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

Gabriel Wlazłowski

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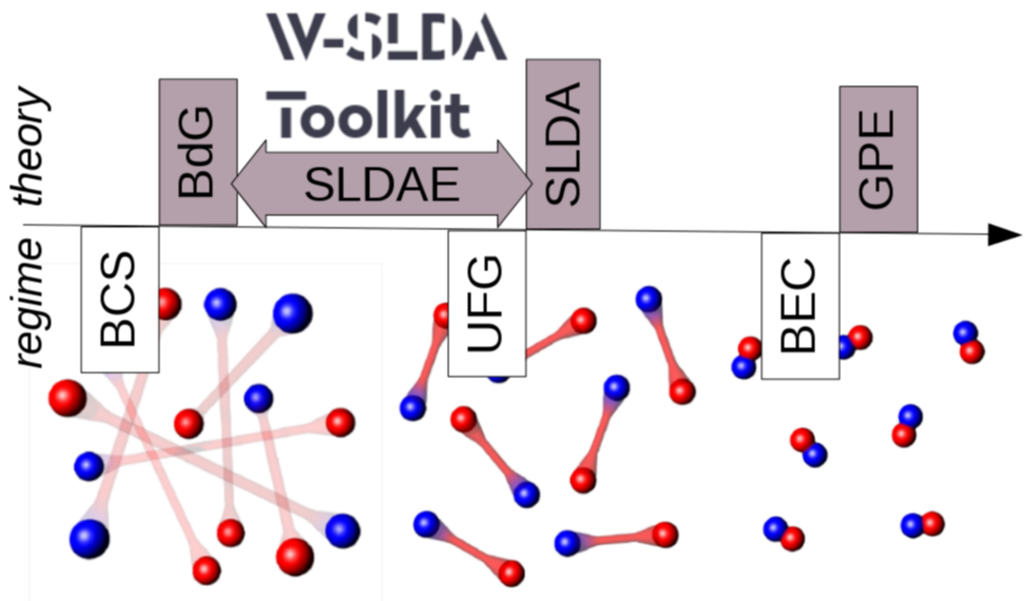
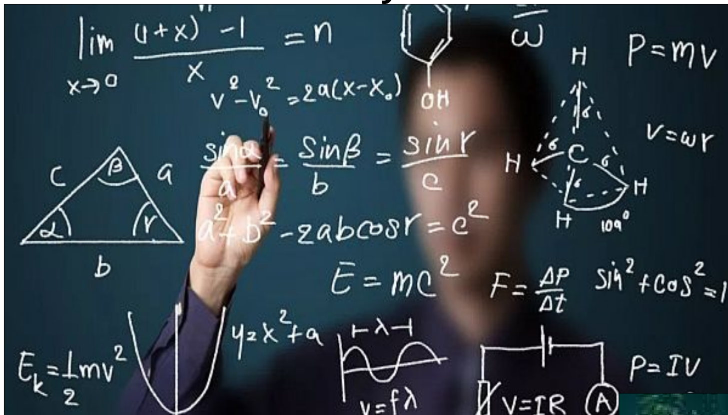
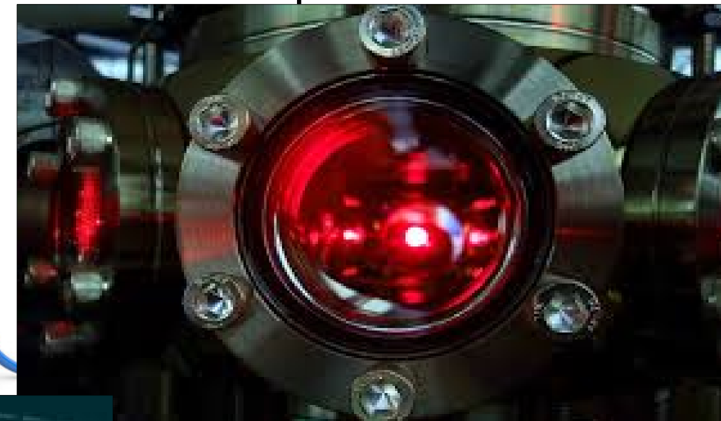


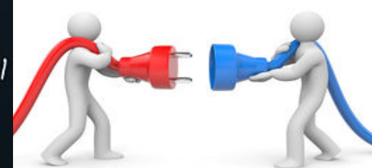
National Science Centre Poland

Theory



Experiment





Computational physics

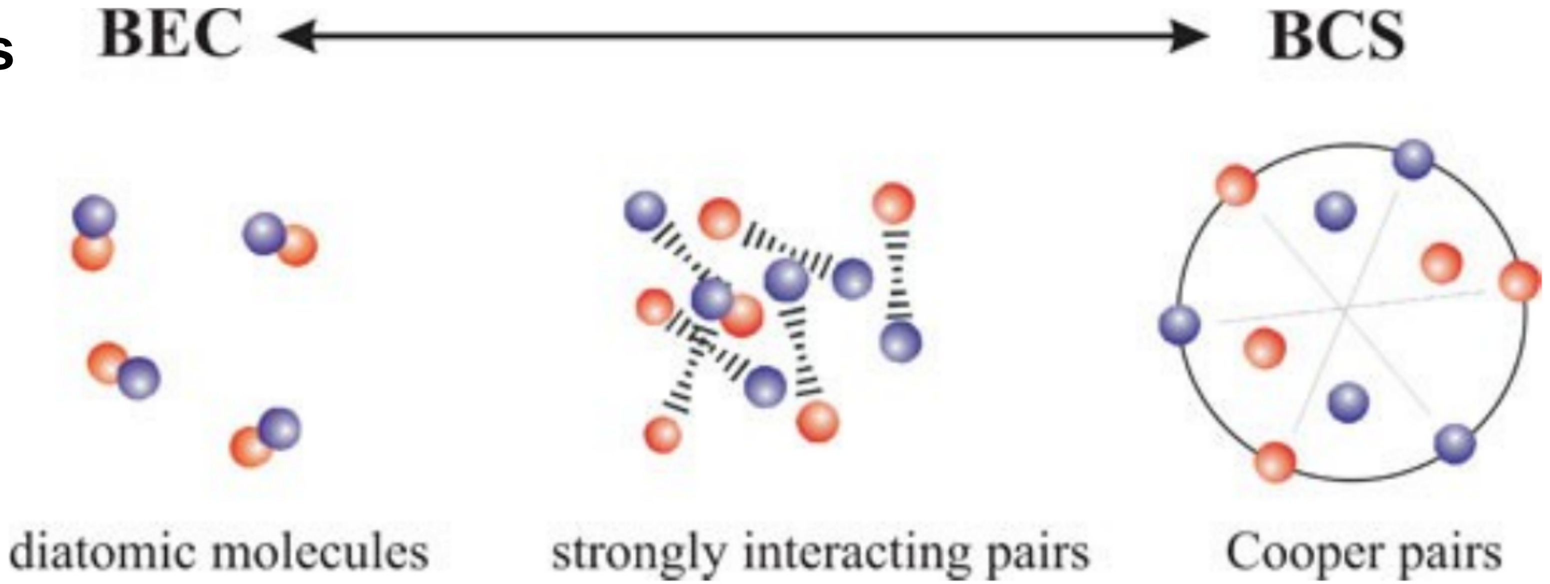
Overview:
*1. Method → DFT**
2. Implementation
3. Applications

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

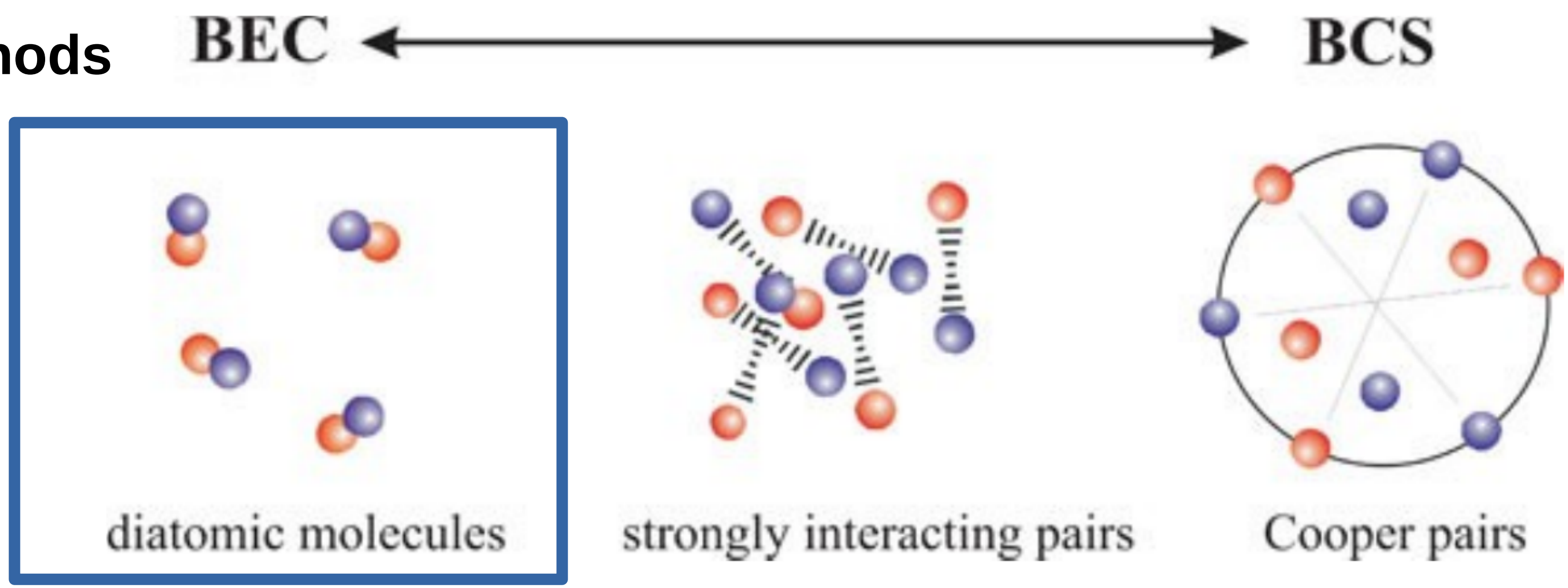
- *General purpose method* → wide range of applicability
  → typically it has numerical complexity at most as a mean-field method
  (example for BECs: Gross-Pitaevskii equation)

- *Specialized methods* → devoted to specific problems / quantities
  → typically *ab initio* methods like QMC, ...

Methods


BEC
BCS
diatomic molecules
strongly interacting pairs
Cooper pairs

Methods



Gross-Pitaevski equation (GPE): $n^{1/3}a_{dd} \ll 1$

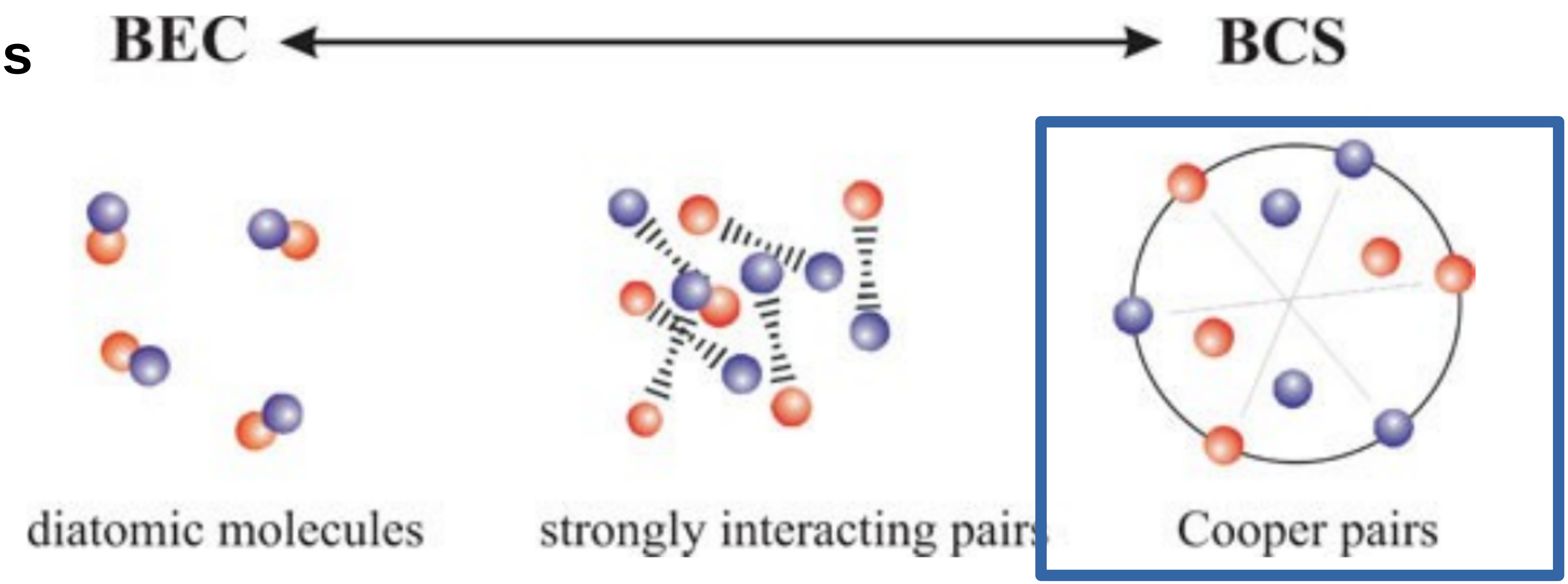
$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2M}\nabla^2 + V_{\mathrm{trap}} + g|\psi(\vec{r},t)|^2\right)\psi(\vec{r},t)$$

mass of dimer = 2m

Depends on dimer-dimer scattering length a_{dd}

Numerical complexity: N logN 

Methods



Bogoliubov-de Gennes equations (BdG):

$|k_F a| \ll 1, \quad k_F = (3\pi^2 n)^{1/3}$

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

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

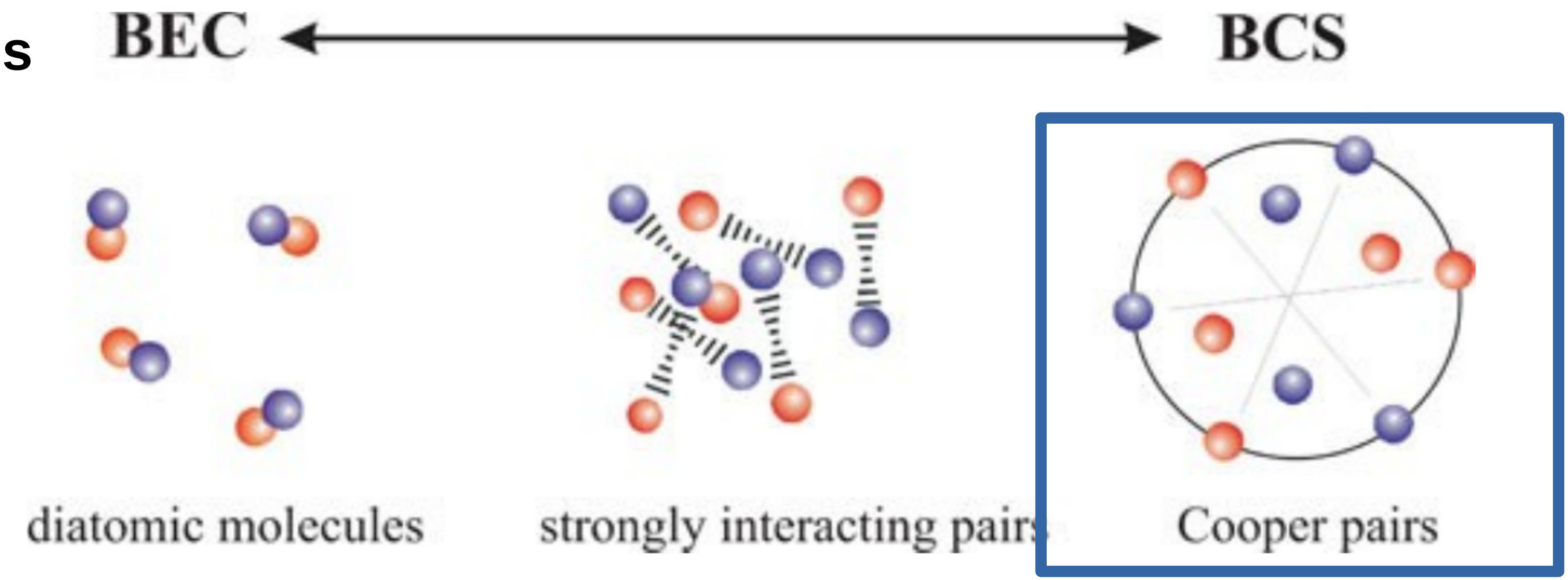
$$h_\sigma(\mathbf{r},t) = -\hbar^2 \nabla^2 / 2m + V_\sigma(\mathbf{r},t)$$ Single particle hamiltonian

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

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

Anomalous density

Methods



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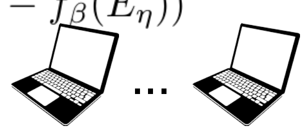
Anomalous density

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



Numerical complexity: N(N logN)*

BdG theory vs experiment

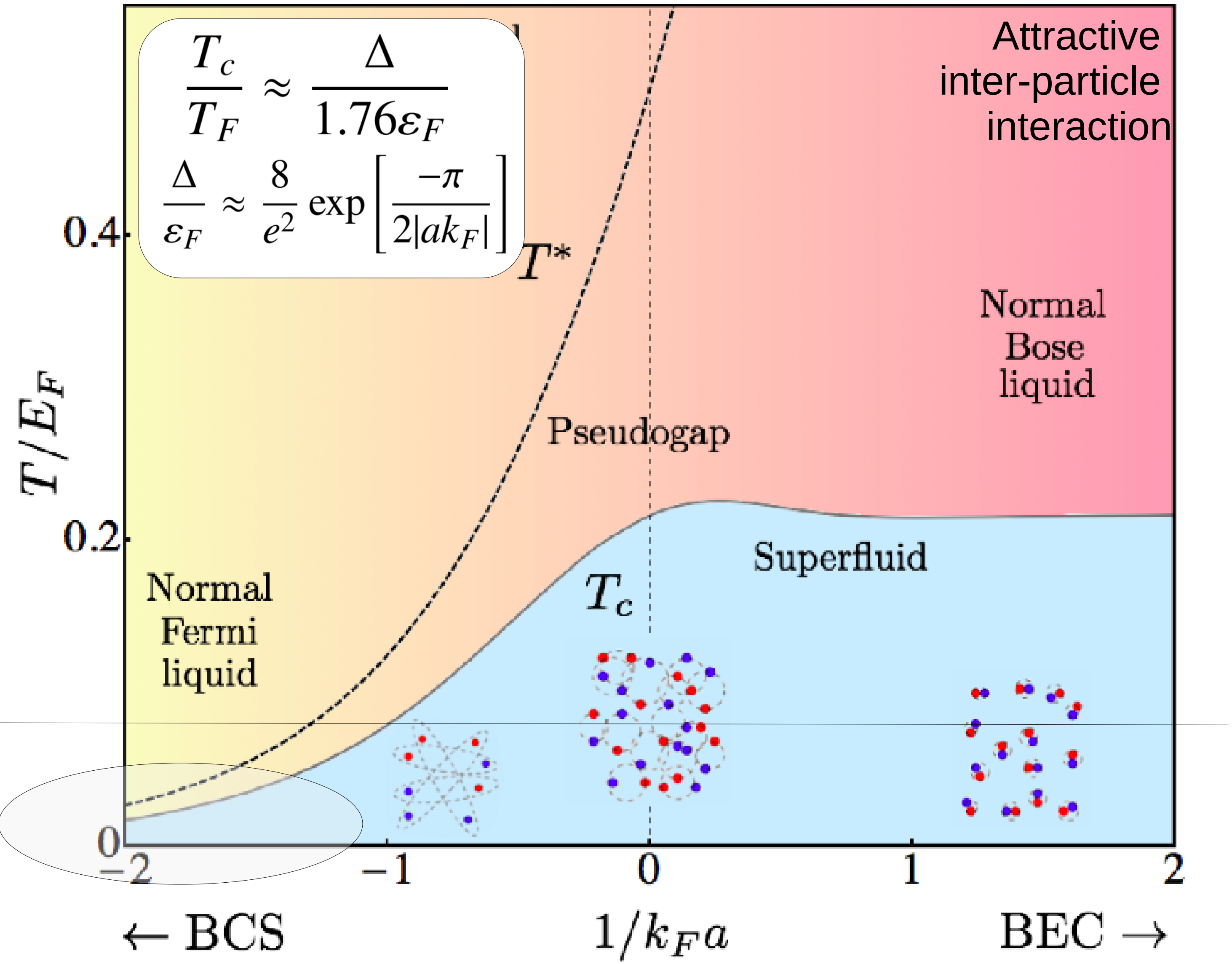
Experiments:

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

↓

$$|ak_F| \gtrsim 1$$

~exp. limitation



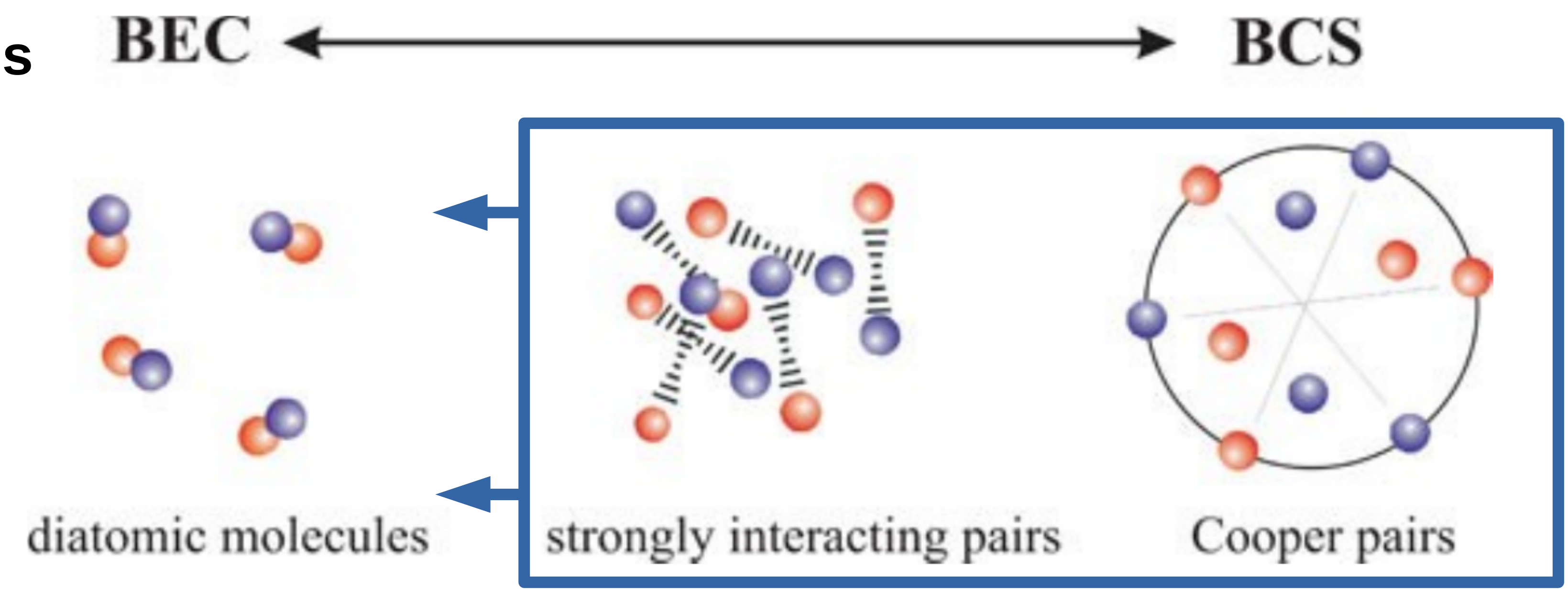
$$\frac{T_c}{T_F} \approx \frac{\Delta}{1.76\varepsilon_F}$$

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

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 $\langle O \rangle = \langle \Psi[\rho] | \hat{O} | \Psi[\rho] \rangle = O[\rho]$
- … 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)

SLDA-type functional

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

Dimensionless functional parameters

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

$$\mathcal{E} = A_\lambda \frac{\tau}{2} + \frac{3}{5} B_\lambda n \varepsilon_{\mathrm{F}} + \frac{C_\lambda}{n^{1/3}} |\nu|^2$$

Kinetic term

Potential term

Pairing term

total = intrinsic + couplings to external fields...

$$E_{tot} = E + \sum_\sigma \int V_\sigma^{(\mathrm{ext})}(\boldsymbol{r}) n_\sigma(\boldsymbol{r})\, d\boldsymbol{r} - \frac{1}{2} \int \left(\Delta^{(\mathrm{ext})}(\boldsymbol{r}) \nu^*(\boldsymbol{r}) + \mathrm{h.c.}\right) d\boldsymbol{r} + \ldots$$

SLDA-type functional

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

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MINIMIZATION

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

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A. Bulgac, M.M. Forbes
Phys. Rev. A 75, 031605(R) (2007)

A. Boulet, G. Wlazłowski, P. Magierski
Phys. Rev. A 106, 013306 (2022)

BdG	ASLDA Asymmetric SLDA, a→∞	SLDAE SLDA Extended, p=0
$A_\lambda \rightarrow 1$	$A_\lambda \rightarrow A[p(\boldsymbol{r})]$	$A_\lambda \rightarrow A[ak_F(\boldsymbol{r})]$
$B_\lambda \rightarrow 0$	$B_\lambda \rightarrow B[p(\boldsymbol{r})]$	$B_\lambda \rightarrow B[ak_F(\boldsymbol{r})]$
$C_\lambda \rightarrow -\frac{4\pi\hbar^2}{(3\pi^2)^{1/3} m} ak_F$	$C_\lambda \rightarrow C[p(\boldsymbol{r})]$	$C_\lambda \rightarrow C[ak_F(\boldsymbol{r})]$

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

→ *ab initio* cals for E/E_{FG}, Δ/ε_F, m^*/m

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

INDUCE →

Functional parameters

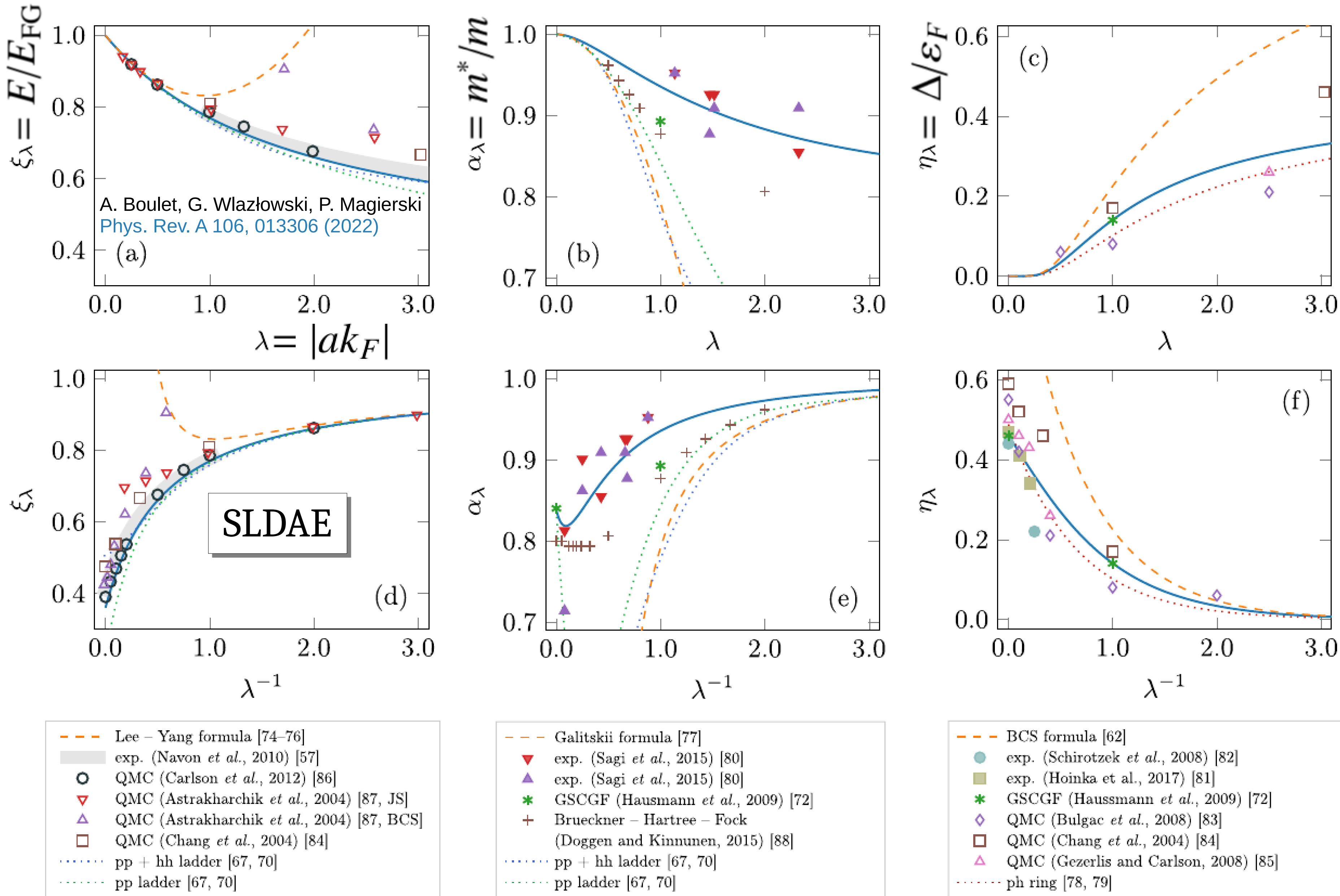
$\{A_\lambda, B_\lambda, C_\lambda\}$

→ *ab initio* cals for E/E_{FG}, Δ/ε_F, m^*/m

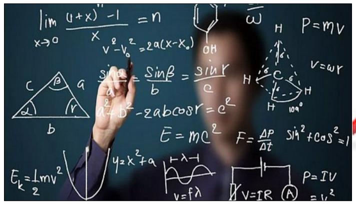
→ limiting cases (EFT, scale invariance, ...)

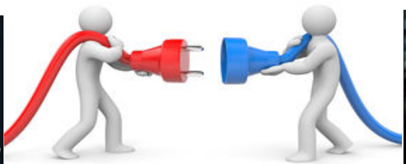
INDUCE

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

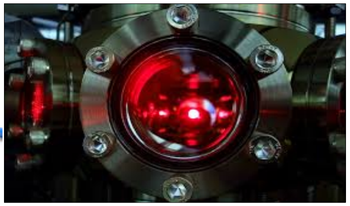


Theoretical method





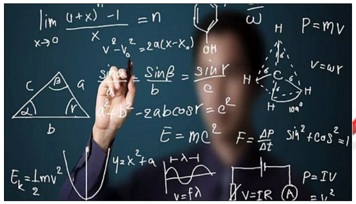
Experiment

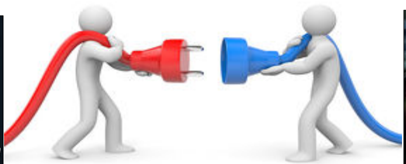


Computer code

PHYSICS.WUT

Theoretical method





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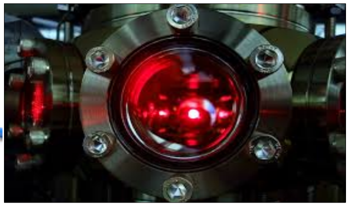

Computer code

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

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

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

time-dependent problems: td-wslda

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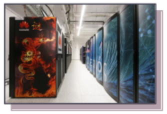

High Performance Computing

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

NVIDIA CUDA AMD ROCm open source

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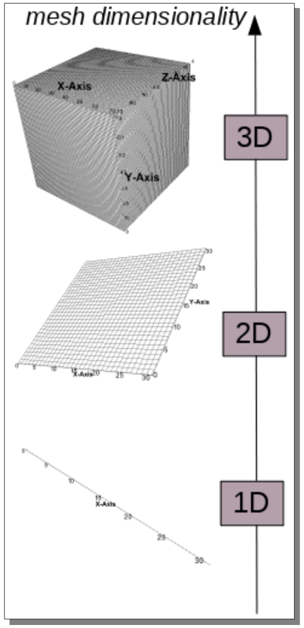

→ BCS-BEC crossover
→ spin-imbalanced systems
→ mass-imbalanced systems
→ finite temperature formalism

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

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PHYSICS.WUT

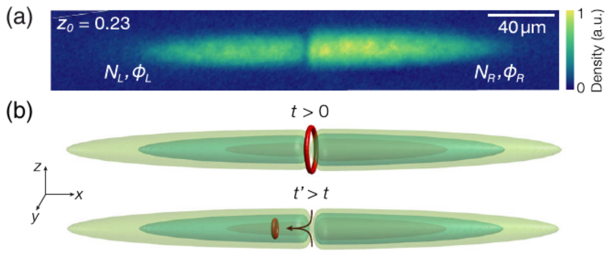
Application #1: Fermionic Josephson Junction

Inspired by LENS ^{6}Li setup (G. Roati's group):

[1] G. Valtolina, et.al., Science **350**, 1505, (2015);

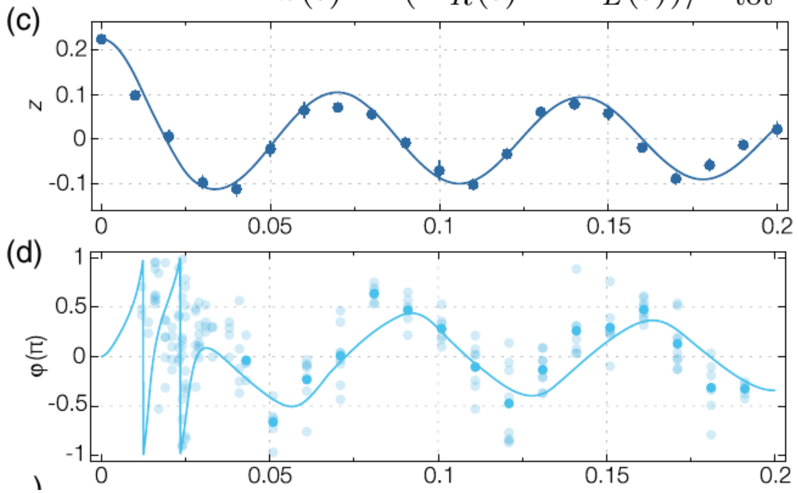
[2] A. Burchianti, et.al., Phys. Rev. Lett. **120**, 025302 (2018)

[3] K. Xhani, et.al., Phys. Rev. Lett. **124**, 045301 (2020)



Figs from [2]

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



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

Experiment

Simulation

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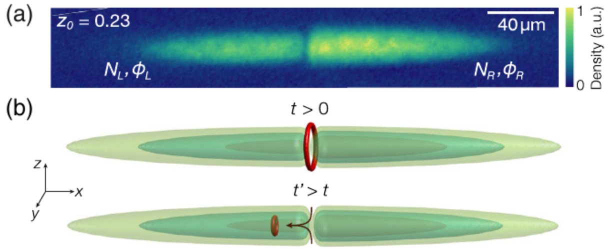

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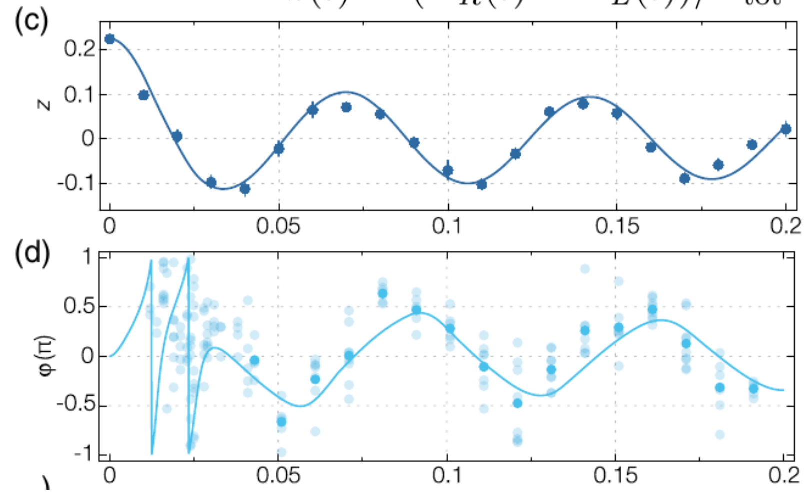


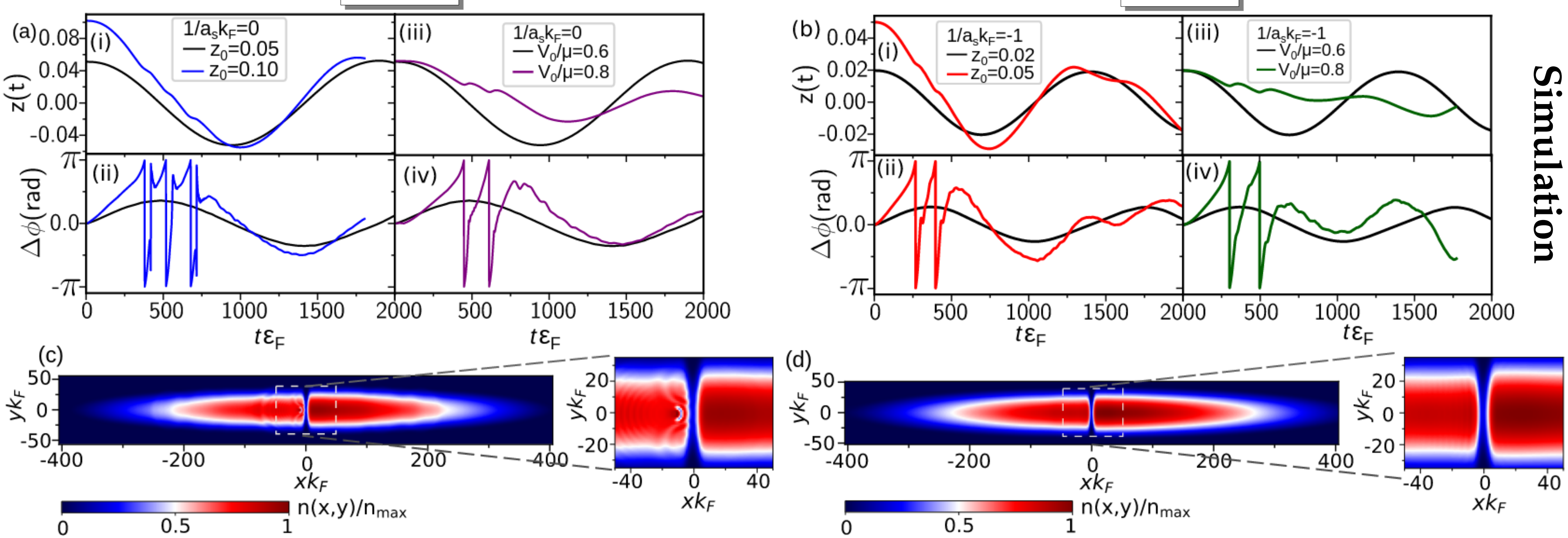
$$\Delta\phi(t) \equiv \phi_L(t) - \phi_R(t)$$ t [ms]

Experiment

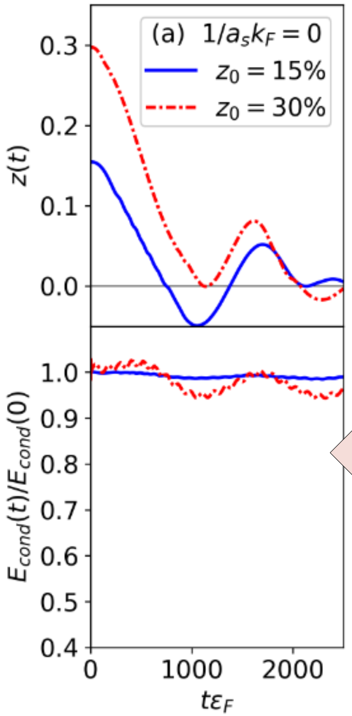
G. Wlazłowski, et.al., arXiv:2207.06059

UFG

BCS

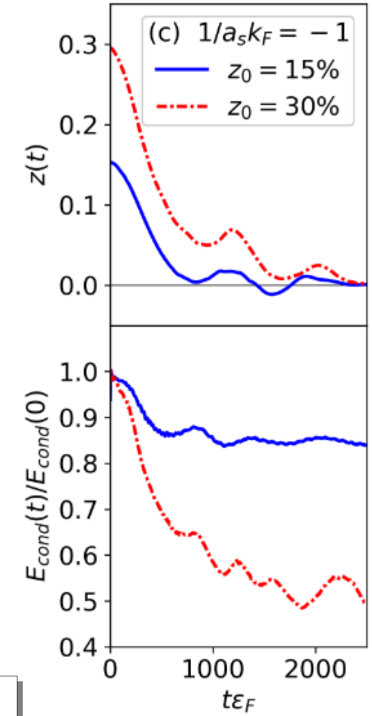


Simulation



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

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

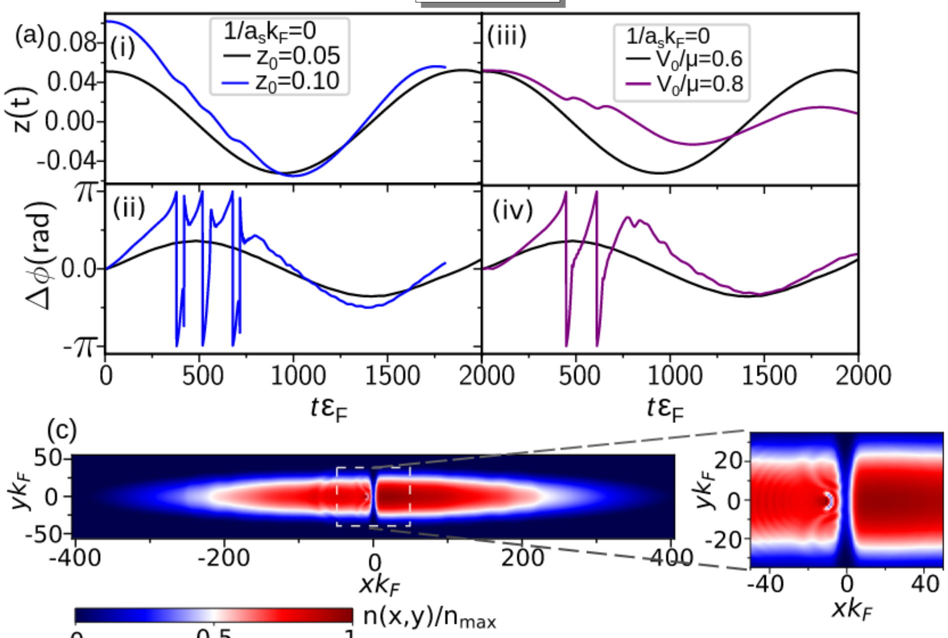


pair breaking is negligible

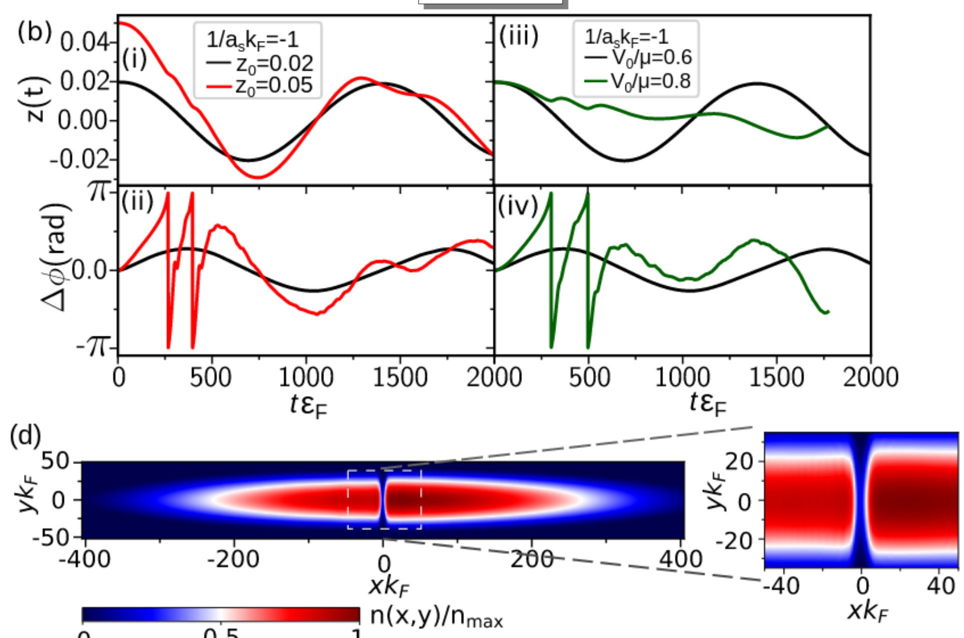
pair breaking!

G. Wlazłowski, K. Xhani, M. Tylutki, N. Proukakis, M. Magierski, arXiv:2207.06059

UFG



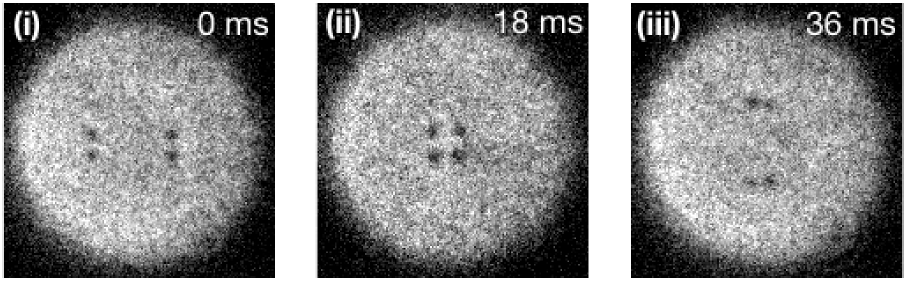
BCS

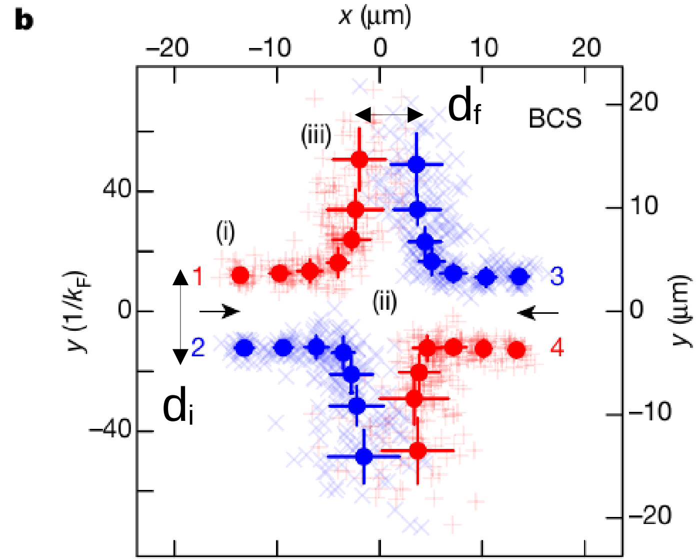


Application #2: Vortex collisions

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

Figs from [1]





Experiment

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

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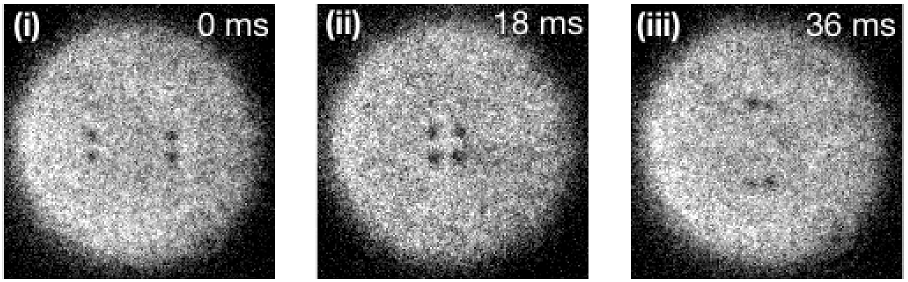

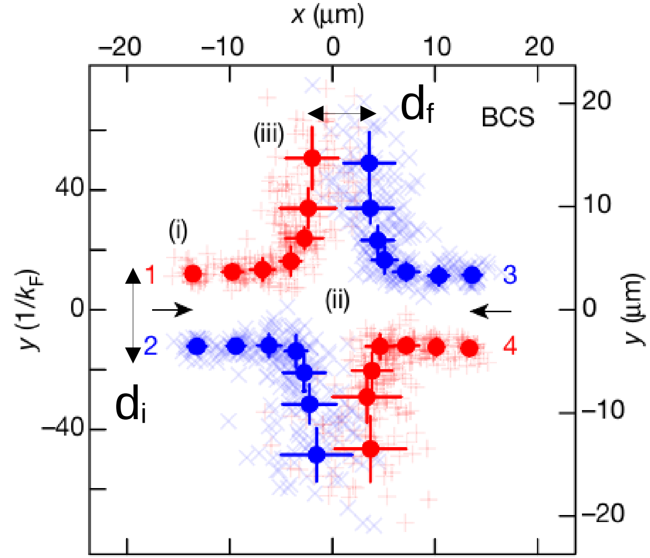

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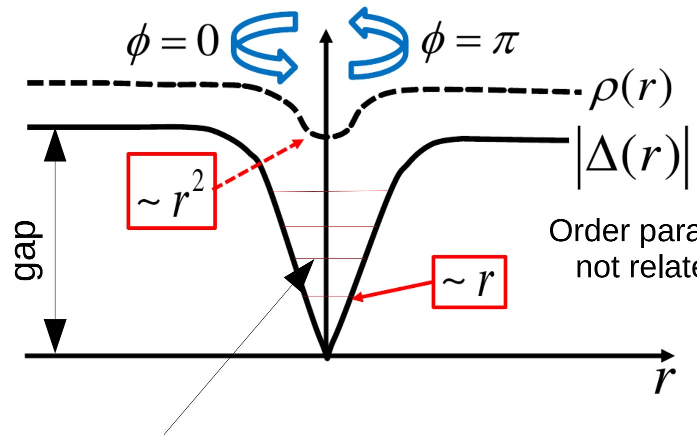
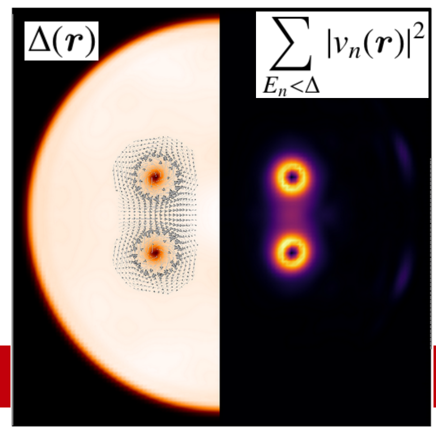
Vortex solution: Fermi gas → BdG



Order parameter:
not related directly to density

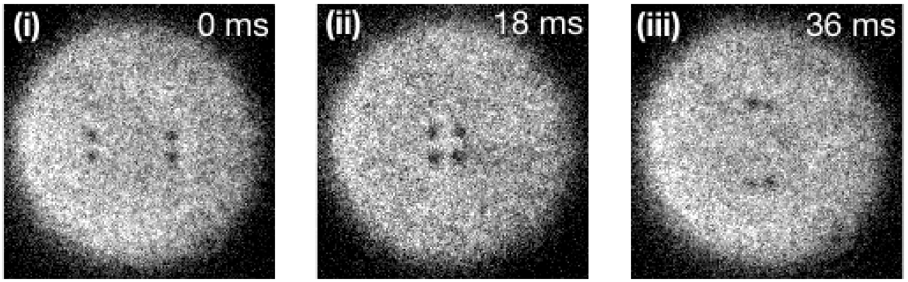
Occupation of Andreev states give rise to significant particle density inside the core.

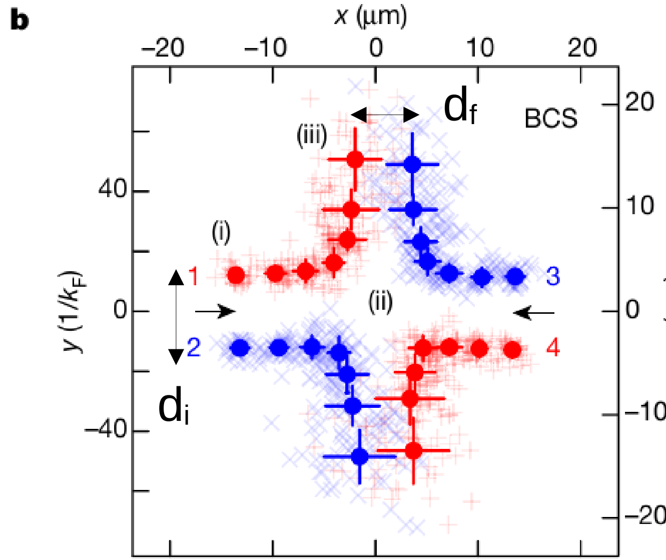


Application #2: Vortex collisions

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

Figs from [1]

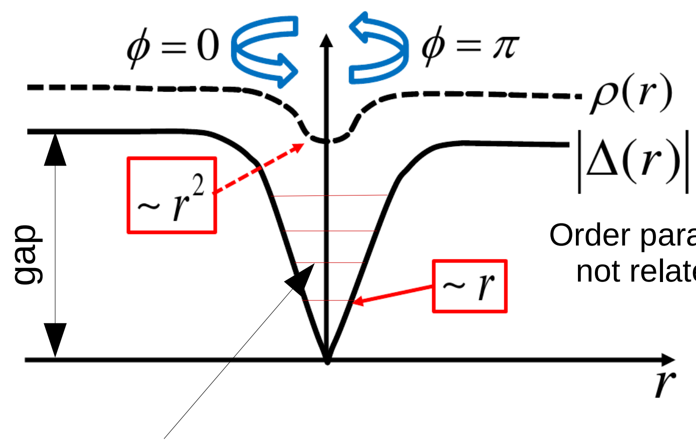




Experiment

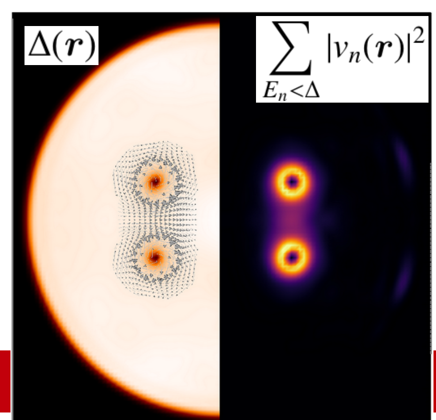
Dissipation during the collision is reflected in $d_f/d_i < 1$.

Vortex solution: Fermi gas → BdG



Order parameter:
not related directly to density

Occupation of Andreev states give rise to significant particle density inside the core.



Do the internal structure of vortices contribute to the dissiption?

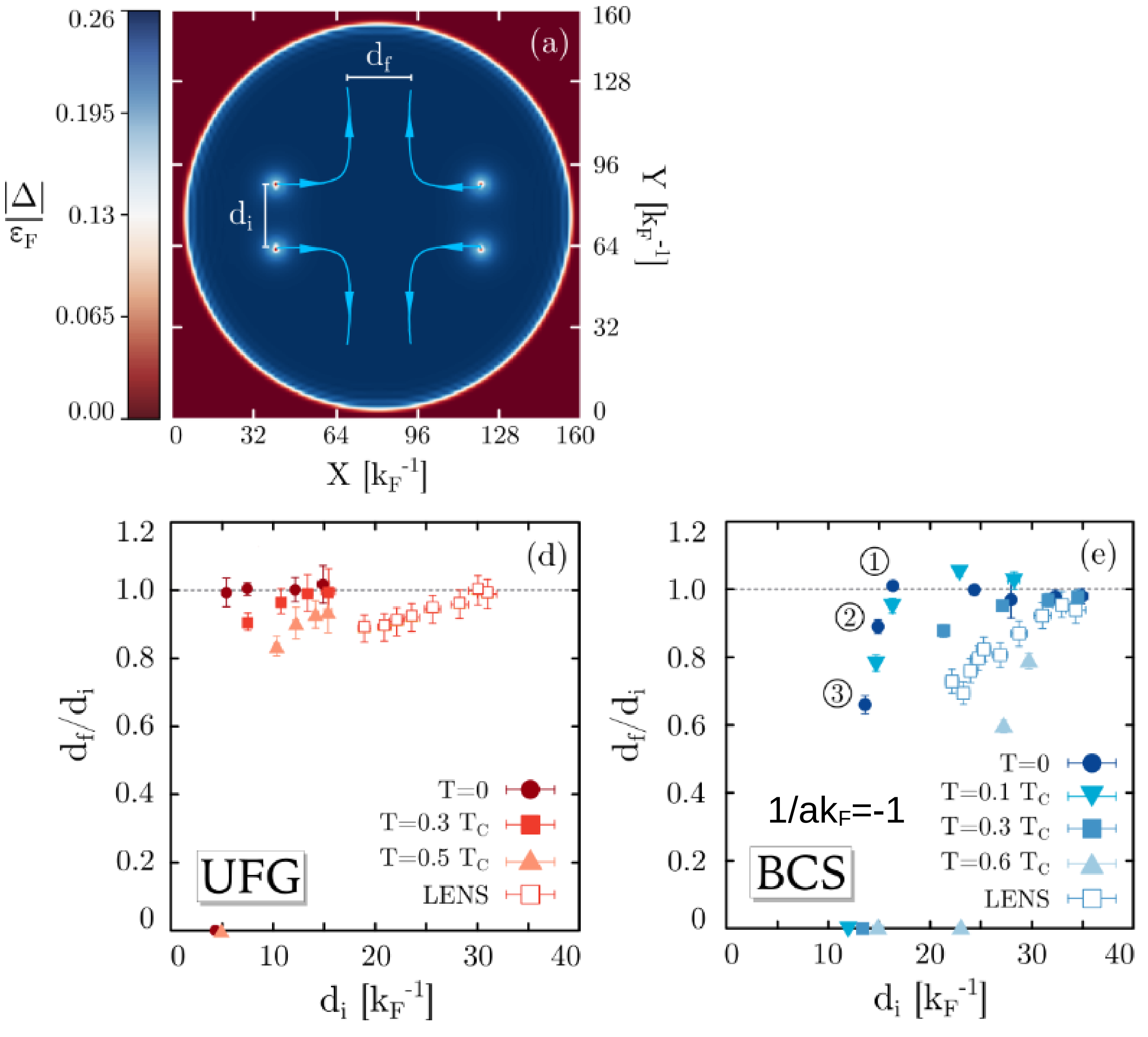
Prediction [M. Silaev, PRL. 108 (2012)]:

→ Andreev quasiparticles can be excited (effective increase of the vortex core temperature), ...

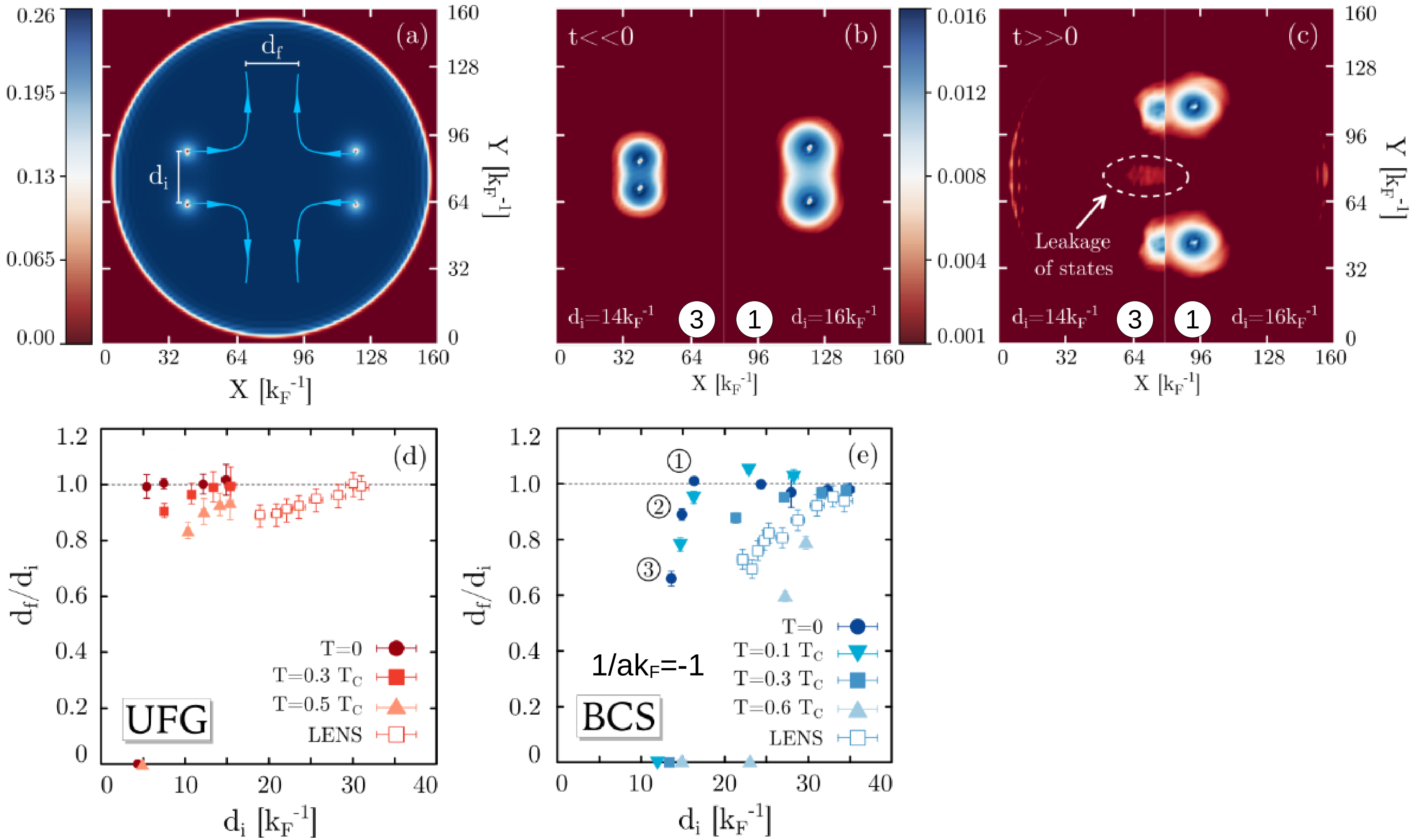
→ and eventually converted into delocalized states

→ the impact of this process gets stronger as we move towards BCS regime

PHYSICS.WUT



A. Barresi, A. Boulet, P. Magierski, G. Wlazłowski, arXiv:2207.00870



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

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

→ *the effect is to weak to explain the experimental measurements*

→ *significant sensitivity of the results to the temperature*

SUMMARY

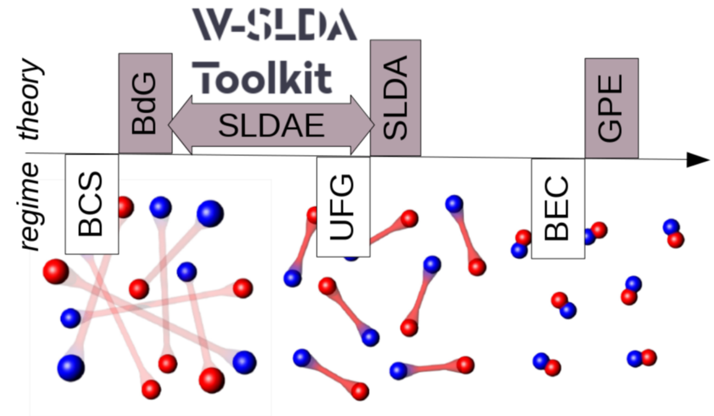
- Microscopic simulations across whole BCS-BEC crossover are presently feasible:

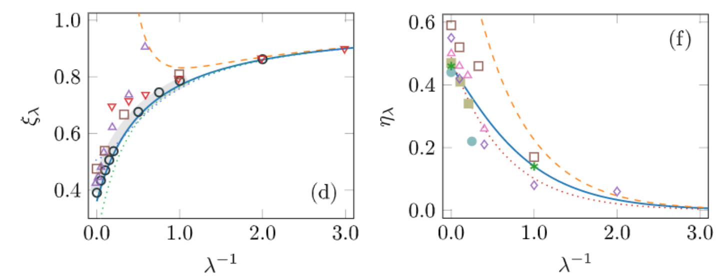
DFT	→	BCS regime;
SLDA		strong interaction;
GPE	→	BEC regime

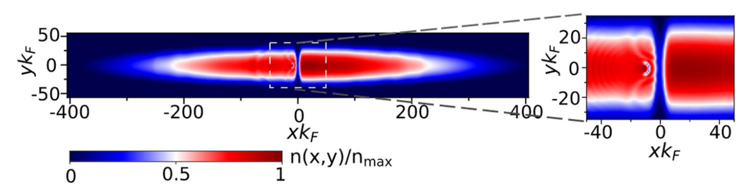
- DFT is general purpose method: it overcomes limitations of mean-field approch, while keeping numerical cost at the same level as BdG calculations.

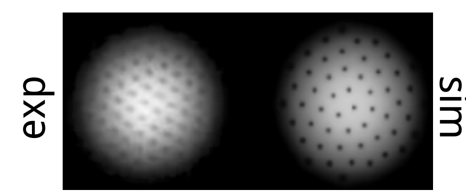
- You do not to be expert in DFT in order to use DFT. Open-source implementation is available.

- DFT can benchmark experiments
  - *Can provide insight into processes that are beyond reach of GPE-like approaches.*
  - *Exotic types of superfluidity (spin-imbalanced, mass-imbalanced…).*









Collaborators: P. Magierski, M. Tylutki, A. Barresi, A. Boulet (WUT); M. Forbes (WSU); A. Bulgac (UW); K. Xhani (LENS); N. Proukakis (Newcastle U.)

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Appendix

Energy

Energy is computed from the formula:

$$E = \int \mathcal{E}_{\text{edf}}(n, \nu, \ldots)\, d^3r + \sum_\sigma \int V_\sigma^{(\text{ext})}(r) n_\sigma(r)\, d^3r$$

$$-\frac{1}{2} \int \left(\Delta^{(\text{ext})}(r)\nu^*(r) + \text{h.c.}\right) d^3r - \sum_\sigma \int \vec{v}_\sigma^{(\text{ext})}(r) \cdot \vec{j}_\sigma(r)\, d^3r$$

The intrinsic energy is assumed to have a generic structure:

$$E_{\text{edf}} = \int \mathcal{E}_{\text{edf}}\, d^3r = \int (\mathcal{E}_{\text{kin}} + \mathcal{E}_{\text{pot}} + \mathcal{E}_{\text{pair}} + \mathcal{E}_{\text{curr}})\, d^3r$$

Potentials

Minimization of the functional with respect to quasiparticle orbitals provides Bogoliubov-de Gennes type equations. Its general form is:

$$\begin{pmatrix} h_{\uparrow}(r) & \Delta(r)+\Delta_{\text{ext}}(r) \\ \Delta^{*}(r)+\Delta^{*}_{\text{ext}}(r) & -h^{*}_{\downarrow}(r) \end{pmatrix} \begin{pmatrix} u_{n\uparrow}(r) \\ v_{n\downarrow}(r) \end{pmatrix} = E_n \begin{pmatrix} u_{n\uparrow}(r) \\ v_{n\downarrow}(r) \end{pmatrix}$$

where single particle hamiltonian is given by

$$h_{\sigma} = -\frac{1}{2}\vec{\nabla}\alpha_{\sigma}(r)\vec{\nabla} + V_{\sigma}(r) - \left(\mu_{\sigma} - V_{\sigma}^{(\text{ext})}(r)\right) - \frac{i}{2}\left\{\vec{A}_{\sigma}(r) - \vec{v}_{\sigma}^{(\text{ext})}(r), \vec{\nabla}\right\}$$

Potentials entering the hamiltonian are:

- `alpha_a` and `alpha_b`:
  $\alpha_{\sigma} = 2\frac{\delta\mathcal{E}_{\text{edf}}}{\delta\tau_{\sigma}}$ -- effective mass,
- `V_a` and `V_b`:
  $V_{\sigma} = \frac{\delta\mathcal{E}_{\text{edf}}}{\delta n_{\sigma}}$ -- mean-field potential,
- `A_a_x`, `A_a_y`, `A_a_z`, `A_b_x`, `A_b_z`, and `A_b_z`:
  $\vec{A}_{\sigma} = \frac{\delta\mathcal{E}_{\text{edf}}}{\delta\vec{j}_{\sigma}}$ -- current potential,
- `delta`:
  $\Delta(r) = -\frac{\delta\mathcal{E}_{\text{edf}}}{\delta\nu^{*}}$ -- paring potential.

Densities

Densities are computed according to formulas:

- `nu`:
  $\nu(r) = \frac{1}{2}\sum_{|E_n|<E_c} u_{n,\uparrow}(r)v^*_{n,\downarrow}(r)(f_\beta(-E_n) - f_\beta(E_n))$
- `rho_a`:
  $n_\uparrow(r) = \sum_{|E_n|<E_c} |u_{n,\uparrow}(r)|^2 f_\beta(E_n)$
- `rho_b`:
  $n_\downarrow(r) = \sum_{|E_n|<E_c} |v_{n,\downarrow}(r)|^2 f_\beta(-E_n)$
- `tau_a`:
  $\tau_\uparrow(r) = \sum_{|E_n|<E_c} |\nabla u_{n,\uparrow}(r)|^2 f_\beta(E_n)$
- `tau_b`:
  $\tau_\downarrow(r) = \sum_{|E_n|<E_c} |\nabla v_{n,\downarrow}(r)|^2 f_\beta(-E_n)$
- `j_a_x`, `j_a_y`, `j_a_z`:
  $\vec{j}_\uparrow(r) = -\sum_{|E_n|<E_c} \mathrm{Im}[u_{n,\uparrow}(r)\nabla u^*_{n,\uparrow}(r)] f_\beta(E_n)$
- `j_b_x`, `j_b_y`, `j_b_z`:
  $\vec{j}_\downarrow(r) = \sum_{|E_n|<E_c} \mathrm{Im}[v_{n,\downarrow}(r)\nabla v^*_{n,\downarrow}(r)] f_\beta(-E_n)$

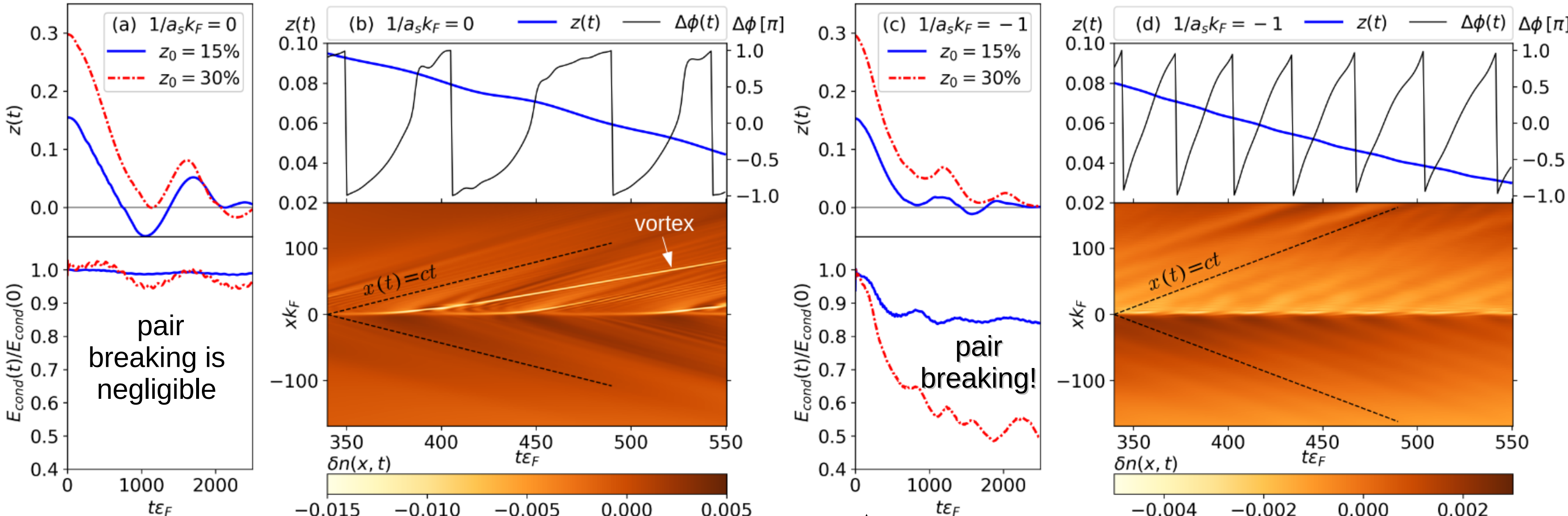
In these formulas E_n denotes quasi-particle energy, and E_c is the energy cut-off scale. Fermi distribution function $f_\beta(E) = 1/(\exp(\beta E) + 1)$ is introduced to model temperature $T = 1/\beta$ effects.

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

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

UFG

BCS

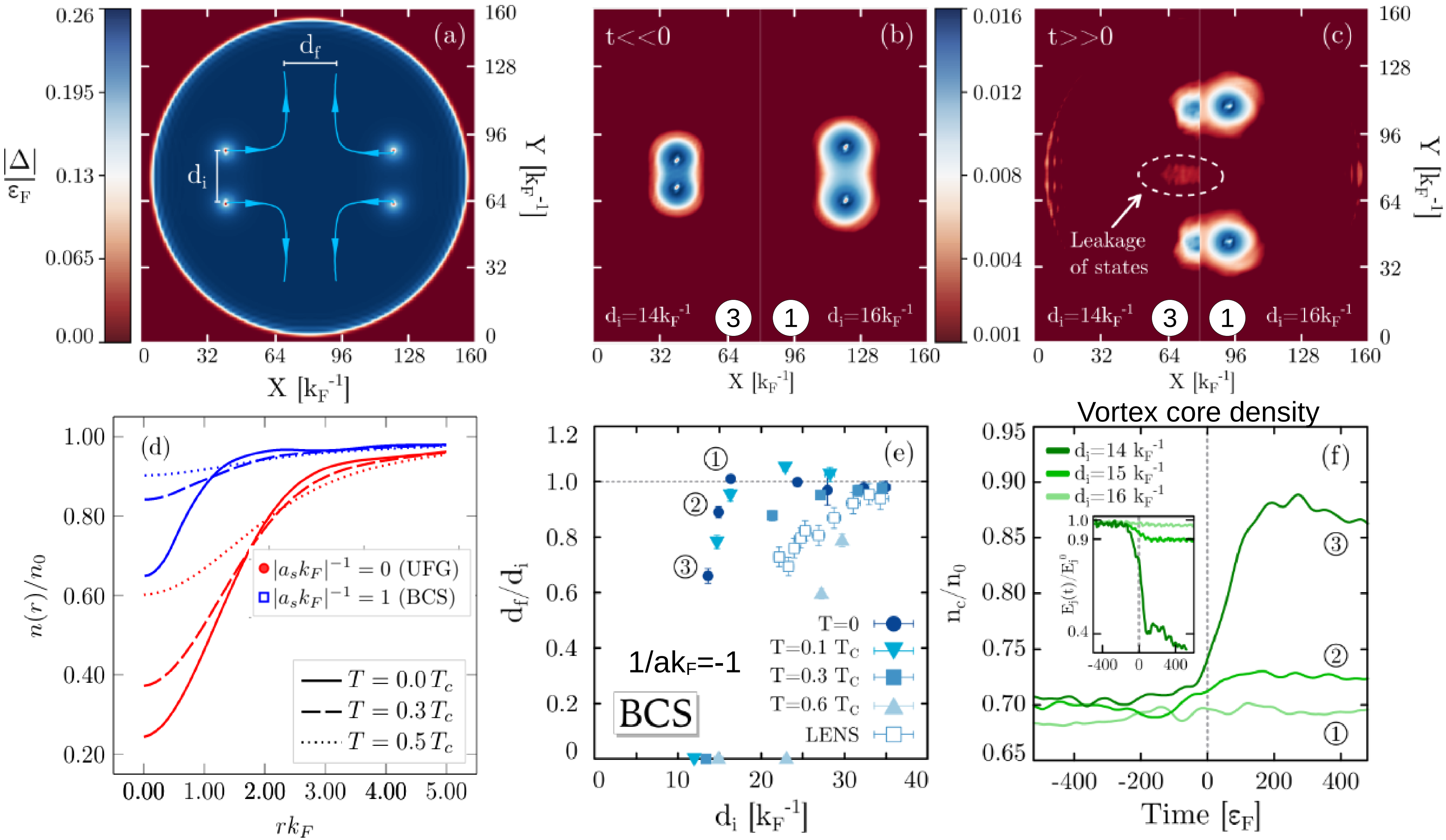


$\delta n(x,t) \equiv n(x,0,t) - n(x,0,0)$

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

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

global characteristics like imbalance or the phase difference, which are used as primary probes in experiments, display **similar patterns irrespectively of the operating dissipation mechanism**



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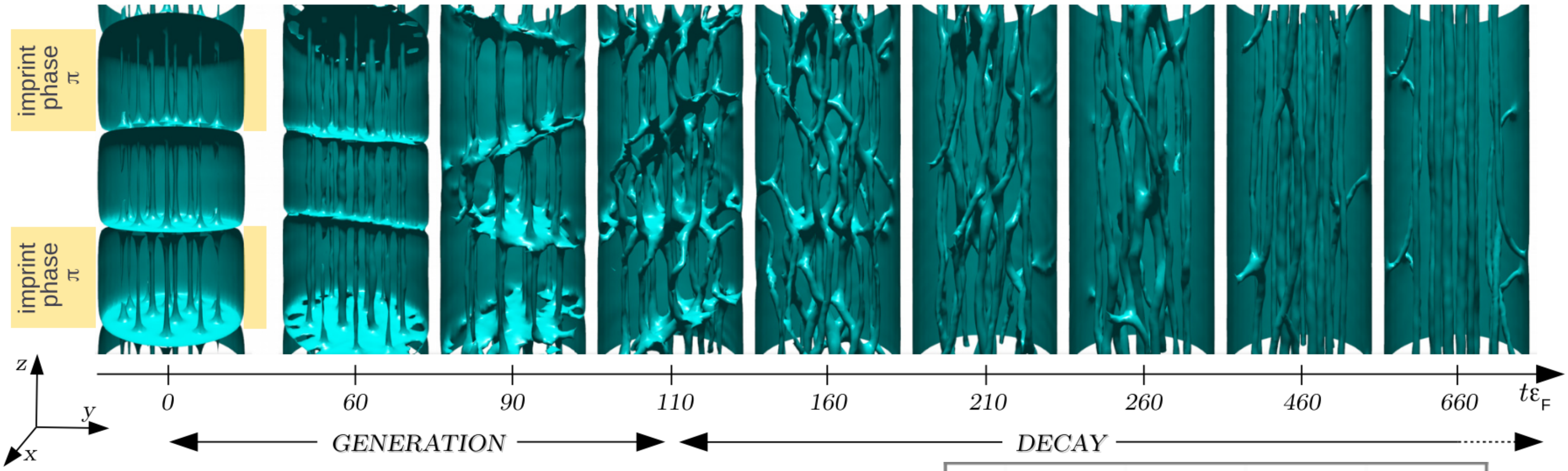
Towards quantum turbulence in strongly interacting Fermi gas

K. Hossain, et.al., Phys. Rev. A 105, 013304 (2022)

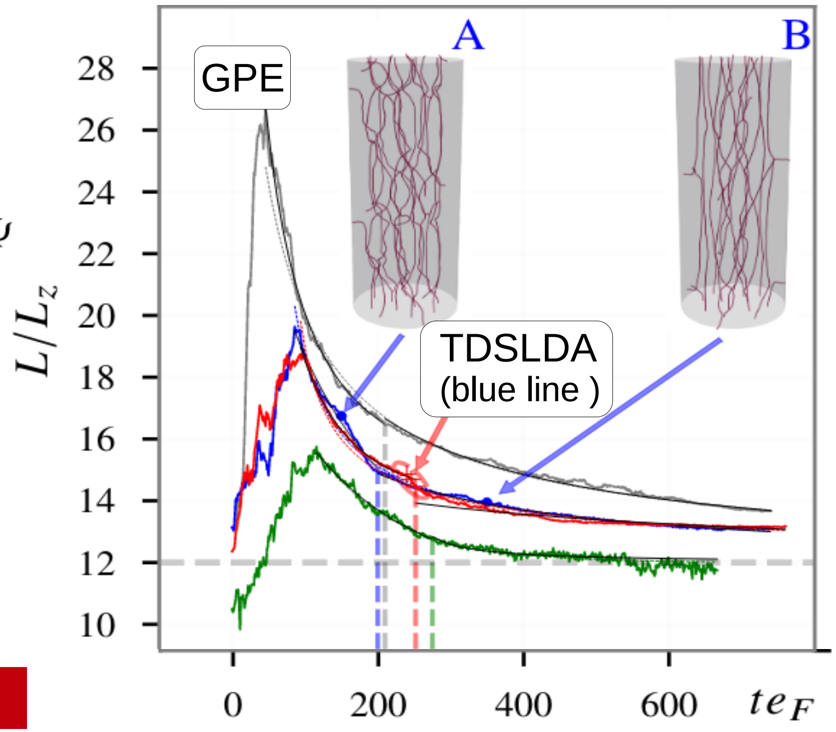


The GPE energy density $gn_D^2/2$ is replaced by the UFG energy density $\xi\mathcal{E}_{FG}(n_F)$:

$$ie^{i\eta}\dot{\Psi} = \left(\frac{-\hbar^2\nabla^2}{4m} + 2(\xi\mathcal{E}'_{FG}(n_F) + V - \mu_F) + \Omega\hat{L}_z\right)\Psi$$

GPE can be tuned to give the same qualitative features, however, the dissipation parameter η (≈ 0.01–0.02) must be tuned appropriately.

→ noticeable differences in energy transfers between GPE and TDSLDA



Theory vs Experiment (unitary regime)

sim: J. Kopyciński, et.al., Phys. Rev. A 104, 053322 (2021)
exp: M. W. Zwierlein, et.al., Science (80). 311, 492 (2006).

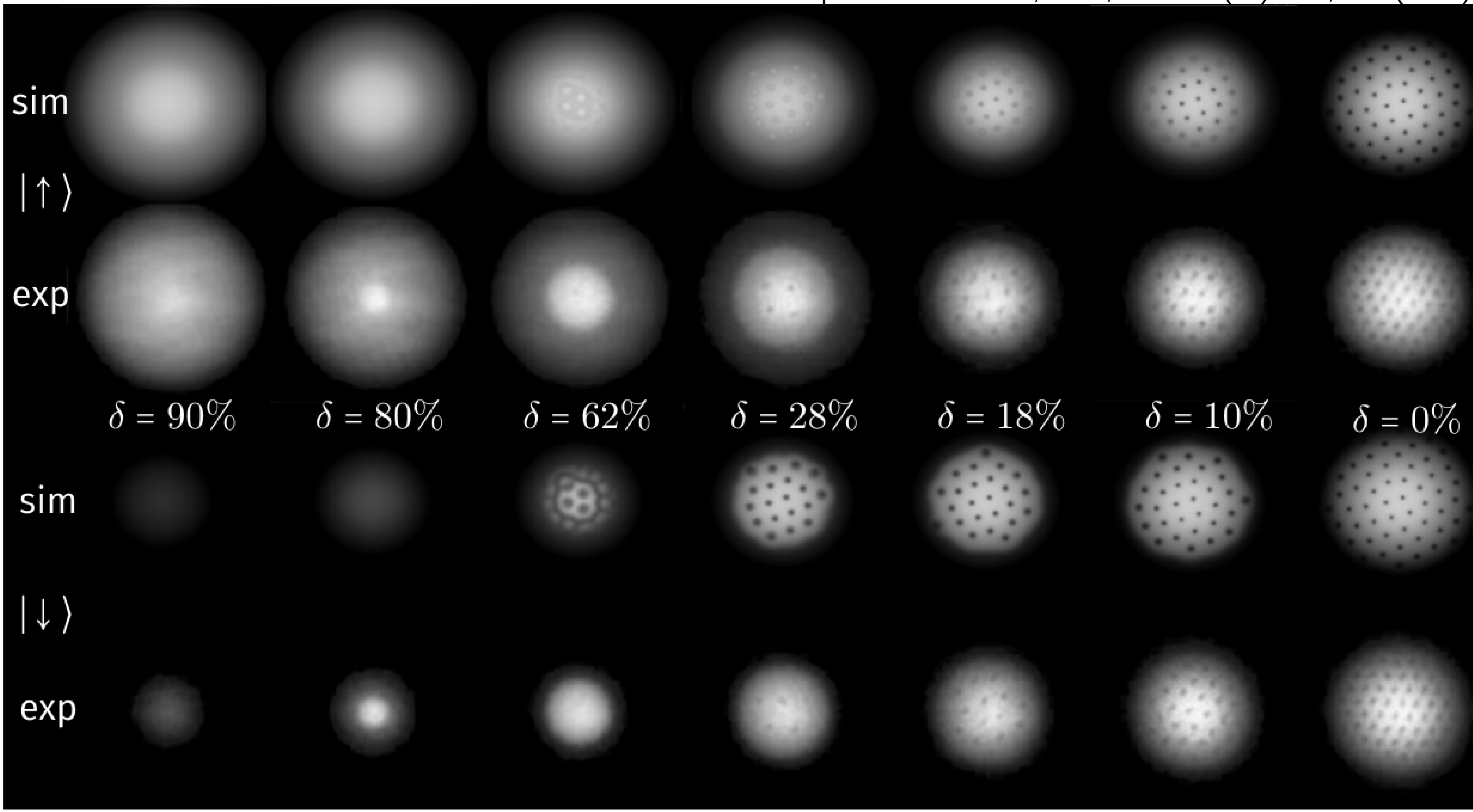


Fig. 4.9: Comparison between the experimental absorption images (exp) of rotating Fermi gas clouds and the simulated densities $n(x,y,z=0)$ (sim) for a rotating system, separately for the majority $|\uparrow\rangle$ and minority $|\downarrow\rangle$ components and different population imbalances δ. Experimental data source: [12].

Experiment

Prepare the system → Ramp to BEC → Take image