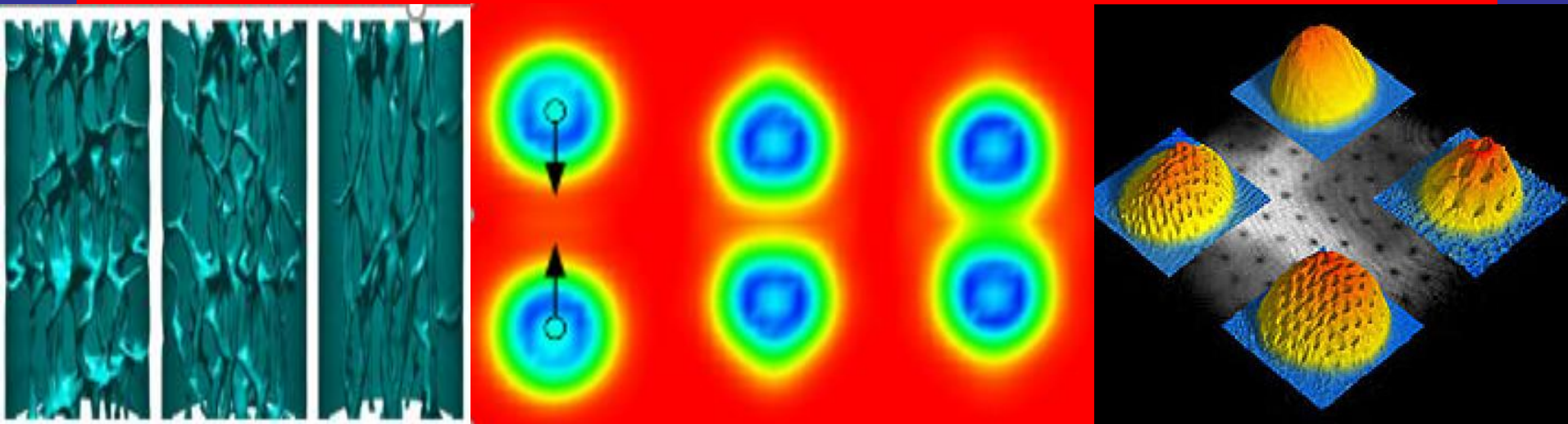


# Exotic Features of Superfluidity in Ultracold Atomic Gases



Piotr Magierski

Warsaw University of Technology

Funding:



NATIONAL  
SCIENCE  
CENTRE  
POLAND

HPC:



東京工業大学  
Tokyo Institute of Technology



Global Scientific Information  
and Computing Center

OAK RIDGE  
National Laboratory | LEADERSHIP  
COMPUTING  
FACILITY



University of Tsukuba

Center for Computational Sciences

筑波大学 計算科学研究センター

# Collaboration

## Warsaw University of Technology

Andrea Barresi

Matthew Barton

Antoine Boulet

Konrad Kobuszewski

Andrzej Makowski

Daniel Pęczak

Buğra Tüzemen

Marek Tylutki

Gabriel Wlazłowski

Tomasz Zawiślak

## Tokyo Institute of Technology

Kazuyuki Sekizawa

## University of Washington

Aurel Bulgac

## Washington State University

Edward Eskew

Khalid Hossain

Michael M. Forbes

Saptarshi R. Sarkar

## Pacific Northwest National Laboratory

Kenneth J. Roche

## Newcastle University

Nikolaos Proukakis

Klejdja Xhani

# What are ultracold atomic gases?

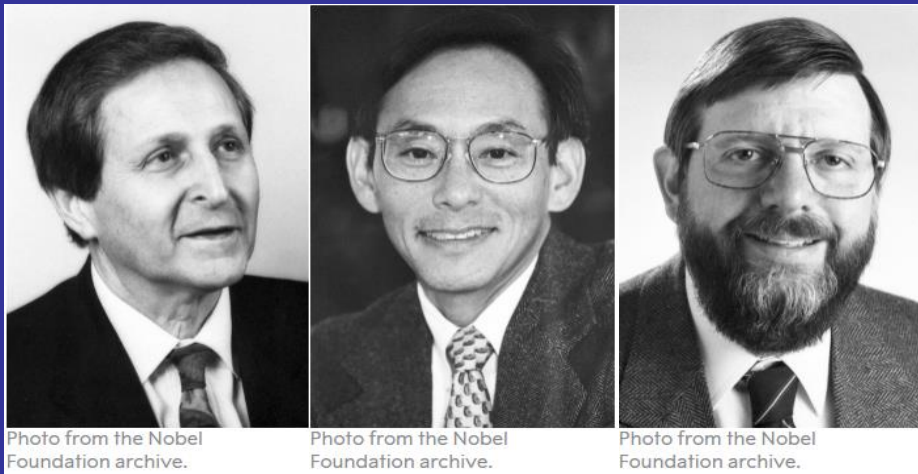


Photo from the Nobel Foundation archive.

Photo from the Nobel Foundation archive.

Photo from the Nobel Foundation archive.

Claude Cohen-Tannoudji

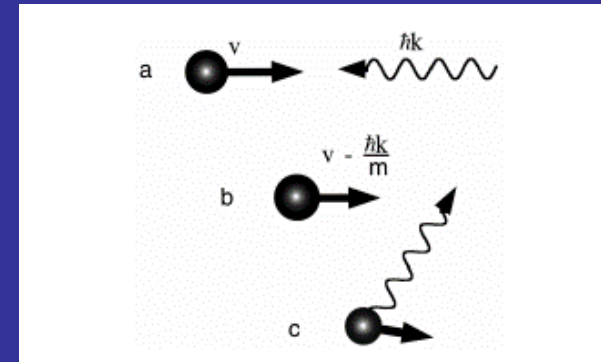
Steven Chu

William D. Phillips

Nobel Prize in Physics 1997

„for development of methods to cool and trap atoms with laser light”

Idea of laser cooling



Schematic realization of optical molasses

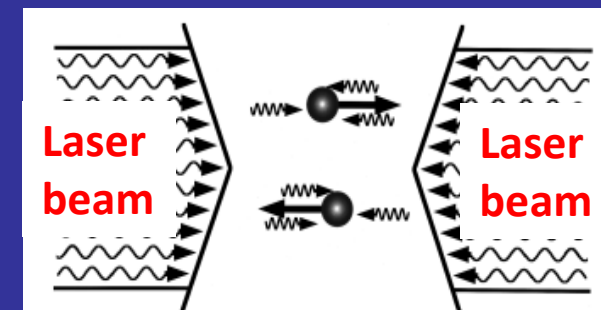
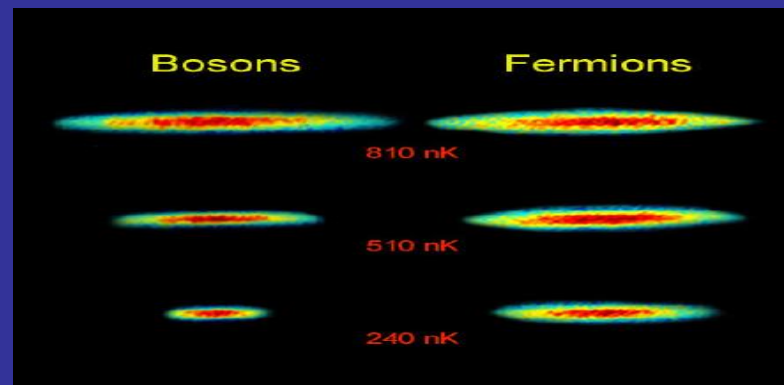
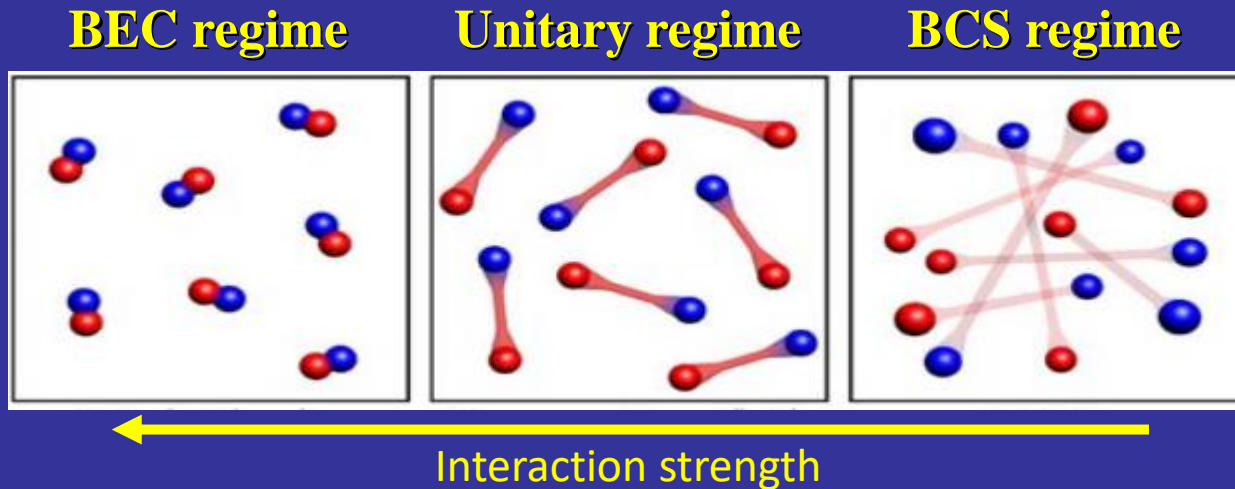


FIG. 12. Doppler cooling in one dimension.

- Alkali atoms (fermions) used for trapping and cooling:  ${}^6\text{Li}$ ,  ${}^{40}\text{K}$
- Laser light (via Doppler effect) is used to create *optical molasses* which decrease the velocity width of atomic cloud and cool it down.
- Sub-doppler cooling is achieved through *Sisyphus cooling* and/or *evaporative cooling* and allows to reach temperatures below microkelvins
- Dilute cloud of  $10^5$ - $10^6$  atoms is kept in magneto-optical trap (MOT)

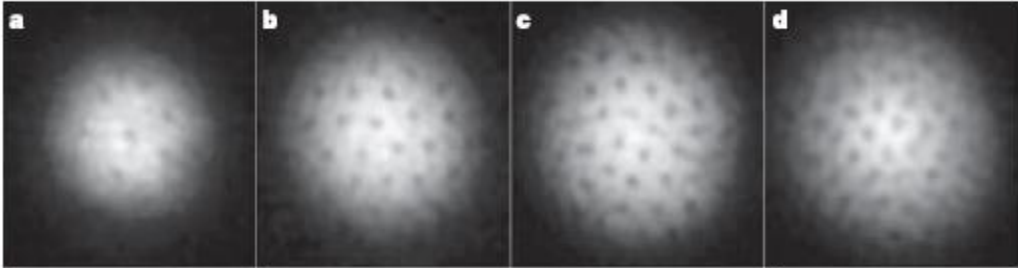
In dilute atomic systems experimenters can control nowadays almost anything:

- The number of atoms in the trap: typically about  $10^5$ - $10^6$  atoms divided 50-50 among the lowest two hyperfine states.
- The density of atoms
- Mixtures of various atoms
- The temperature of the atomic cloud
- **The strength of this interaction is fully tunable!**

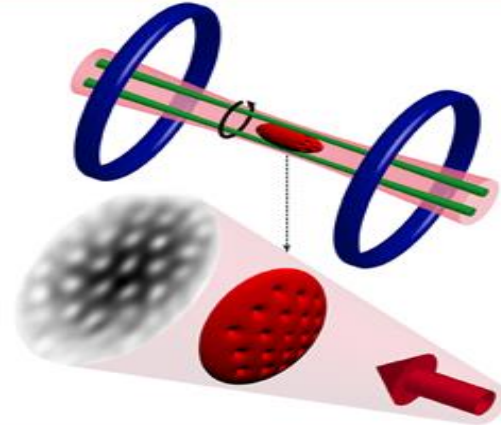
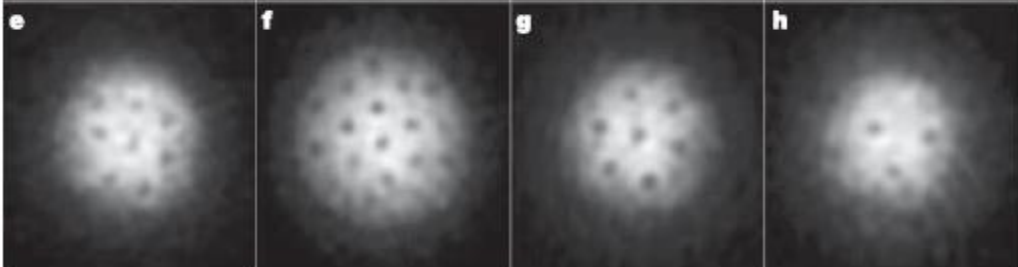


# Evidence for fermionic superfluidity in ultracold atomic gases.

BEC regime:



BCS regime:

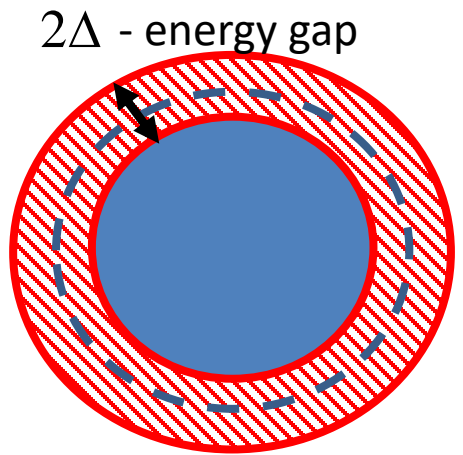
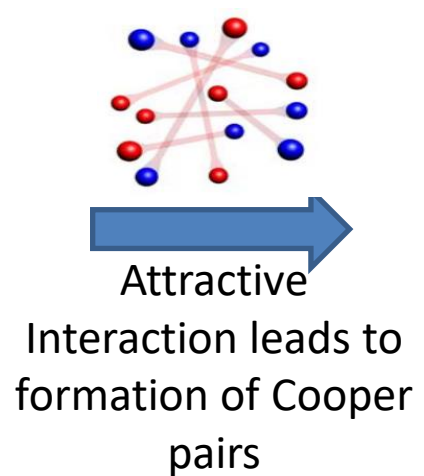
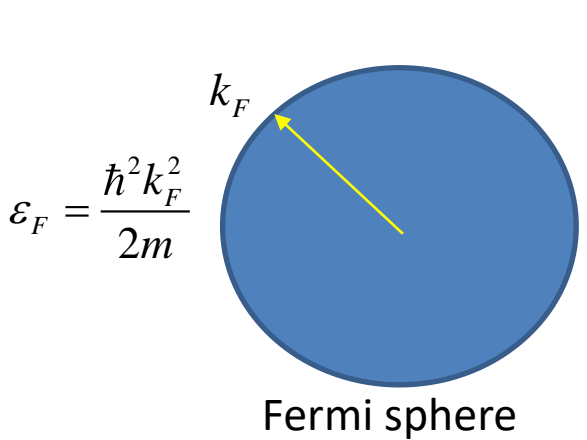


Rotation of a superfluid cloud leads to generation of **quantum vortices**

**M.W. Zwierlein et al., Nature, 435, 1047 (2005)**

Figure 2 | Vortices in a strongly interacting gas of fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (a) or 500 ms (b–h) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, the

magnetic field was ramped to 735 G for imaging (see text for details). The magnetic fields were 740 G (a), 766 G (b), 792 G (c), 812 G (d), 833 G (e), 843 G (f), 853 G (g) and 863 G (h). The field of view of each image is 880 μm × 880 μm.



# Why do we need supercomputers to simulate ultracold gases?

Evolution of Cooper pair field (pairing field) is at the heart of theoretical description of superfluids :

$$\Delta(\vec{r}, t) = |\Delta(\vec{r}, t)| e^{i\phi(\vec{r}, t)}$$

## Method: Time Dependent Density Functional Theory

Replacing hard-to-solve linear Schroedinger eq.

$$i\hbar \frac{\partial}{\partial t} \psi = \hat{H} \psi$$

by huge set ( $10^5$  -  $10^6$ ) partial differential, nonlinear eqs.

(Superfluid Local Density Approximation):

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} u_{n,a}(\mathbf{r}, t) \\ u_{n,b}(\mathbf{r}, t) \\ v_{n,a}(\mathbf{r}, t) \\ v_{n,b}(\mathbf{r}, t) \end{pmatrix} = \begin{pmatrix} h_a(\mathbf{r}, t) & 0 & 0 & \Delta(\mathbf{r}, t) \\ 0 & h_b(\mathbf{r}, t) & -\Delta(\mathbf{r}, t) & 0 \\ 0 & -\Delta^*(\mathbf{r}, t) & -h_a^*(\mathbf{r}, t) & 0 \\ \Delta^*(\mathbf{r}, t) & 0 & 0 & -h_b^*(\mathbf{r}, t) \end{pmatrix} \begin{pmatrix} u_{n,a}(\mathbf{r}, t) \\ u_{n,b}(\mathbf{r}, t) \\ v_{n,a}(\mathbf{r}, t) \\ v_{n,b}(\mathbf{r}, t) \end{pmatrix}$$

where  $h$  and  $\Delta$  depends on “densities”:

$$n_\sigma(\mathbf{r}, t) = \sum_{E_n < E_c} |v_{n,\sigma}(\mathbf{r}, t)|^2, \quad \tau_\sigma(\mathbf{r}, t) = \sum_{E_n < E_c} |\nabla v_{n,\sigma}(\mathbf{r}, t)|^2,$$

$$v(\mathbf{r}, t) = \sum_{E_n < E_c} u_{n,\uparrow}(\mathbf{r}, t) v_{n,\downarrow}^*(\mathbf{r}, t), \quad \mathbf{j}_\sigma(\mathbf{r}, t) = \sum_{E_n < E_c} \text{Im}[v_{n,\sigma}^*(\mathbf{r}, t) \nabla v_{n,\sigma}(\mathbf{r}, t)],$$

More details:

A. Bulgac, M.M. Forbes, P. Magierski,  
*The Unitary Fermi Gas: From Monte Carlo to Density Functionals*,  
 Lecture Notes in Physics 836  
 ed. W. Zwerger, Springer (2011).

## W-SLDA Toolkit

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

static problems: st-wslda

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

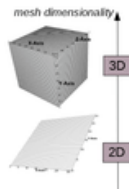
time-dependent problems: td-wslda

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

Speed-up calculations by  
exploiting High Performance  
Computing

Functionals for studies of  
BCS and unitary regimes

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



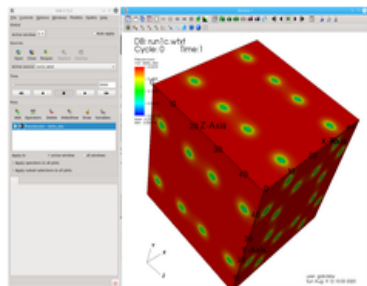
W-SLDA allows to solve problems

in 3D without any symmetry restrictions:  $\Psi = \varphi(x, y, z)$

in 2D with translational invariance along  $z$  direction:  $\Psi = \varphi(x, y)$

in 1D with translational invariance along  $y$  and  $z$  direction:  $\Psi = \varphi(x)$

## Integration with VisIt: visualization, animation and analysis tool



W-SLDA is integrated with open-source VisIt tool. It allows for:

visualizing 3D, 2D and 1D results,

data processing,

creating animations for time-dependent simulations.

### Contributors

#### Project leader

Gabriel Wlazłowski

🏠 Warsaw University of Technology, Faculty of Physics  
👤 Main developer of the W-SLDA Toolkit

#### Theory expertise

Aurel Bulgac

🏠 Department of Physics, University of Washington  
👤 Aurel Bulgac derived Superfluid Local Density Approximation (SLDA) equations for cold atoms, presently implemented in W-SLDA Toolkit. He also supervised implementation of core algorithms of td-wslda codes.

Piotr Magierski

🏠 Warsaw University of Technology, Faculty of Physics  
👤 Piotr Magierski contributed to development of Superfluid Local Density Approximation (SLDA) method.

Michael McNeil Forbes

🏠 Department of Physics and Astronomy, Washington State University  
👤 Michael Forbes together with Aurel Bulgac developed Asymmetric Superfluid Local Density Approximation (ASLDA) for spin-imbalanced atomic gases.

#### HPC expertise

Kenneth J. Roche

🏠 Pacific Northwest National Laboratory  
👤 Kenneth J. Roche supervised parallelization process (MPI + CUDA) of main engine of td-wslda codes.

Maciej Marchwiany

🏠 Interdisciplinary Centre for Mathematical and Computational Modelling (ICM)  
👤 implementation of parallel I/O in td-wslda codes (2016-2018)



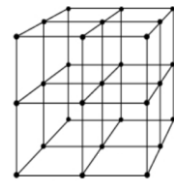
# To execute superfluid TDDFT we need supercomputers...

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	<b>Summit</b> - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM DOE/SC/Oak Ridge National Laboratory United States	2,397,824	143,500.0	200,794.9	9,783
2	<b>Sierra</b> - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM DOE/NNSA/LLNL United States				
3	<b>Sunway TaihuLight</b> - Sunway TaihuLight, NRCPC National Supercomputing Center, China				
4	<b>Tianhe-2A</b> - TH-IVB-FE1600, TH Express-2, Matrix-2000, National Super Computer Center, China				
5	<b>Piz Daint</b> - Cray XC50, Xeon E5-2680v4, Mellanox EDR interconnect , NVIDIA Tesla M40, Swiss National Supercomputing Center, Switzerland				
6	<b>Trinity</b> - Cray XC40, Xeon E5-2680v4, Aries interconnect, DOE/NNSA/LANL/SNL United States				
7	<b>AI Bridging Cloud Infrastructure (ABCI)</b> - PRIMERGY CX2570 M4, Xeon Gold 6148 20C 2.4GHz, NVIDIA Tesla V100 SXM2, Infiniband EDR , Fujitsu National Institute of Advanced Industrial Science and Technology	391,680	19,880.0	32,576.6	1,649



## Present computing capabilities:

- ▶ full 3D (unconstrained) superfluid dynamics
- ▶ spatial mesh up to  $100^3$
- ▶ max. number of particles of the order of  $10^4$
- ▶ up to  $10^6$  time steps (for cold atomic systems it gives a trajectory of length of a few ms)

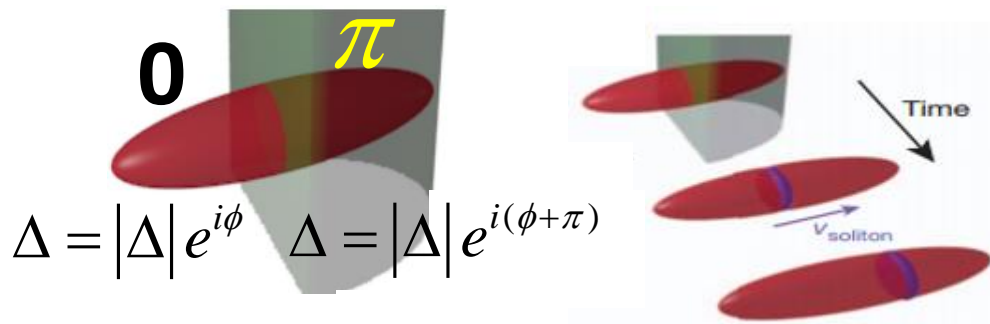


All further results shown here were generated on Piz Daint (CSCS)



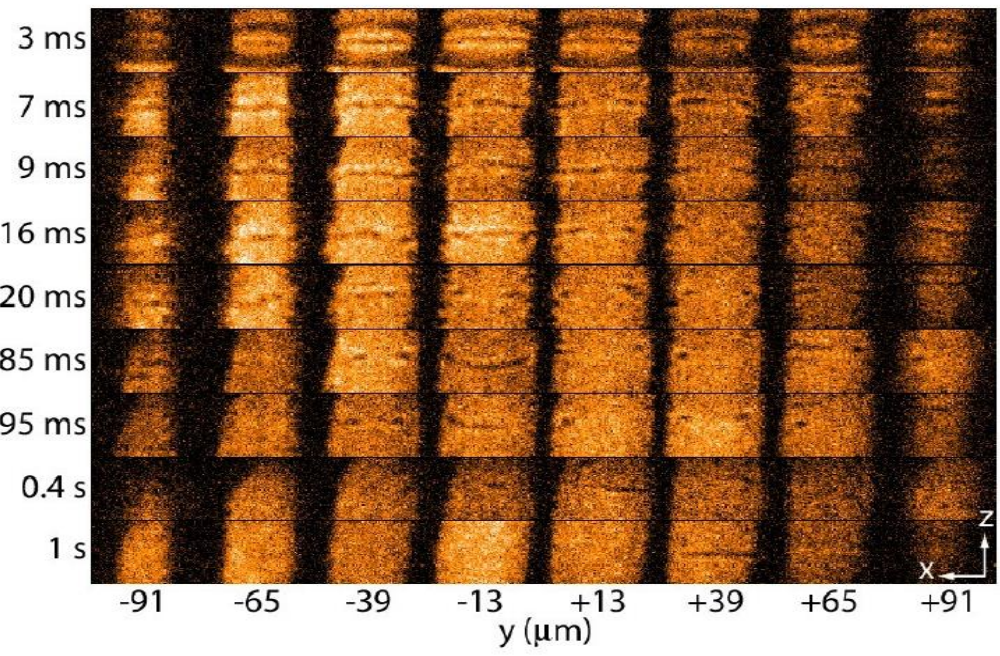


# Example 1: Atomic cloud collisions - decay of solitonic excitations



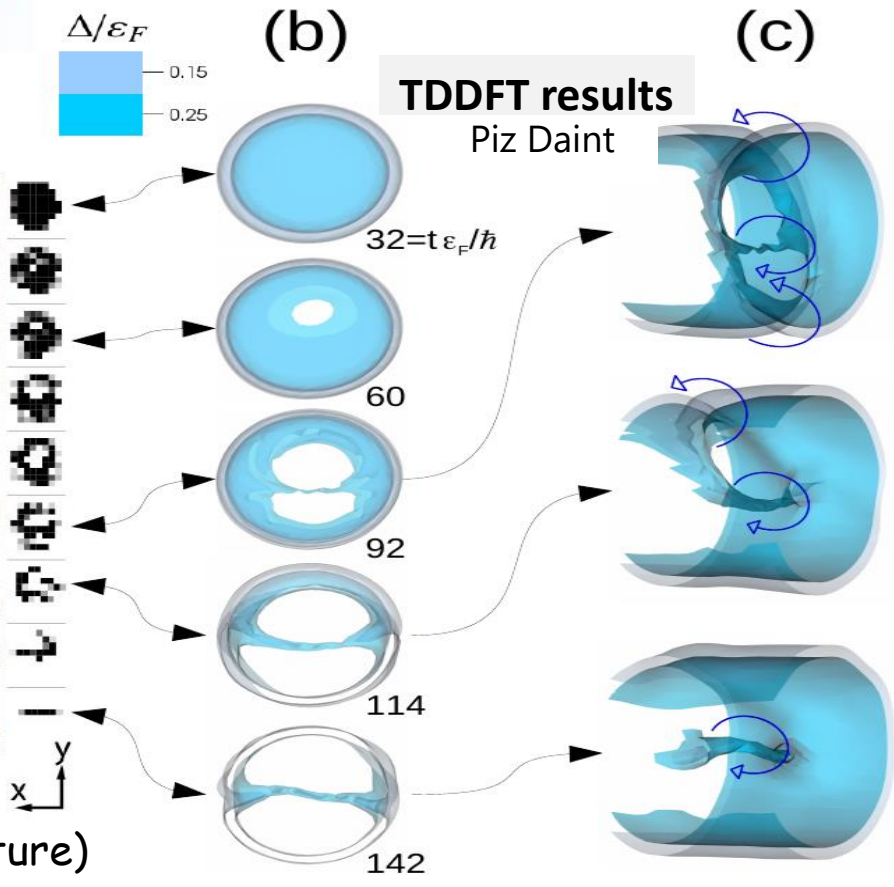
**MIT experiment**

Phys. Rev. Lett. 116, 045304 (2016)



Decay of solitonic excitation (pairing nodal structure) generates a sequence of topological excitations involving: "Phi"-soliton and vortex line.

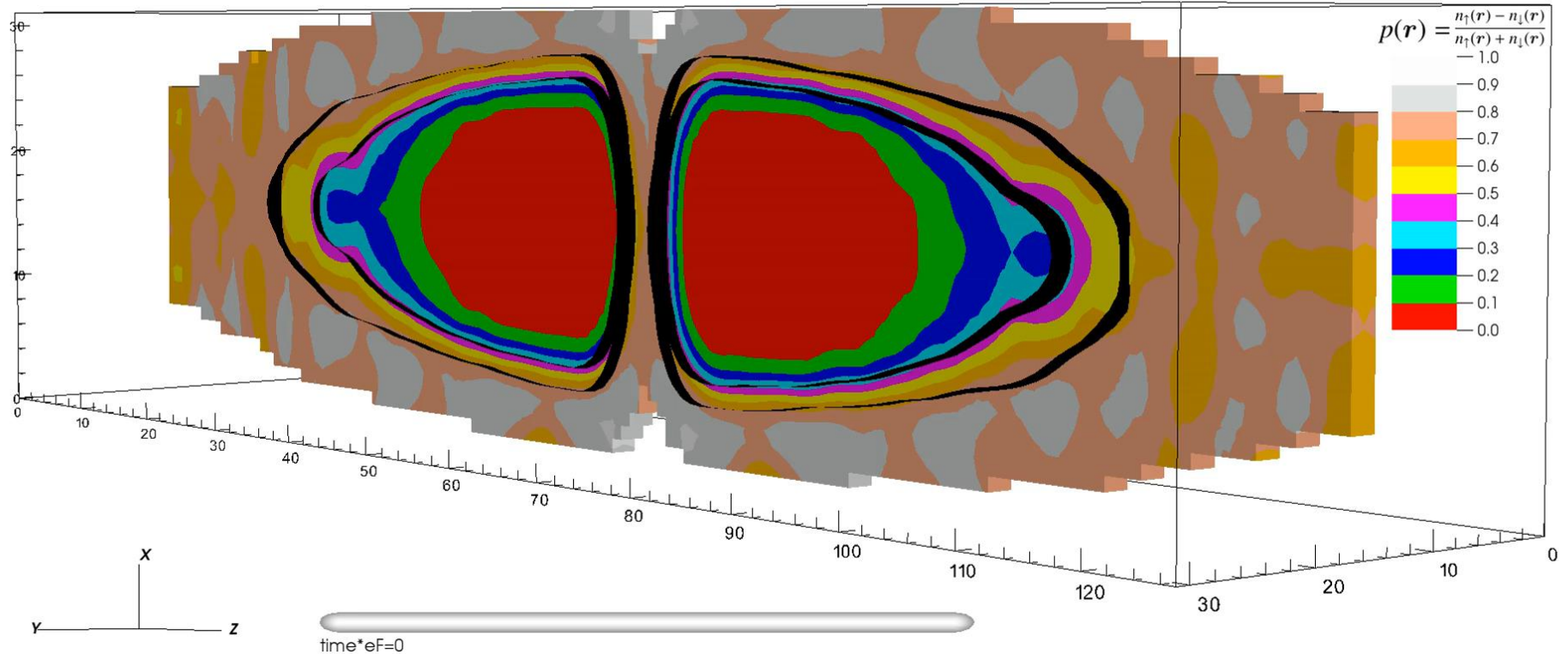
Series of MIT experiments:  
 Nature 499, 426 (2013);  
 PRL 113, 065301 (2014);  
 PRL 116, 045304 (2016);  
 → observation of decay of a dark soliton into a vortex line



G. Wlazłowski, K. Sekizawa, M. Marchwiany, P. Magierski, Phys. Rev. Lett. **120**, 253002 (2018)

# Spin imbalanced ultracold atomic gas in the unitary regime

$$N_{\uparrow} = 304, N_{\downarrow} = 202, P = 20\%$$



The vortex core becomes polarized.

This may be understood noting that the most energetically favorable place to store excess of unpaired spins is at the core of the vortex where,  $\Delta = 0$  - no Cooper pairs need to be broken.

## ➤ New effects predicted for spin-polarized systems:

*Impact on the solitonic cascade:*

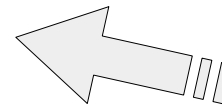
*final product of the cascade depends on the spin imbalance in the system*

(can be verified experimentally with present setups)

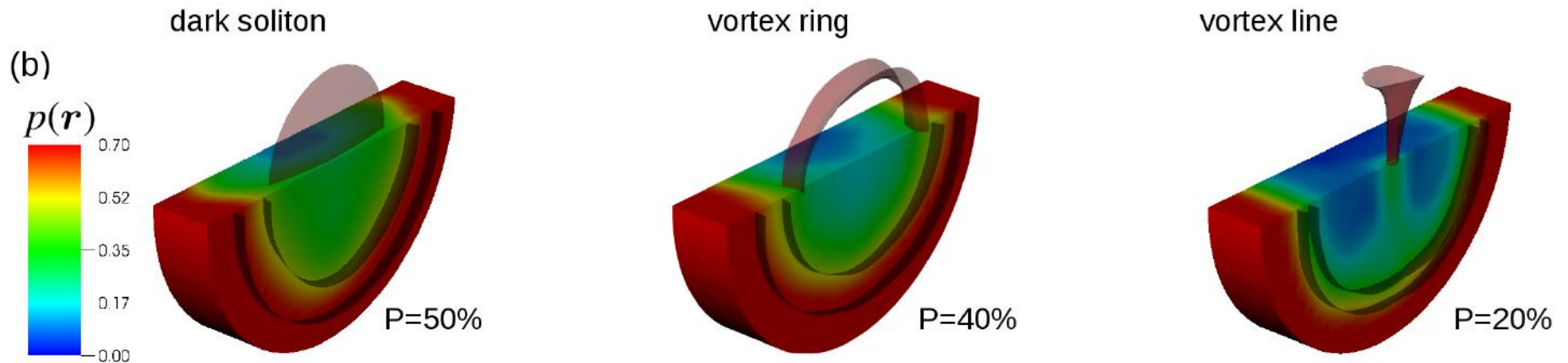
P=20%: Dark soliton  $\Rightarrow$  Vortex ring  $\Rightarrow$  Vortex line

P=40%: Dark soliton  $\Rightarrow$  Vortex ring

P=50%: Dark soliton



**Cascade is suppressed  
by the polarization  
effects**



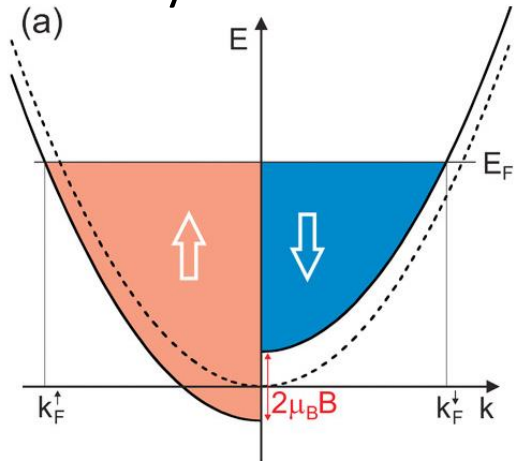
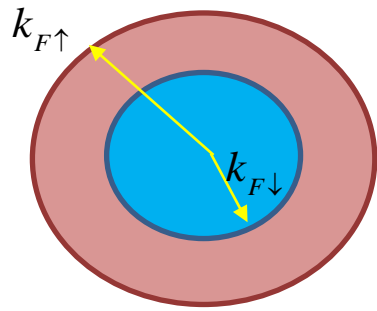
Stability of topological defect depends on its internal structure...

→ For sufficiently large spin-imbalance dark solitons become stable

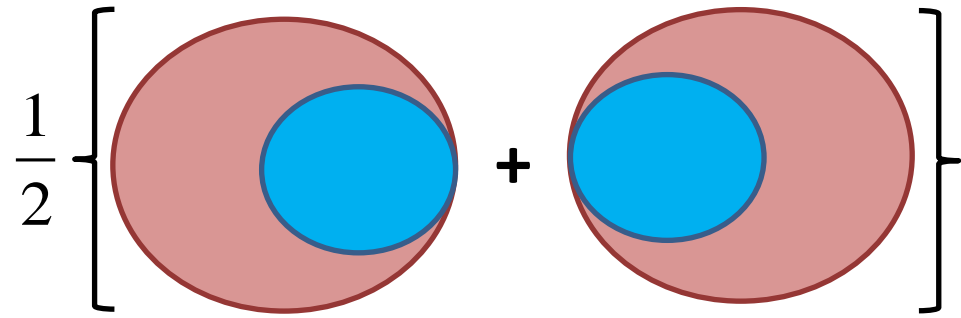
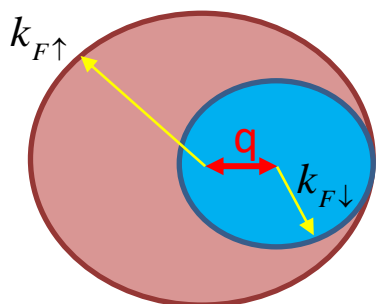
(no snake instability) (see also: Reichl & Mueller, PRA 95, 053637; Lombardi, et. al., PRA 96, 033609)

# Example 2: Spin polarized impurities in superfluids

Pairing in spin imbalanced systems



**INSTABILITY**



**Fulde-Ferrell phase:**

**Larkin-Ovchinnikov phase:**

Translational symmetry is broken:

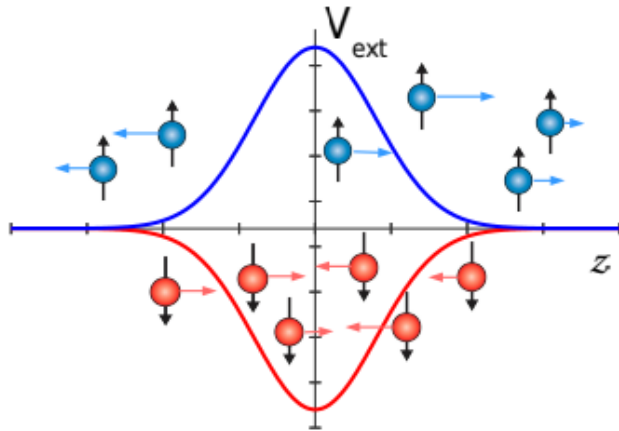
**Larkin-Ovchinnikov (LO):**  $\Delta(r) \sim \cos(\vec{q} \cdot \vec{r})$

**Fulde-Ferrell (FF):**  $\Delta(r) \sim \exp(i\vec{q} \cdot \vec{r})$

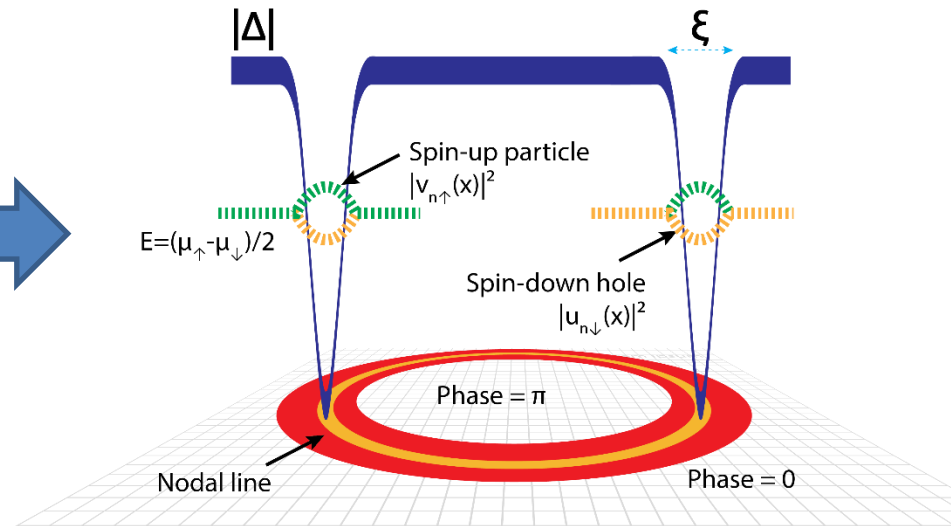
A.I. Larkin and Y. N. Ovchinnikov, Sov. Phys. JETP 20, 762 (1965)  
 P. Fulde and R. A. Ferrell, Phys. Rev. 135, A550 (1964)

# Engineering the structure of nodal surfaces in ultracold atomic gas

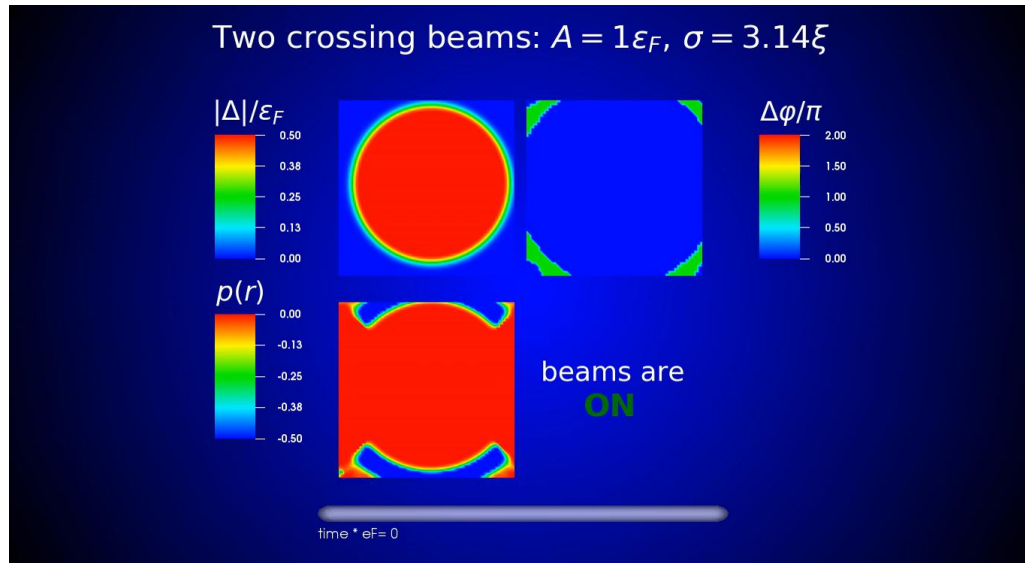
Spin-selective potential applied locally leads to Cooper pair breaking



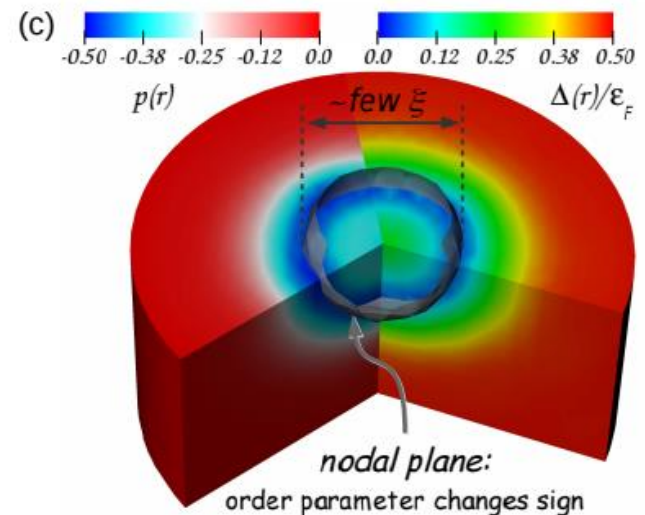
Pairing field nodal structure



Generation of *ferron* in the unitary regime



*Ferron* structure



# Non-central collision of two impurities

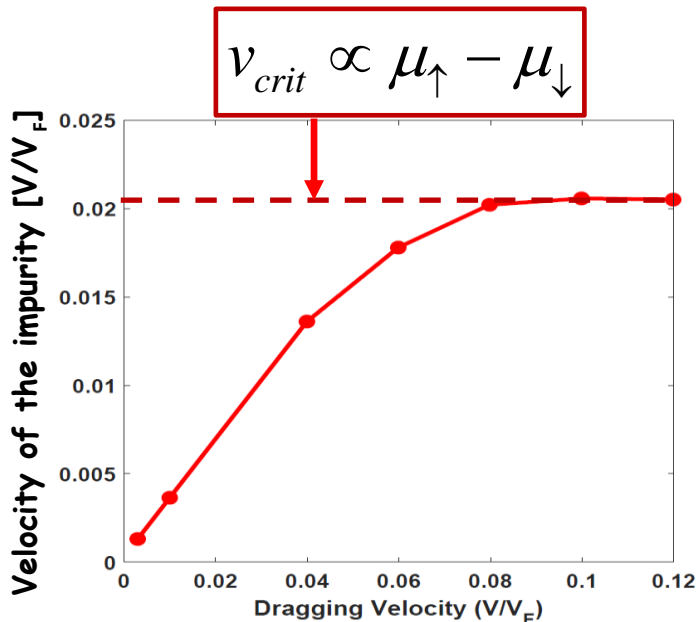


Surprisingly, the nodal structure remains stable even during collisions

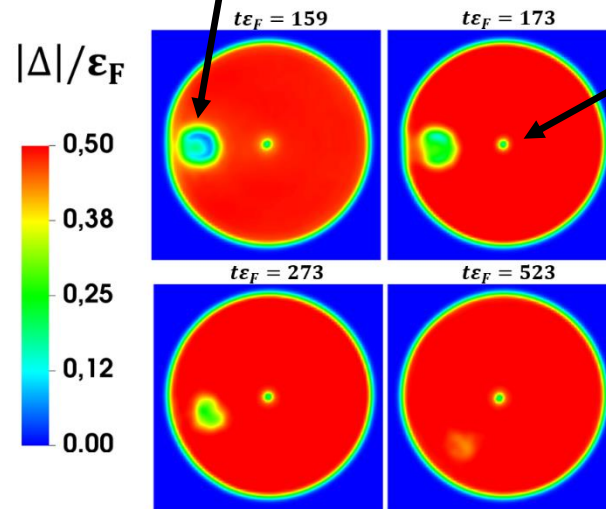
P. Magierski, B. Tüzemen, G. Wlazłowski, Phys. Rev. A100, 033613 (2019)

The velocities of impurities are about 30% of the velocity of sound.

**Peculiarity of ferron dynamics: there is a limiting velocity proportional to its polarization.**



Instability of ferron in the vicinity of quantum vortex

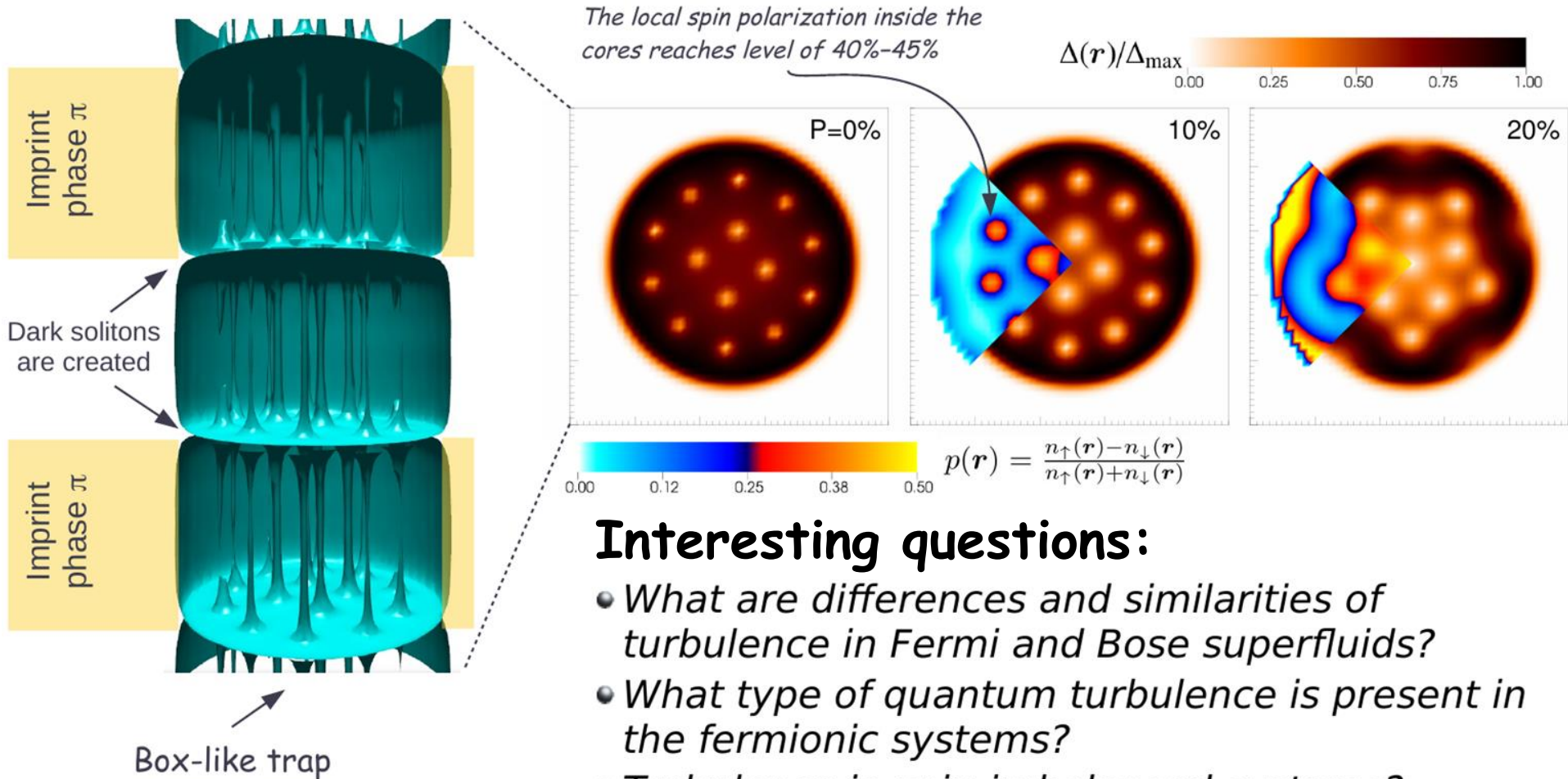


P. Magierski, B. Tüzemen, G. Wlazłowski, arXiv:2102.04833

# Example 3: Generation and decay of quantum turbulent state

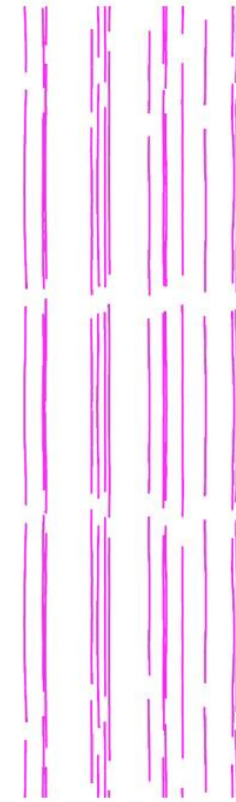
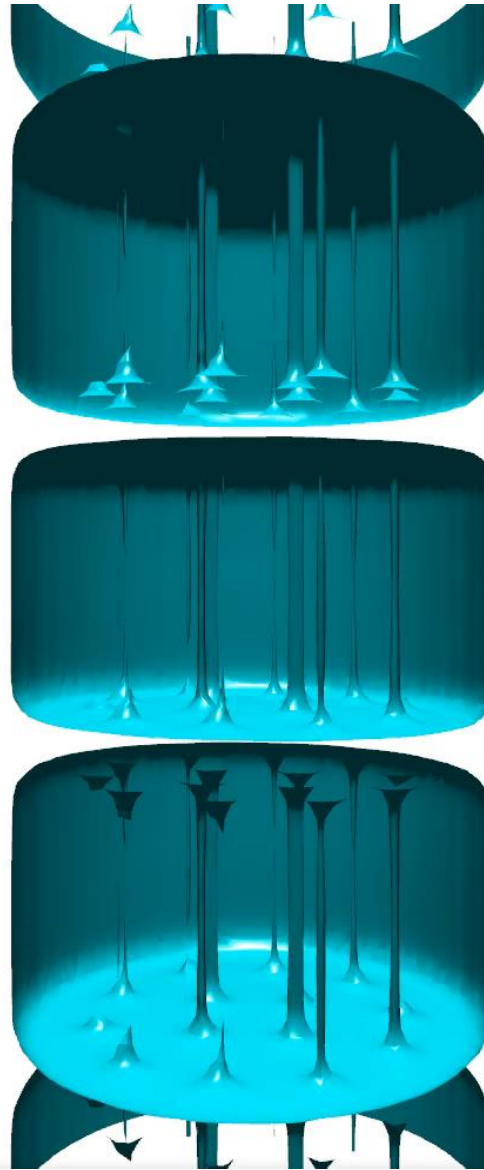
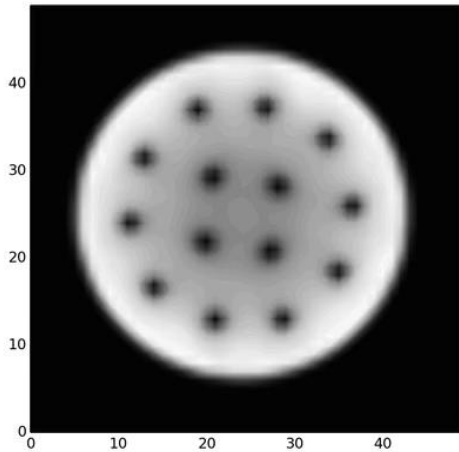
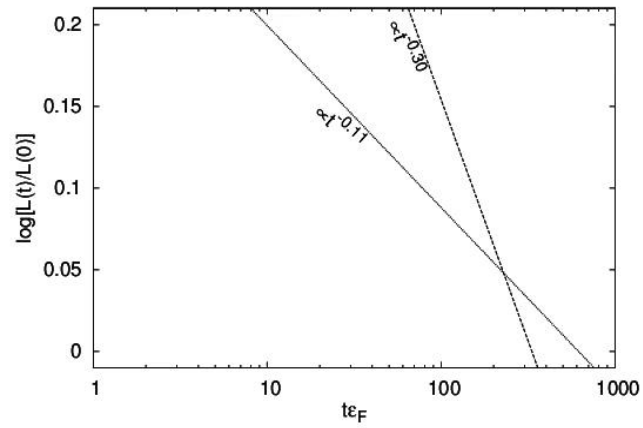
Problem: how to generate the turbulence?

→ Our suggestion: *imprint few dark solitons on existing vortex lattice*  
 → *rotating turbulence* (nonzero total angular momentum)



## Interesting questions:

- What are differences and similarities of turbulence in Fermi and Bose superfluids?
- What type of quantum turbulence is present in the fermionic systems?
- Turbulence in spin-imbalanced systems?



time = 0  $[\epsilon_F^{-1}]$



