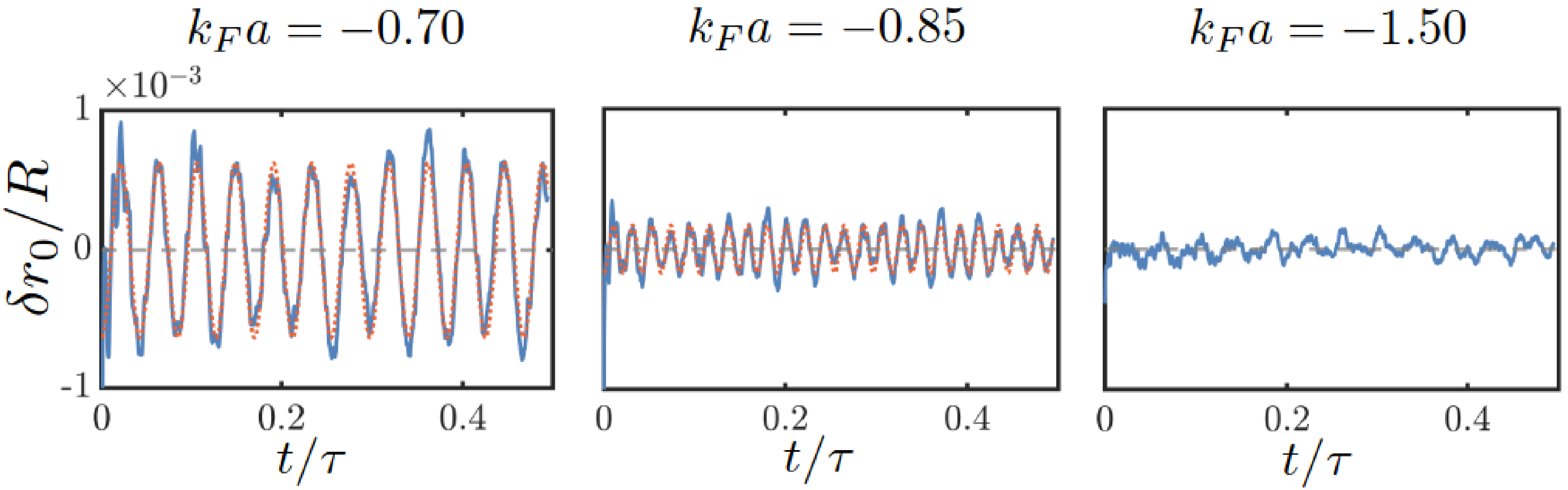
Vortex mass: numerical simulation with time-dependent BdG

A. Richaud M. Caldara, M. Capone, P. Massignan, G. Wlazłowski, arXiv:2410.12417



Blue: numerical result for distance of vortex core from the disk center; Orange: fit of sin function

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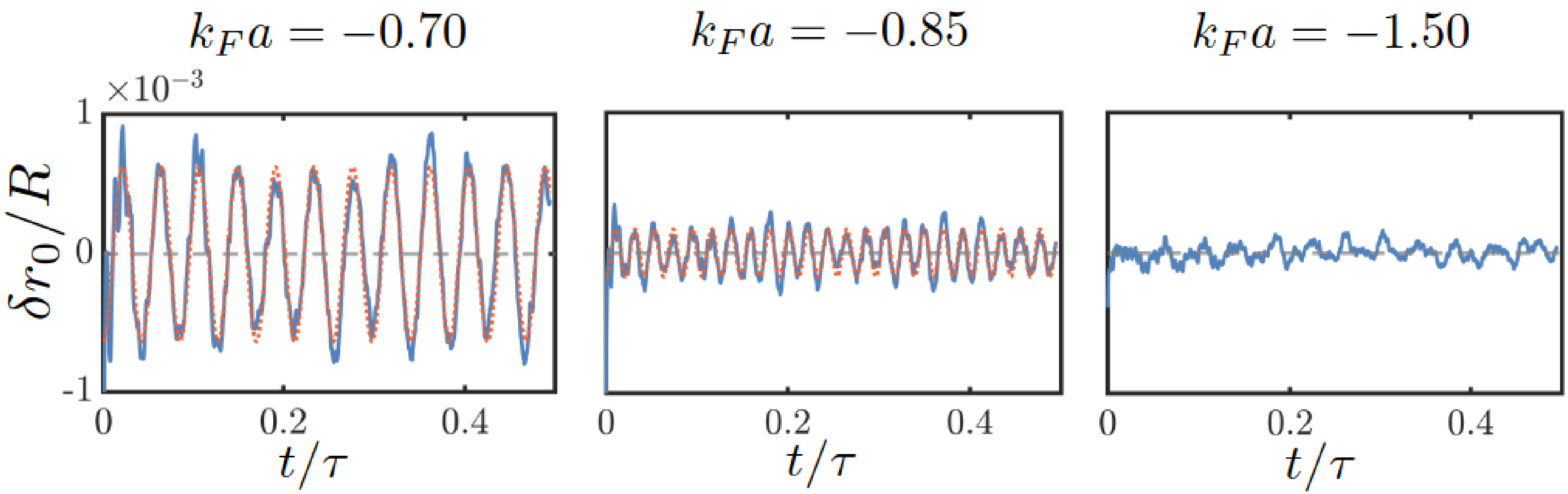

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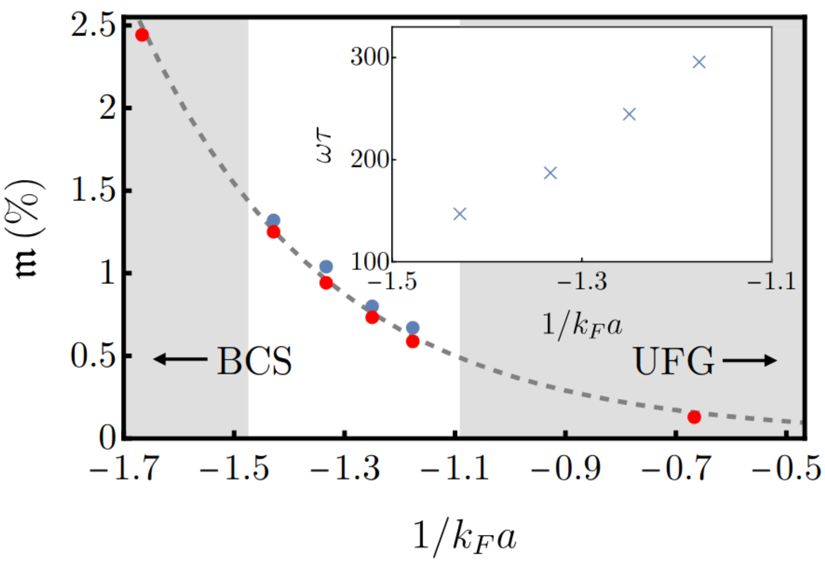

- Dynamics: Mass extracted from measurement of ω (fit of the point vortex model trajectory to data)
- N_n/N_s: Mass extracted as amount of normal component in the vortex core

Dashed line:

$$\mathfrak{m} = \alpha \times (\xi/R)^2 \qquad \xi = \frac{\hbar^2 k_F}{m\pi\bar{\Delta}},$$

vortex mass is proportional to the area of the core
($\propto \xi^2$, where ξ is the coherence or healing length)

Vortex mass: numerical simulation with time-dependent BdG

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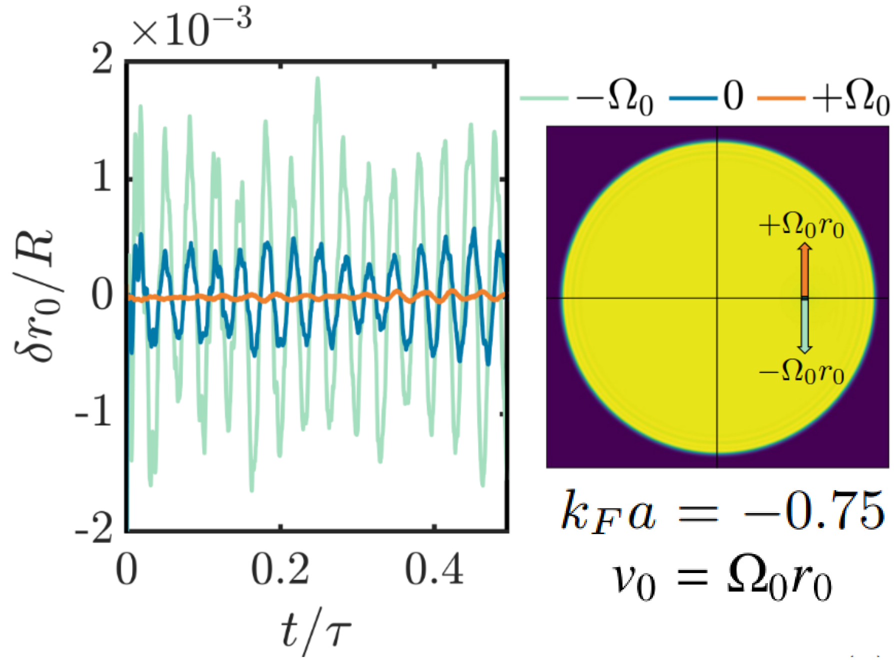

$$r(t) = r_0 + A(v_0, \mathfrak{m}) \sin(\omega(\mathfrak{m})t)$$

The sensitivity of the vortex trajectory with respect to the initial velocity is a clear indicator that the equation of motion is of the second order

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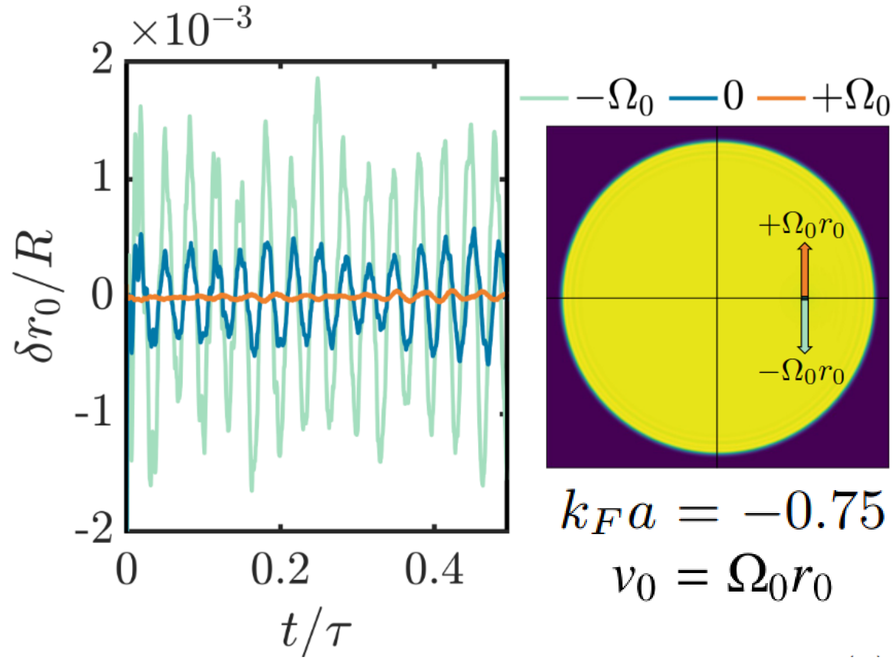

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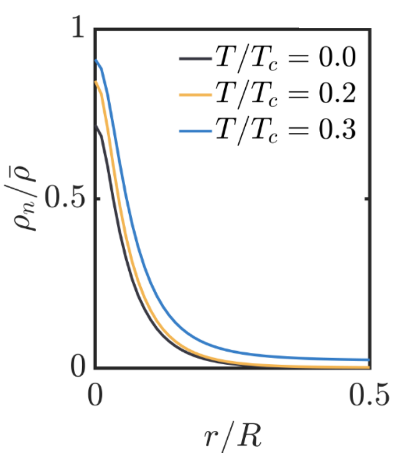
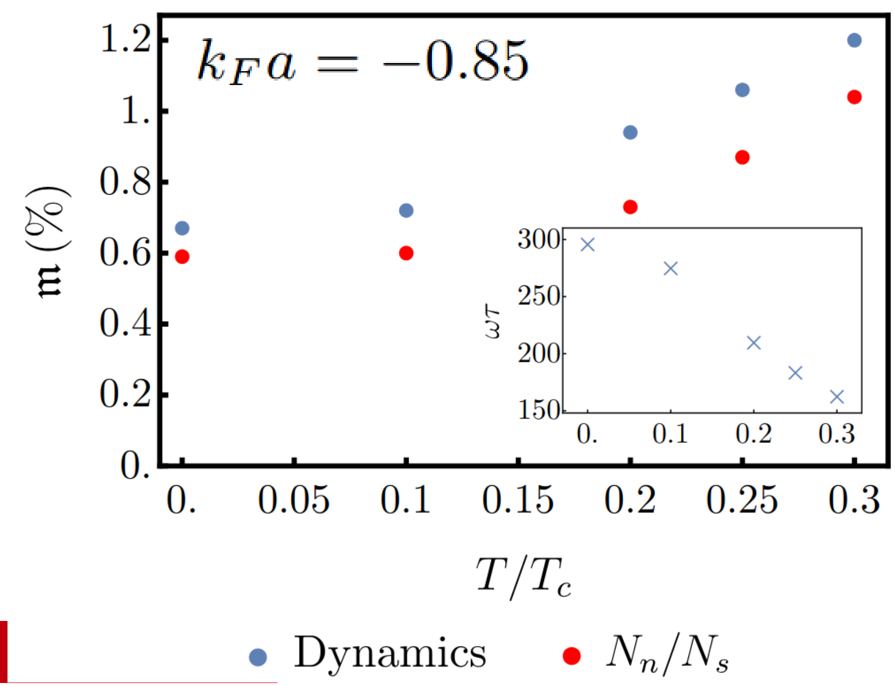


As expected,
the vortex mass grows
as we increase the
temperature.



Dissipative effects $\mathbf{F}_{\text{dissipative}} = -D(\mathbf{v}_V - \mathbf{v}_n) - D'\hat{\mathbf{z}} \times (\mathbf{v}_V - \mathbf{v}_n)$

GPE (Bose): dissipation via emission of phonons (sound)

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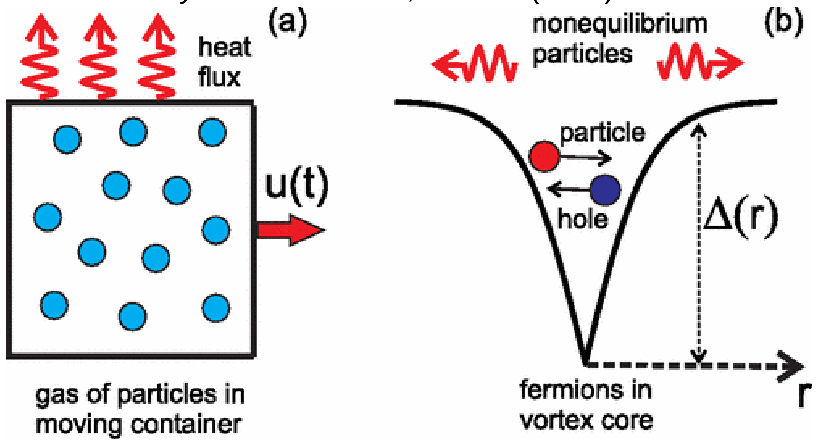
BdG (Fermi):
→ in-core excitations (present event at T=0)

Source: Phys. Rev. Lett. 108, 045303 (2012)



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

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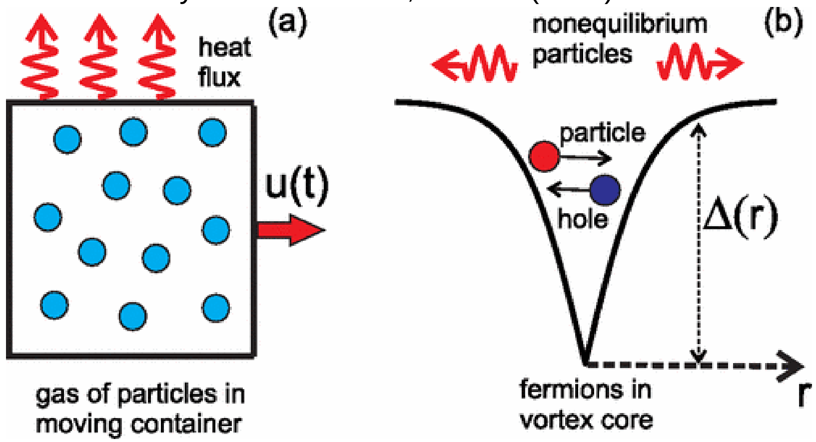
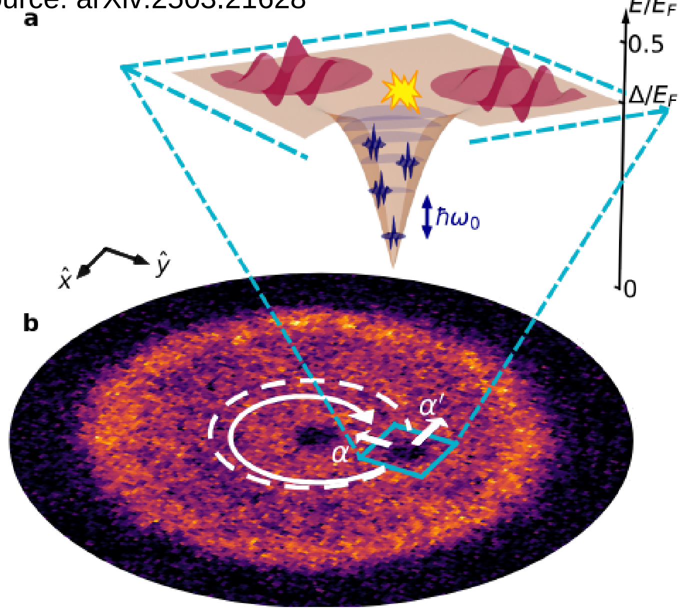


M.A. Silaev, *Universal Mechanism of Dissipation in Fermi Superfluids at Ultralow Temperatures*, Phys. Rev. Lett. 108, 045303 (2012)

→ dissipation mechanism via excitations of the vortex core

→ vortex-core – bulk interactions (T>0)

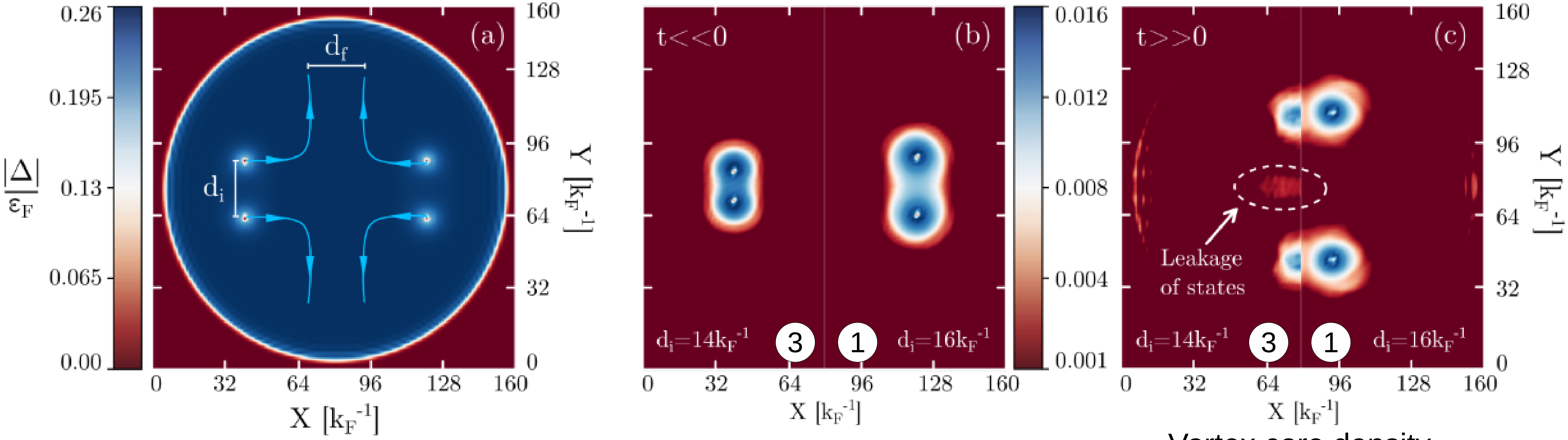
Source: arXiv:2503.21628



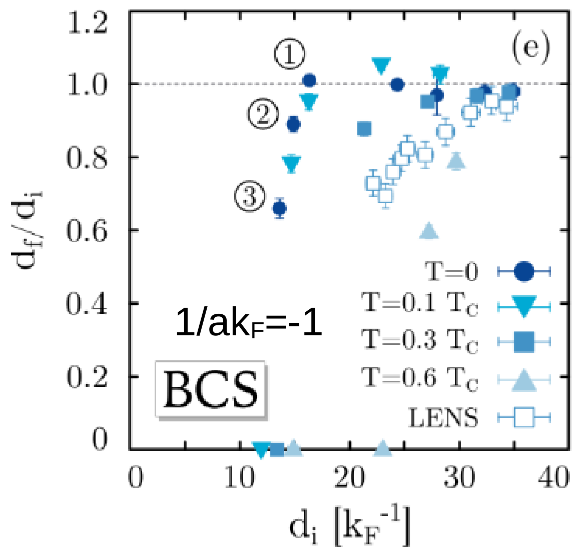
B. Kopnin, *Vortex dynamics and mutual friction in superconductors and Fermi superfluids*, Rep. Prog. Phys. 65, 1633 (2002)

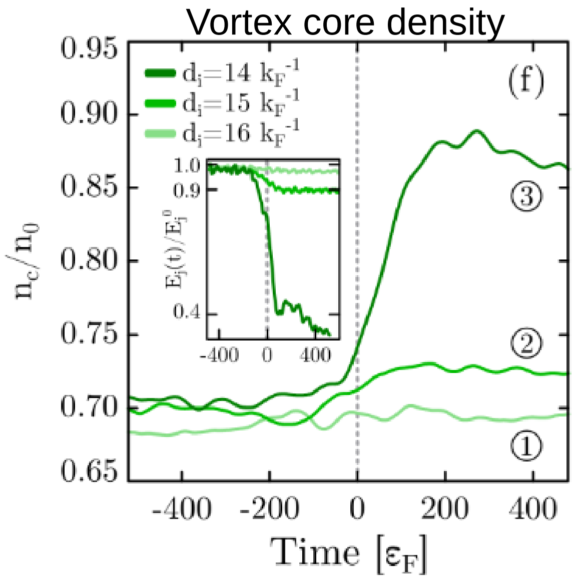
→ dissipation mechanism via scattering of thermal excitations on the CdGM states.

Dissipative effects: results of time-dependent BdG



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

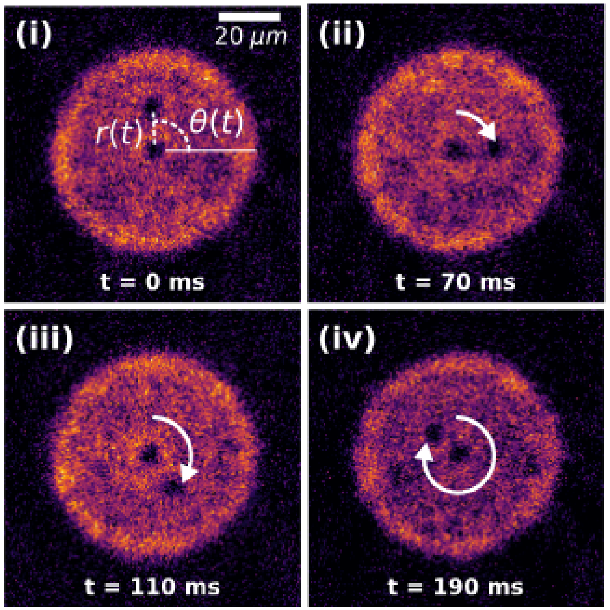


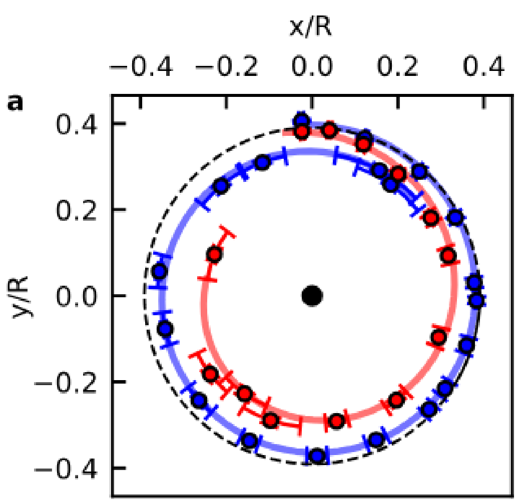


→ *the dissipation due to CdGM states is detected in BCS regime*

(it can be interpreted as effective increase of the vortex core temperature)

Dissipative effects: measurements for strongly interacting Fermi gas & numerical predictions by SLDA [N. Grani et al, arXiv:2503.21628]





T/T_c = 0.36(4) (blue); T/T_c = 0.50(6) (red)

→ *ultracold gas of ^{6}Li atoms confined by disk-shaped trap $ak_F=\infty$ (unitary Fermi gas)*

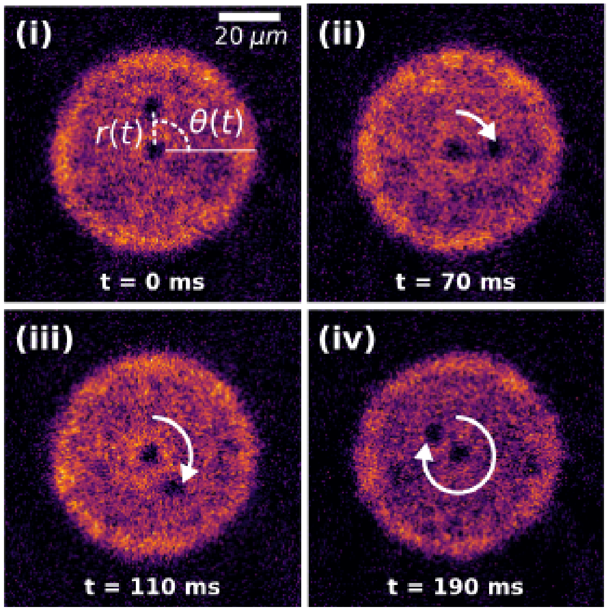
→ *antivortex is pinned by extarnal potential (laser beam) in center of the disk*

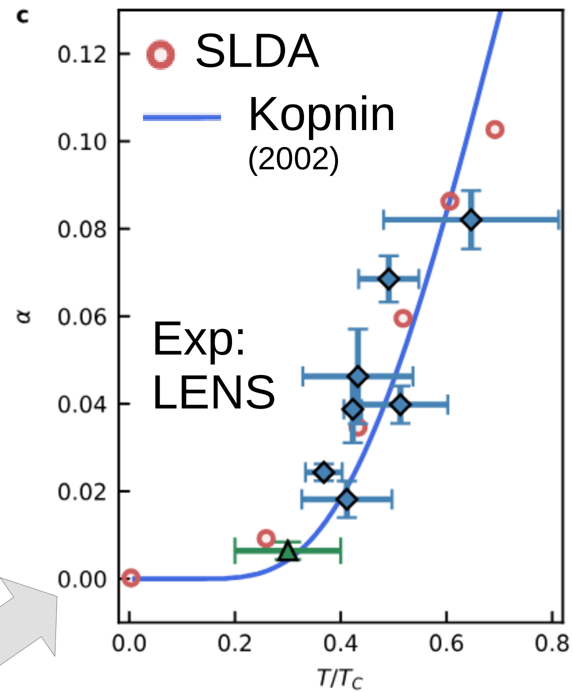
→ *vortex is allowed to orbit around the antivortex*

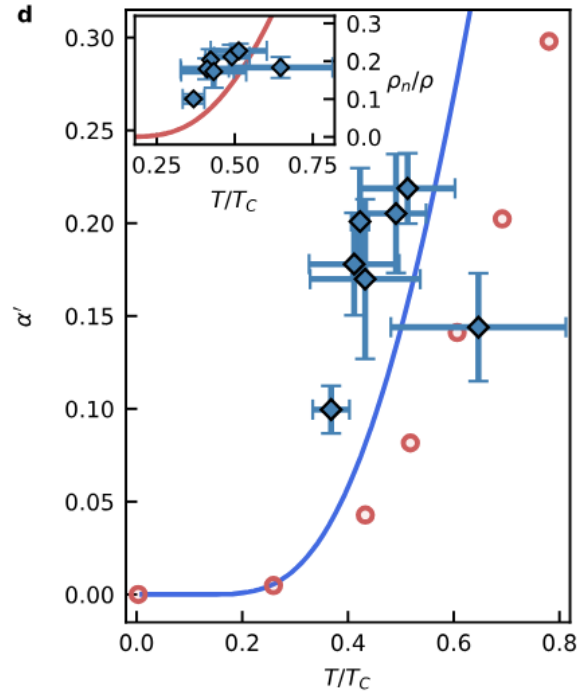
→ *the vortex trajectory is measured as a function of time for different temperatures*

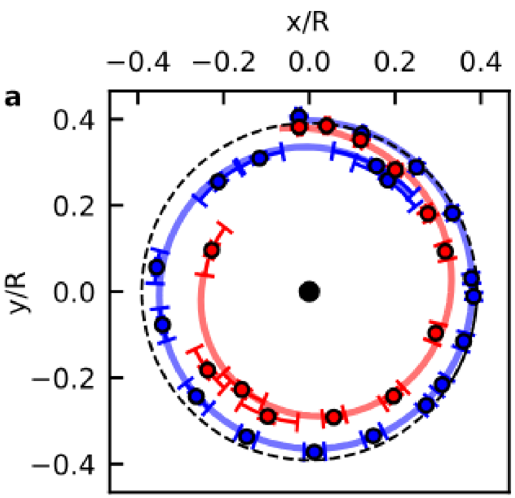
→ *fit of Vortex Point Model trajectory with respect of D and D' ($m_V \approx 0$).*

Dissipative effects: measurements for strongly interacting Fermi gas & numerical predictions by SLDA [N. Grani et al, arXiv:2503.21628]









T/T$_c$ = 0.36(4) (blue); T/T$_c$ = 0.50(6) (red)

SLDA – Extension of BdG equations to strongly interacting regime (formally the same structure of equations as for time-dependent BdG)

$$\alpha = \frac{\tilde{D}}{\tilde{D}^2+(1-\tilde{D}')^2},$$

$$1-\alpha' = \frac{1-\tilde{D}'}{\tilde{D}^2+(1-\tilde{D}')^2}$$

$$\tilde{D} = \frac{D}{\kappa n_s},\ \tilde{D}' = \frac{D'}{\kappa n_s}$$

→ *interplay between vortex-bound quasiparticles and delocalized thermal excitations drives the dissipation*

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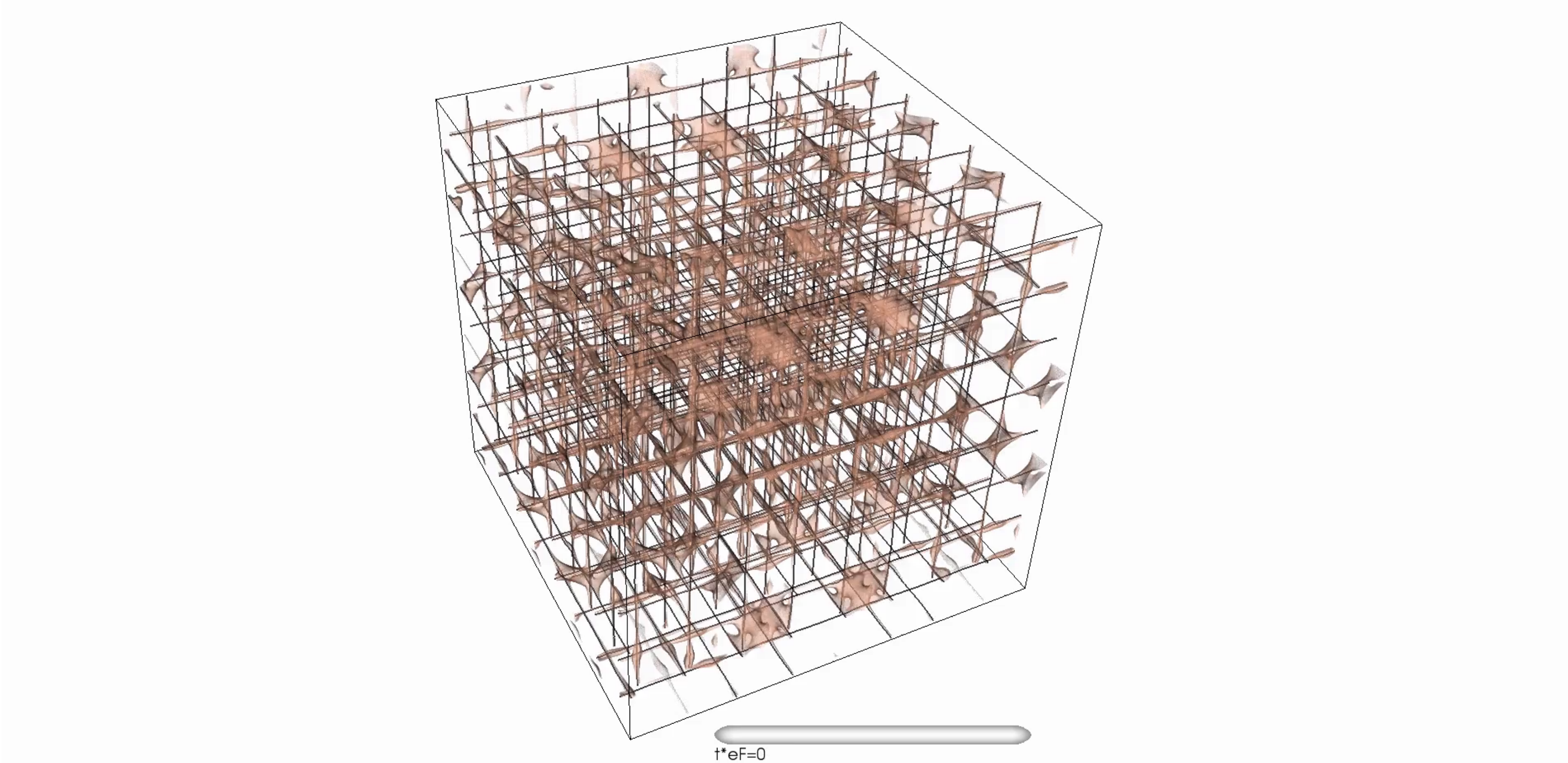
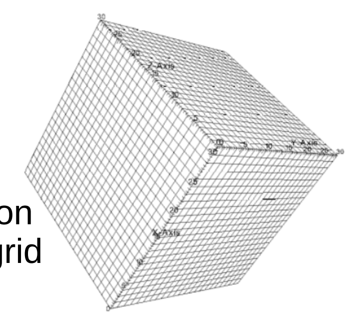
BdG-type equations & Computational physics



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

Quantum turbulence in the unitary Fermi gas
PNAS Nexus, pgae160 (2024)



Computation on spatial grid

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

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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

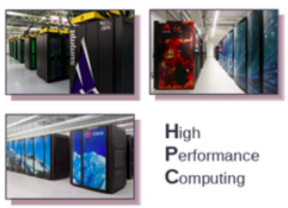
$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}u_n(\boldsymbol{r},t)\\ v_n(\boldsymbol{r},t)\end{pmatrix} = \begin{pmatrix} h_a(\boldsymbol{r},t)-\mu_a & \Delta(\boldsymbol{r},t) \\ \Delta^*(\boldsymbol{r},t) & -h_b^*(\boldsymbol{r},t)+\mu_b \end{pmatrix}\begin{pmatrix}u_n(\boldsymbol{r},t)\\ v_n(\boldsymbol{r},t)\end{pmatrix}$$

Extension to nuclear matter in neutron stars

Unified solvers for static and time-dependent problems

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

Speed-up calculations by exploiting High Performance Computing



W-SLDA is designed to exploit capabilities of leadership-class supercomputers.

Depending on the type of the code the toolkit can be executed on:

static codes: standard CPU machines, GPU accelerated machines,
time-dependent codes: only GPU accelerated machines.

To learn more about a computer that you need for calculations see Requirements

ALL FUNCTIONALITIES →

Integration with VisIt: visualization, animation and analysis tool

Speed-up calculations by exploiting High Performance Computing

Functionals for studies of BCS and unitary regimes

We release the data generated by the W-SLDA Toolkit to maximize the knowledge gained from simulations run on costly HPC systems and to share research opportunities with other groups.

Example: (approx 70GB of raw data)

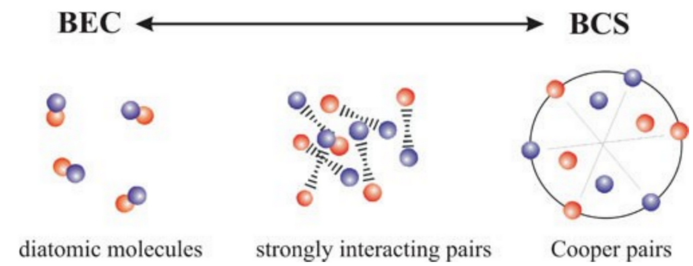
September 25, 2023 (v1) | Dataset | Open

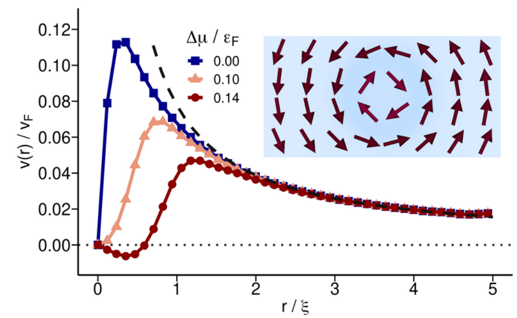
Quantum turbulence in superfluid Fermi gas: results of numerical simulation

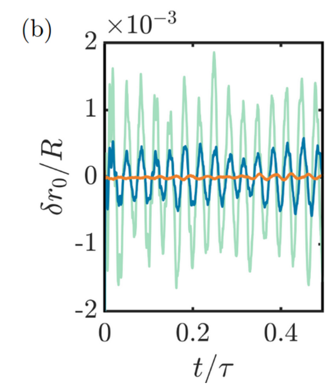
Gabriel Wlazłowski; Michael McNeil Forbes; Saptarshi Rajan Sarkar; and 2 others

SUMMARY

- Microscopic simulations across whole BCS-BEC crossover are presently feasible:
  - TDBdG → BCS regime;
  - TDSLDA → strong interaction;
  - GPE → BEC regime
- Many properties of quantized vortices are determined by the topology of the order parameter
- Vortices acquire internal structure in Fermi superfluids
  - → origin of vortex mass
    (normal component in the vortex core)
  - → origin of new dissipation mechanism
    (excitations of the vortex core, ...)







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Thank you

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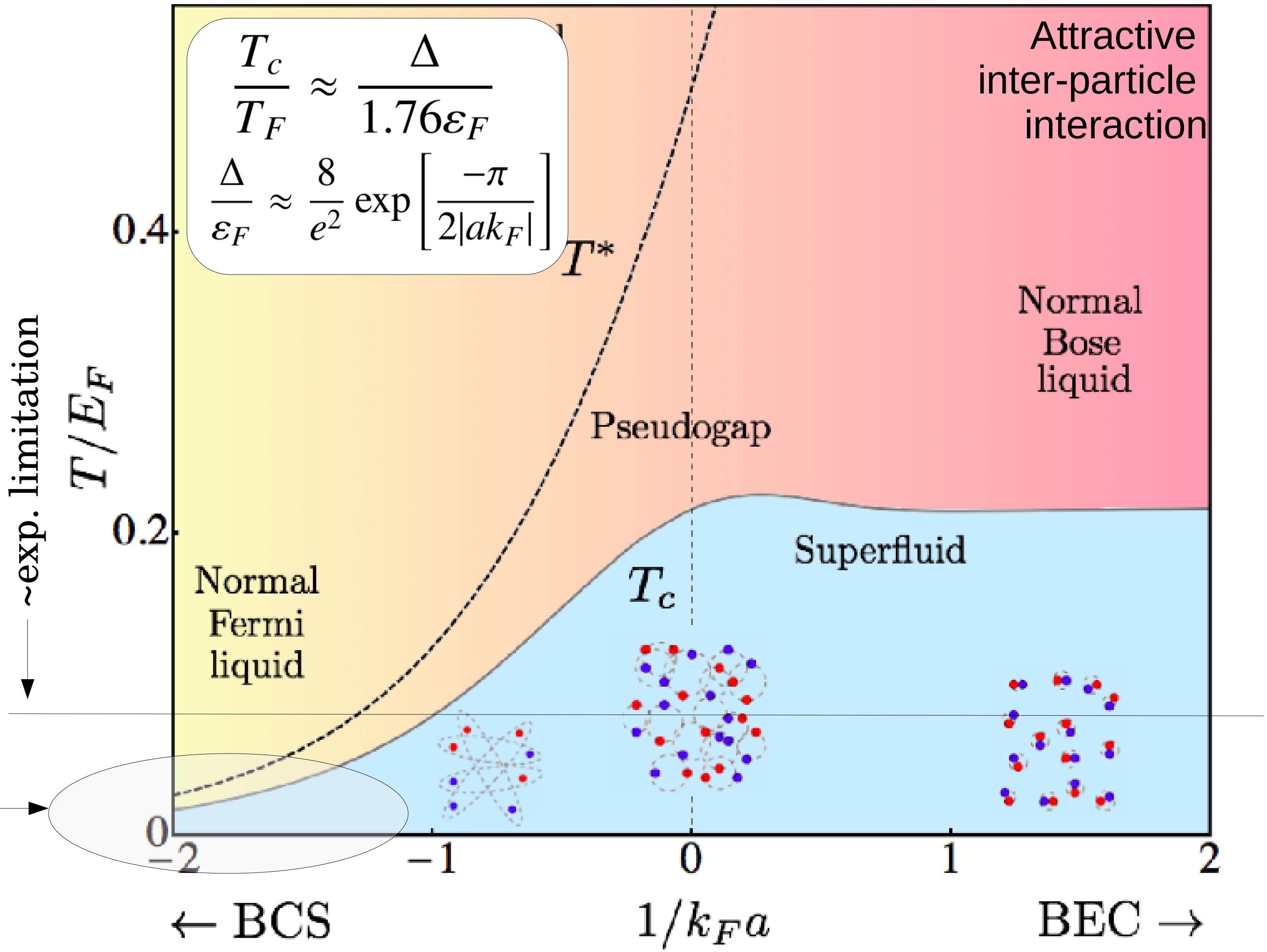
physics wut

Synergy: theory & experiment

Experiments:

$$\frac{T}{T_F} \gtrsim 0.05$$

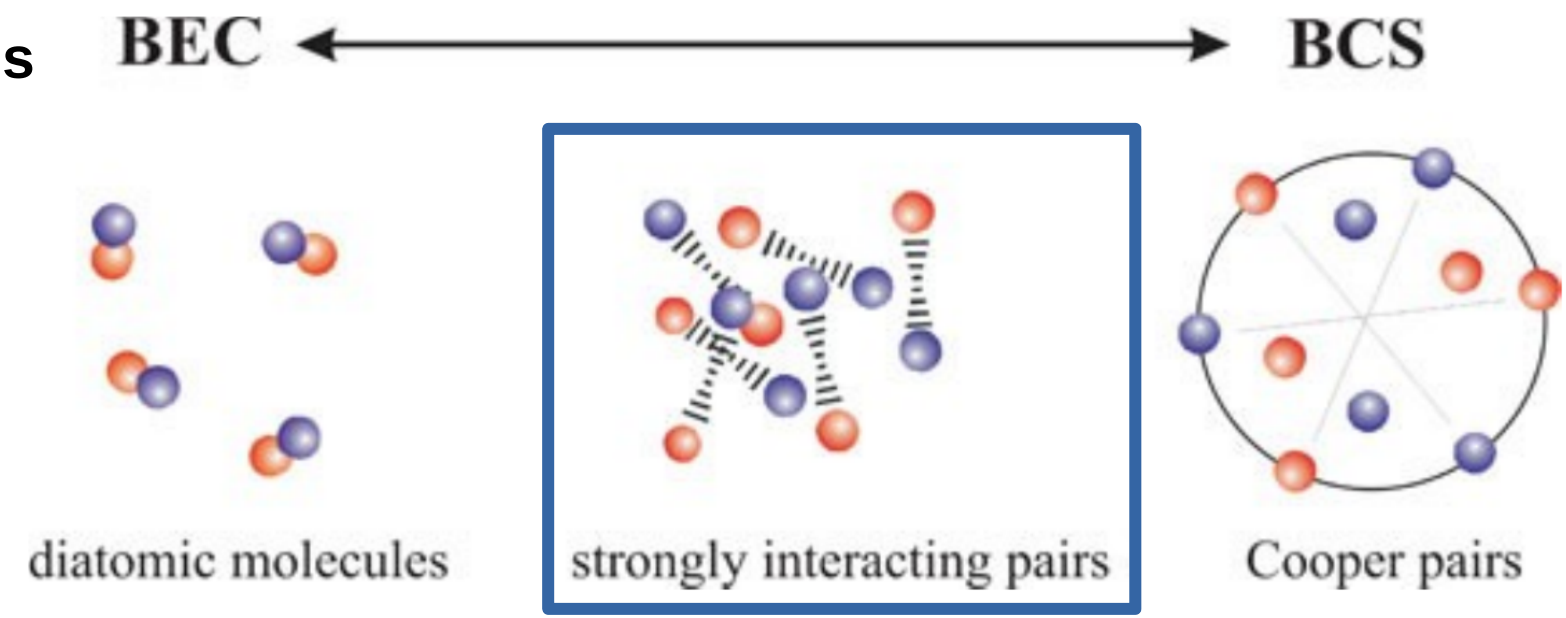
$$|ak_F| \gtrsim 1$$



Regime of validity of BdG theory

(note: BdG for uniform system = BCS theory)

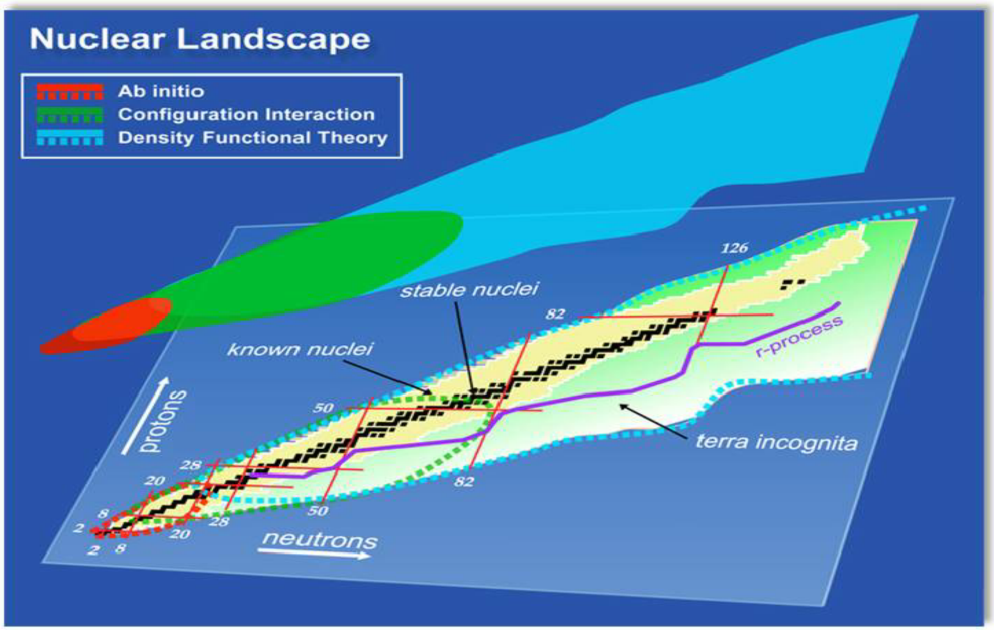
Methods



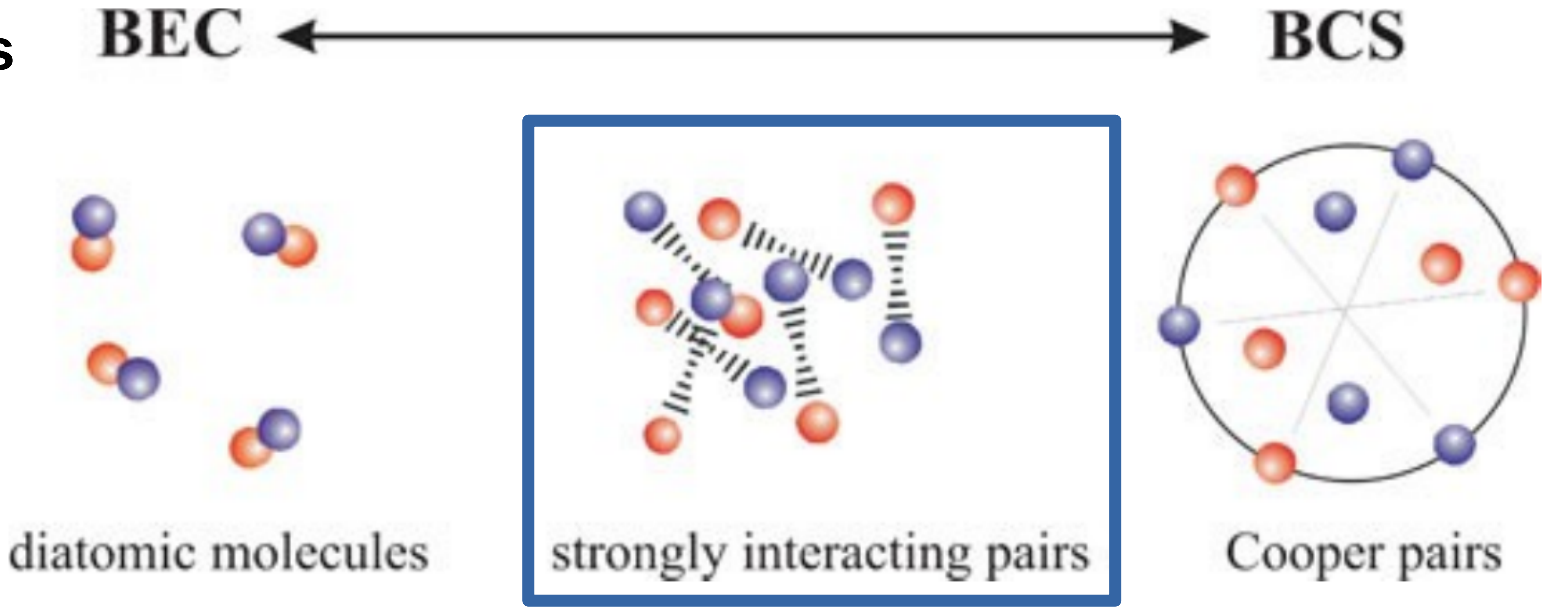
Density Functional Theory:
Superfluid Local Density Approximation (SLDA)

Workhorse for:

- Solid state physics…
- Quantum chemistry…
- Nuclear physics…
- …atomic gases…



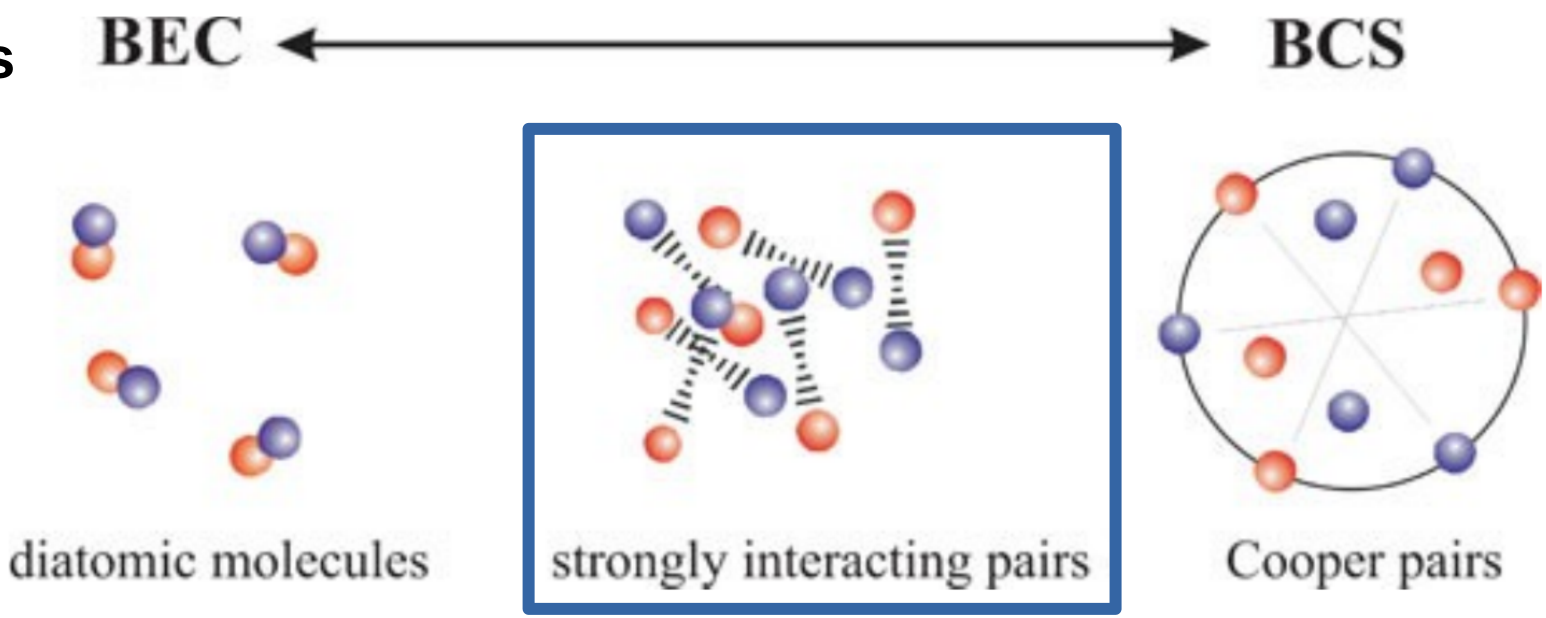
Methods



Density Functional Theory:
Superfluid Local Density Approximation (SLDA)

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

Methods



Density Functional Theory:
Superfluid Local Density Approximation (SLDA)

Formally equations are the same as for BdG:

Current corrections

$$h_\sigma(\boldsymbol{r},t) = -\nabla\frac{\hbar^2}{2m^*(n)}\nabla + U_\sigma(n,\nu) + V_\sigma(\boldsymbol{r},t) - \frac{i}{2}\{\boldsymbol{A}(n,\boldsymbol{j}),\nabla\}$$

Effective mass

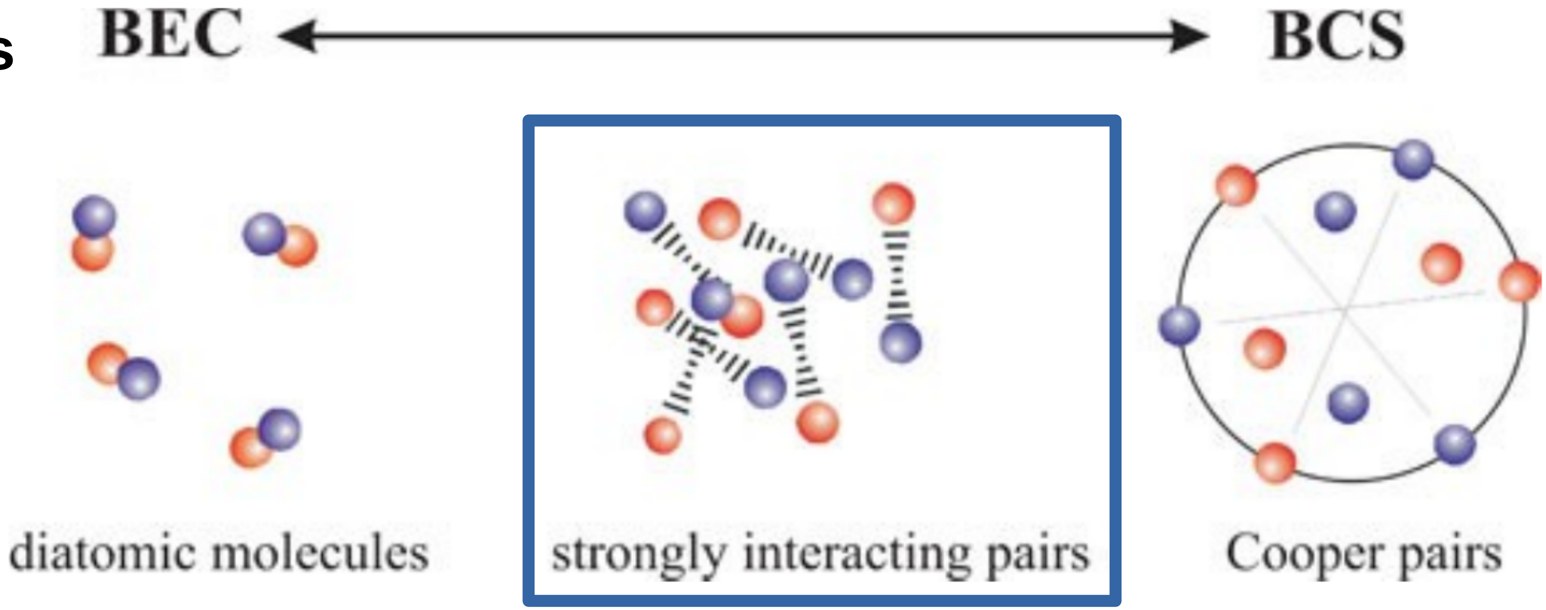
Potential simulating effects of interactions

$$\Delta(\boldsymbol{r},t) = g(n)\nu$$

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_\eta(\mathbf{r},t) \\ v_\eta(\mathbf{r},t)\end{pmatrix} = \mathcal{H}_{\mathrm{SLDA}}\begin{pmatrix} u_\eta(\mathbf{r},t) \\ v_\eta(\mathbf{r},t)\end{pmatrix}$$

$$\mathcal{H}_{\mathrm{SLDA}} = \begin{pmatrix} h_\uparrow(\mathbf{r},t) - \mu_\uparrow & \Delta(\mathbf{r},t) \\ \Delta^*(\mathbf{r},t) & -h^*_\downarrow(\mathbf{r},t) + \mu_\downarrow \end{pmatrix}$$

Methods



Density Functional Theory:
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Effective mass

Potential simulating effects of interactions

Explicit coupling between density modes and pairing modes

$$\Delta(\boldsymbol{r},t) = \underline{g(n)}\nu$$

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SLDA-type functional

Superfluid Local Density Approximation

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

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

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

quasiparticle = mixture of hole particle

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

current density

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

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

+ orthonormality condition (Pauli principle)

anomalous density

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

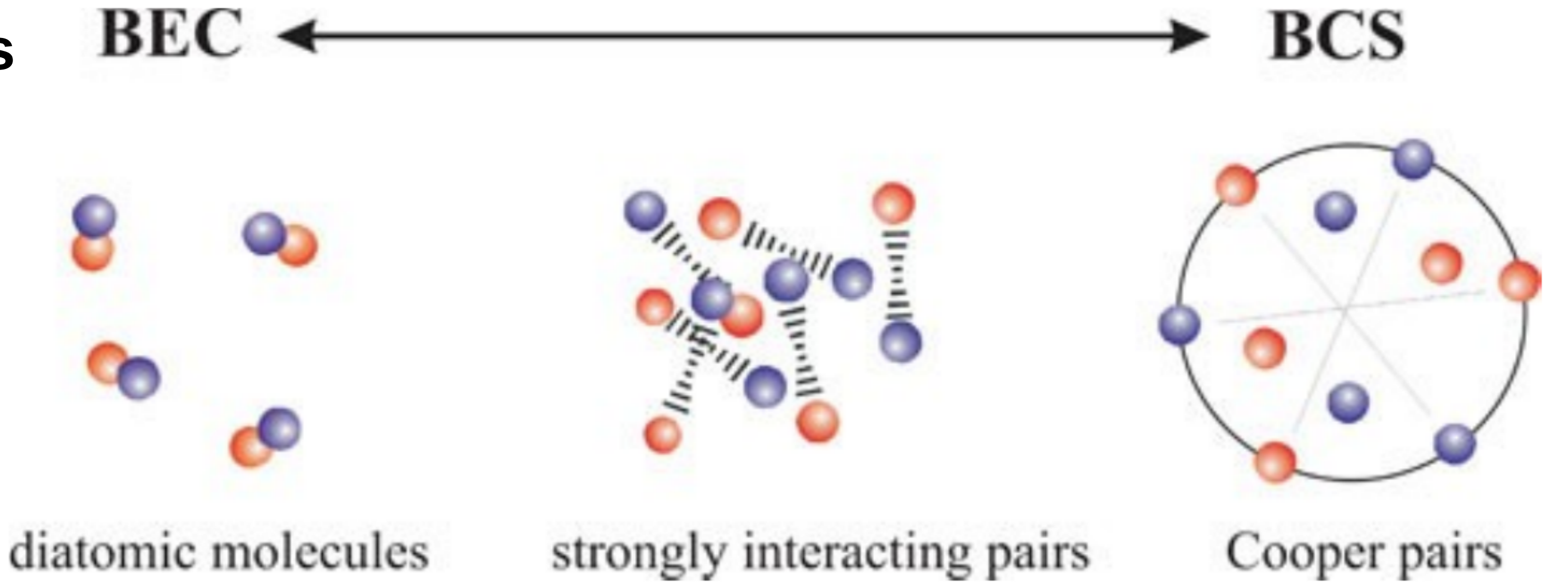
Additional density required by DFT theorem for systems with broken U(1) symmetry

Energy cut-off scale (need for regularization)

SLDA (and BdG) allows for solutions: **n≠0 and ν=0**

→ ***Cooper pair breaking*** → ***effectively normal component***

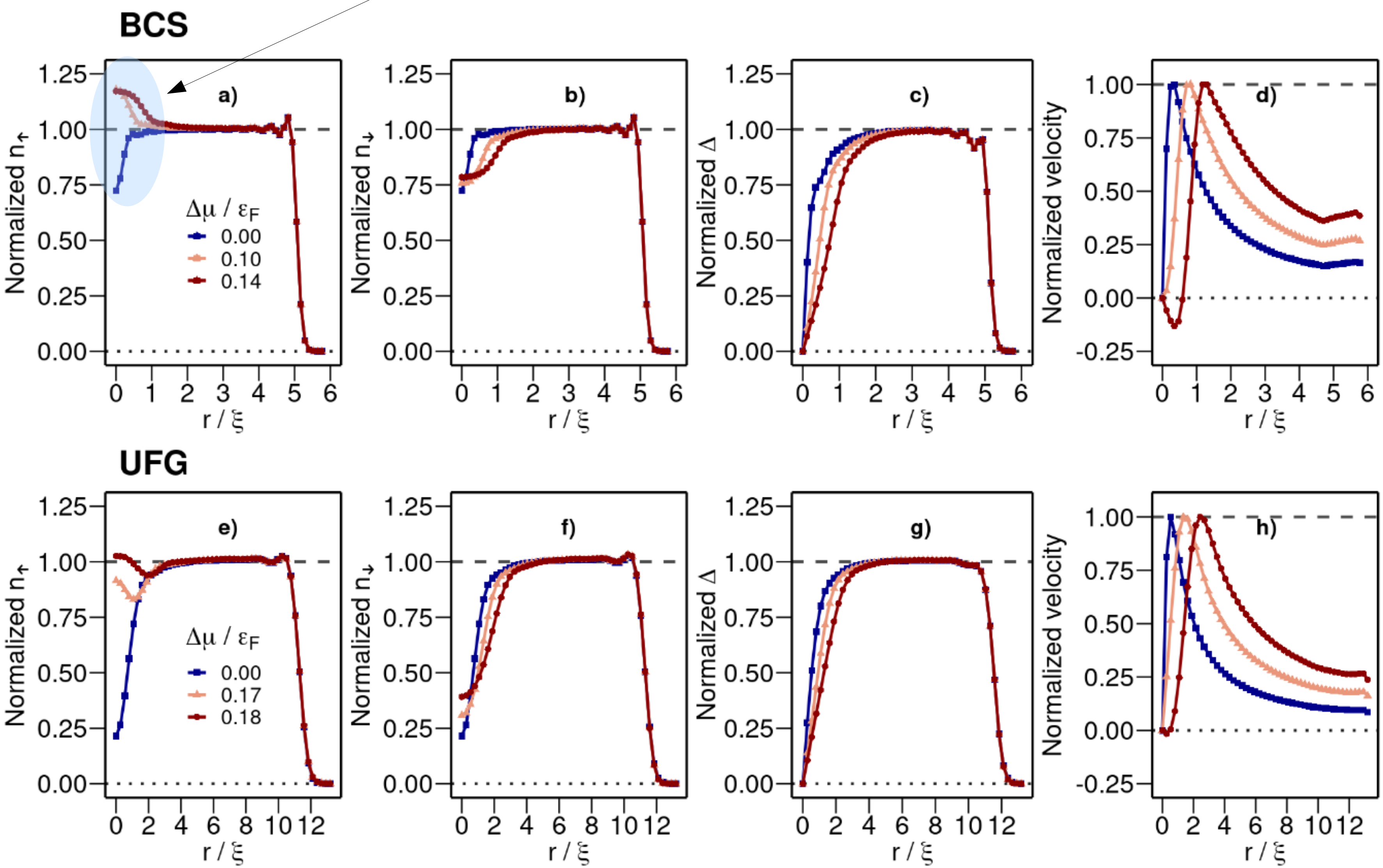
Methods



	GPE	SLDA	BdG
dof	Dimers (bosons)	Fermions	Fermions
wave-function	Condensate wave-function $\psi(r,t)$	Quasiparticle states $\varphi_n(r,t)=\{u_n(r,t),v_n(r,t)\}$	Quasiparticle states $\varphi_n(r,t)=\{u_n(r,t),v_n(r,t)\}$
Dynamics depends on	$n=\lvert\psi\rvert^2$	n – normal density, ν – anomalus density **j** – current density	ν – anomalus density (all interaction effects are modeled by pairing term)

Vortex structure

Majority component accumulates in the core.



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