Nierównowagowe procesy w nadciekłych układach kwantowych: zimnych gazach atomów i jądrach atomowych

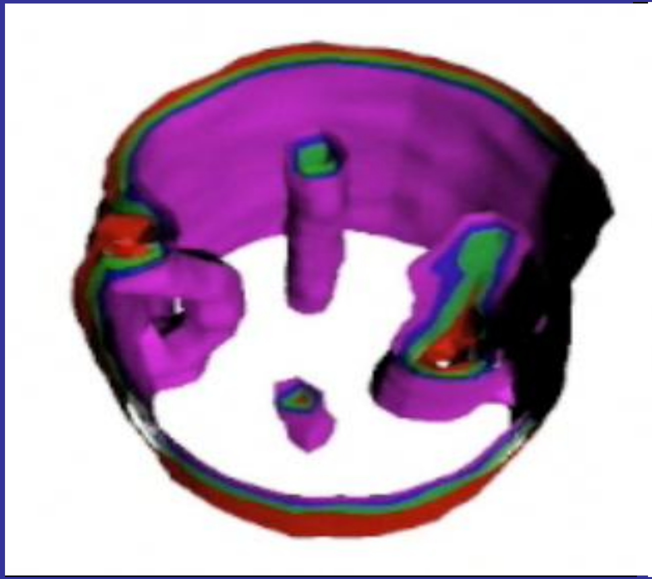
Piotr Magierski (*Politechnika Warszawska*)

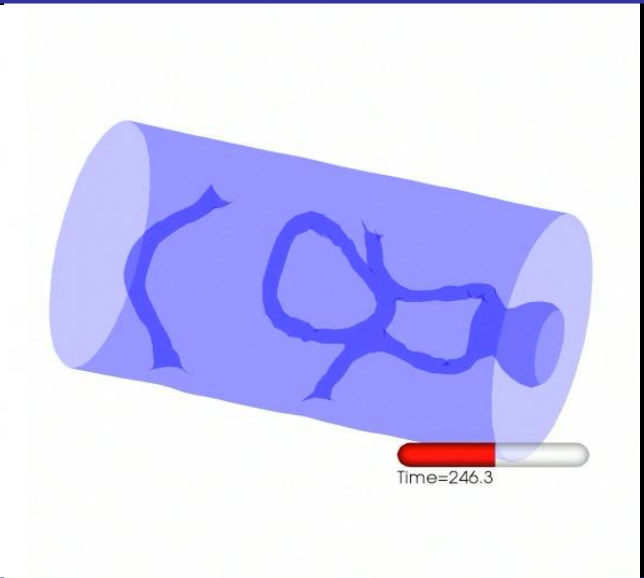
Uczestnicy grantu G31-12: Jacek Dobaczewski (IFT UW)
Gabriel Wlazłowski (Wydział Fizyki PW)
Krzysztof Zberecki (Wydział Fizyki PW)

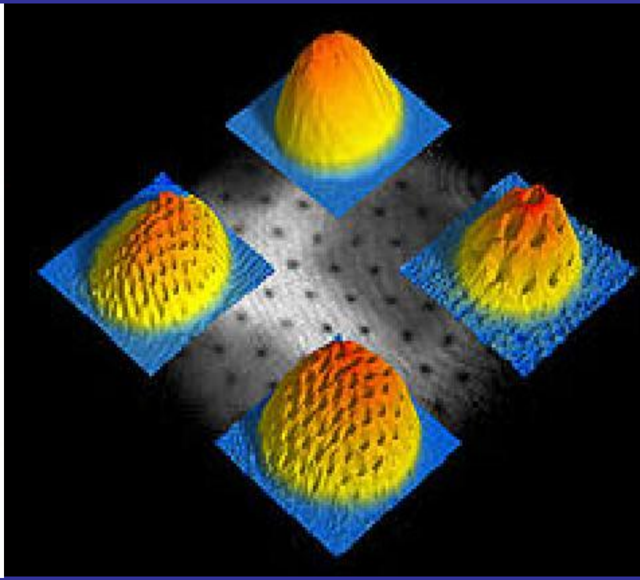
<u>Zastosowanie metod:</u>

- całek po trajektoriach (Monte Carlo),
- funkcjonału gęstości energii (stacjonarnej i zależnej od czasu),

do badania kwantowych gazów atomowych i układów jądrowych (jądra atomowe, materia neutronowa, materia jądrowa.)







What is a unitary gas?

A gas of interacting fermions is in the unitary regime if the average separation between particles is large compared to their size (range of interaction), but small compared to their scattering length.

$\boxed{n\, r_0^3 \ll 1}$ $\boxed{n\, |a|^3 \gg 1}$

n - particle density

a - scattering length

r_0 - effective range

$$\boxed{\text{i.e. } r_0 \to 0, a \to \pm\infty}$$

NONPERTURBATIVE REGIME

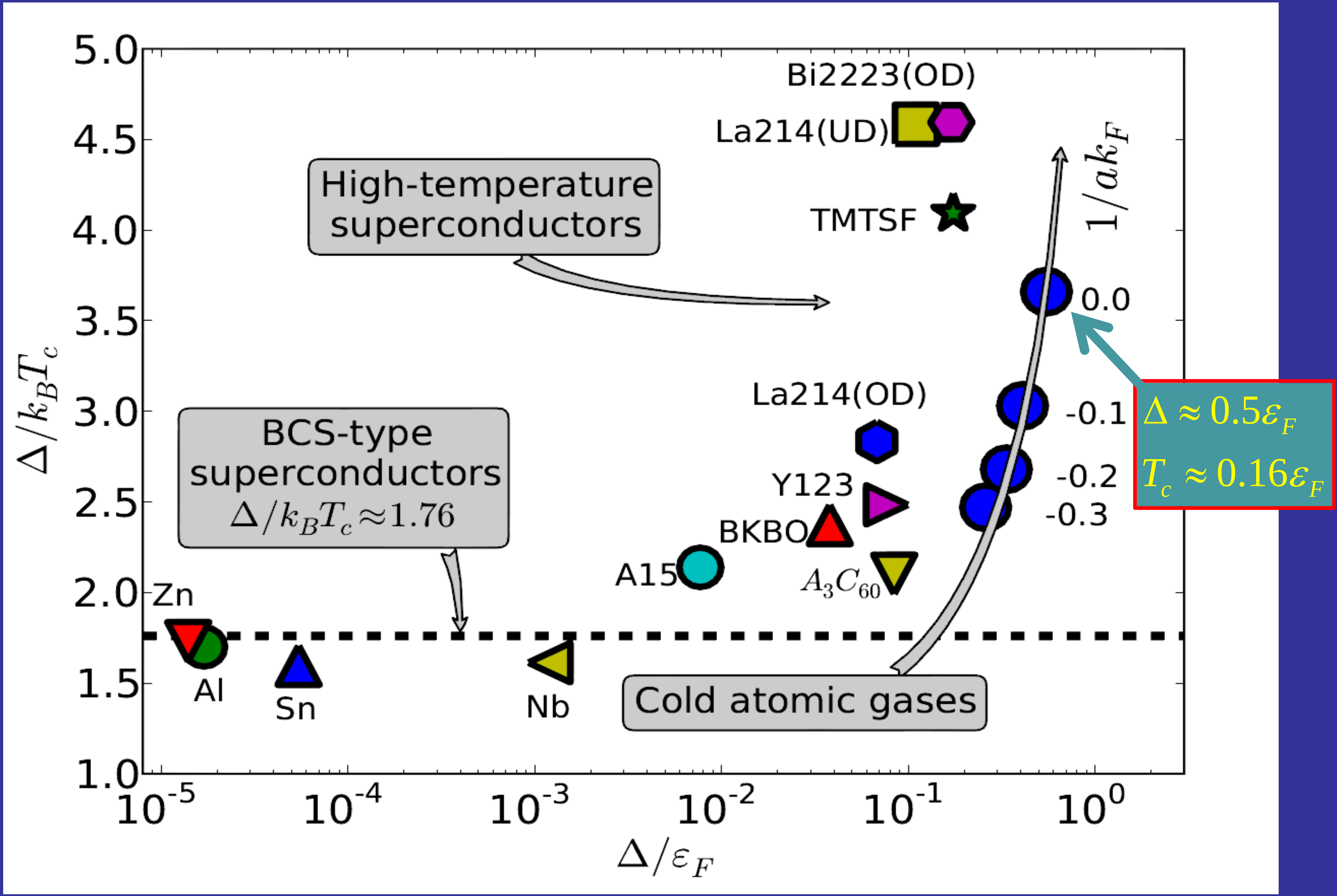
System is dilute but strongly interacting!

Universality: $E(x) = \xi(x) E_{FG};\ x = T/\varepsilon_F$

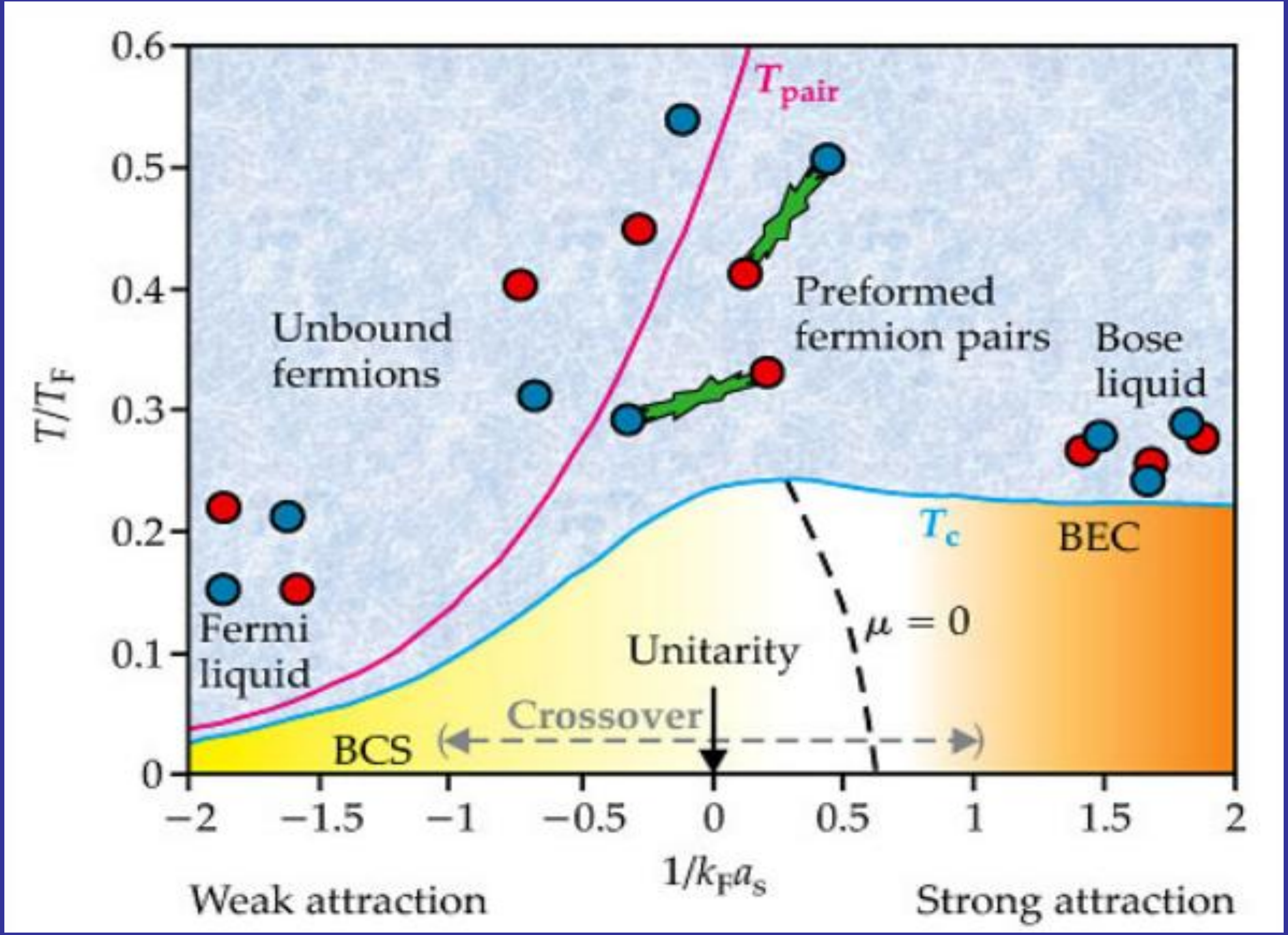
$\xi(0) = 0.3(1)$ - Exp. estimate

E_{FG} - Energy of noninteracting Fermi gas

Cold atomic gases and high Tc superconductors



From Fischer et al., Rev. Mod. Phys. 79, 353 (2007) & P. Magierski, G. Wlazłowski, A. Bulgac, Phys. Rev. Lett. 107, 145304 (2011)



From Sa de Melo, Physics Today (2008)

<u>Pairing pseudogap:</u> suppression of low-energy spectral weight function due to incoherent pairing in the normal state ($T > T_c$)

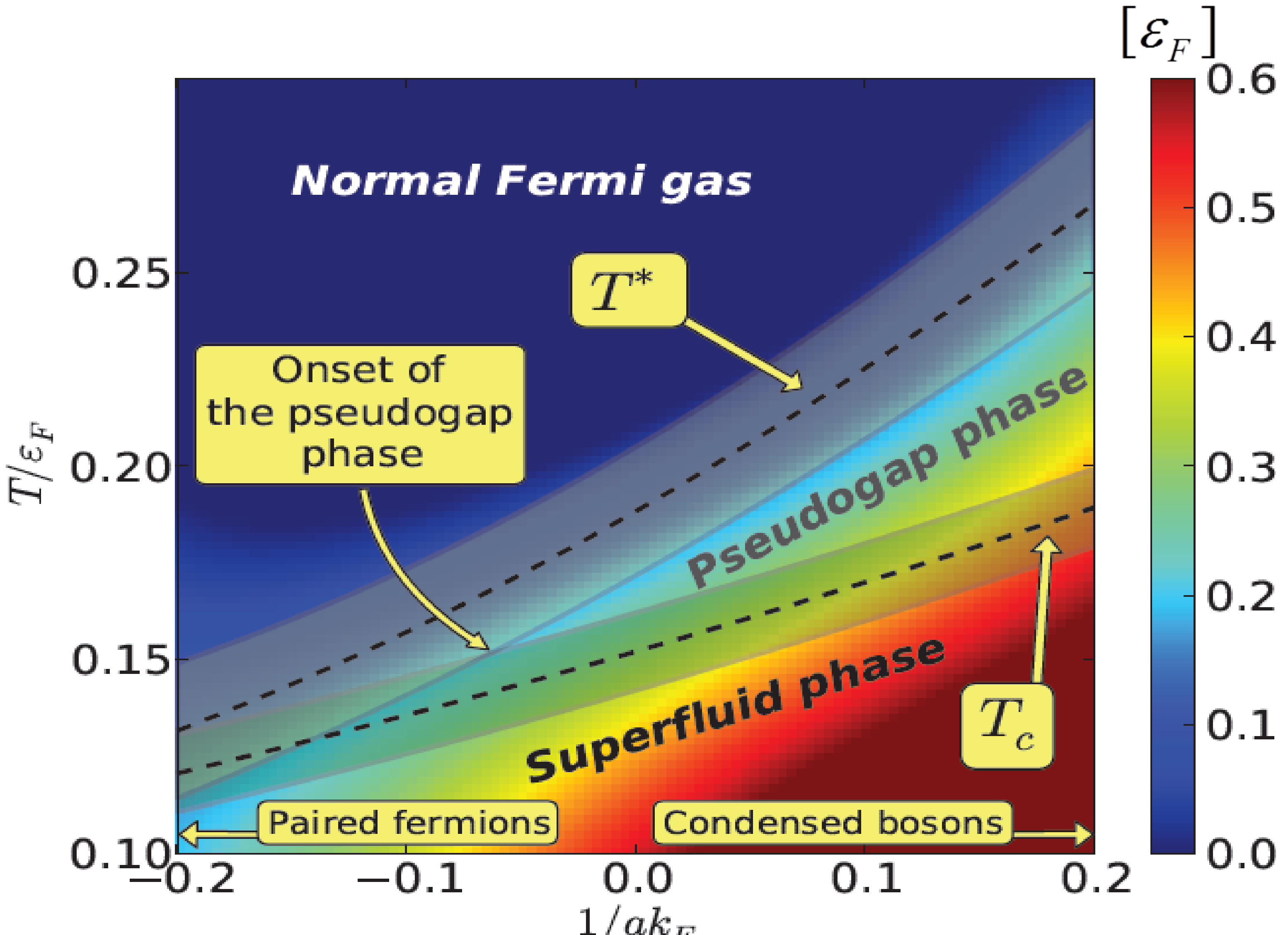
<u>Important issue related to pairing pseudogap:</u>

- Are there sharp gapless quasiparticles in a normal Fermi liquid

YES: Landau's Fermi liquid theory;

NO: breakdown of Fermi liquid paradigm

Gap in the single particle fermionic spectrum - theory



Ab initio **result: The onset of pseudogap phase at $1/ak_F \approx -0.05$.**

Magierski, Wlazłowski, Bulgac, *Phys. Rev. Lett.*107,145304(2011)
Magierski, Wlazłowski, Bulgac, Drut, *Phys. Rev. Lett.*103,210403(2009)

Spin susceptibility and spin drag rate

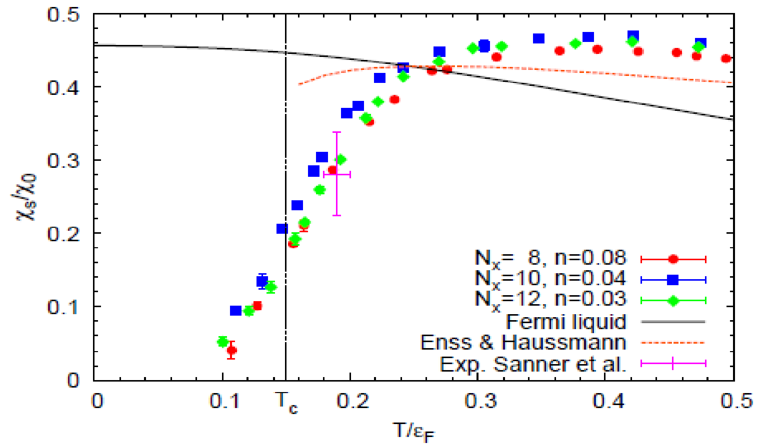


FIG. 2: (Color online) The static spin susceptibility as a function of temperature for an 8^3 lattice solid (red) circles, 10^3 lattice (blue) squares and 12^3 lattice (green) diamonds. Vertical black dotted line indicates the critical temperature of superfluid to normal phase transition $T_c = 0.15\,\varepsilon_F$. For comparison Fermi liquid theory prediction and recent results of the T-matrix theory produced by Enss and Haussmann [25] are plotted with solid and dashed (brown) lines, respectively. The experimental data point from Ref. [15] is also shown.

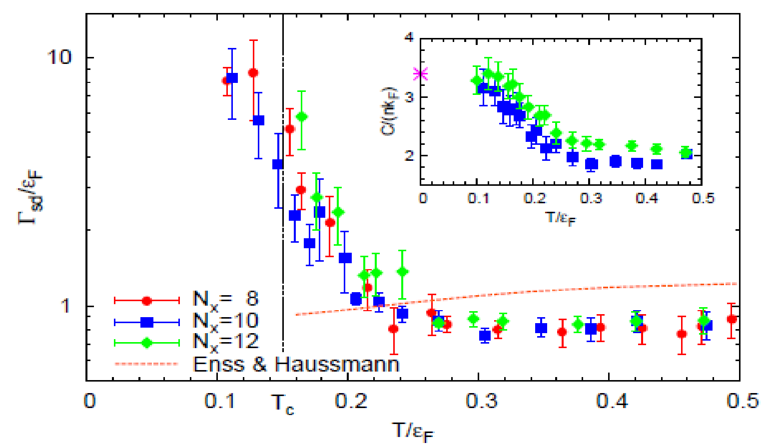


FIG. 3: (Color online) The spin drag rate $\Gamma_{sd} = n/\sigma_s$ in units of Fermi energy as a function of temperature for an 8^3 lattice solid (red) circles, 10^3 lattice (blue) squares and 12^3 lattice (green) diamonds. Vertical black dotted line locates the critical temperature of superfluid to normal phase transition. Results of the T-matrix theory are plotted by dashed (brown) line [25]. The inset shows extracted value of the contact density as function of the temperature. The (purple) asterisk shows the contact density from the QMC calculations of Ref. [29] at $T = 0$.

$\Gamma = \dfrac{n}{\sigma_s}$ - spin drag rate

$\sigma_s(\omega) = \pi\rho_s(q=0,\omega)/\omega$ - spin conductivity

$$G_s(q,\tau) = \frac{1}{V}\left\langle \left(\hat{j}^z_{q\uparrow}(\tau) - \hat{j}^z_{q\downarrow}(\tau)\right)\left(\hat{j}^z_{-q\uparrow}(0) - \hat{j}^z_{-q\downarrow}(0)\right)\right\rangle$$

$$G_s(q,\tau) = \int_0^\infty \rho_s(q,\omega)\frac{\cosh[\omega(\tau-\beta/2)]}{\sinh[\omega\beta/2]}d\omega$$

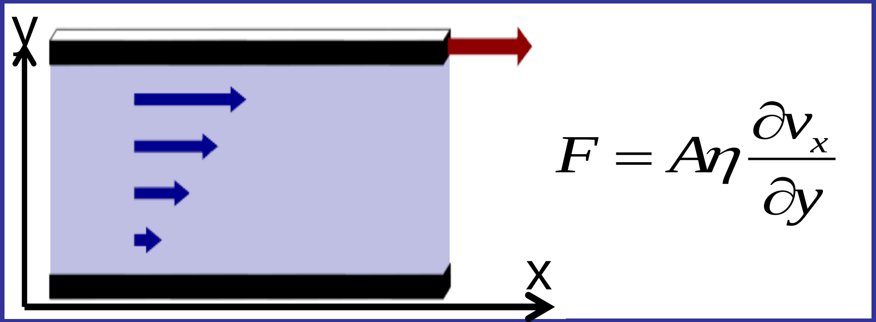
Wlazłowski, Magierski, Bulgac, Drut, Roche, Phys. Rev. Lett. 110, 090401,(2013)

Hydrodynamics at unitarity

No intrinsic length scale $\Rightarrow$ **Uniform expansion keeps the unitary gas in equilibrium**

Consequence:

uniform expansion does not produce entropy = bulk viscosity is zero!



Shear viscosity:

For any physical fluid:

$$\frac{\eta}{S} \geq \frac{\hbar}{4\pi k_B}$$

KSS conjecture
Kovtun, Son, Starinets, Phys.Rev.Lett. 94, 111601, (2005)
from AdS/CFT correspondence

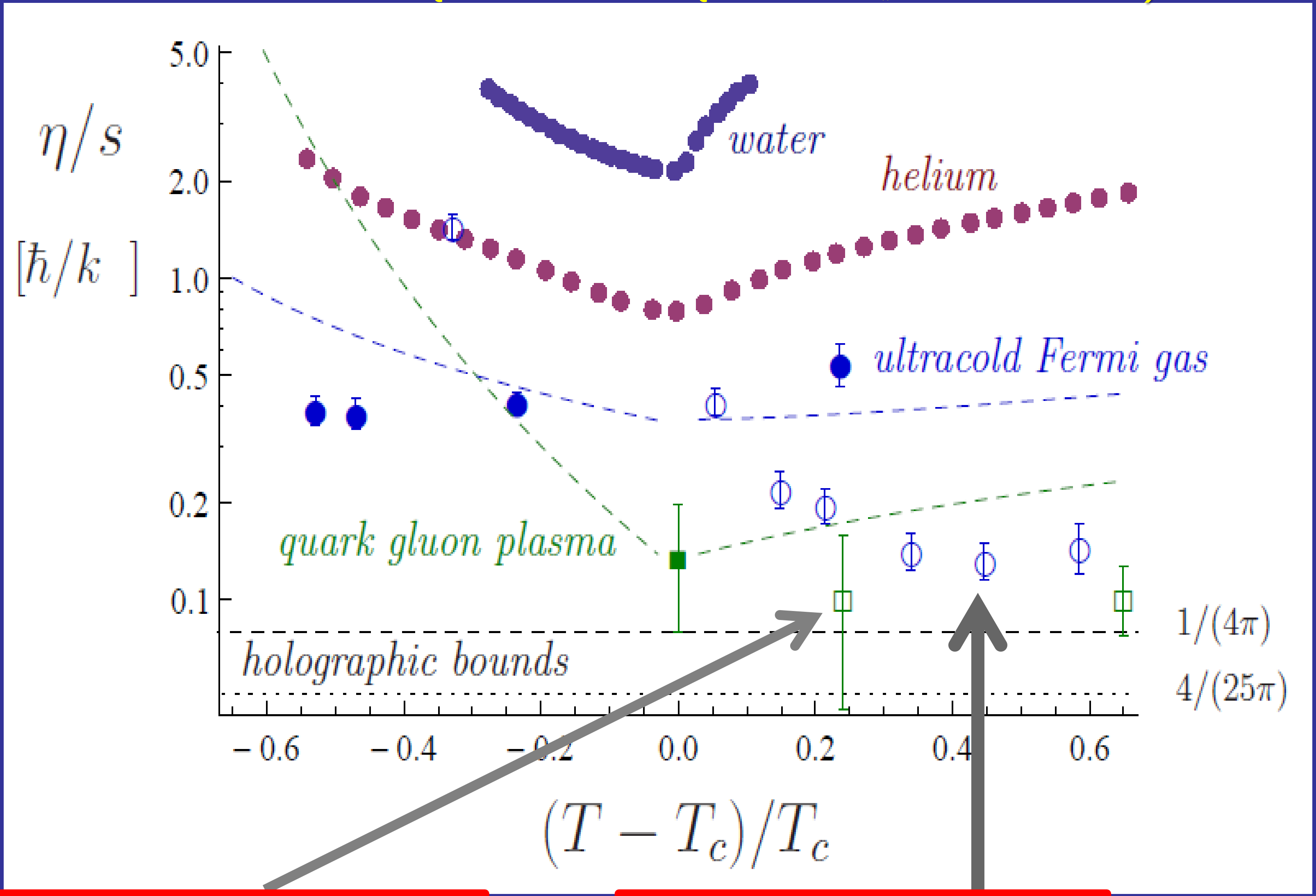
Maxwell classical estimate: [illegible]

Perfect fluid $\frac{\eta}{S} = \frac{\hbar}{4\pi k_B}$ - strongly interacting quantum system = No well defined quasiparticles

Candidates: unitary Fermi gas, quark-gluon plasma

Shear viscosity to entropy ratio – experiment vs. theory

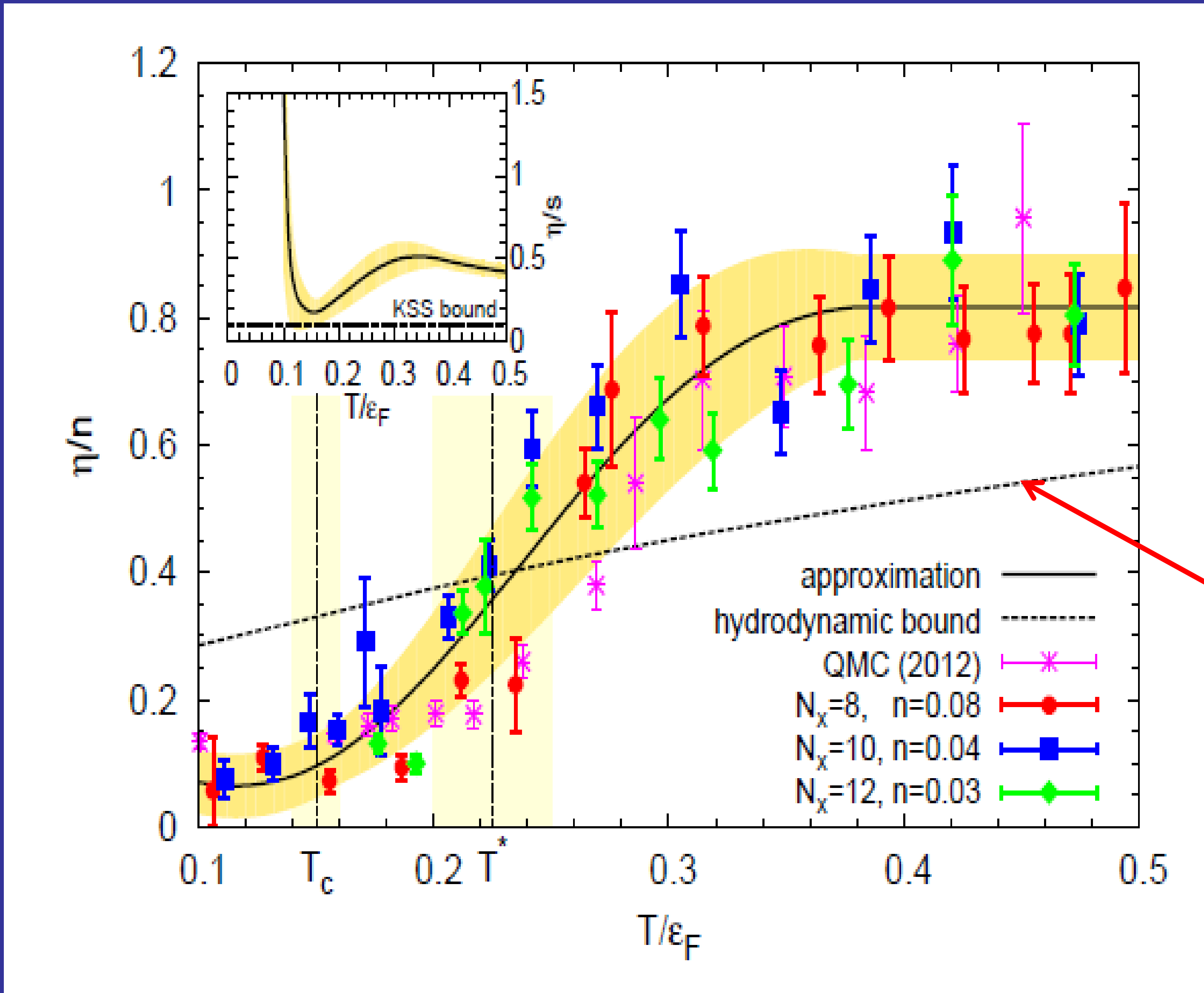
(from A. Adams et al. New Journal of Physics, "Focus on Strongly Correlated Quantum Fluids: from Ultracold Quantum Gases to QCD Plasmas„ arXive:***1205.5180)***



Lattice QCD (SU(3) gluodynamics):
H.B. Meyer, Phys. Rev. D 76, 101701 (2007)

QMC calculations for UFG:
G. Wlazłowski, P. Magierski, J.E. Drut,
Phys. Rev. Lett. 109, 020406 (2012)

Shear viscosity per unit density as a function of temperature



C. Chafin, T. Schafer, PRA87,023629(2013)
P.Romatschke, R.E. Young, arXiv:1209.1604

Wlazłowski, Magierski, Bulgac, Roche

Formalism for Time Dependent Phenomena: TDSLDA

A.K. Rajagopal and J. Callaway, Phys. Rev. B 7, 1912 (1973)
V. Peuckert, J. Phys. C 11, 4945 (1978)
E. Runge and E.K.U. Gross, Phys. Rev. Lett. 52, 997 (1984)

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

Density functional contains normal densities, anomalous density (pairing) and currents:

$$E(t) = \int d^3r \left[\varepsilon(n(\vec{r},t), \tau(\vec{r},t), \nu(\vec{r},t), \underline{\vec{j}(\vec{r},t)}) + V_{ext}(\vec{r},t)n(\vec{r},t) + \ldots \right]$$

Density functional for unitary Fermi gas

Nuclear energy functional: SLy4, SkP, SkM*,…

Both codes: SLDA and TDSLDA are formulated on the 3D lattice without any symmetry restrictions.

SLDA generates initial conditions for TDSLDA.

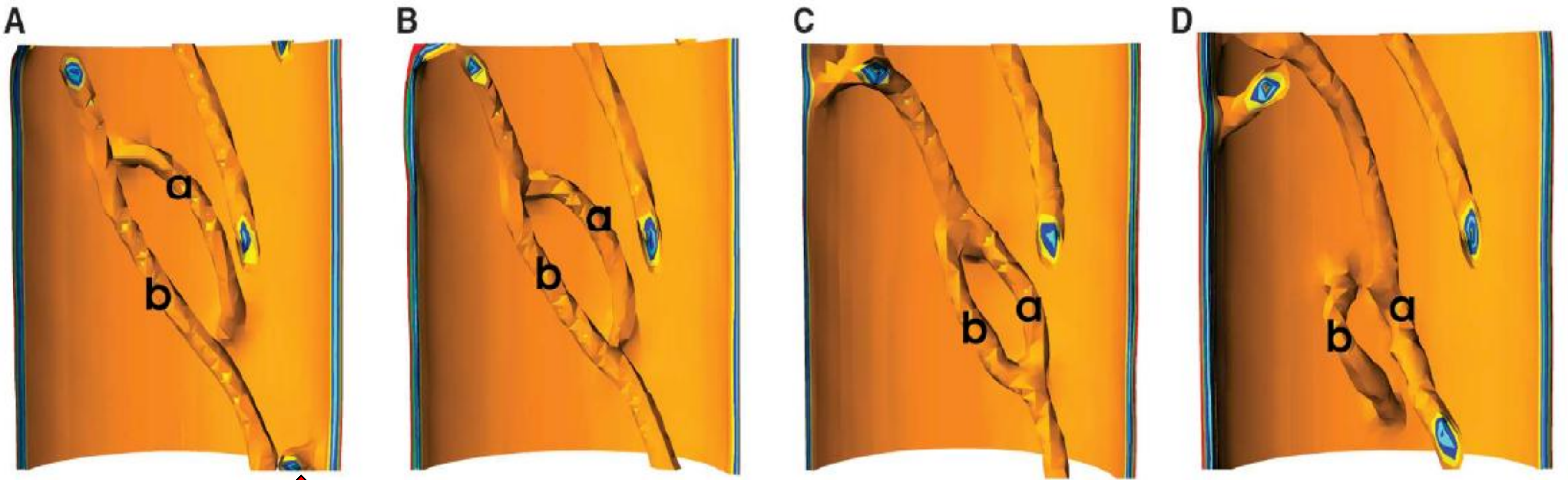
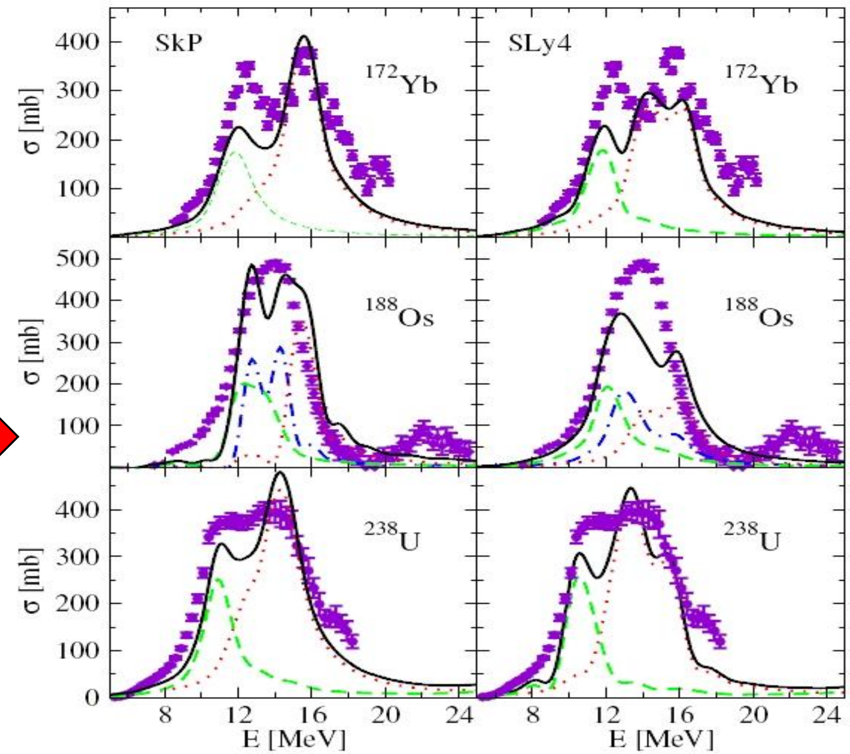


Fig. 3. (**A** to **D**) Two vortex li… …proach each other, connect at two points, form a ring and exchange between them a portion of the vortex line, and subsequently separate. Segment (a), which i… …y belonged to the vortex line attached to t…

Vortex dynamics:
Bulgac, Luo, Magierski, Roche, Yu,
Science 332, 1288 (2011)

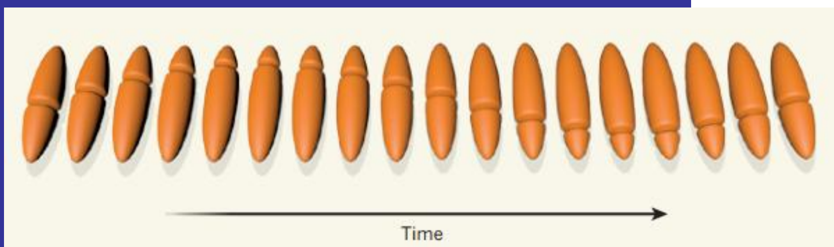
Photoabsorption cross section for heavy, deformed nuclei.

(gamma,n) reaction
through the excitation of GDR



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

Soliton dynamics vs ring vortex – a controversy



MIT Experiment:
Nature 499 (2013) 426

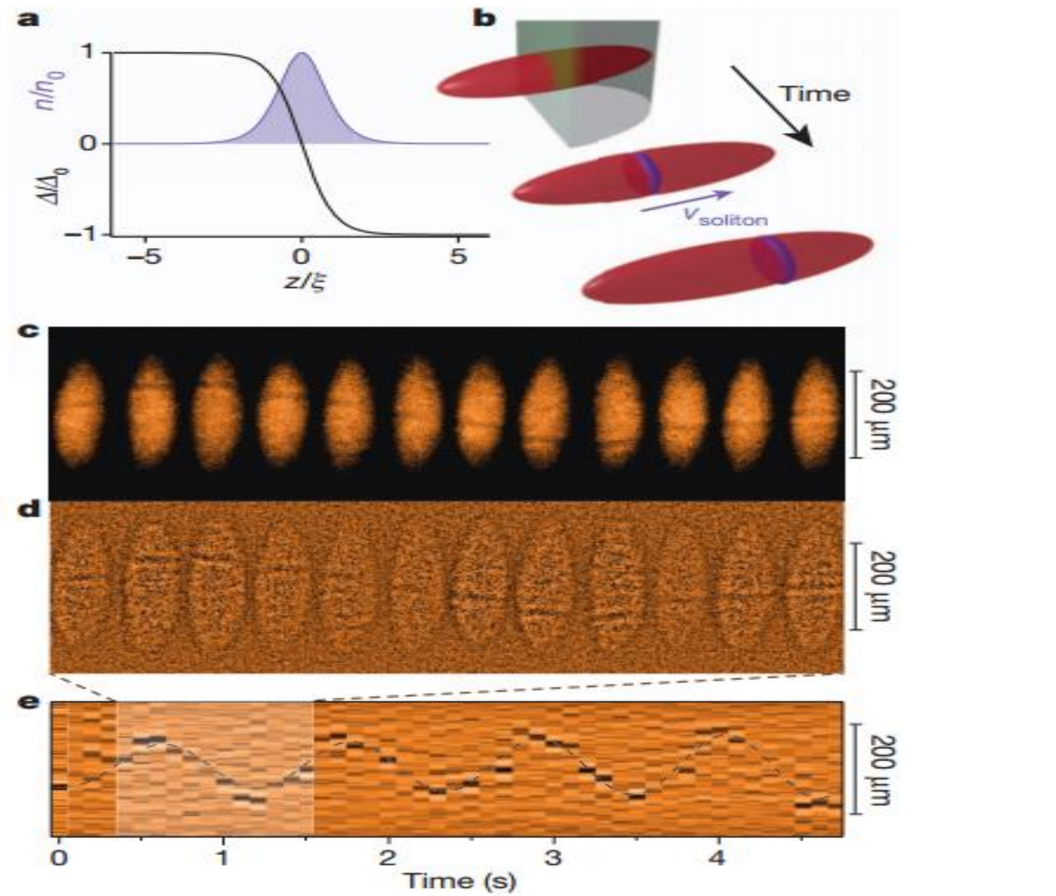


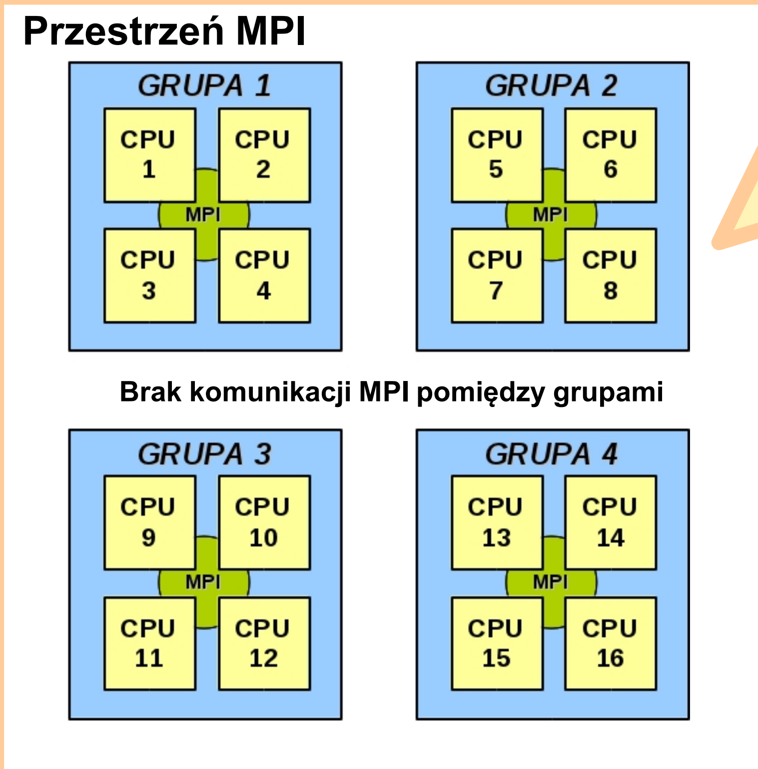
Figure 1 | Creation and observation of solitons in a fermionic superfluid. **a**, Superfluid pairing gap $\Delta(z)$ for a stationary soliton, normalized by the bulk pairing gap Δ_0, and density $n(z)$ of the localized bosonic (fermionic) state versus position z, in the BEC (BCS) regime of the crossover, 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)

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: $O(10^4)$- $O(10^6)$
- 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
- 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 for nuclear systems (a few million time steps)
- Presented calculations for unitary Fermi gas required over 200,000 cores of Titan (Oak Ridge Nat. Lab.)
- Recently the TDSLDA code for the unitary gas has been rewritten for GPUs (reaching the speed up of factor 10)

Aspekty techniczne obliczeń

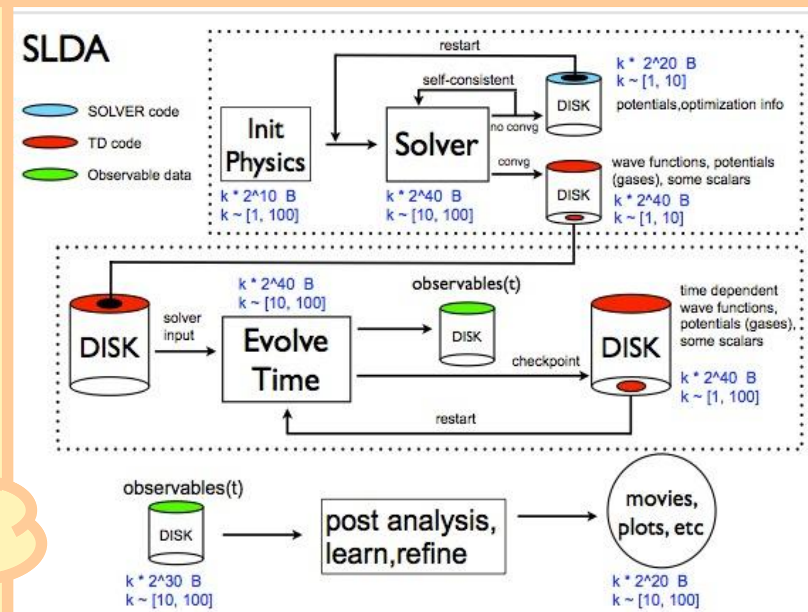


Organizacja obliczeń typu „*Kwantowe Monte Carlo*”

- ✓Przestrzeń MPI zostaje podzielona na grupy
- ✓Każda grupa niezależnie wykonuje próbkowanie Monte Carlo
- ✓ W ramach każdej grupy procesory tworzą sieć kwadratową
- ✓ Funkcje falowe oraz elementy macierzowe zostają rozdzielone pomiędzy rdzenie (*Block Cyclic Data Distribution)*
- ✓ Na koniec symulacji wyniki są zbierane z poszczególnych grup i generowany jest końcowy wynik

Komputery: halo2
Języki programowania: FOTRAN, C, C++
Biblioteki: MPI, LAPACK, FFTW,
SCALAPACK, BLACS

Organizacja obliczeń typu „***Funkcjonał gęstości***”

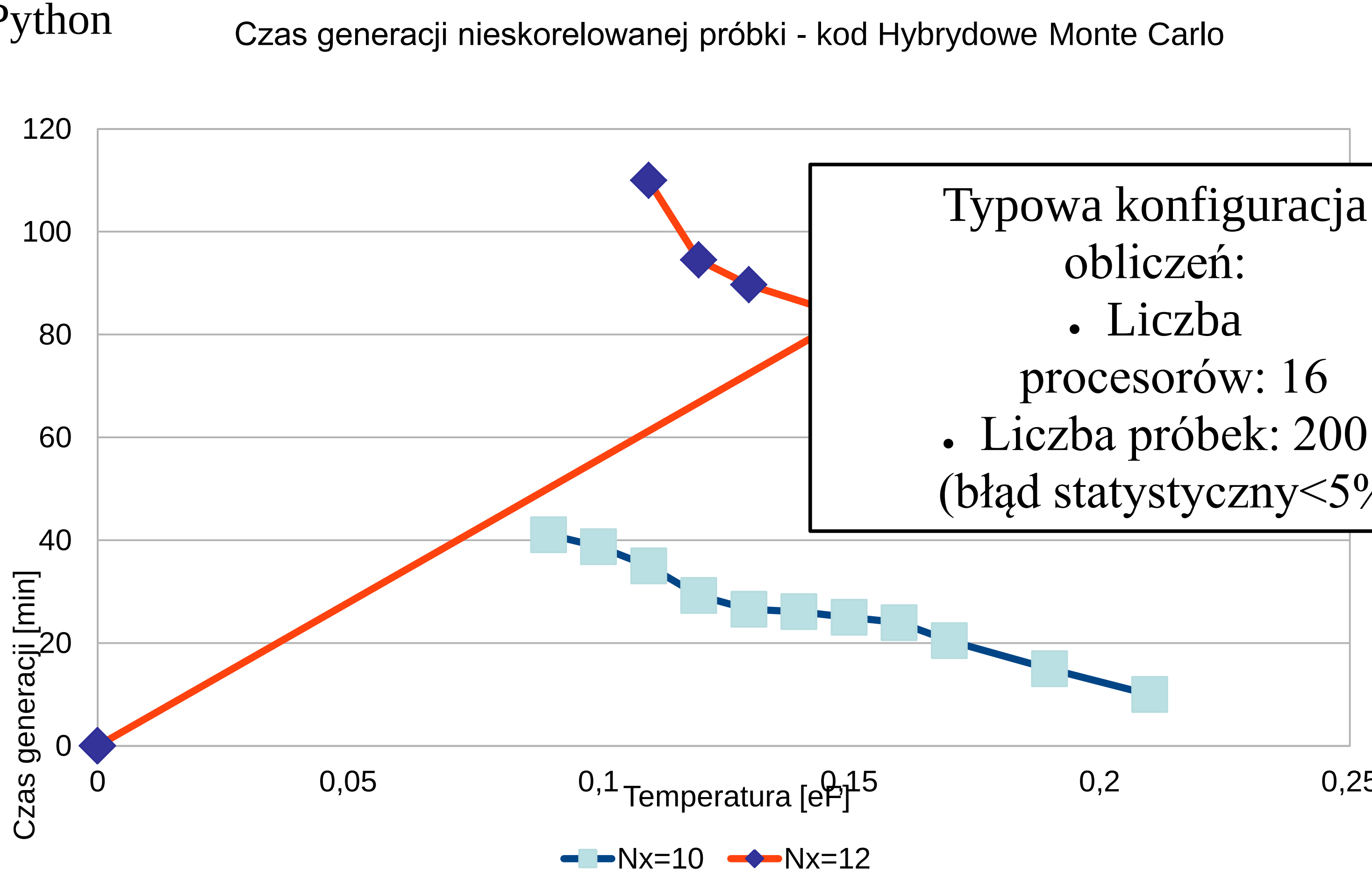


Wykorzystane oprogramowanie dla obliczeń QMC:

- Kompilator Fortran 90

  (module pgi/10.9)
- OpenMPI

  (module openmpi/1.4.2/pgi10.9)
- BLAS/LAPACK
- AMD Core Math Library (ACML)
- FFTW
- Python

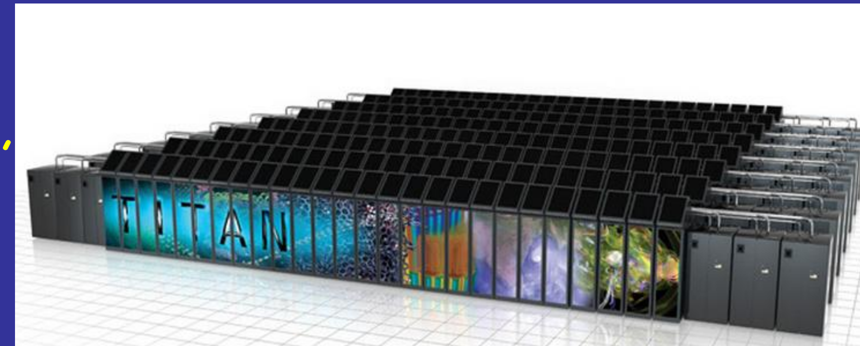


Typowa konfiguracja obliczeń:

- Liczba procesorów: 16
- Liczba próbek: 200 (błąd statystyczny<5%)

Computational resources

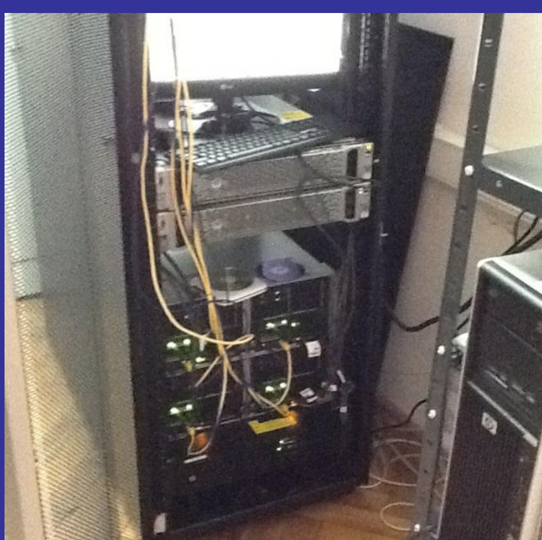
Titan, Oak Ridge USA,
Hybrid architecture (CPU+GPU),



Various CPU machines at NERSC (USA) :
mainly Edison and Hopper

icm
interdyscyplinarne centrum
modelowania matematycznego
i komputerowego

Halo2 at the moment



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)

Postdoc and doctoral positions (either for physicists or computer scientists) available at the Faculty of Physics (WUT):

Field: Nonequilibrium processes in superfluid Fermi systems: ultracold atomic gases, atomic nuclei and neutron stars.

Tools: Time dependent DFT for superfluid systems and Quantum Monte Carlo

Computational issues: Parallel programming (MPI), programming for hybrid architectures (CUDA).

Interested persons should contact Piotr Magierski,
Faculty of Physics, (email: piotrm @ uw.edu, http://nuclear.fizyka.pw.edu.pl)