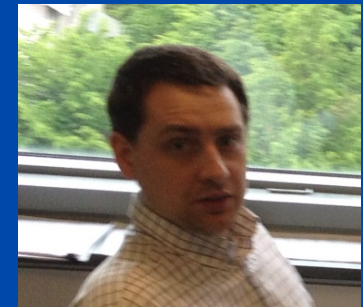


Fermions in the unitary regime at finite temperatures

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Gabriel Wlazlowski (Warsaw/Seattle)



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References:

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- *Quantum Monte Carlo study of dilute neutron matter at finite temperatures*, G. Wlazlowski and P. Magierski, Phys. Rev. C 83, 012801(R) (2011)
- *Finite-temperature pairing gap of a unitary Fermi gas by quantum Monte Carlo calculations*, P. Magierski, G. Wlazlowski, A. Bulgac, and J.E. Drut, Phys. Rev. Lett. 103, 210403 (2009)
- *Quantum Monte Carlo simulations of the BCS-BEC crossover at finite temperatures*, A. Bulgac, J.E. Drut, and P. Magierski, Phys. Rev. A 78, 023625 (2008)
- *Thermodynamics of a trapped unitary Fermi gas*, A. Bulgac, J.E. Drut, and P. Magierski, Phys. Rev. Lett. 99, 120401 (2007)
- *Spin $\frac{1}{2}$ fermions in the unitary regime: a superfluid of a new type*, A. Bulgac, J.E. Drut, and P. Magierski, Phys. Rev. Lett. 96, 090404 (2006)

Why would one want to study this system?

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 $\frac{1}{2}$ fermions interacting via a zero-range, infinite scattering-length contact interaction.

What are the scattering length and the effective range?

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

$$\sigma = \frac{4\pi}{k^2} \sin^2 \delta_0 + \dots = 4\pi a^2 + \dots$$

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

Let me consider 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 $\frac{1}{2}$ 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:

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

$$\frac{N}{V} = \frac{k_F^3}{3\pi^2},$$

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$$

Pure number



What are the ground state properties of the many-body system composed of spin $\frac{1}{2}$ fermions interacting via a zero-range, infinite scattering-length contact interaction.

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

In 1999 it was not yet clear, either theoretically or experimentally, whether such fermion matter is stable or not! A number of people argued that under such conditions Fermionic matter is unstable.

- *systems of bosons are unstable (Efimov effect)***
 - *systems of three or more fermion species are unstable (Efimov effect)***
 - Baker (LANL, winner of the MBX challenge) concluded that the system is stable. See also Heiselberg (entry to the same competition)**
 - Carlson et al (2003) Fixed-Node Green Function Monte Carlo and Astrakharchik et al. (2004) FN-DMC provided the best theoretical estimates for the ground state energy of such systems.**
- Carlson et al (2003) have also shown that the system has a huge pairing gap !**
- Thomas' Duke group (2002) demonstrated experimentally that such systems are (meta)stable.**

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 !

$$E_{gs} = \frac{3}{5} \varepsilon_F N \times \xi \quad \Delta = \varepsilon_F \times \zeta$$
$$\xi = 0.40(1), \quad \zeta = 0.50(1)$$

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

The system is very dilute, but strongly interacting!

$$n r_0^3 \ll 1$$

$$n |a|^3 \gg 1$$

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

n - number density

r_0 - range of interaction

a - scattering length

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

${}^6\text{Li}$ ground state in a magnetic field

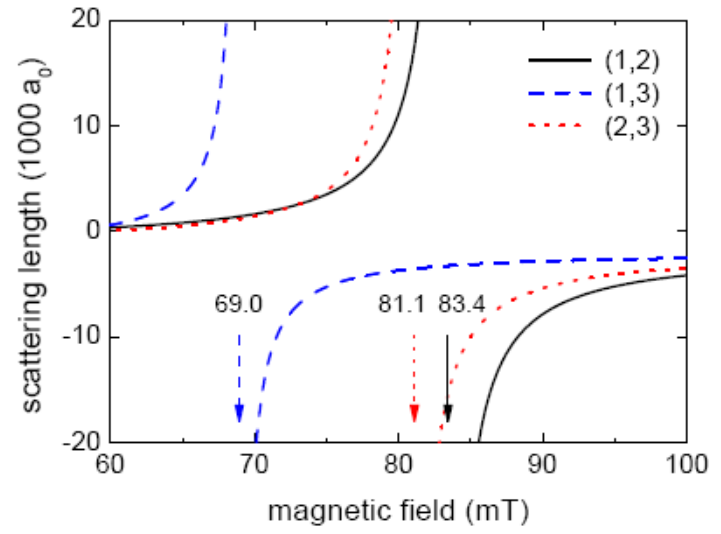
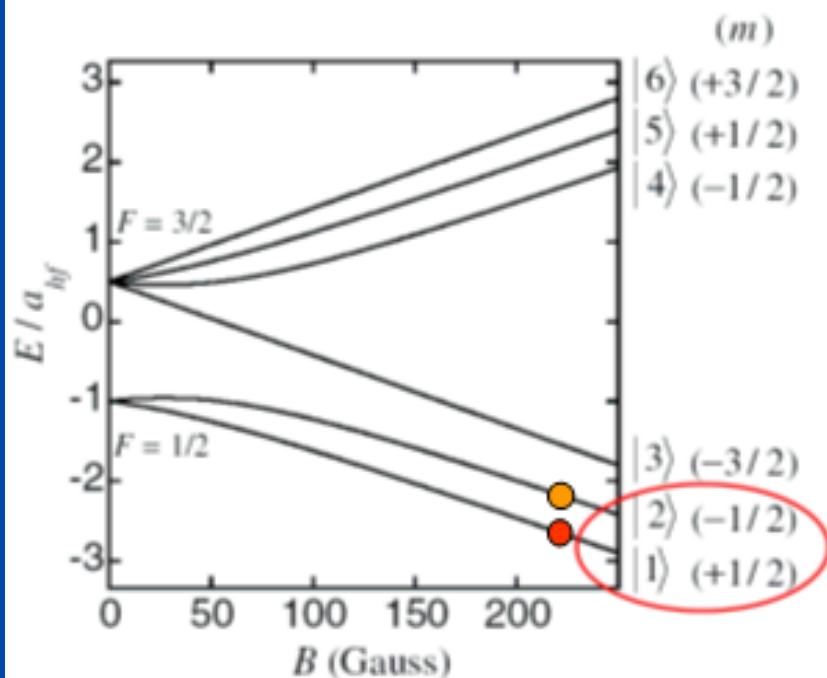


FIG. 4: Scattering lengths versus magnetic field from multi-channel quantum scattering calculations for the (1,2), (1,3), and (2,3) scattering channels. The arrows indicate the resonance positions.

Bartenstein *et al.* Phys. Rev. Lett. **94**, 103201 (2005)

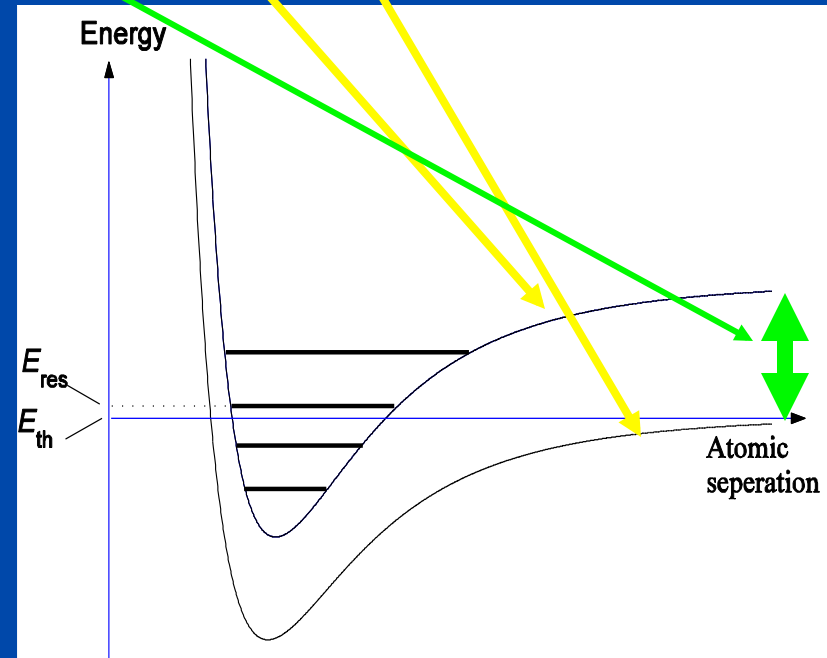
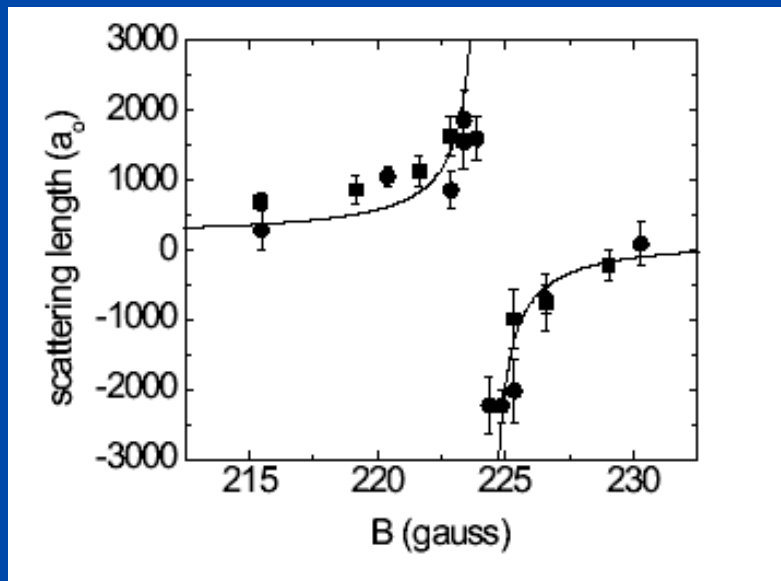
Feshbach resonance

$$H = \frac{\vec{p}^2}{2\mu_r} + \sum_{i=1}^2 (V_i^{hf} + V_i^Z) + V_0(\vec{r})P_0 + V_1(\vec{r})P_1 + \cancel{V^d}$$

$$V^{hf} = \frac{a_{hf}}{\hbar^2} \vec{S}^{elec} \cdot \vec{S}^{nucl}, \quad V^Z = (\gamma_e S_z^{elec} - \gamma_n S_z^{nucl}) B$$

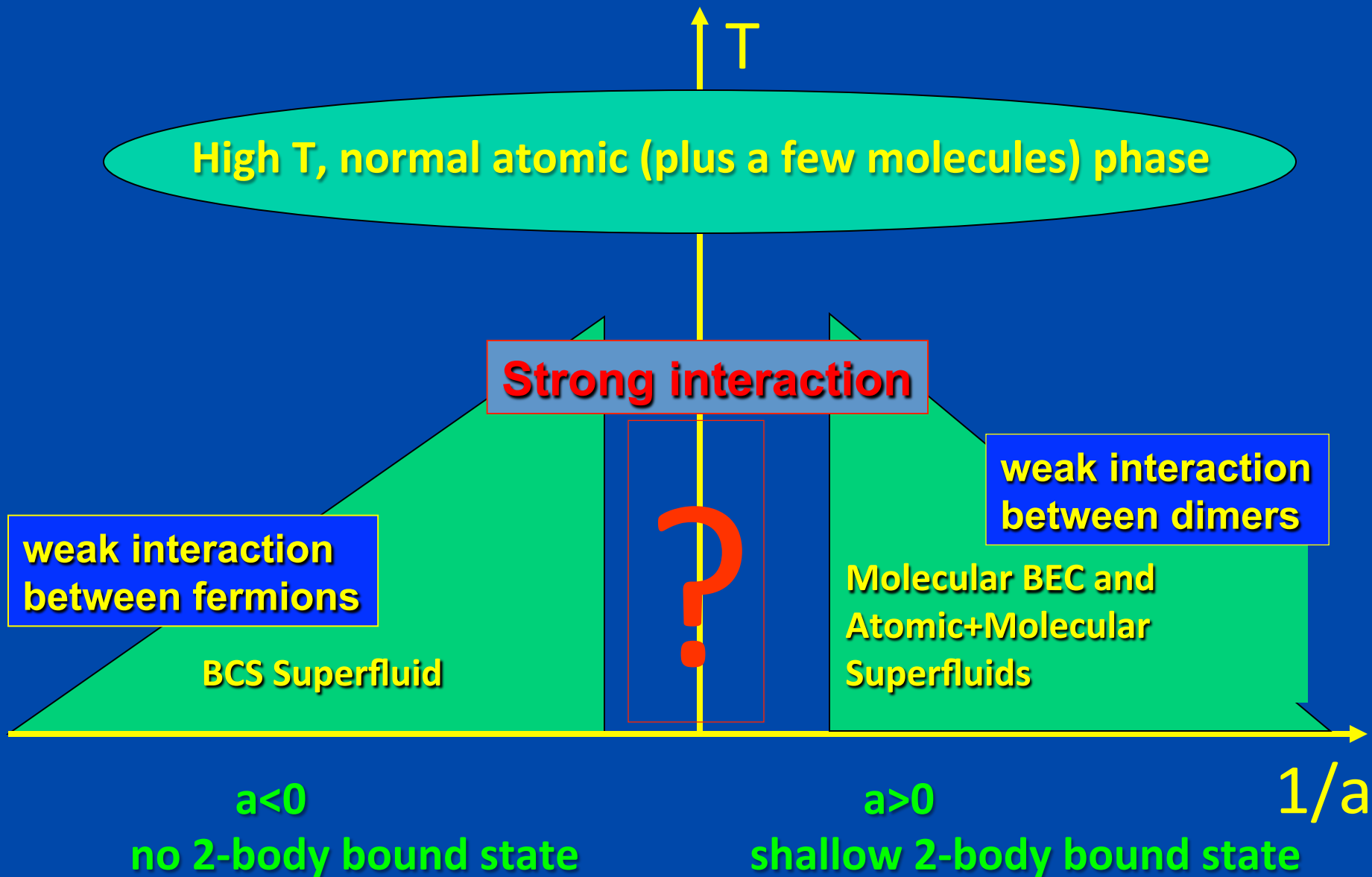
Channel coupling

Tiesinga, Verhaar, and Stoof
 Phys. Rev. A 47, 4114 (1993)



Regal and Jin
 Phys. Rev. Lett. 90, 230404 (2003)

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



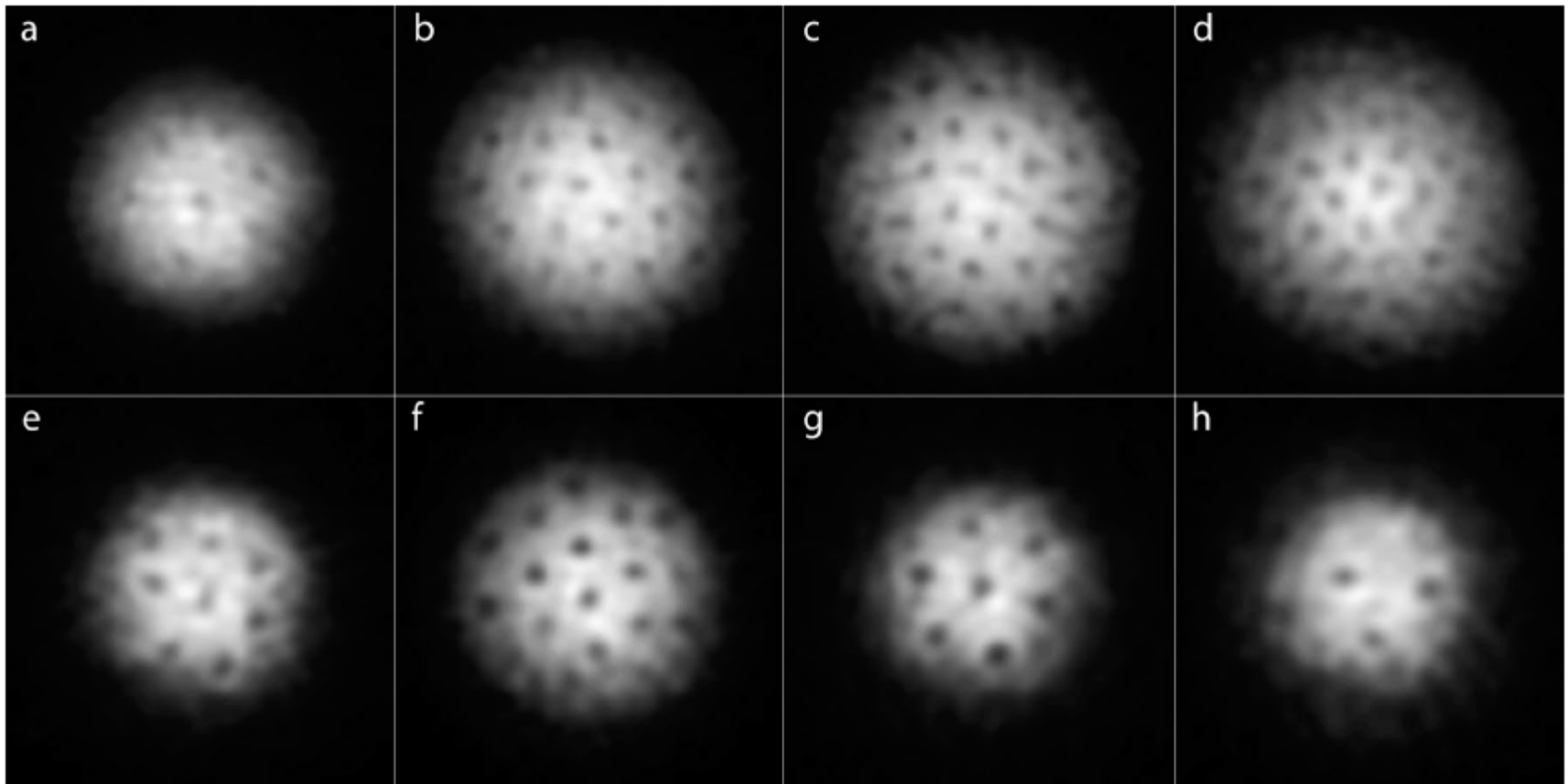


Fig. 2: Vortices in a strongly interacting gas of fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (a) to 500 ms (b-h) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, the magnetic 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 $880 \mu\text{m} \times 880 \mu\text{m}$.

Finite Temperatures

Grand Canonical Path-Integral Monte Carlo

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

Trotter expansion (*trotterization* of the propagator)

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

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

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

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 $L=N_1l$, with periodic boundary conditions

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

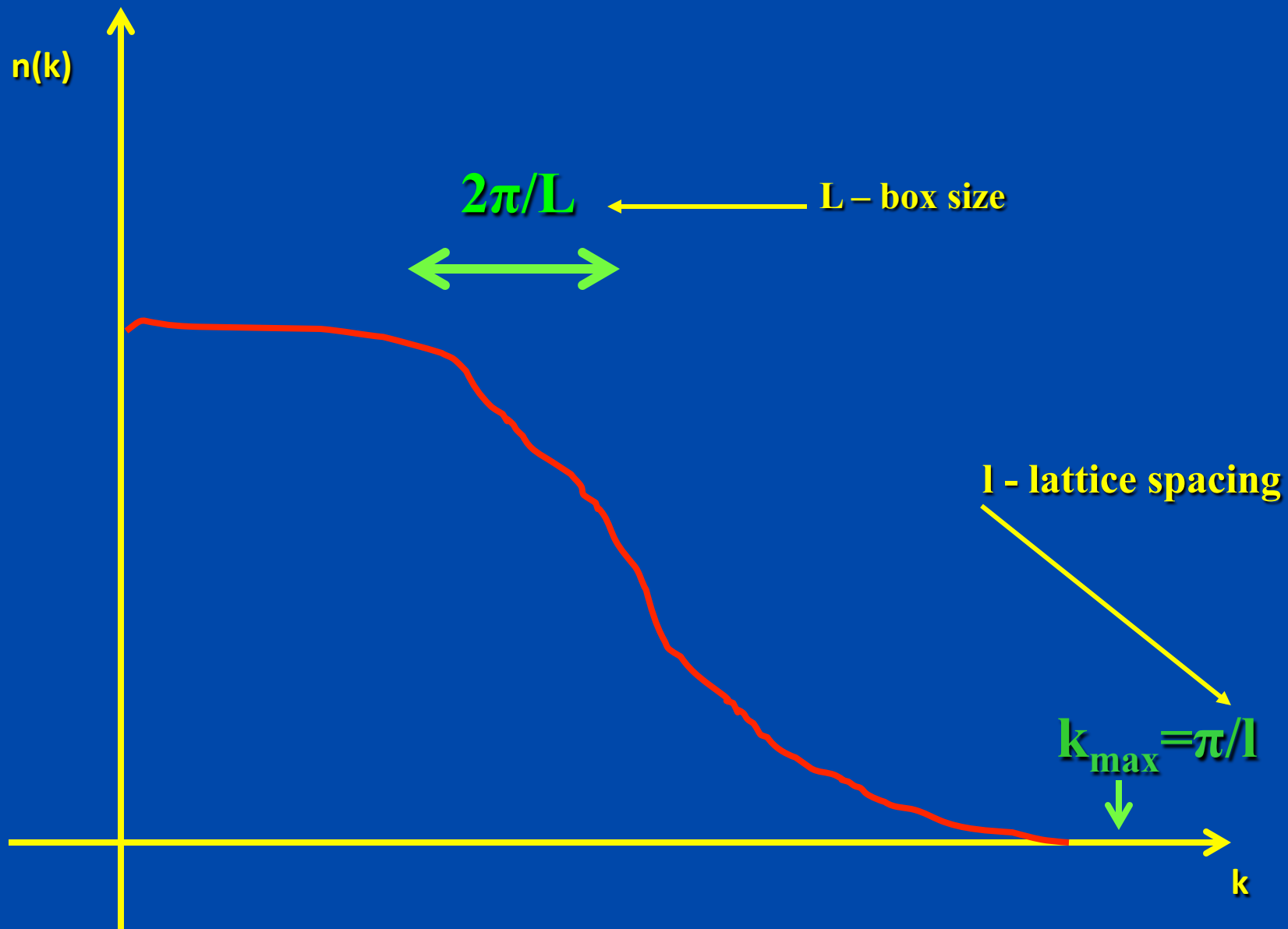
Discrete Hubbard-Stratonovich transformation

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

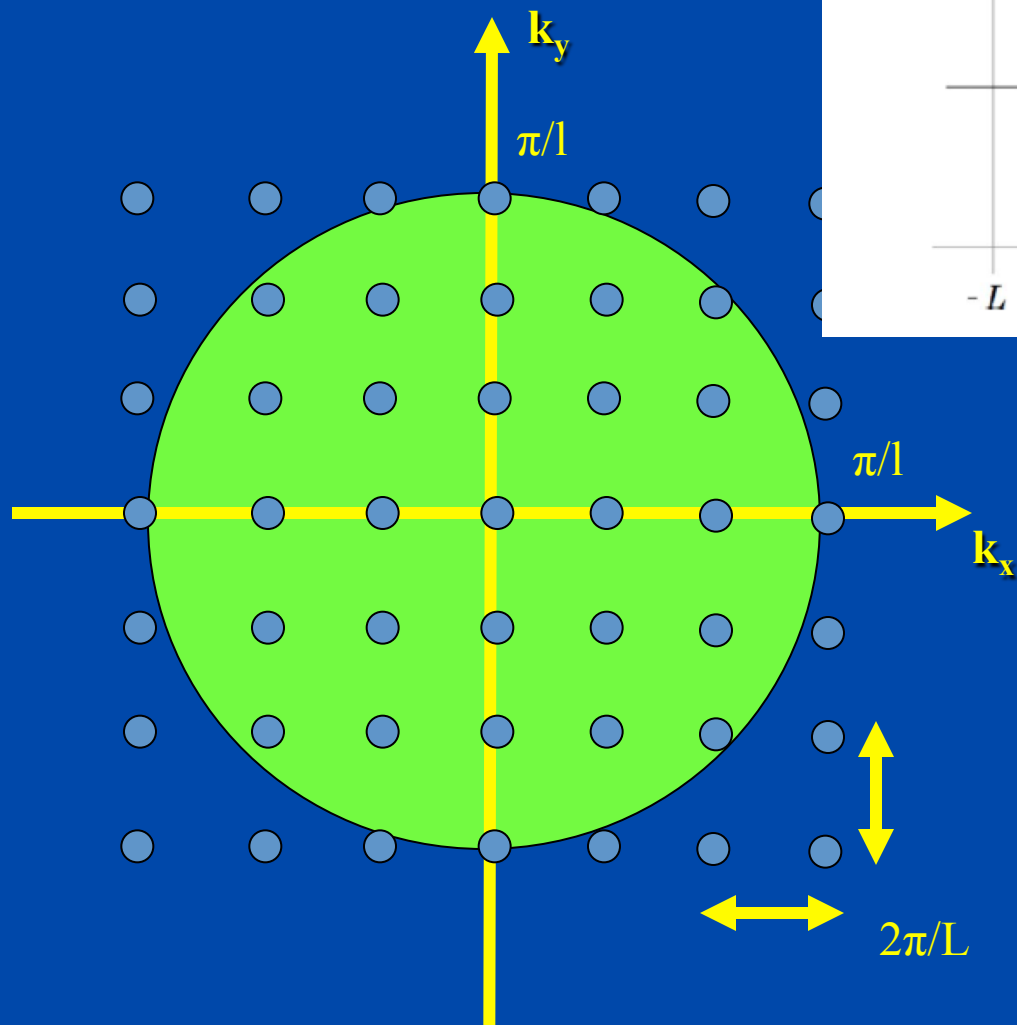
σ -fields fluctuate both in space and imaginary time

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

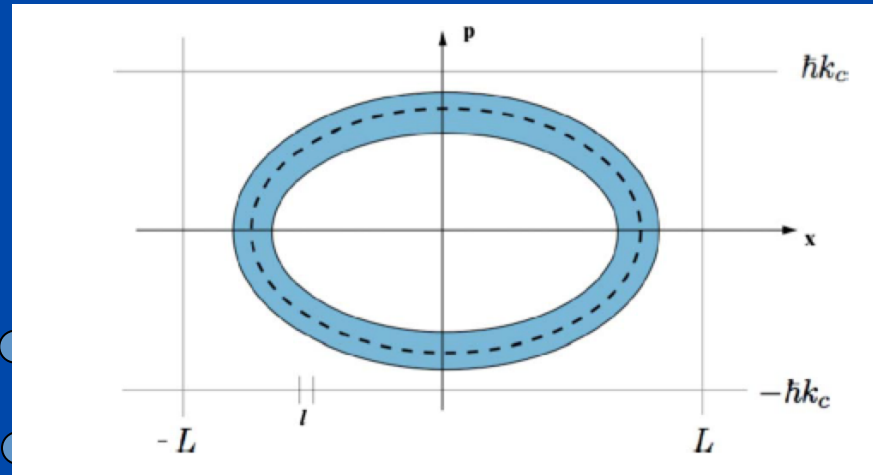
Running coupling constant g defined by lattice



How to choose the lattice spacing and the box size?



Momentum space



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

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

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

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

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

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

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

One-body evolution operator in imaginary time

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

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

No sign problem!

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

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

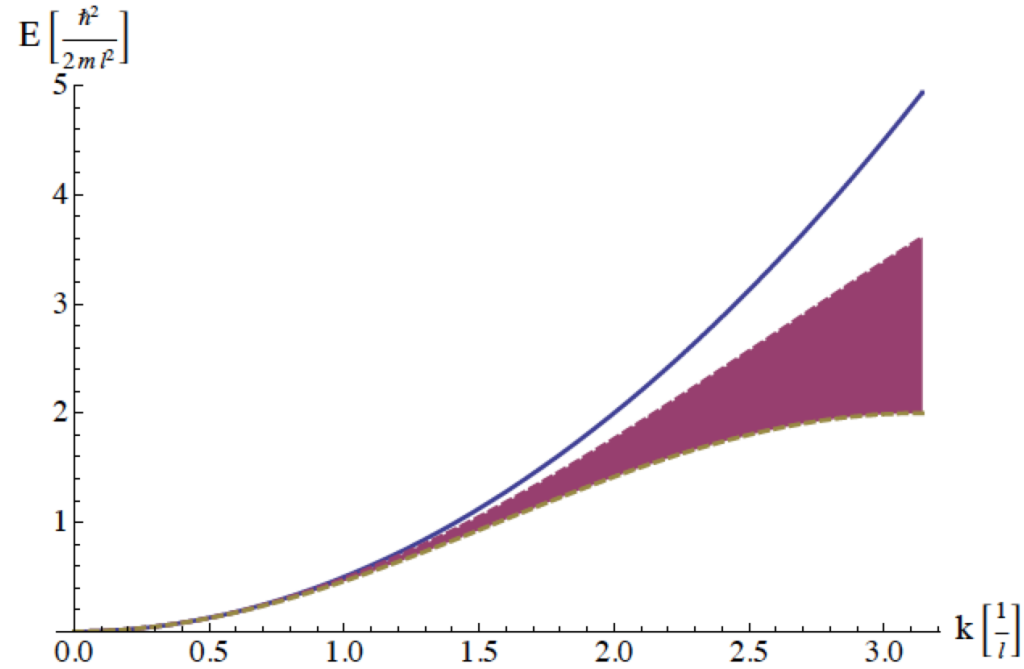


FIG. 3: (Color online) The solid blue line shows the dispersion relation used in this work and the dashed lines and purple area result from a lowest order second difference discrete derivative (see text for discussion). The units in this plot are set by the lattice spacing: the wavevector k is in units of $1/l$ and the energy in units of $\hbar^2/2ml^2$.

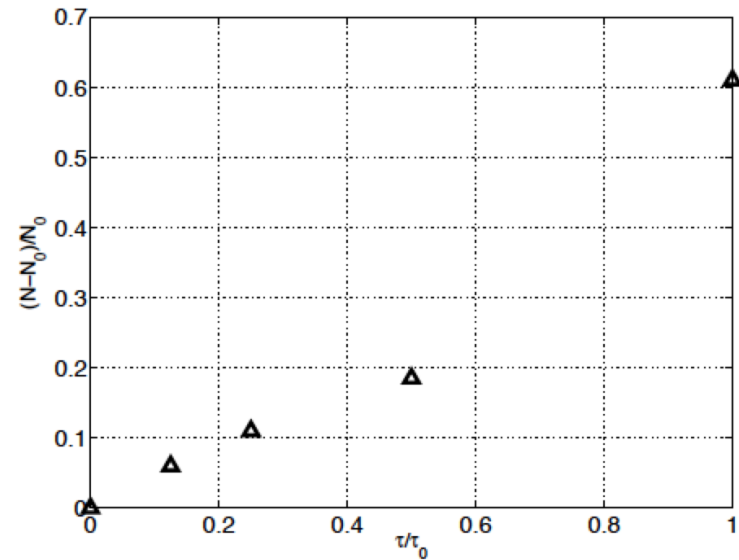
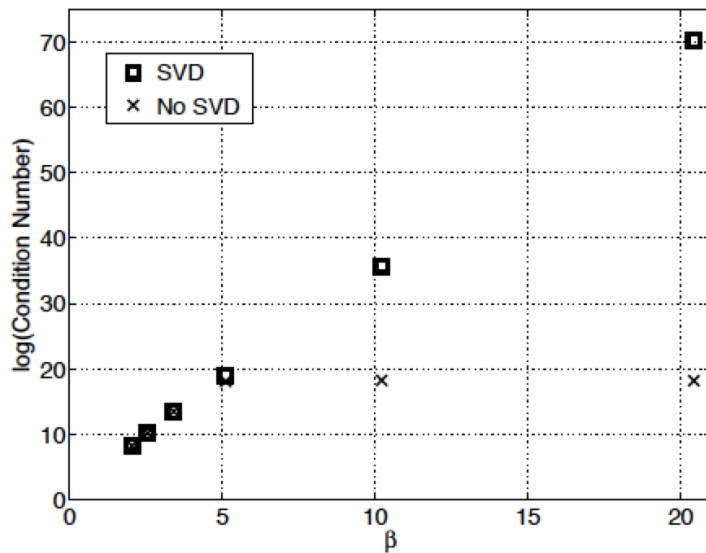


FIG. 4: Left Panel: Condition number of \mathcal{U} as a function of β . Squares: with SVD. Crosses: without SVD. Right Panel: Convergence of simulated particle number N relative to exact solution N_0 , as a function of time step τ in units of τ_0 , defined in the text.

$$\mathcal{U}_0 = 1$$

$$\mathcal{U}_1 = \mathcal{W}_1$$

$$\mathcal{U}_2 = \mathcal{W}_2 \mathcal{W}_1$$

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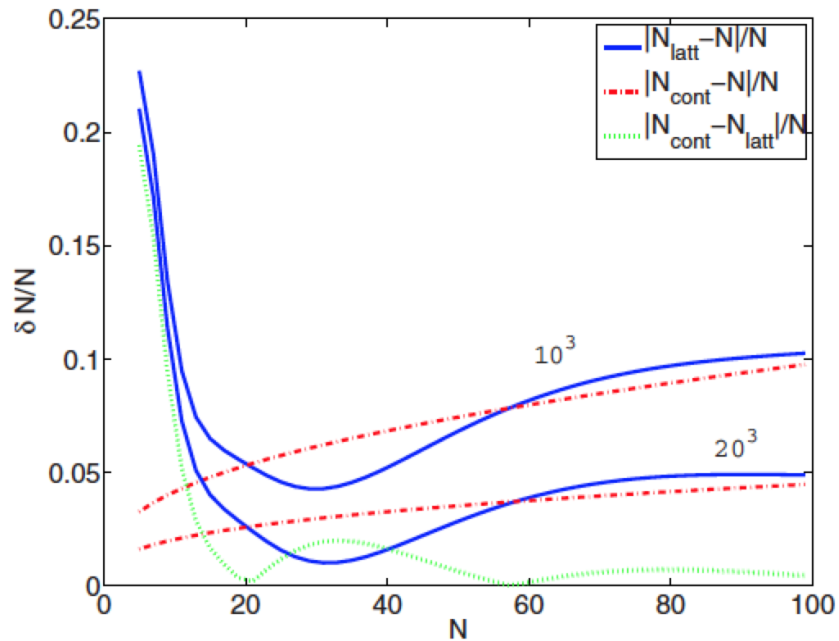
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$$\mathcal{U}_n = \mathcal{W}_n \mathcal{W}_{n-1} \dots \mathcal{W}_1 = \mathcal{W}_n \mathcal{U}_{n-1}.$$

$$\mathcal{U}_0 = 1$$

$$\mathcal{U}_1 = \mathcal{W}_1 = \mathcal{S}_1 \mathcal{D}_1 \mathcal{V}_1$$

$$\mathcal{U}_2 = \mathcal{W}_2 \mathcal{W}_1 = (\mathcal{W}_2 \mathcal{S}_1 \mathcal{D}_1) \mathcal{V}_1 = \mathcal{S}_2 \mathcal{D}_2 \mathcal{V}_2 \mathcal{V}_1$$



$$N = L^3 \int \frac{d^3k}{(2\pi)^3} \left[1 - \frac{\epsilon(k) + U - \mu}{\sqrt{[\epsilon(k) + U - \mu]^2 + \Delta^2}} \right], \quad (3.11)$$

$$N_{\text{cont}} = L^3 \int_{k \leq k_c} \frac{d^3k}{(2\pi)^3} \left[1 - \frac{\epsilon(k) + U - \mu}{\sqrt{[\epsilon(k) + U - \mu]^2 + \Delta^2}} \right], \quad (3.12)$$

$$N_{\text{latt}} = \sum_{\mathbf{k}}^{k \leq k_c} \left[1 - \frac{\epsilon(k) + U - \mu}{\sqrt{[\epsilon(k) + U - \mu]^2 + \Delta^2}} \right], \quad (3.13)$$

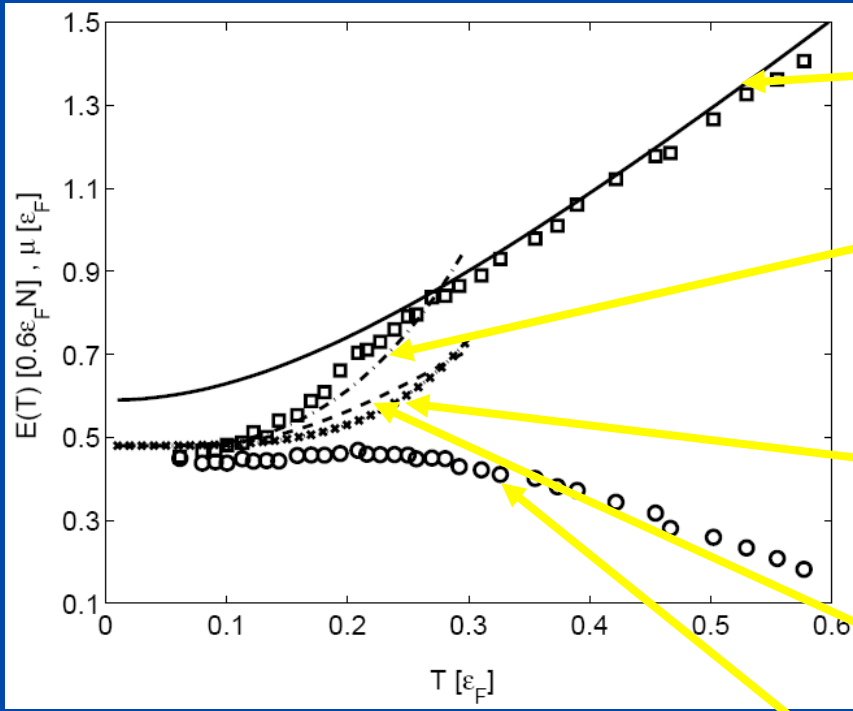
Error in particle number due to discretization for a 10^3 and a 20^3 lattices.

More details of the calculations:

- Typical spatial lattice sizes used from $N_s^3 = 8^3$ to 16^3 , number of spwf retained $\approx O(N_s^3)$, imaginary time steps up to $N_\tau = 1000s$
- 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
- Change randomly at a fraction of all space and time sites the signs the auxiliary fields $\sigma(x,\tau)$ so as to maintain a running average of the acceptance rate between 0.4 and 0.6
- Thermalize for 50,000 – 100,000 MC steps or/and use as a start-up field configuration a $\sigma(x,\tau)$ -field configuration from a different T
- At low temperatures use Singular Value Decomposition of the evolution operator $U(\{\sigma\})$ to stabilize the numerics
- Generate 1,000,000s $\sigma(x,\tau)$ - field configurations for calculations
- MC correlation “time” $\approx 250 - 300$ time steps at $T \approx T_c$

$$a = \pm\infty$$

Bulgac, Drut, and Magierski
 Phys. Rev. Lett. 96, 090404 (2006)



Normal Fermi Gas
 (with vertical offset, solid line)

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

Bogoliubov-Anderson phonons
 contribution only

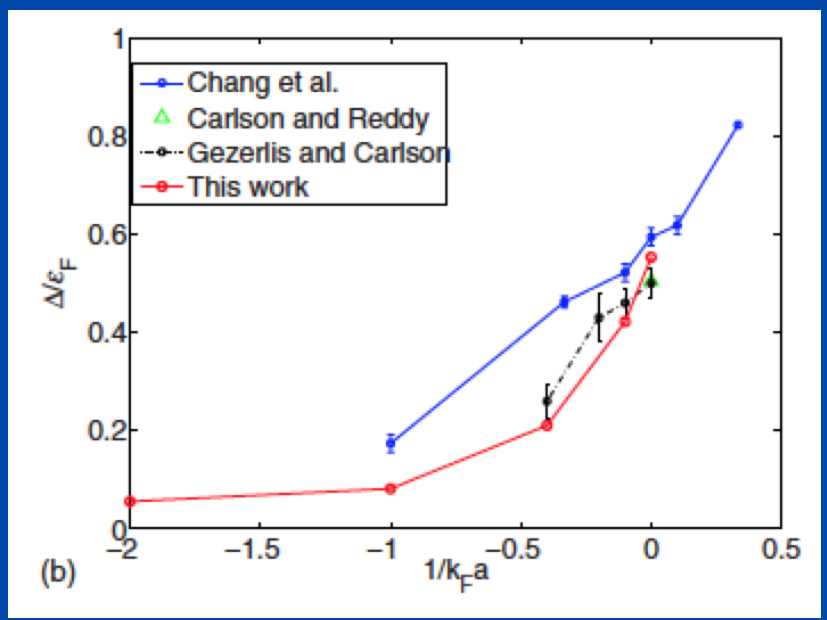
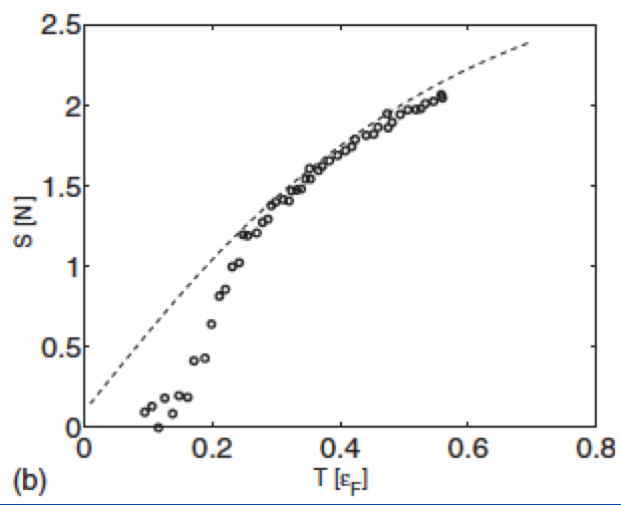
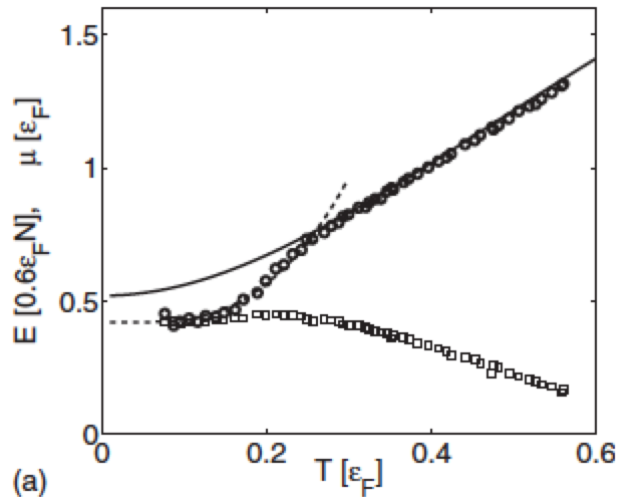
Quasi-particles contribution only
 (dashed line)

μ - chemical potential (circles)

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

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

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



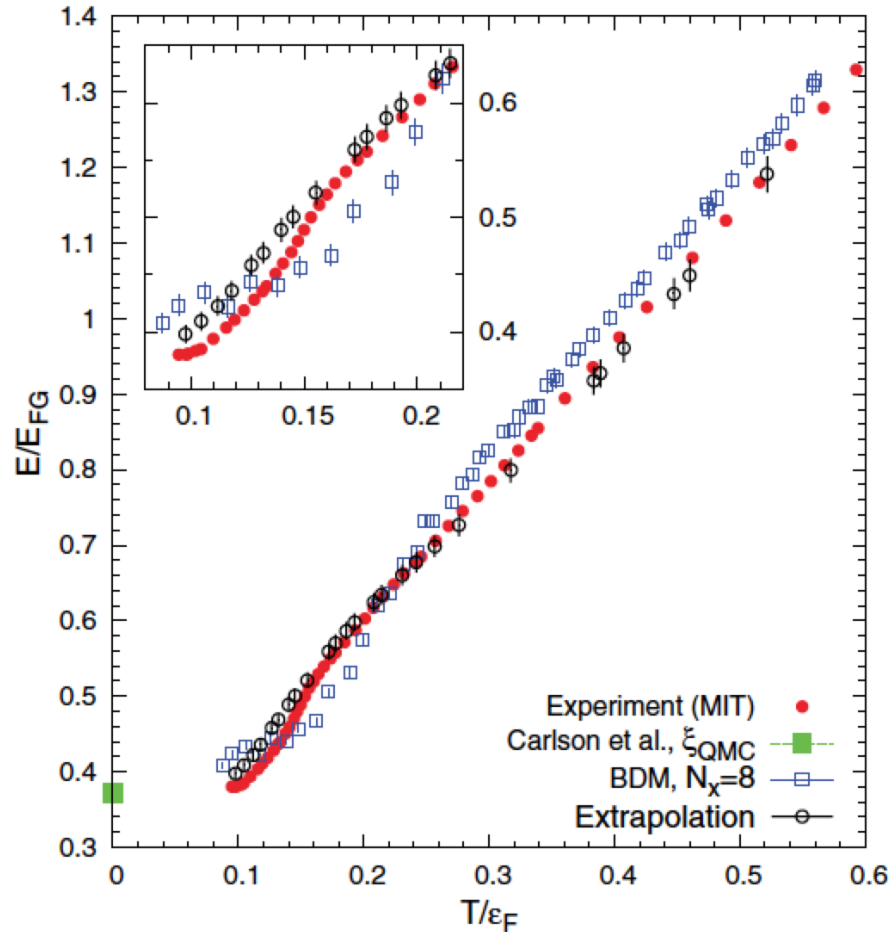


FIG. 2. (Color online) Energy E/E_{FG} (red dots), as obtained by Ku *et al.* [8]. Our AFQMC results extrapolated to infinite volume are shown by open black circles. The results for $N_x = 8$ (open blue squares) were obtained with the DMC algorithm in Ref. [9]. The green square shows the QMC result of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

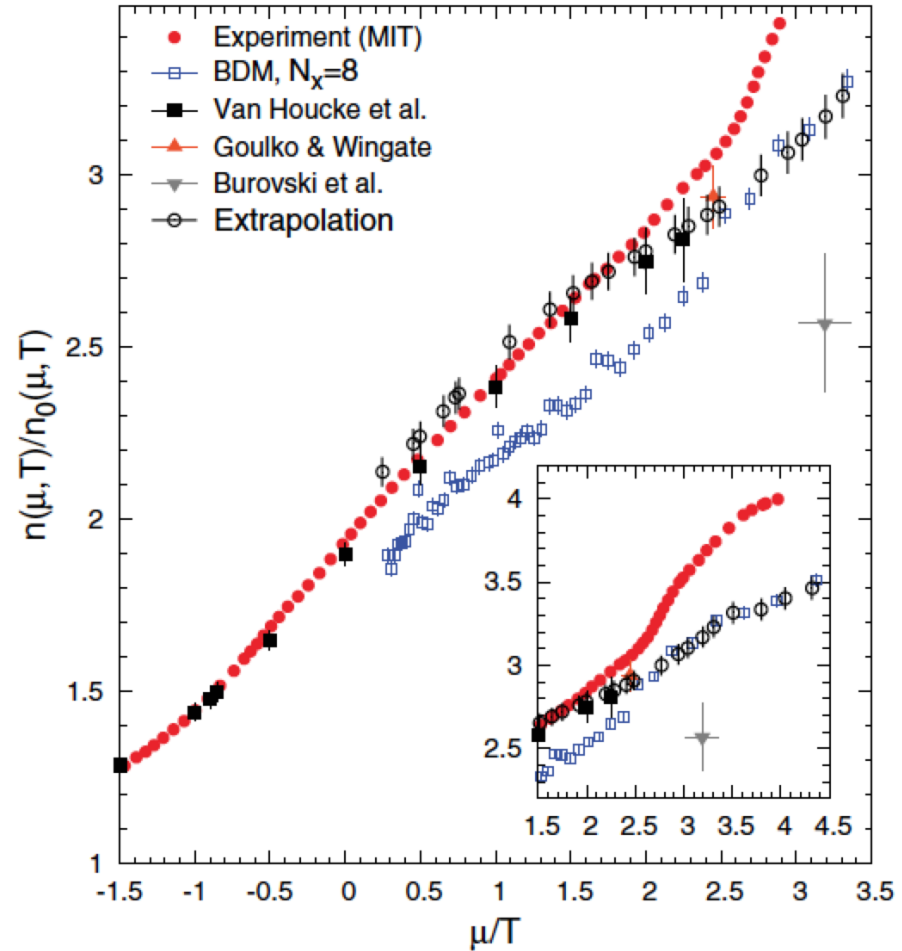
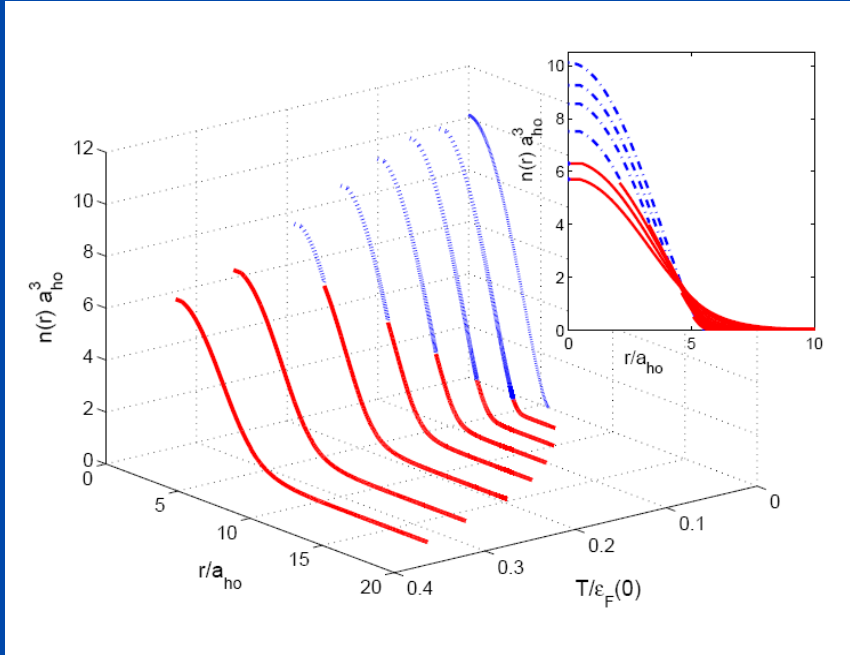
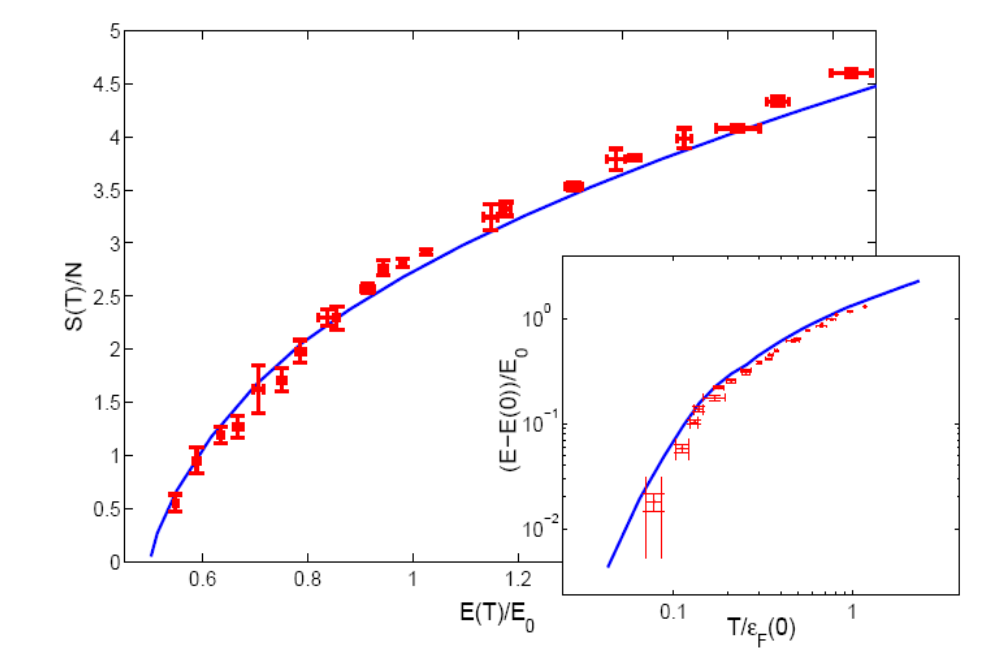


FIG. 4. (Color online) Density $n(\mu, T)$ of the UFG (red circles) as obtained by Ku *et al.* [8], normalized to the density $n_0(\mu, T)$ of a noninteracting Fermi gas. The notation for the AFQMC results is identical to Fig. 2. The diagrammatic MC results of Refs. [21,22] (solid up and down triangles)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

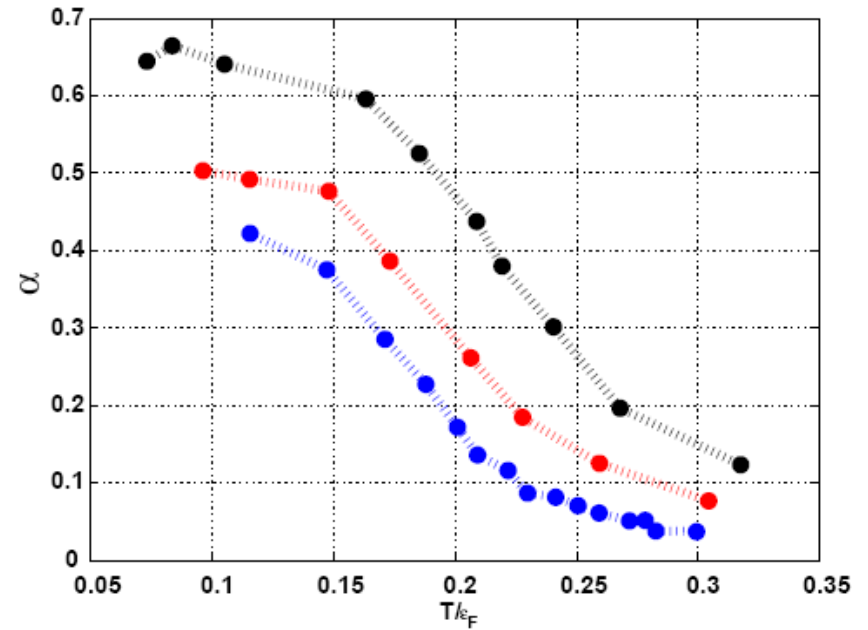
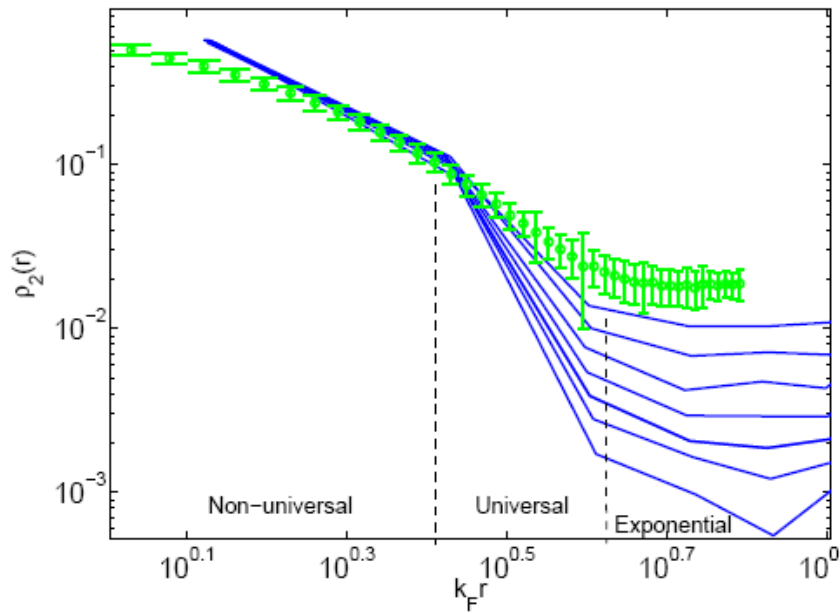
Experiment (about 100,000 atoms in a trap):

Measurement of the Entropy and Critical Temperature of a Strongly Interacting Fermi Gas, Luo, Clancy, Joseph, Kinast, and Thomas, Phys. Rev. Lett. 98, 080402 (2007)



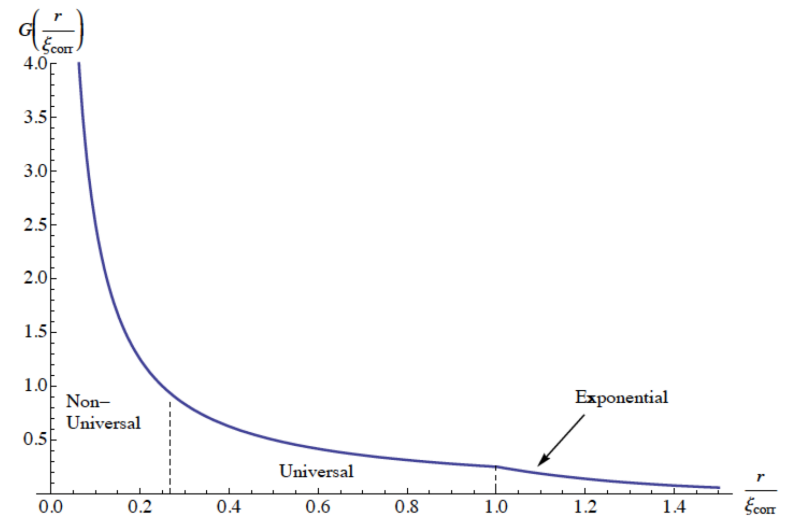
Ab initio theory (no free parameters)
Bulgac, Drut, and Magierski, Phys. Rev. Lett. 99, 120401 (2007)

Long range order and condensate fraction

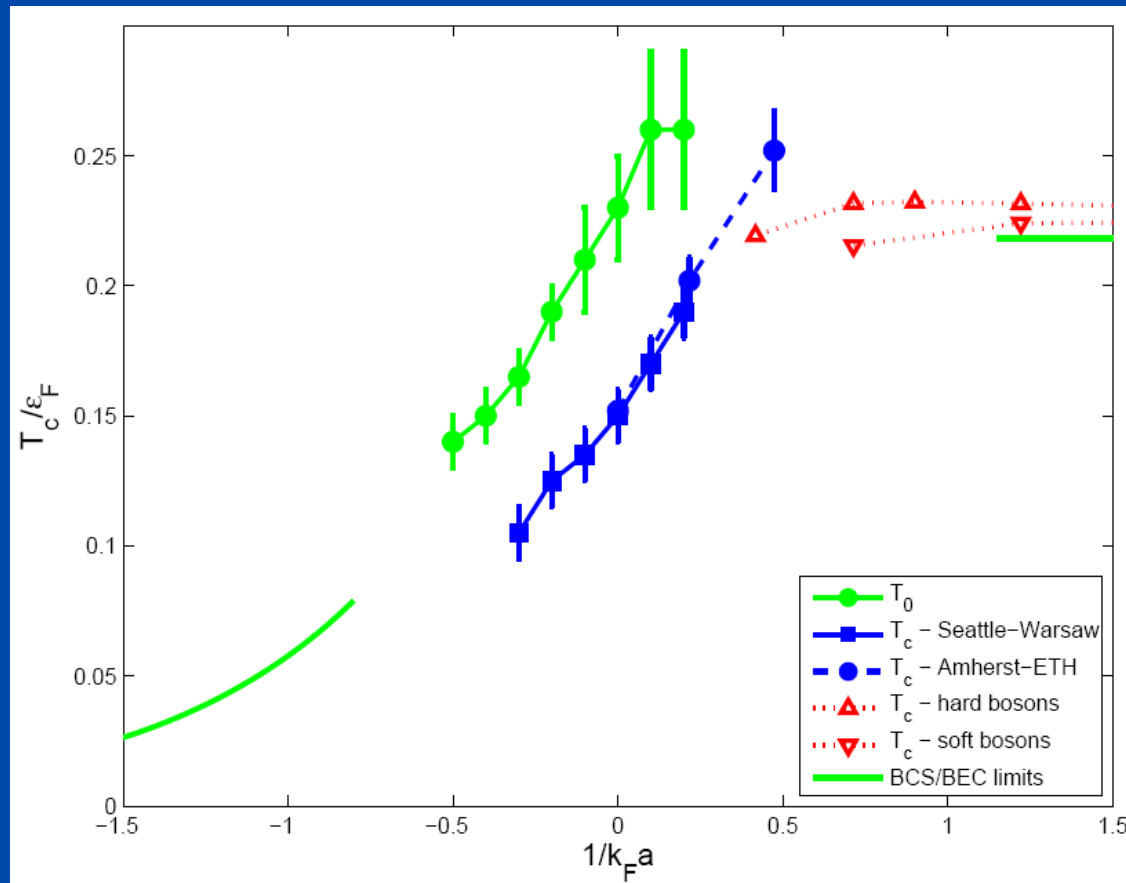


$$G(\vec{r}) = \left(\frac{2}{N}\right)^2 \int d^3\vec{r}_1 \int d^3\vec{r}_2 \langle \psi_{\uparrow}^{\dagger}(\vec{r}_1 + \vec{r}) \psi_{\downarrow}^{\dagger}(\vec{r}_2 + \vec{r}) \psi_{\downarrow}(\vec{r}_2) \psi_{\uparrow}(\vec{r}_1) \rangle$$

$$\alpha = \lim_{r \rightarrow \infty} \frac{N}{2} G(\vec{r}) - n(\vec{r})^2, \quad n(\vec{r}) = \frac{2}{N} \int d^3\vec{r}_1 \langle \psi_{\uparrow}^{\dagger}(\vec{r}_1 + \vec{r}) \psi_{\uparrow}(\vec{r}_1) \rangle$$



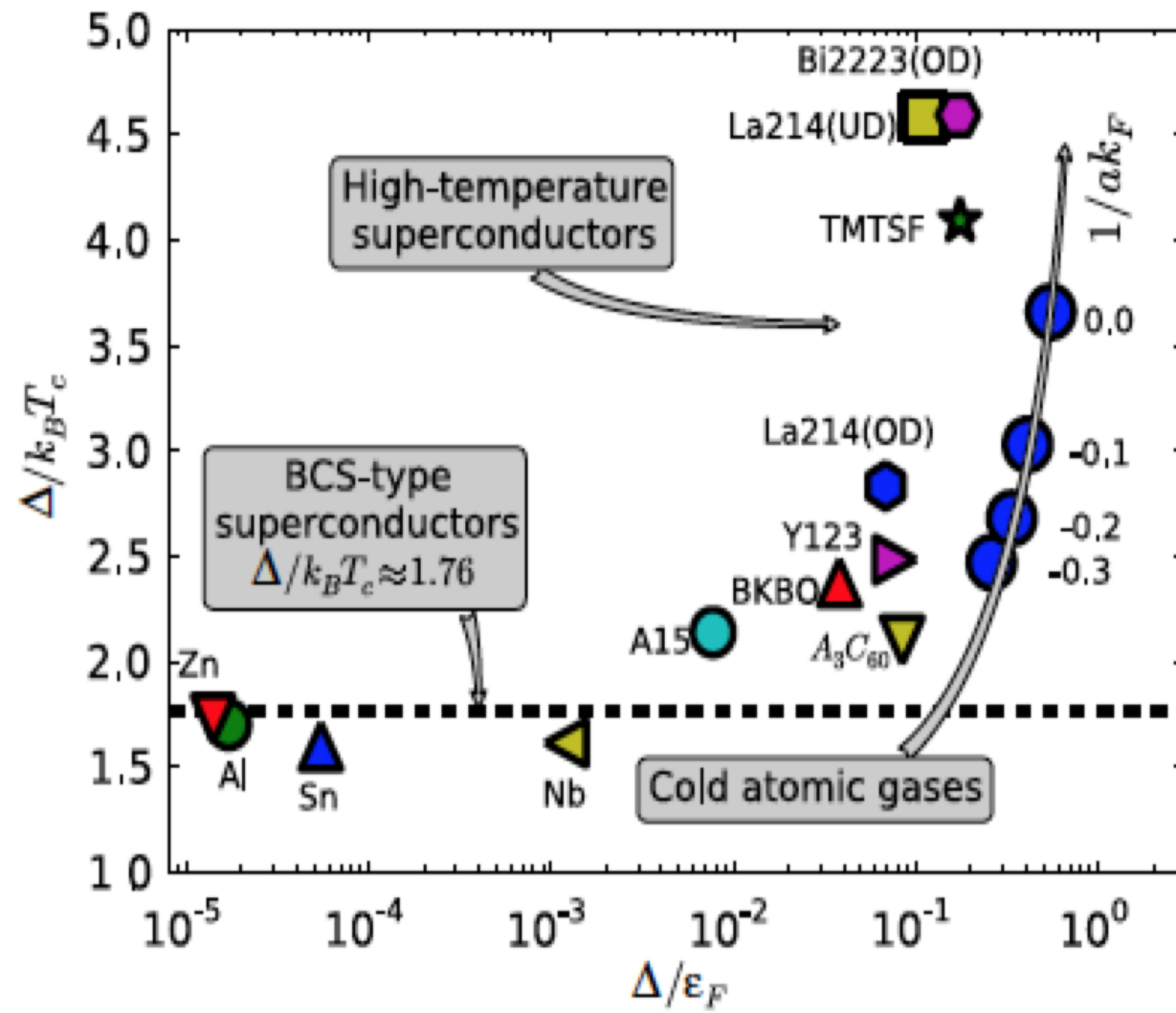
Critical temperature for superfluid to normal transition



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

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

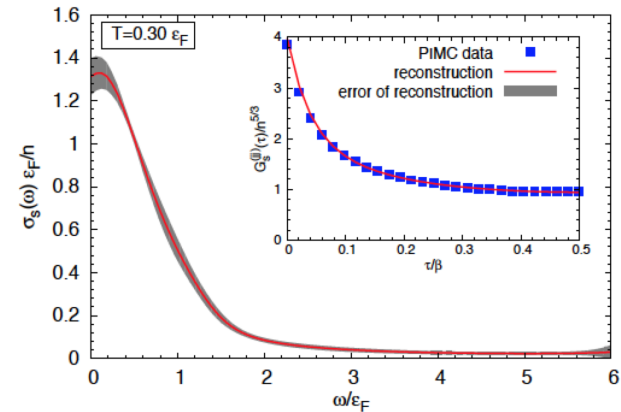
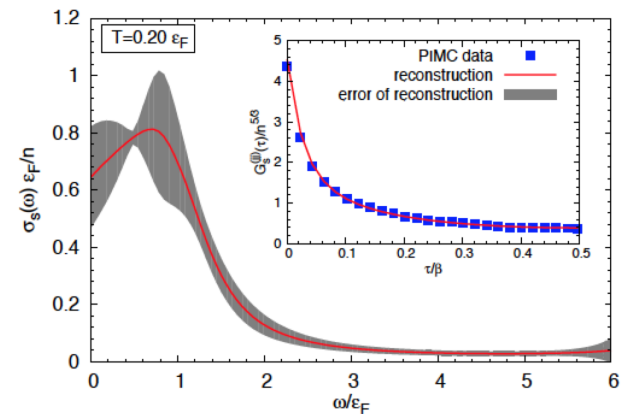
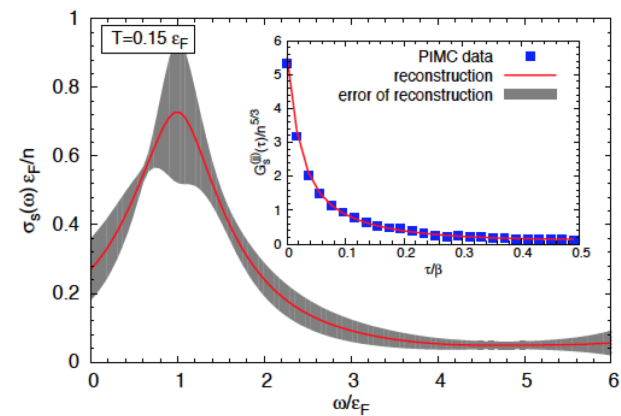
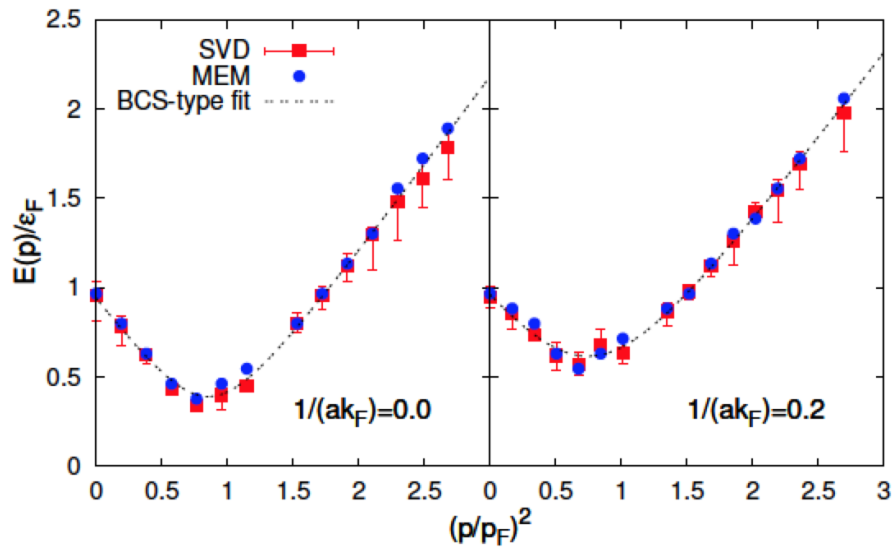
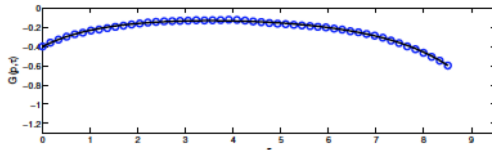
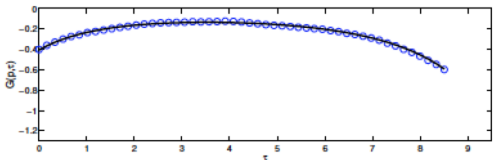
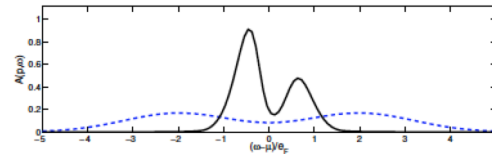
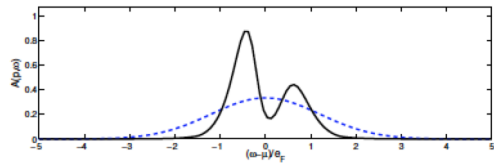
Hard and soft bosons: Pilati et al. PRL 100, 140405 (2008)



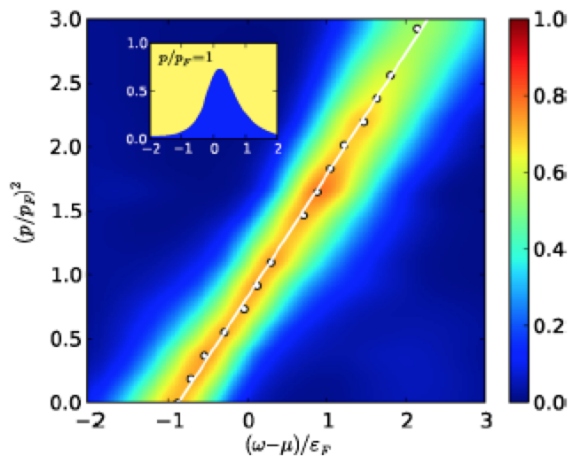
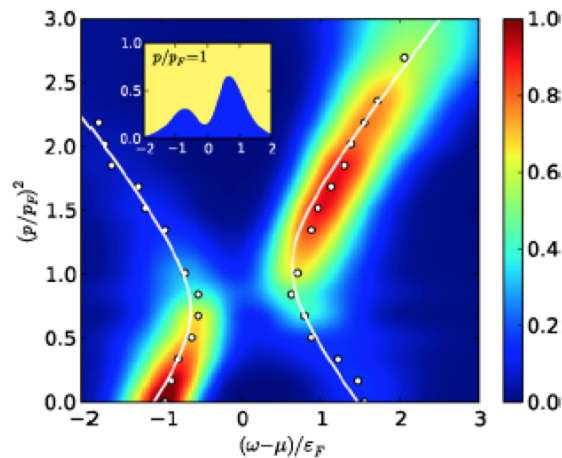
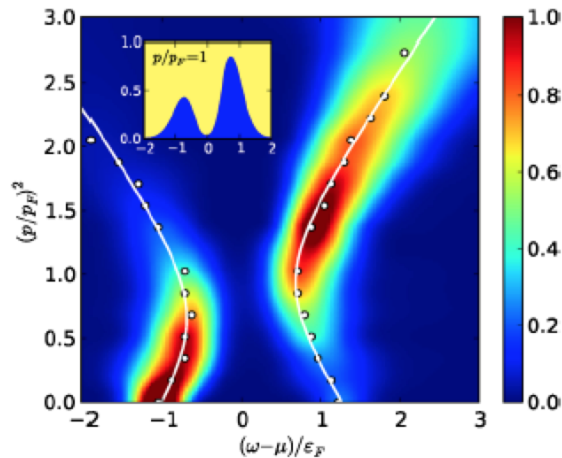
$$\begin{aligned}
G(\vec{p}, \tau) &= \frac{1}{Z} \text{Tr} \left\{ \exp \left[-(\beta - \tau)(H - \mu N) \right] \psi^\dagger(\vec{p}) \exp \left[-\tau(H - \mu N) \right] \psi(\vec{p}) \right\} \\
&= -\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega A(\omega, \vec{p}) \frac{\exp(-\omega\tau)}{1 + \exp(-\omega\beta)} \\
\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega A(\omega, \vec{p}) &= 1, \quad \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega A(\omega, \vec{p}) \frac{1}{1 + \exp(\omega\beta)} = n(\vec{p}), \quad A(\omega, \vec{p}) \geq 0
\end{aligned}$$

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

Matsubara propagator, spectral function and linear response

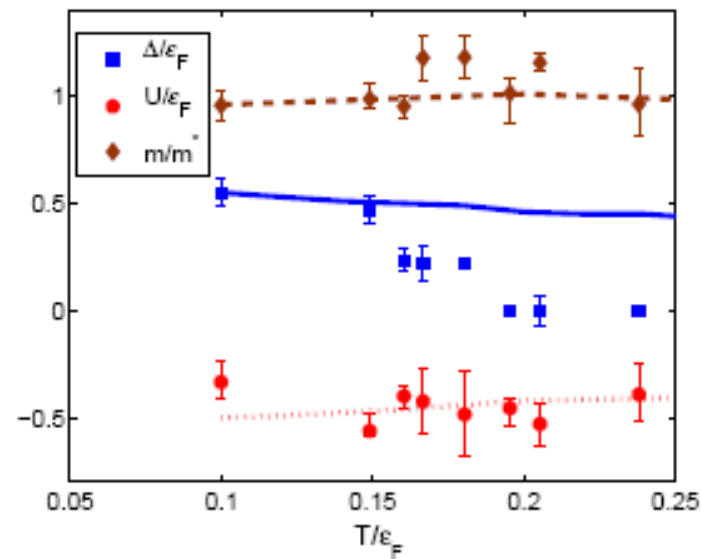
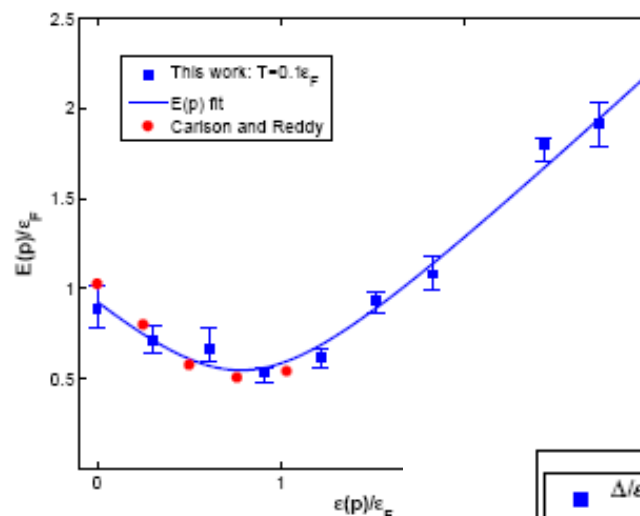


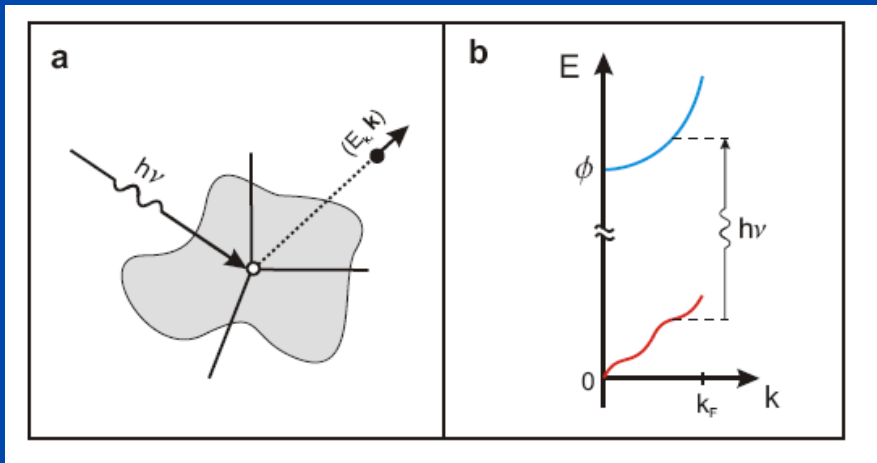
Singular value decomposition and maximum entropy method reconstruction of the spectral function



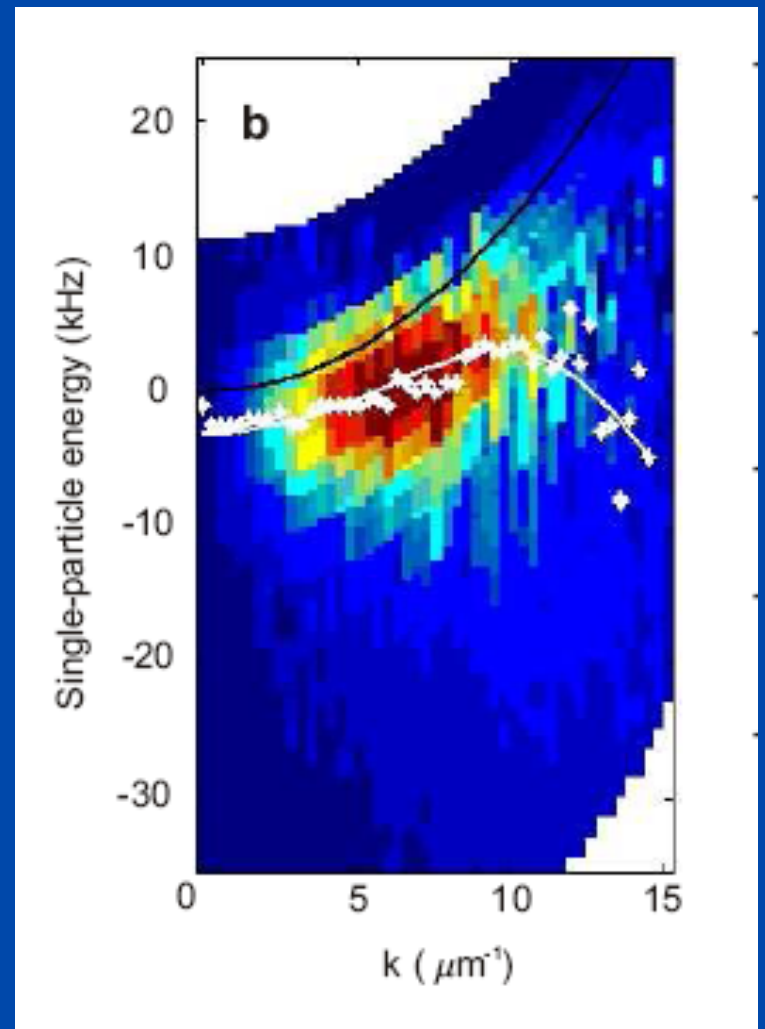
$$G(p, \tau) = \frac{1}{Z} \text{Tr} \left\{ \exp[-(\beta - \tau)(H - \mu N)] \psi^\dagger(p) \exp[-\tau(H - \mu N)] \psi(p) \right\}$$

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

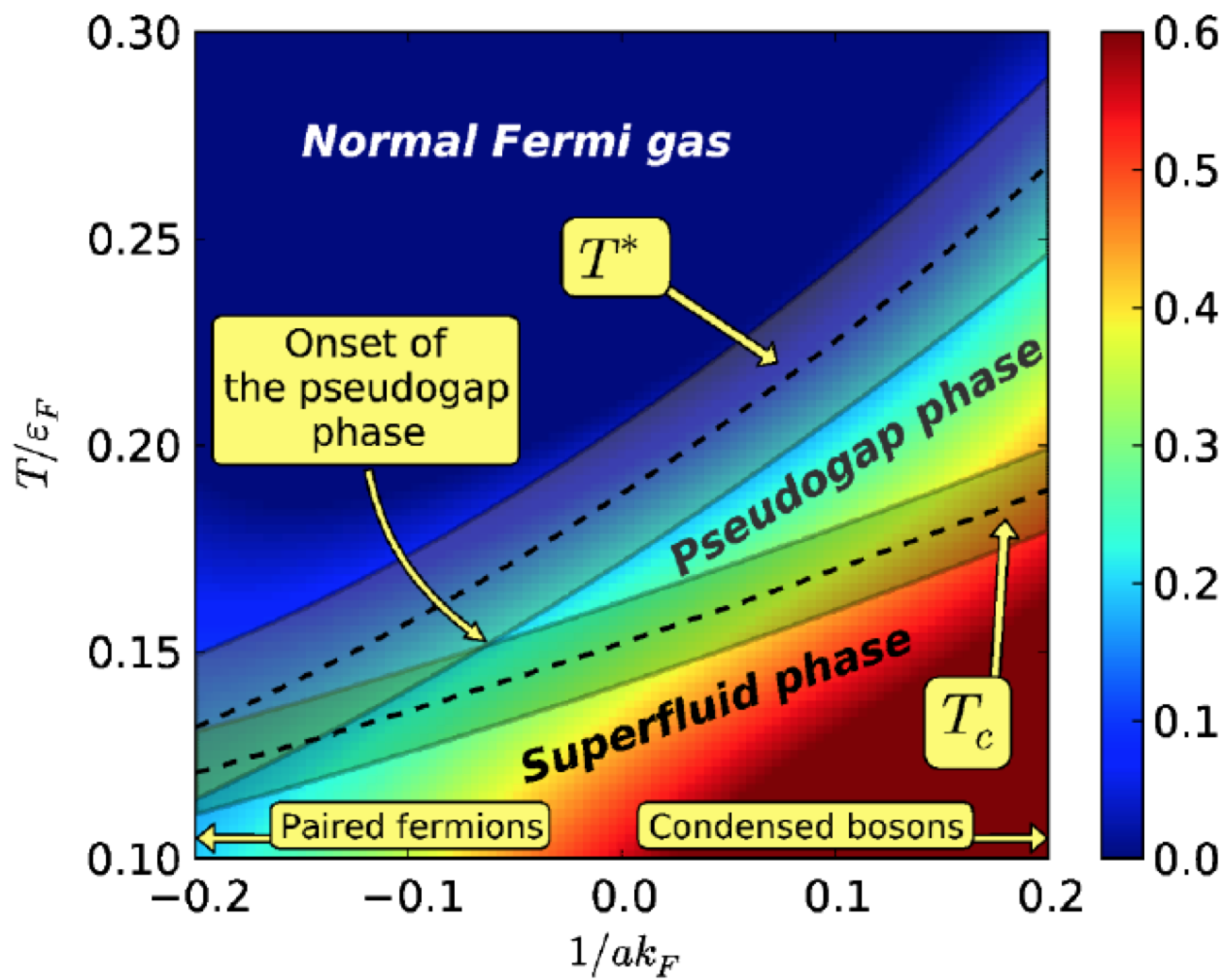


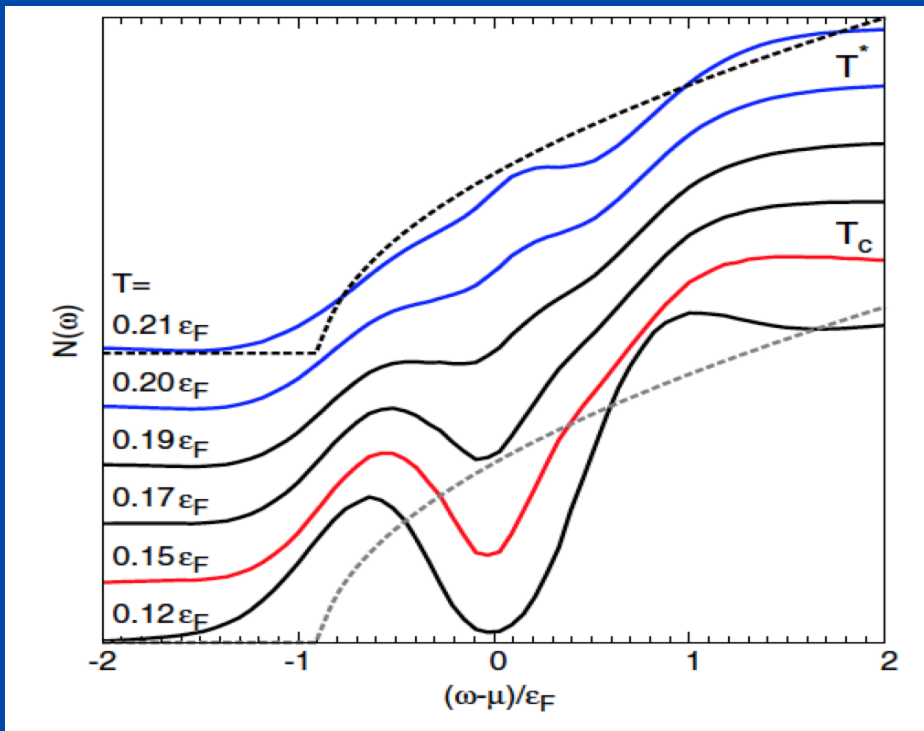


$$E(N) + h\nu = E(N-1) + E_k + \frac{\hbar^2 k^2}{2m} + \phi$$

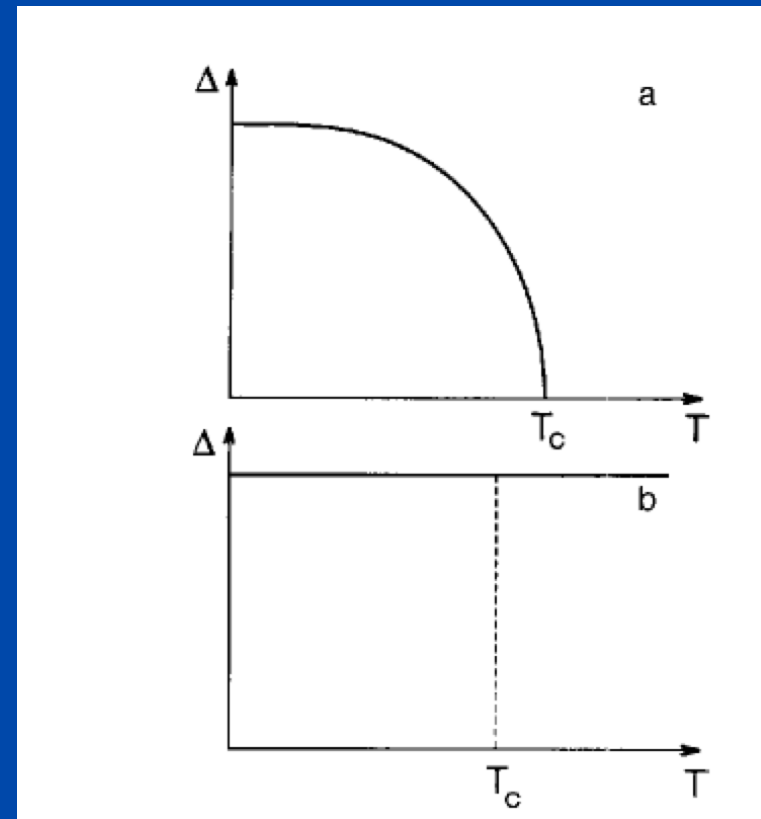
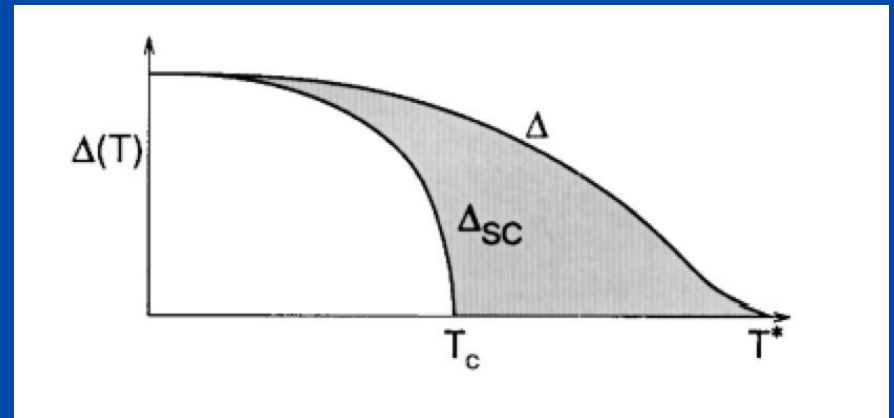


Using photoemission spectroscopy to probe a strongly interacting Fermi gas
 Stewart, Gaebler, and Jin, *Nature*, **454**, 744 (2008)

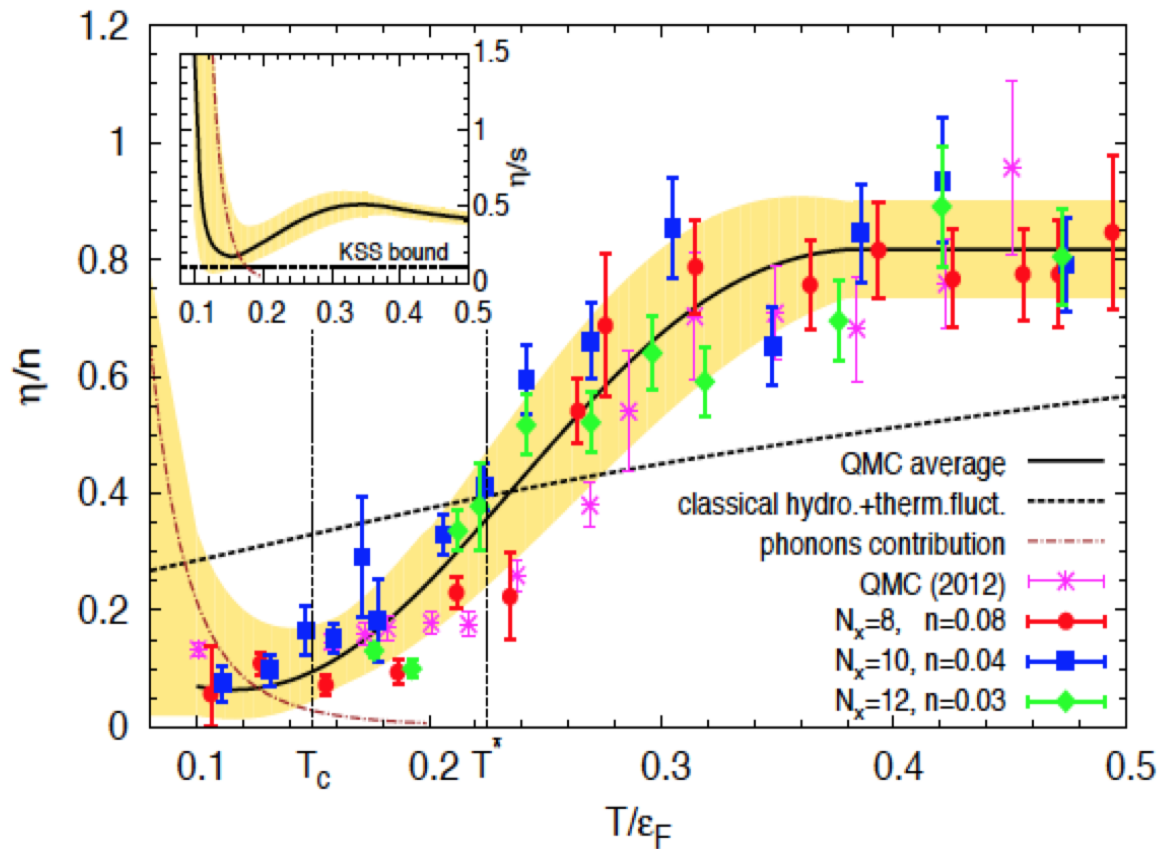




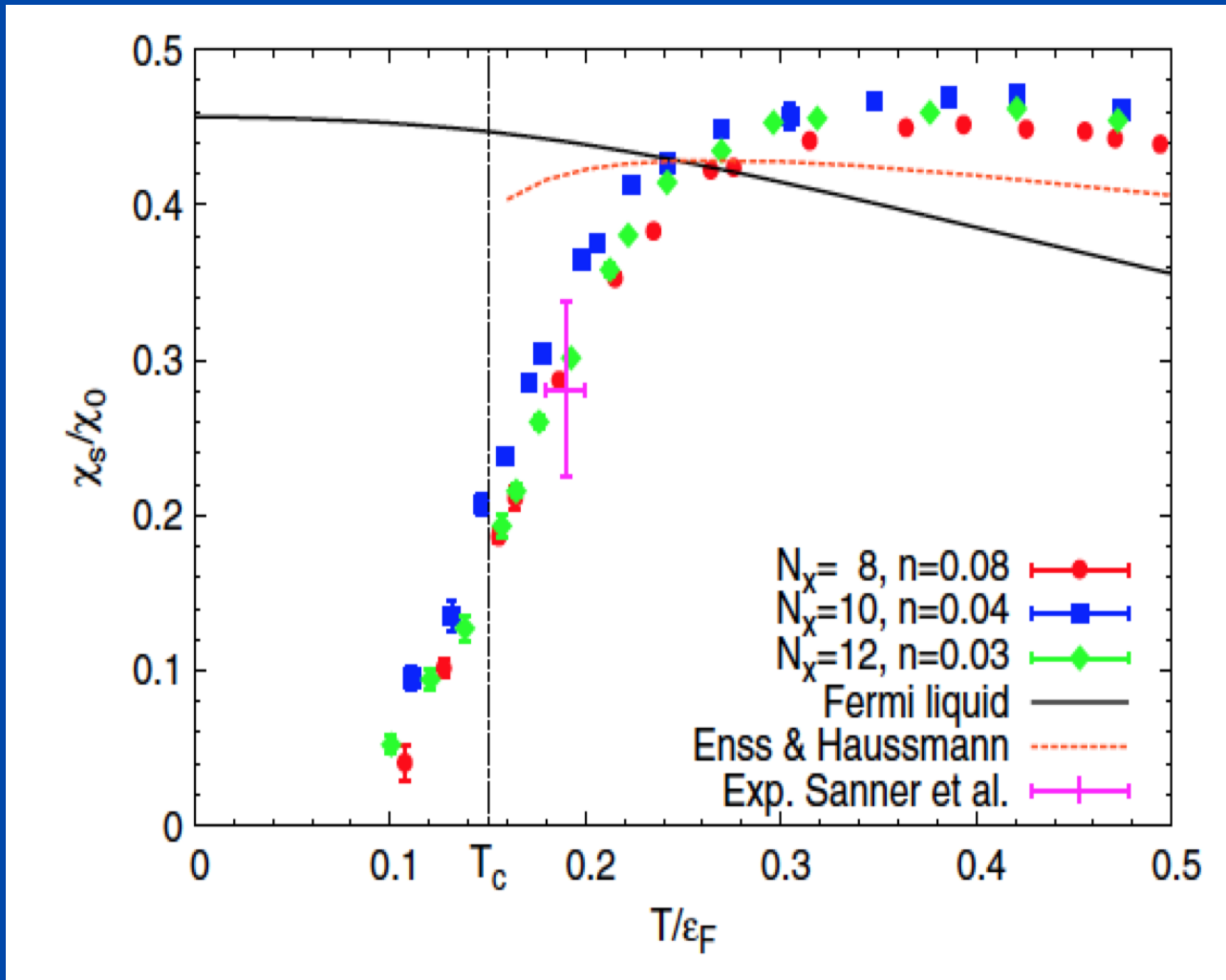
G. Wlazlowski, et al., Phys. Rev. Lett. 110, 090401 (2013)



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



Shear viscosity of a unitary Fermi gas



Spin susceptibility