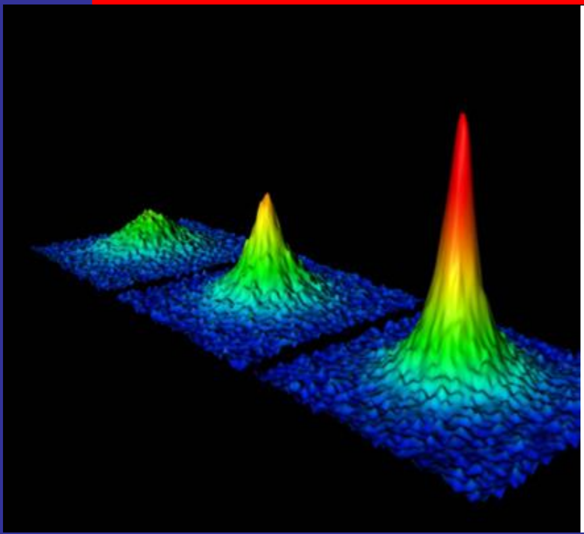
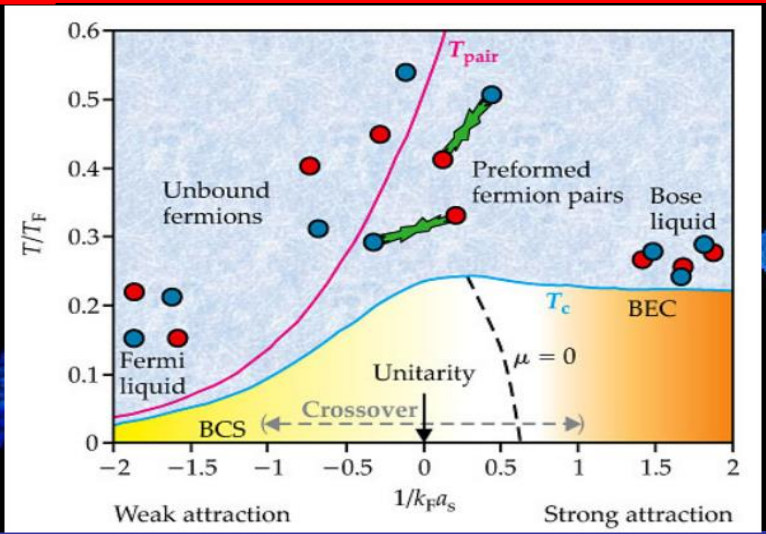
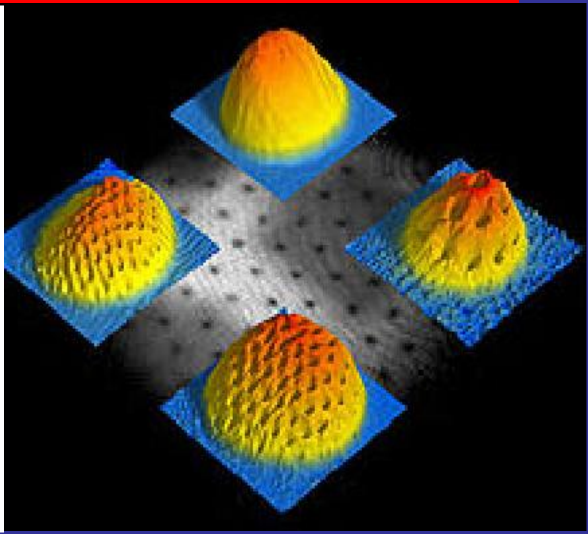
Equilibrium and nonequilibrium properties of unitary Fermi gas from Quantum Monte Carlo







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G. Wlazłowski - Univ. of Washington/Warsaw Univ. of Techn.

Outline

- BCS-BEC crossover. Unitary regime.
- Theoretical approach: Path Integral Monte Carlo (QMC)
- Equation of state for the Fermi gas in the unitary regime.
- Pairing gap and pseudogap. Spin susceptibility, conductivity and diffusion.
- Viscosity.

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

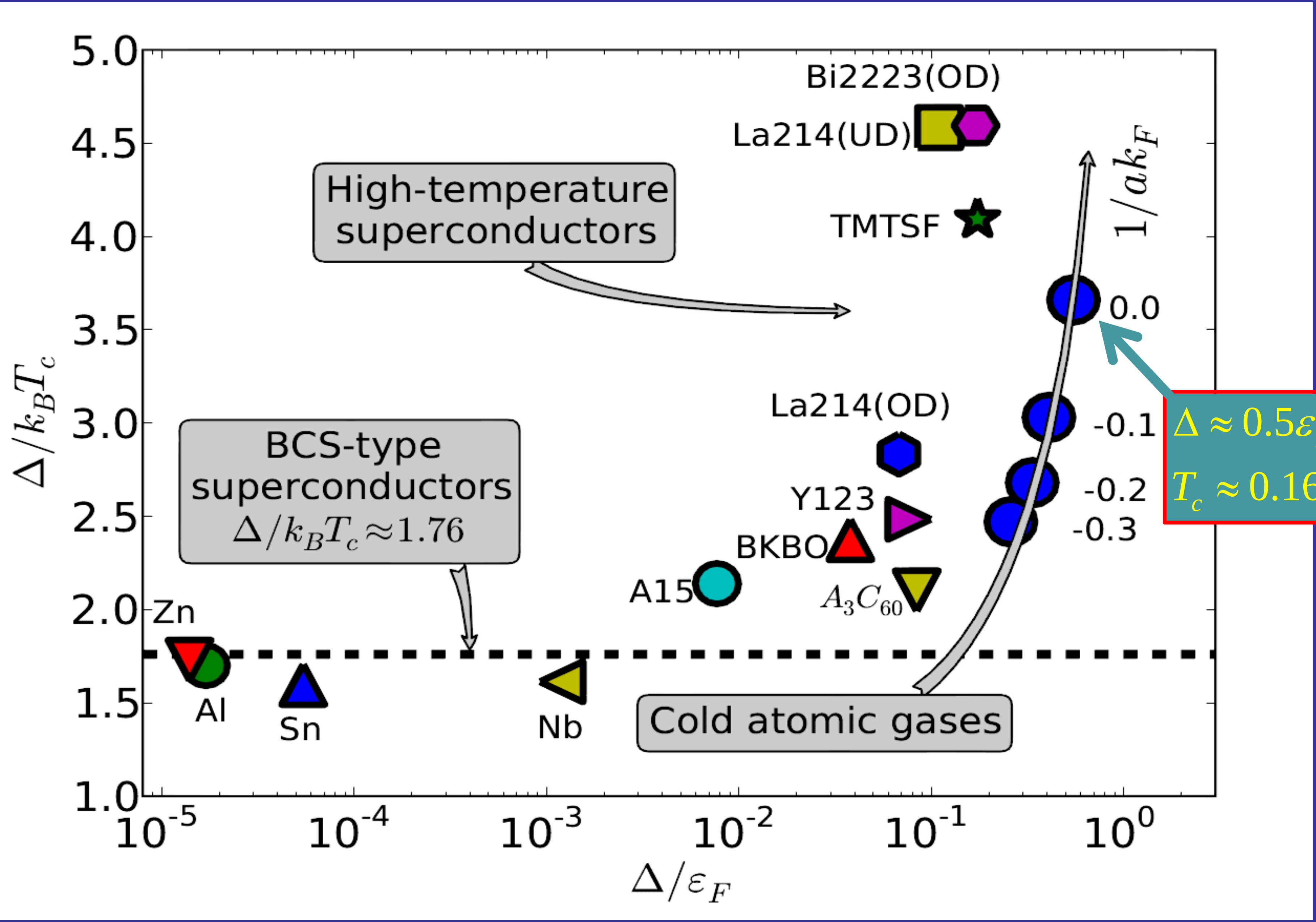
System is dilute but strongly interacting!

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

$\xi(0) = 0.37(1)$ - **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)

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

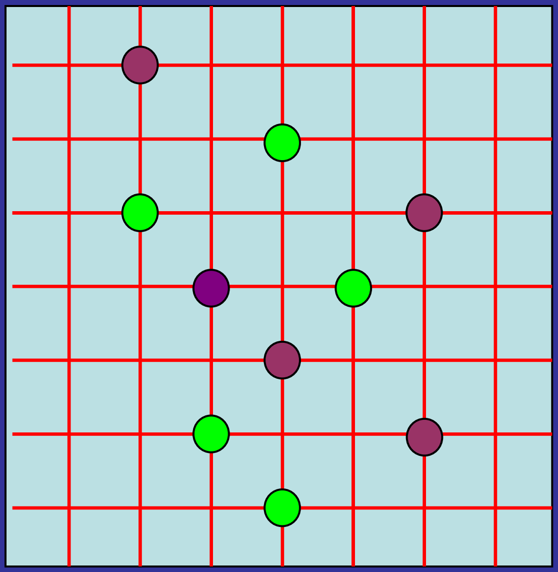
$Volume = L^3$

$lattice\ spacing = \Delta x$

Coordinate space

L –limit for the spatial correlations in the system

$k_{cut} = \frac{\pi}{\Delta x}$; Δx



- Spin up fermion: ↑

- Spin down fermion: ↓

External conditions:

T - temperature

μ - chemical potential

Periodic boundary conditions imposed

Basics of Auxiliary Field Monte Carlo (Path Integral MC)

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

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

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

Running coupling constant g defined by lattice

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

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

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

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

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

$$\mathrm{Tr}\,\hat{U}(\{\sigma\}) = \{\det[1 + \hat{U}_\uparrow(\sigma)]\}^2 = \exp[-S(\{\sigma\})] > 0$$

- No sign problem for spin symmetric system!

Details of calculations, improvements and problems

• Currently we can reach 14^3 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%.

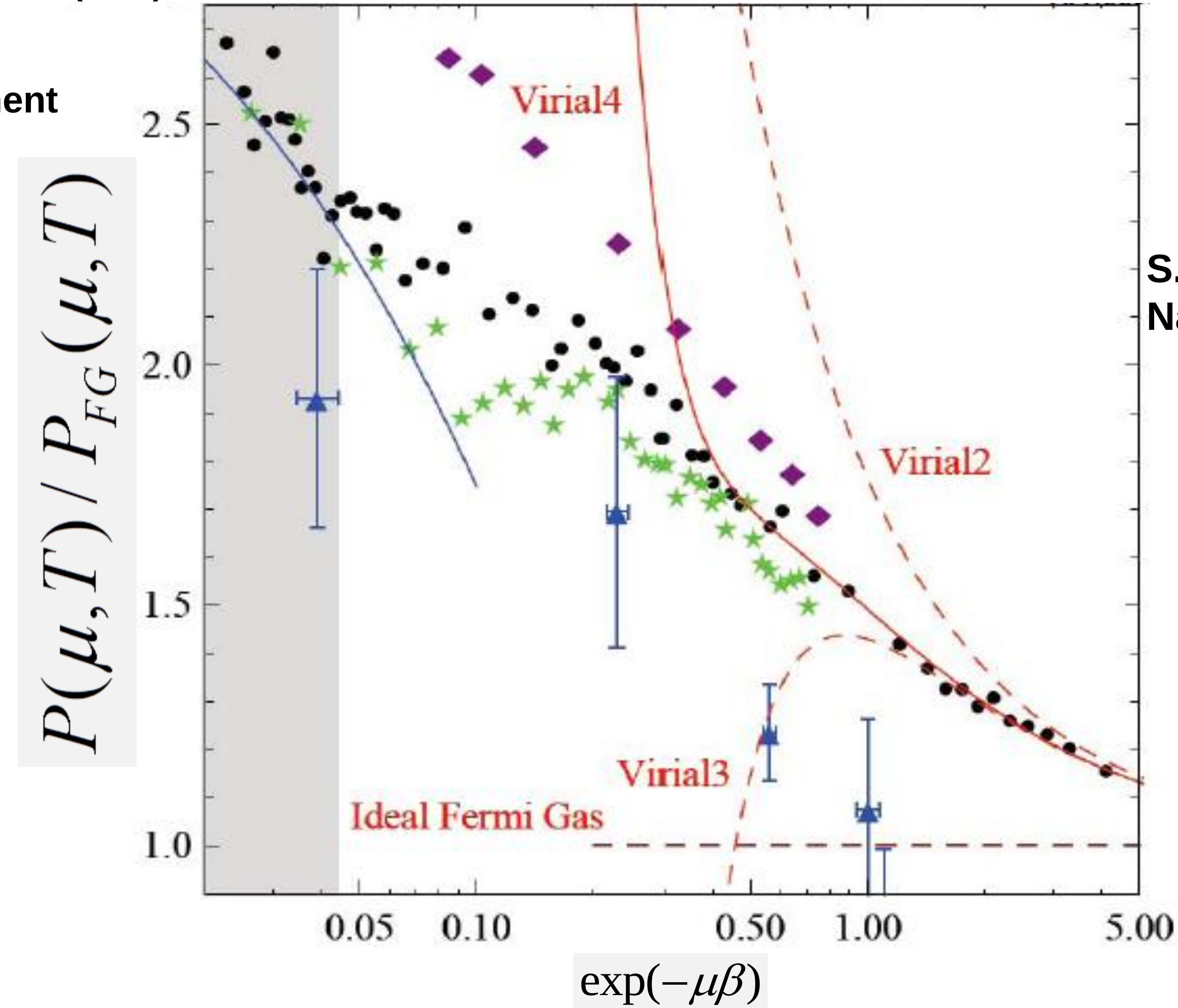
Comparison with Many-Body Theories (1)

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

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

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

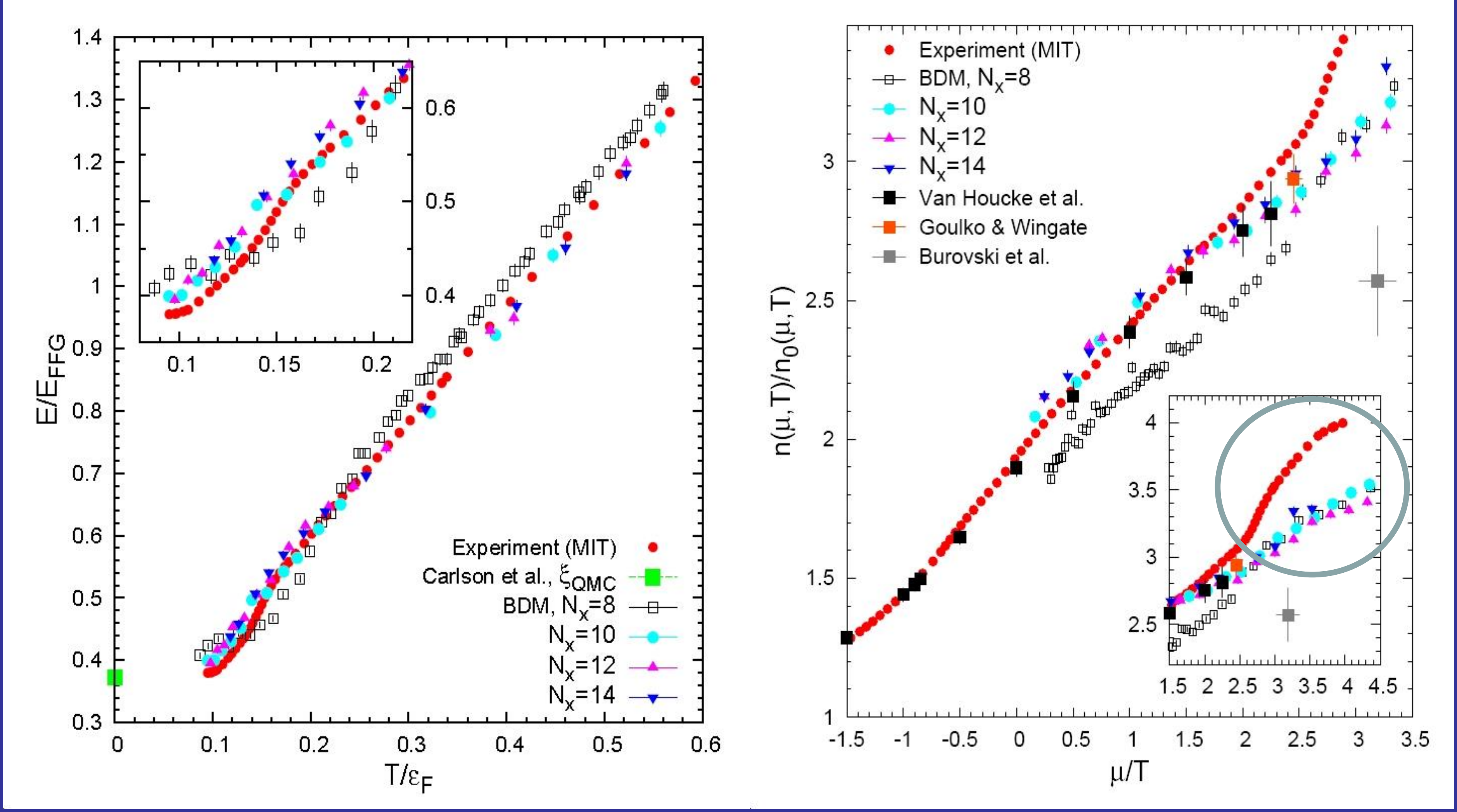
● **Experiment**



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

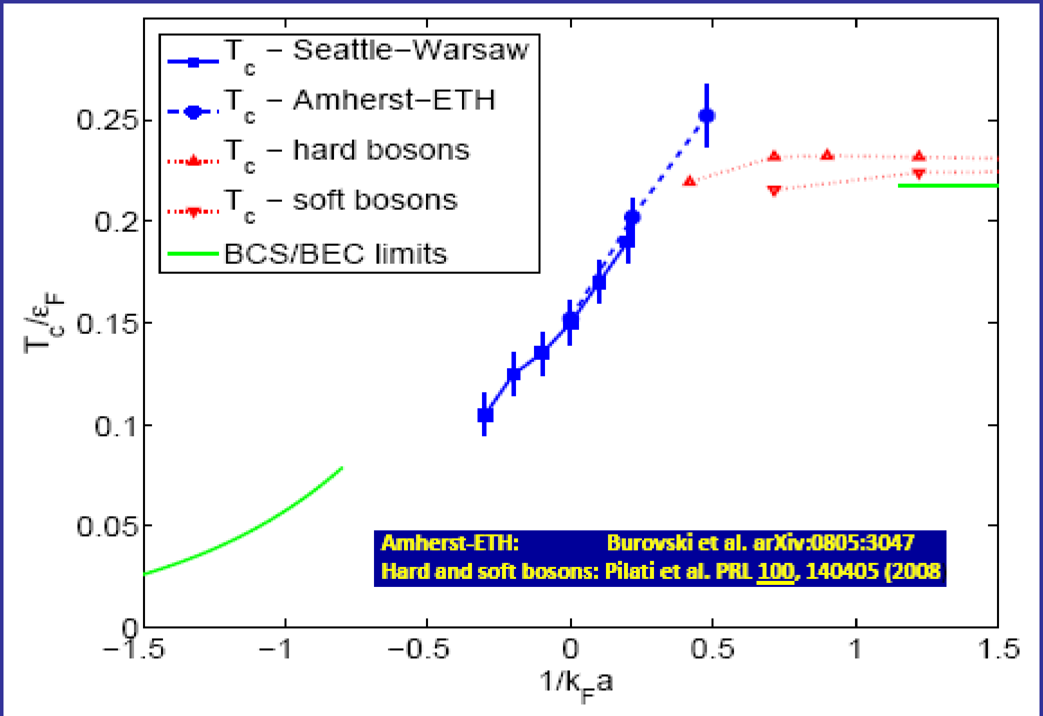
Courtesy of C. Salomon

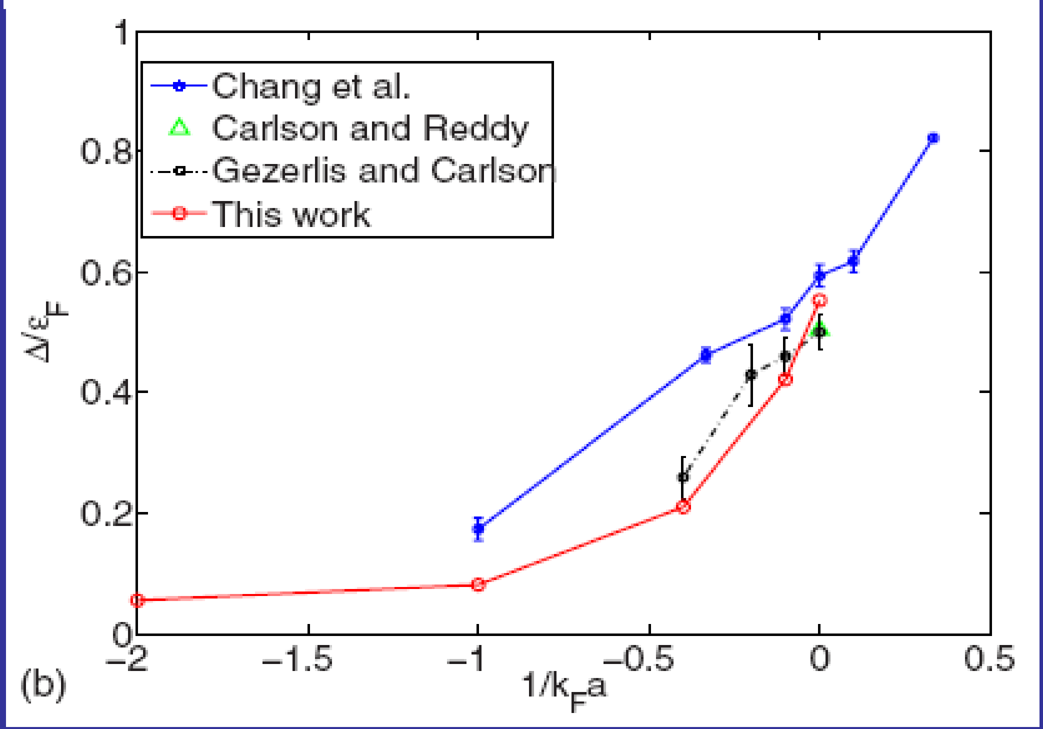
Equation of state of the unitary Fermi gas - current status



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)





Results in the vicinity of the unitary limit:

-Critical temperature

-Pairing gap

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)

Pairing gap from spectral function::

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.

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

Constraints

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

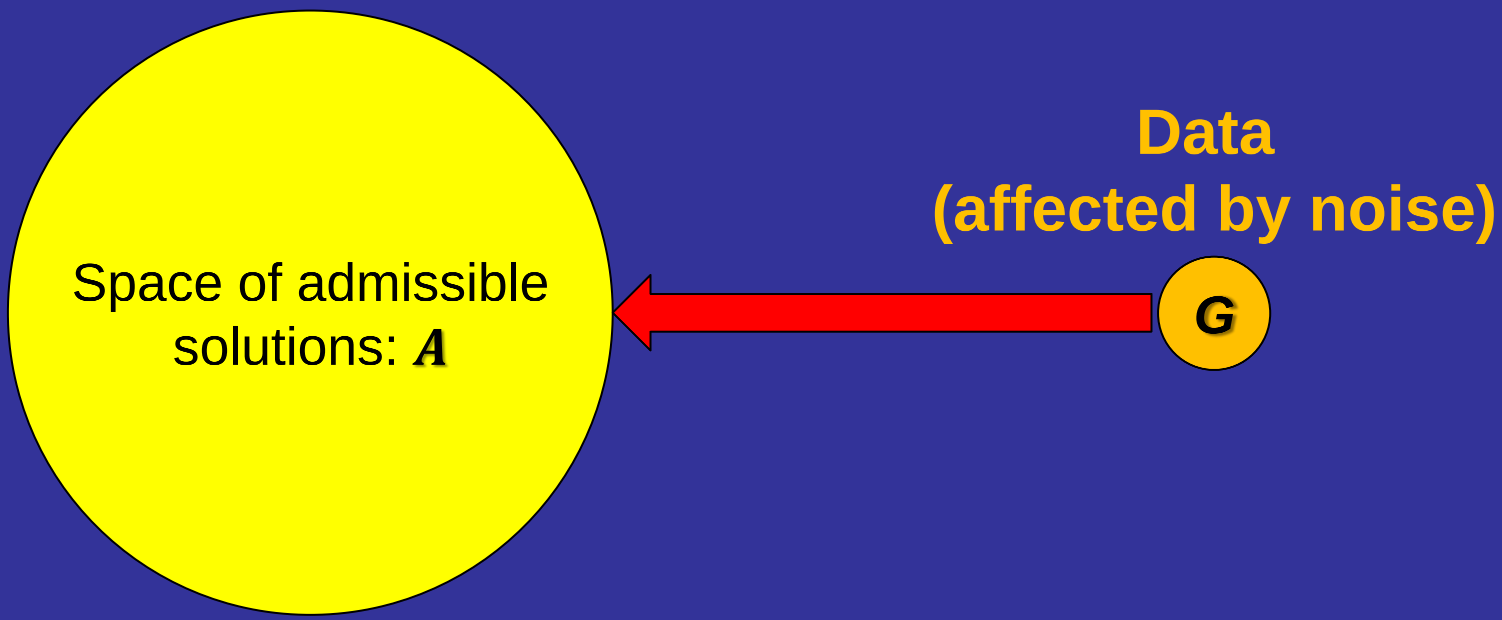
$$\int_{-\infty}^{+\infty} A(\vec{p},\omega)(1+e^{\beta\omega})^{-1}\frac{d\omega}{2\pi} = n(\vec{p})$$

In the limit of independent quasiparticles: $A(\vec{p},\omega) = 2\pi\delta(\omega - E(p))$

<u>Linear inverse problem</u>

$$G(y) = \int_{-\infty}^{\infty} K(x, y) A(x) dx,$$

G is known from QMC with some error for a number of values of y, usually uniformly distributed within the interval: (0, 1/T)



One needs to associate a probability distribution in the space of solutions under condition that G is known with certain accuracy: P(A|$\tilde{G}$)

Maximum entropy method (MEM):

Bayes' theorem:

$$p(\vec{A}|\vec{\tilde{G}}) = \frac{p(\vec{\tilde{G}}|\vec{G})p(\vec{A})}{p(\vec{\tilde{G}})},$$

Maximization of conditional probability leads to minimization of:

$$F(\vec{A}) = \frac{1}{2}\sum_{i=1}^{N_\tau}\left(\frac{\tilde{G}_i - G_i}{\sigma_i}\right)^2 + \alpha \sum_{i=1}^{N} A_i \log \frac{A_i}{\mathcal{M}_i}.$$

Relative entropy term

<u>Problem:</u> if „alpha" is too small then the procedure is numerically unstable.
If it is too large then the entropy term is too restrictive.

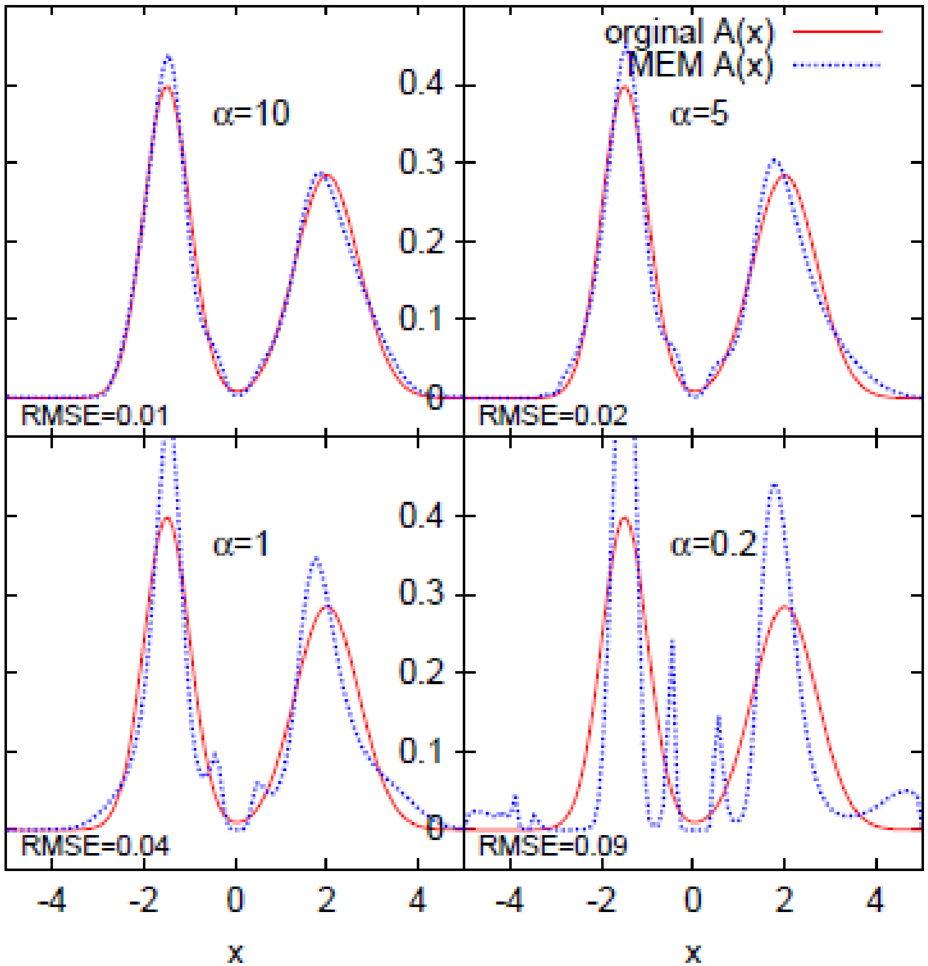
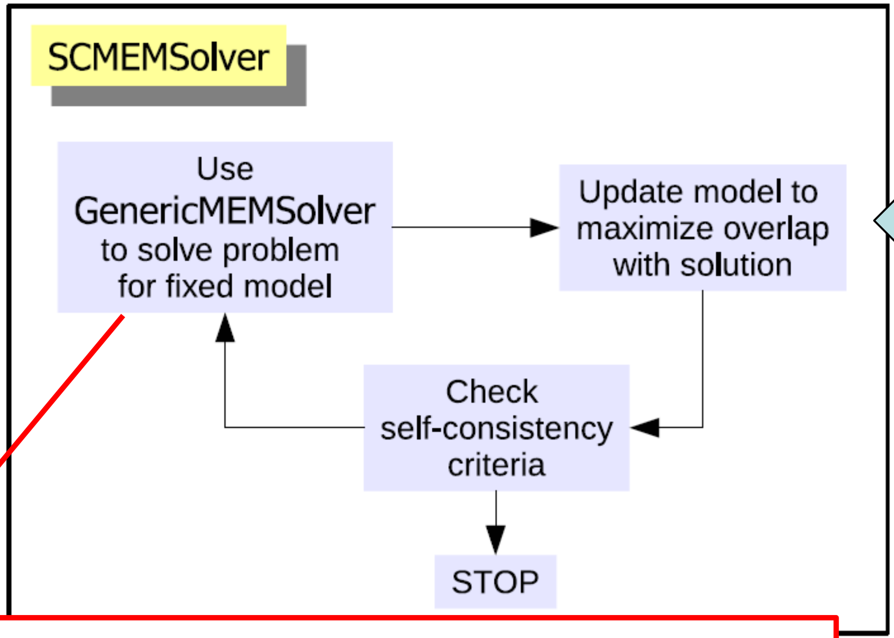


Figure 5: (Color online) Reconstruction of the artificial object function $A(x)$ by self-consistent MEM for different values of parameter α.

Magierski, Wlazłowski,
Comp. Phys. Comm. 183 (2012) 2264

Solution: construct the class of models depending on a set of parameters which are adjusted selfconsistently.



EMSolver.

$$O(\vec{f}) = \frac{\left(\sum_{i=1}^{N} A_i \mathcal{M}_i(\vec{f})\right)^2}{\sum_{i=1}^{N} A_i^2 \sum_{i=1}^{N} \mathcal{M}_i^2(\vec{f})}.$$

It can be transformed into an iterative process of consecutive least square problems:

$$F(\vec{A}^0 + \delta\vec{A}) = F(\vec{A}^0, \vec{A})$$

$$= \frac{1}{2}\sum_{i=1}^{N_\tau}\left(\frac{\tilde{G}_i - G_i}{\sigma_i}\right)^2$$

$$+\alpha \sum_{i=1}^{N}\left(\frac{1}{2A_i^0}(\gamma_i - A_i)^2 + \omega_i\right) + O(|\delta\vec{A}|^3),$$

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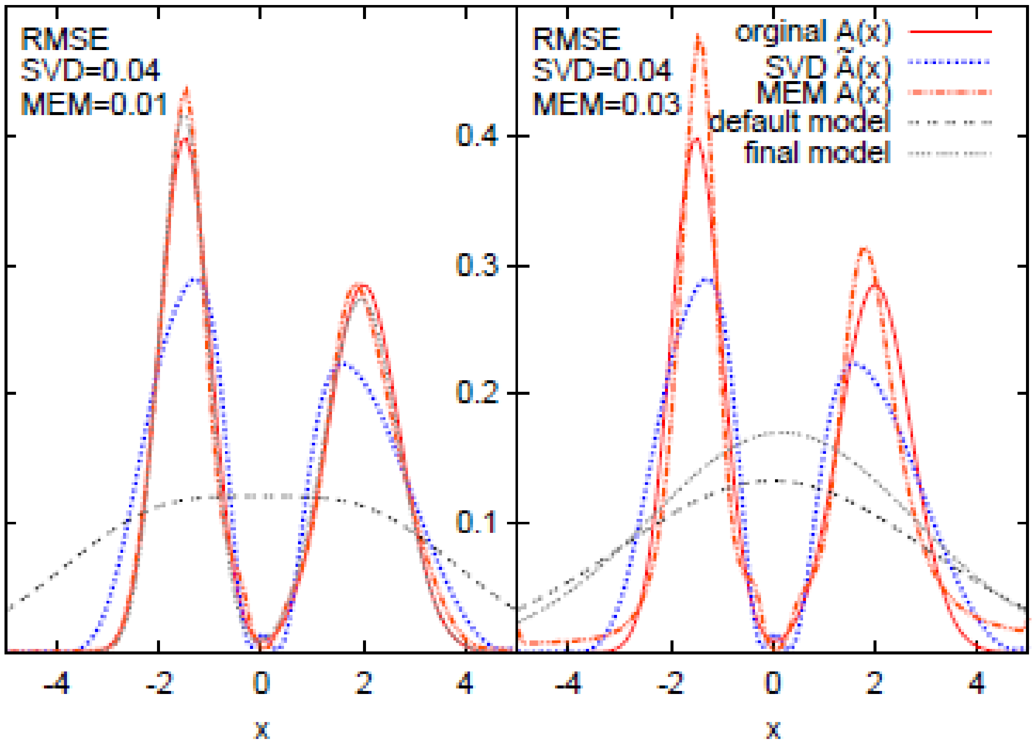

Figure 6: (Color online) The reconstruction ability of the spectral function for the full problem (data with noise + external constraints) of the SVD and MEM methods. The left panel shows the solution of the self-consistent MEM with a combination of two Gaussians functions as a default model class. The right panel shows the solution of the self-consistent MEM with Gaussian functions as a default model class.

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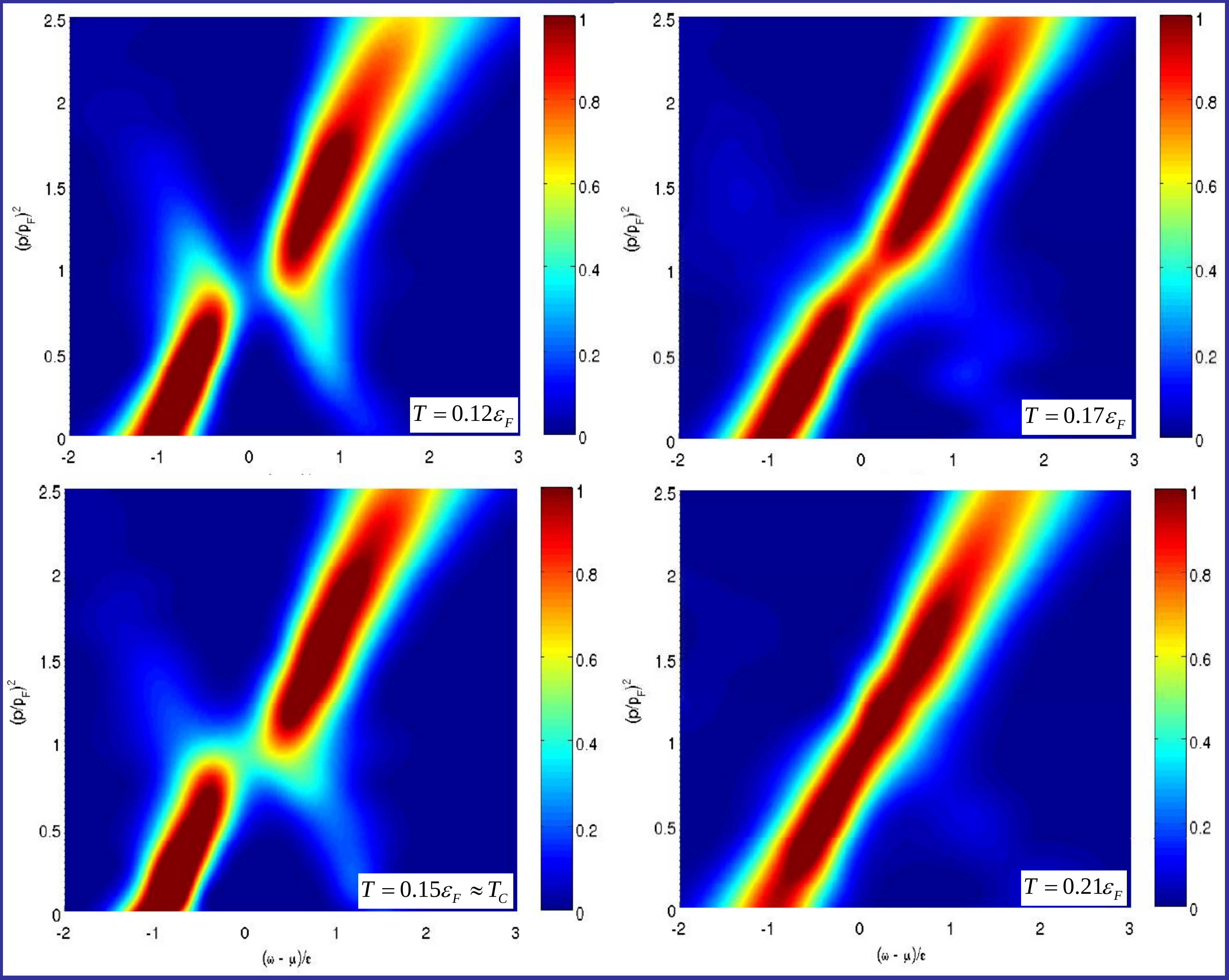
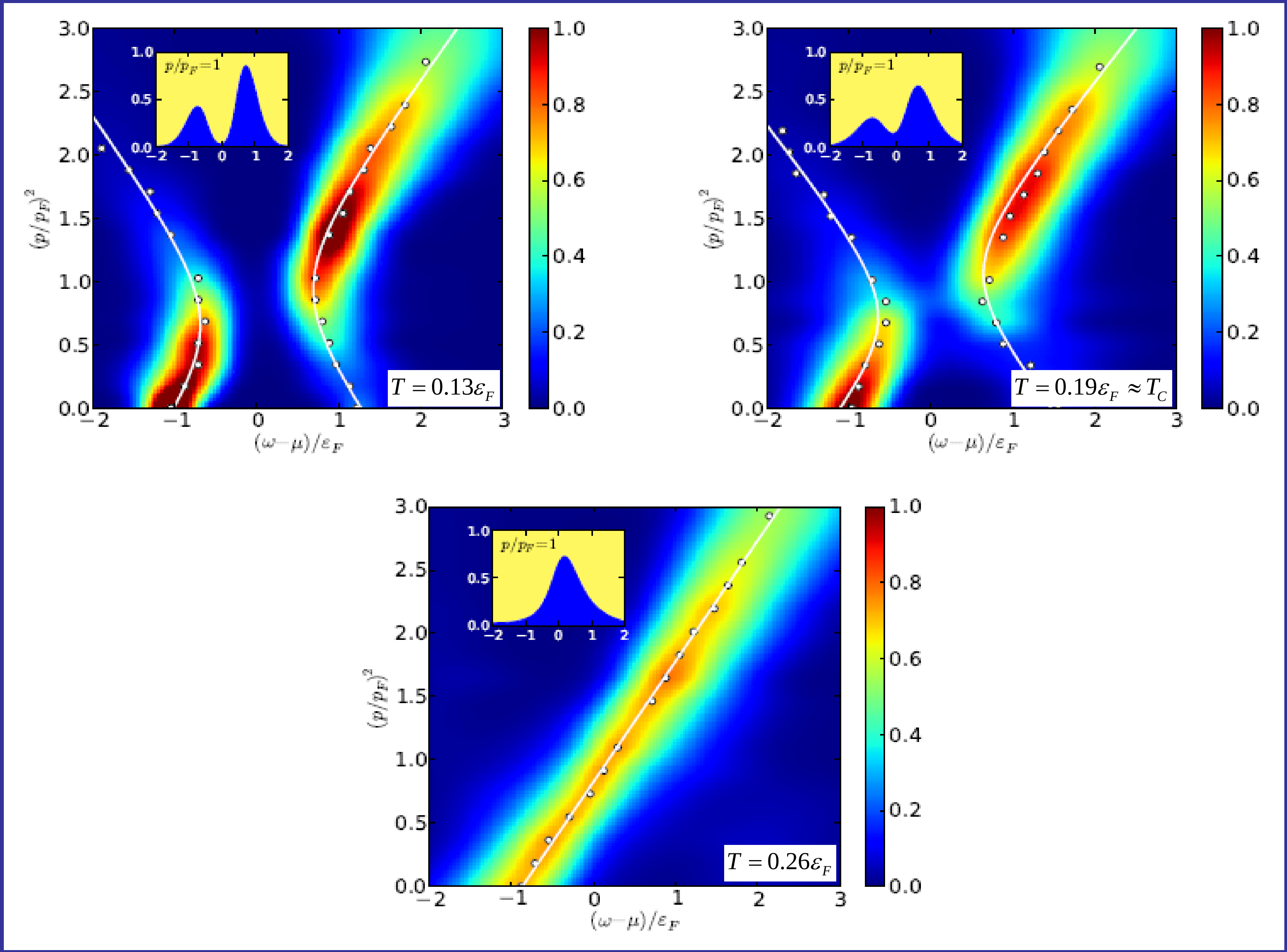
Spectral weight function at unitarity: $(k_F a)^{-1} = 0$



Spectral weight function at the BEC side: $(k_F a)^{-1} = 0.2$

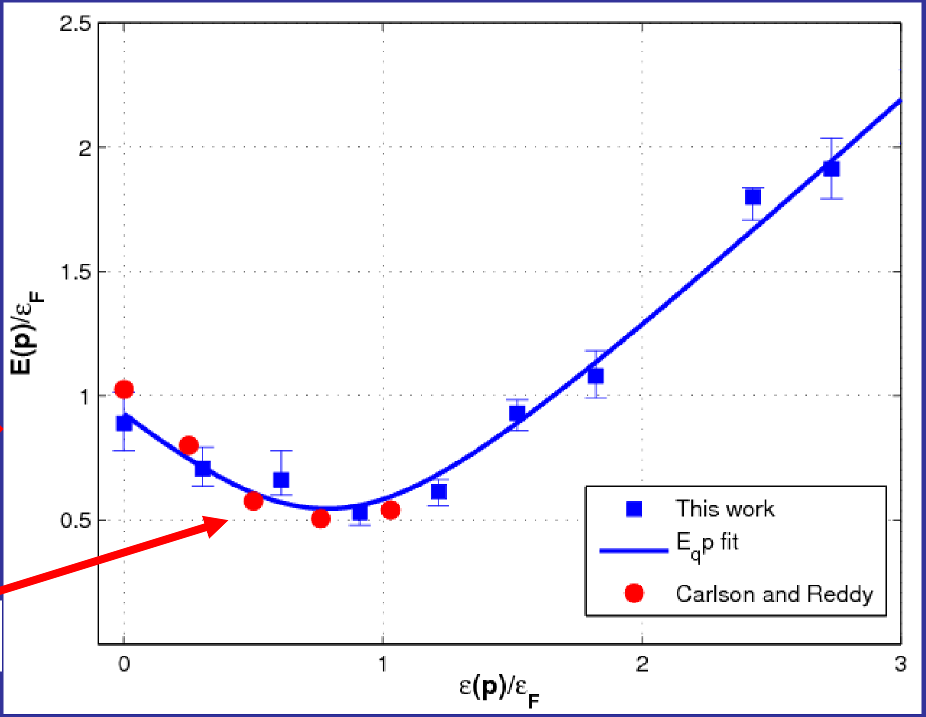


Single-particle properties

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

Quasiparticle spectrum extracted from spectral weight function at $T=0.1\varepsilon_F$

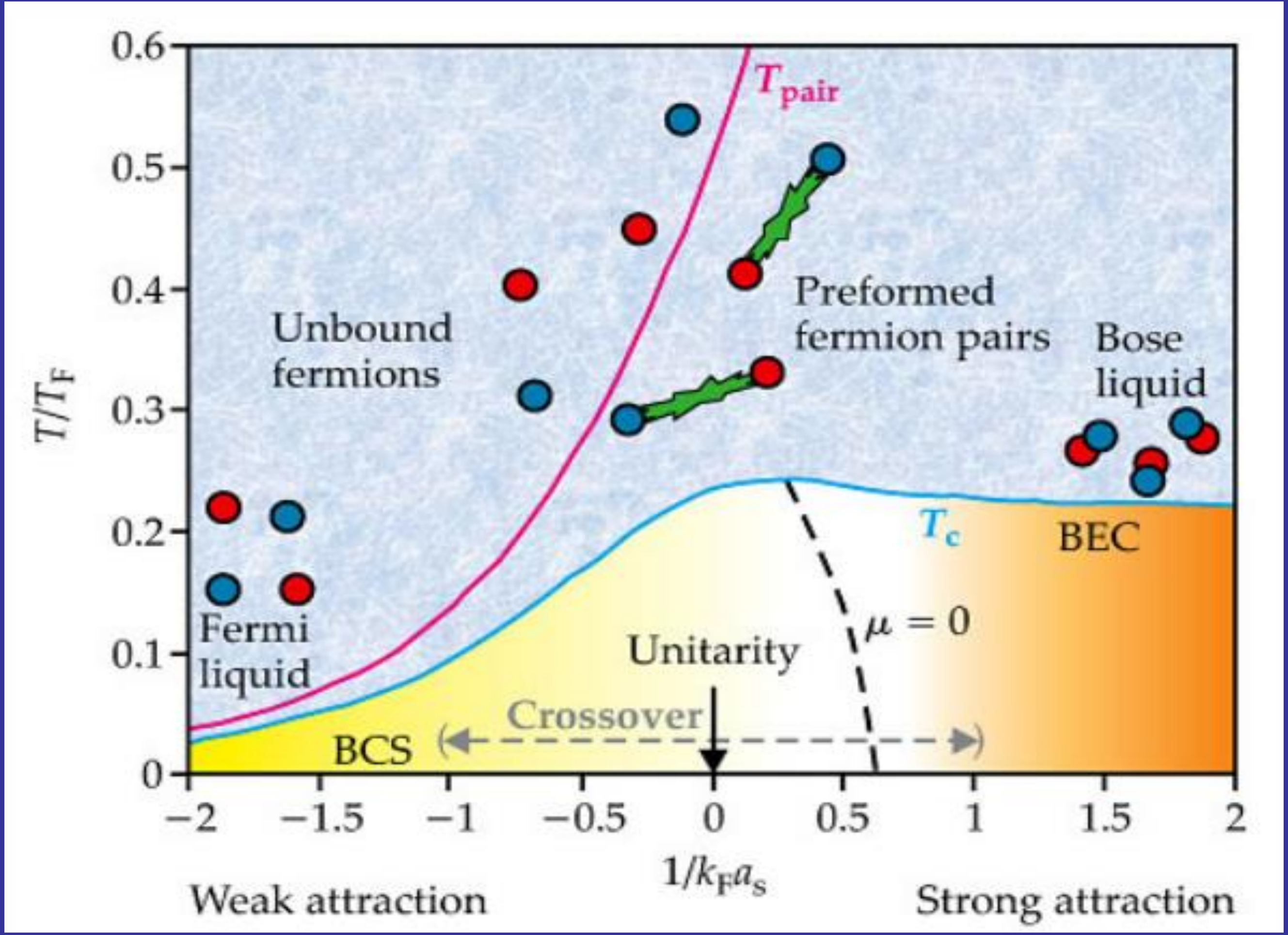
Fixed node MC calcs. at T=0



Effective mass: $m^*=(1.0\pm0.2)m$

Mean-field potential: $U=(-0.5\pm0.2)\varepsilon_F$

Weak temperature dependence!



From Sa de Melo, Physics Today (2008)

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

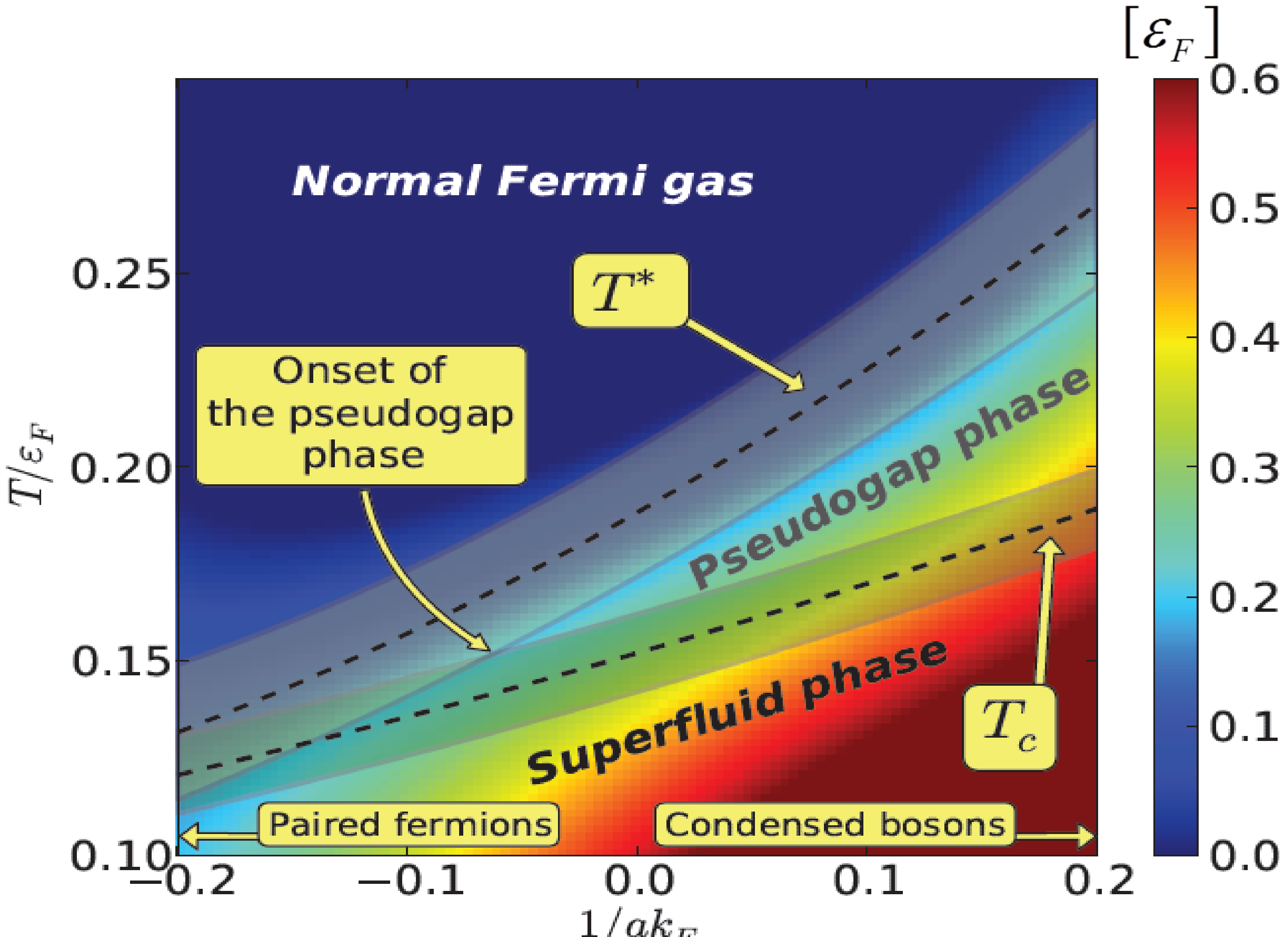
Important issue related to pairing pseudogap:

- 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

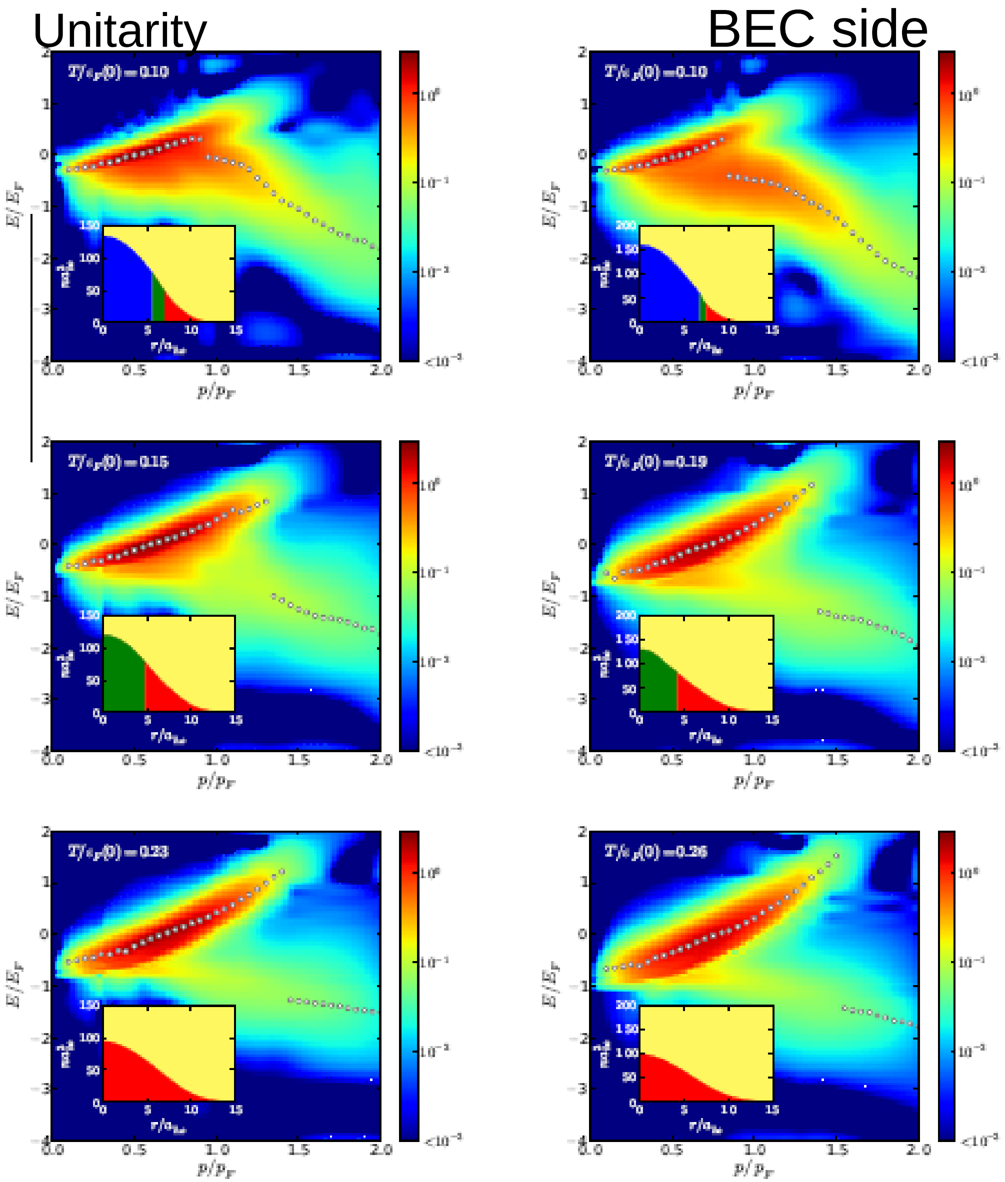


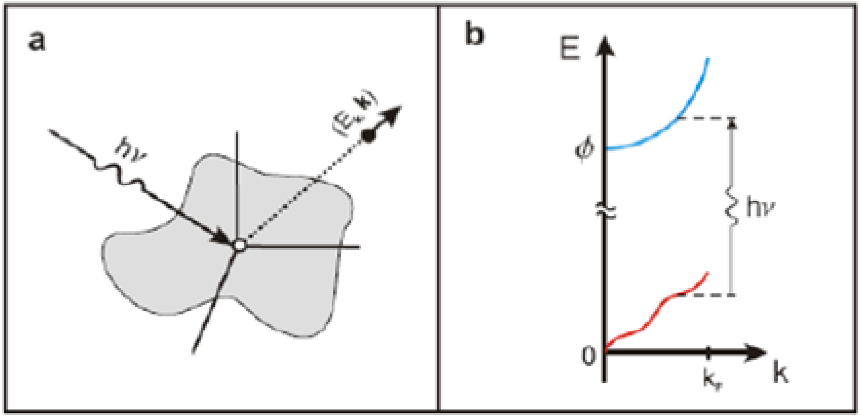
Ab initio result: The onset of pseudogap phase at $1/ak_F \approx -0.05$.

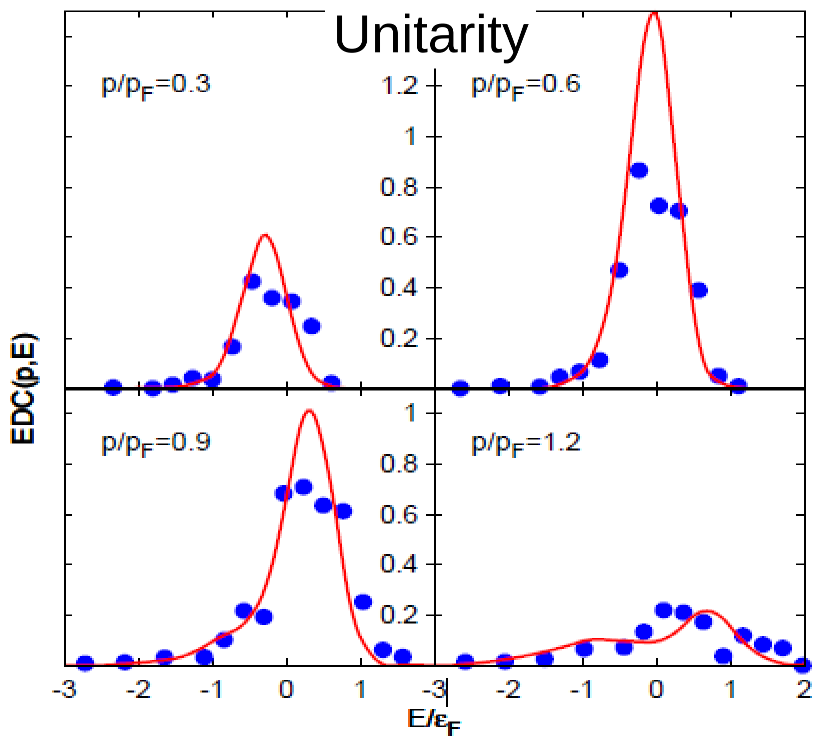
Magierski, Wlazłowski, Bulgac, *Phys. Rev. Lett.* 107,145304(2011)
Magierski, Wlazłowski, Bulgac, Drut, *Phys. Rev. Lett.* 103,210403(2009)

Energy distribution curves (EDC) from the spectral weight function

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







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

Local density approximation (LDA) from QMC

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.

Spin susceptibility and spin drag rate

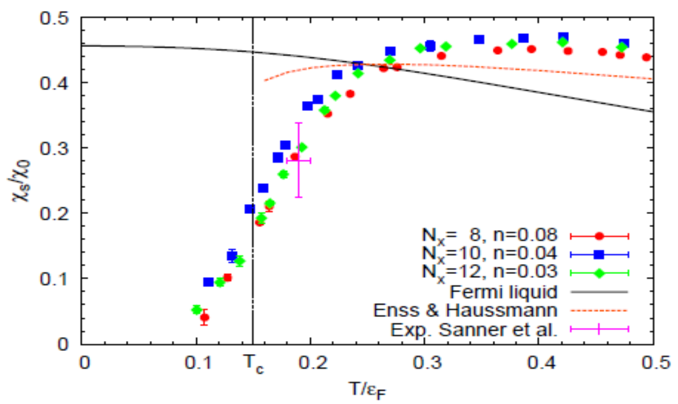


FIG. 2: (Color online) The static spin susceptibility as a function of temperature for an 8^3 lattice solid (red) circles, 10^3 lattice (blue) squares and 12^3 lattice (green) diamonds. Vertical black dotted line indicates the critical temperature of superfluid to normal phase transition $T_c = 0.15\,\varepsilon_F$.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

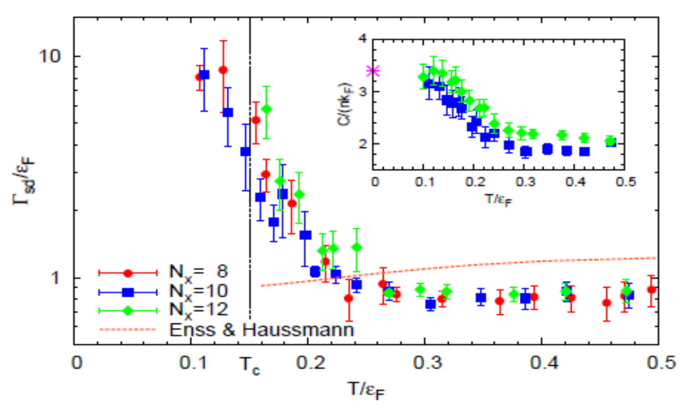


FIG. 3: (Color online) The spin drag rate $\Gamma_{sd} = n/\sigma_s$ in units of Fermi energy as a function of temperature for an 8^3 lattice solid (red) circles, 10^3 lattice (blue) squares and 12^3 lattice (green) diamonds. Vertical black dotted line locates the critical temperature of superfluid to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

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

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

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

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

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

$$D_s = \frac{\sigma_s}{\chi_s}$$

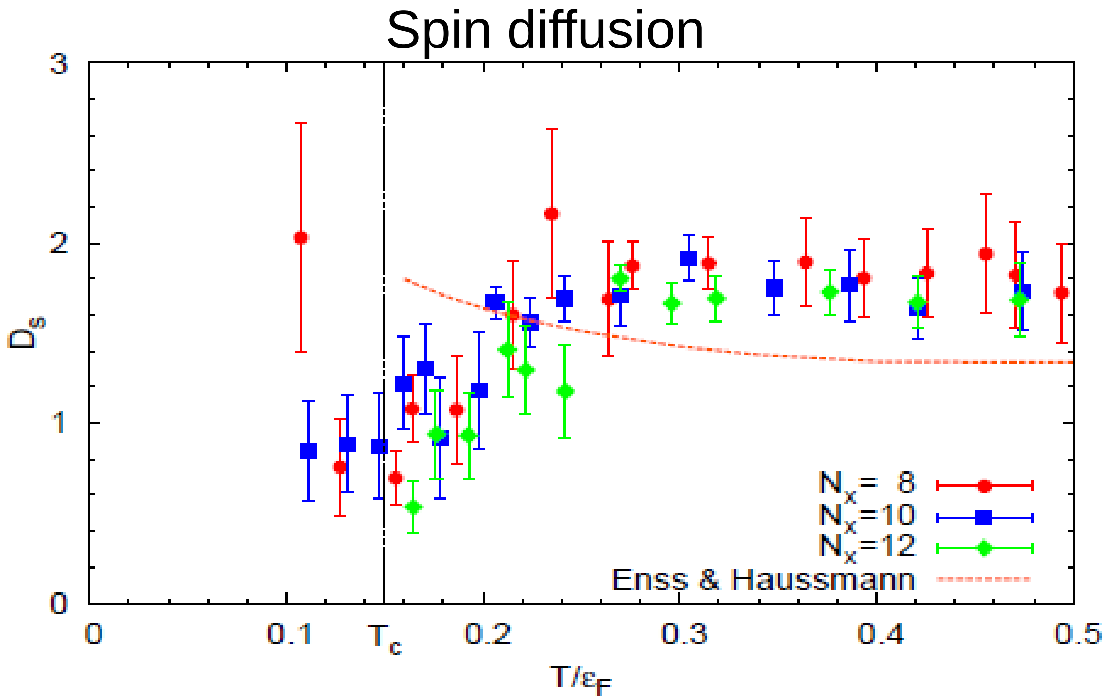


FIG. 4: (Color online) The spin diffusion coefficient obtained by the Einstein relation $D_s = \sigma_s/\chi_s$ as function of temperature. The notation is identical to Fig. 3.

No minimum is seen in QMC down to 0.1 of Fermi energy

Estimate from kinetic theory at low T: $D_s \sim p_F l \sim n^{1/3} n^{-1/3} \sim 1$

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

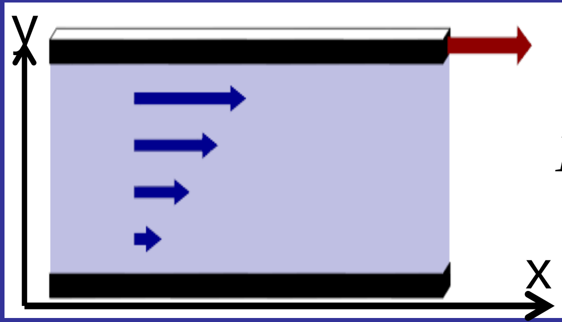
Pseudogap at unitarity – theoretical predictions

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

Hydrodynamics at unitarity

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

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



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

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: $\eta \sim$ 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, quark-gluon plasma

Shear viscosity

$$\eta(\omega) = \pi \rho_{xyxy}(q=0,\omega)/\omega$$

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

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

$$i\left[\hat{j}_k(r),\hat{H}\right] = \partial_l \hat{\Pi}_{kl}(r)$$

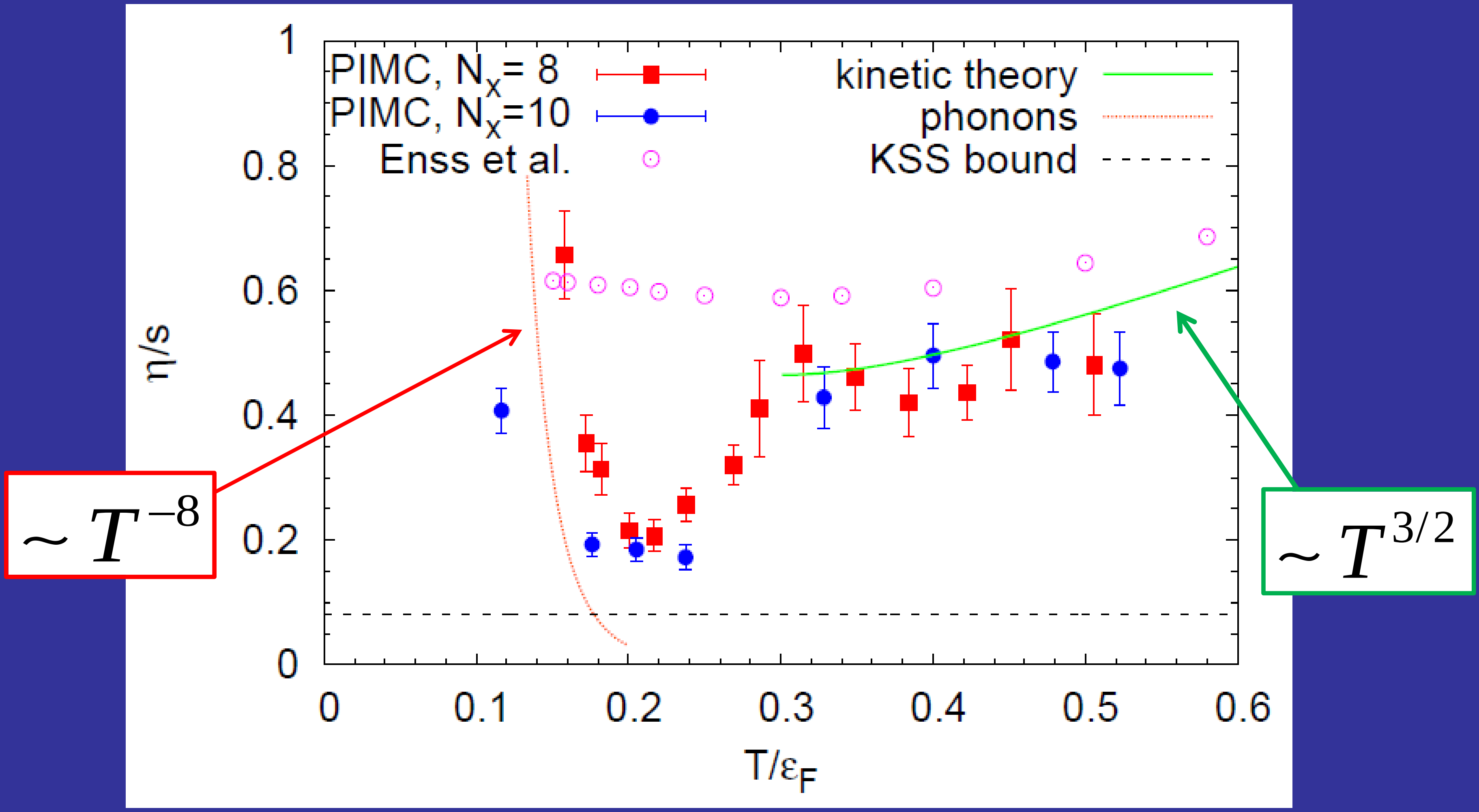
Additional symmetries and sum rules:

$$G(\tau) = G(\beta-\tau)$$

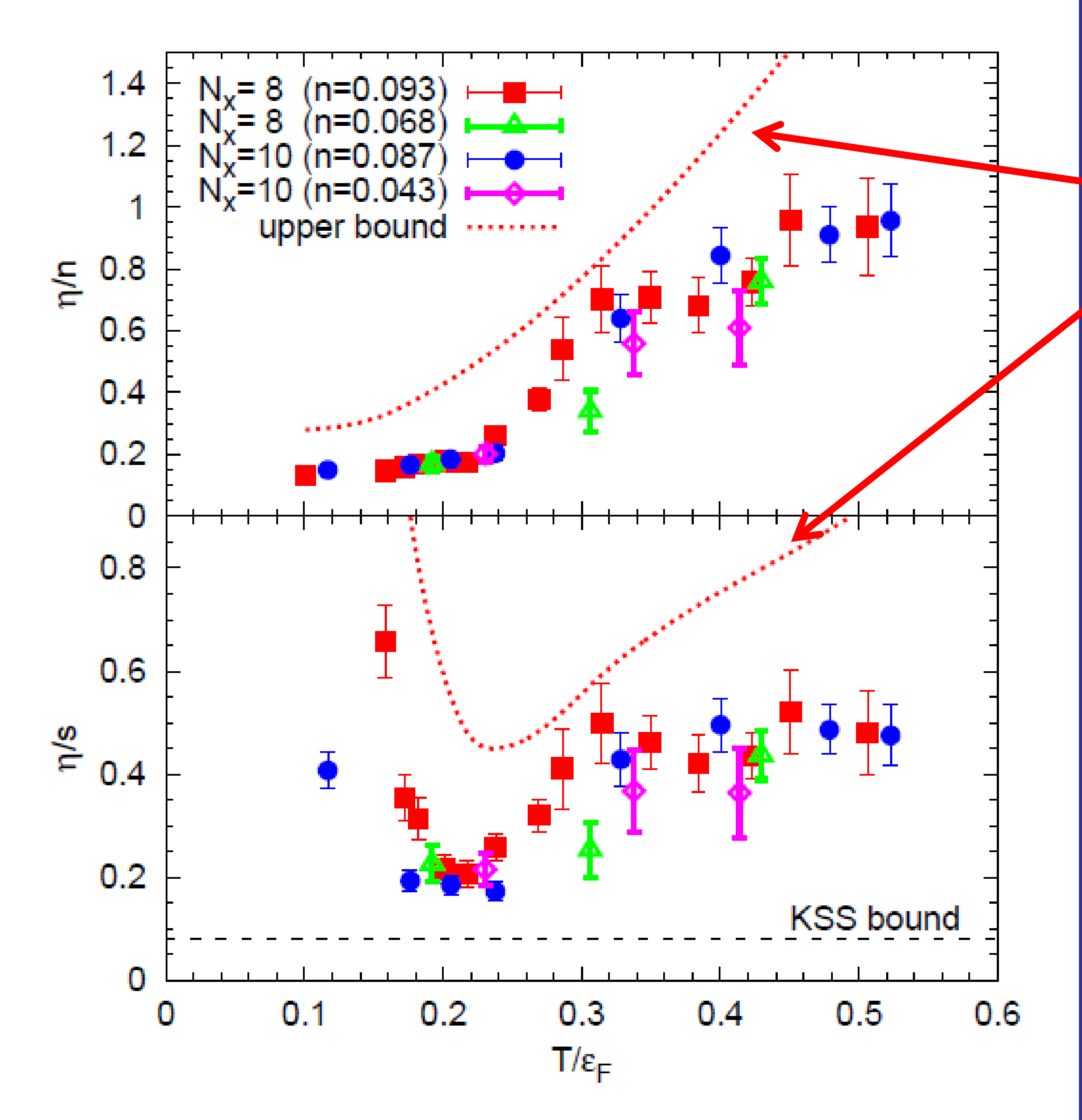
$$\frac{1}{\pi}\int_0^\infty d\omega\left[\eta(\omega) - \frac{C}{15\pi\sqrt{m\omega}}\right] = \frac{\varepsilon}{3},$$ ε – *energy density*

$$\eta(\omega\to\infty) \simeq \frac{C}{15\pi\sqrt{m\omega}}.$$

Shear viscosity to entropy density ratio

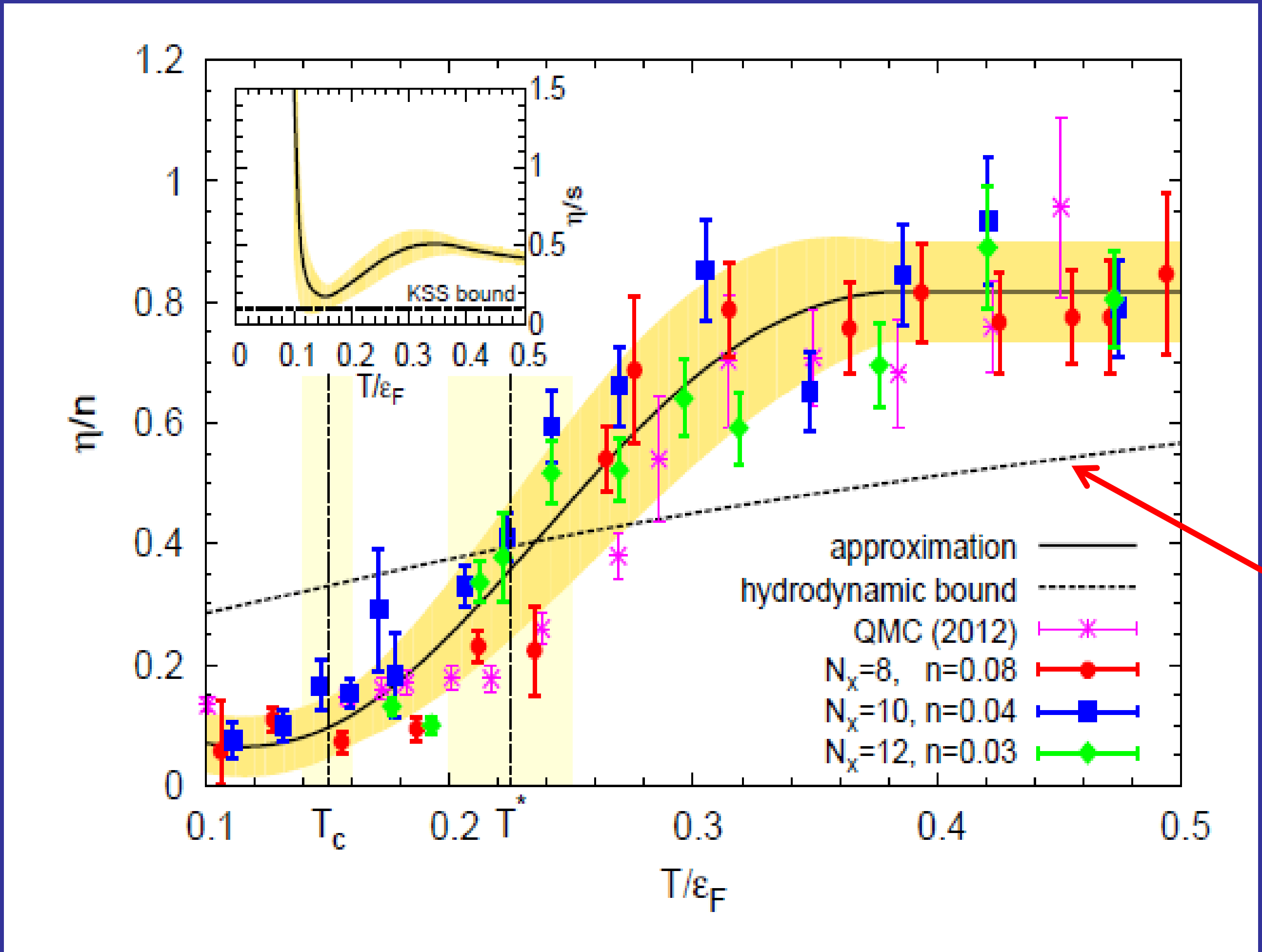


G.Wlazłowski, P.Magierski,J.E.Drut,
Phys. Rev. Lett. 109, 020406 (2012)



Uncertainties related to numerical analytic continuation

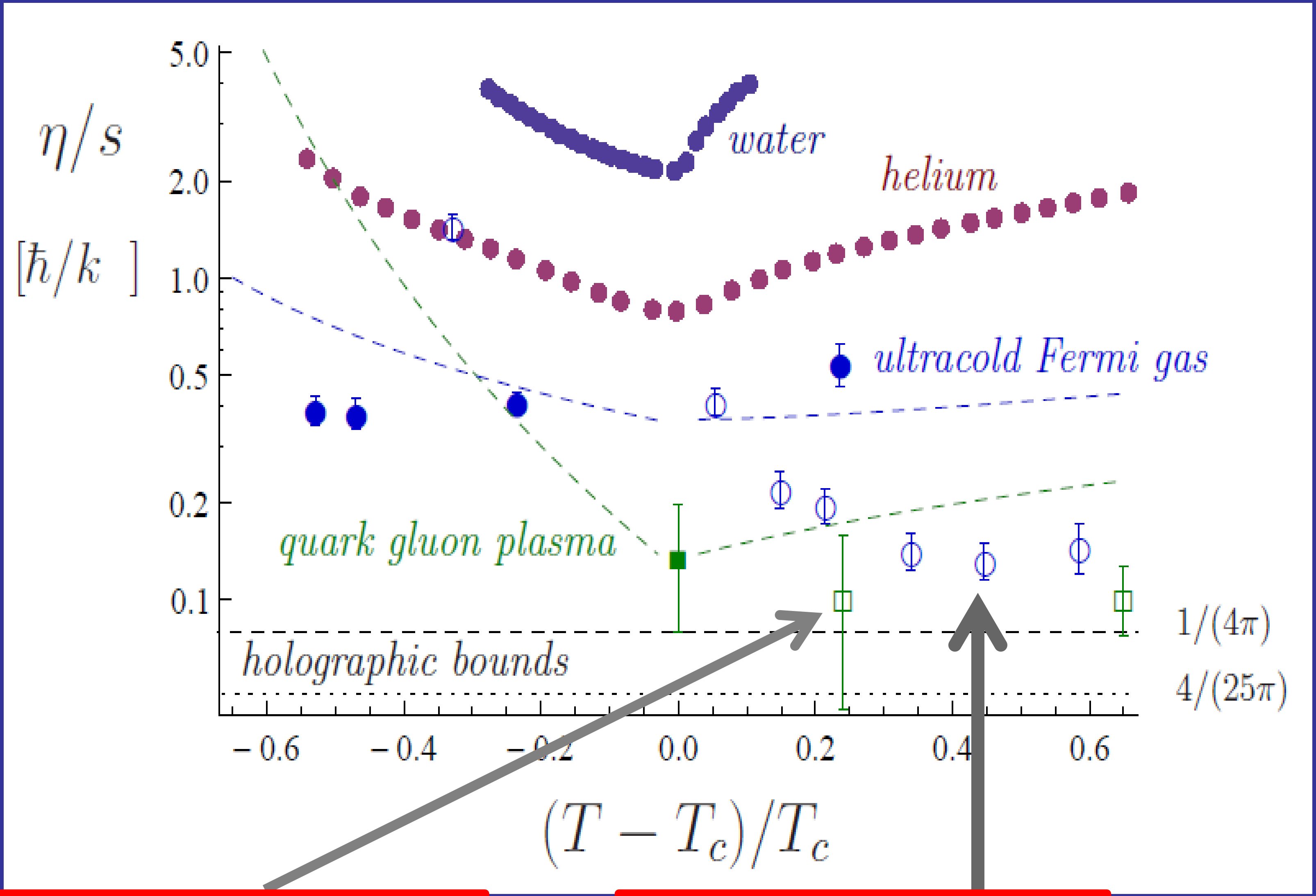
G.Wlazłowski, P.Magierski,J.E.Drut, Phys. Rev. Lett. 109, 020406 (2012)



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

Wlazłowski, Magierski, Bulgac, Roche. arXiv:1304.2283

Shear viscosity to entropy ratio – experiment vs. theory
(from A. Adams et al.1205.5180)



Lattice QCD (SU(3) gluodynamics):
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QMC calculations for UFG:
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