Ab-initio approaches to strongly correlated Fermi systems

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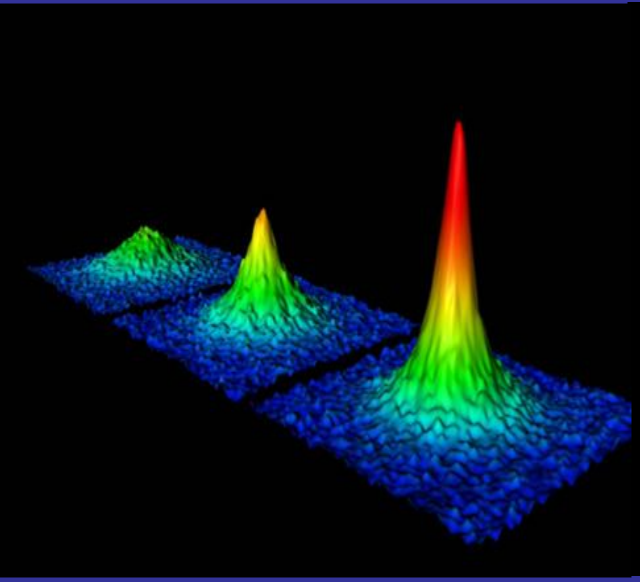
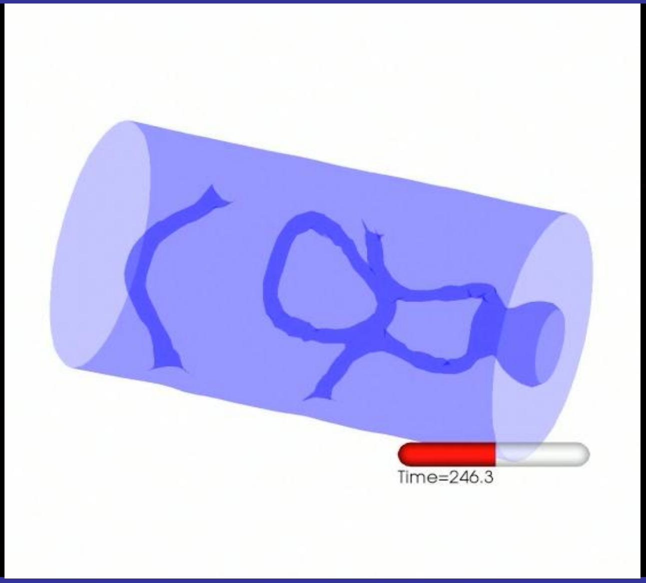
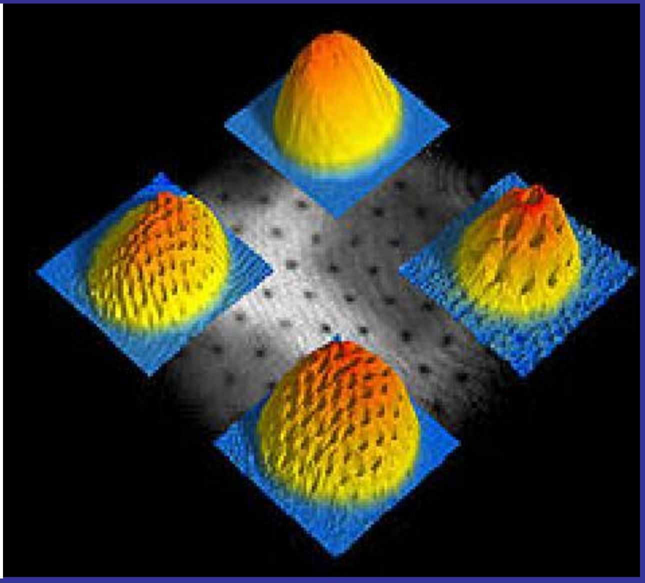





Collaborators:

A. Bulgac - Seattle
J.E. Drut - LANL
T. Lähde - Helsinki
Y-L. (Alan) Luo - Seattle
K.J. Roche - PNNL
I. Stetcu - LANL
G. Wlazłowski - Seattle/Warsaw
Y. Yu - Wuhan

By strongly correlated Fermi systems I mean:

- **Unitary Fermi gas**
- **Nuclear systems: atomic nuclei, neutron matter, neutron stars**

By *ab-initio* approach I mean:

- **Path Integral Monte Carlo on a lattice (at finite T)**
- **Density Functional Theory (both static and time dependent, extended to superfluid systems)**

BCS – BEC crossover

Eagles (1969), Leggett (1980): Variational approach

$$|gs\rangle = \prod_k \left(u_k + v_k \hat{a}^\dagger_{k\uparrow} \hat{a}^\dagger_{-k\downarrow}\right)|vacuum\rangle \quad \text{BCS wave function}$$

BCS limit: $1/k_F a_s \to -\infty$

a_s - scattering length

$\mu \to \varepsilon_F$ chemical potential

$$\Delta \to \frac{8}{e^2}\varepsilon_F \exp\left(\frac{\pi}{2k_F a_s}\right)$$ pairing gap

Usual BCS solution for small and negative scattering lengths, with exponentially small pairing gap describing the system of spatially overlapping Cooper pairs.

BEC limit: $1/k_F a_s \to +\infty$

$$\mu \to -\frac{\hbar^2}{2m a_s^2} = -\frac{E_b}{2}$$

$$\Delta \to \frac{4\varepsilon_F}{\sqrt{3\pi k_F a_s}}$$

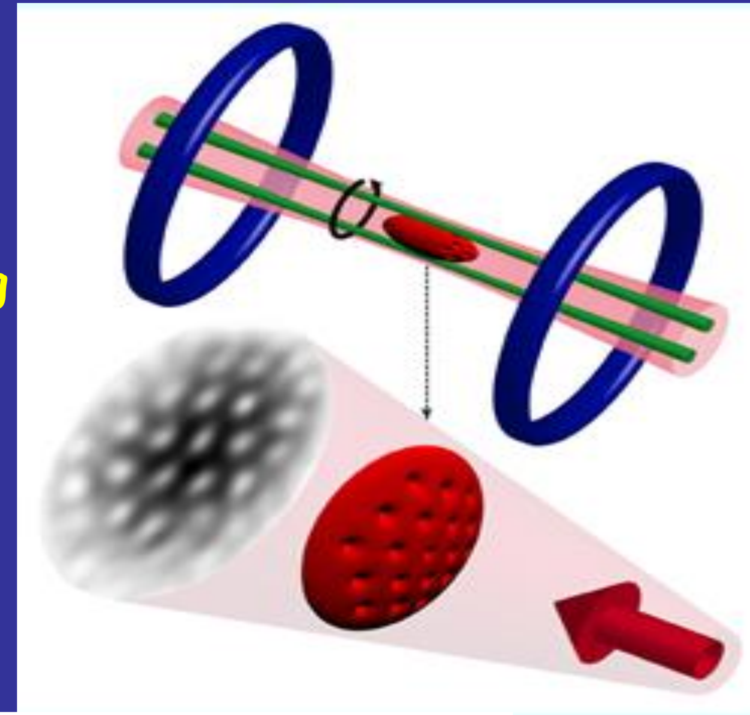
Gas of weakly repelling molecules with binding energy E_b, essentially all at rest (almost pure BEC state)

No singularity within the whole range of scattering length!
Smooth crossover from spatially overlapping Cooper pairs to tightly bound difermionic molecules

Beyond mean field: Nozieres, Schmitt-Rink (1985), Randeria et al.(1993)

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!

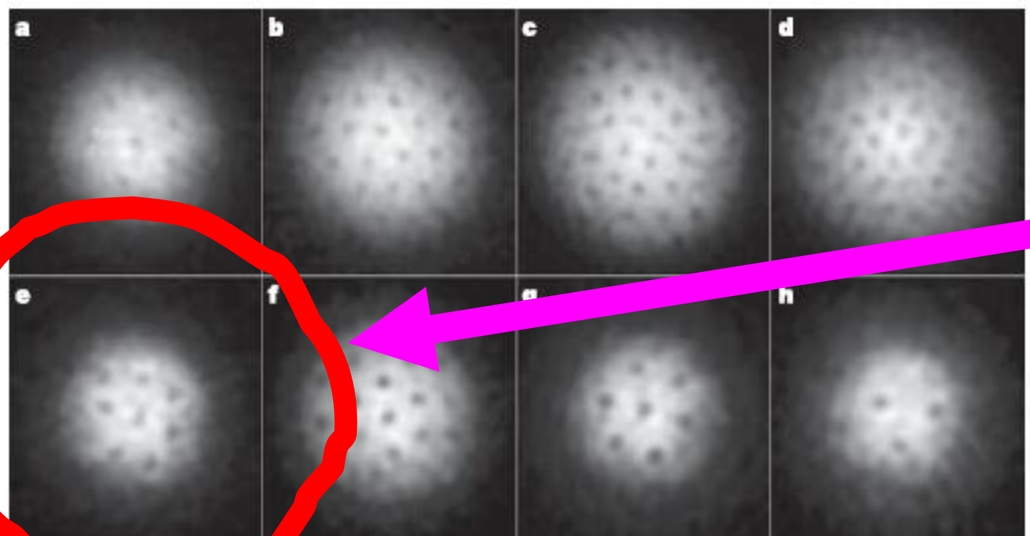


system of fermionic ^{6}Li atoms

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 (s[illegible] magnetic fields were 740 G (**a**), 766 G (**b**), 792 G (**c**[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)

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

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

NONPERTURBATIVE REGIME

System is dilute but strongly interacting!

Universality: $E = \xi_0 E_{FG} \quad \text{for } T = 0$

$\xi_0 = 0.376(5)$ - **Exp. estimate**

E_{FG} - **Energy of noninteracting Fermi gas**

Thermodynamics of the unitary Fermi gas

ENERGY: $E(x) = \frac{3}{5}\xi(x)\varepsilon_F N; \quad x = \frac{T}{\varepsilon_F}$

ENTROPY/PARTICLE: $\sigma(x) = \frac{S(x)}{N} = \frac{3}{5}\int_0^x \frac{\xi'(y)}{y}dy$

FREE ENERGY: $F = E - TS = \frac{3}{5}\varphi(x)\varepsilon_F N$

$$\varphi(x) = \xi(x) - x\sigma(x)$$

PRESSURE: $P = -\frac{\partial E}{\partial V} = \frac{2}{5}\xi(x)\varepsilon_F \frac{N}{V}$

$$PV = \frac{2}{3}E$$

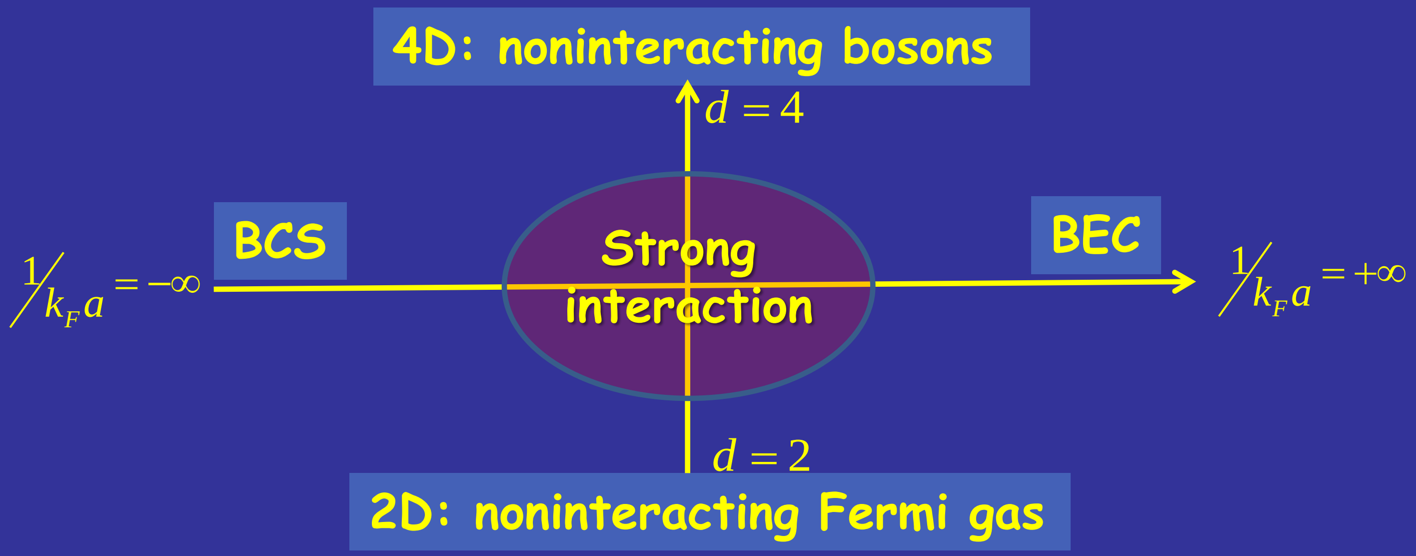
Note the similarity to the ideal Fermi gas

Unitary limit in 2 and 4 dimensions:

$$a \to \infty: \; R(r) \propto \frac{1}{r^{d-2}} + O(r^{4-d}), \quad \textit{Two body wave function for } r \to 0.$$

Intuitive arguments:

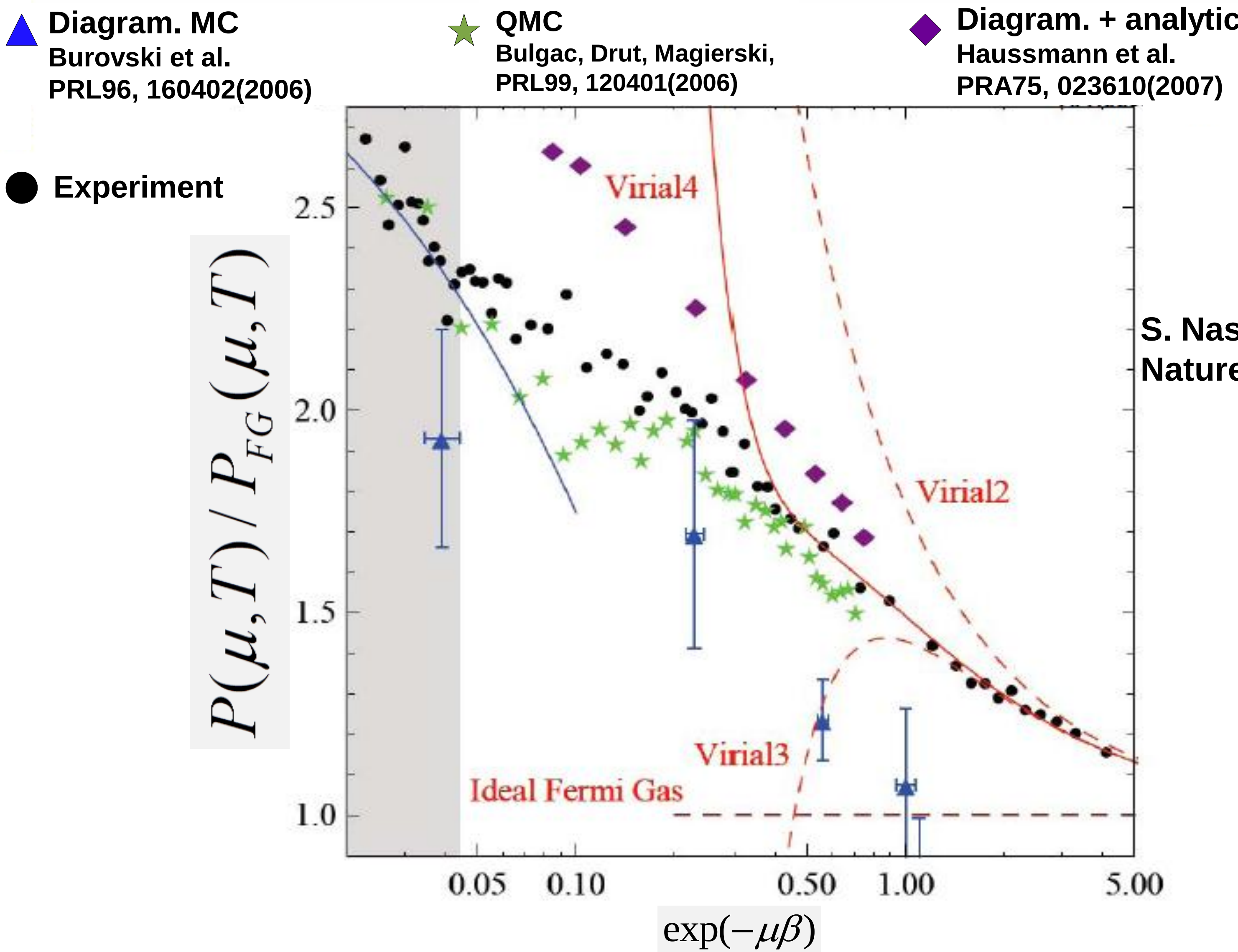
- For d=4 $\int R(r)^2 d^d r$ diverges at the origin
- For d=2 the singularity of the wave function disappears = interaction also disappears.



The only nontrivial case of unitary regime is in 3D

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

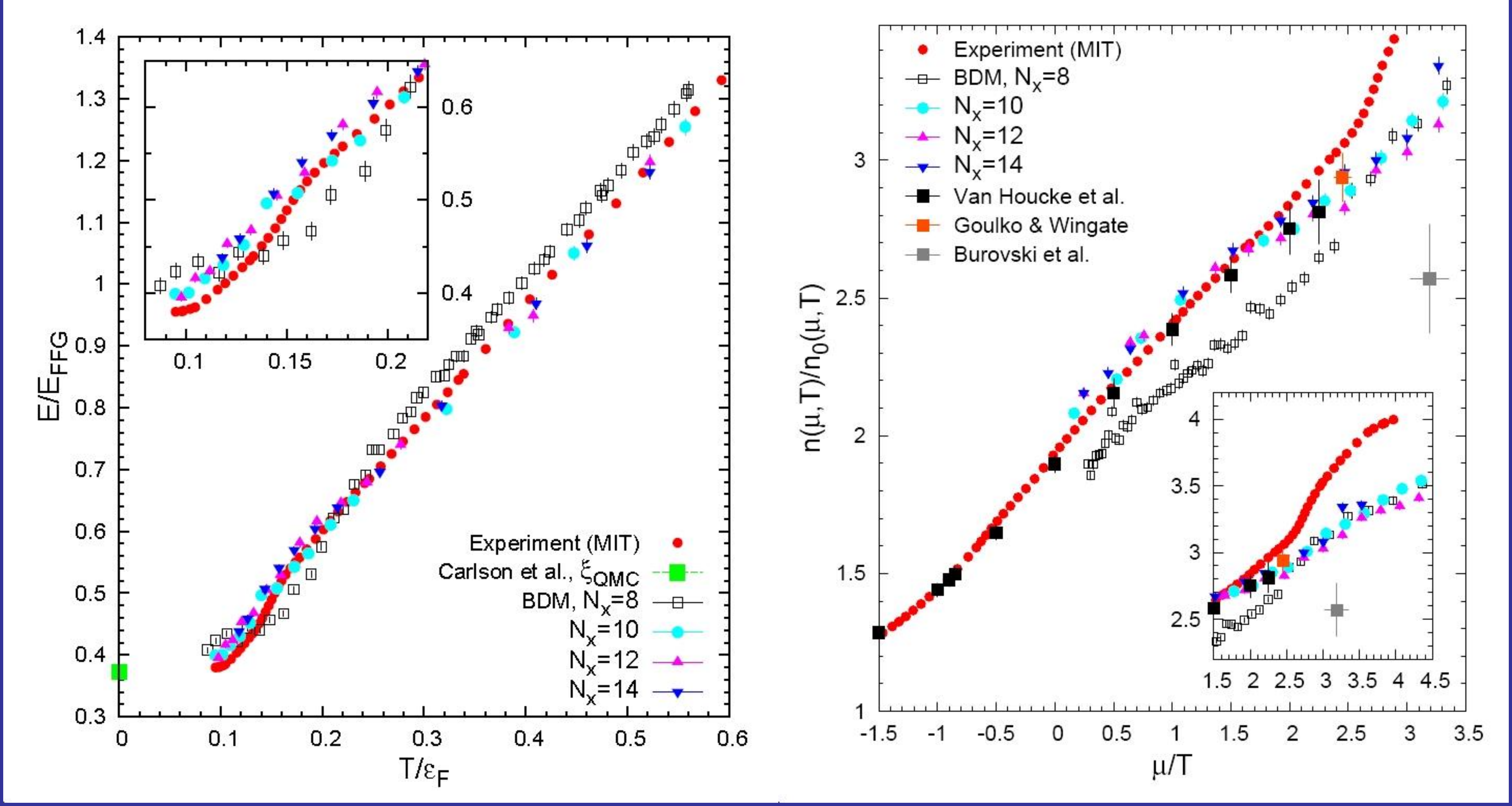
Comparison with Many-Body Theories (1)



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

Courtesy of C. Salomon

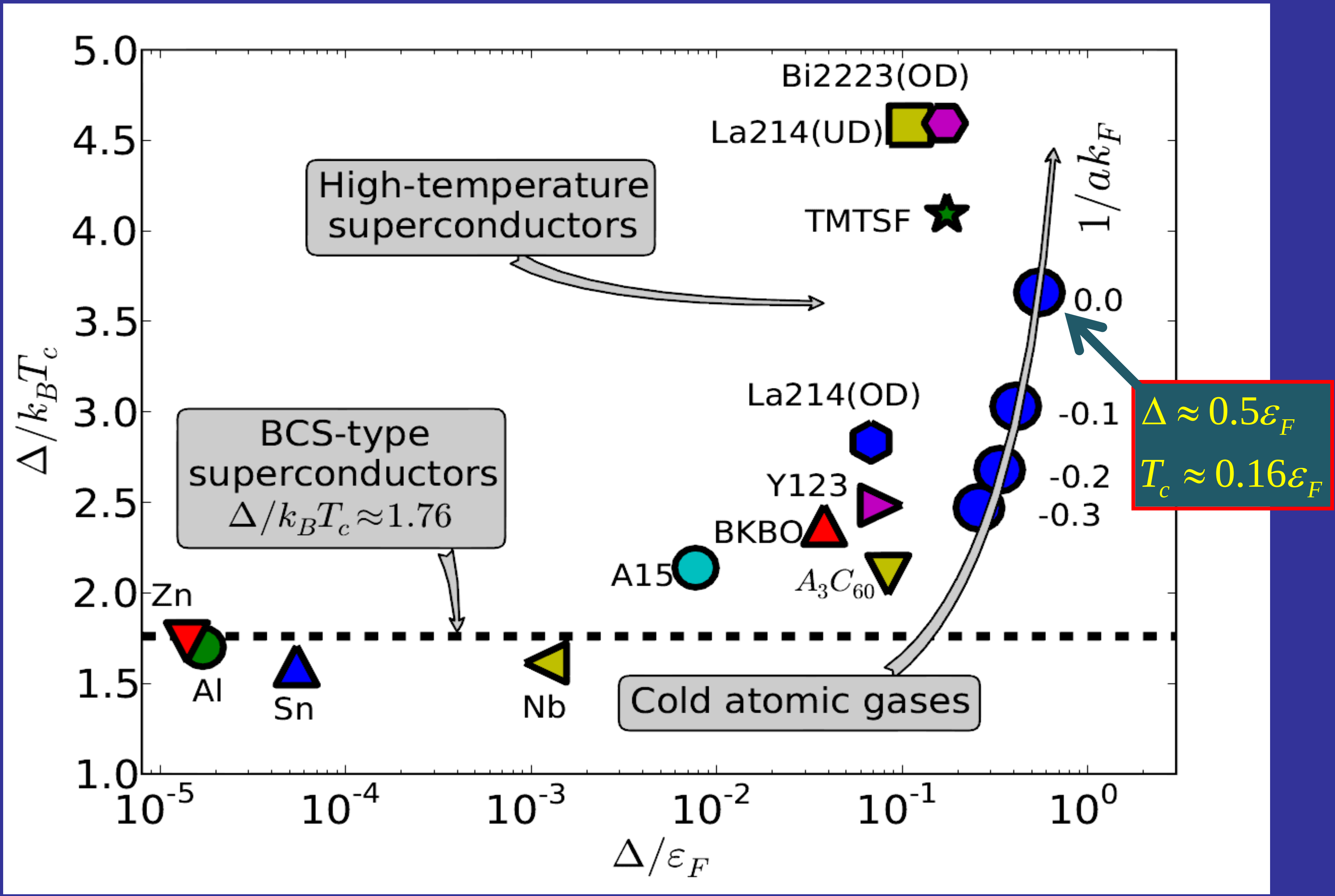
Equation of state of the unitary Fermi gas



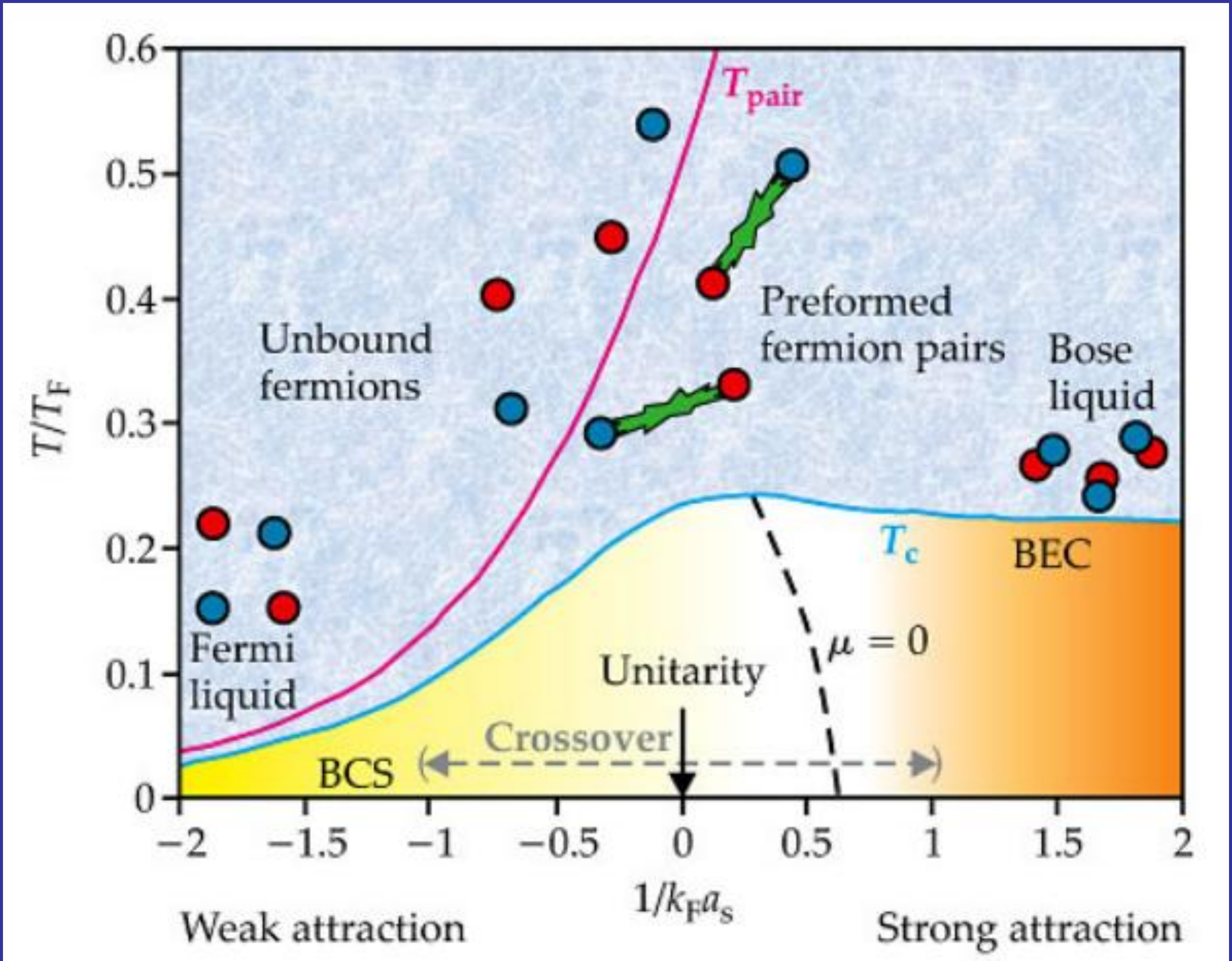
J.E.Drut, T.Lähde, G.Wlazłowski, P.Magierski, arXive:1111.5079

Experiment: M.J.H. Ku *et al.* , arXive:1110.3309

Cold atomic gases and high Tc superconductors



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



From Sa de Melo, Physics Today (2008)

Pseudogap

Suppression of low-energy spectral weight function in the normal state ($T > T_c$) = single particle density of states at the Fermi level is lowered

Origin of terminology:
Ding et al., „Spectroscopic evidence for a pseudogap in the normal state of underdoped high- T_c superconductors, Nature 382, 51 (1996)

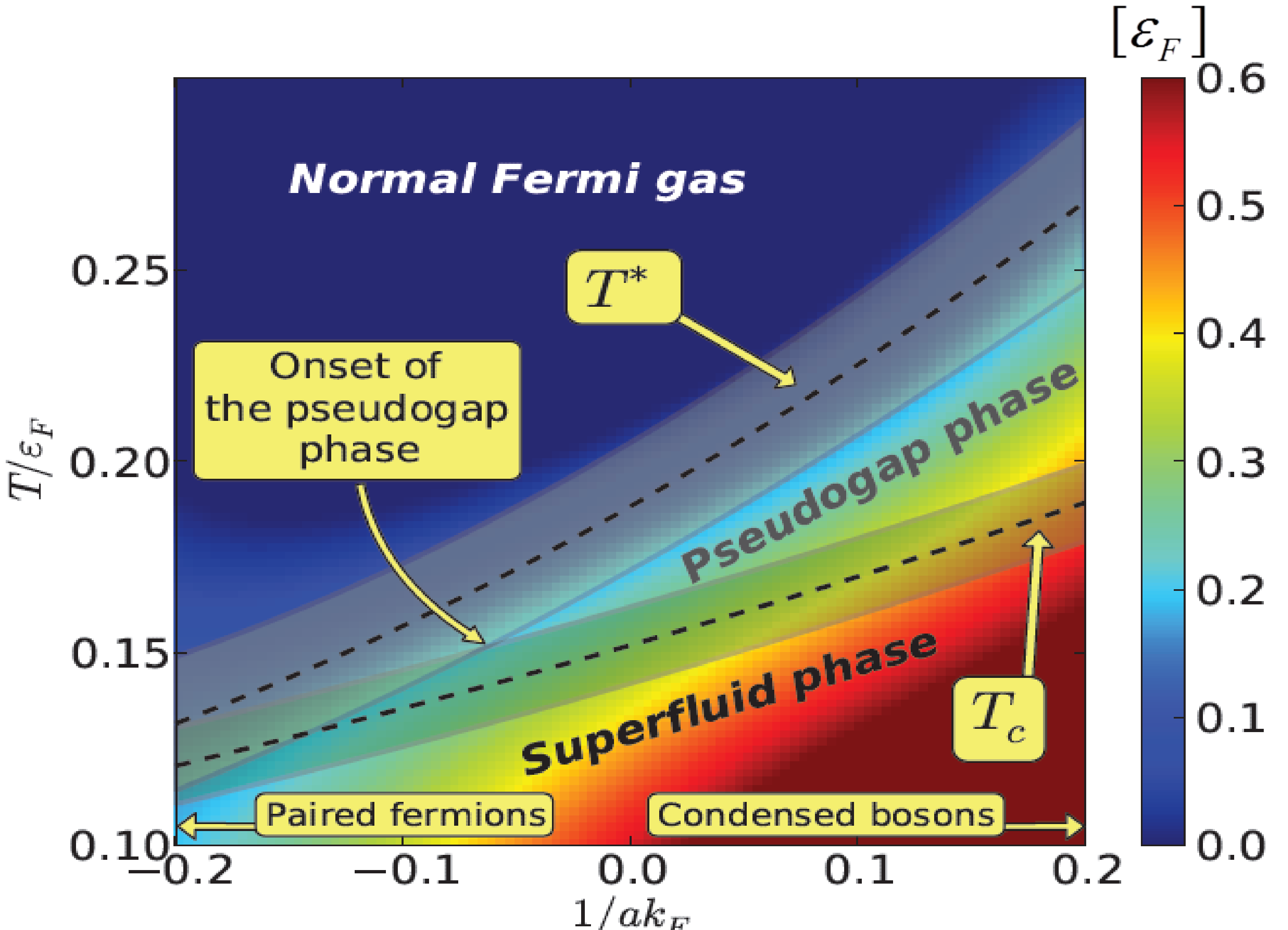
Pairing pseudogap

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

Two important issues related to pairing pseudogap:

- What drives the transition to the superconducting state, amplitude (BCS theory) or phase fluctuations?
- Are there sharp gapless quasiparticles in a normal Fermi liquid (**YES**: Landau's Fermi liquid theory; **NO**: breakdown of Fermi liquid paradigm)

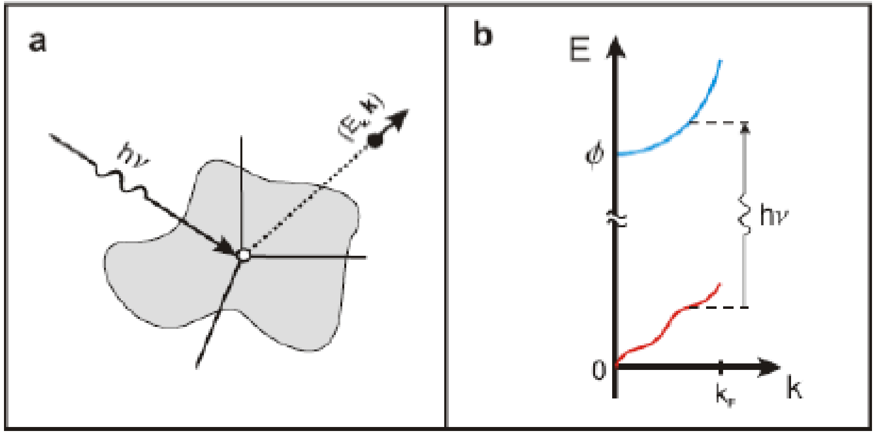
Gap in the single particle fermionic spectrum - theory



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

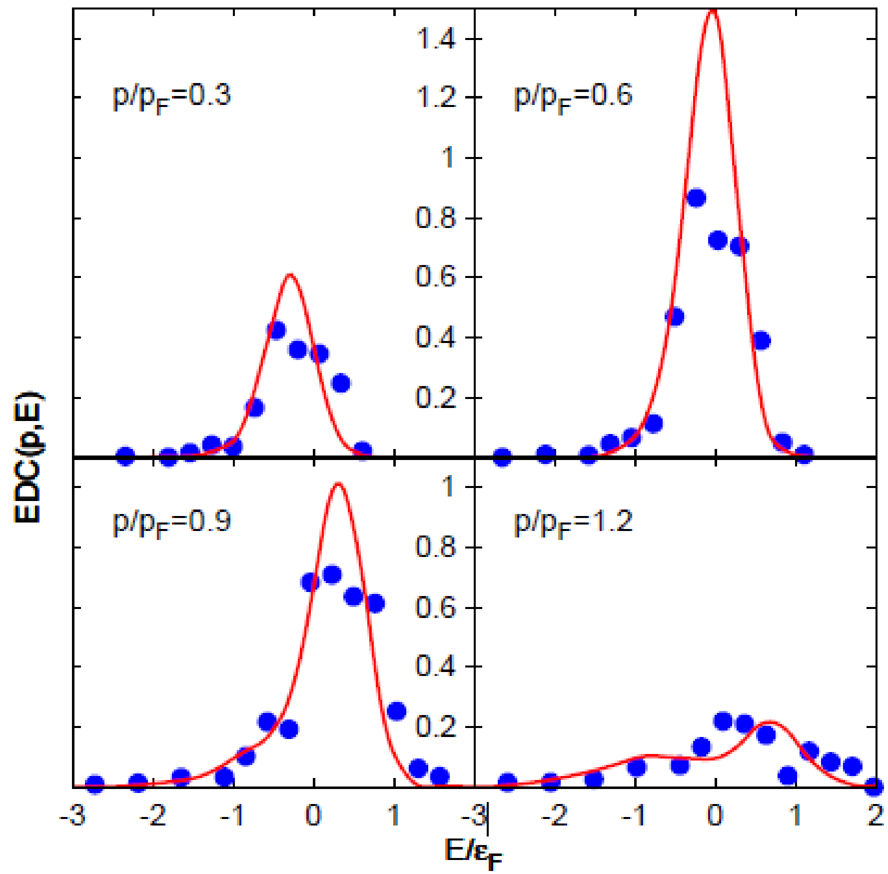


$$-E_s + h\nu = \frac{\hbar^2 k^2}{2m} + \phi$$

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

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)

Experimental status of pseudogap measurements around unitarity

Spectroscopy → **YES**

(D. Jin's group, JILA)

Thermodynamics → **NO**

(C.Salomon's group, Paris
M. Zwierlein's group, MIT)

Pseudogap at unitarity – theoretical predictions

Path Integral Monte Carlo - YES
Dynamic Mean Field - YES
Selfconsistent T-matrix - NO
Nonselfconsistent T-matrix - YES

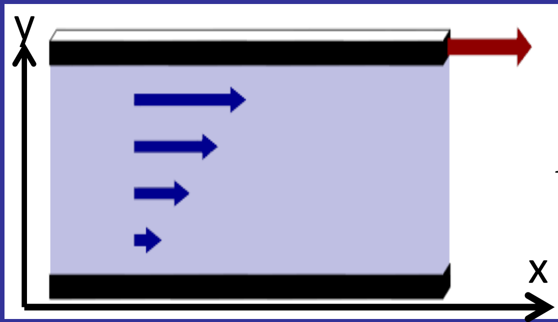
Hydrodynamics at unitarity

Scaling: $\psi_i(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N) \rightarrow \frac{1}{\lambda^{3N/2}}\psi_i\left(\vec{r}_1/\lambda, \vec{r}_2/\lambda, \ldots, \vec{r}_N/\lambda\right); E_i \rightarrow E_i/\lambda^2$

No intrinsic length scale ⇒ Uniform expansion keeps the unitary gas in equilibrium

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

Shear viscosity:



$$F = A\eta \frac{\partial v_x}{\partial y}$$

For any physical fluid:

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

KSS conjecture

Kovtun,Son,Starinets, (2005) from AdS/CFT correspondence

Maxwell classical estimate: $\eta \sim$ mean free path

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

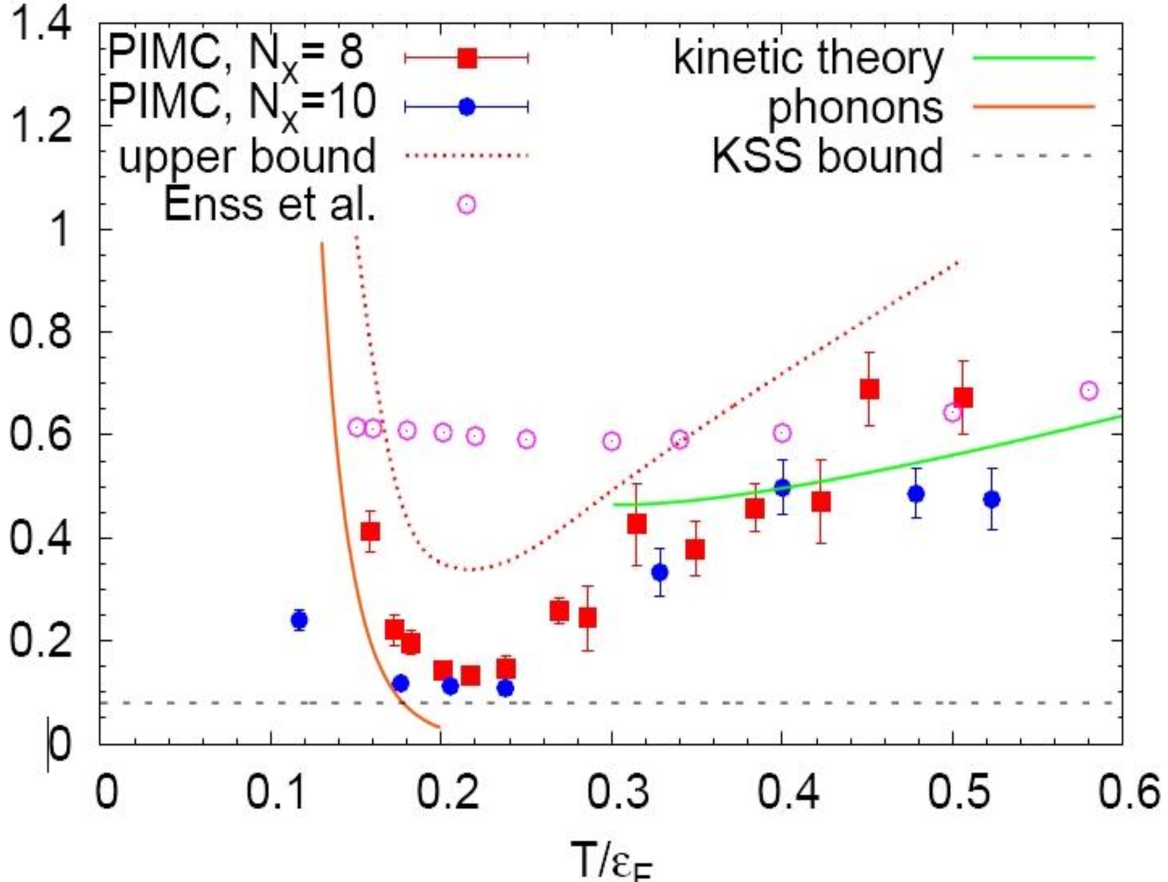
Candidates: unitary Fermi gas, QGP

Shear viscosity from PIMC

$$\eta(\omega) = \pi \frac{\rho_{xy,xy}(\vec{q}=0,\omega)}{\omega}$$

$$G_{xy,xy}(\vec{q},\tau) = \int_0^\infty \rho_{xy,xy}(\vec{q},\omega) \frac{\cosh(\omega(\tau-\beta/2))}{\sinh(\omega\beta/2)}$$

$$G_{xy,xy}(\vec{q},\tau) = \int d^3r e^{-i\vec{q}\cdot\vec{r}} \left\langle \hat{\Pi}_{xy}(\vec{r},\tau)\hat{\Pi}_{xy}(0,0) \right\rangle$$



G.Wlazłowski, P.Magierski,J.E.Drut, to be published

Formalism for Time Dependent Phenomena

The time-dependent density functional theory is viewed in general as a reformulation of the exact quantum mechanical time evolution of a many-body system when only one-body properties are considered.

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)

http://www.tddft.org

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

$$\begin{cases} [h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu]\mathrm{u}_i(\vec{r},t) + [\Delta(\vec{r},t) + \Delta_{ext}(\vec{r},t)]\mathrm{v}_i(\vec{r},t) = i\hbar \dfrac{\partial \mathrm{u}_i(\vec{r},t)}{\partial t} \\ [\Delta^*(\vec{r},t) + \Delta^*_{ext}(\vec{r},t)]\mathrm{u}_i(\vec{r},t) - [h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu]\mathrm{v}_i(\vec{r},t) = i\hbar \dfrac{\partial \mathrm{v}_i(\vec{r},t)}{\partial t} \end{cases}$$

In each case we solved on JaguarPf or Franklin the TDSLDA equations for a 32^3 , 48^3 and 32^2 *96 spatial lattices (approximately for 30k to 40k quasiparticle wavefunctions) for about 10k to 100k time steps using from about 30k to 40k PEs

Fully symmetry unrestricted calculations!

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

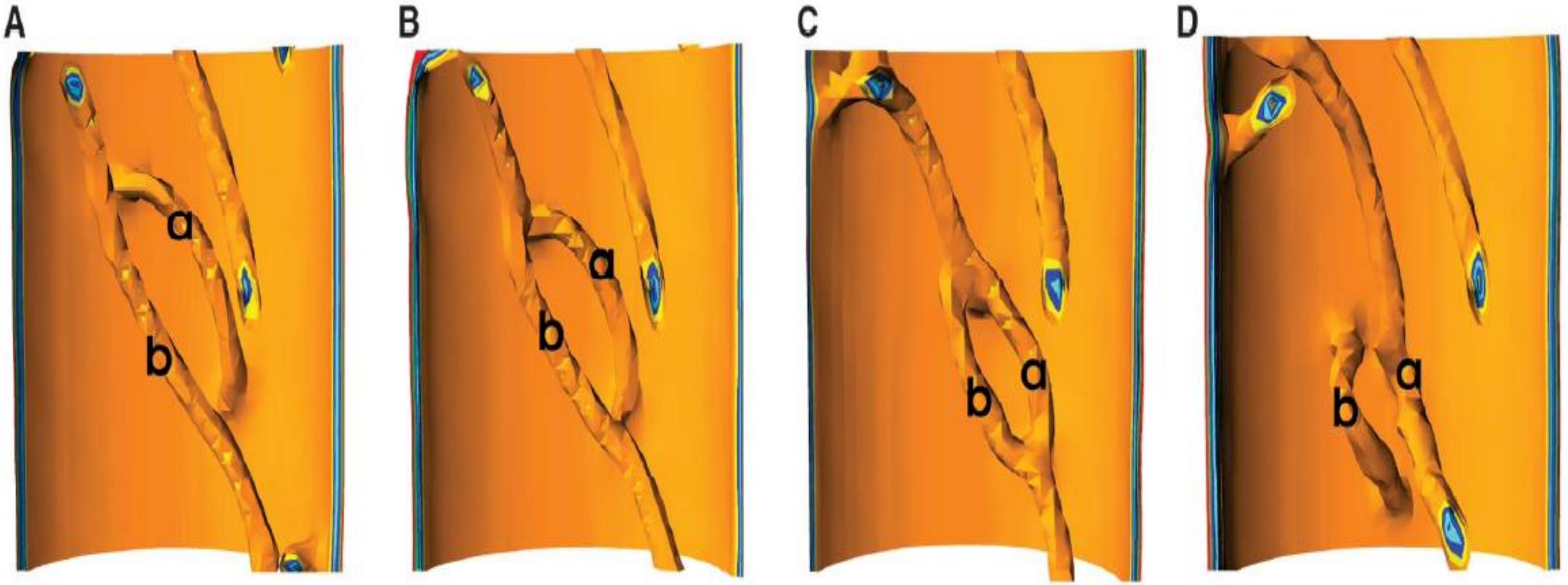


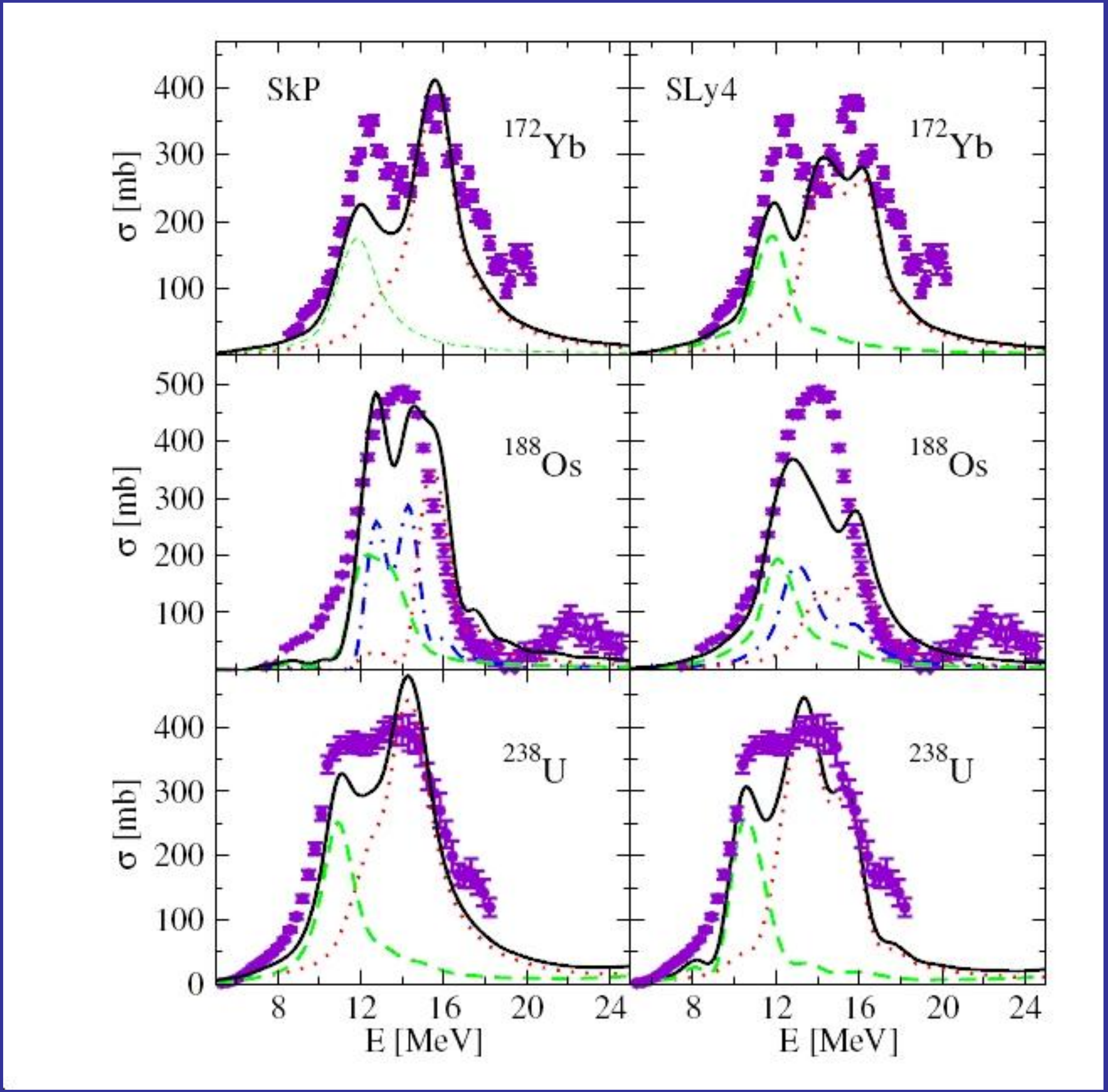
Fig. 3. (**A** to **D**) Two vortex lines approach each other, connect at two points, form a ring and exchange between them a portion of the vortex line, and subsequently separate. Segment (a), which initially belonged to the vortex line attached to the wall, is transferred to the long vortex line (b)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

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

Nuclear dynamics from time dependent density functional theory

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)

We created a set of accurate and efficient tools for studies of large, superfluid Fermi systems.

They have been successfully implemented on leadership class computers (Franklin, JaguarPF)

- **Currently capable of treating large volumes with up to 40,000-50,000 fermions , and for long times, fully self-consistently and with no symmetry restrictions under the action of complex spatio-temporal external probes.**

- **There is a clear path towards exascale applications and implementation of Stochastic TD(A)SLDA**

APPLICATIONS: - Dynamics of unitary Fermi gas
- Dynamics of atomic nuclei:
  neutron capture, induced fission, fussion,
  low energy nuclear reaction,
  dynamics of vortices in neutron star crust, etc.