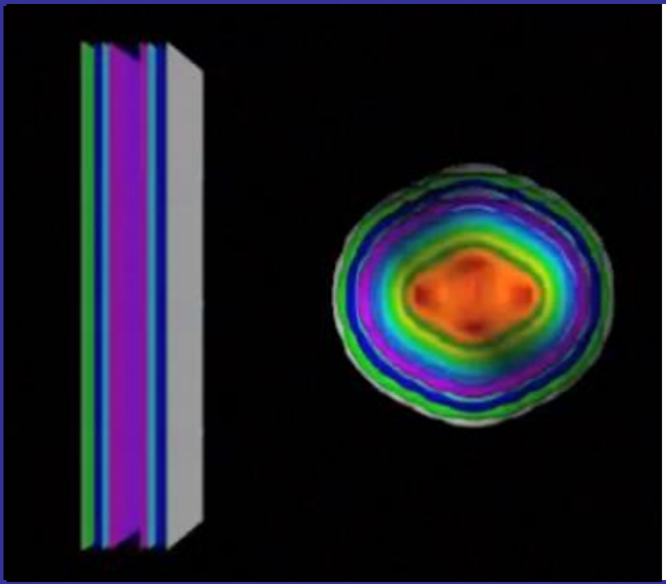
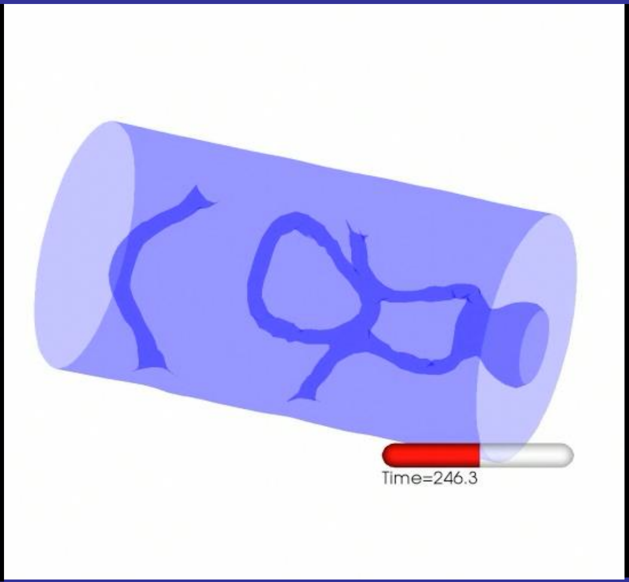
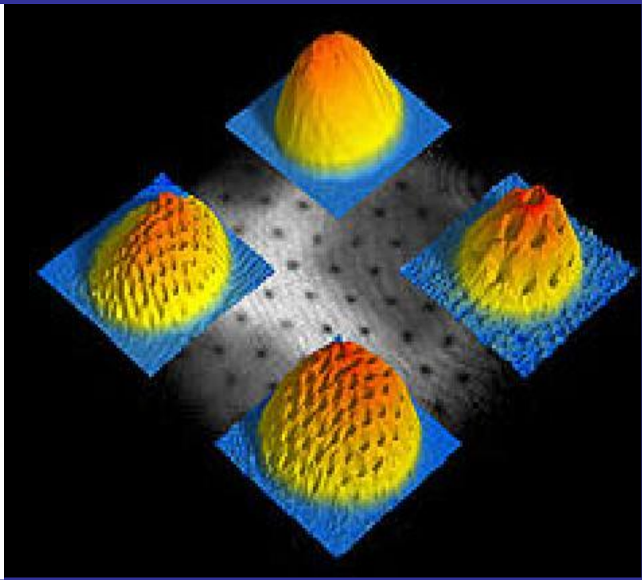
Nierównowagowe procesy w nadciekłych układach kwantowych.







Piotr Magierski
Wydział Fizyki PW

100 years of superconductivity and superfluidity

<u>Discovery</u>: H. Kamerlingh Onnes in 1911 cooled a metallic sample of mercury at T<4.2K

20 orders of magnitude over a century of (low temperature) physics

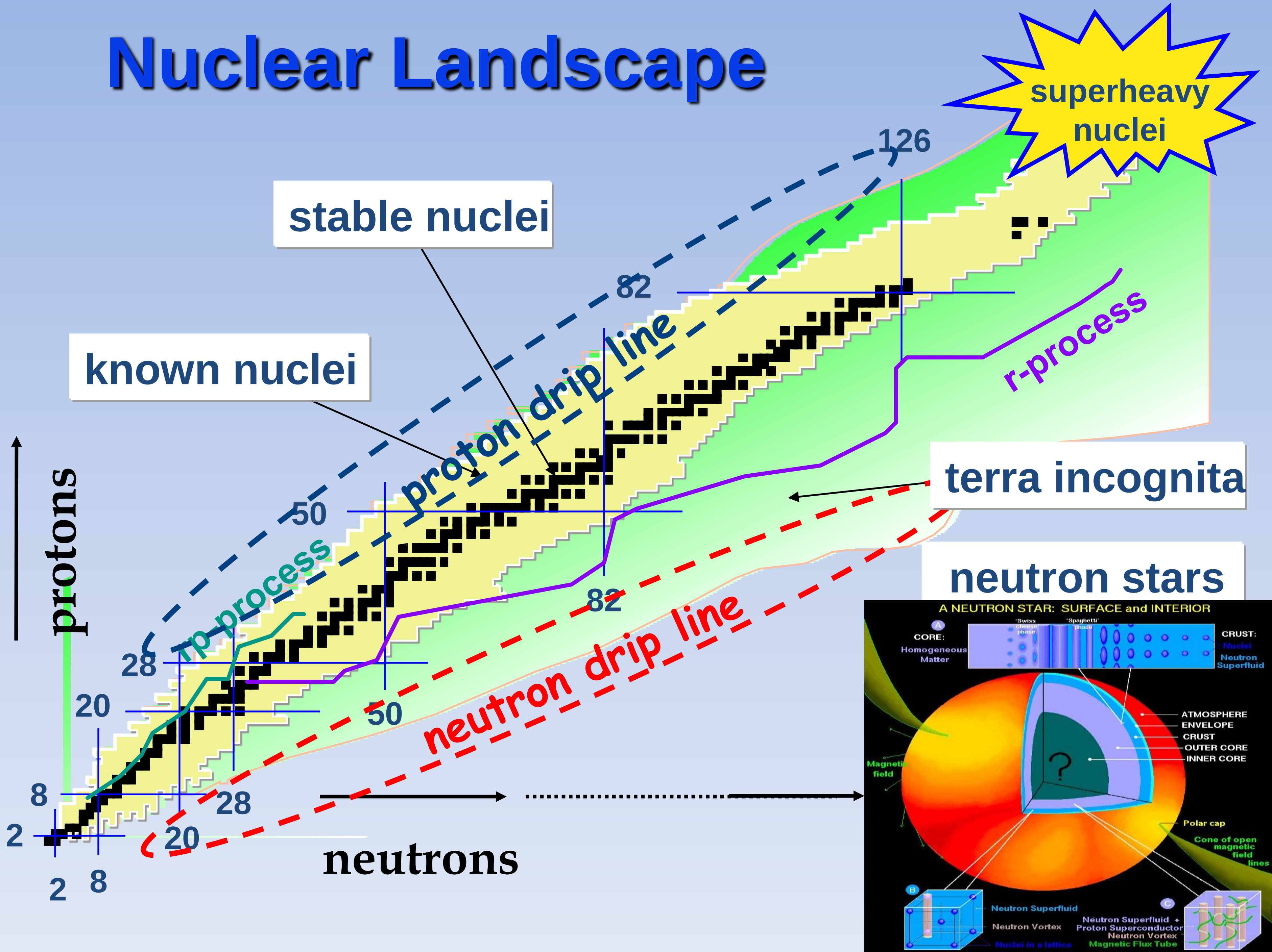
- ✓ **Dilute atomic Fermi gases** $T_c \approx 10^{-12} - 10^{-9}$ eV
- ✓ **Liquid ^{3}He** $T_c \approx 10^{-7}$ eV
- ✓ **Metals, composite materials** $T_c \approx 10^{-3} - 10^{-2}$ eV
- ✓ **Nuclei, neutron stars** $T_c \approx 10^{5} - 10^{6}$ eV
- **QCD color superconductivity** $T_c \approx 10^{7} - 10^{8}$ eV

units (1 eV $\approx 10^4$ K)

I will focus on two quantum systems:

- *atomic nuclei*
- *quantum atomic gases*

Nuclear Landscape



Questions that Drive the Field

- How do protons and neutrons make stable nuclei and rare isotopes?
- What is the origin of simple patterns in complex nuclei?
- What is the equation of state of matter made of nucleons?
- What are the heaviest nuclei that can exist?

Physics of nuclei

- When and how did the elements from iron to uranium originate?
- How do stars explode?
- What is the nature of neutron star matter?

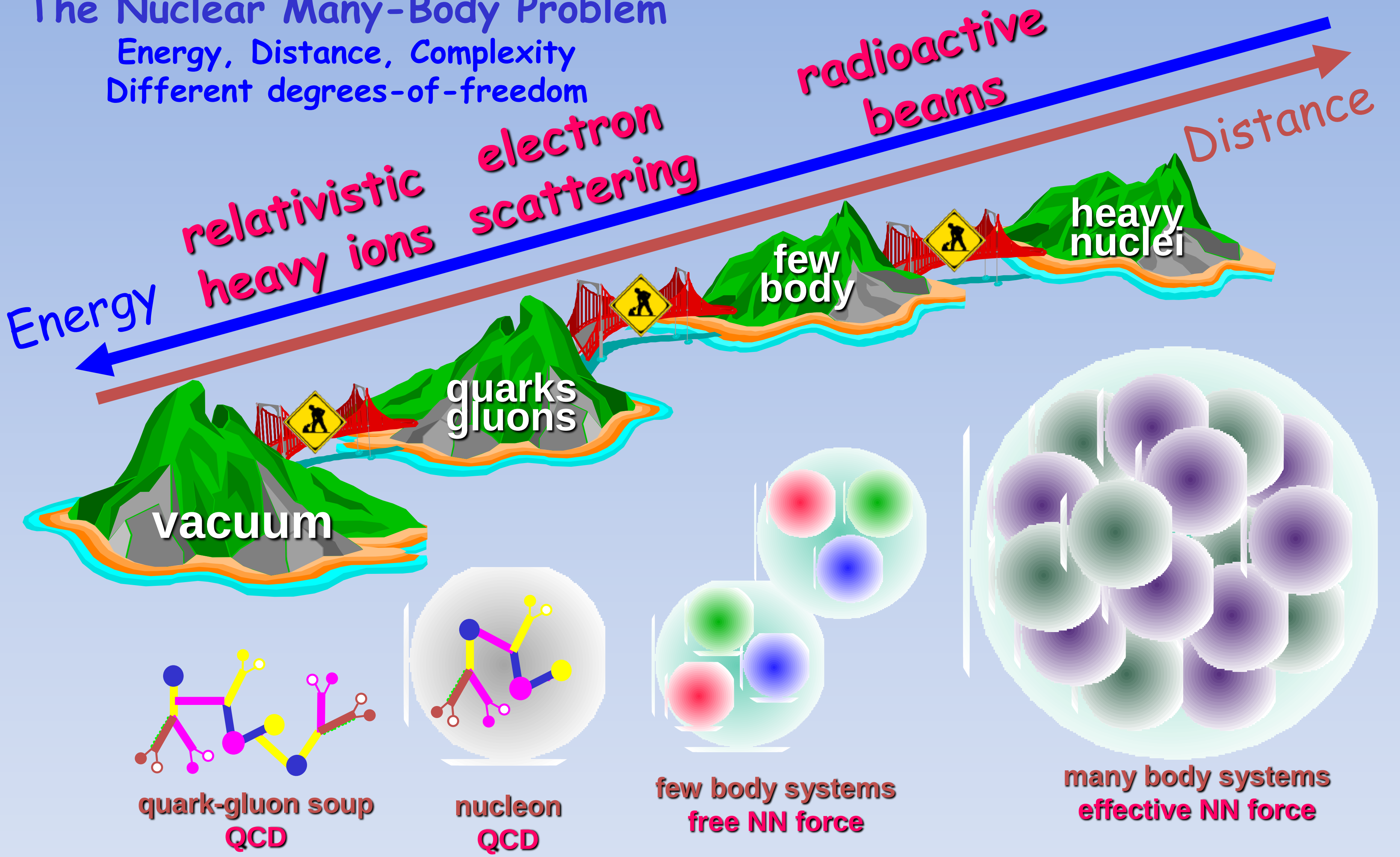
Nuclear astrophysics

- How can our knowledge of nuclei and our ability to produce them benefit the humankind?
  - Life Sciences, Material Sciences, Nuclear Energy, Security

Applications of nuclei

The Nuclear Many-Body Problem

Energy, Distance, Complexity
Different degrees-of-freedom



There is no "one size fits all" theory for nuclei, but all our theoretical approaches need to be linked. We are making great progress in this direction.

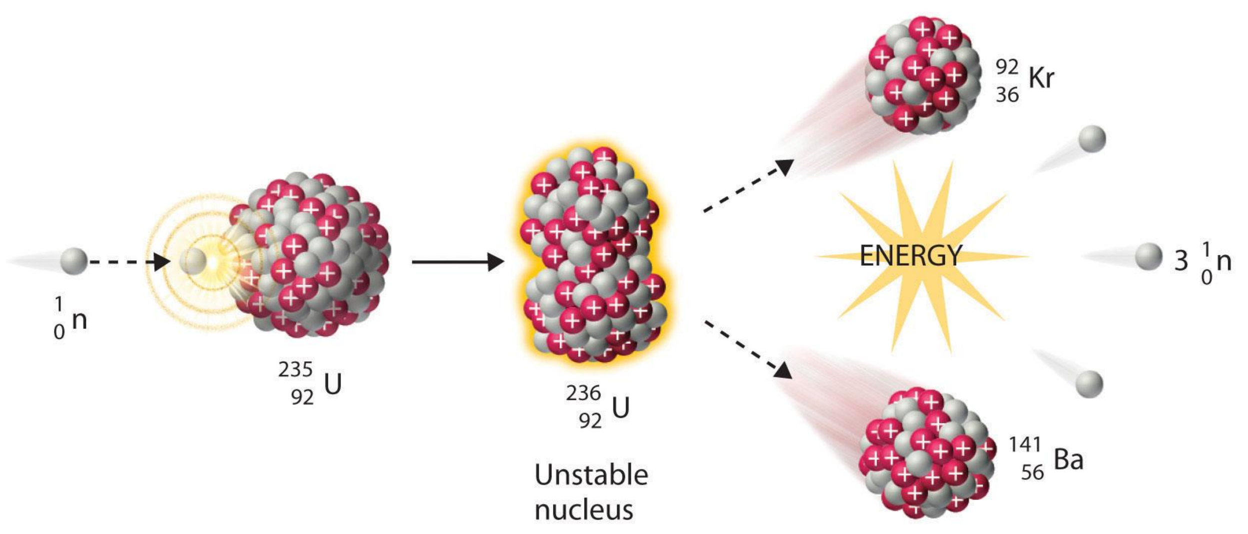
Nuclear theory challenge:

To arrive at a comprehensive and unified microscopic description of all nuclei and low-energy reactions from the basic interactions between the constituent protons and neutrons

Our goal:

Microscopic description of nuclear dynamics far from equilibrium from the basic interactions between the constituent protons and neutrons

- *Nuclear large amplitude collective motion (induced fission)*
- *Coulomb excitation with realtivistic heavy ions*
- *Excitation of nuclei with gamma rays and neutrons*
- *Nuclear reactions, fusion between colliding heavy ions*
- *Nuclear dynamics in the neutron star crust, dynamics of vortices and their pinning mechanism.*



Neutron induced fission

Quantum atomic gases – manipulating atoms with light

Recipe:

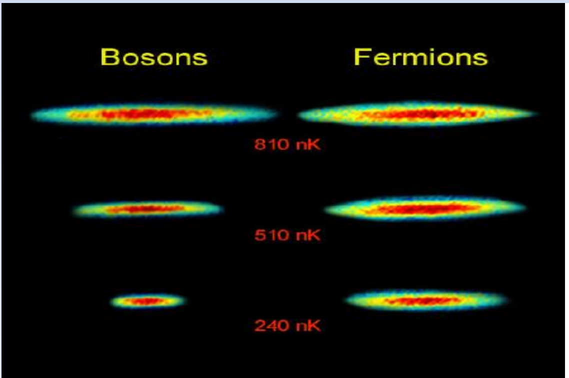
- Take a bunch of atoms (0.1-1 milion) eg. Li, K, Rb. You may consider mixtures of various atoms as well.
- Keep them in a magneto-optical trap as a dilute gas (average distance > thousands of the atomic size) – metastable state.
- Cool them down using light to *nK* so it becomes a quantum gas.

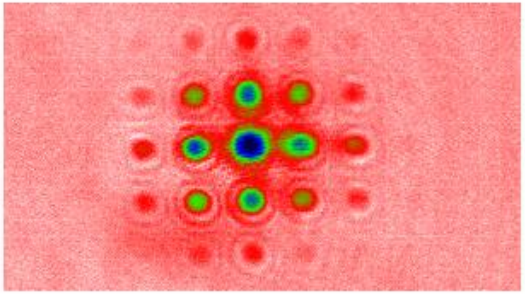
Now you may:

- change the interaction between atoms using external magnetic field
- modify the trapping potential: if you have many laser beams you can produce optical lattices of various geometries
- switch off and on the trapping potential and see how the cloud expands
- introduce external perturbation of whatever type you like using laser beams: steer it , shake it, etc.
- take mixture of various atoms (eg. Bose-Fermi mixtures)

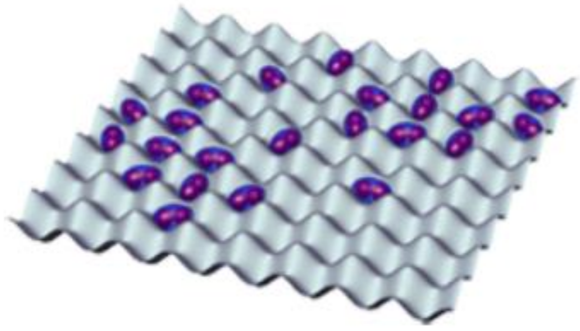
Have fun!

Cooling bosons and fermions (Anglin&Ketterle)





Rubidium BEC on an optical lattice (Denschlag&Limmer)



Why the excitement?

The reason that ultracold atoms have generated enormous scientific excitement is that they make it possible to study basic properties of matter with almost unbelievable clarity and control.

These include phase transitions to exotic states of matter such as superfluidity and superconductivity.

Manipulation of atoms offer new inroads to quantum entanglement and new possibilities for quantum computation. They are also finding applications in metrology, including atomic clocks.

<u>Nobel Prizes for achievements in the field of ultracold atomic gases.</u>

1998 – Steven Chu, Claude Cohen-Tannoudji, William D. Phillips

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

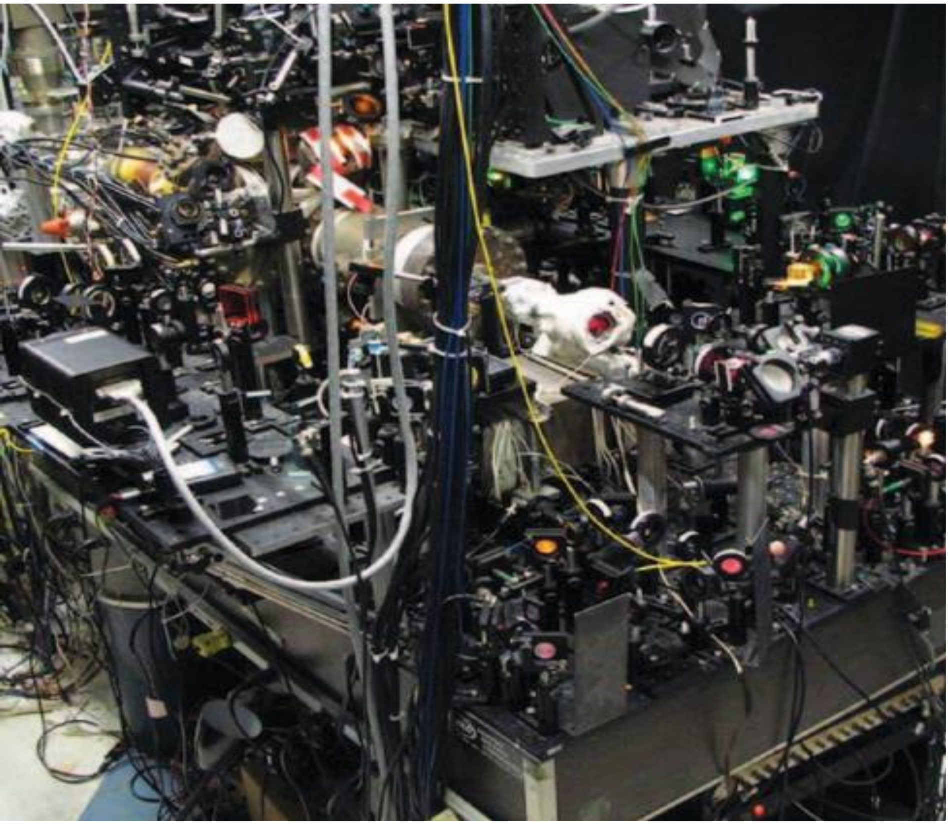
2001 – Eric A. Cornell, Wolfgang Ketterle, Carl E. Wieman

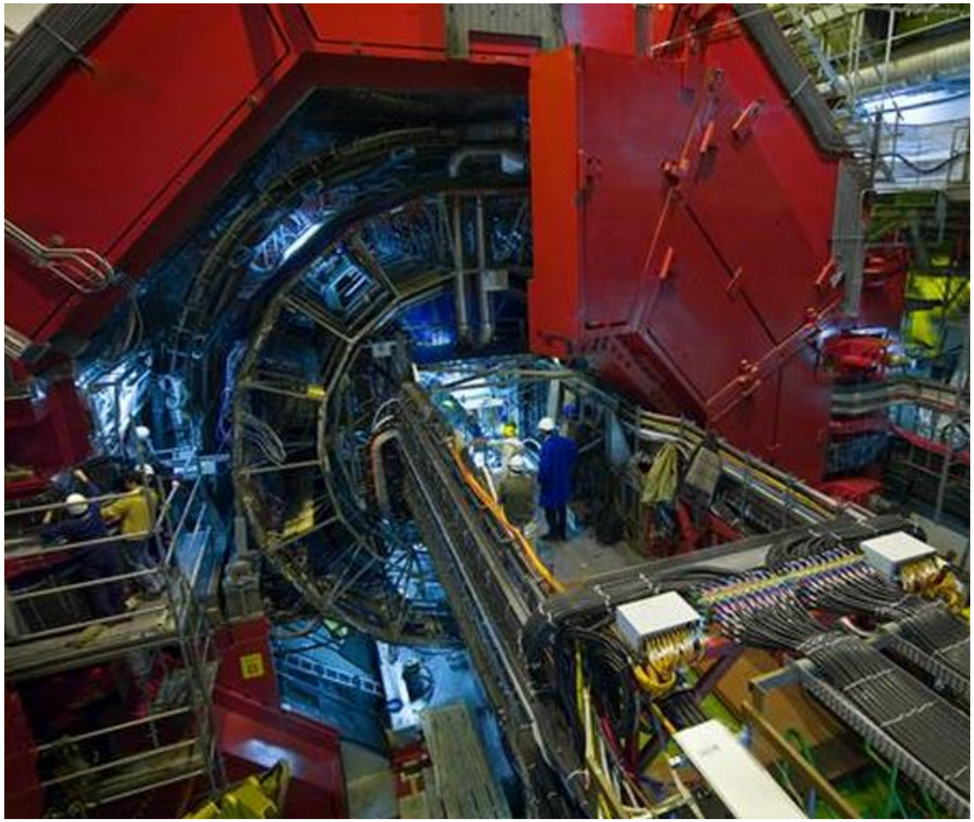
"for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates"

Gases of ultracold atoms and quark gluon plasma teach us how matter behaves under the strongest interactions that nature allows

Little Fermi Collider (MIT)
Cooling and trapping of 0.1-1 million of atoms

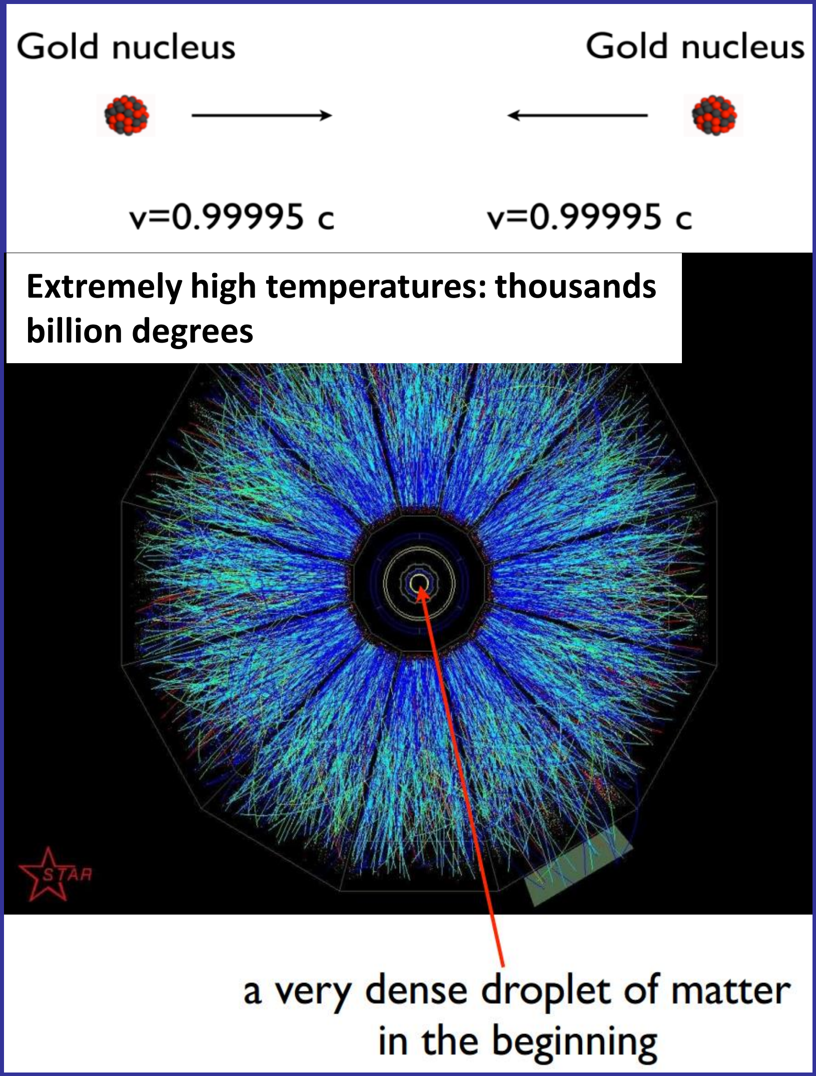
Large Hadron Collider (CERN)
Collision of heavy nuclei in order to create quark gluon plasma

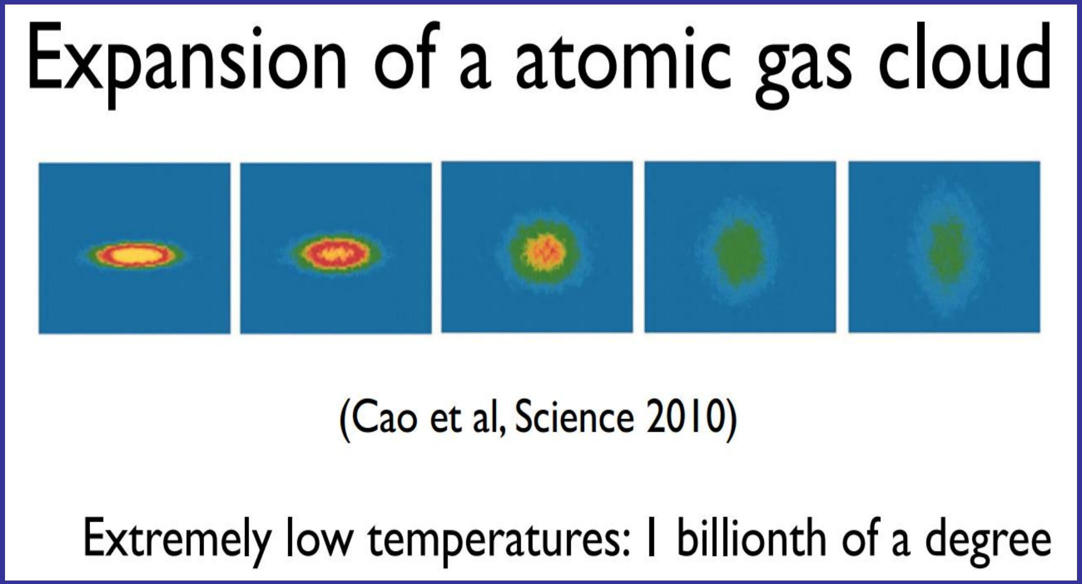




Vacuum chamber, countless mirrors, magnetic coils, water cooling, CCD cameras and lasers for laser cooling of atomic gases (human size)

ALICE experiment: search for quark gluon plasma view of the ALICE detector: 26m x 16m x 16 m + particle collider in a tunnel of 27 km circumference





Despite of energy scales differing by many orders of magnitude, expansion of both system is pretty much similar and in particular exhibts the so-called <u>elliptic flow</u>.

How to describe quantum processes far from equilibrium

From quantum mechanics:

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

However even if we know the Hamiltonian can we solve in practice the above equation?

But the wave function depends on A variables (disregarding spin):

$$\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A, t)$$

and to store the wave function (at fixed *t*) we need to store A^A **complex numbers.**

For $A \approx 100$ **it means** 10^{200} **complex numbers!**

Not possible now and most likely will never be!!!

But the situation is even worse because we need to evolve this wave function in time…

Time evolution

If we are interested in nuclear processes involving excitations up to several hundreds MeV (for nuclei) we need to adjust the time step accordingly:

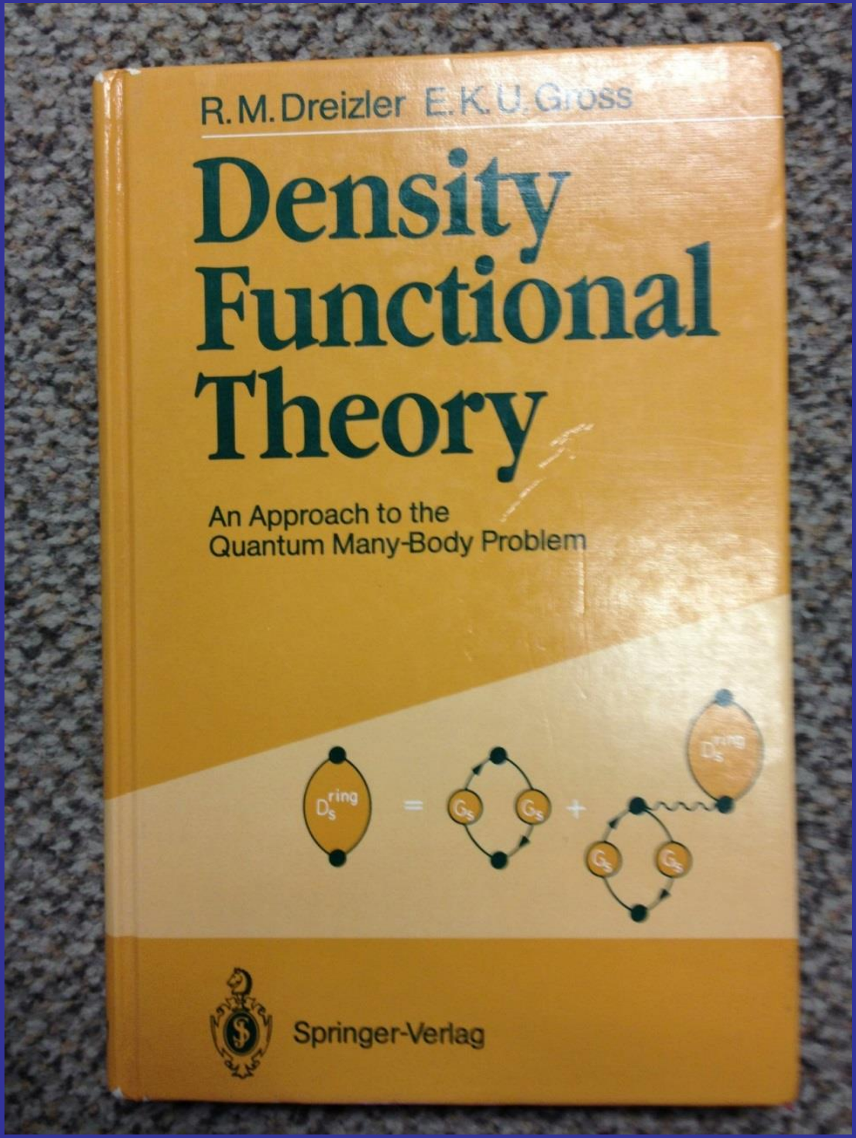
$$\Delta t = \frac{\hbar}{E_{exc}} \approx 0.1\, {}^{fm}\!/_{c}$$

And in order to get the energy resolution of the order of *keVs* the length of the time evolution should be:

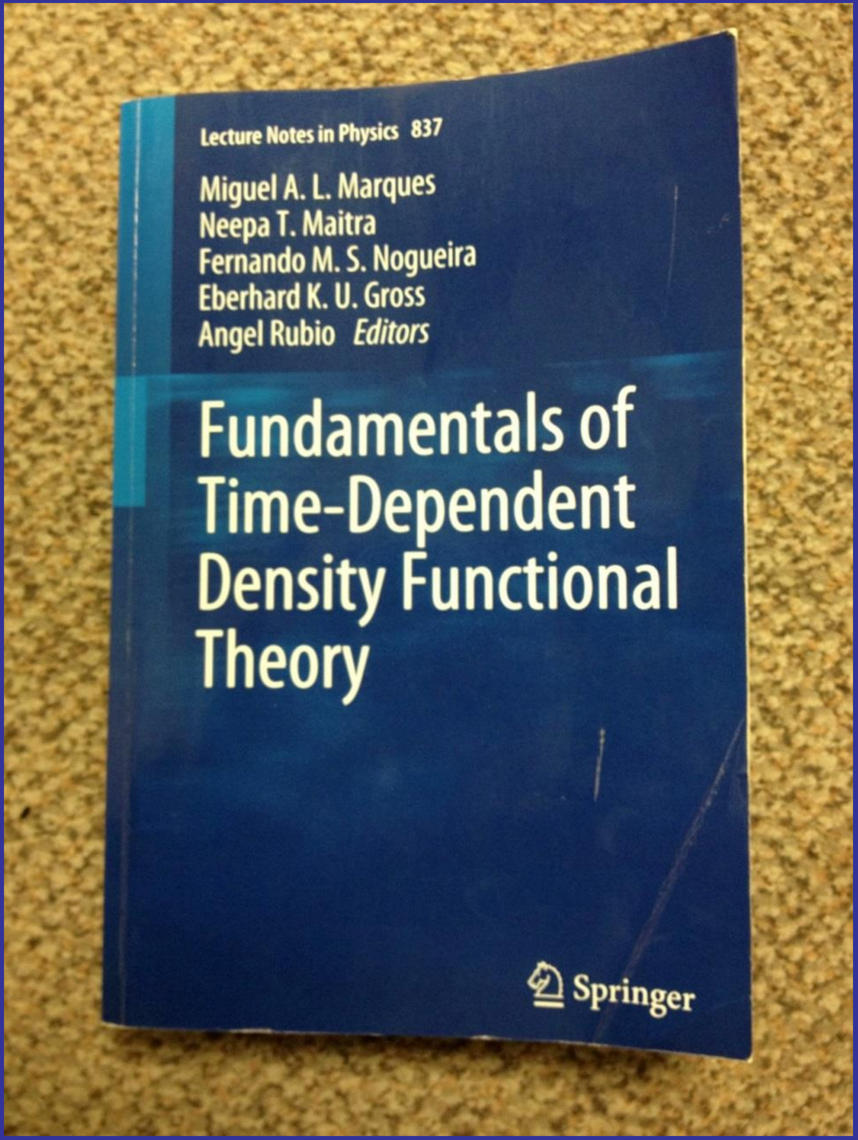
$$T = \frac{\hbar}{\Delta E} \approx 10^5\, {}^{fm}\!/_{c}$$

Summarizing: we need to evolve the wave function through 1 million time steps without loosing numerical precision!

Density Functional Theory (DFT)



1990



2012

Kohn-Sham approach

Suppose we are given the density of an interacting system.
There exists a unique noninteracting system with the same density.

Interacting system

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = (\hat{T}+\hat{V}(t)+\hat{W})\left|\psi(t)\right\rangle$$

Noninteracting system

$$i\hbar\frac{\partial}{\partial t}\left|\varphi(t)\right\rangle = (\hat{T}+\hat{V}_{KS}(t))\left|\varphi(t)\right\rangle$$

$$\rho(\vec{r},t) = \left\langle\psi(t)\right|\hat{\rho}(\vec{r})\left|\psi(t)\right\rangle = \left\langle\varphi(t)\right|\hat{\rho}(\vec{r})\left|\varphi(t)\right\rangle$$

Hence the DFT approach is essentially exact.

However as always there is a price to pay:

- **Kohn-Sham potential in principle depends on the past (memory).**
  Very little is known about the memory term and usually it is disregarded (adiabatic TDDFT).
- **Only one body observables can be reliably evaluated within standard DFT.**

E. Runge, E.K.U Gross, PRL 52, 997 (1984)
B.-X. Xu, A.K. Rajagopal, PRA 31, 2682 (1985)
G. Vignale, PRA77, 062511 (2008)

For superfluid systems one needs:
- to find an energy functional
- extend it to superfluid systems (SLDA)
- extend it to time dependent phenomena.

Then one need to solve the set of nonlinear differential equations:

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{k\uparrow}(\mathbf{r},t) \\ u_{k\downarrow}(\mathbf{r},t) \\ v_{k\uparrow}(\mathbf{r},t) \\ v_{k\downarrow}(\mathbf{r},t) \end{pmatrix} = \begin{pmatrix} h_{\uparrow,\uparrow}(\mathbf{r},t) & h_{\uparrow,\downarrow}(\mathbf{r},t) & 0 & \Delta(\mathbf{r},t) \\ h_{\downarrow,\uparrow}(\mathbf{r},t) & h_{\downarrow,\downarrow}(\mathbf{r},t) & -\Delta(\mathbf{r},t) & 0 \\ 0 & -\Delta^*(\mathbf{r},t) & -h^*_{\uparrow,\uparrow}(\mathbf{r},t) & -h^*_{\uparrow,\downarrow}(\mathbf{r},t) \\ \Delta^*(\mathbf{r},t) & 0 & -h^*_{\uparrow,\downarrow}(\mathbf{r},t) & -h^*_{\downarrow,\downarrow}(\mathbf{r},t) \end{pmatrix} \begin{pmatrix} u_{k\uparrow}(\mathbf{r},t) \\ u_{k\downarrow}(\mathbf{r},t) \\ v_{k\uparrow}(\mathbf{r},t) \\ v_{k\downarrow}(\mathbf{r},t) \end{pmatrix}$$

- **The system is placed on a large 3D spatial lattice.**
- **No symmetry restrictions**
- **Number of PDEs is of the order of the number of spatial lattice points**

Selected capabilities of the SLDA/TDSLDA codes:

- ✓ full 3D simulations with no symmetry restrictions
- ✓ number of evolved quasiparticle wave functions is of the order of the lattice size: $O(10^4)$- $O(10^6)$
- ✓ high numerical accuracy for spatial derivatives using FFTW
- ✓ for TD high-accuracy and numerically stable Adams–Bashforth–Milne 5th order predictor-corrector-modifier algorithm with only 2 evaluations of the rhs per time step and with no matrix operations
- ✓ The time step is adjusted so the relative error in ABM method is between 10^{-7} -10^{-15}

  Eg. we evolve 4x136626=546504 coupled eigenvectors for ^{238}U on the lattice: 50x50x80 fm (mesh size: 1.25fm) with energy cutoff 100MeV to an accuracy 10^{-8}
- ✓ very fast I/O capabilities
- ✓ volumes of the order of ($L = 80^3$) capable of simulating time evolution of 42000 neutrons at saturation density (possible application: neutron stars)
- ✓ capable of simulating up to times of the order of 10^{-19} s (a few million time steps)
- ✓ Presented calculations for unitary Fermi gas required over 200,000 cores on Titan
- ✓ CPU vs GPU on Titan ≈ 15 speed-up (likely an additional factor of 4 possible)

  Eg. for 137062 two component wave functions:

  CPU version (4096 nodes x 16 PEs) - 27.90 sec for 10 time steps

  GPU version (4096 PEs + 4096GPU) - 1.84 sec for 10 time step

Selected results

Photoabsorption cross section for heavy, deformed nuclei.

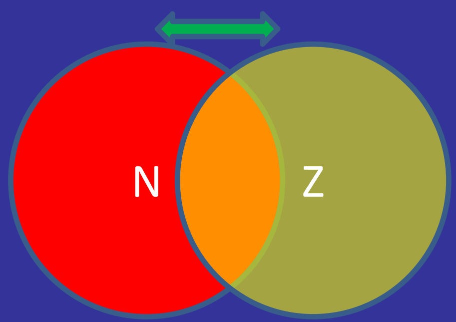
$$h_{\tau,\sigma\sigma}(\mathbf{r},t) \Rightarrow h_{\tau,\sigma\sigma}(\mathbf{r},t) + F_\tau(\mathbf{r})f(t) \quad F_\tau(\mathbf{r}) = N_\tau \sin(\mathbf{k}\cdot\mathbf{r}_\tau)/|\mathbf{k}|,$$

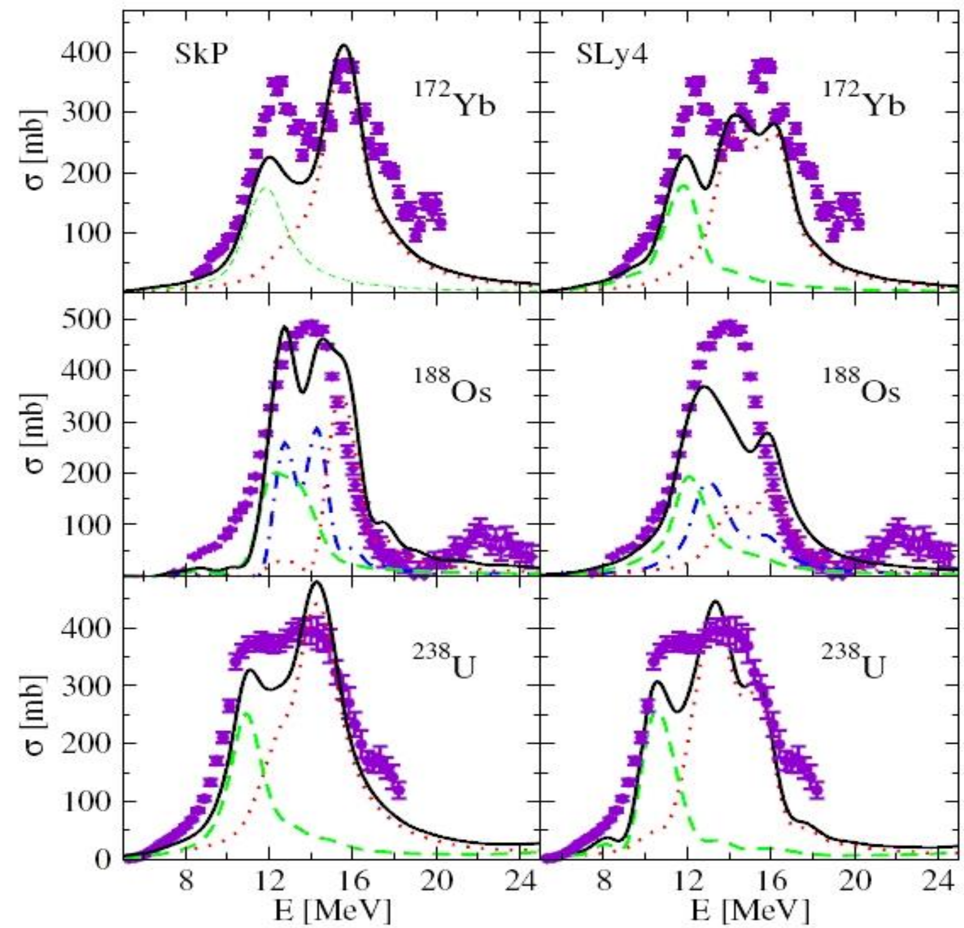
$$S(E) = \sum_\nu |\langle\nu|\hat{F}|0\rangle|^2 \delta(E - E_\nu)$$

$$S(\omega) = \mathrm{Im}\{\delta F(\omega)/[\pi f(\omega)]\}$$

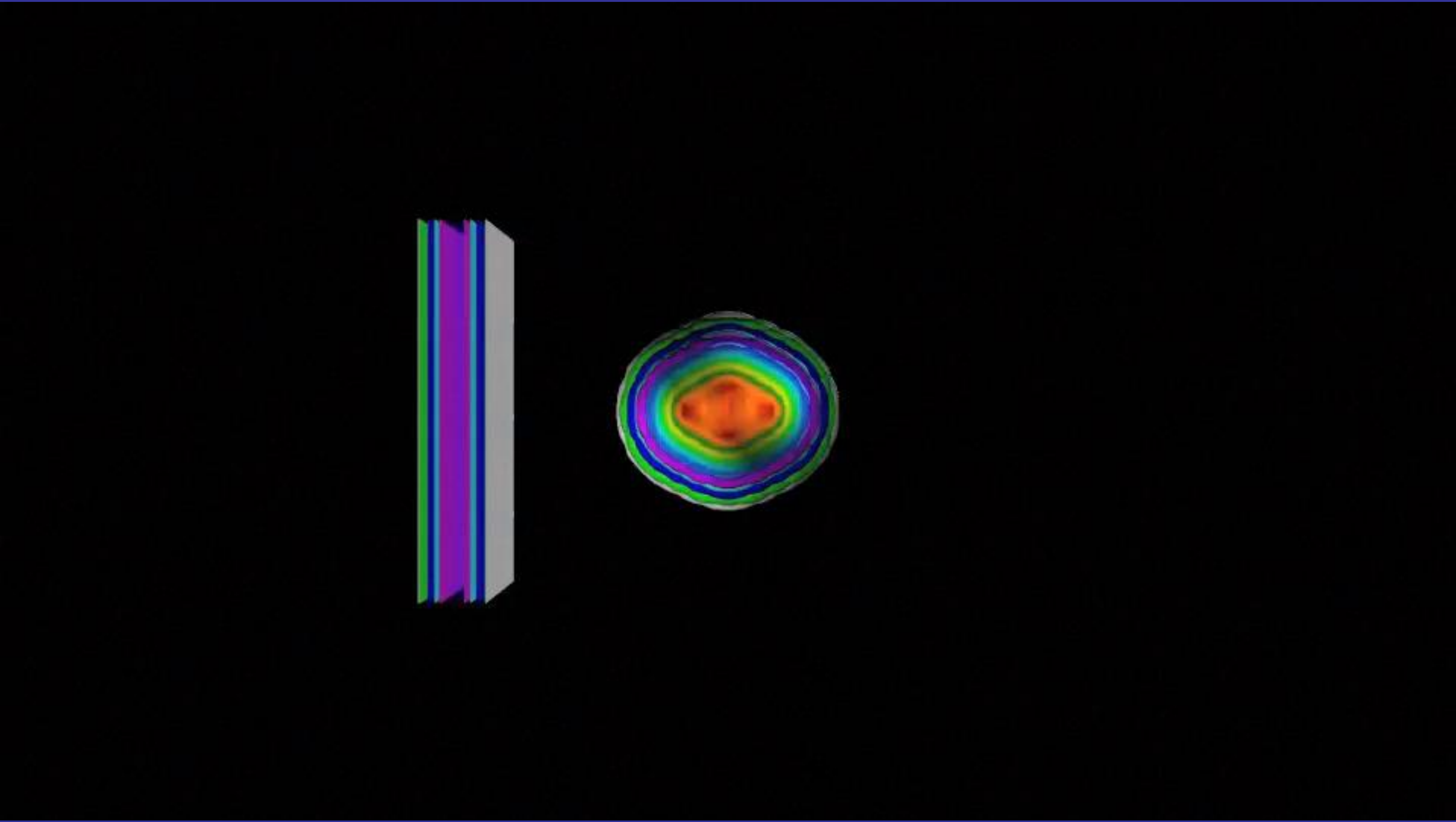
$$\delta F(t) = \langle\hat{F}\rangle_t - \langle\hat{F}\rangle_0 = \int d^3r\,\delta\rho(\mathbf{r},t)F(\mathbf{r}) \quad f(t) = C\exp[-(t-10)^2/2]$$

Excitation of giant dipole resonance:





I.Stetcu, A.Bulgac, P. Magierski, K.J. Roche, Phys. Rev. C84 051309 (2011)



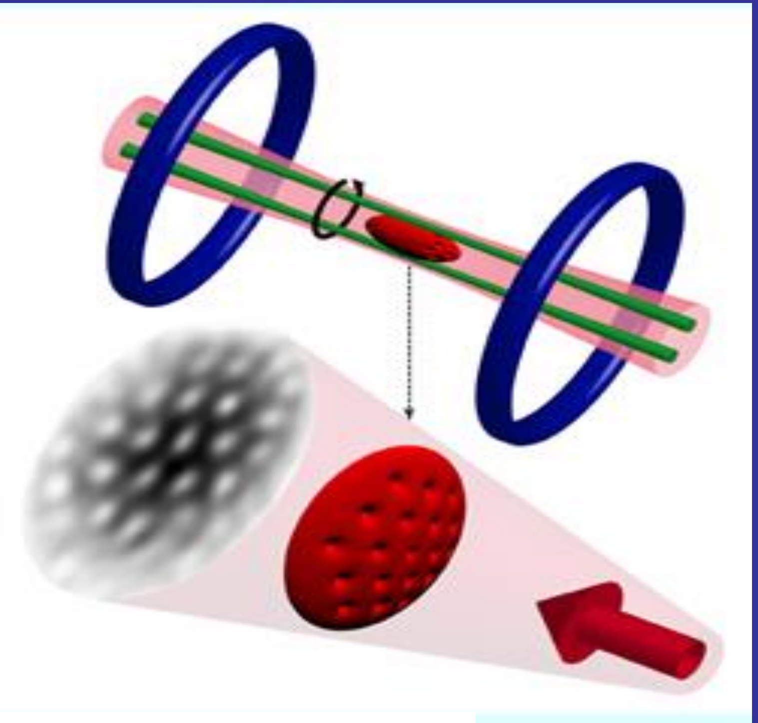
Neutron scattering of ^{238}U computed in TDSLDA with absorbing boundary conditions

Movie

I. Stetcu *et al.*

Superfluidity in atomic Fermi gases:

✓In 2005 Zwierlein/Ketterle group observed quantum vortices which survived when passing from BEC to unitarity – <u>evidence for superfluidity!</u>

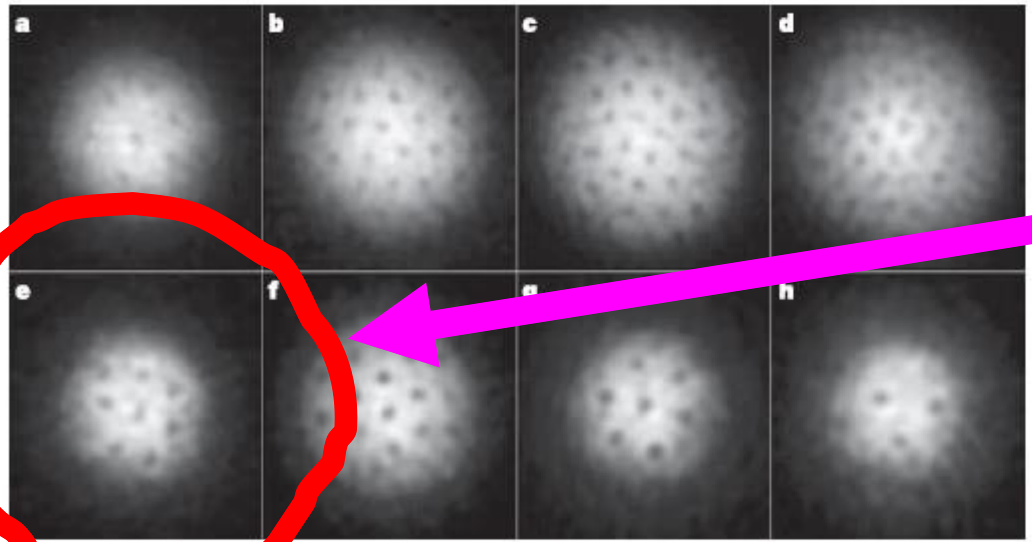


system of fermionic ^6Li atoms

Feshbach resonance: B=834G

BEC side: a>0

BCS side a<0

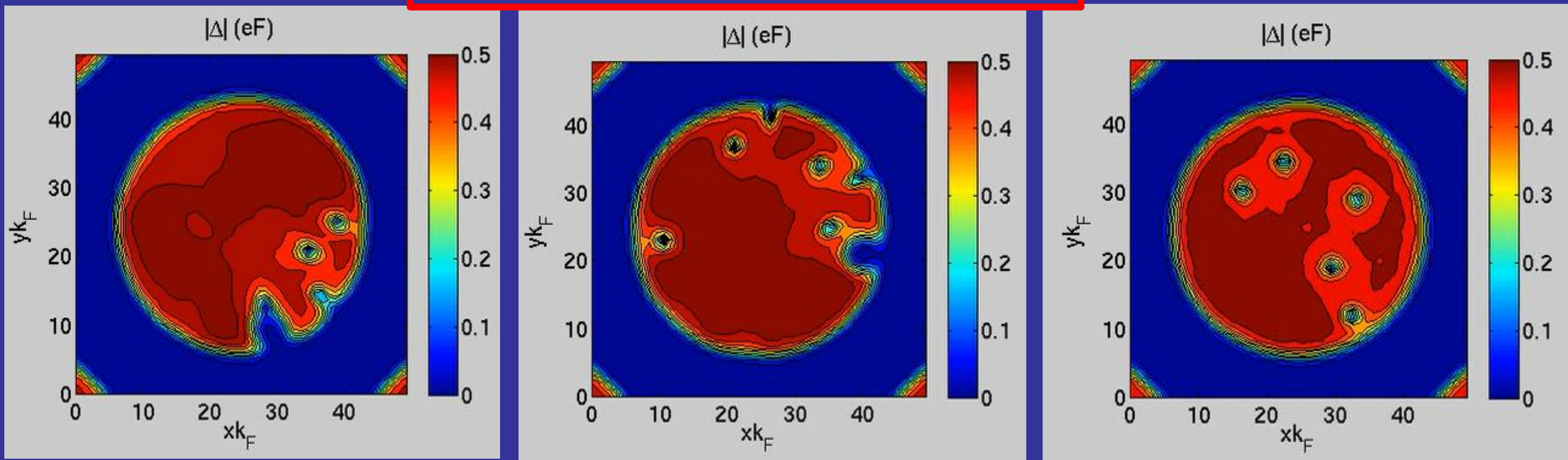


UNITARY REGIME

Figure 2 | Vortices in a strongly ... 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 (s... magnetic fields were 740 G (**a**), 766 G (**b**), 792 G (**c** ... 843 G (**f**), 853 G (**g**) and 863 G (**h**). The field of vie... 880 μm × 880 μm.

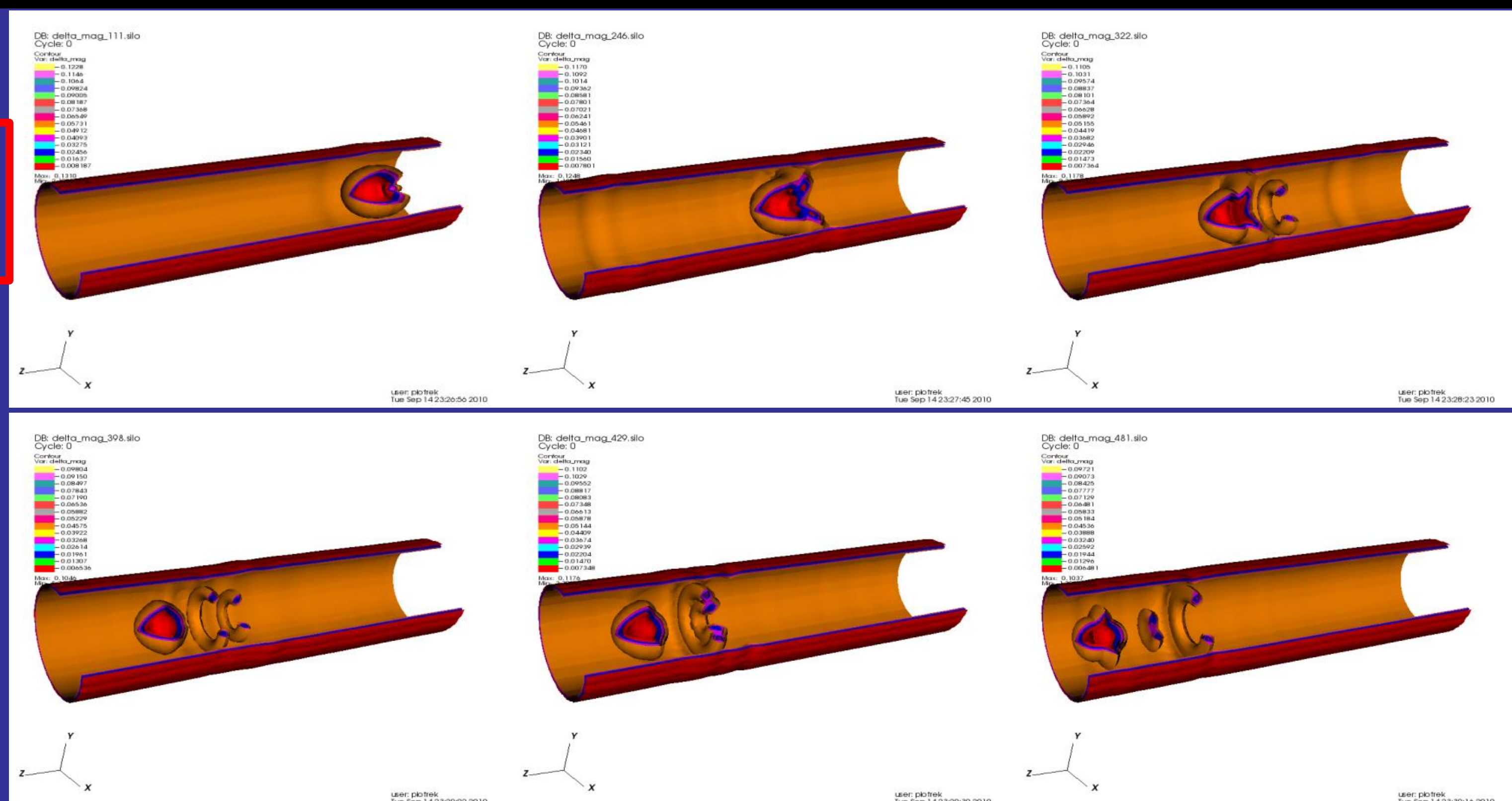
M.W. Zwierlein *et al*., Nature, 435, 1047 (2005)

Excitation of vortices through stirring

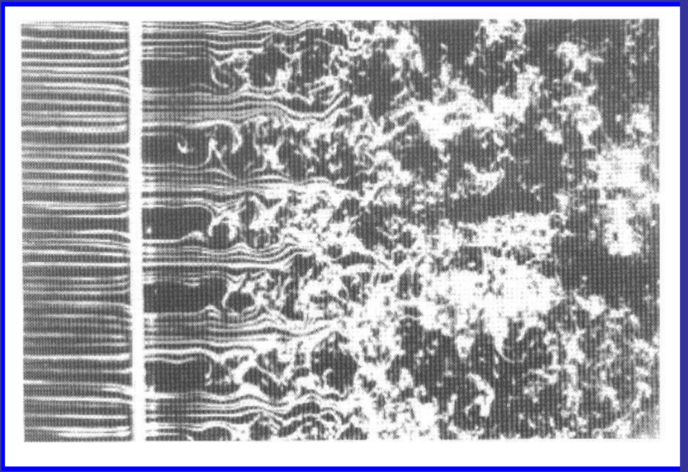


dynamics of vortex rings

Heavy spherical object moving through the superfluid unitary Fermi gas



Road to quantum turbulence



Classical turbulence: energy is transfered from large scales to small scales where it eventually dissipates.

Kolmogorov spectrum: $E(k)=C\,\varepsilon^{2/3}\,k^{-5/3}$

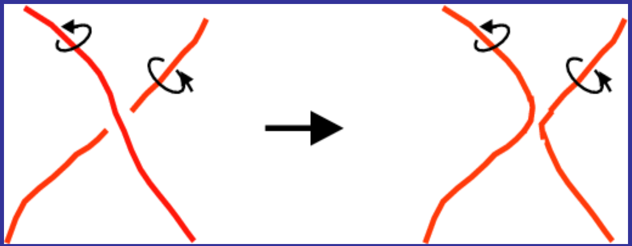
E – kinetic energy per unit mass associated with the scale 1/k
ε - energy rate (per unit mass) transfered to the system at large scales.
k - wave number (from Fourier transformation of the velocity field).
C – dimensionless constant.

Superfluid turbulence (quantum turbulence): disordered set of quantized vortices. The friction between the superfluid and normal part of the fluid serves as a source of energy dissipation.

Problem: how the energy is dissipated in the superfluid system at small scales at T=0? - „pure" quantum turbulence

Possibility: vortex reconnections → Kelvin waves → phonon radiation

Vortex reconnections



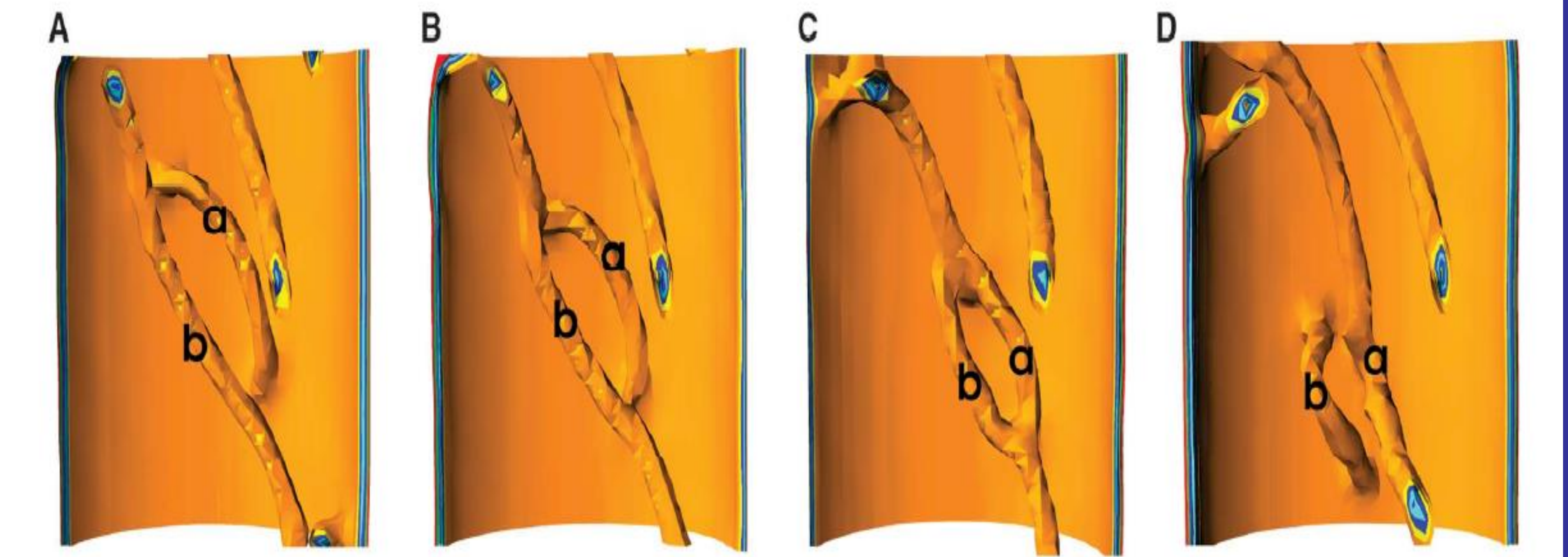
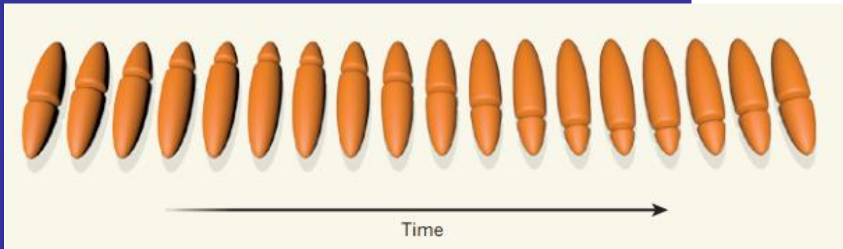


Fig. 3. (**A** to **D**) Two vortex lines approach each other, connect at two points, form a ring and exchange between them a portion of the vortex line, and subsequently separate. Segment (a), which initially belonged to the vortex line attached to the wall, is transferred to the long vortex line (b) after reconnection and vice versa.

Bulgac, Luo, Magierski, Roche, Yu, *Science* 332, 1288 (2011)

Soliton dynamics vs ring vortex – a controversy



MIT Experiment:
Nature 499 (2013) 426

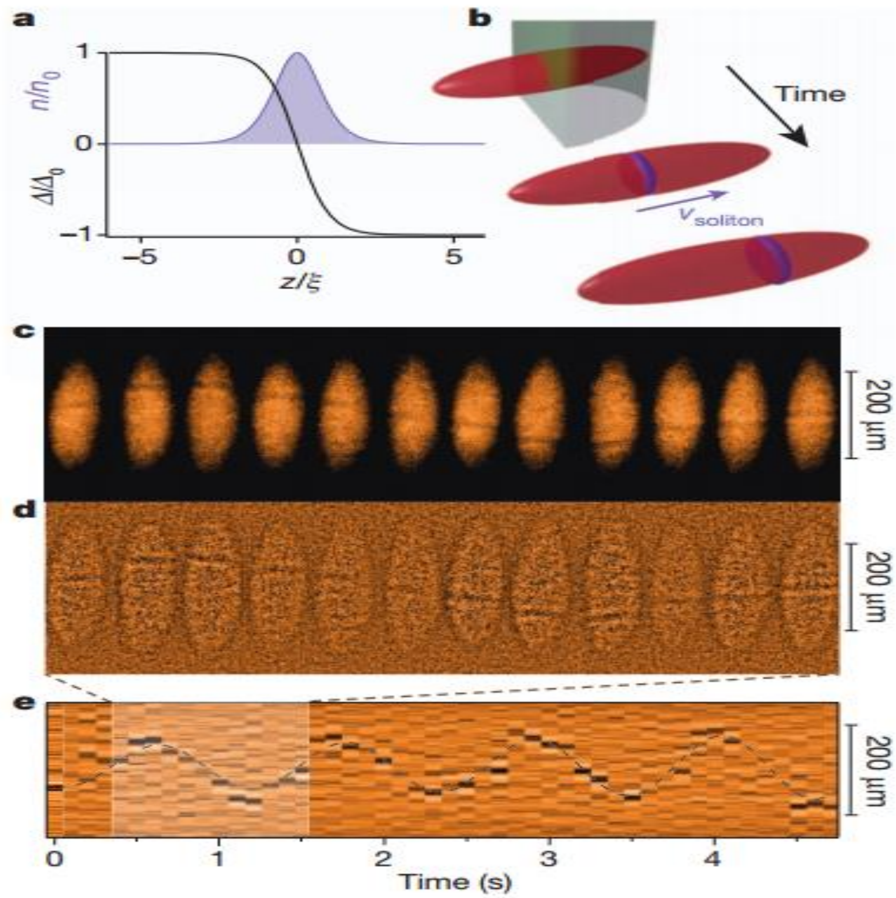
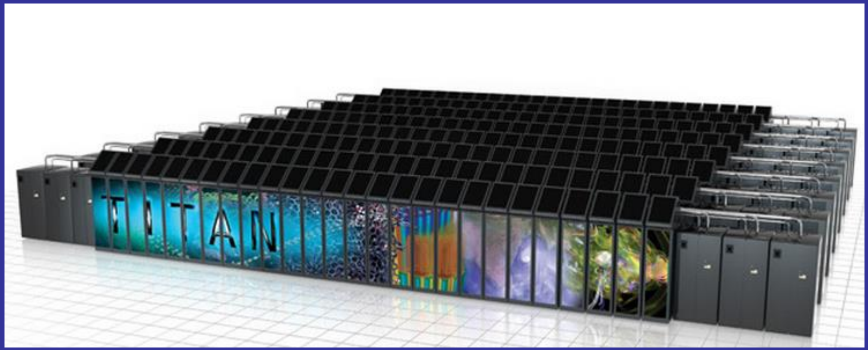


Figure 1 | Creation and observation of solitons in a fermionic superfluid. **a**, Superfluid pairing gap $\Delta(z)$ for a stationary soliton, normalized by the bulk pairing gap Δ_0, and density $n(z)$ of the localized bosonic (fermionic) state versus position z, in the BEC (BCS) regime of the crossover, in units of the BEC healing length (BCS coherence length) ξ. **b**, Diagram of the experiment. A phase-imprinting laser beam twists the phase of one-half of the trapped superfluid by approximately π. The soliton generally moves at non-zero velocity $v_{soliton}$. **c**, Optical density and **d**, residuals (optical density minus a smoothed copy of the same image) of atom clouds at 815 G, imaged via the rapid ramp method[34], showing solitons at various hold times after creation. One period of soliton oscillation is shown. The in-trap aspect ratio was $\lambda = 6.5(1)$. **e**, Radially integrated residuals as a function of time revealing long-lived soliton oscillations. The soliton period is $T_s = 12(2)T_z$, much longer than the trapping period of $T_z = 93.76(5)$ ms, revealing an extreme enhancement of the soliton's relative effective mass, M^*/M.

Theory prefers ring vortices:
A. Bulgac, et al.,
Phys. Rev. Lett. 112, 025301 (2014)
G. Wlazłowski, et al.
Phys. Rev. Lett. (in press)

Computational resources

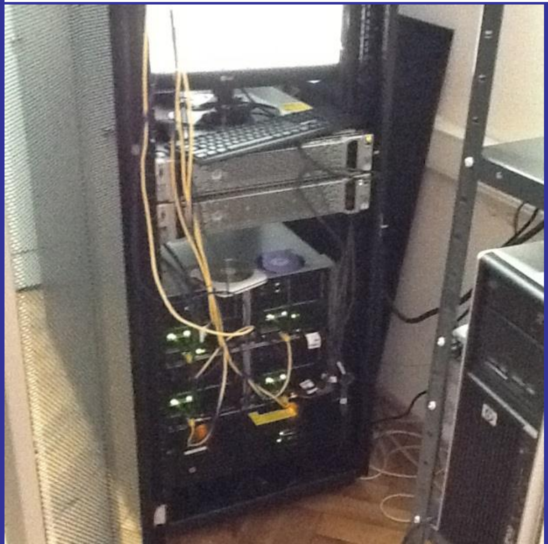
Titan, Oak Ridge USA,
Hybrid architecture (CPU+GPU),
Ranking: no. 1



Various CPU machines at NERSC (USA) :
mainly Edison and Hopper. Ranking: no. around 20

interdyscyplinarne centrum
modelowania matematycznego
i komputerowego

K Computer, Kobe, Japan
CPU architecture , Ranking: no. 4



Personal toy (being installed): DWARF (Faculty of Physics)
Phase I (2014) : 12 Nvidia K40 tesla GPUs in 4 servers
+ memory server for 36TB
Phase II (2015) : additional 8 GPUs (20 in total)

Collaborators:

Aurel Bulgac
(U. Washington)

Michael M. Forbes
(INT)

Kenneth J. Roche
(PNNL)

Ionel Stetcu
(LANL)

Gabriel Wlazłowski
(PW/ U. Washington)

TDSLDA applications:

1) Nuclear physics:

- **Electromagnetic response**
- **Pairing vibrations**
- **Heavy ion collisions**
- **Induced fission**
- **Neutron scattering/capture**

2) Neutron stars:

- **Dynamics of vortices**
- **Vortex pinning mechanism in the neutron star crust (glitches)**

3) Various applications in cold atom physics:

Vortex and soliton dynamics, atomic cloud collisions, dynamics in optical lattices.