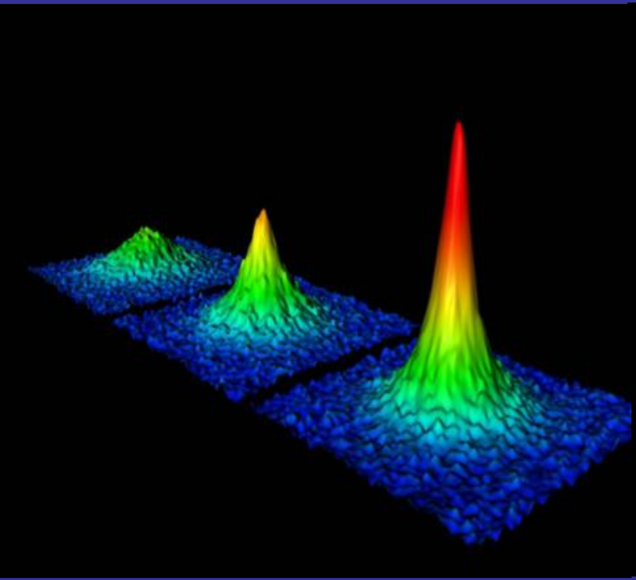
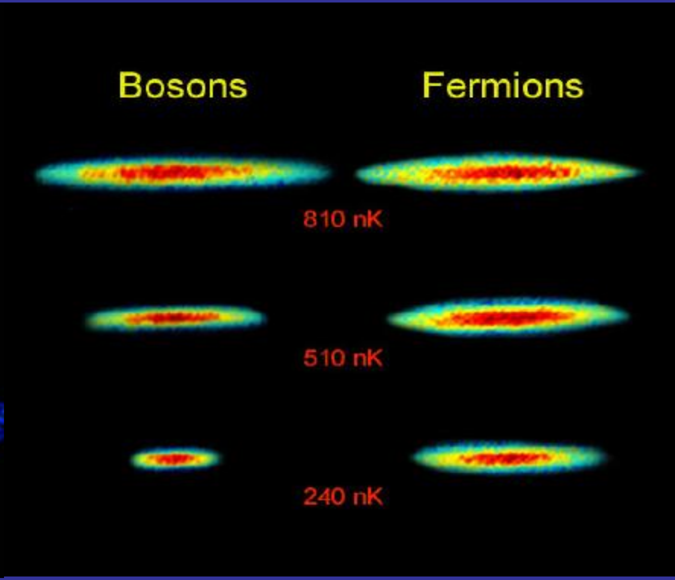
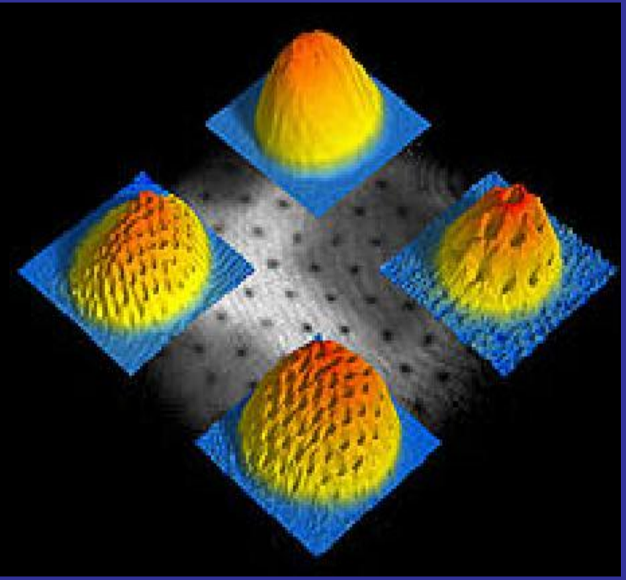
Unitarny gaz atomów – pomiędzy nadprzewodnikiem a kondensatem Bosego-Einsteina

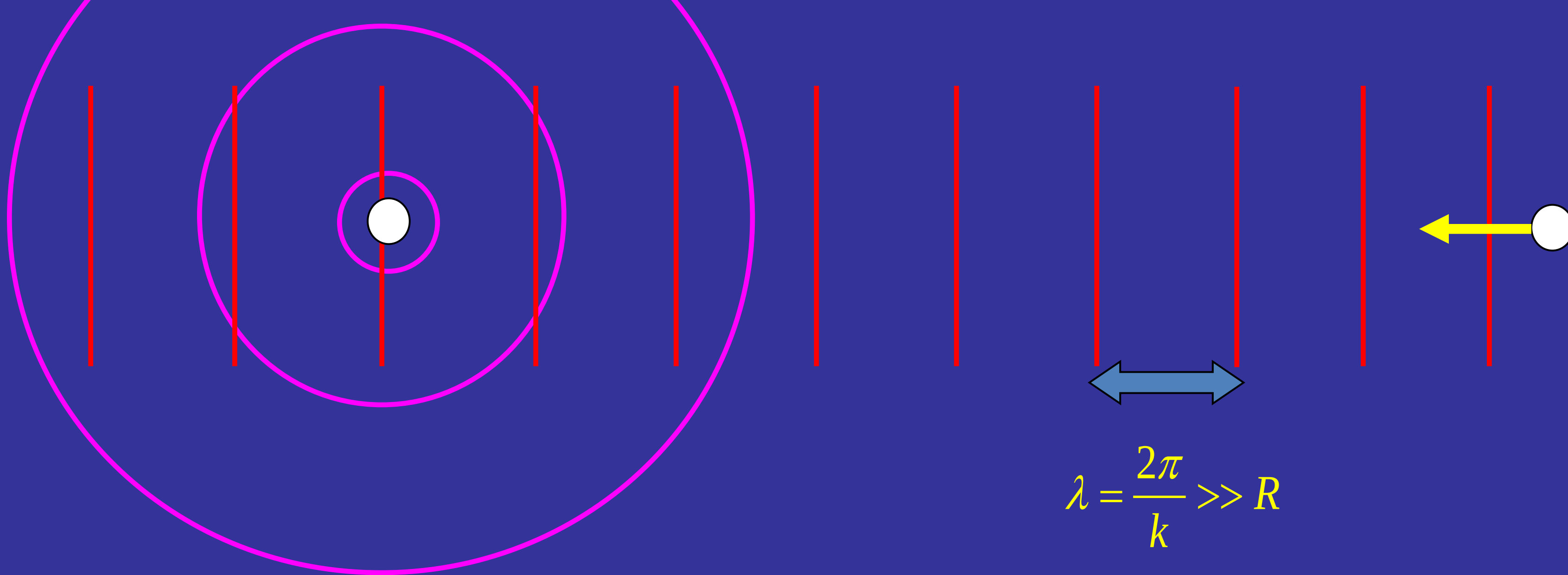






Piotr Magierski
Wydział Fizyki PW

Scattering in quantum mechanics at low energies (s-wave scattering)



$$\lambda = \frac{2\pi}{k} >> R$$

R - radius of the interaction potential

$$\psi(\vec{r}) = e^{i\vec{k}\vec{r}} + f(\theta)\frac{e^{ikr}}{r}; \quad f \text{ - scattering amplitude}$$

$$f(k) = \frac{1}{-\frac{1}{a} + \frac{1}{2} r_0 k^2 - ik}, \quad a \text{ - scattering length}, \; r_0 \text{ - effective range}$$

If $k \rightarrow 0$ then the interaction is determined by the scattering length alone.

Expected phases of a two species dilute Fermi system
BCS-BEC crossover

T

Characteristic temperature:
T_C superfluid-normal
phase transition

Strong interaction
UNITARY REGIME

Characteristic temperatures:
T_C superfluid-normal
phase transition
T^* break up of Bose molecule
$T^* > T_c$

weak interaction

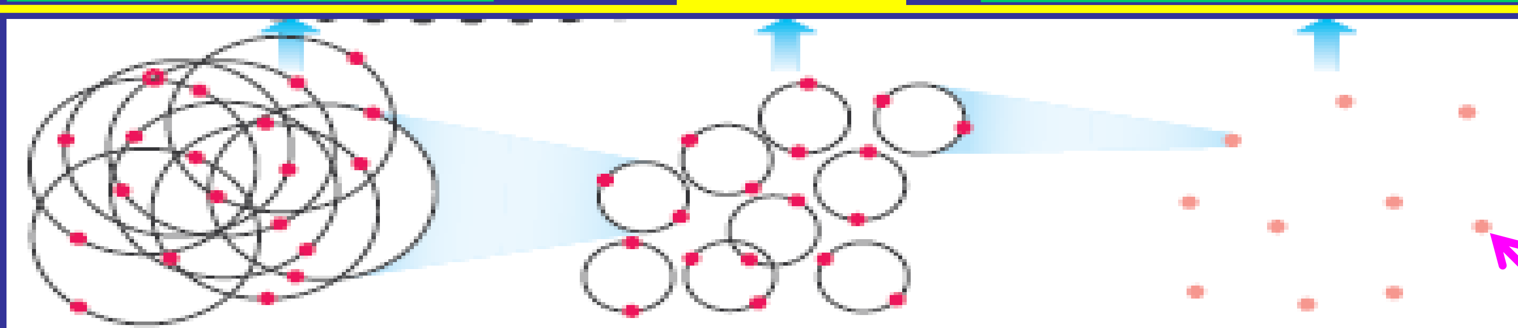
weak interactions

?

BCS Superfluid

Molecular BEC and Atomic+Molecular Superfluids

1/a



Bose molecule

a<0
no 2-body bound state

a>0
shallow 2-body bound state

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.

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

n - particle density
a - scattering length
r_0 - effective range

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

NONPERTURBATIVE REGIME

System is dilute but strongly interacting!

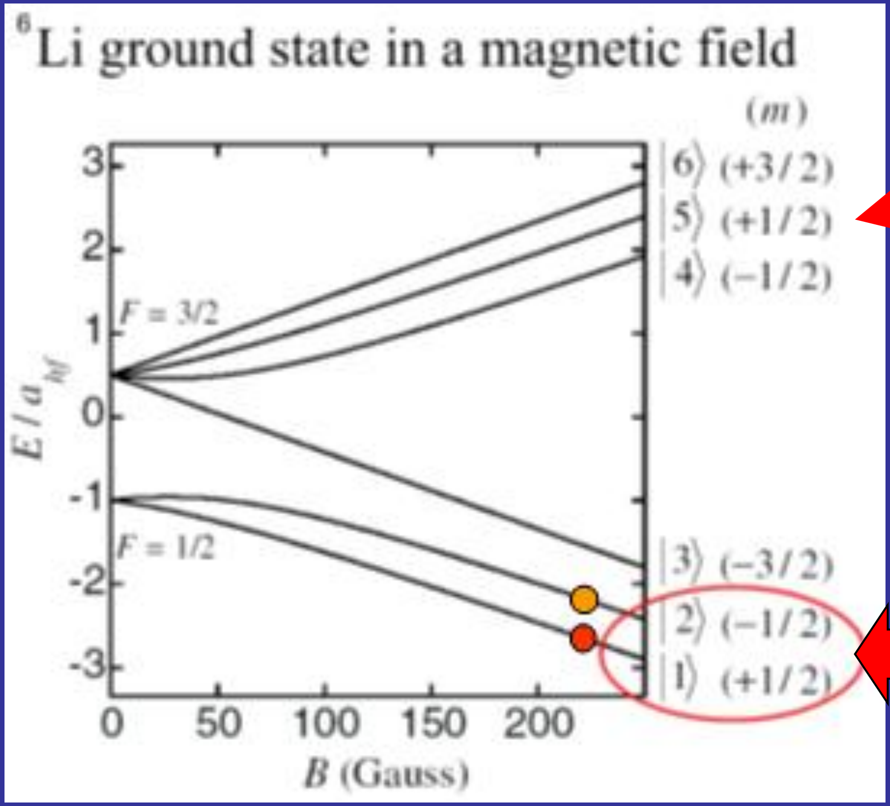
UNIVERSALITY:

$$E(T) = \xi\left(\frac{T}{\varepsilon_F}\right) E_{FG}$$

QUESTIONS:

What is the shape of $\xi(T/\varepsilon_F)$?
What is the critical temperature for the superfluid-to-normal transition?
...

One fermionic atom in magnetic field



$$\left| F \; m_F \right\rangle$$

$$\vec{F} = \vec{I} + \vec{J} \; ; \; \vec{J} = \vec{L} + \vec{S}$$

Nuclear spin Electronic spin

Two hypefine states are populated in the trap

Collision of two atoms:

At low energies (low density of atoms) only L=0 (s-wave) scattering is effective.

- Due to the high diluteness atoms in the same hyperfine state do not interact with one another.
- Atoms in different hyperfine states experience interactions only in s-wave.

Effective Hamiltonian of an atom-atom system

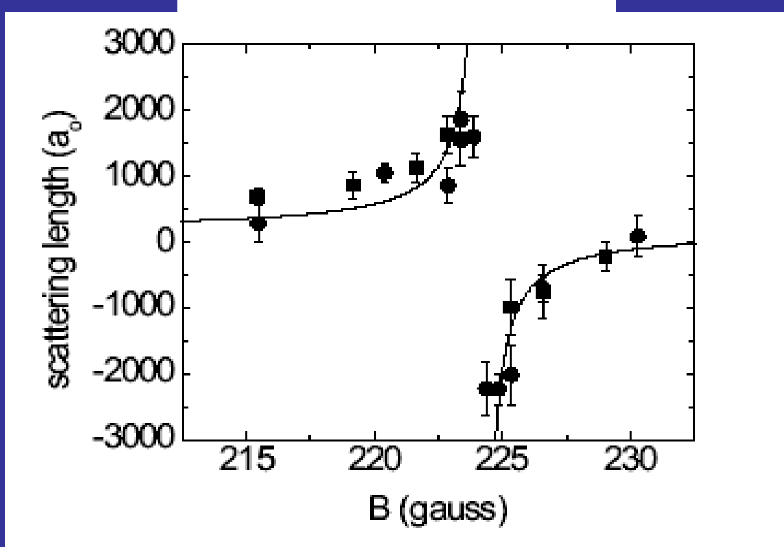
$$H = \frac{\vec{p}^{\,2}}{2\mu} + \sum_{i=1}^{2} \left(V_i^{hf} + V_i^{Z}\right) + V_0(\vec{r})P_0 + V_1(\vec{r})P_1 + \ldots$$

$$V^{hf} = \frac{a_{hf}}{\hbar^2}\vec{I}\cdot\vec{J},\ V_i - \text{Coulomb term}$$

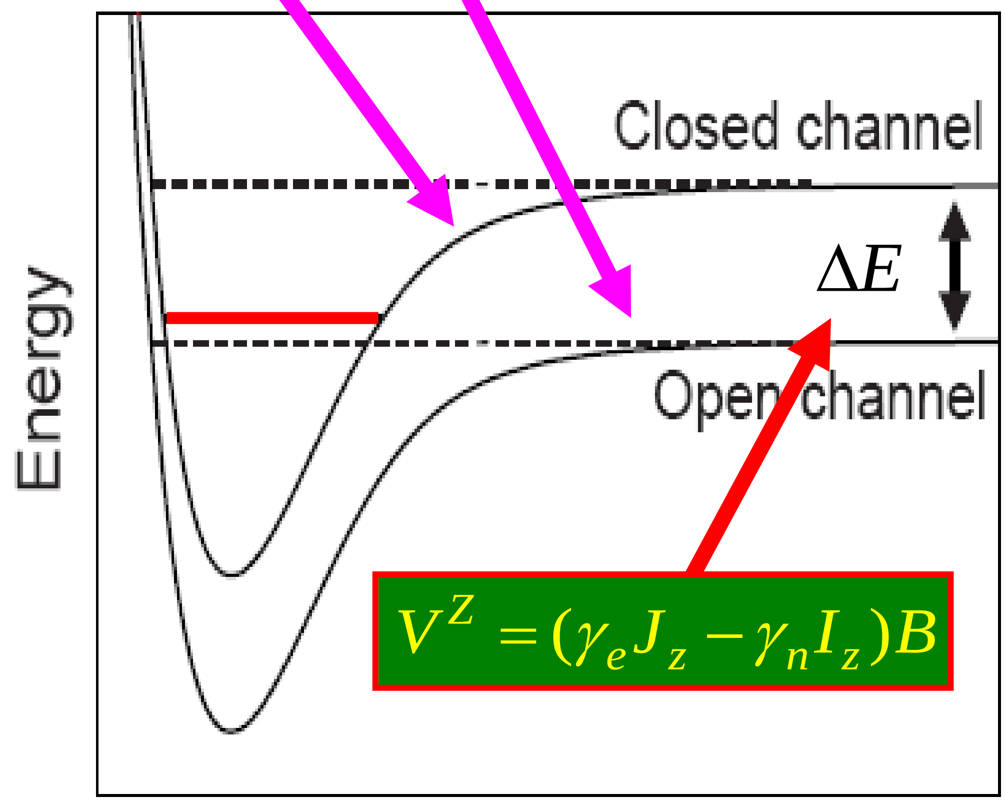
Tiesinga, Verhaar, Stoof, Phys. Rev. A<u>47</u>, 4114 (1993)

Channel coupling

Feshbach resonance



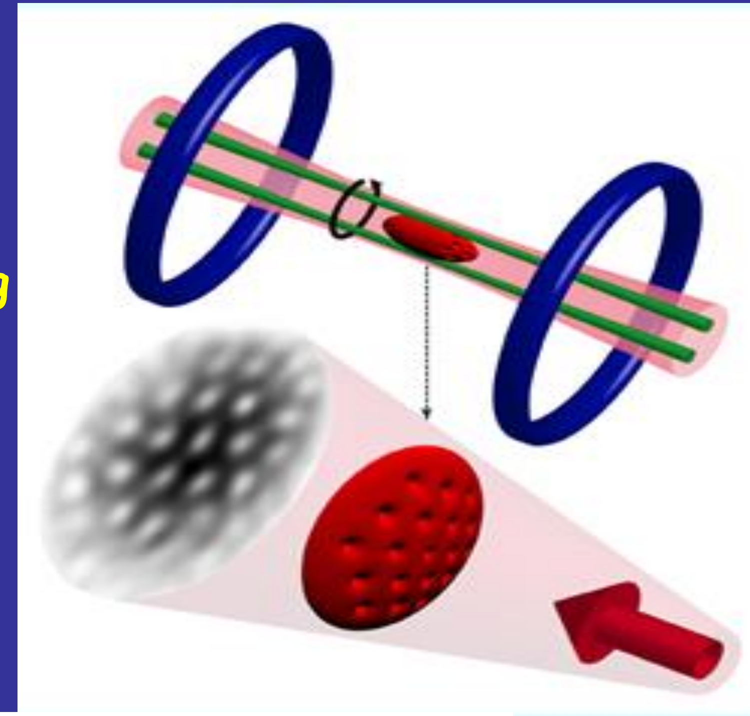
Regal and Jin, PRL <u>90</u>, 230404 (2003)



Interatomic distance

Short (selective) history:

- ✓In 1999 DeMarco and Jin created a degenerate atomic Fermi gas.
- ✓In 2005 Zwierlein/Ketterle group observed quantum vortices which survived when passing from BEC to unitarity – evidence for superfluidity!

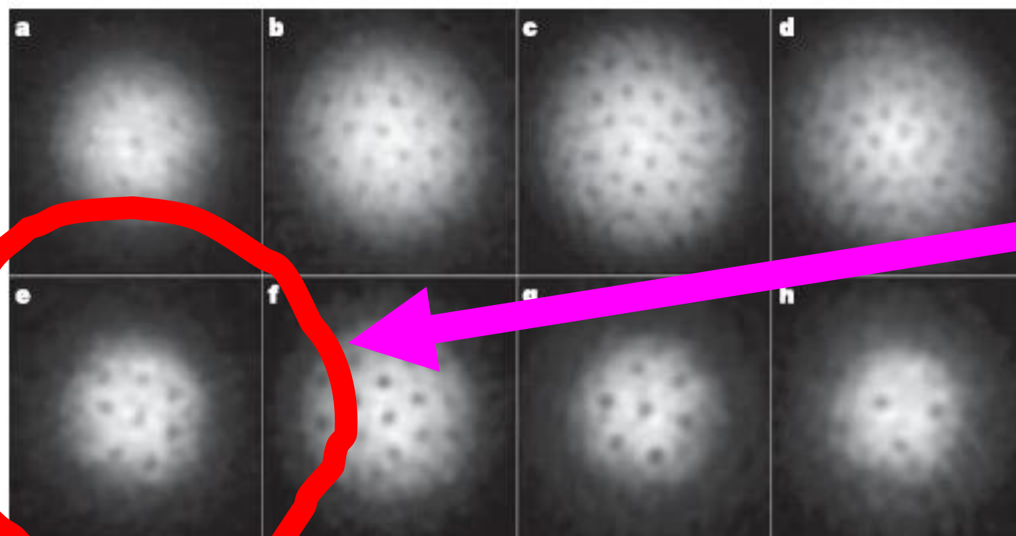


system of fermionic ^6Li atoms

Feshbach resonance: B=834G

BEC side: a>0

BCS side: a<0



UNITARY REGIME

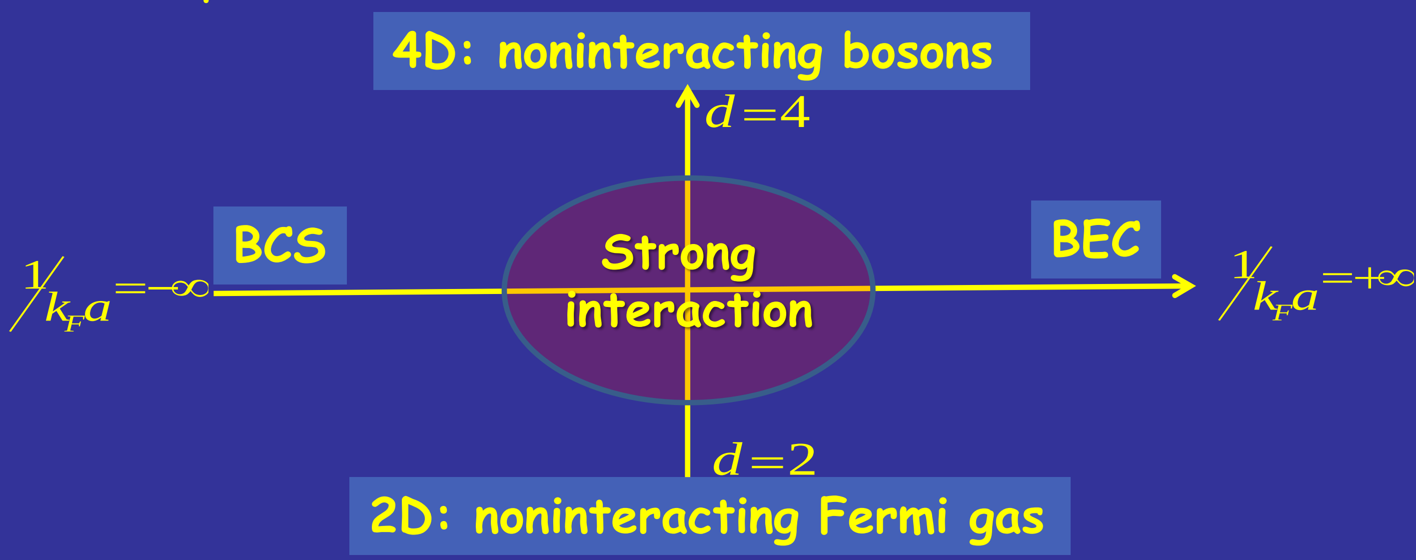
Figure 2 | Vortices in a strongly [illegible] fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (**a**) or 500 ms (**b**–**h**) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, the magnetic field was ramped to 735 G for imaging ([illegible] magnetic fields were 740 G (**a**), 766 G (**b**), 792 G ([illegible] 843 G (**f**), 853 G (**g**) and 863 G (**h**). The field of vie[illegible] 880 μm × 880 μm.

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

Unitary limit in 2 and 4 dimensions:

Intuitive arguments:

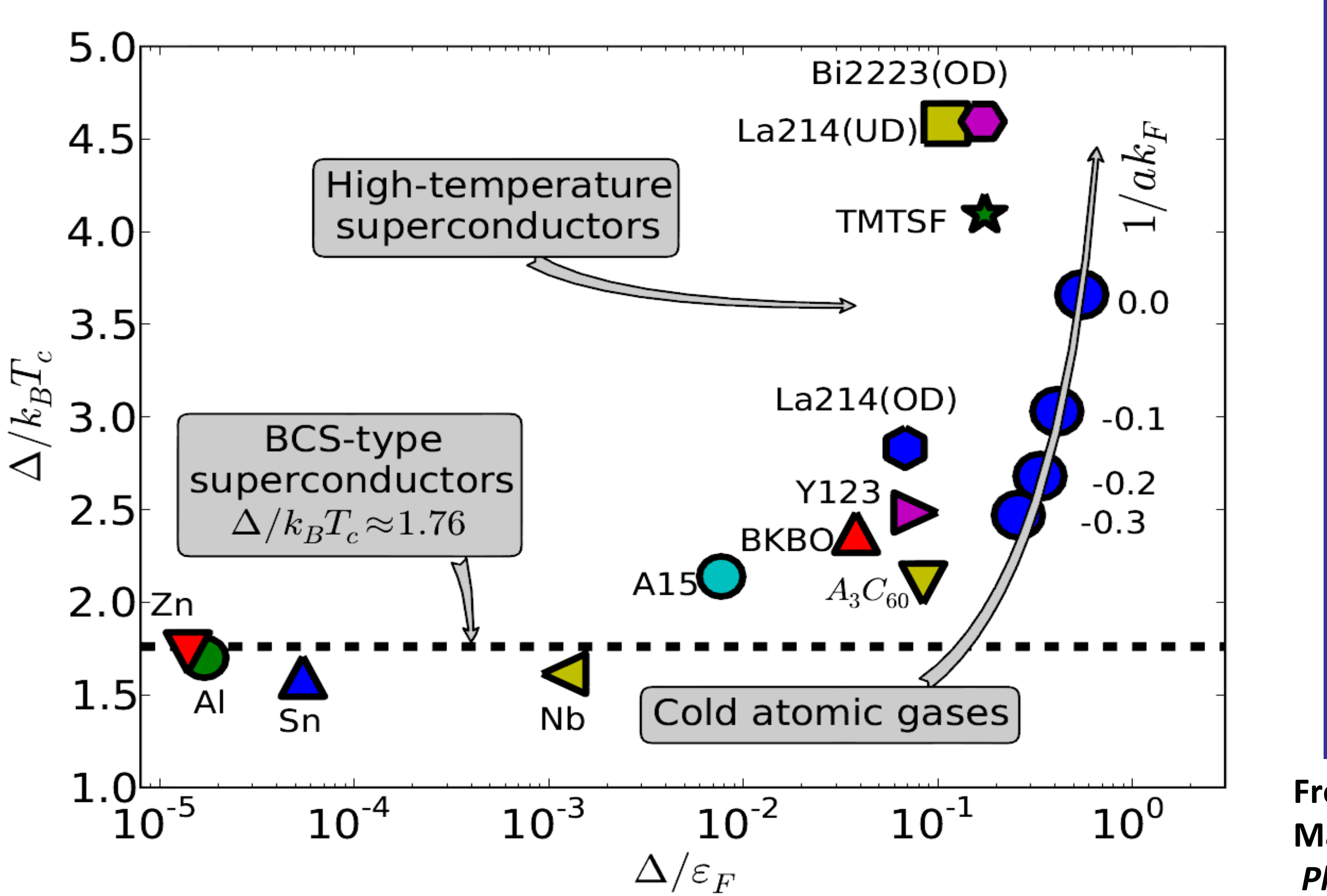
- For d=4 $\int R(r)^2 d^d r$ diverges at the origin
- For d=2 the singularity of the wave function disapears = interaction also disapears.



The only nontrivial case of unitary regime is in 3D

Nussinov,Nussinov, Phys.Rev. A74, 053622(2006)

Cold atomic gases and high Tc superconductors



From:
Magierski, Wlazłowski, Bulgac, *Phys. Rev. Lett.* 107,145304(2011)

Δ/ε_F – Ratio of the strength of two interparticle correlations to the kinetic energy of the fastest particle in the system.

Standard theory of superconductivity (BCS theory) fails!
Qualitatively new phenomena occur like e.g. <u>pseudogap characteristic for high-Tc superconductors</u>

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

Hamiltonian

$$\hat{H} = \hat{T} + \hat{V} = \int d^3r \sum_{s=\uparrow\downarrow} \hat{\psi}_s^\dagger(\vec{r}) \left(-\frac{\hbar^2 \Delta}{2m} \right) \hat{\psi}_s(\vec{r}) \; - \; g \int d^3r \; \hat{n}_\uparrow(\vec{r}) \hat{n}_\downarrow(\vec{r})$$

$$\hat{N} = \int d^3r \; \left(\hat{n}_\uparrow(\vec{r}) + \hat{n}_\downarrow(\vec{r}) \right); \;\; \hat{n}_s(\vec{r}) = \hat{\psi}_s^\dagger(\vec{r}) \hat{\psi}_s(\vec{r})$$

Path Integral Monte Carlo for fermions on 3D lattice

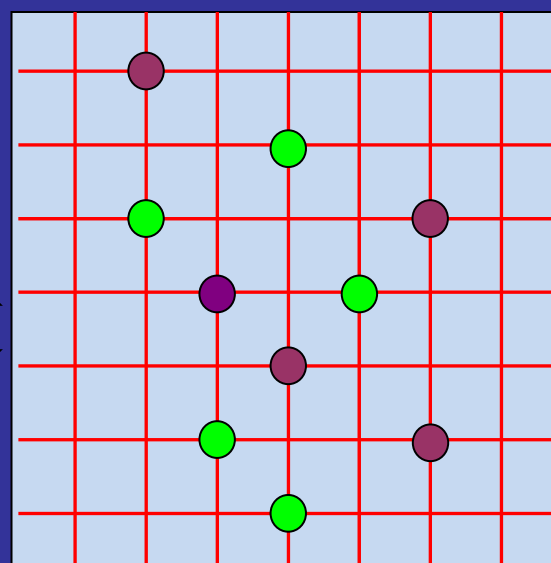
$$Volume = L^3$$

$$lattice\ spacing = \Delta x$$

Coordinate space

L –limit for the spatial correlations in the system

$$k_{cut} = \frac{\pi}{\Delta x} \; ; \;\; \Delta x$$



- Spin up fermion:

- Spin down fermion:

External conditions:

T - temperature

μ - chemical potential

Periodic boundary conditions imposed

Hamiltonian

$$\hat{H} = \hat{T} + \hat{V} = \int d^3r \sum_{s=\uparrow\downarrow} \hat{\psi}_s^{\dagger}(\vec{r}) \left(-\frac{\hbar^2 \Delta}{2m} \right) \hat{\psi}_s(\vec{r}) \; - \; g \int d^3r \; \hat{n}_{\uparrow}(\vec{r}) \hat{n}_{\downarrow}(\vec{r})$$

$$\hat{N} = \int d^3r \; \left(\hat{n}_{\uparrow}(\vec{r}) + \hat{n}_{\downarrow}(\vec{r}) \right); \;\; \hat{n}_s(\vec{r}) = \hat{\psi}_s^{\dagger}(\vec{r}) \hat{\psi}_s(\vec{r})$$

$$\frac{1}{g} = -\frac{m}{4\pi\hbar^2 a} + \frac{m k_{cut}}{2\pi^2\hbar^2}$$

Running coupling constant g defined by lattice

$$\frac{1}{g} = \frac{m}{2\pi\hbar^2 \Delta x}$$ - UNITARY LIMIT

Grand-canonical ensemble:

$$E(T) = \langle \hat{H} \rangle = \frac{1}{Z(T)} Tr \left\{ \hat{H} \rho(\hat{H}, \hat{N}, T) \right\} = \frac{1}{Z} \sum_n E_n e^{-\frac{1}{kT}(E_n - \mu N_n)}$$

$$Z(T) = Tr \left\{ \rho(\hat{H}, \hat{N}, T) \right\} = \sum_n e^{-\frac{1}{kT}(E_n - \mu N_n)}; \;\; \rho(\hat{H}, \hat{N}, T) = e^{-\frac{1}{kT}(\hat{H} - \mu \hat{N})}$$

Eigenenergies of the Hamiltonian are unknown!

Basics of Auxiliary Field Monte Carlo (Path Integral MC)

$$Z(\beta) = Tr\left\{\exp(-\beta(\hat{H} - \mu\hat{N})\right\} = \sum_{\substack{n-many \\ body\ states}} \left\langle n \middle| \exp(-\beta(\hat{H} - \mu\hat{N}) \middle| n \right\rangle$$

$\beta = 1/kT$; imaginary time: $\tau = it$

$$Z(\beta) = \int D\left[\sigma(\vec{r},\tau)\right]\ e^{\ln\{\det[1+\hat{U}(\{\sigma\})]\}}$$

$$S[\sigma(\vec{r},\tau)] = -\ln\{\det[1 + \hat{U}(\{\sigma\})]\}$$ - action

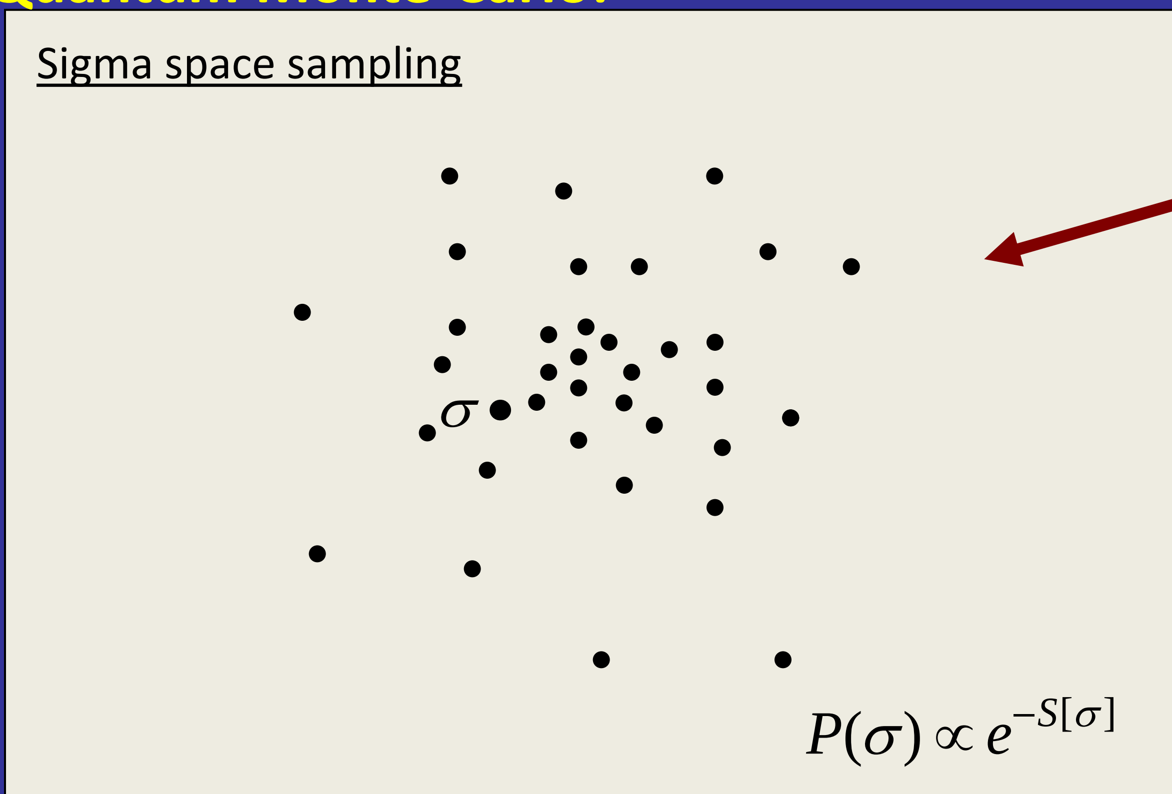
$$\hat{U}(\{\sigma\}) = T_\tau \exp\{-\int_0^\beta d\tau[\hat{h}(\{\sigma\}) - \mu]\};\ \hat{h}(\{\sigma\}) - \text{one-body operator}$$

$$U(\{\sigma\})_{kl} = \langle \psi_k | \hat{U}(\{\sigma\}) | \psi_l \rangle; \quad |\psi_l\rangle \text{- single-particle wave function}$$

$$E(T) = \langle \hat{H} \rangle = \int \frac{D[\sigma(\vec{r},\tau)] e^{-S[\sigma]}}{Z(T)} E[U(\{\sigma\})]$$

$E[U(\{\sigma\})]$- energy associated with a given sigma field

Quantum Monte-Carlo:



$$\bar{E}(T) = \frac{1}{N_\sigma} \sum_{k=1}^{N_\sigma} E\left(U(\{\sigma_k\})\right)$$

$\bar{E}(T)$ - stochastic variable

$\langle \bar{E}(T) \rangle = E(T)$

$\sqrt{\langle \bar{E}(T)^2 \rangle - \langle \bar{E}(T) \rangle^2} \propto 1/\sqrt{N_\sigma}$

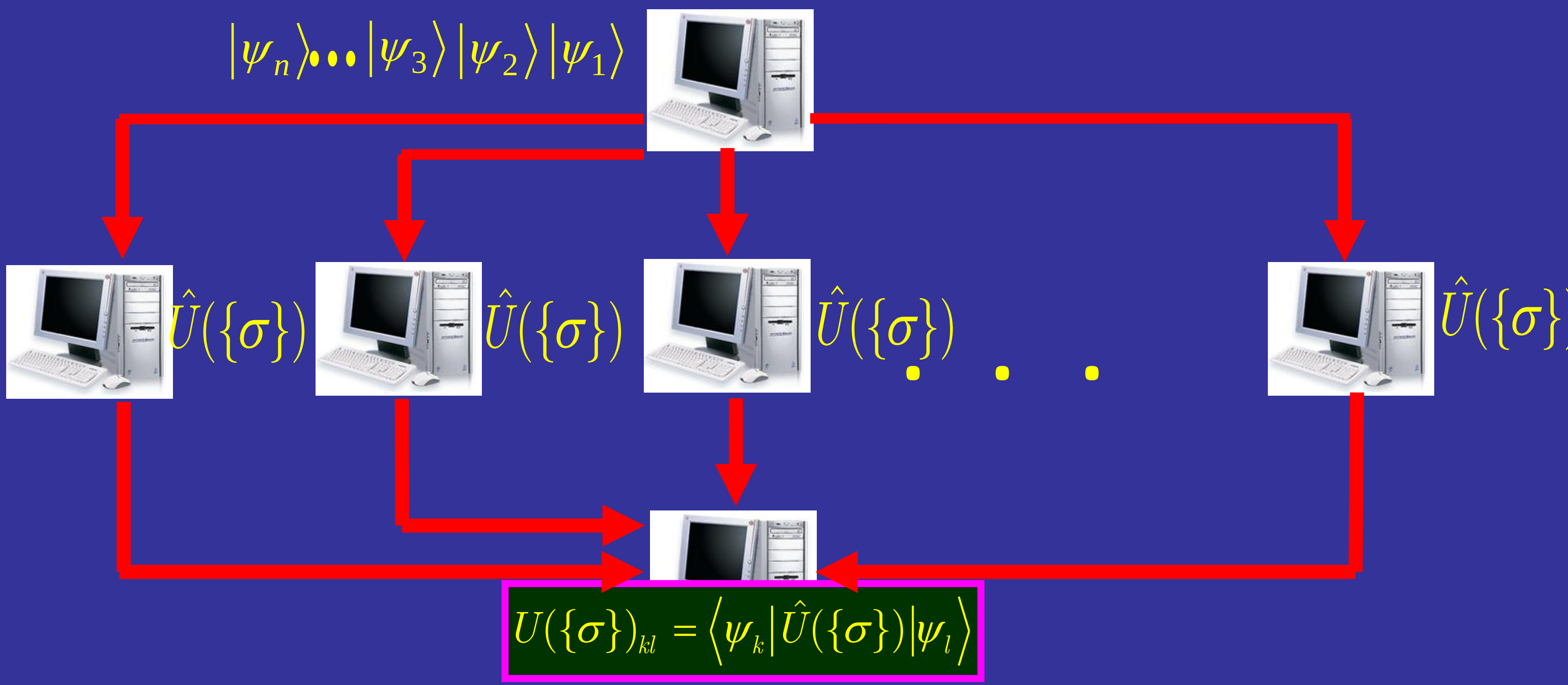
N_σ - number of uncorrelated samples

Quantum Monte-Carlo: parallel computing

$$\hat{U}(\{\sigma\}) = T_\tau \exp\{-\int_0^\beta d\tau[\hat{h}(\{\sigma\}) - \mu]\};\ \hat{h}(\{\sigma\}) - \text{one-body operator}$$

$$U(\{\sigma\})_{kl} = \langle \psi_k | \hat{U}(\{\sigma\}) | \psi_l \rangle; \quad |\psi_l\rangle \text{- single-particle wave function}$$

For each sigma *n* single particle states have to be evolved.



Details of calculations, improvements and problems

- Currently we can reach 16^3 lattice and perform calcs. down to x = 0.06 (x – temperature in Fermi energy units) at the densities of the order of 0.03.

- Effective use of FFT(W) makes all imaginary time propagators diagonal (either in real space or momentum space) and there is no need to store large matrices.

- Update field configurations using the Metropolis importance sampling algorithm. QMC calculations can be split into two independent processes:
  1) sample generation (generation of sigma fields),
  2) calculations of observables.

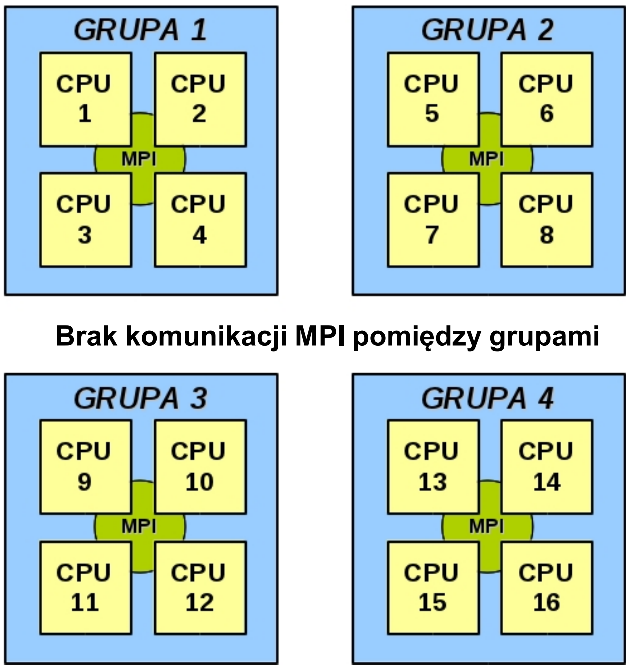
- Change randomly at a fraction of all space and time sites the signs the auxiliary fields $\sigma(r,\tau)$ so as to maintain a running average of the acceptance rate between 0.4 and 0.6 .

- At low temperatures use Singular Value Decomposition of the evolution operator $U(\{\sigma\})$ to stabilize the numerics.

- MC correlation "time" ≈ 200 time steps at $T \approx T_c$ for lattices 10^3 . Unfortunately when increasing the lattice size the correlation time also increases. One needs few thousands uncorrelated samples (we usually take about 10 000) to decrease the statistical error to the level of 1%.

Aspekty techniczne obliczeń

Przestrzeń MPI



Komputery: halo2
Języki programowania: FOTRAN, C, C++
Biblioteki: MPI, LAPACK, FFTW, SCALAPACK, BLACS
Zużycie CPU (2012): 1,211,673

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

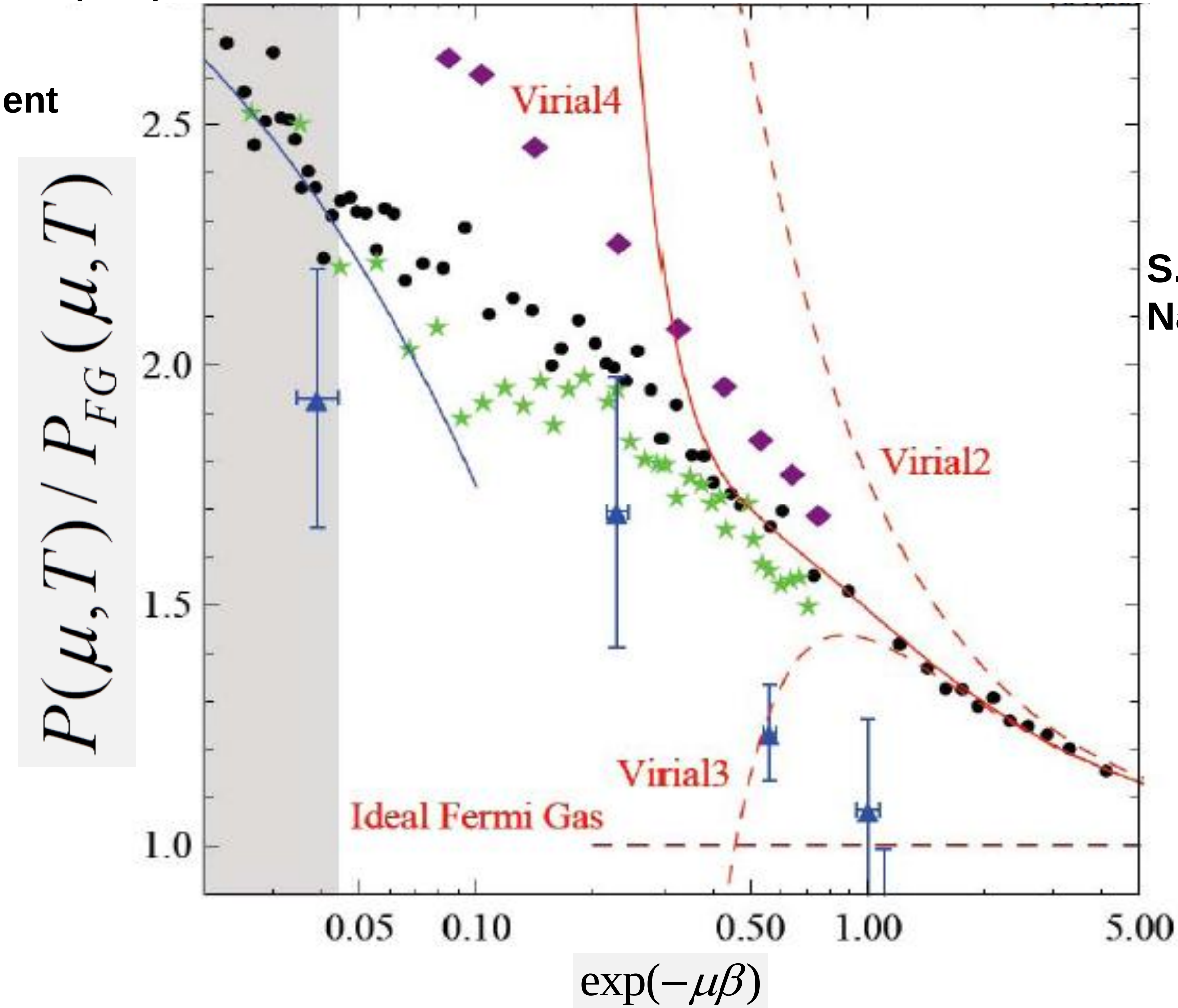
Comparison with Many-Body Theories (1)

▲ **Diagram. MC**
Burovski et al.
PRL96, 160402(2006)

★ **QMC**
Bulgac, Drut, Magierski,
PRL99, 120401(2006)

◆ **Diagram. + analytic**
Haussmann et al.
PRA75, 023610(2007)

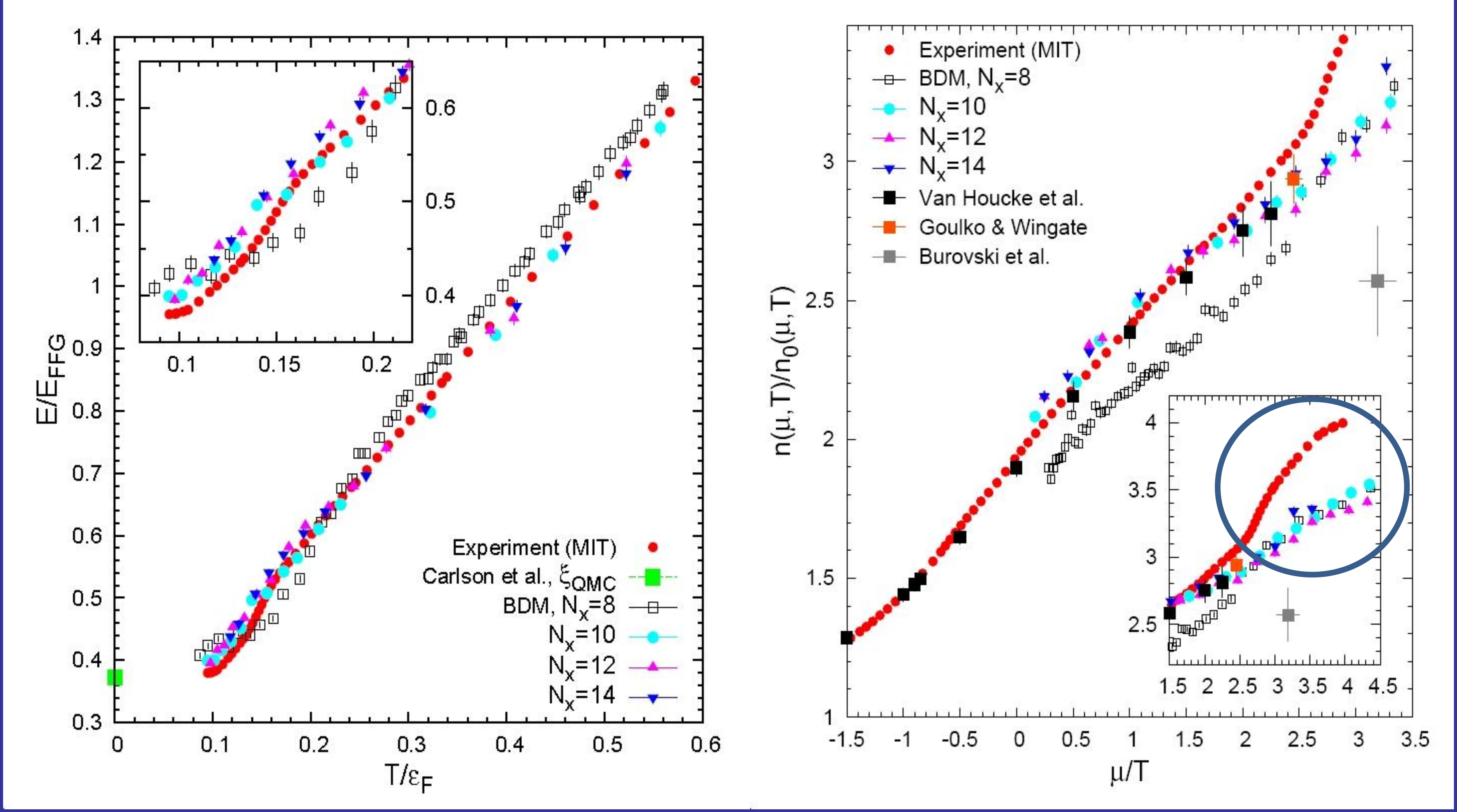
● **Experiment**



S. Nascimbene et al.
Nature 463, 1057 (2010)

Courtesy of C. Salomon

Equation of state of the unitary Fermi gas - current status



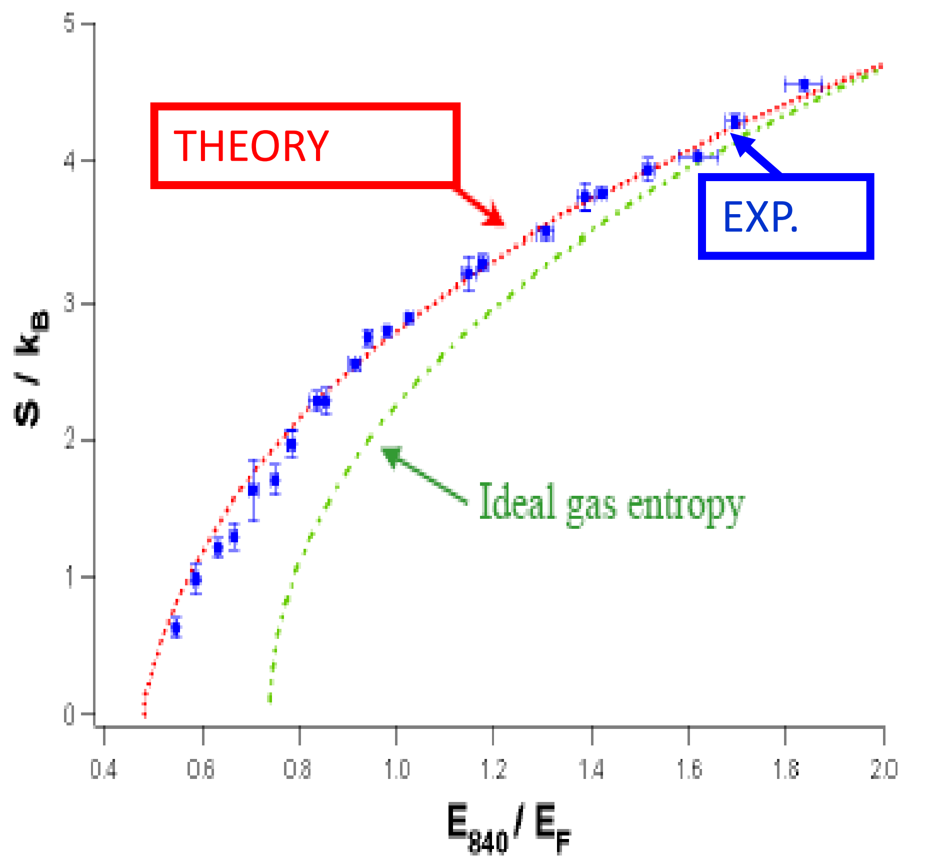
Experiment: M.J.H. Ku, A.T. Sommer, L.W. Cheuk, M.W. Zwierlein , Science 335, 563 (2012)

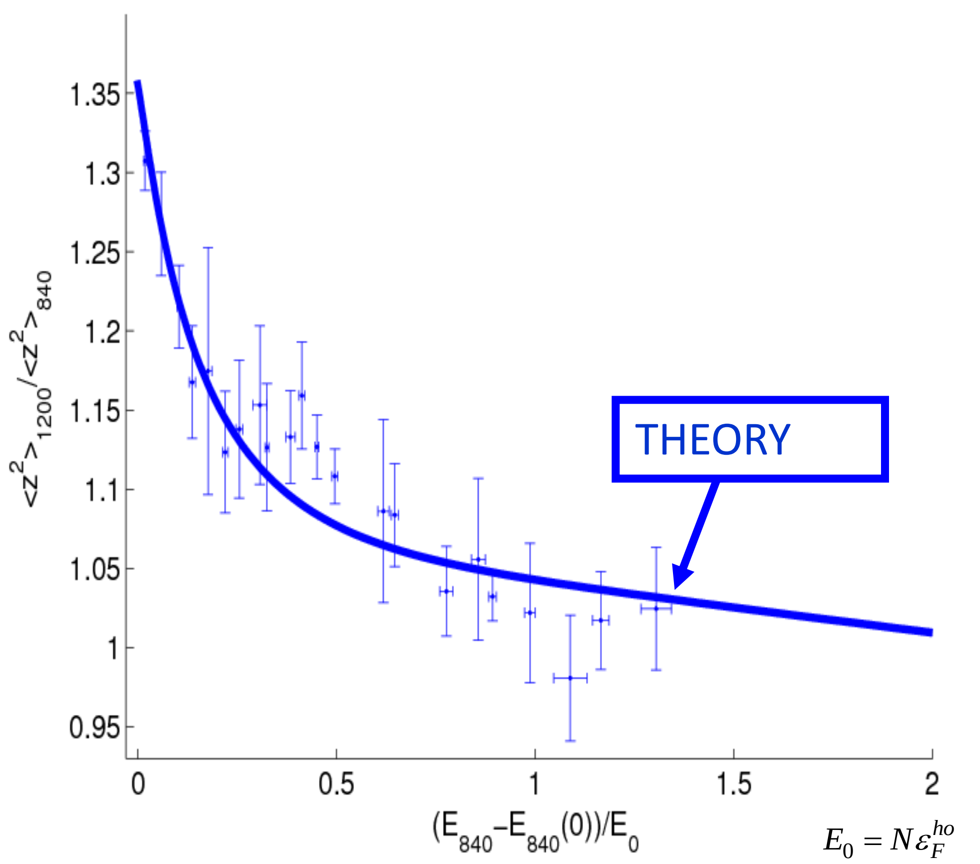
QMC (PIMC + Hybrid Monte Carlo): J.E.Drut, T.Lähde, G.Wlazłowski, P.Magierski, Phys. Rev. A 85, 051601 (2012)

Comparison with experiment

John Thomas' group at Duke University,

L.Luo, et al. Phys. Rev. Lett. 98, 080402, (2007)



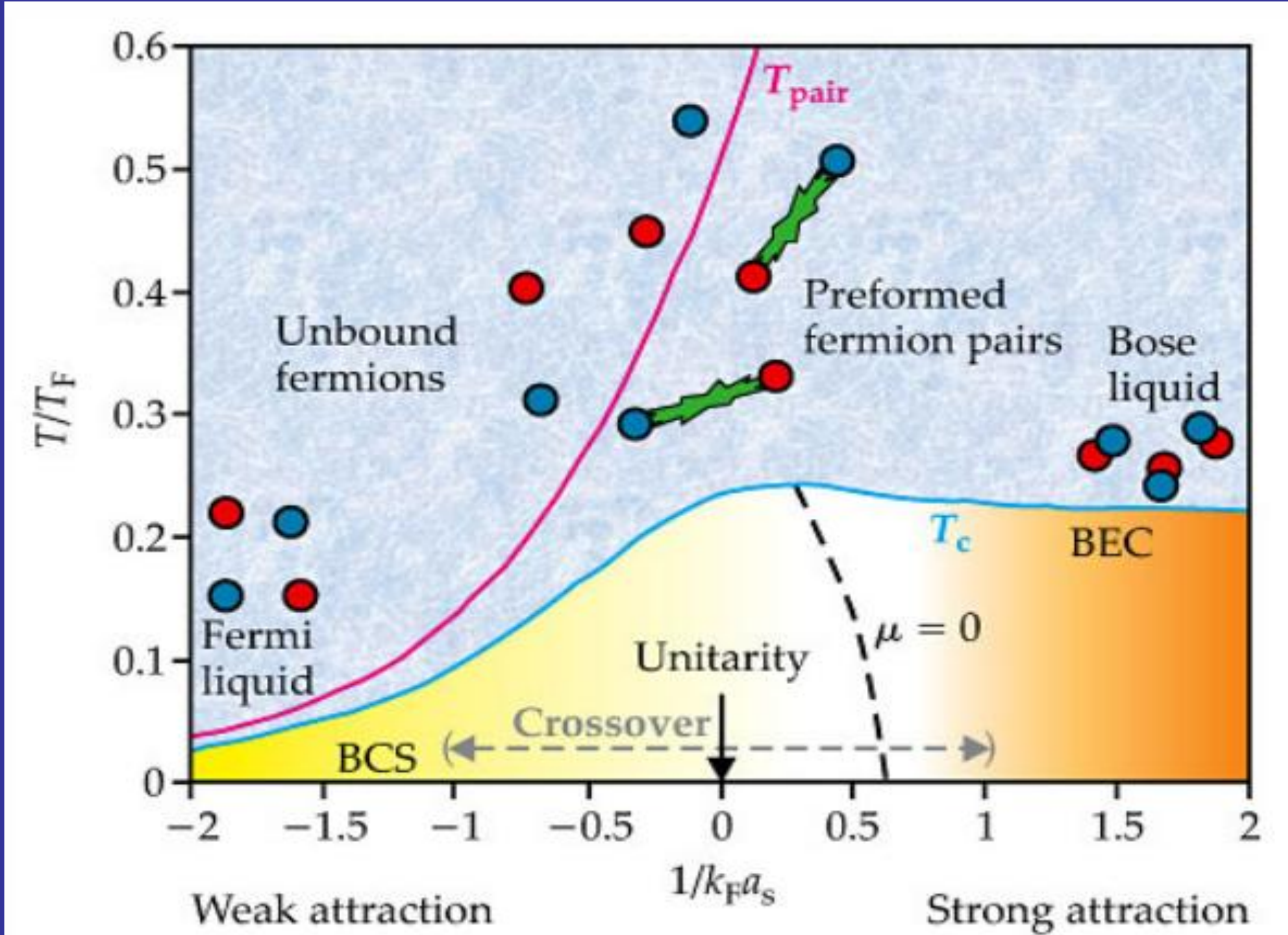


Entropy as a function of energy (relative to the ground state) for the unitary Fermi gas in the harmonic trap.

Ratio of the mean square cloud size at B=1200G to its value at unitarity (B=840G) as a function of the energy. Experimental data are denoted by point with error bars.

$B = 1200G \Rightarrow 1/k_F a \approx -0.75$

Theory: **Bulgac, Drut, and Magierski PRL 99, 120401 (2007)**



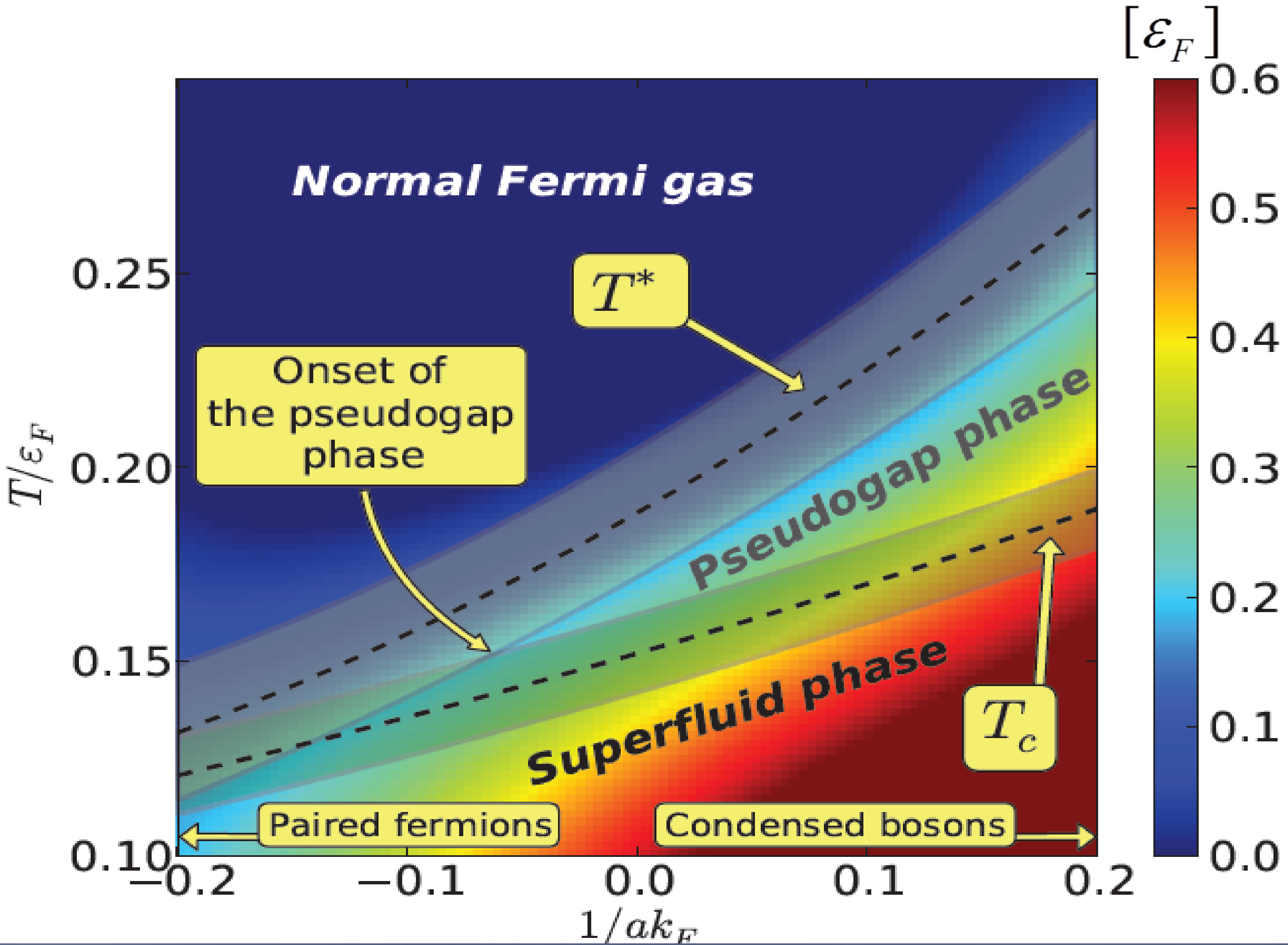
From Sa de Melo, Physics Today (2008)

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

Important issue related to pairing pseudogap:

- Are there sharp gapless quasiparticles in a normal Fermi liquid
  YES: Landau's Fermi liquid theory;
  NO: breakdown of Fermi liquid paradigm

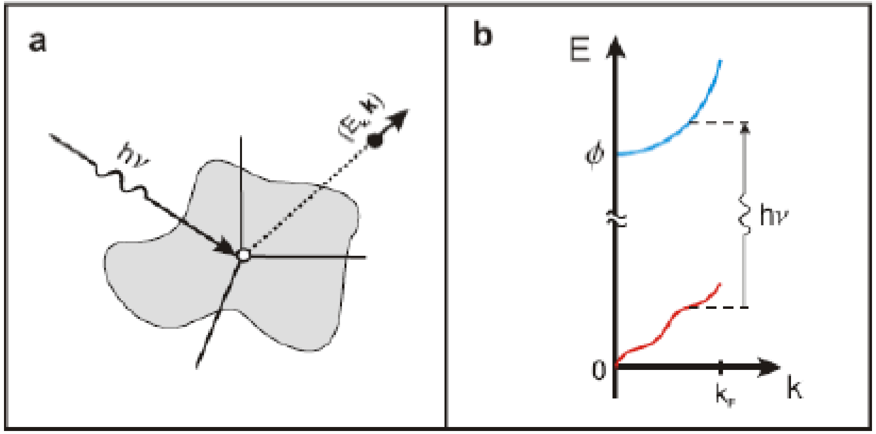
Gap in the single particle fermionic spectrum - theory



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)

RF spectroscopy in ultracold atomic gases

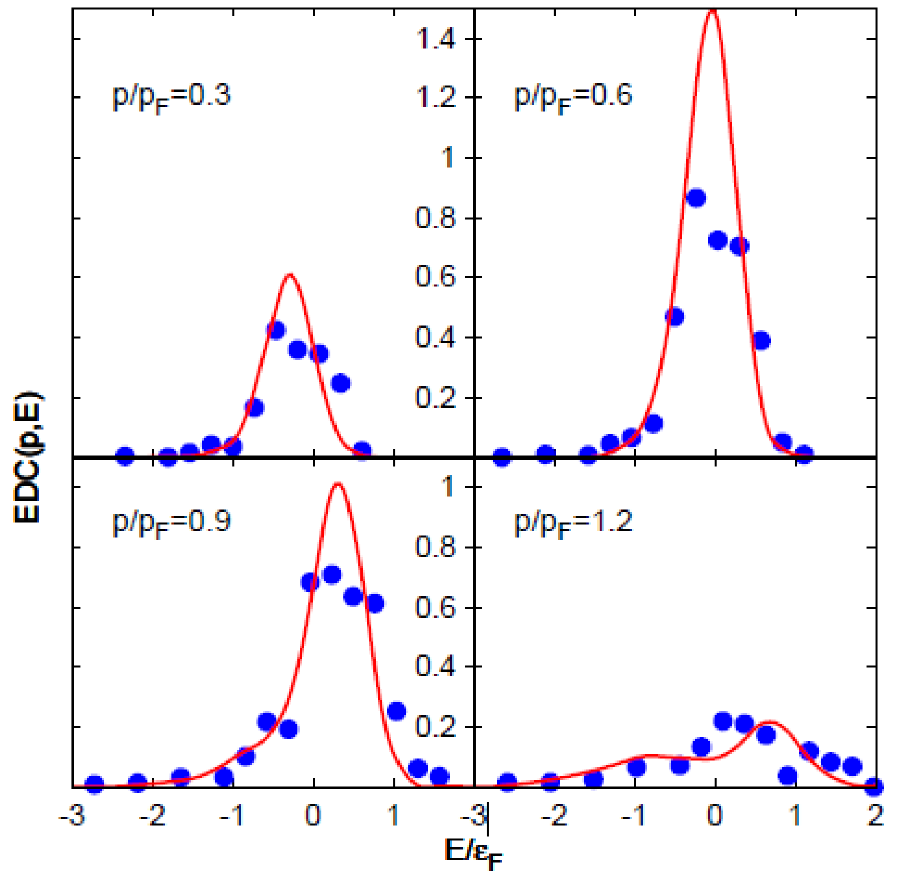


$$-E_s + h\nu = \frac{\hbar^2 k^2}{2m} + \phi$$

$$E(N) = E(N-1) + E_s$$

Stewart, Gaebler, Jin, Using photoemission spectroscopy to probe a strongly interacting Fermi gas, Nature, 454, 744 (2008)

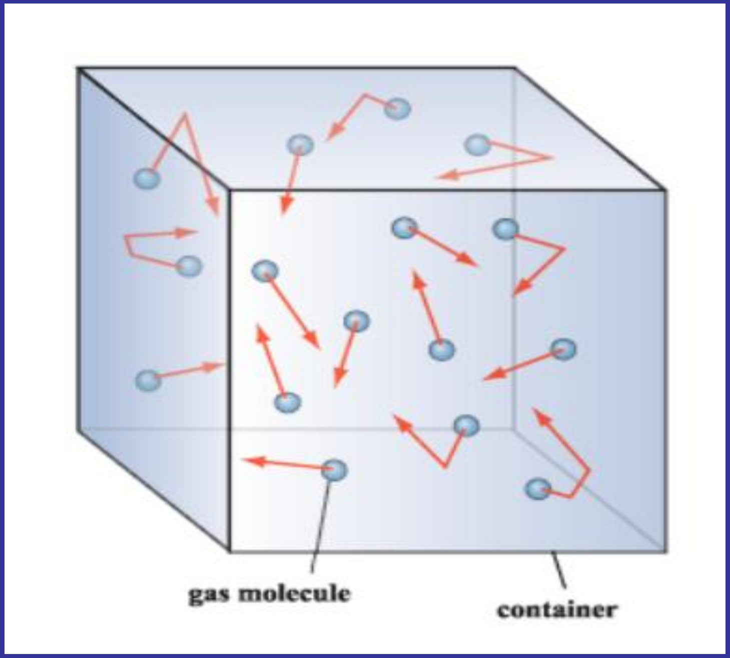
$$\mathrm{EDC}(p,E,T) = \mathcal{C}p^2 \int_0^\infty dr\, r^2 \frac{1}{\varepsilon_F(r)} A\left[\frac{p}{p_F(r)}, \frac{E-\mu(r)}{\varepsilon_F(r)}, \frac{T}{\varepsilon_F(r)}\right] f(E-\mu(r)),$$



Experiment (blue dots): D. Jin's group
Gaebler et al. *Nature Physics 6, 569(2010)*
Theory (red line):
Magierski, Wlazłowski, Bulgac, Phys.Rev.Lett.107,145304(2011)

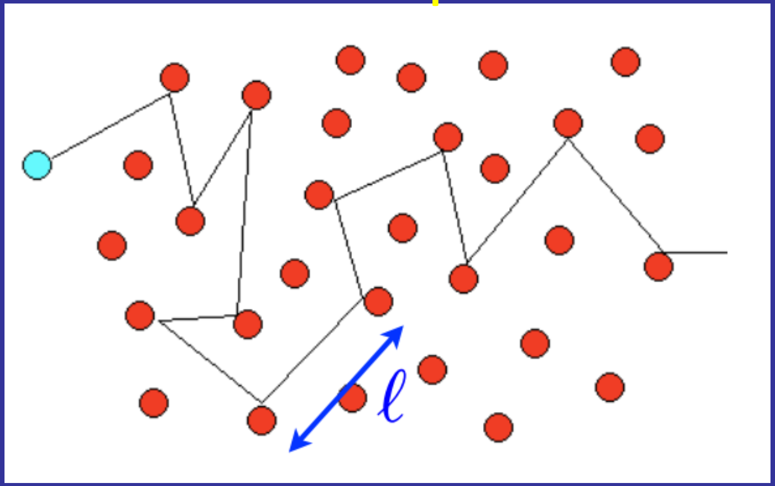
Viscosity in strongly correlated quantum systems:

Water and honey flow with different rates:
different viscosity



In the light of the kinetic theory of gases molecules are moving mostly along straight lines and occasionally bump onto each other.

Mean free path



This leads to the Maxwell's formula for viscosity (1860):

$$\eta \sim \rho v \ell = \text{mass density} \times \text{velocity} \times \text{mean free path}$$

Consequences:

- Non interacting gas is a pathological example of the system with an <u>infinite viscosity</u>
- Strongly interacting system can have low viscosity since the mean free path is short **but…**

…but when the system is strongly correlated then the kinetic theory fails!

However:
If we blindly use this formula we may notice that the Heisenberg uncertainty principle would give the following relation:

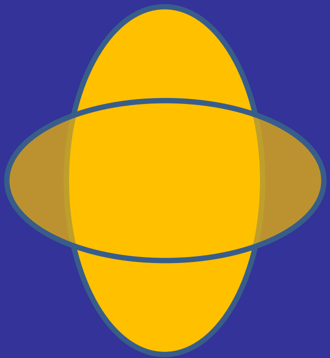
$$\frac{\eta}{\rho} \sim \overline{p} l \geq \hbar$$

$\overline{p}$ - average momentum

Can we make the above statement more precise?

How do we measure the viscosity of a system?

- Viscosity = response of the fluid under shear
- Theorist: send gravitational wave through the system

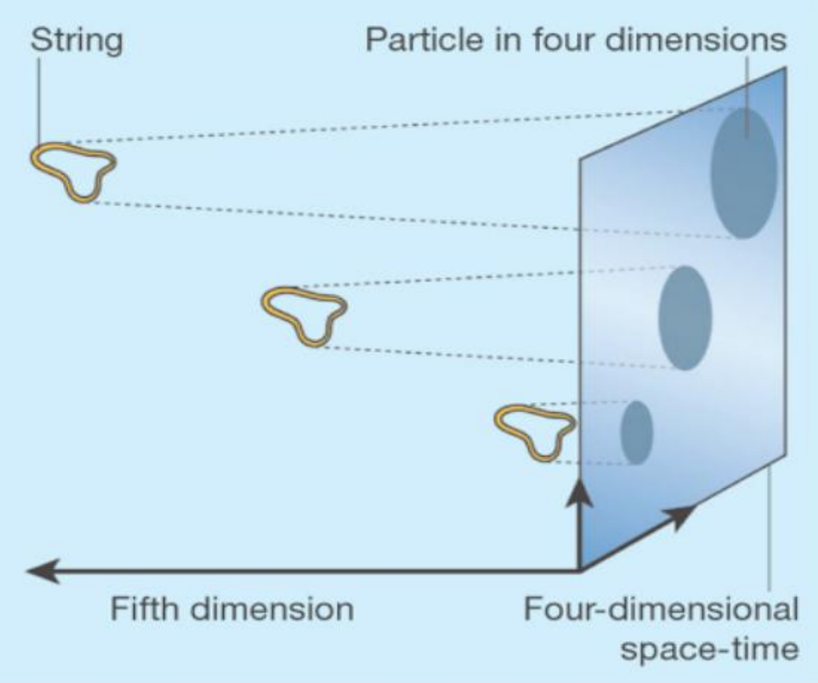


Maldacena's breakthrough (1997):

1997: gauge/gravity duality

particles in 4 dimensions = strings in 5 dimensions

Sometimes, the string picture is clearer than the particle picture!



(from Nature)

Consequence of Maldacena's hypothesis
(string theory turned out to be useful in a very unexpected way)

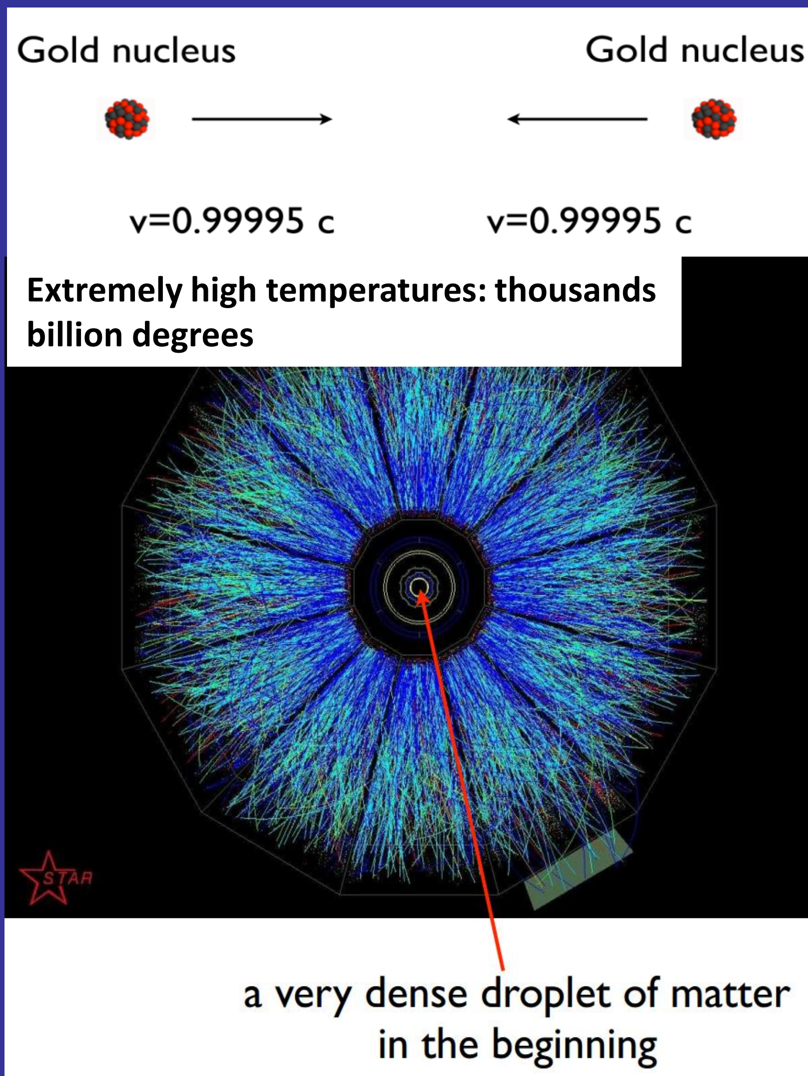
$$\frac{\eta}{S} = \frac{\hbar}{4\pi}$$

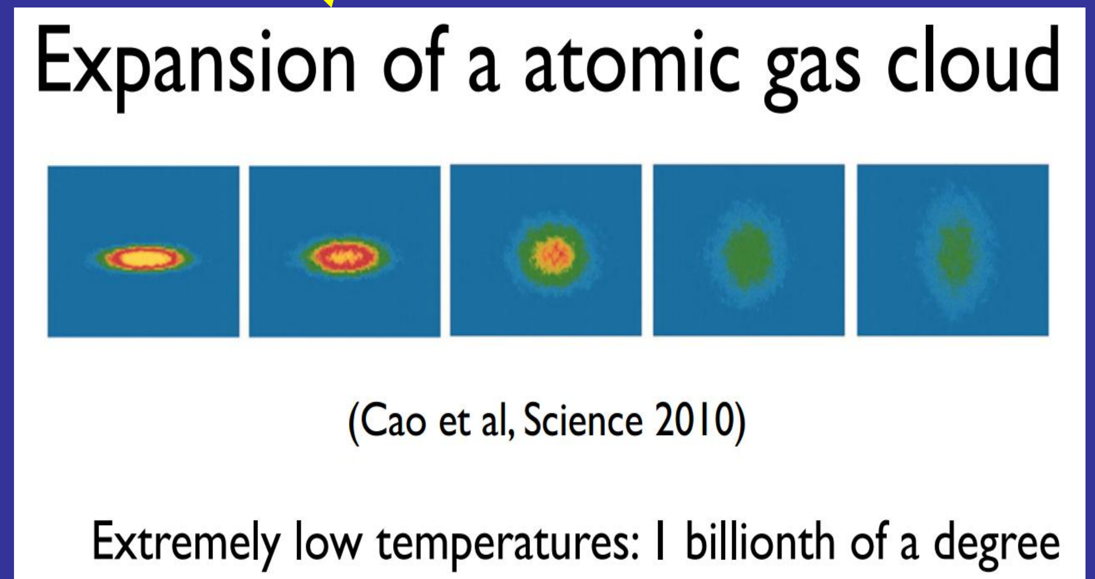
Kovtun,Son,Starinets, (2005) from AdS/CFT correspondence
S – entropy density

KSS conjecture: all known fluids satisfy: $$\frac{\eta}{S} \geq \frac{\hbar}{4\pi}$$

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

Candidates: quark gluon plasma, atomic gas

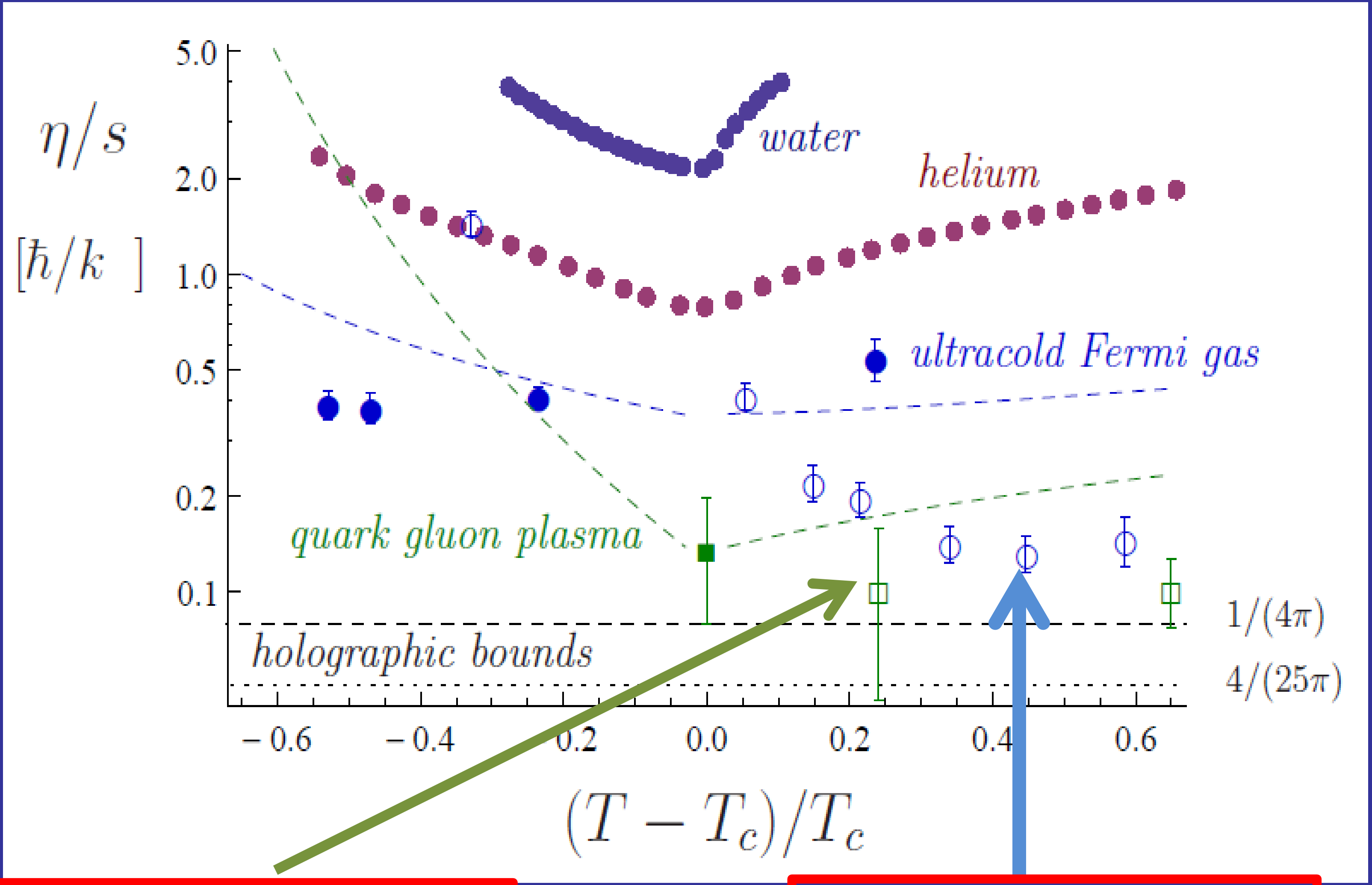




Despite of energy scales differing by many orders of magnitude, expansion of both system is pretty much similar and in particular exhibts the so-called <u>elliptic flow</u>.

Shear viscosity to entropy ratio – experiment vs. theory

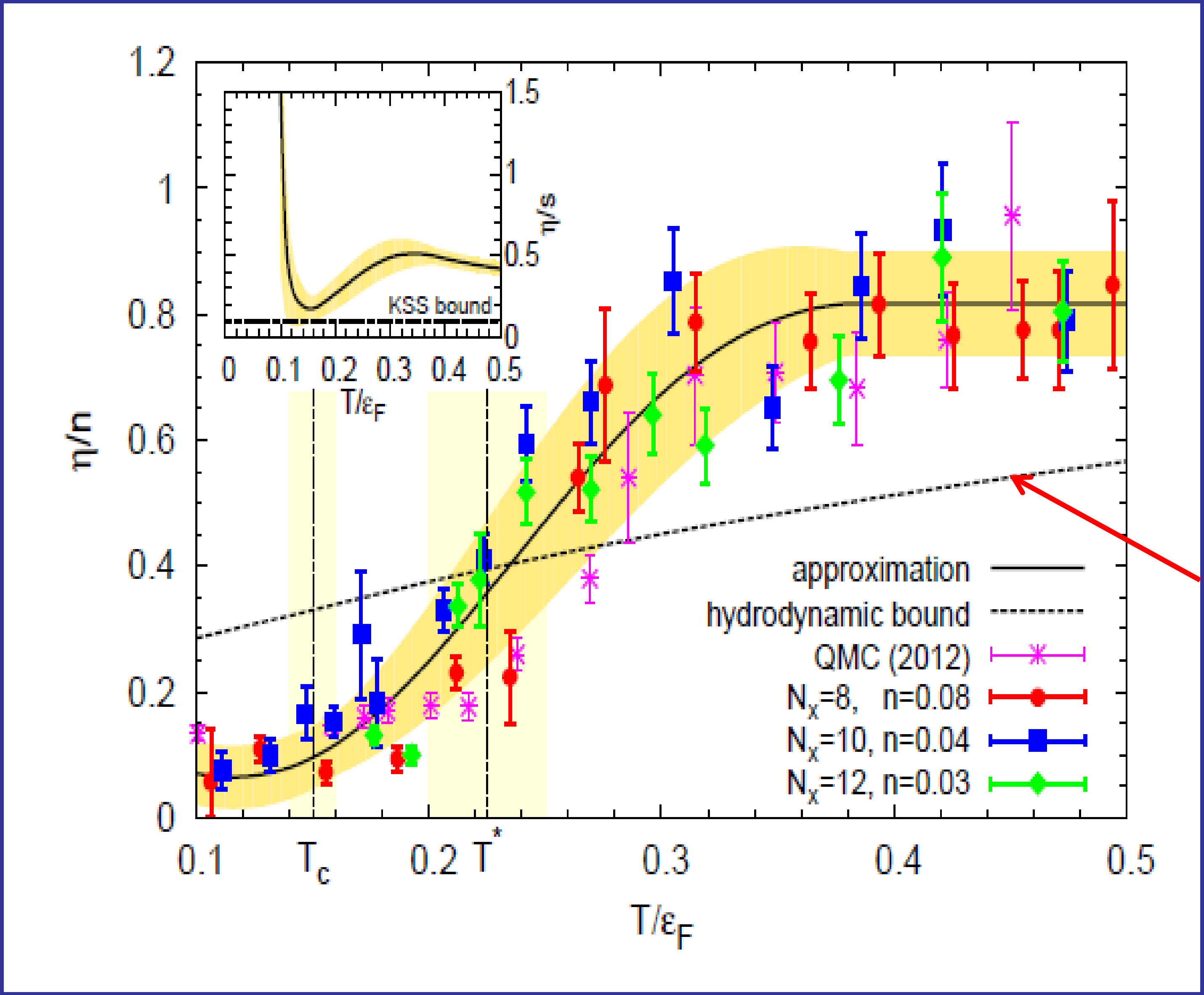
(from A. Adams et al. New Journal of Physics, "Focus on Strongly Correlated Quantum Fluids: from Ultracold Quantum Gases to QCD Plasmas,, arXive:***1205.5180)***



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, Phys. Rev. A88, 013639 (2012)

Spin susceptibility and spin drag rate

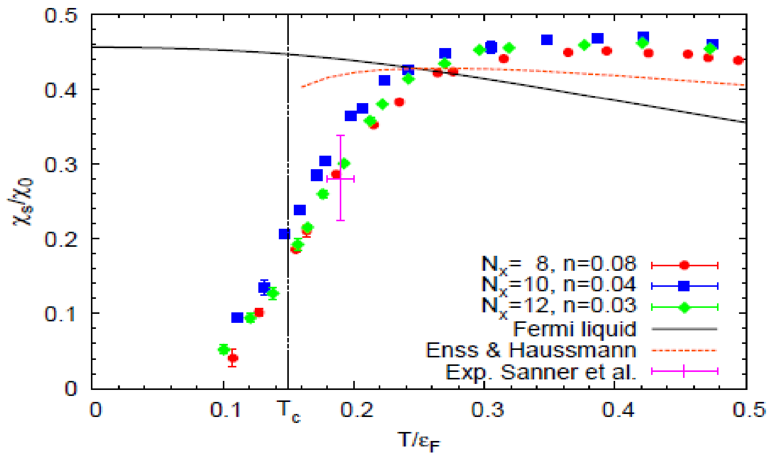


FIG. 2: (Color online) The static spin susceptibility as a function of temperature for an 8^3 lattice solid (red) circles, 10^3 lattice (blue) squares and 12^3 lattice (green) diamonds. Vertical black dotted line indicates the critical temperature of superfluid to normal phase transition $T_c = 0.15\,\varepsilon_F$. 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.

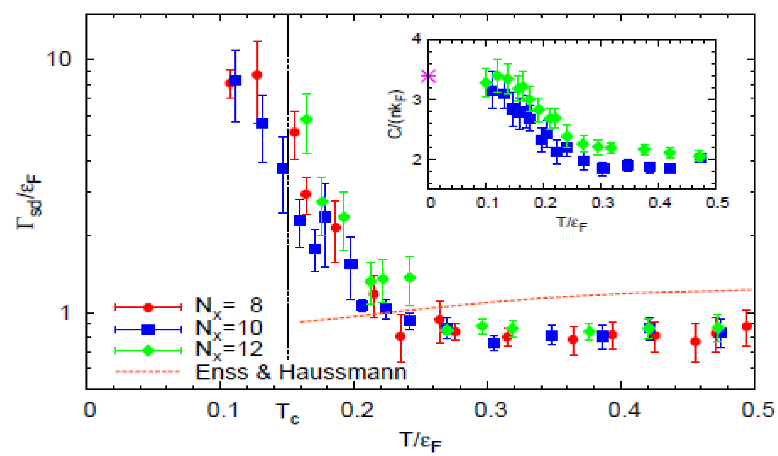


FIG. 3: (Color online) The spin drag rate $\Gamma_{sd} = n/\sigma_s$ in units of Fermi energy as a function of temperature for an 8^3 lattice solid (red) circles, 10^3 lattice (blue) squares and 12^3 lattice (green) diamonds. Vertical black dotted line locates the critical temperature of superfluid to 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 $T = 0$.

$$\Gamma = \frac{n}{\sigma_s} \quad \text{- spin drag rate}$$

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

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

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

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