Thermodynamics, pairing properties of a unitary Fermi gas

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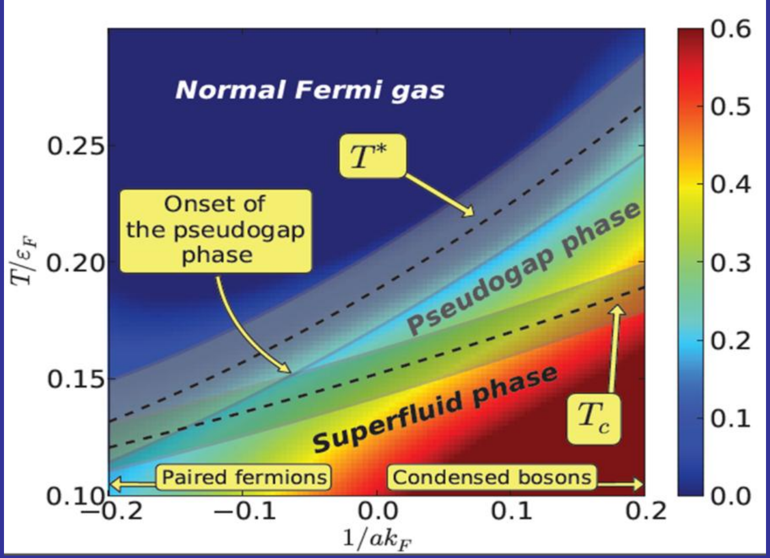


Outline

Path Integral Monte Carlo (PIMC) on the lattice.

Equation of state at unitarity. Thermodynamics. Contact.

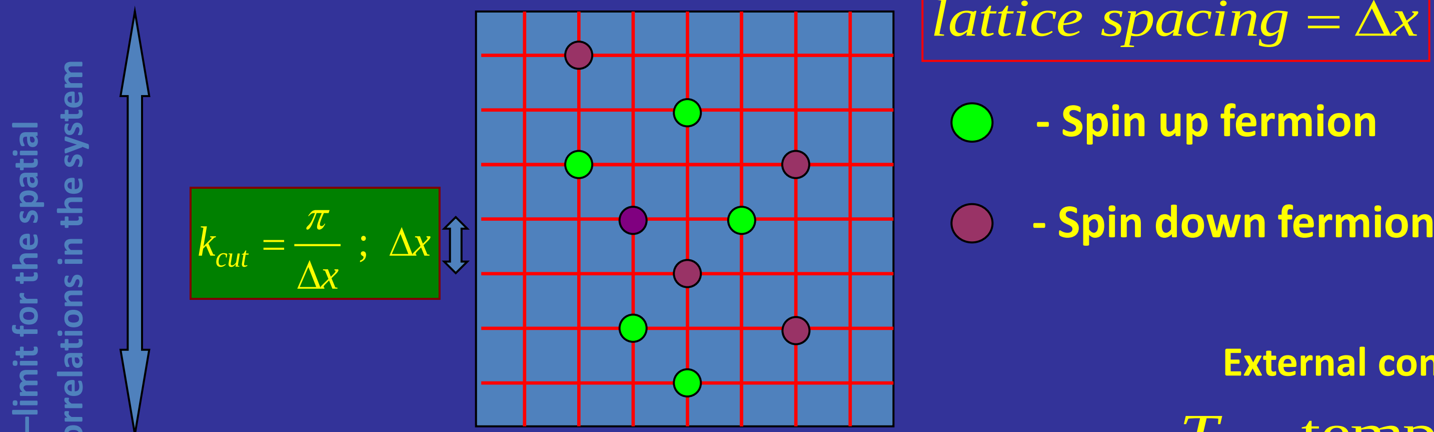
Superfluid to normal phase transition. Critical temperature.

Pairing properties. Spectral weight function. Pseudogap.

Coordinate space

$Volume = L^3$

$lattice\ spacing = \Delta x$



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

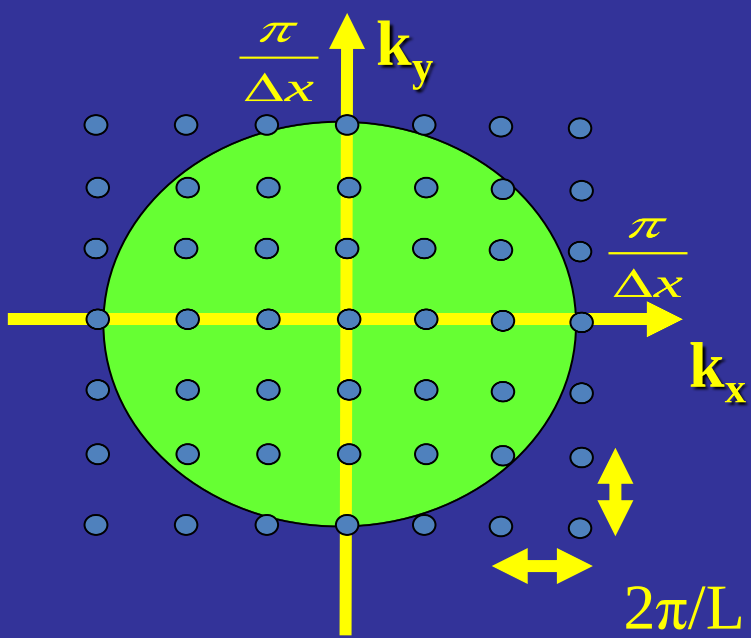
Periodic boundary conditions imposed

External conditions:

T - temperature

μ - chemical potential

Momentum space



UV momentum cutoff $\Lambda_{UV} = \frac{\pi}{\Delta x}$

IR momentum cutoff $\Lambda_{IR} = \frac{2\pi}{L}$

$$\frac{\hbar^2 \Lambda_{IR}{}^2}{2m} << \varepsilon_F,\ \Delta << \frac{\hbar^2 \Lambda_{UV}{}^2}{2m}$$

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

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

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

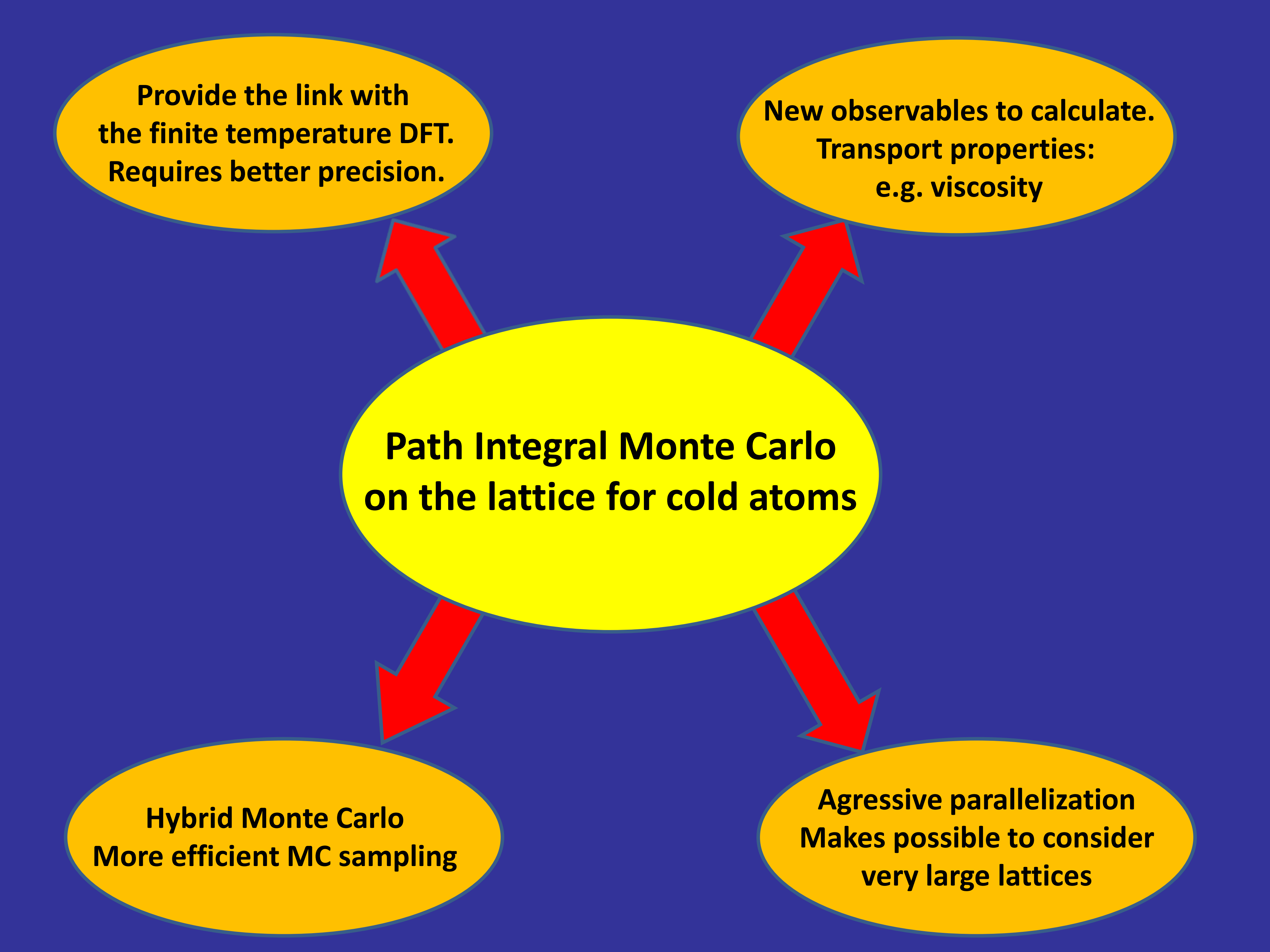
Running coupling constant g defined by lattice in the case of spherical momentum cutoff.

Trotter expansion (*trotterization* of the propagator)

$$Z(\beta) = \mathrm{Tr}\;\exp\left[-\beta\left(\hat{H} - \mu\hat{N}\right)\right] = \mathrm{Tr}\;\left\{\exp\left[-\tau\left(\hat{H} - \mu\hat{N}\right)\right]\right\}^{N_\tau}, \qquad \beta = \frac{1}{T} = N_\tau \tau$$

$$E(T) = \frac{1}{Z(T)}\mathrm{Tr}\;\hat{H}\exp\left[-\beta\left(\hat{H} - \mu\hat{N}\right)\right]$$

$$N(T) = \frac{1}{Z(T)}\mathrm{Tr}\;\hat{N}\exp\left[-\beta\left(\hat{H} - \mu\hat{N}\right)\right]$$


Provide the link with
the finite temperature DFT.
Requires better precision.
New observables to calculate.
Transport properties:
e.g. viscosity
Path Integral Monte Carlo
on the lattice for cold atoms
Hybrid Monte Carlo
More efficient MC sampling
Agressive parallelization
Makes possible to consider
very large lattices

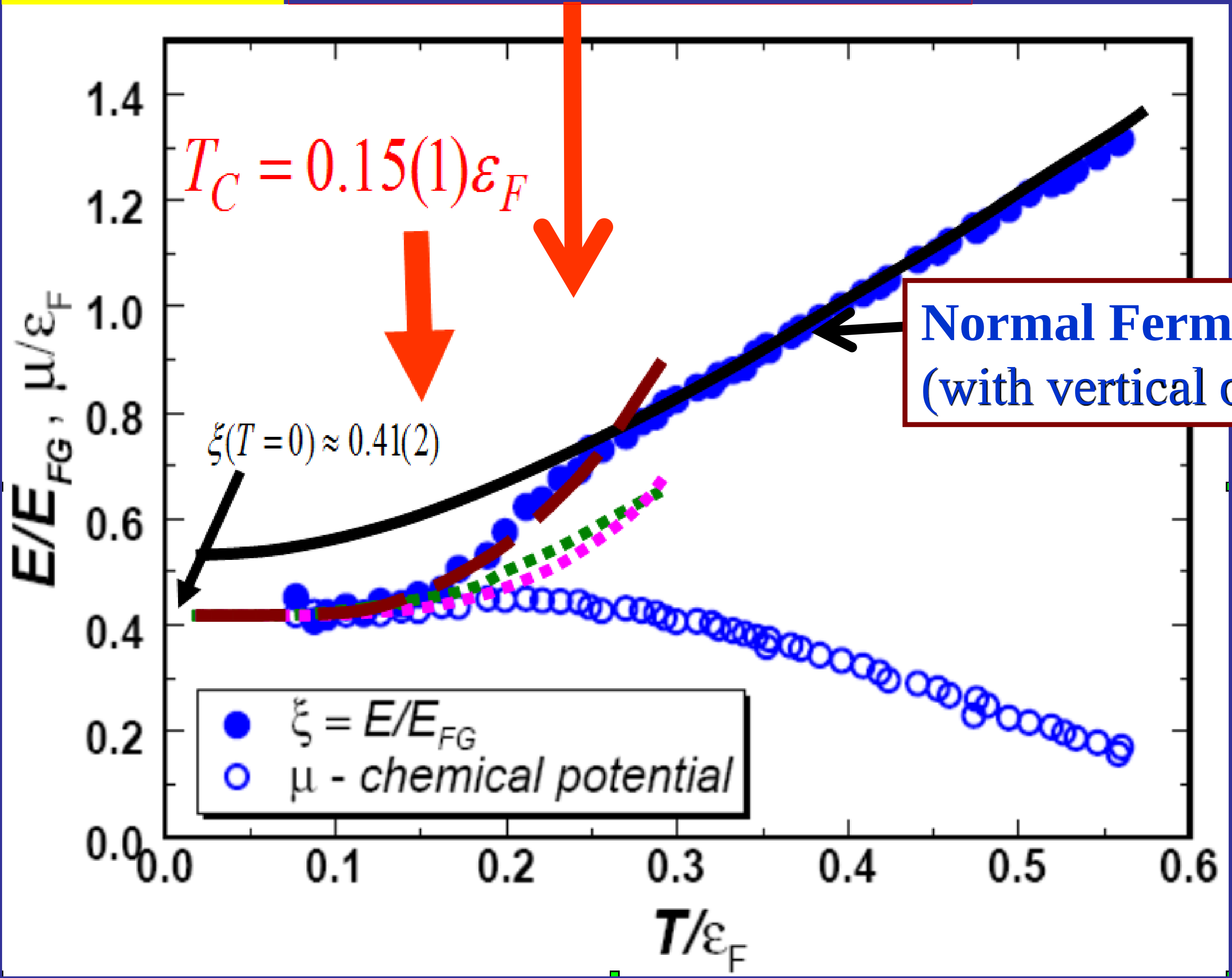
Equation of state from PIMC (Path Integral Monte Carlo)

$a = \pm\infty$

Deviation from Normal Fermi Gas

$L = 8$

$\rho \approx 0.1$



Normal Fermi Gas
(with vertical offset, solid line)

A. Bulgac, J.E. Drut, P. Magierski, PRL96,090404(2006)

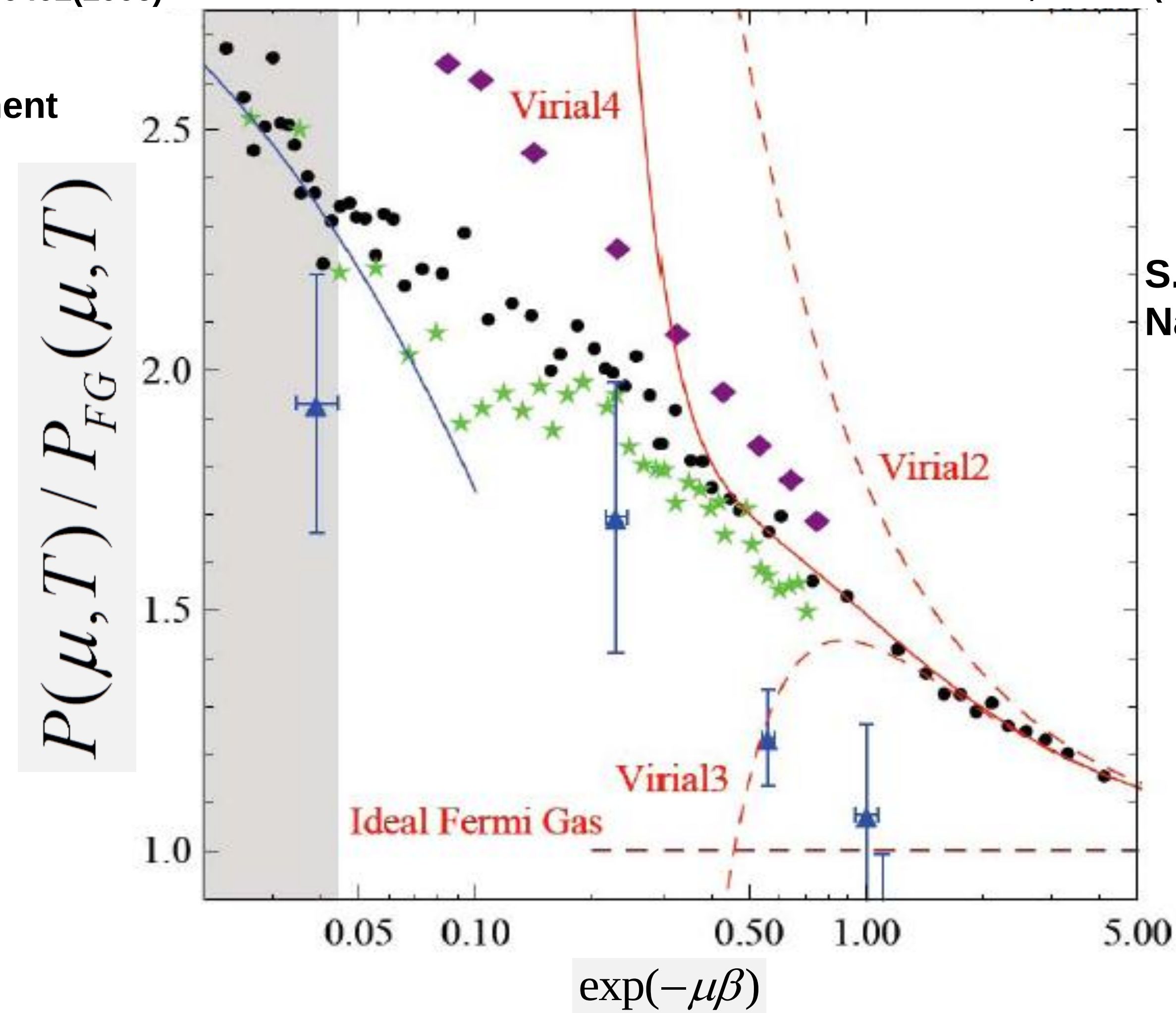
Comparison with Many-Body Theories (1)

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

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

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

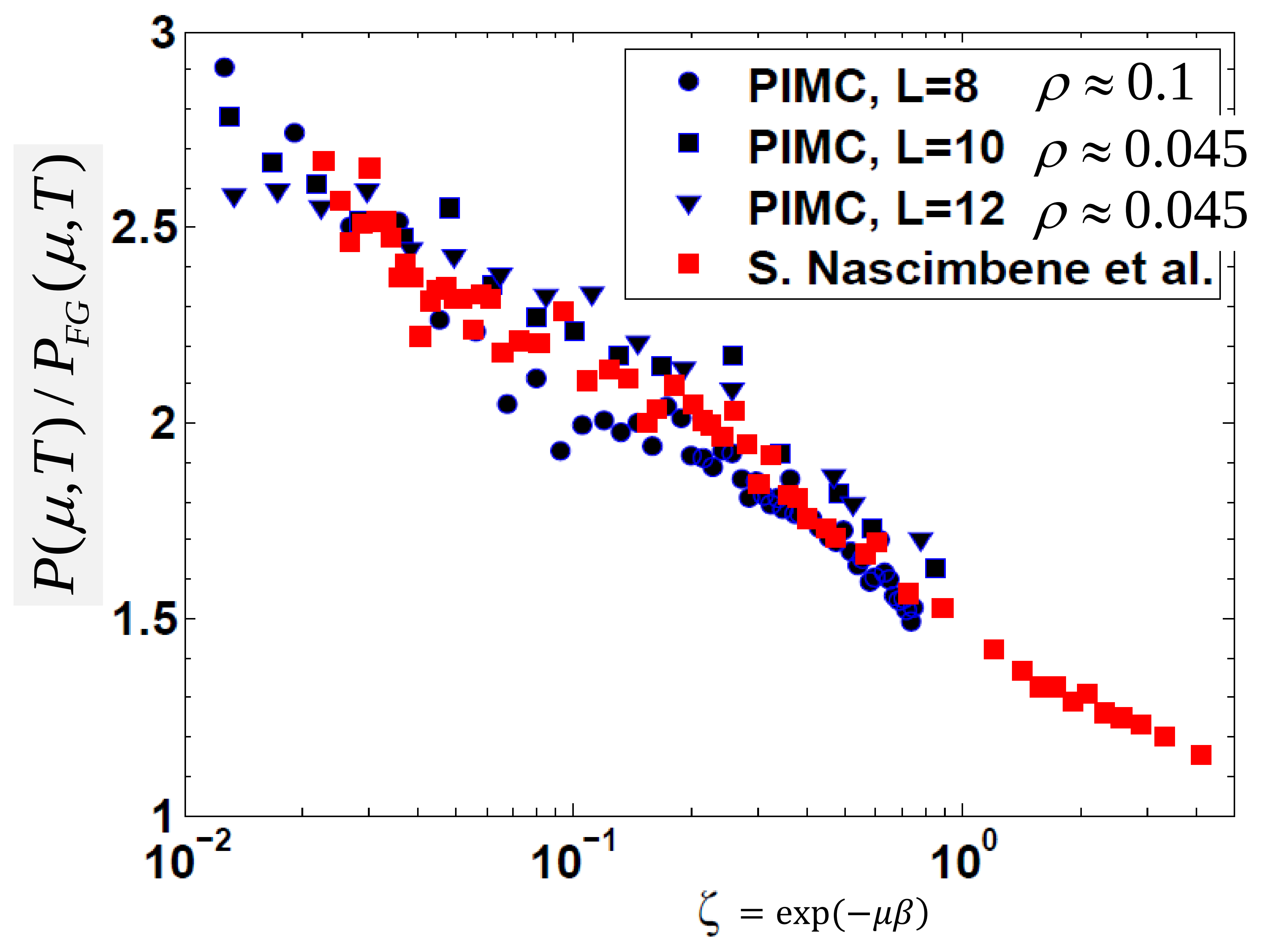
● **Experiment**

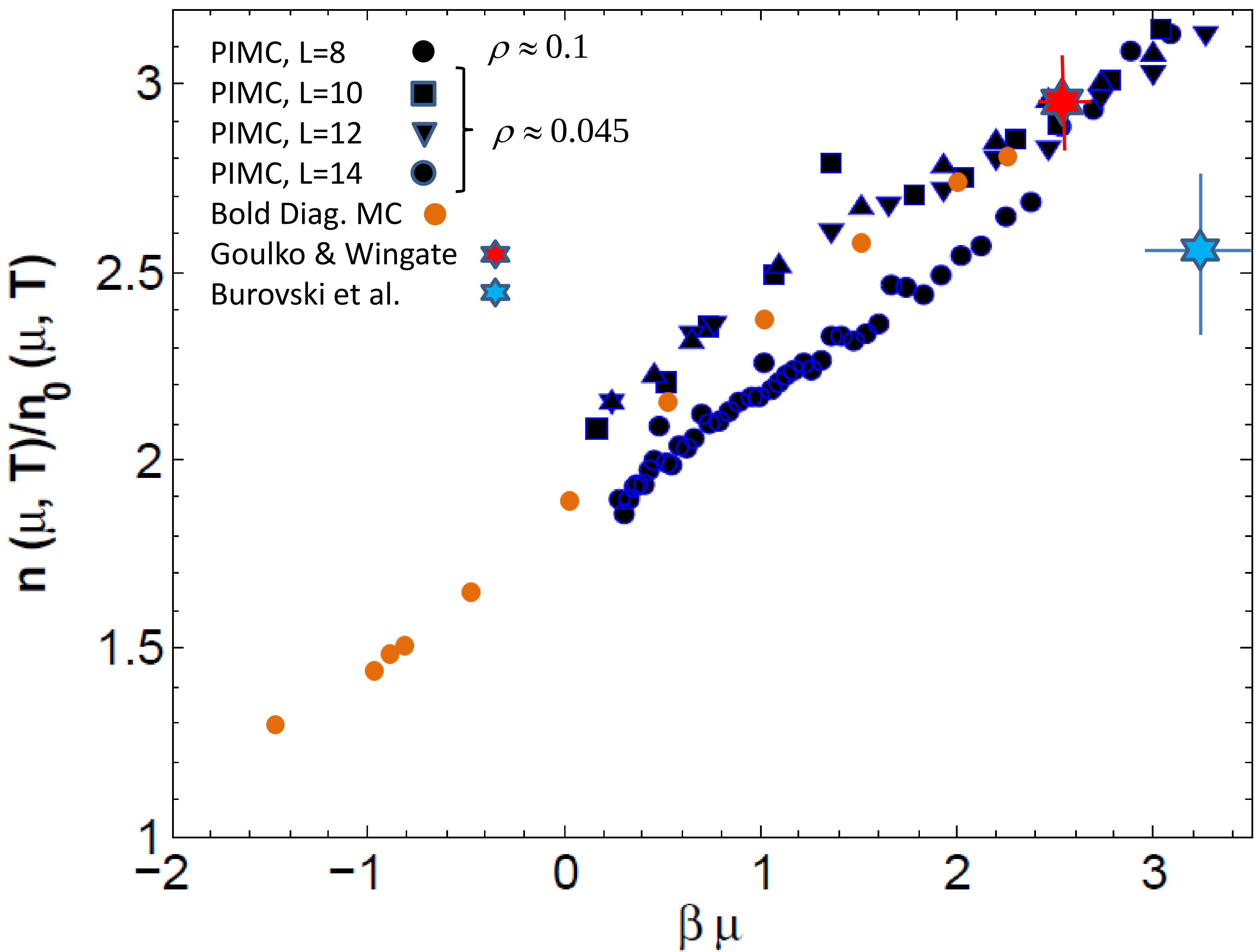


S. Nascimbene et al.
Nature 463, 1057 (2010)

Courtesy of C. Salomon

Pressure vs temperature:
experiment and PIMC theory for various lattice sizes

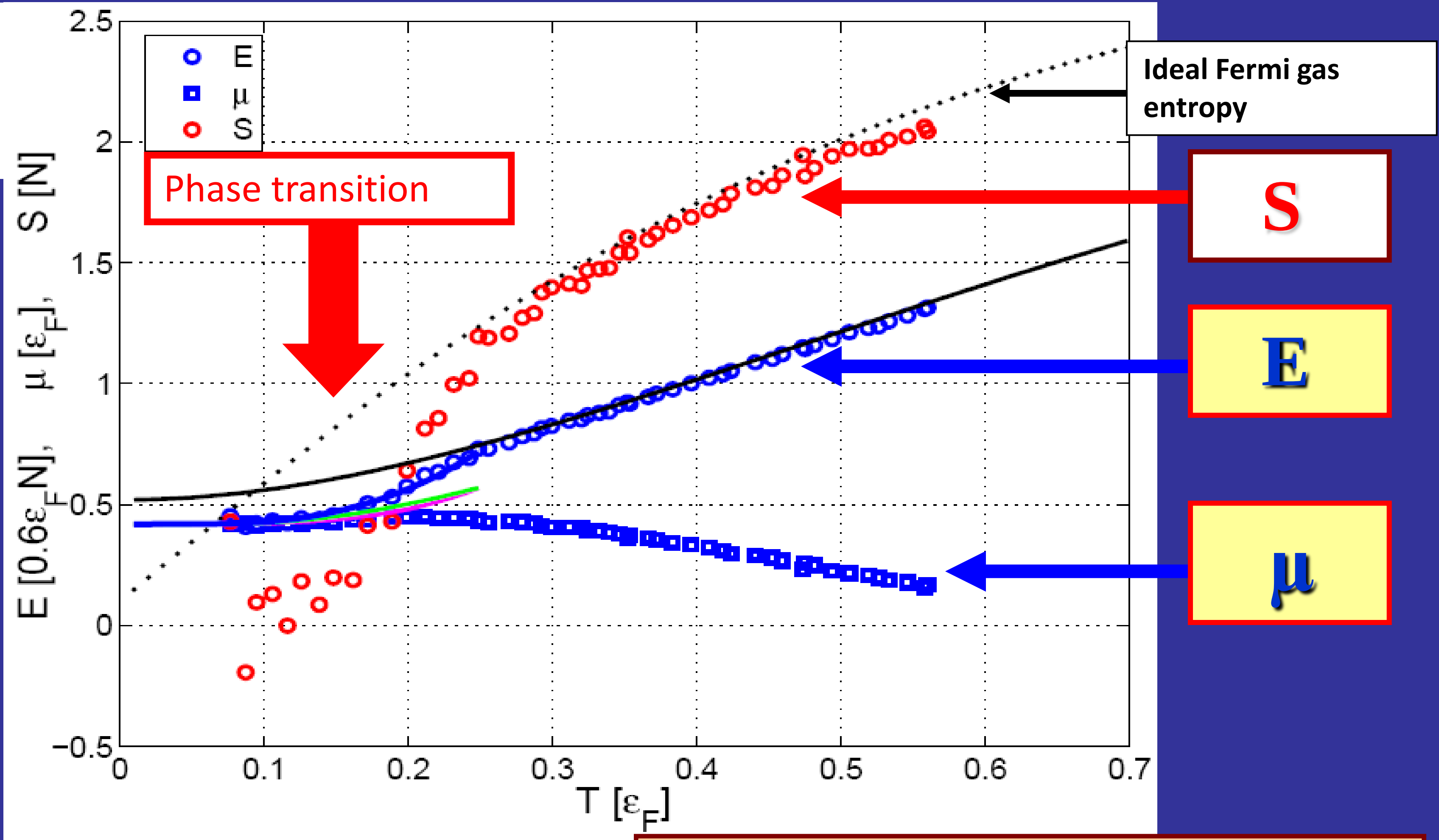




PIMC, L=8
PIMC, L=10
PIMC, L=12
PIMC, L=14
Bold Diag. MC
Goulko & Wingate
Burovski et al.
$\rho \approx 0.1$
$\rho \approx 0.045$
n (μ, T)/n_0 (μ, T)
β μ
1
1.5
2
2.5
3
−2
−1
0
1
2
3

$L = 8$

$\rho \approx 0.1$



$$E = \frac{3}{5}\varepsilon_F(n)N\ \xi\left(\frac{T}{\varepsilon_F(n)}\right)$$

$$n = \frac{N}{V} = \frac{k_F^3}{3\pi^2}, \qquad \varepsilon_F(n) = \frac{\hbar^2 k_F^2}{2m}$$

$$S(T) = S(0) + \int_0^T \frac{\partial E}{\partial T}\frac{dT}{T}$$

$$S(T) = \frac{3}{5}N\int_0^{T/e_F} dy\,\frac{\xi'(y)}{y}$$

Theory: local density approximation (LDA)

Uniform system

$$\Omega = F - \lambda N = \frac{3}{5}\varphi(x)\varepsilon_F N - \lambda N$$

Nonuniform system

(gradient corrections neglected)

$$\Omega = \int d^3 r \left[\frac{3}{5}\varepsilon_F(\vec{r})\varphi(x(\vec{r})) + U(\vec{r}) - \lambda\right] n(\vec{r})$$

$$x(\vec{r}) = \frac{T}{\varepsilon_F(\vec{r})}; \quad \varepsilon_F(\vec{r}) = \frac{\hbar^2}{2m}\left[3\pi^2 n(\vec{r})\right]^{2/3}$$

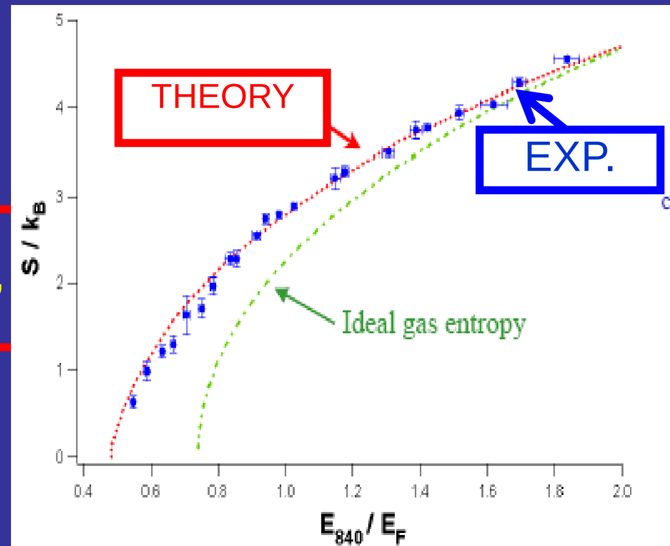
The overall chemical potential λ and the temperature *T* are constant throughout the system. The density profile will depend on the shape of the trap as dictated by:

$$\frac{\delta\Omega}{\delta n(\vec{r})} = \frac{\delta(F - \lambda N)}{\delta n(\vec{r})} = \mu(x(\vec{r})) + U(r) - \lambda = 0$$

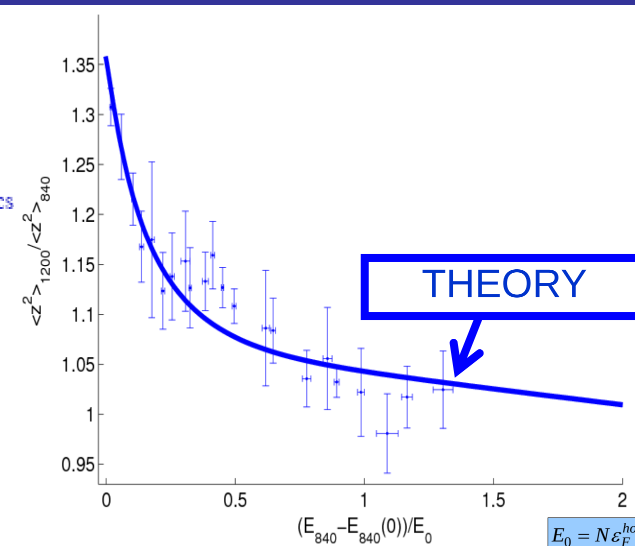
Using as an input the Monte Carlo results for the uniform system and experimental data (trapping potential, number of particles), we determine the density profiles.

Unitary Fermi gas (^{6}Li atoms) in a harmonic trap

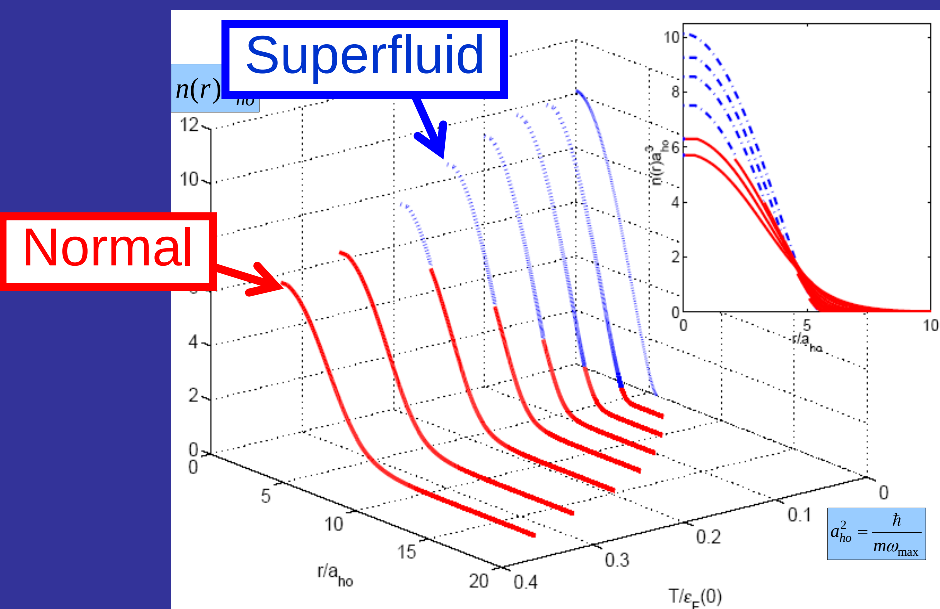
Experiment:
Luo, Clancy, Joseph, Kinast, Thomas, Phys. Rev. Lett. 98, 080402, (2007)



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.



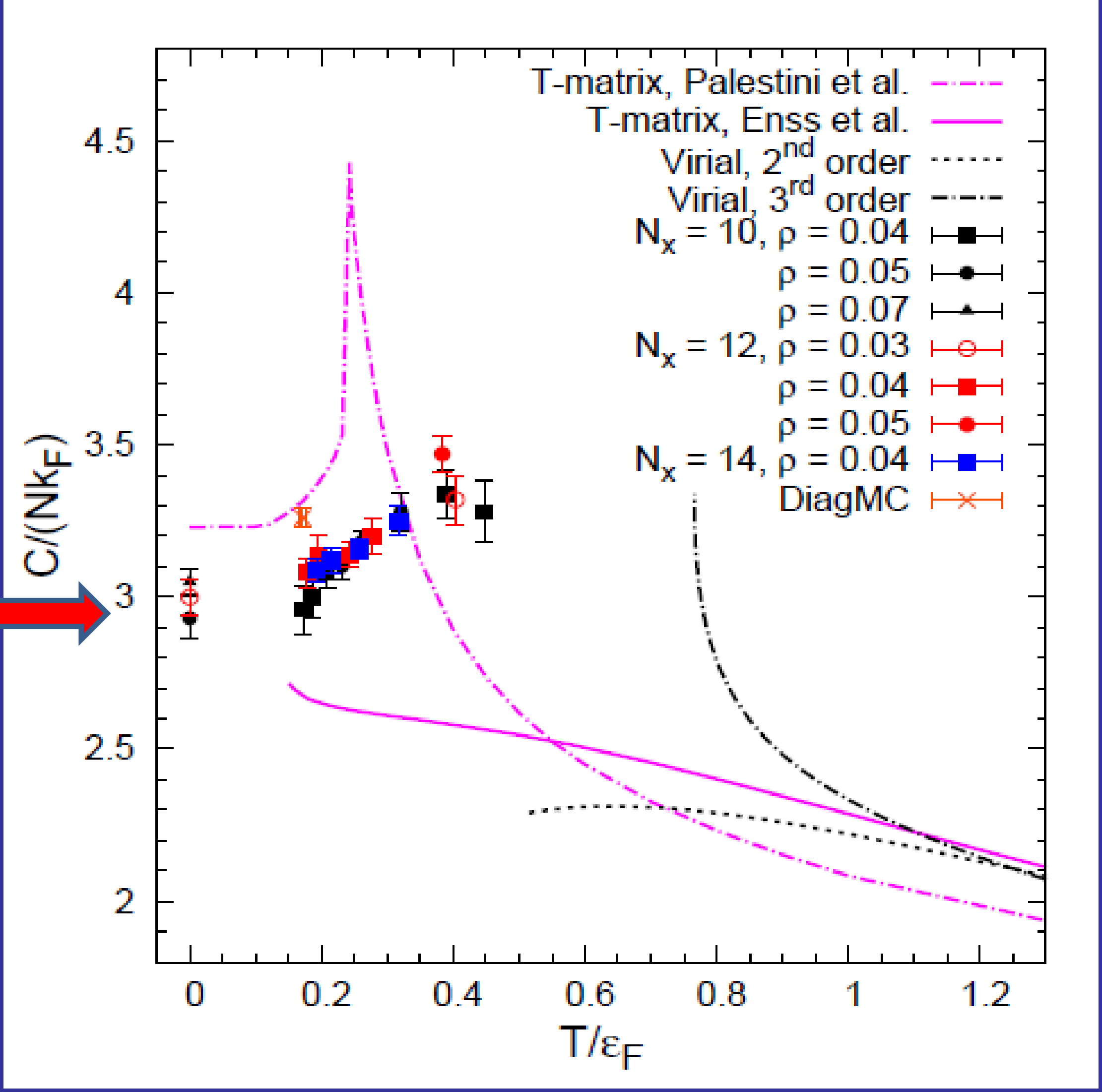
Full *ab initio* theory (no free parameters): LDA + QMC input
Bulgac, Drut, Magierski, Phys. Rev. Lett. 99, 120401 (2007)

$\varepsilon_F(0)$ - Fermi energy at the center of the trap

The radial (along shortest axis) density profiles of the atomic cloud at various temperatures.

Contact at finite T: $C(T) = \lim_{k\to\infty} k^4 n(k,T)$

$C(T=0)/(Nk_F) \simeq 2.9 \pm 0.1$



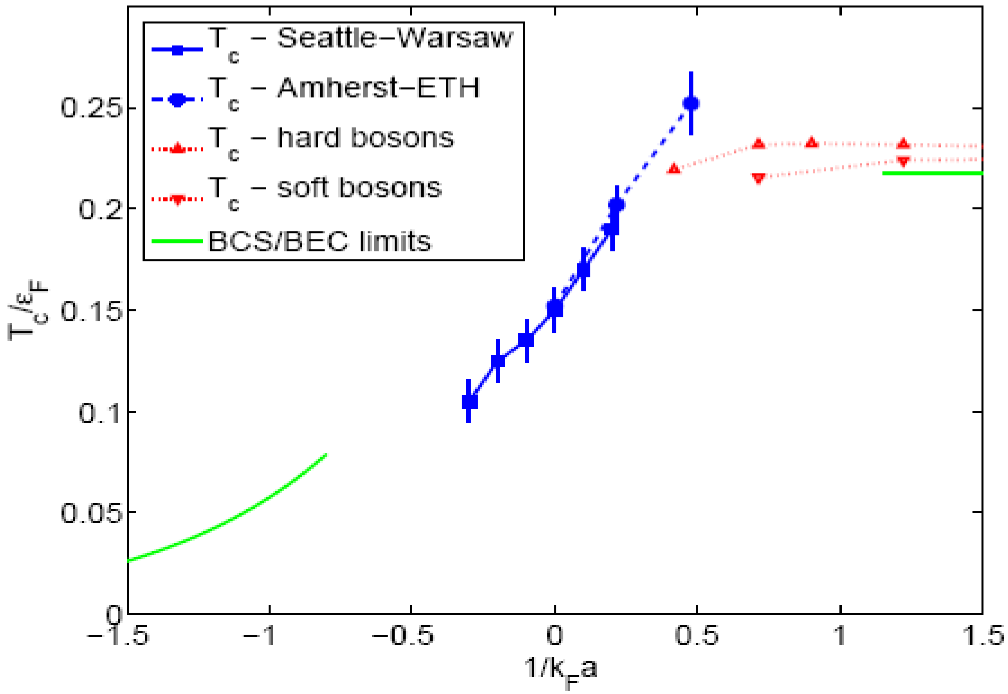
Diffusion Monte Carlo results:

$C(T=0)/(Nk_F) \simeq 3.4$

Combescot, Giorgini,Stringari Europhys.Lett.75,695(2006)

Lobo et al. PRL 97,100405(2006

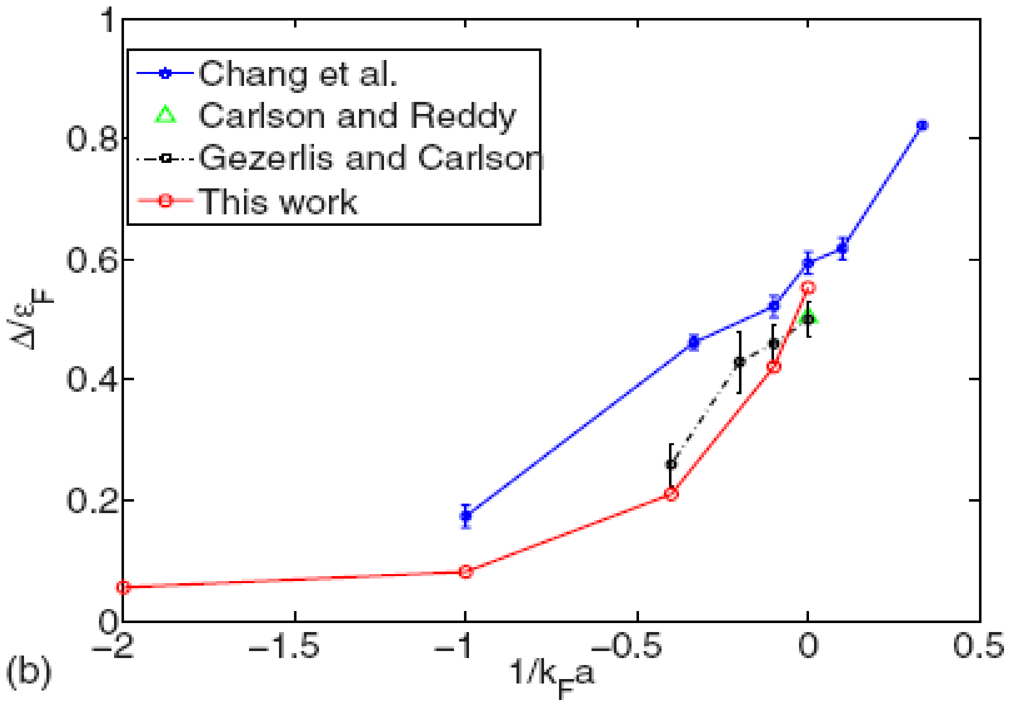
Drut, Lähde,Ten, arXiv:1012.5474, PRL in press



Results in the vicinity of the unitary limit:

-Critical temperature

-Pairing gap at T=0



BCS theory predicts:

$$\Delta(T=0)/T_C \approx 1.7$$

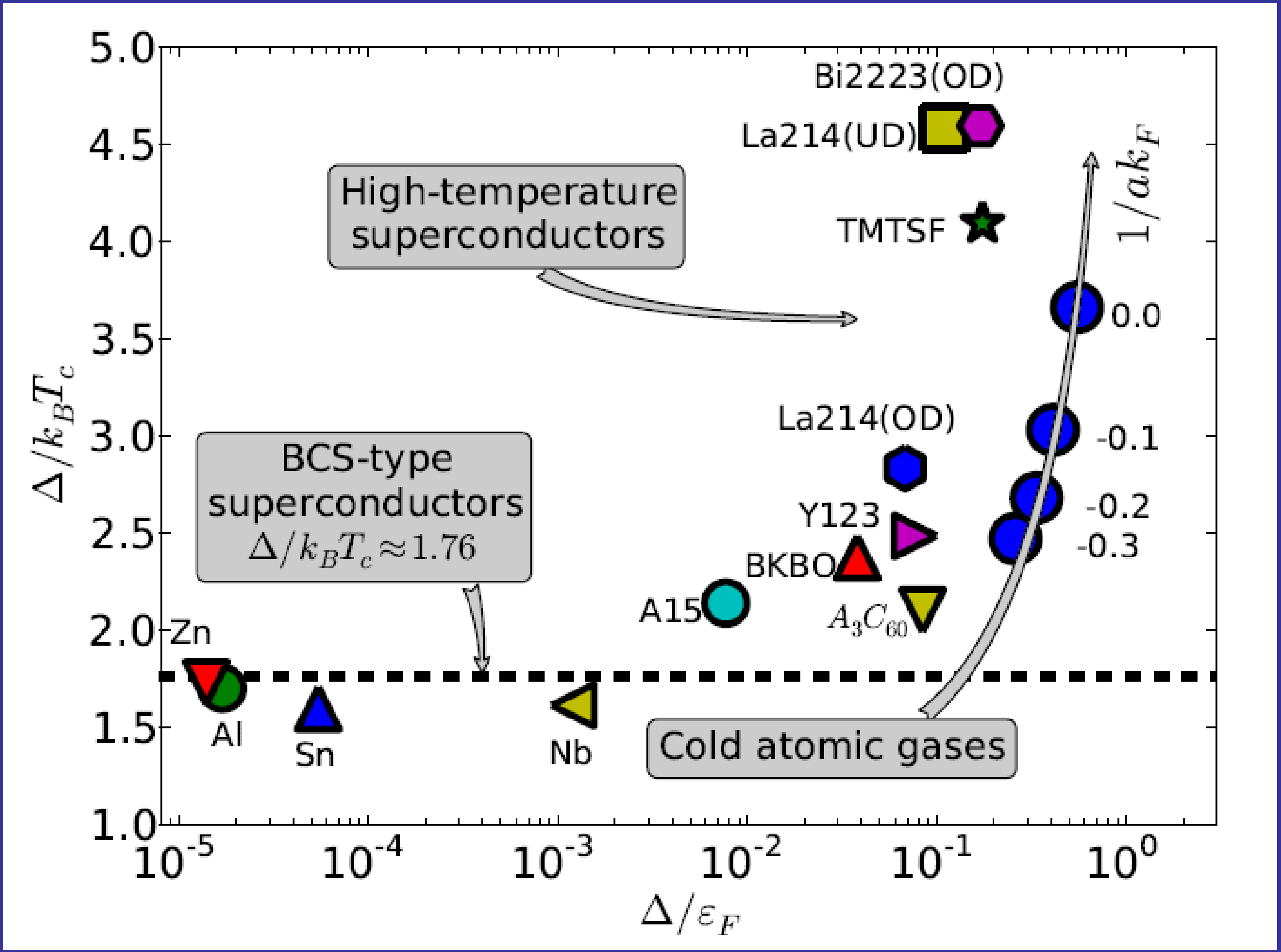
At unitarity:

$$\Delta(T=0)/T_C \approx 3.3$$

This is NOT a BCS superfluid!

Bulgac, Drut, Magierski, PRA78, 023625(2008)

Cold atomic gases and high Tc superconductors



Spectral weight function: $A(\vec{p},\omega)$

$$G^{ret/adv}(\vec{p},\omega)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}d\omega'\frac{A(\vec{p},\omega')}{\omega-\omega'\pm i0^{+}}$$

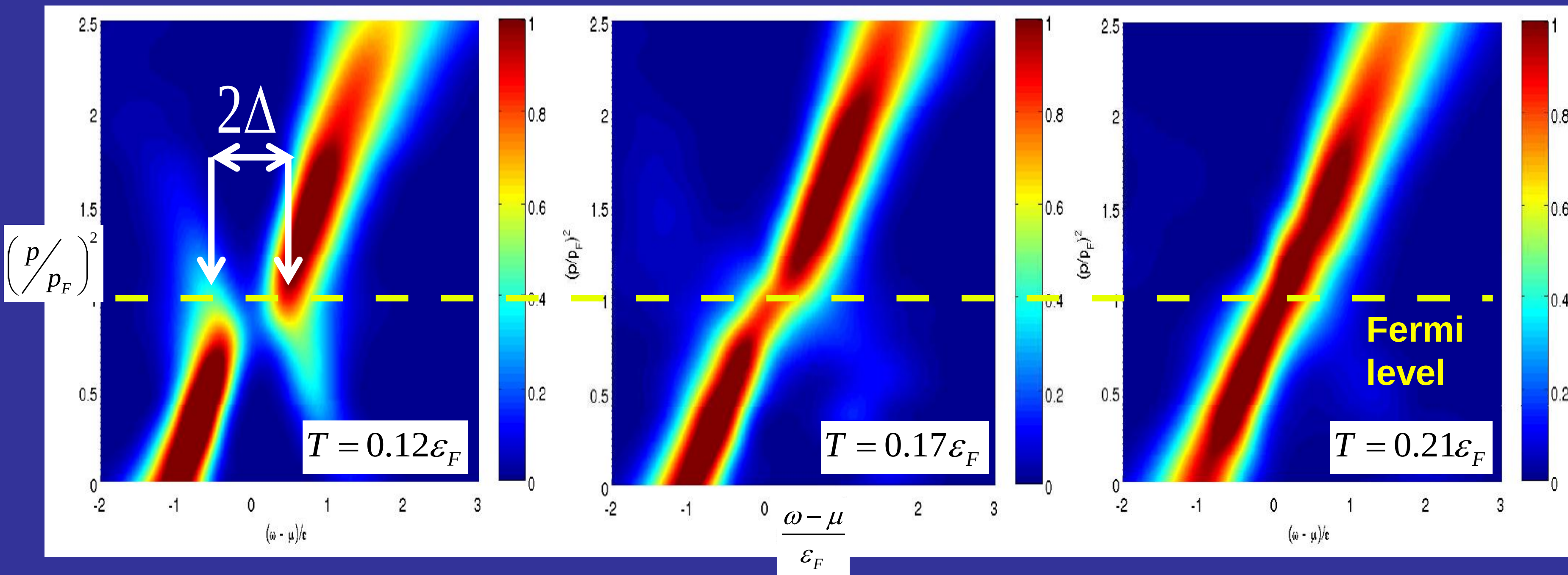
$$G(\vec{p},\tau)=-\frac{1}{2\pi}\int_{-\infty}^{+\infty}d\omega A(\vec{p},\omega)\frac{e^{-\omega\tau}}{1+e^{-\beta\omega}}$$

From Monte Carlo calcs.

$$G(\vec{p},\tau)=\frac{1}{Z}Tr\{e^{-(\beta-\tau)(\hat{H}-\mu\hat{N})}\hat{\psi}_{\uparrow}(\vec{p})e^{-\tau(\hat{H}-\mu\hat{N})}\hat{\psi}^{+}_{\uparrow}(\vec{p})\}$$

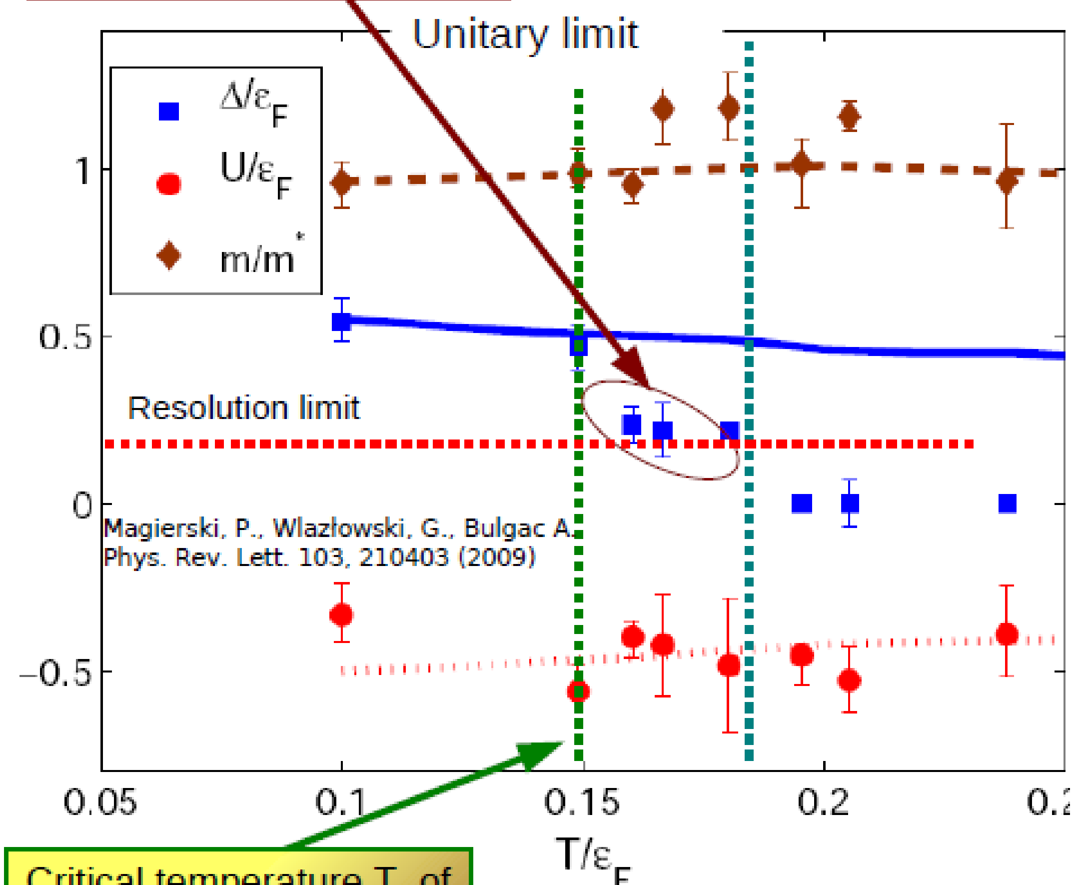
Spectral weight function from PIMC at unitarity

Superfluid phase | Pseudogap regime | Normal Fermi gas



Energy gap for unitary limit

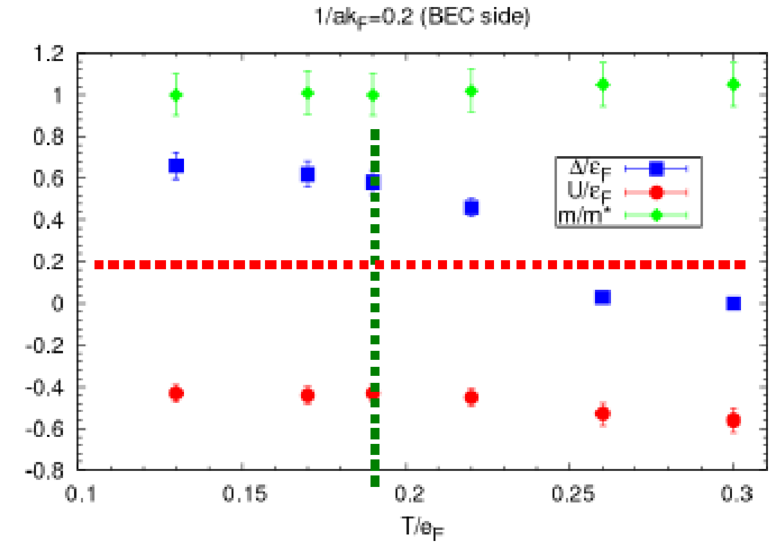
The energy gap exists above the critical temperature!

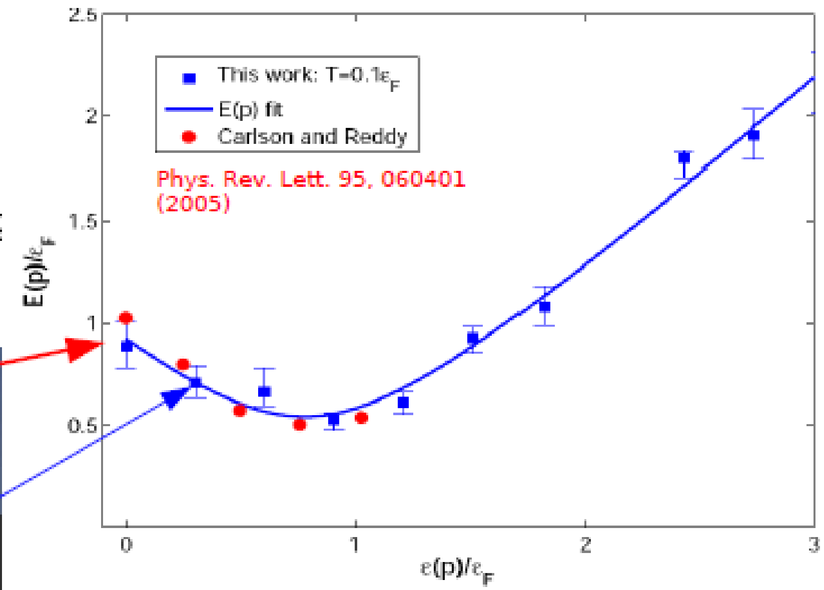


Critical temperature T_c of the superfluid-normal phase transition

Fix node MC calculations at T=0

Quasiparticle spectrum extracted from the spectral function at $T=0.1e_F$





Single-particle properties

$$E(p) = \sqrt{\left(\frac{p^2}{2m^*} + U - \mu\right)^2 + \Delta^2}$$

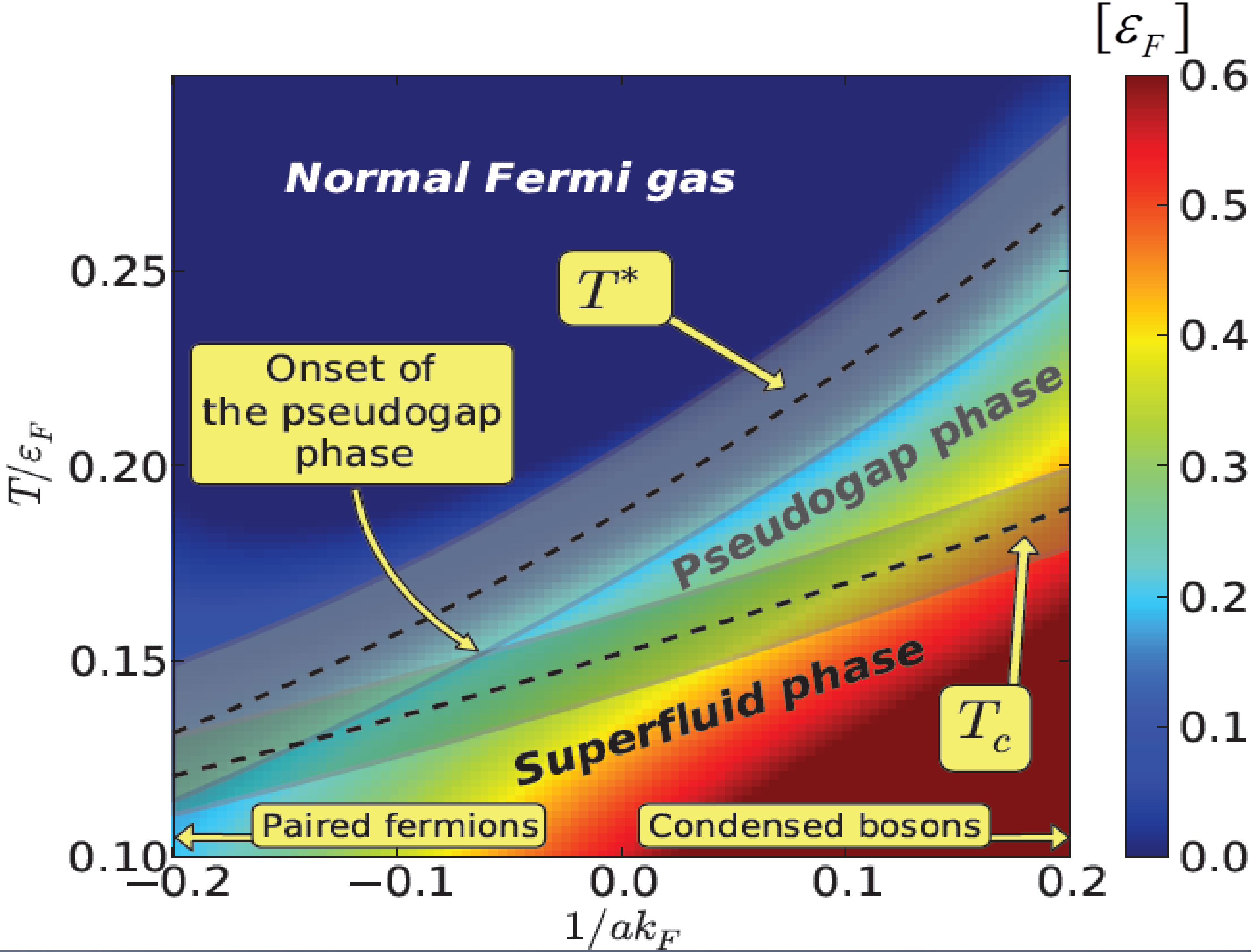
Effective mass: $m^* = (1.0 \pm 0.2)m$

Self energy: $U = (0.5 \pm 0.2)m$

Weak temperature dependence!

P.Magierski, G. Wlazłowski, A. Bulgac, J.E. Drut, PRL103, 210403 (2009)

Gap in the single particle fermionic spectrum from MC calcs.



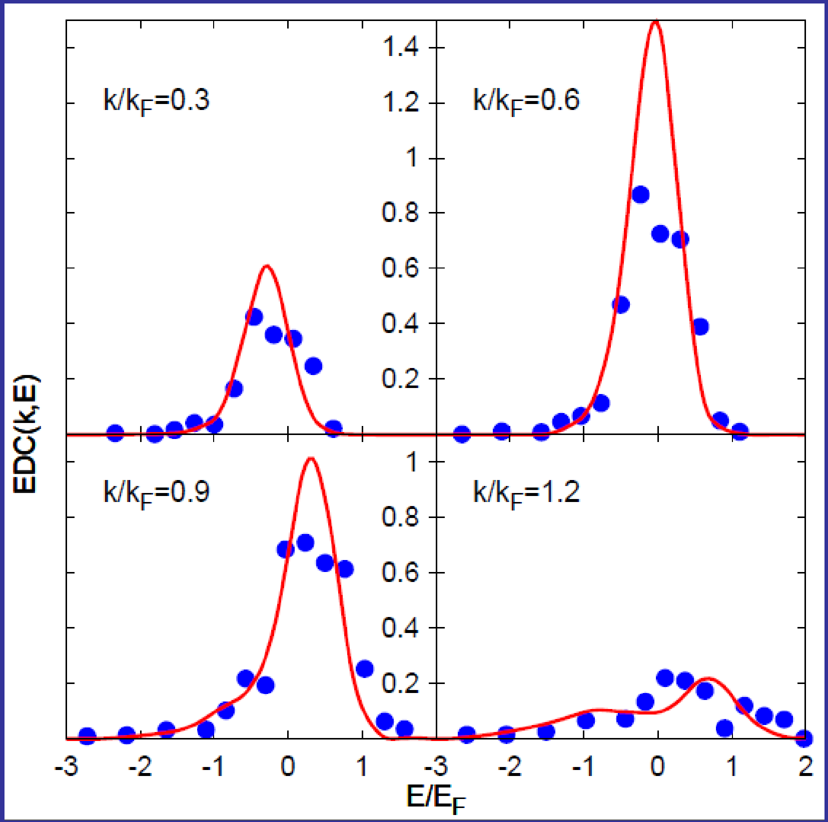
Ab initio **result: The onset of pseudogap phase at $1/ak_F \approx -0.05$.**

Magierski, Wlazłowski, Bulgac, arXiv1103.4382

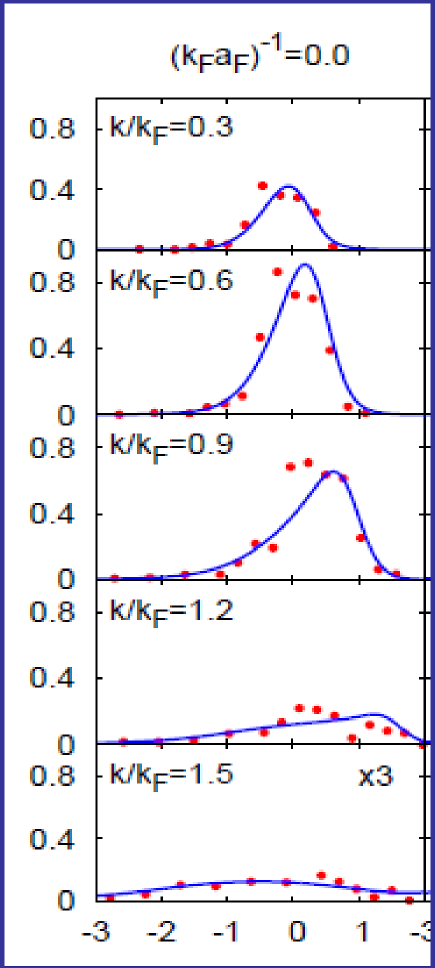
Theory vs Experiment (photoemission spectr.)

$$EDC(k,E) \sim A(k,\omega) f(\omega)$$

PIMC



Non selfconsistent t-matrix approx.



Perali, A., Palestini, F., Pieri, P., Strinati, G.C., Stewart, J.T., Gaebler, J.P., Drake, T.E. & Jin, Phys. Rev. Lett. 106, 060402 (2011)

Pseudogap in cold atoms - summary :

Theory:

Selfconsistent t-matrix approach	-	NO
Nonselfconsistent t-matrix approach	-	YES (large)
Dynamic Mean Field Theory	-	YES
PIMC (AFMC)	-	YES (moderate)