Auxiliary-Field QMC Simulations of Neutron Matter in Chiral Effective Field Theory

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Collaborators:

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Piotr Magierski - Warsaw and Seattle
Sergej Moroz - Seattle, Boulder (now)
Kenneth J. Roche - Seattle and PNNL
Gabriel Wlazłowski* - Seattle and Warsaw

A long detour at first:

Cold gases and the Unitary Fermi gas.

In the Autumn of 2003 Joaquín Drut walked into my office asking whether he can work with me.

All I knew about MC is that many people do it and that they used random numbers to calculate infinite dimensional integrals …

and that there was a very challenging problem still unsolved in theoretical physics:

The properties of the unitary Fermi gas!

Why would one want to study cold Fermi gases?

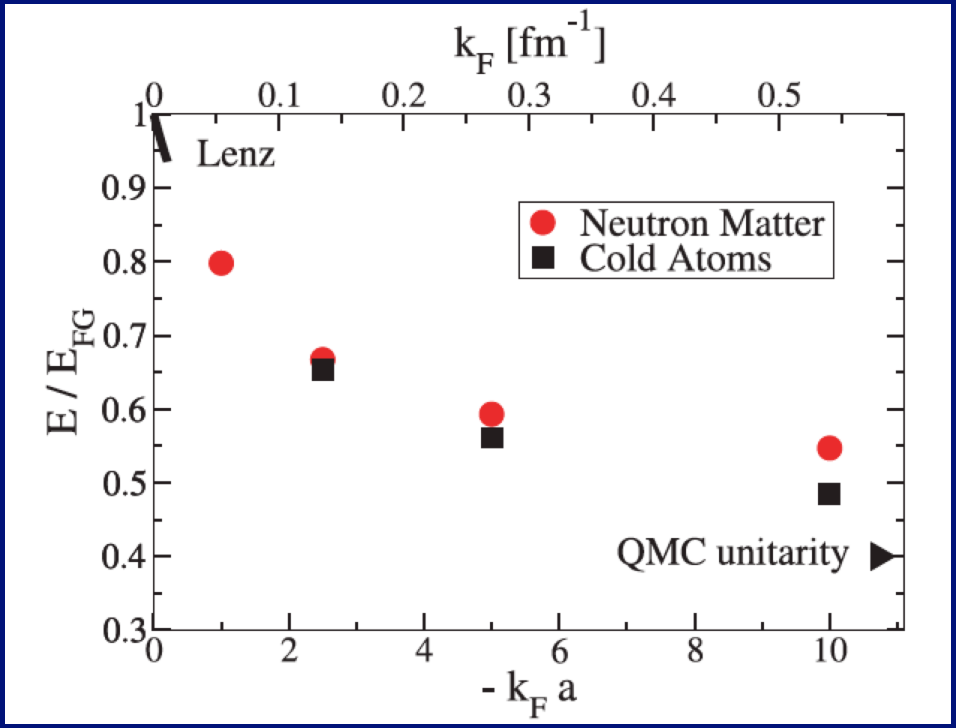
One reason:

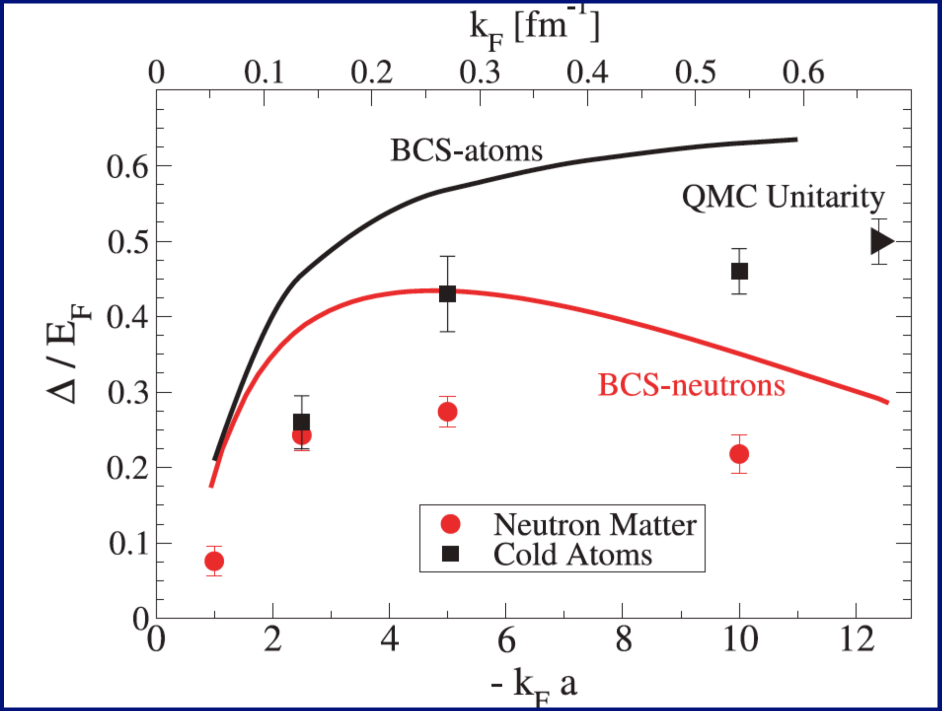
**(for the nerds, I mean the hard-core theorists,
not for the phenomenologists)**

Bertsch's Many-Body X challenge, Seattle, 1999

What are the ground state properties of the many-body system composed of spin ½ fermions interacting via a zero-range, infinite scattering-length contact interaction?

Besides pure theoretical curiosity, this problem is relevant to neutron stars!





Gezerlis and Carlson,
Phys. Rev. C 77, 032801(R) (2008)

What are the scattering length and the effective range?

$$k \ \text{cotan}\ \delta_0 = -\frac{1}{a} + \frac{1}{2} r_{eff} k^2 + \cdots$$

$$\sigma = \frac{4\pi}{k^2}\sin^2\delta_0 + \cdots = 4\pi \frac{a^2}{1+k^2a^2} + \cdots \underset{k\to 0}{=} 4\pi a^2 + \cdots$$

If the energy is small only the s-wave is relevant.

Let me consider at first as an instructive example the hydrogen atom.

The ground state energy could only be a function of:

- ✓ Electron charge
- ✓ Electron mass
- ✓ Planck's constant

and then trivial dimensional arguments lead to

$$E_{gs} = \frac{e^4 m}{\hbar^2} \times \frac{1}{2}$$

Only the factor ½ requires some hard work (Quantum Mechanics).

Let me now turn to dilute fermion matter

The ground state energy is given by such a function:

$$E_{gs} = f(N, V, \hbar, m, a, r_0)$$

Taking the scattering length to infinity and the range of the interaction to zero, we are left with:

$$E_{gs} = F(N, V, \hbar, m) = \frac{3}{5}\varepsilon_F N \times \xi$$

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

Pure number

What George Bertsch essentially asked in 1999 is:

What is the value of ξ ?! Is it positive?

But he wished to know the properties of the system as well:

The system turned out to be superfluid !

$$E_{gs} = \frac{3}{5}\varepsilon_F N \times \xi \qquad \Delta = \varepsilon_F \times \varsigma$$

$$\xi = 0.372(5), \qquad \zeta = 0.45(5)$$

Now these results are a bit unexpected.

✓ The energy looks almost like that of *a non-interacting system*!
(there are no other dimensional parameters in the problem)

✓ The system has *a huge pairing gap*!

✓ This system is a very strongly interacting one,
since the *elementary cross section is huge*!

The initial Bertsch's Many Body challenge has evolved over time and became the problem of *Fermions in the Unitary Regime.*
(And this is part of the BCS-BEC crossover problem)

In cold old gases one can control the strength of the interaction!

The system is very dilute, but strongly interacting!

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

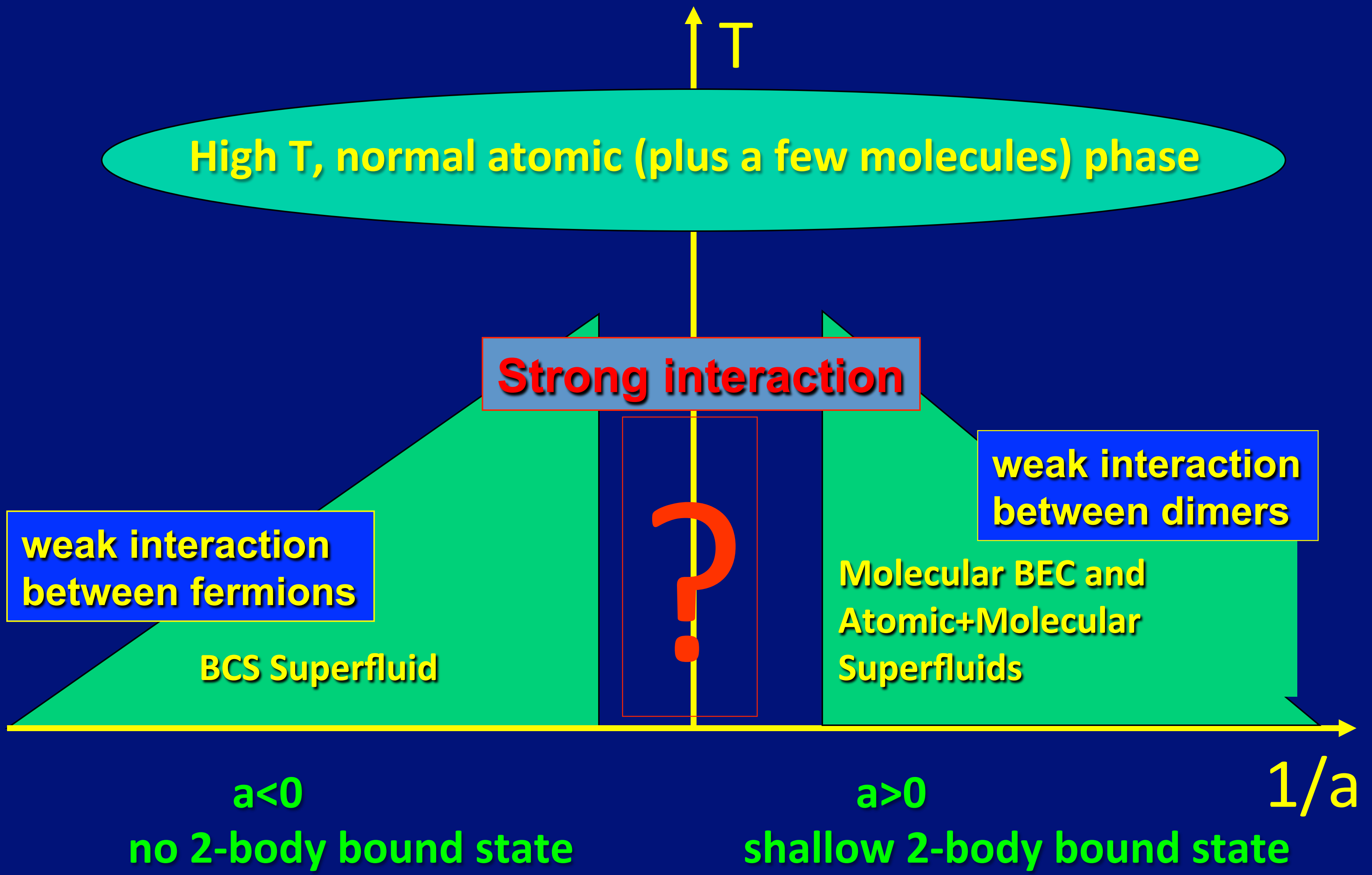
n - number density

$$r_0 \ll n^{-1/3} \approx \lambda_F/2 \ll |a|$$

r_0 - range of interaction

a - scattering length

Phases of a two species dilute Fermi system in the BCS-BEC crossover



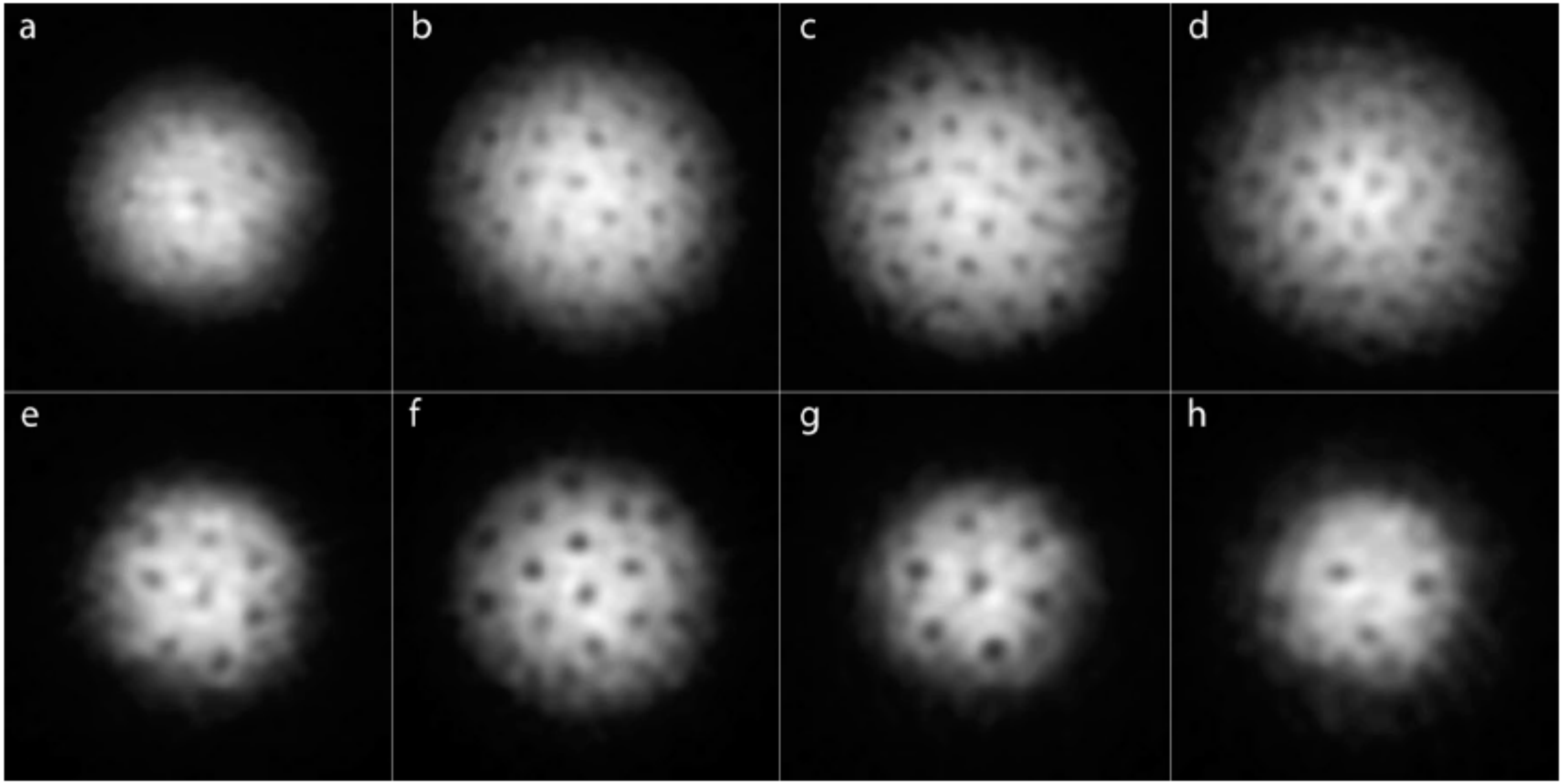


Fig. 2: Vortices in a strongly interacting gas of fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (a) to 500 ms (b-h) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, the magnetic field was ramped to 735 G for imaging (see text for details). The magnetic fields were (a) 740 G, (b) 766 G, (c) 792 G, (d) 812 G, (e) 833 G, (f) 843 G, (g) 853 G and (h) 863 G. The field of view of each image is $880\ \mu m \times 880\ \mu m$.

Zweirlein et al. Nature <u>435</u>, 1047 (2005)

Finite Temperatures

Grand Canonical Path-Integral Monte Carlo

$$\hat{H} = \hat{T} + \hat{V} = \int d^3x \left[\psi_\uparrow^\dagger(\vec{x}) \left(-\frac{\hbar^2 \Delta}{2m} \right) \psi_\uparrow(\vec{x}) + \psi_\downarrow^\dagger(\vec{x}) \left(-\frac{\hbar^2 \Delta}{2m} \right) \psi_\downarrow(\vec{x}) \right] - g \int d^3x \; \hat{n}_\uparrow(\vec{x}) \hat{n}_\downarrow(\vec{x})$$

$$\hat{N} = \int d^3x \left[\hat{n}_\uparrow(\vec{x}) + \hat{n}_\downarrow(\vec{x}) \right], \qquad \hat{n}_s(\vec{x}) = \psi_s^\dagger(\vec{x}) \psi_s(\vec{x}), \qquad s = \uparrow, \downarrow$$

Trotter expansion

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

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

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

No approximations so far, except for the fact that the interaction is not well defined!

Recast the propagator at each time slice and put the system on a 3D-spatial lattice, in a cubic box of side $L=N_s l$, with periodic boundary conditions

$$\exp\left[-\tau\left(\hat{H}-\mu\hat{N}\right)\right]\approx\exp\left[-\tau\left(\hat{T}-\mu\hat{N}\right)/2\right]\exp(-\tau\hat{V})\exp\left[-\tau\left(\hat{T}-\mu\hat{N}\right)/2\right]+O(\tau^3)$$

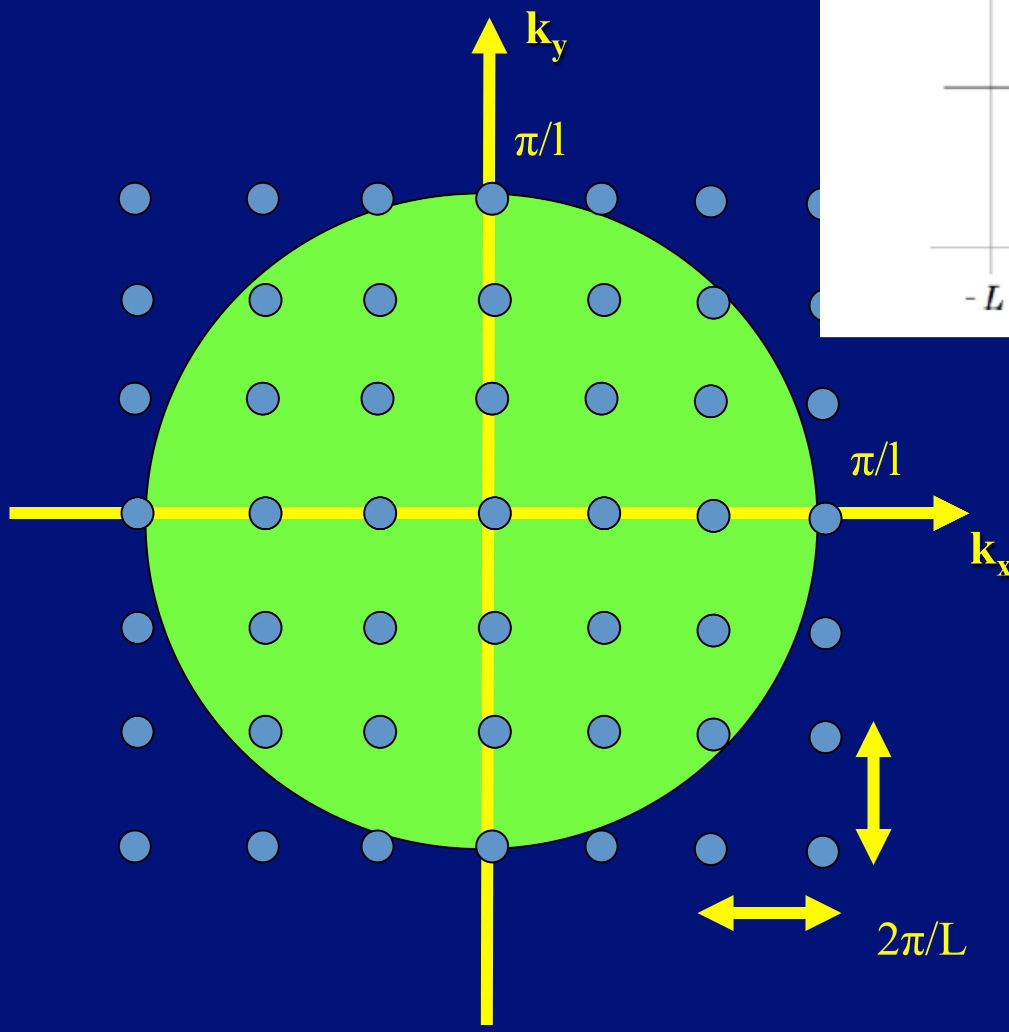
Discrete Hubbard-Stratonovich transformation

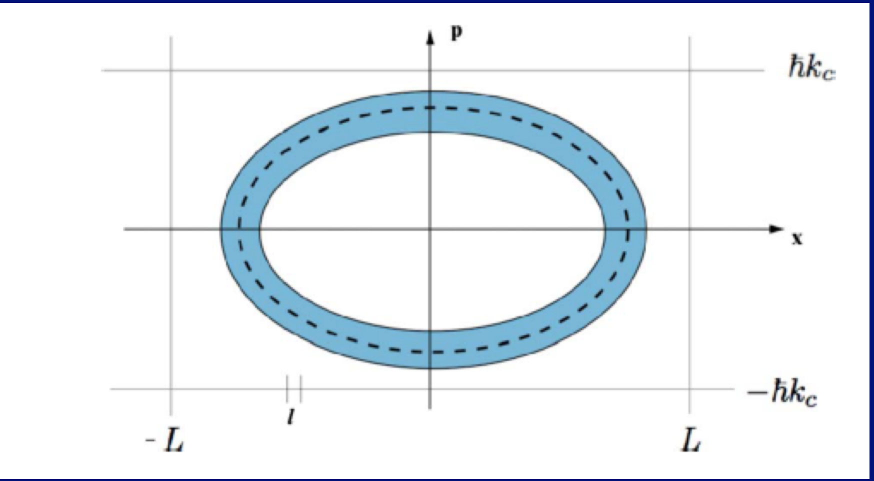
$$\exp(-\tau\hat{V})=\prod_{\vec{x}}\sum_{\sigma_\pm(\vec{x})=\pm1}\frac{1}{2}\left[1+\sigma_\pm(\vec{x})A\hat{n}_\uparrow(\vec{x})\right]\left[1+\sigma_\pm(\vec{x})A\hat{n}_\downarrow(\vec{x})\right],\qquad A=\sqrt{\exp(\tau g)-1}$$

σ-fields fluctuate both in space and imaginary time

$$\frac{m}{4\pi\hbar^2 a}=-\frac{1}{g}+\frac{mk_c}{2\pi^2\hbar^2},\qquad k_c<\frac{\pi}{l}.\qquad r_{eff}=\frac{4}{\pi k_c}$$

Running coupling constant g defined by lattice





$$\varepsilon_F,\ \Delta,\ T \ll \frac{\hbar^2\pi^2}{2ml^2}$$

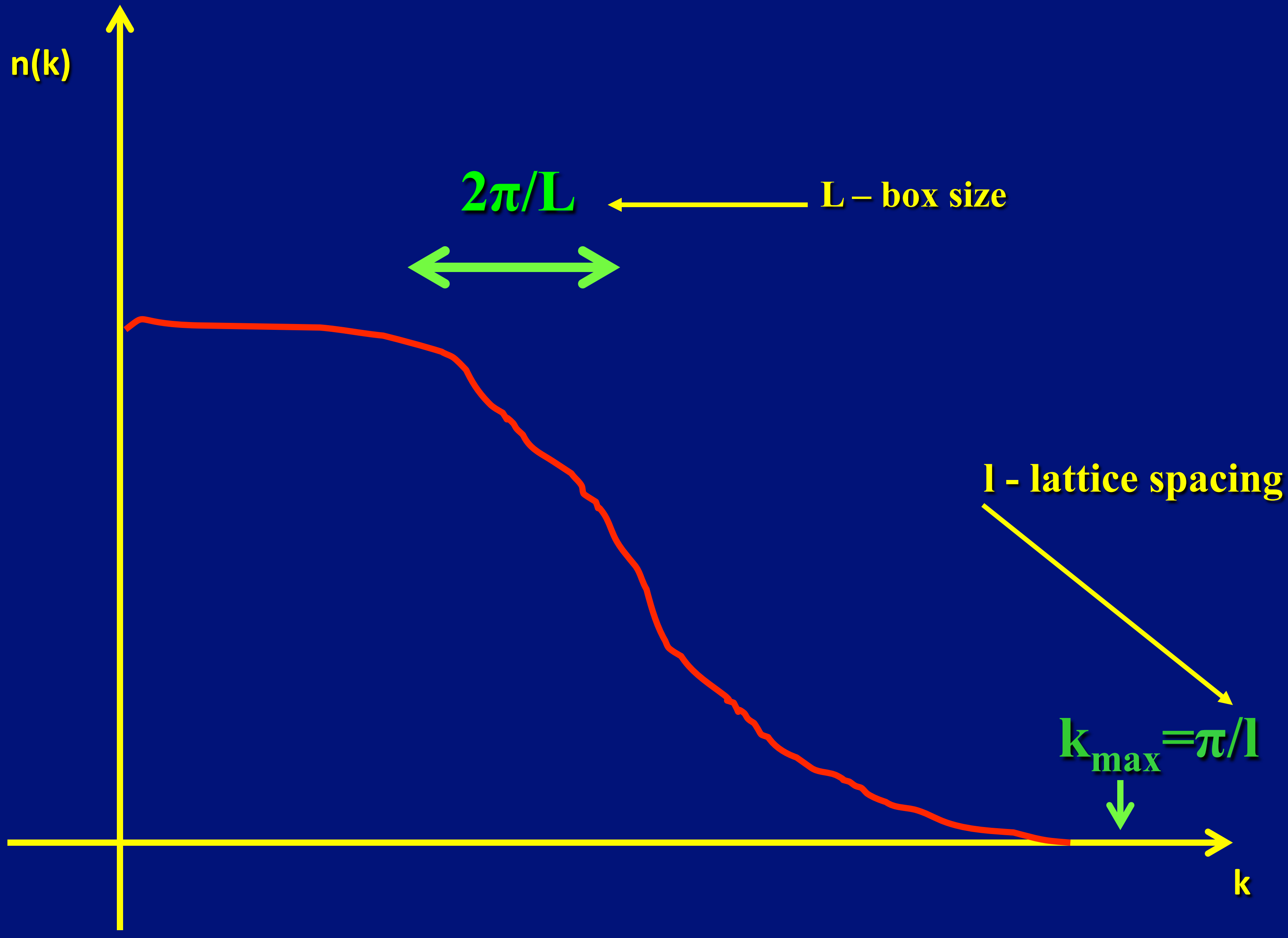
$$\delta\varepsilon > \frac{2\hbar^2\pi^2}{mL^2}$$

$$\varepsilon_F,\ \Delta \gg \frac{2\hbar^2\pi^2}{mL^2}$$

$$\xi_{coh} \ll L = N_s l$$

$$\delta p > \frac{2\pi\hbar}{L}$$

Momentum space



How to choose the lattice spacing and the box size?

$$Z(T) = \int \prod_{\vec{x},\tau} D\sigma(\vec{x},\tau)\ \mathrm{Tr}\,\hat{U}(\{\sigma\})$$

$$\hat{U}(\{\sigma\}) = T_\tau \prod_{\tau} \exp\{-\tau[\hat{h}(\{\sigma\}) - \mu]\}$$

One-body evolution operator in imaginary time

$$E(T) = \int \frac{\prod_{\vec{x},\tau} D\sigma(\vec{x},\tau) \mathrm{Tr}\,\hat{U}(\{\sigma\})}{Z(T)} \ \frac{\mathrm{Tr}\left[\hat{H}\hat{U}(\{\sigma\})\right]}{\mathrm{Tr}\,\hat{U}(\{\sigma\})}$$

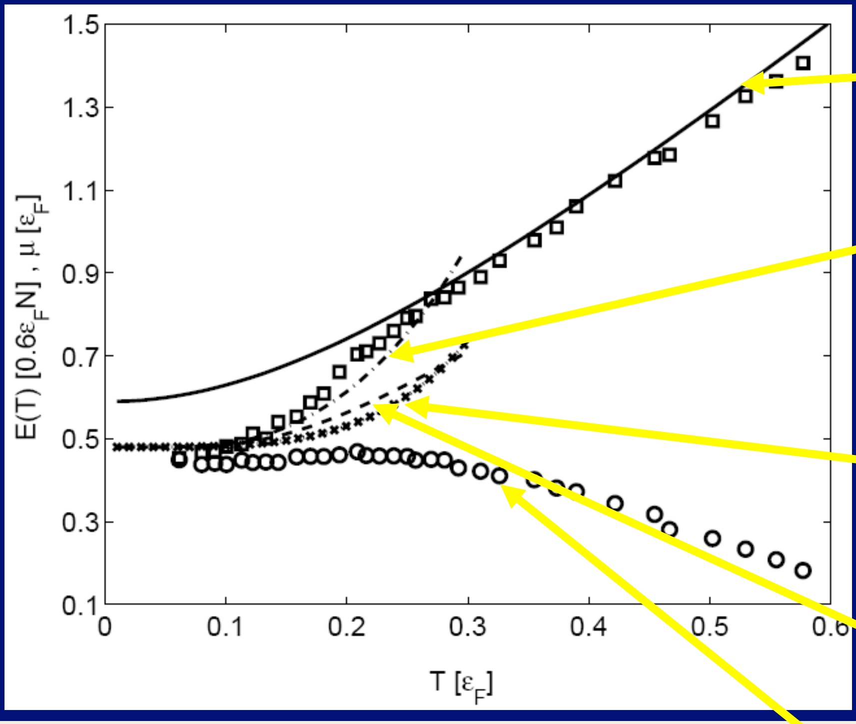
$$\mathrm{Tr}\,\hat{U}(\{\sigma\}) = \{\det[1 + \hat{U}(\{\sigma\})]\}^2 = \exp[-S(\{\sigma\})] > 0$$

No sign problem!

$$n_\uparrow(\vec{x},\vec{y}) = n_\downarrow(\vec{x},\vec{y}) = \sum_{k,l<k_c} \varphi_{\vec{k}}(\vec{x}) \left[\frac{\hat{U}(\{\sigma\})}{1+\hat{U}(\{\sigma\})}\right]_{\vec{k}\vec{l}} \varphi^*_{\vec{l}}(\vec{y}), \qquad \varphi_{\vec{k}}(\vec{x}) = \frac{\exp(i\vec{k}\cdot\vec{x})}{\sqrt{V}}$$

All traces can be expressed through these single-particle density matrices

$a = \pm\infty$



Normal Fermi Gas (with vertical offset, solid line)

Bogoliubov-Anderson phonons and quasiparticle contribution (dot-dashed line)

Bogoliubov-Anderson phonons contribution only

Quasi-particles contribution only (dashed line)

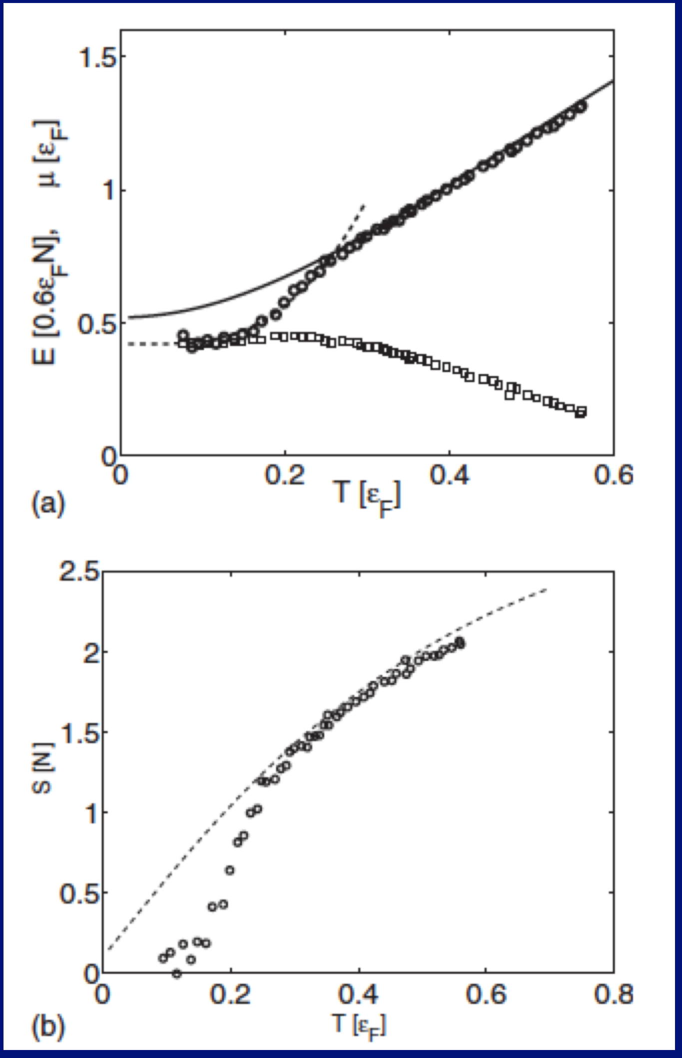
μ - chemical potential (circles)

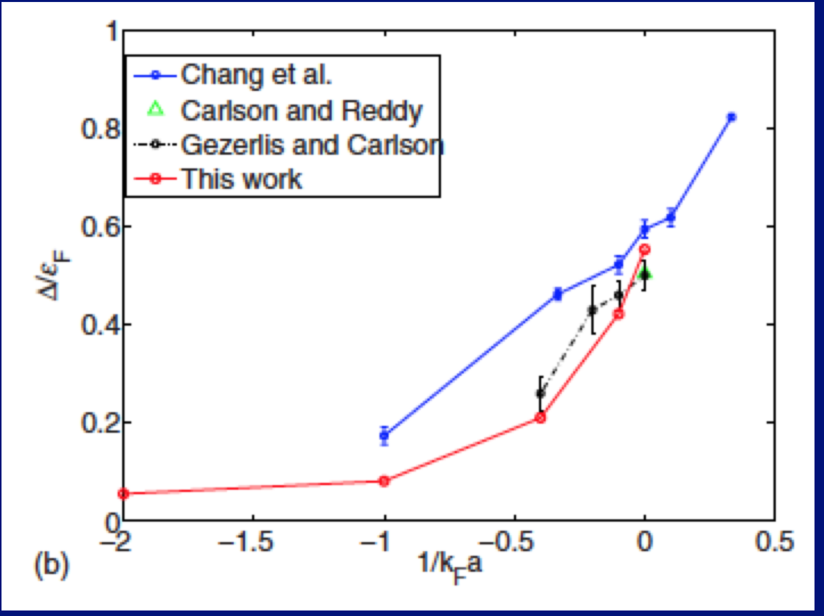
$$E_{\text{phonons}}(T) = \frac{3}{5}\varepsilon_F N \; \frac{\sqrt{3}\pi^4}{16\xi_s^{3/2}}\left(\frac{T}{\varepsilon_F}\right)^4, \qquad \xi_s \approx 0.44$$

$$E_{\text{quasi-particles}}(T) = \frac{3}{5}\varepsilon_F N \; \frac{5}{2}\sqrt{\frac{2\pi\Delta^3 T}{\varepsilon_F^4}}\exp\left(-\frac{\Delta}{T}\right)$$

$$\Delta = \left(\frac{2}{e}\right)^{7/3}\varepsilon_F \exp\left(\frac{\pi}{2k_F a}\right)$$

Bulgac, Drut, and Magierski
Phys. Rev. Lett. 96, 090404 (2006)
Received: 16 May, 2004
Published: 10 March, 2006


E [0.6ε_F N], μ [ε_F]
T [ε_F]
(a)
S [N]
T [ε_F]
(b)


Chang et al.
Carlson and Reddy
Gezerlis and Carlson
This work
Δ/ε_F
1/k_F a
(b)

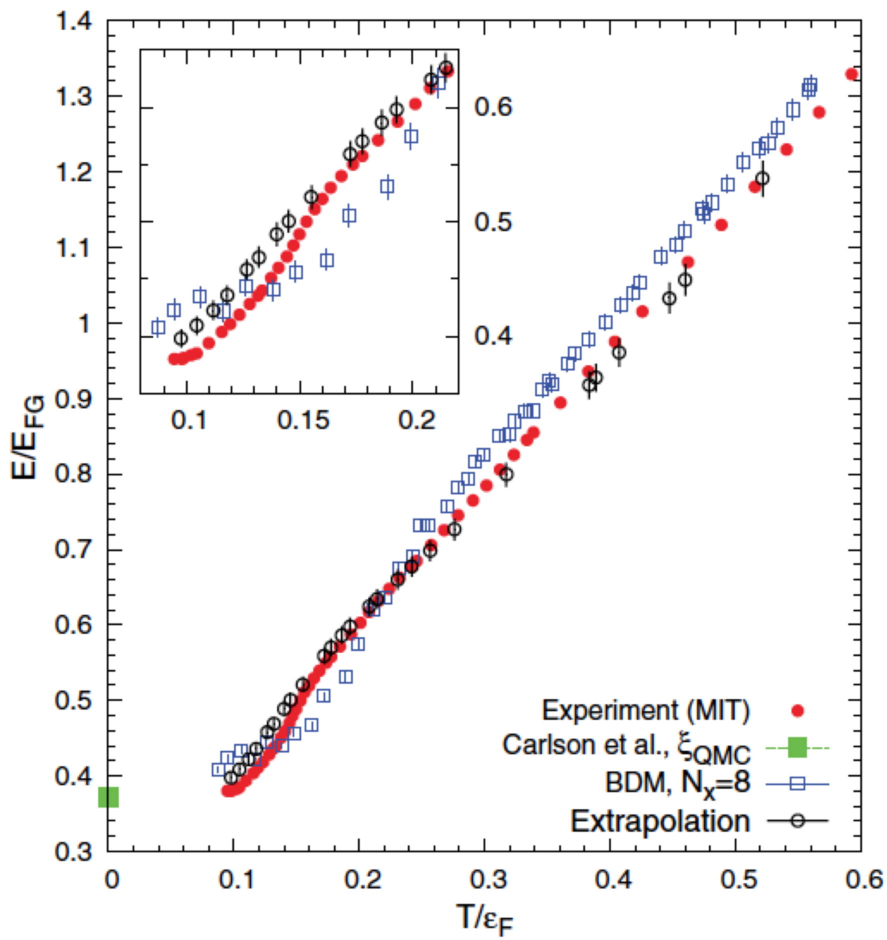


FIG. 2. (Color online) Energy $E/E_{\rm FG}$ (red dots), as obtained by Ku *et al.* [8]. Our AFQMC results extrapolated to infinite volume are shown by open black circles. The results for $N_x = 8$ (open blue squares) were obtained with the DMC algorithm in Ref. [9]. The green square shows the QMC result of Ref. [20] for ξ at $T = 0$. The inset shows the vicinity of the superfluid phase transition at $T_c/\epsilon_F \simeq 0.15$.

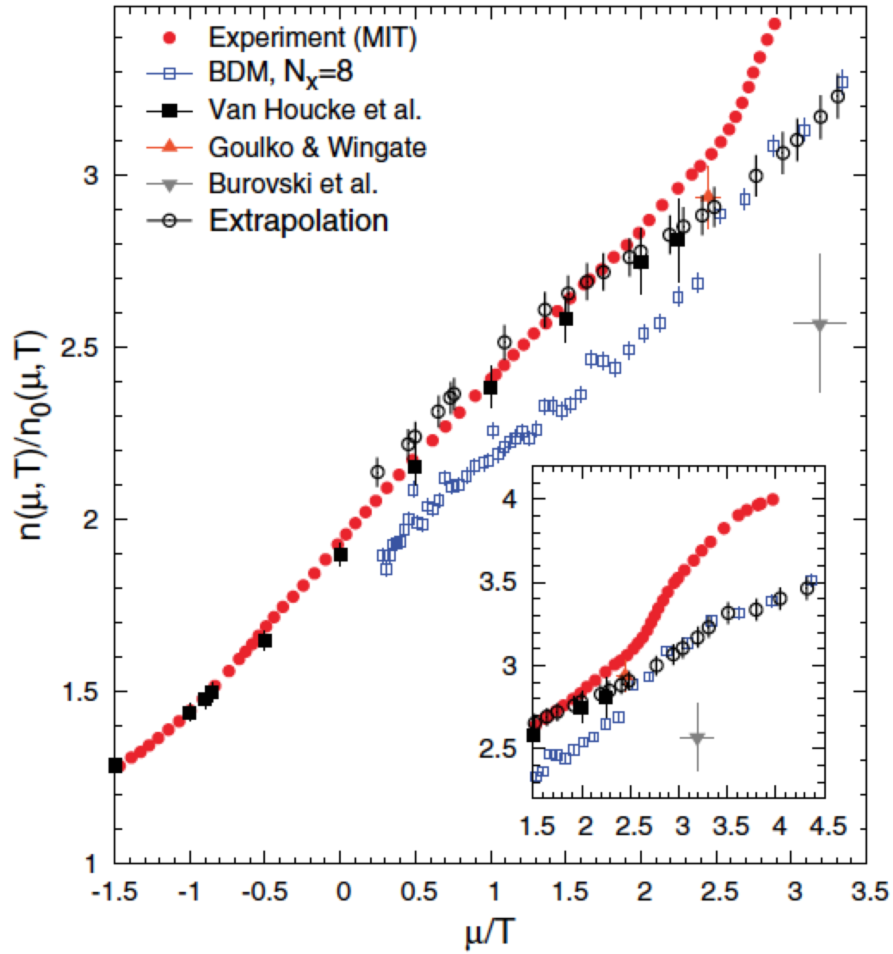
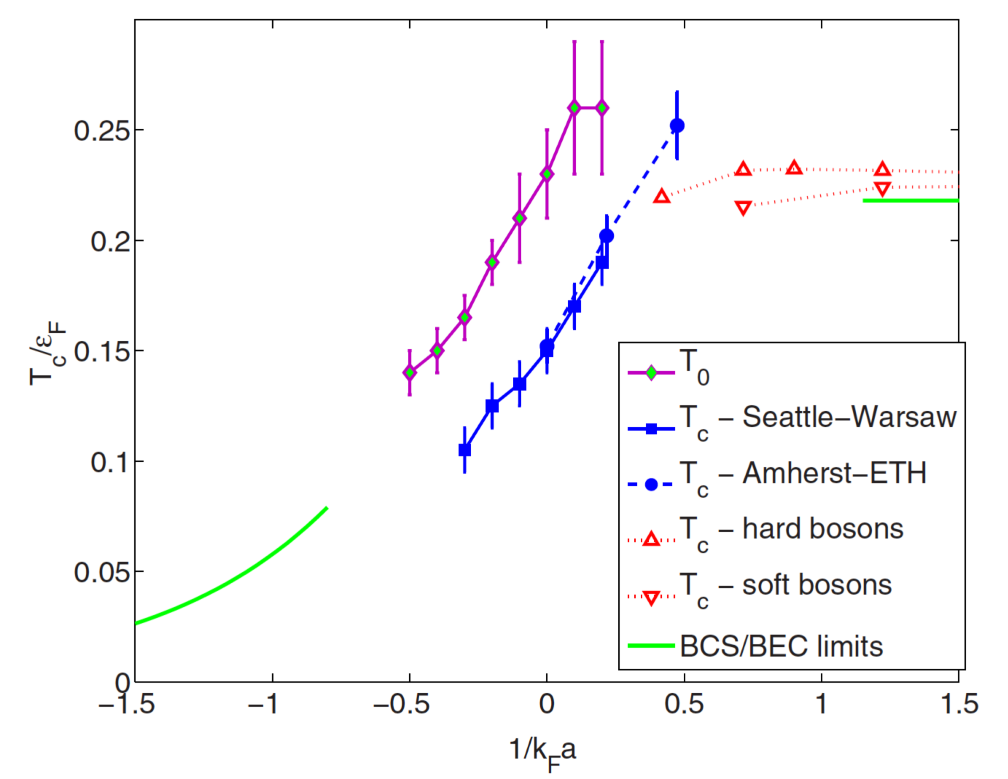


FIG. 4. (Color online) Density $n(\mu,T)$ of the UFG (red circles) as obtained by Ku *et al.* [8], normalized to the density $n_0(\mu,T)$ of a noninteracting Fermi gas. The notation for the AFQMC results is identical to Fig. 2. The diagrammatic MC results of Refs. [21,22] (solid up and down triangles) and the Bold Diagrammatic MC results of Ref. [23] are shown as well (solid squares). The inset shows the vicinity of the superfluid phase transition at $T_c/\epsilon_F \simeq 0.15$.

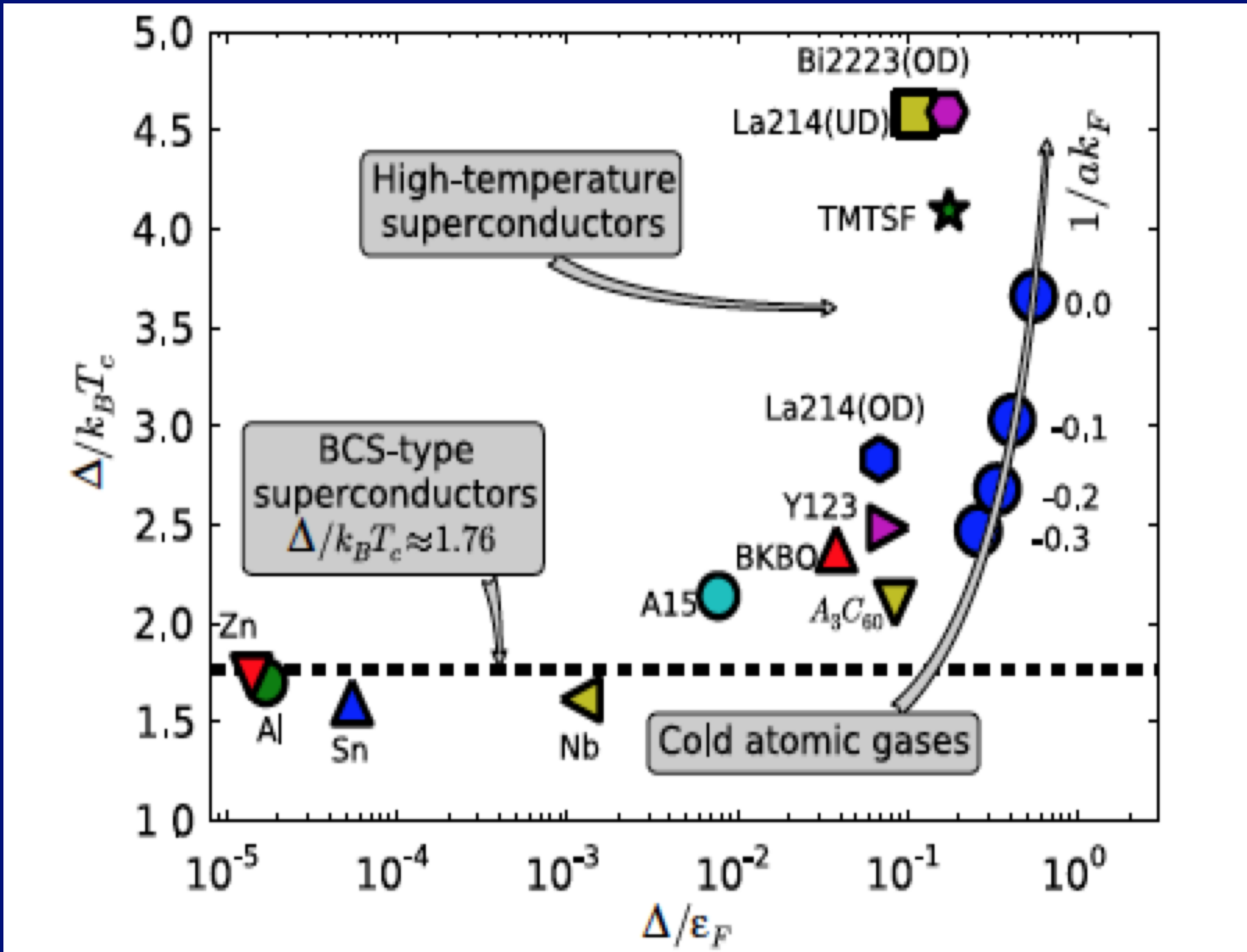
Critical temperature for superfluid to normal transition



Bulgac, Drut, and Magierski, Phys. Rev. A 78, 023625 (2008)

Amherst-ETH: Burovski et al. Phys. Rev. Lett. 101, 090402 (2008)

Hard and soft bosons: Pilati et al. PRL 100, 140405 (2008)



Bi2223(OD)
La214(UD)
High-temperature superconductors
TMTSF
$1/ak_F$
0.0
La214(OD)
-0.1
BCS-type superconductors
$\Delta/k_BT_c \approx 1.76$
Y123
-0.2
-0.3
BKBO
A15
A_3C_{60}
Zn
Al
Sn
Nb
Cold atomic gases
Δ/k_BT_c
Δ/ε_F
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}

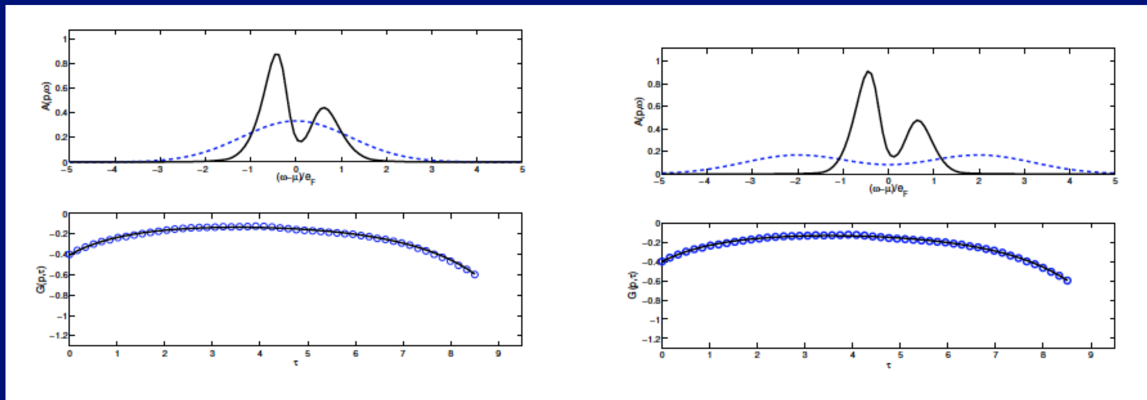
Matsubara propagator, spectral function and linear response

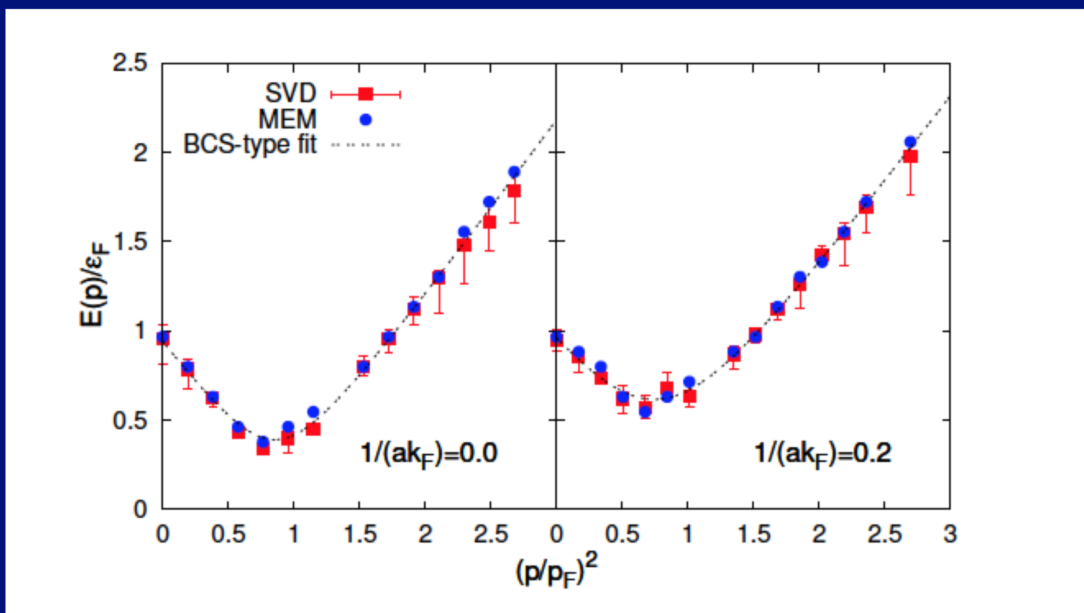
$$G(\vec{p},\tau)=\frac{1}{Z}\mathrm{Tr}\left\{\exp\left[-\left(\beta-\tau\right)\left(H-\mu N\right)\right]\psi^{\dagger}(\vec{p})\exp\left[-\tau\left(H-\mu N\right)\right]\psi(\vec{p})\right\}$$

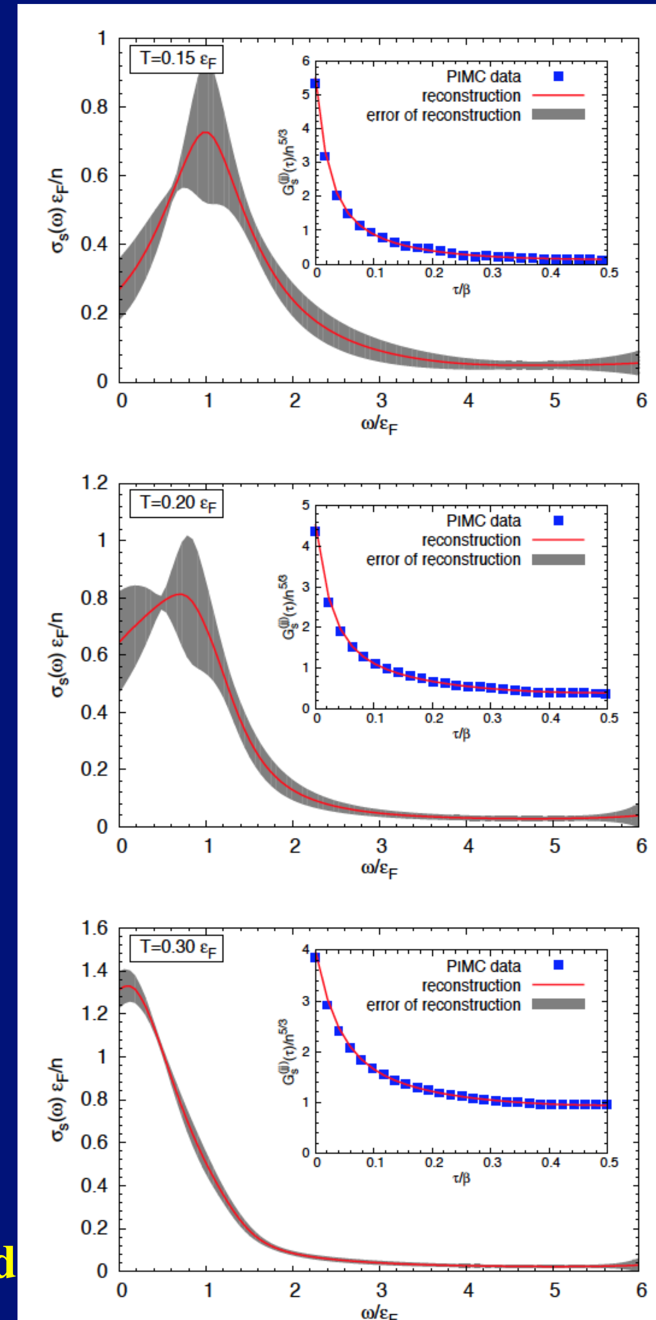
$$=-\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\, A(\omega,\vec{p})\frac{\exp(-\omega\tau)}{1+\exp(-\omega\beta)}$$

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\, A(\omega,\vec{p})=1,\qquad \frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\, A(\omega,\vec{p})\frac{1}{1+\exp(\omega\beta)}=n(\vec{p}),\quad A(\omega,\vec{p})\geq 0$$

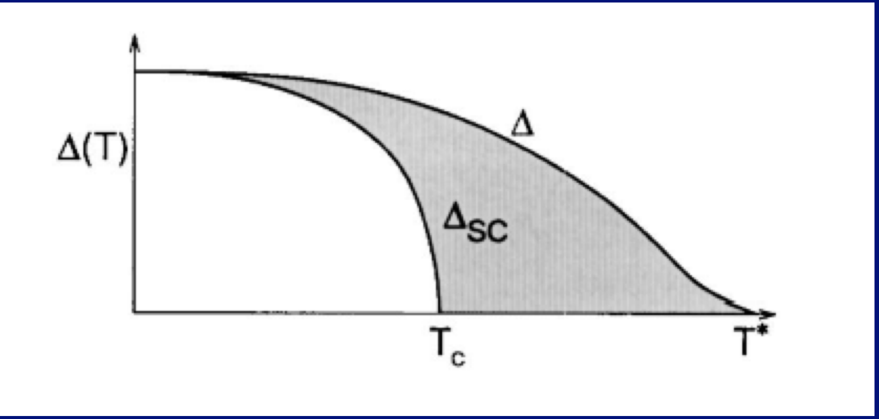
$$\chi_{s}=\lim_{p\to 0}\frac{1}{V}\int_{0}^{\beta}d\tau\left\langle s_{z}(\vec{p},\tau)s_{z}(-\vec{p},0)\right\rangle,\qquad s_{z}(\vec{p},\tau)=n_{\uparrow}(\vec{p},\tau)-n_{\downarrow}(\vec{p},\tau)$$

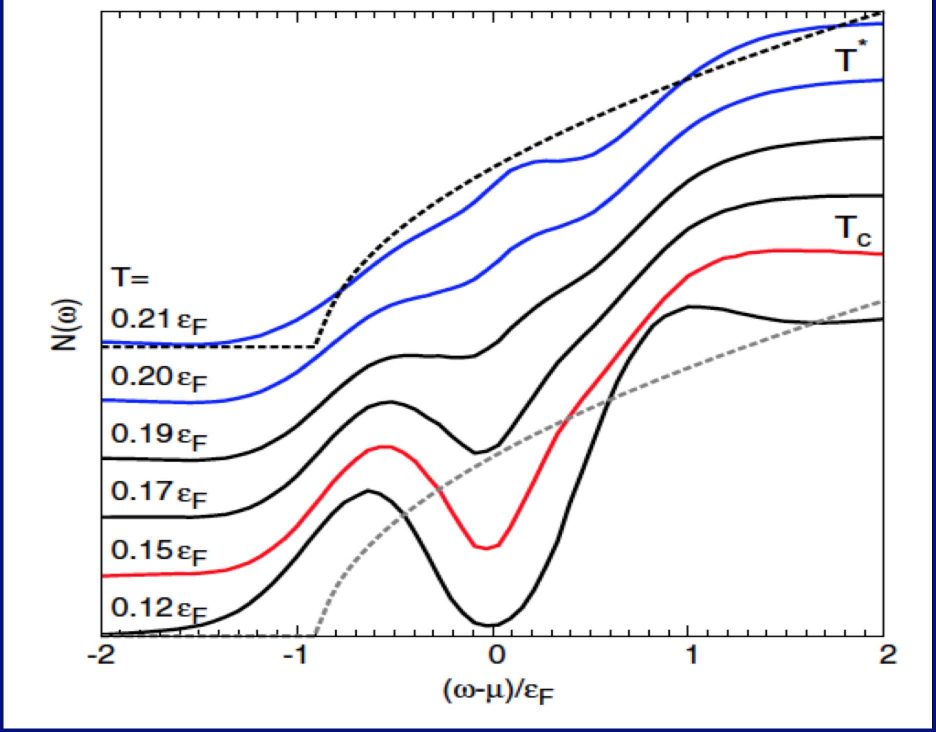




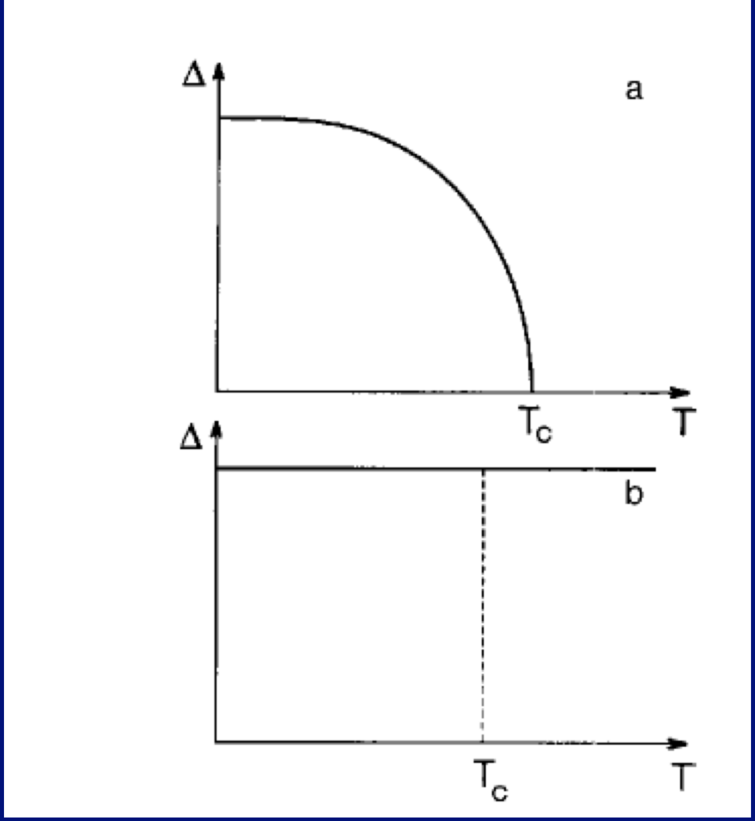


Singular value decomposition and maximum entropy method reconstruction of the spectral function

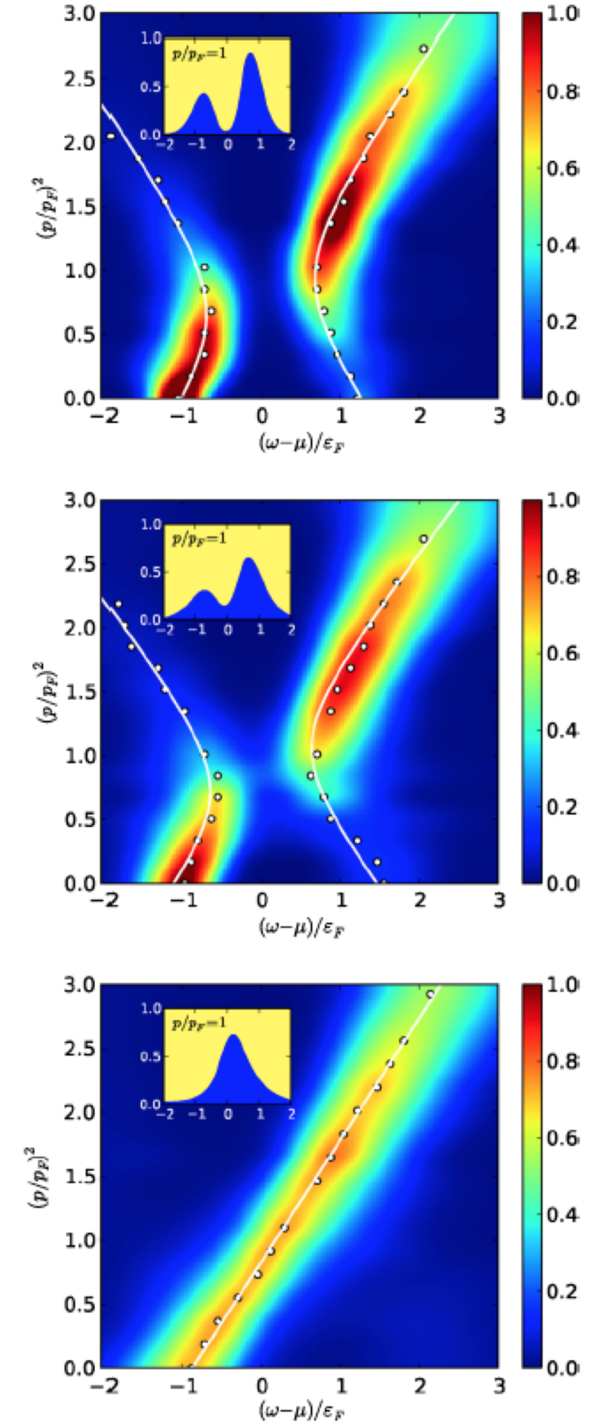




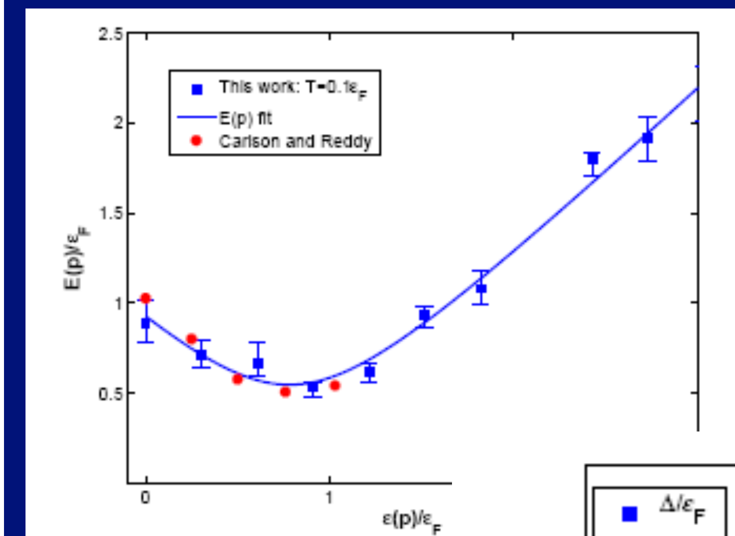
G. Wlazlowski, et al., Phys. Rev. Lett. 110, 090401 (2013)

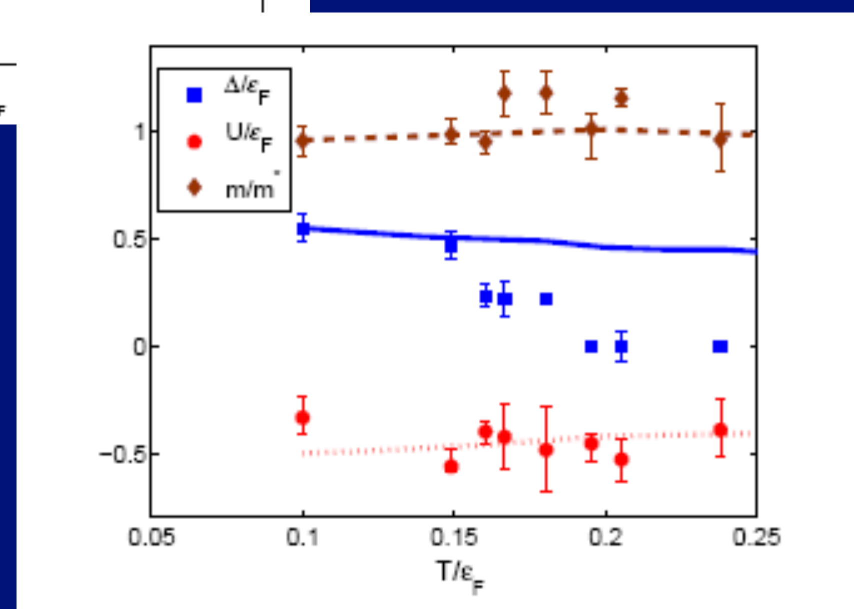


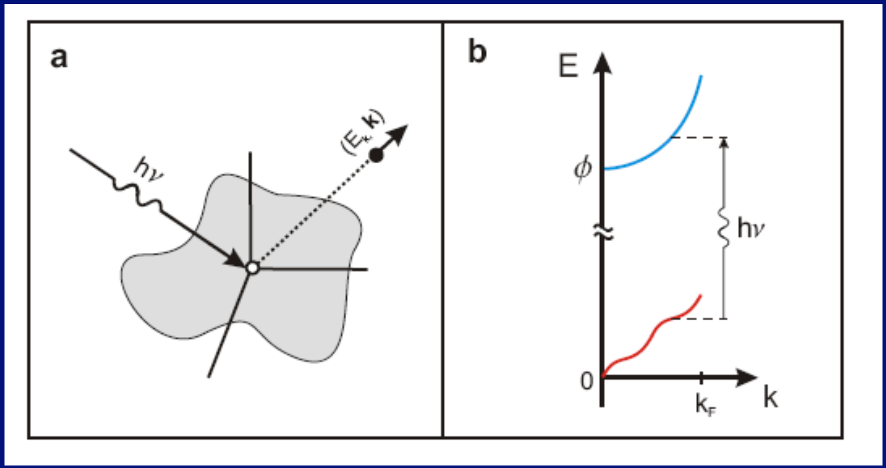
Chen et al, Low Temp. Phys. 32, 406 (2006)

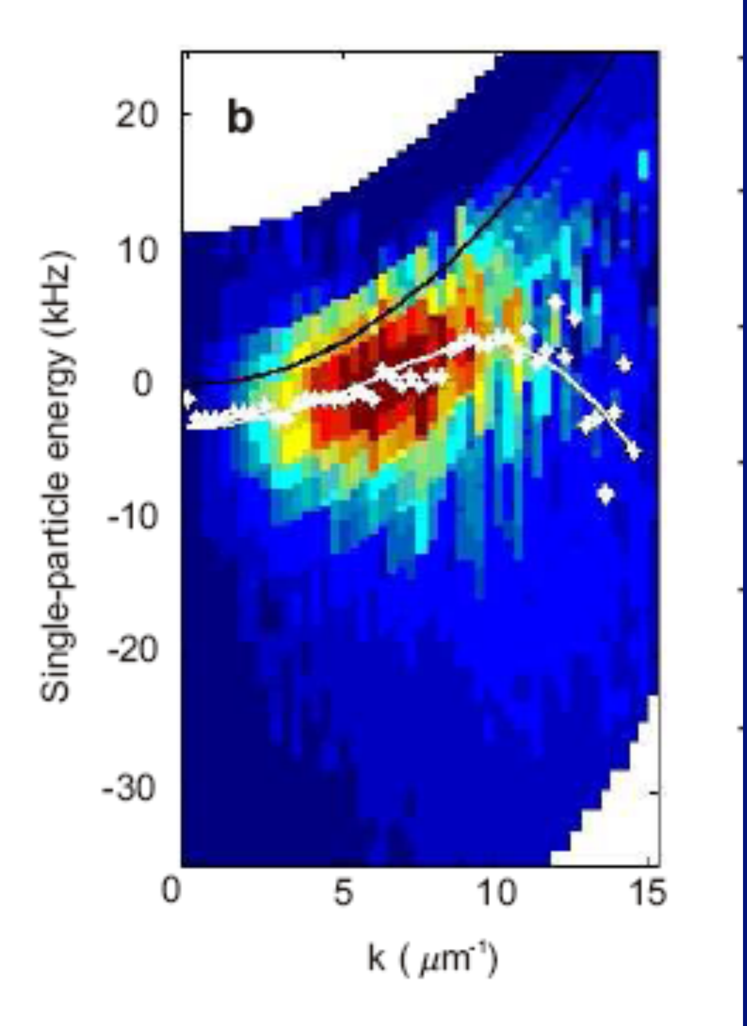


$$G(p,\tau) = \frac{1}{Z}\mathrm{Tr}\left\{\exp\left[-(\beta-\tau)(H-\mu N)\right]\psi^{\dagger}(p)\exp\left[-\tau(H-\mu N)\right]\psi(p)\right\}$$
$$= -\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega A(p,\omega)\frac{\exp(-\omega\tau)}{1+\exp(-\omega\beta)}$$





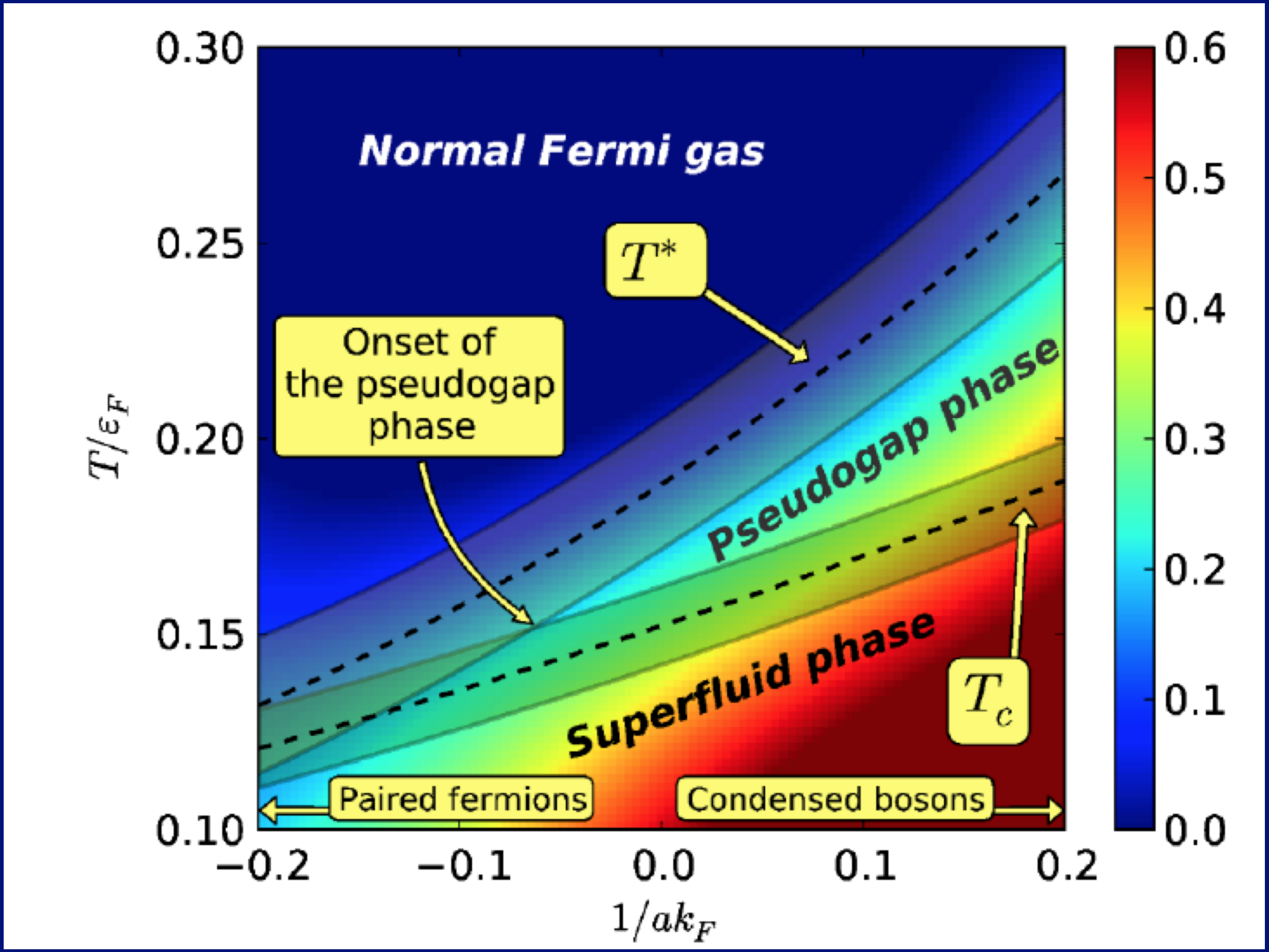




$$E(N) + h\nu = E(N-1) + E_k + \frac{\hbar^2 k^2}{2m} + \phi$$

Using photoemission spectroscopy to probe a strongly interacting Fermi gas

Stewart, Gaebler, and Jin, Nature, 454, 744 (2008)


Normal Fermi gas
T^*
Onset of the pseudogap phase
Pseudogap phase
Superfluid phase
T_c
Paired fermions
Condensed bosons
0.30
0.25
0.20
0.15
0.10
T/ε_F
−0.2
−0.1
0.0
0.1
0.2
$1/ak_F$
0.6
0.5
0.4
0.3
0.2
0.1
0.0

KSS conjecture

[Kovtun, Son, Starinets, PRL (2005)]

$$\frac{\eta}{s} \geq \frac{1}{4\pi}\frac{\hbar}{k_B}$$

shear viscosity → η

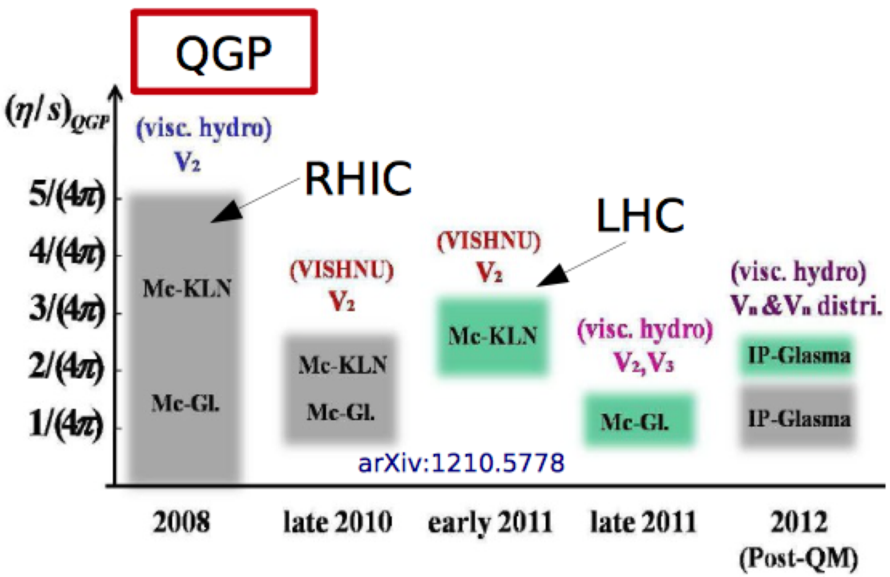
entropy density → s

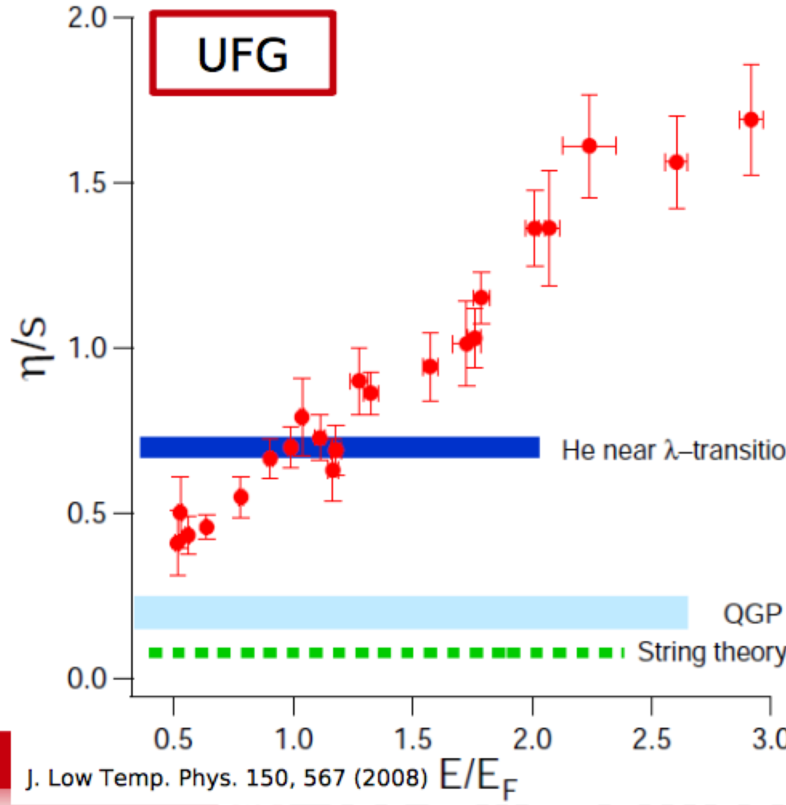
Minimum defines a "perfect" fluid

Bound has been proposed on the basis of string theory.

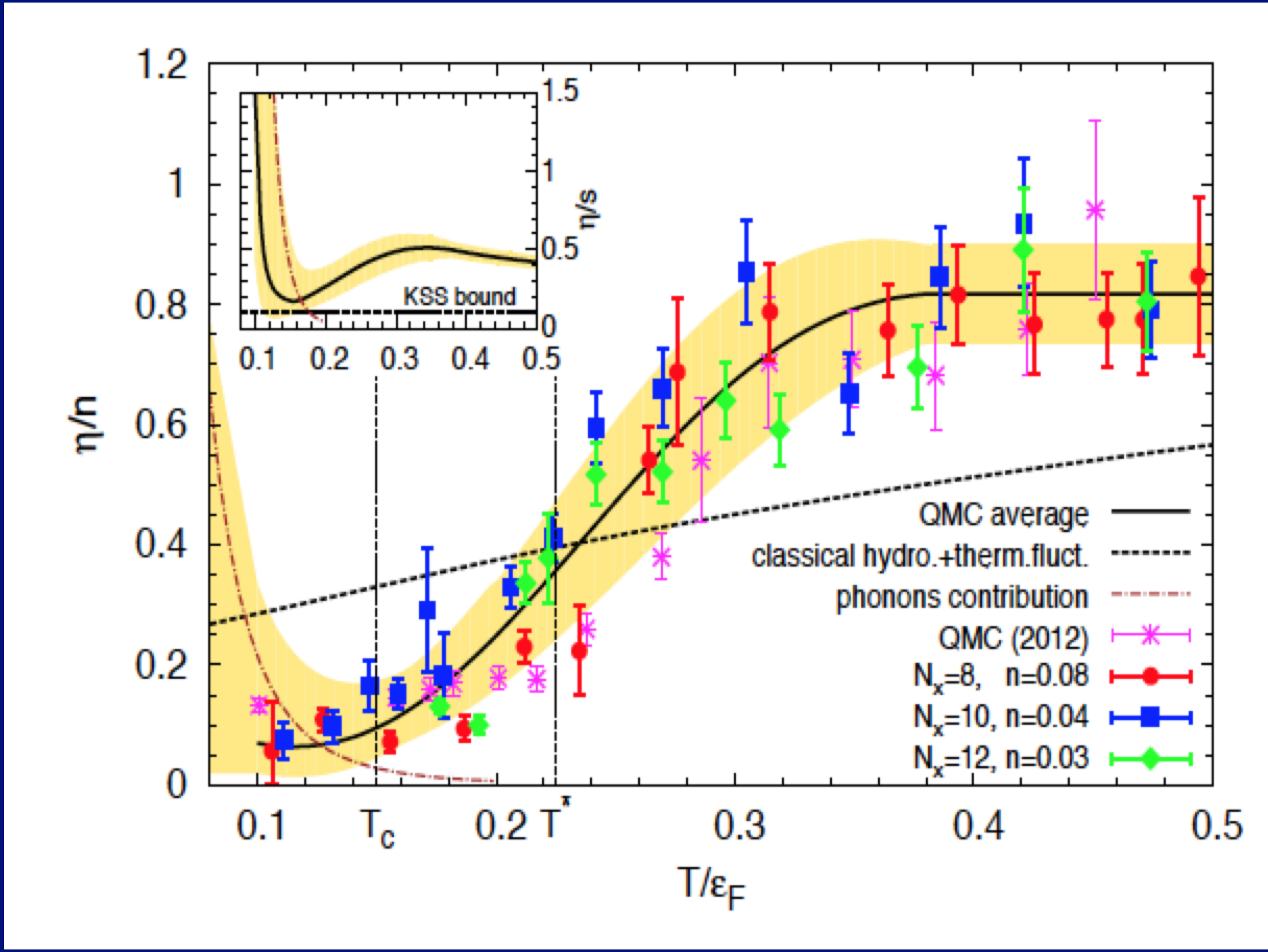
Valid for large class of (string) theories.

Saturated for the case of strongly coupled theory.

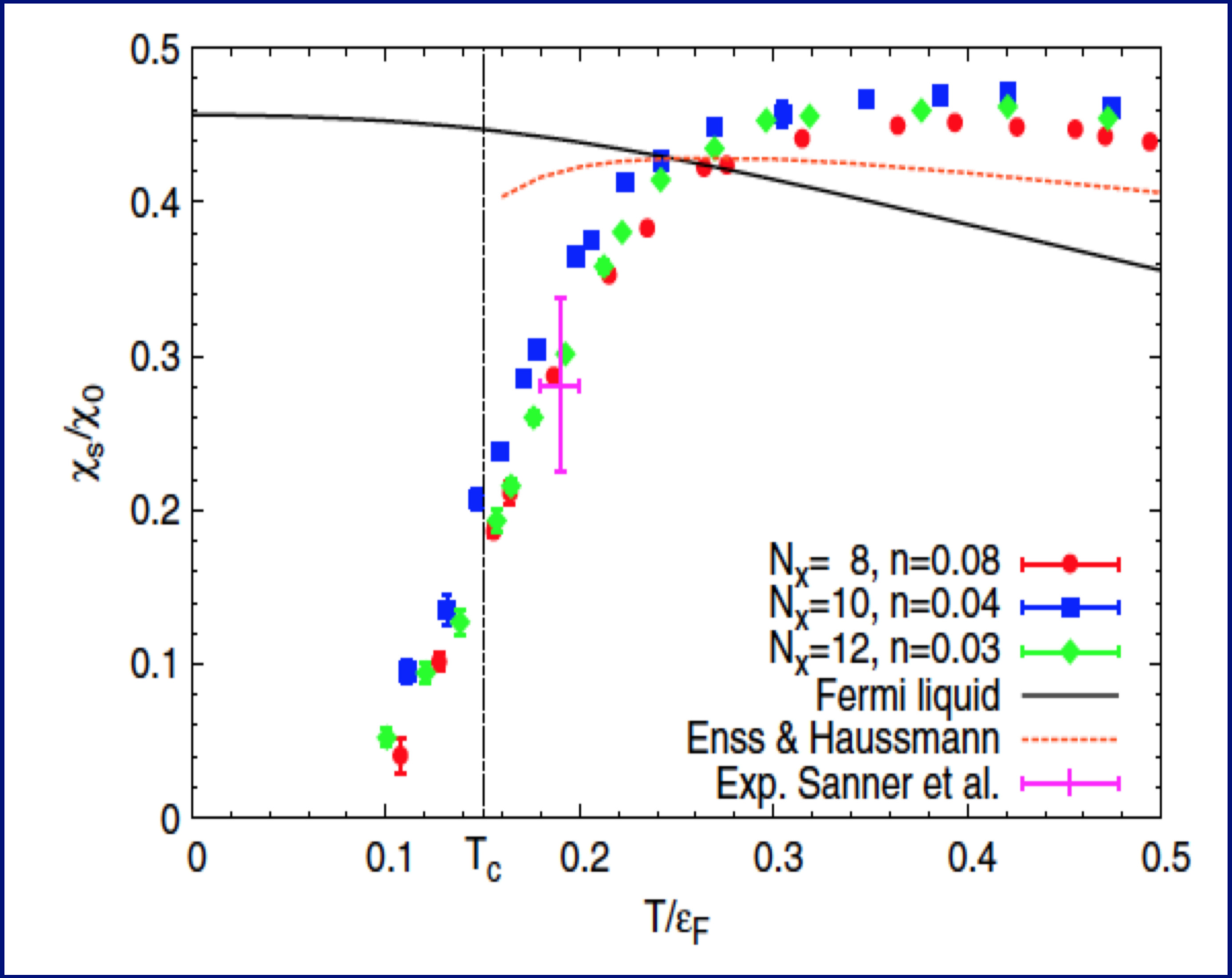




Slide from a talk given by G. Wlazlowski



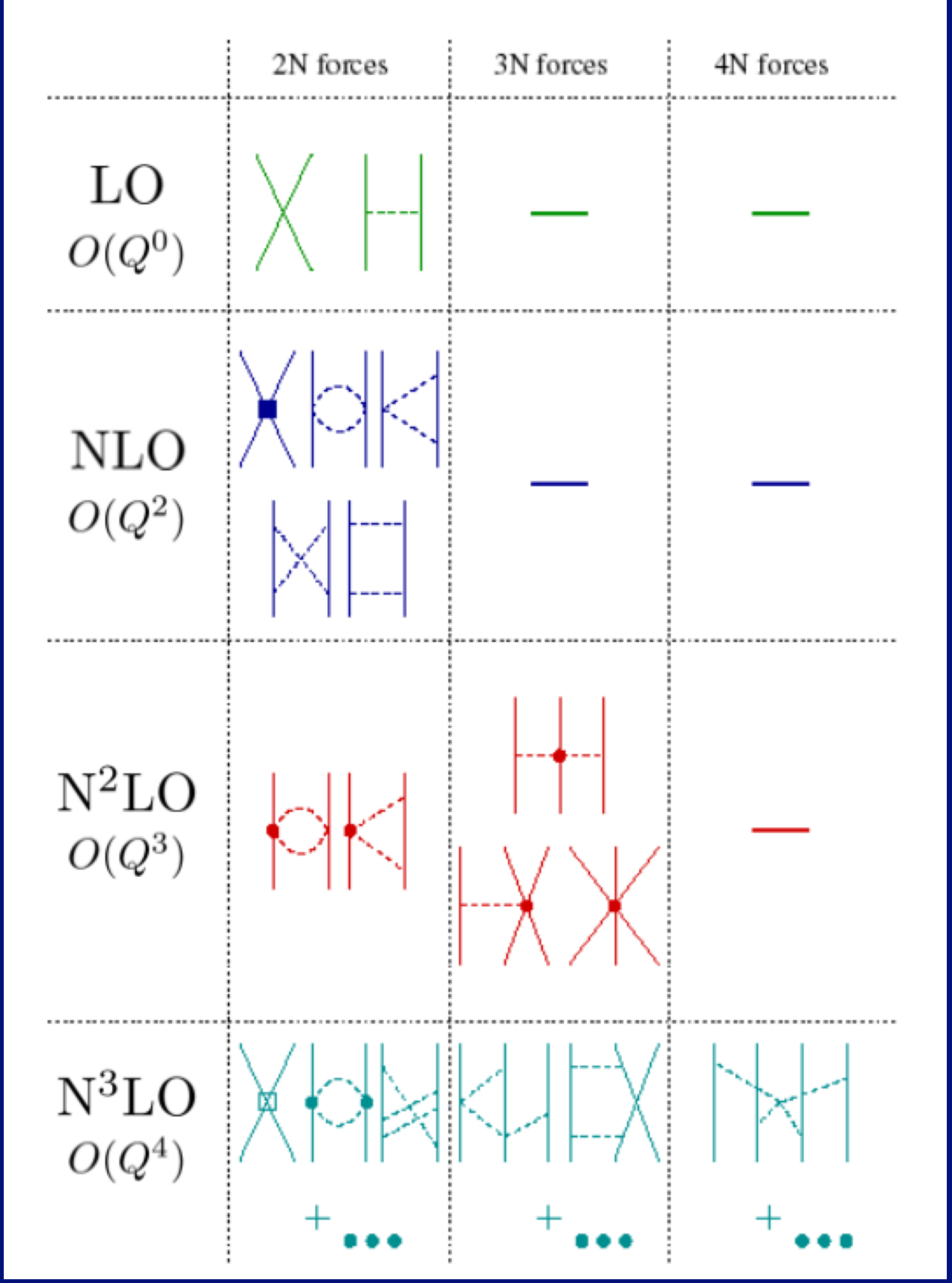
Shear viscosity of a unitary Fermi gas



$$\chi_s = \lim_{p\to 0} \frac{1}{V}\int_0^\beta d\tau \left\langle s_z(\vec{p},\tau)s_z(-\vec{p},0)\right\rangle, \qquad s_z(\vec{p},\tau) = n_\uparrow(\vec{p},\tau) - n_\downarrow(\vec{p},\tau)$$

Spin susceptibility

Now back to realistic Nuclear Physics



Somebody else's slide

Entem and Machleidt parameterization of the NN and NNN interaction with Λ=414 MeV/c

- NN phase shifts up to lab energies 200 MeV with χ^2/DOF = 1.44
- Binding energy and lifetime of ^3H
- Empirical nuclear matter saturation point and critical point of liquid-gas phase transition

see Corragio et al, Phys. Rev. C 75, 024311 (2007)
Phys. Rev. C 87, 014322 (2013)
Machleidt and Entem, Phys. Rep. 503, 1 (2011)

$\Delta\tau = 0.1\ \text{MeV}^{-1}$ and about 300 imaginary time steps

$$\Delta \text{x} = \frac{\pi\hbar}{\Lambda} = 1.5\ \text{fm and}\ \Lambda = 414\ \text{MeV/c}$$

$$N_x = N_y = N_z = 10,\ 12, 14, 16$$

$$N_{\text{part}} = 38 - 340$$

$$\langle\psi|O|\psi\rangle^{\text{cont}} \approx \langle\psi|O|\psi\rangle \frac{\langle\psi_0|O|\psi_0\rangle^{\text{cont}}}{\langle\psi_0|O|\psi_0\rangle}$$

$$f(p,p') = \exp\left(-\left(\frac{p}{\Lambda}\right)^{20} - \left(\frac{p'}{\Lambda}\right)^{20} \right), \quad \Lambda = 414 \text{ Mev/c}$$

$$H = T + V_{\text{evol}} + \left(V - V_{\text{evol}}\right)$$

$$V = V_{2N} + V_{3N}$$

$$\psi\left(\tau \to \infty\right) \propto \exp\left(-\tau H_{\text{evol}}\right)\psi_0$$

$$V_{\text{evol}} = \sum_{\alpha=\pi,\sigma,\omega} \frac{V_\alpha}{m_\alpha^2 + q^2} f(q), \quad f(q) = \exp\left(-\left(\frac{q}{\Lambda}\right)^{30} \right)$$

$$\chi^2 = \sum_{i,j} w^{(j)} \left[\delta^j_{\text{EFT}}(E_i) - \delta^j_{\text{evol}}(E_i)\right]^2 + \alpha\left[\text{E}^{\text{pert}}_{\text{EFT}} - \text{E}^{\text{pert}}_{\text{evol}}\right]^2, \quad j = \text{s- and p-waves}$$

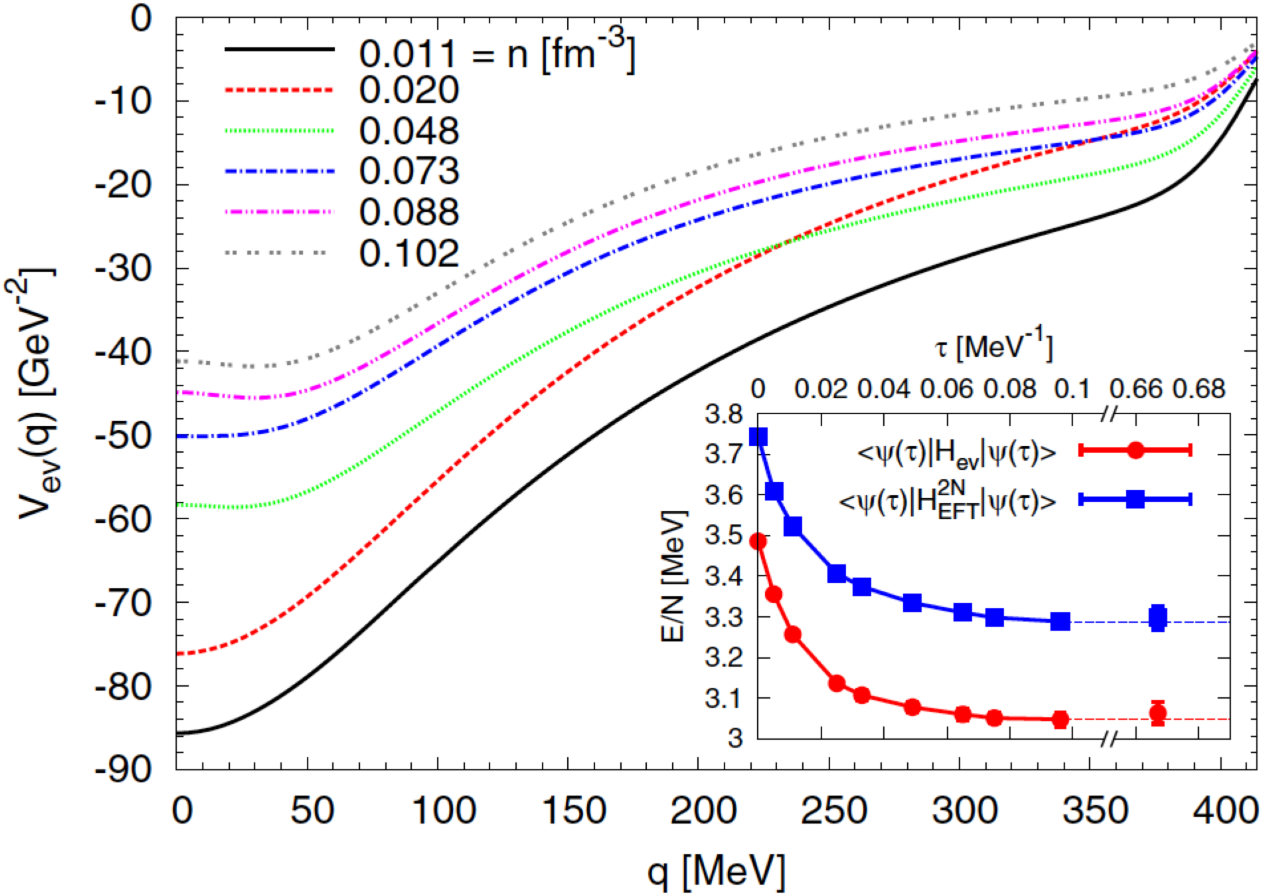


FIG. 1 (color online). Momentum-space evolution potentials [see Eq. (4)] employed in the imaginary-time propagation of the trial wave function, corresponding to different densities. In the inset is shown the expectation values of the evolution potential (red solid circles) and the two-body chiral potential (blue squares) computed for the density $n = 0.011\ \mathrm{fm}^{-3}$.

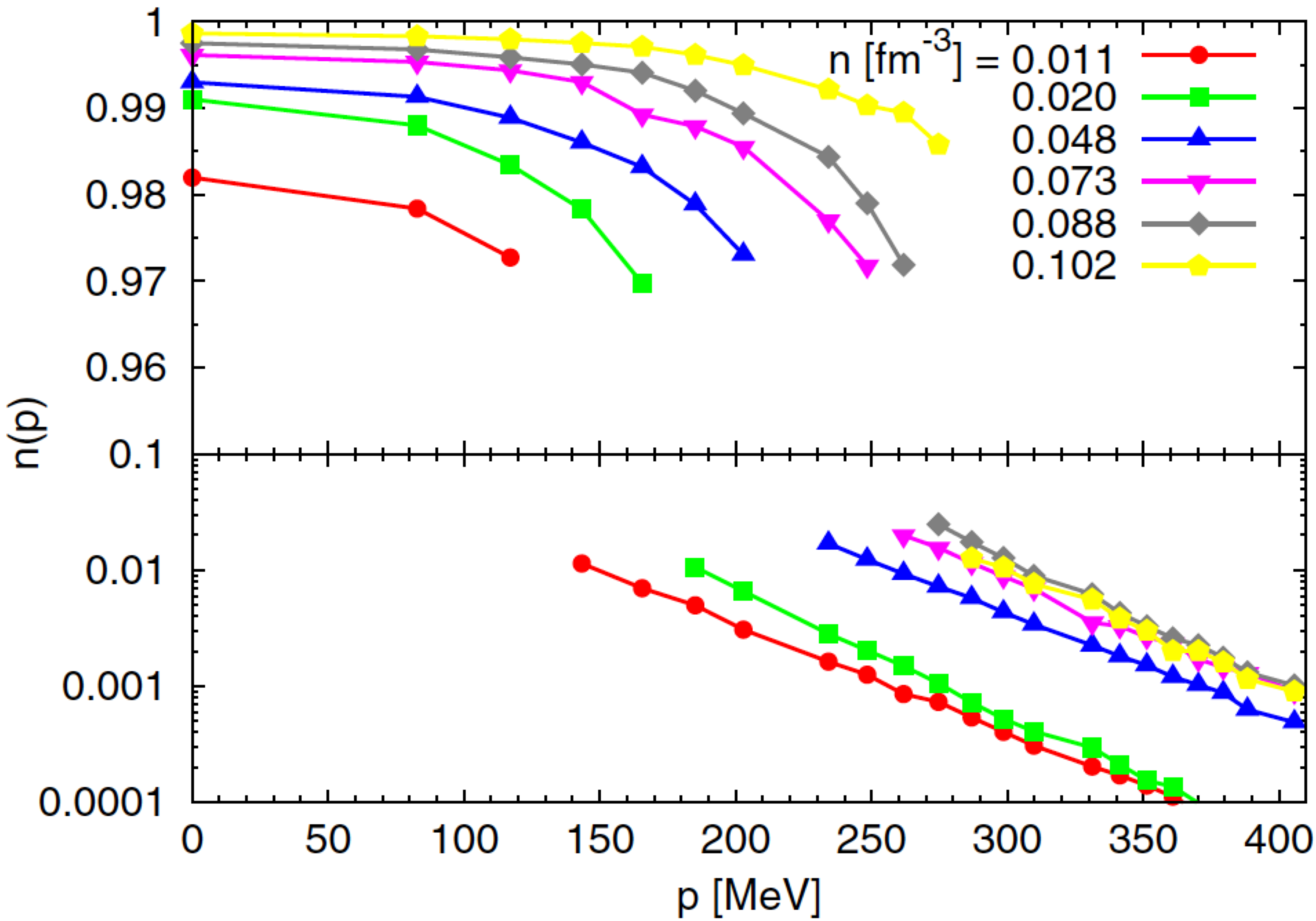
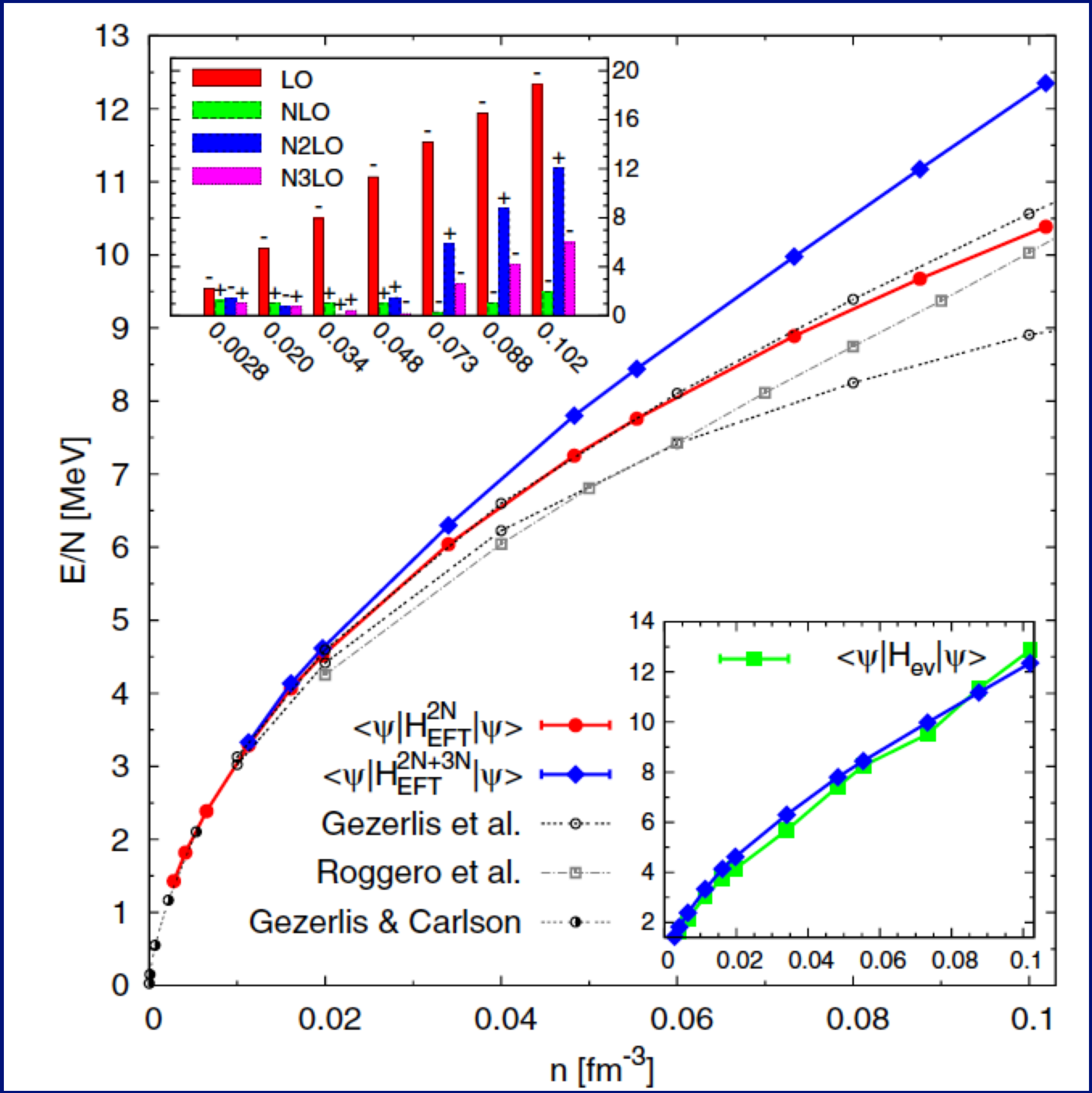


FIG. 2 (color online). Occupation probabilities of neutron matter as a function of momentum for selected densities.

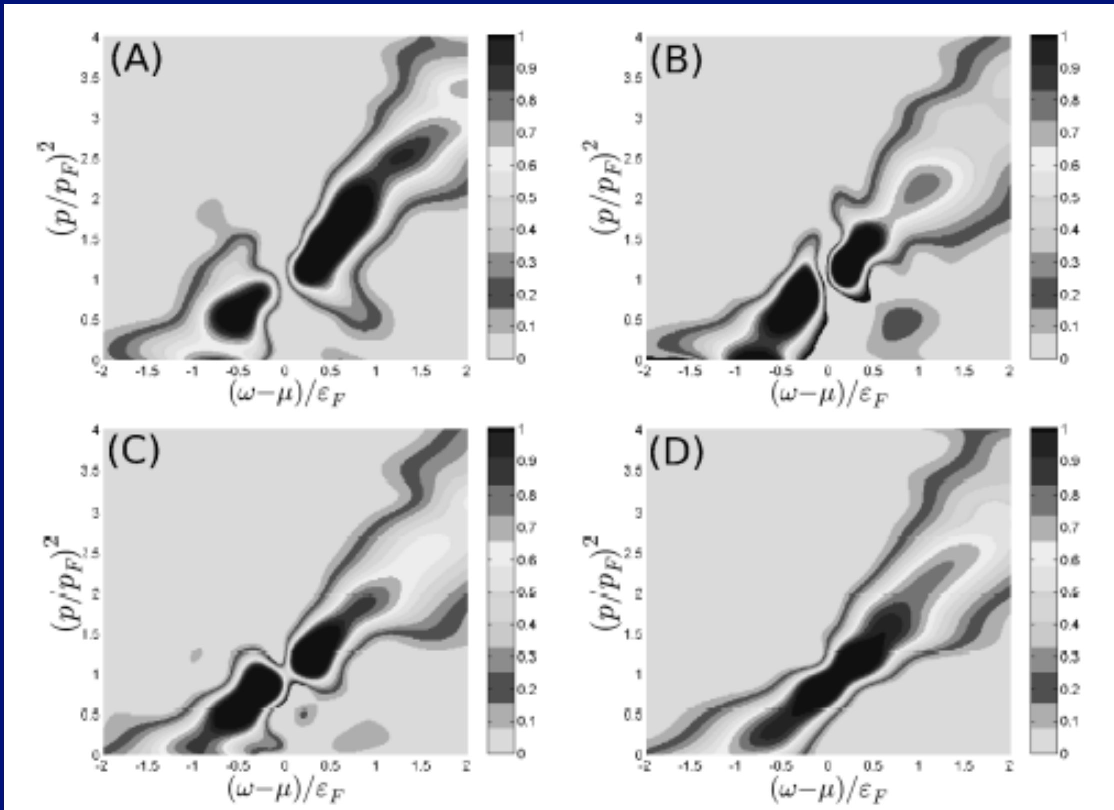
- Gezerlis, Tews, Epelbaum, Gandolfi, Hebeler, Nogga, and Schwenk,
Phys. Rev. Lett. 111, 032501 (2013)
AFQMC/GFMC with two-body NN–interaction LO+NLO+NNLO

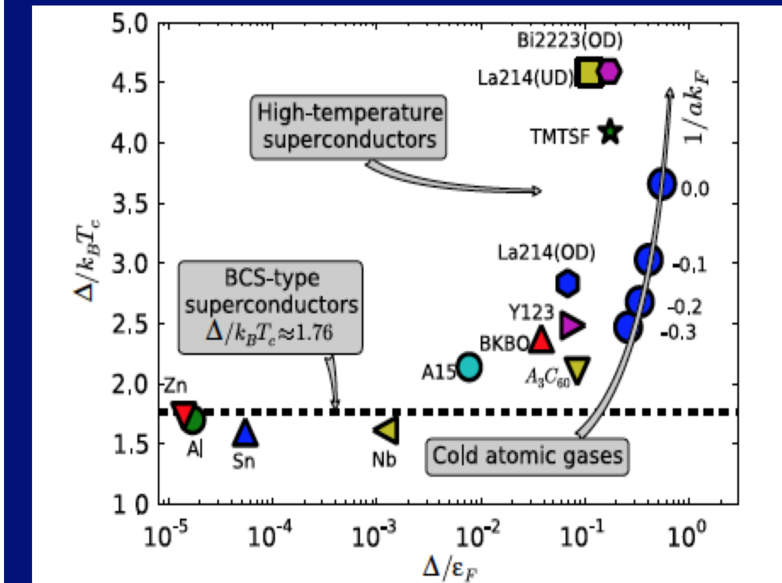
- Roggero, Mukherjee, and Pederiva,
Phys. Rev. Lett. 112, 221103 (2014)
CIMC with two-body NN–interaction LO+NLO+NNLO

- Gezerlis and Carlson,
Phys. Rev. C 77, 032801(R) (2008)
GFMC with s-wave part of AV18 NN–interaction



We have included NN (up to NNNLO) and NNN (NNLO)

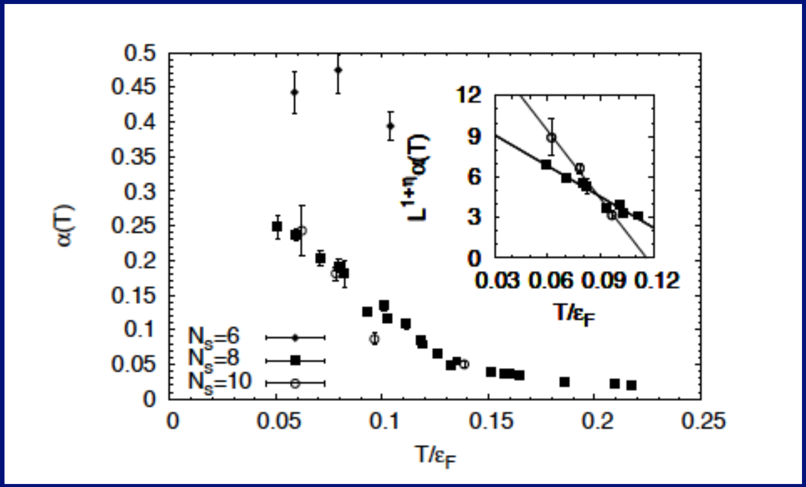


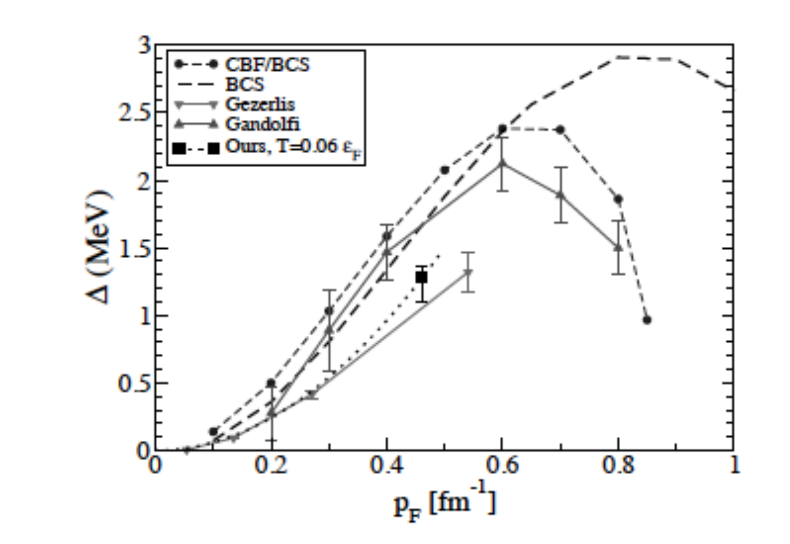


A) T = 0.06 ε_F, B) T = 0.08 ε_F, C) T = 0.1 ε_F, D) T = 0.12 ε_F

Wlazlowski and Magierski, PRC 83, 012801 (2011), Int. J. Mod. Phys. E20, 569 (2011)

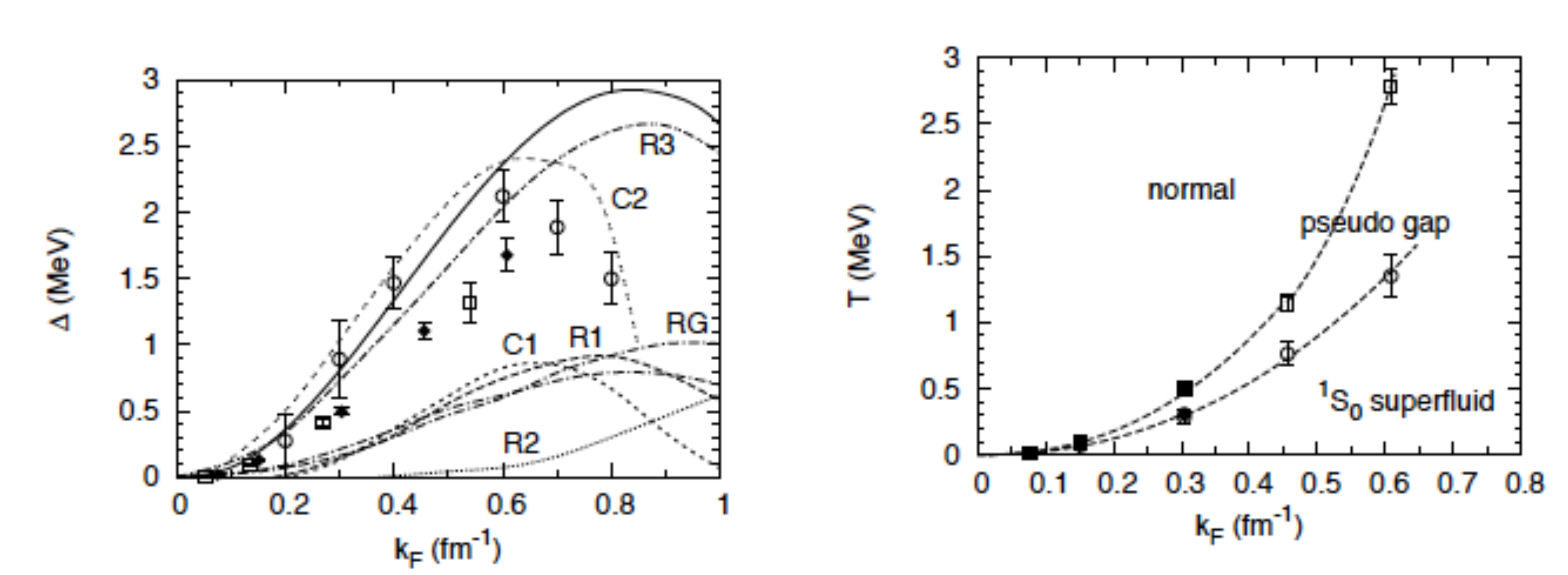
$T_c = 0.09\ \varepsilon_{F,}$ $\Delta = 0.25\ \varepsilon_{F,}$ <u>$\Delta/T_c = 2.8$</u>





A) T = 0.06 T_F, B) T = 0.08 T_F, C) T = 0.1 T_F, D) T = 0.12 T_F - Tc = 0.09 T_F

Wlazlowski and Magierski, PRC 83, 012801 (2011), Int. J. Mod. Phys. E18, 919 (2010)



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