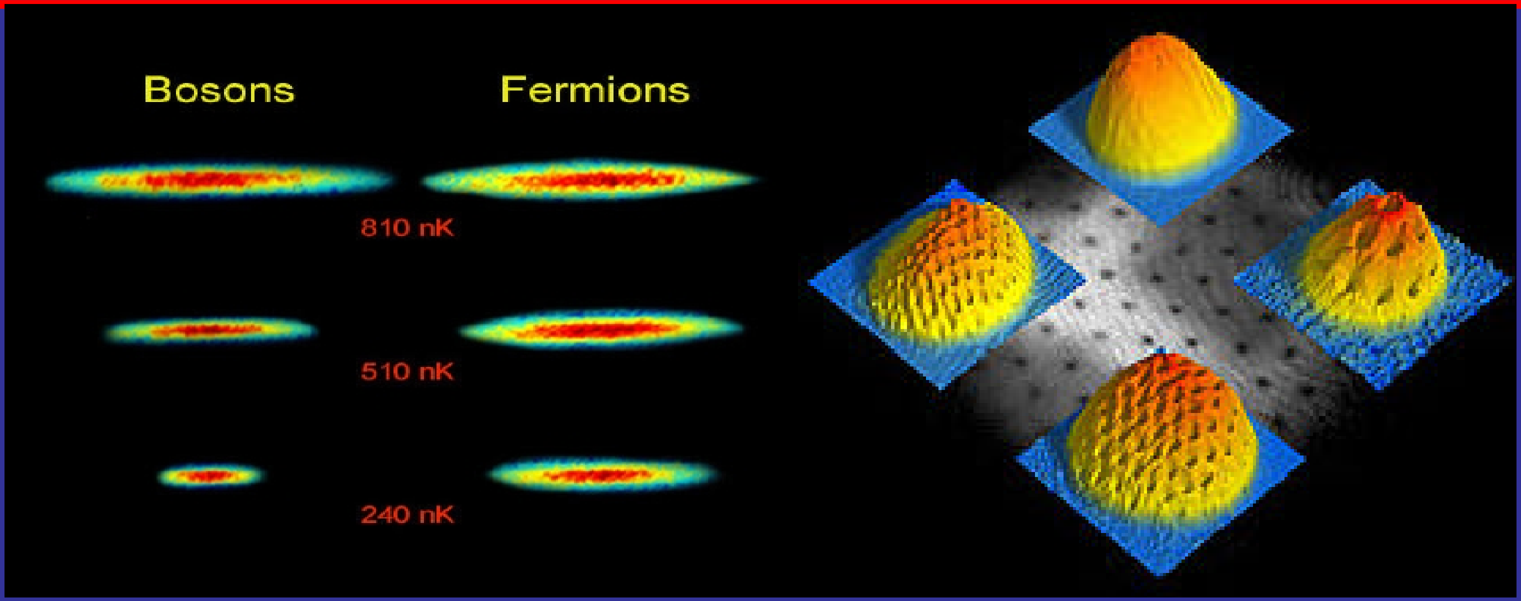
# *Pairing in cold atoms from Monte Carlo calculations; finite temperature aspects.*

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## Setting the problem:

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**

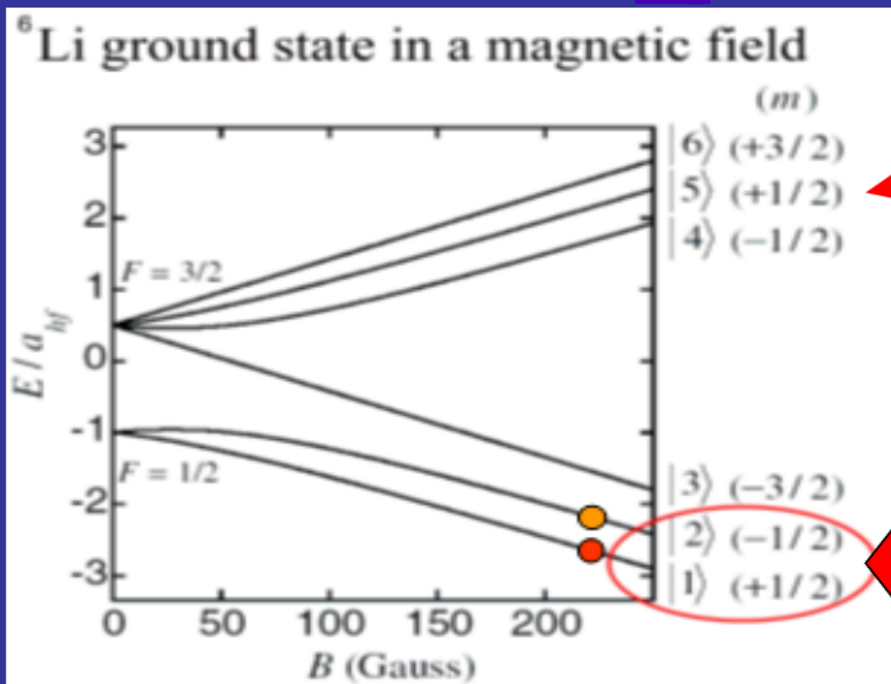
**System is dilute but strongly interacting!**

**UNIVERSALITY:** $E = \xi_0 E_{FG}$

**AT FINITE TEMPERATURE:** $E(T) = \xi\left(\frac{T}{\varepsilon_F}\right) E_{FG},\quad \xi(0) = \xi_0$

<u>Physical realization:</u> e.g. dilute system of $^6Li$ atoms in a trap

- The number of atoms in the trap: typically about $10^5$-$10^6$ atoms divided 50-50 among the lowest two hyperfine states.
- The strength of this interaction is fully tunable!




$$|F\ m_F\rangle$$

$$\vec{F} = \vec{I} + \vec{J}\ ;\ \ \vec{J} = \vec{L} + \vec{S}$$

**Nuclear spin** **Electronic spin**

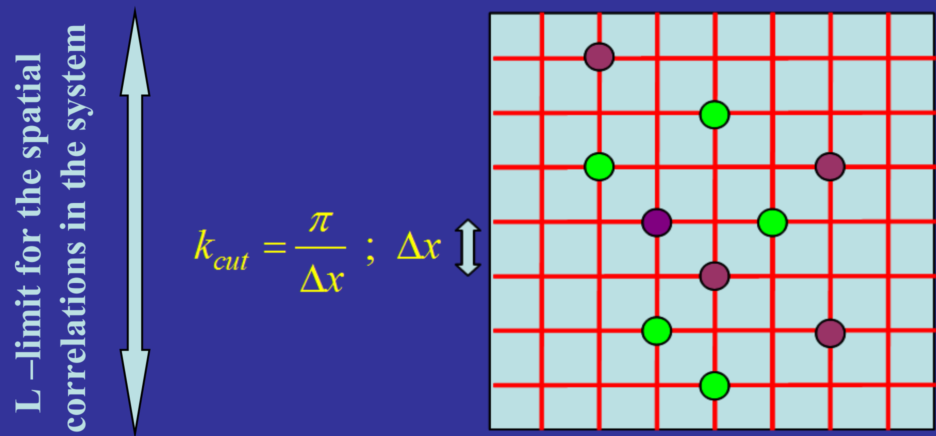
**Two hypefine states are populated in the trap**

**Collision of two atoms:**

**At low energies (low density of atoms) only L=0 (s-wave) scattering is effective.**

- **Due to the high diluteness atoms in the same hyperfine state do not interact with one another.**
- **Atoms in different hyperfine states experience interactions only in s-wave.**

# Coordinate space




$Volume = L^3$

$lattice\ spacing = \Delta x$

- Spin up fermion

- Spin down fermion

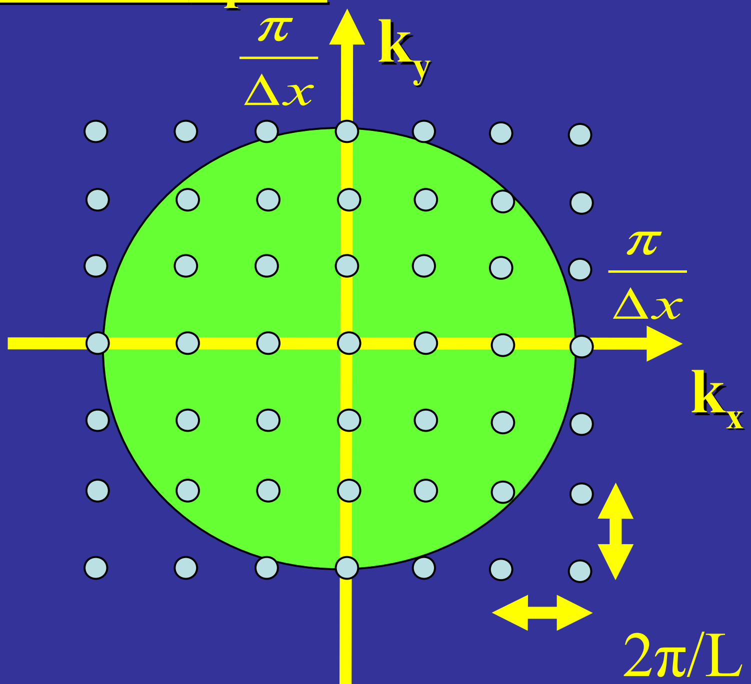
**Periodic boundary conditions imposed**

**External conditions:**

$T$ - temperature

$\mu$ - chemical potential

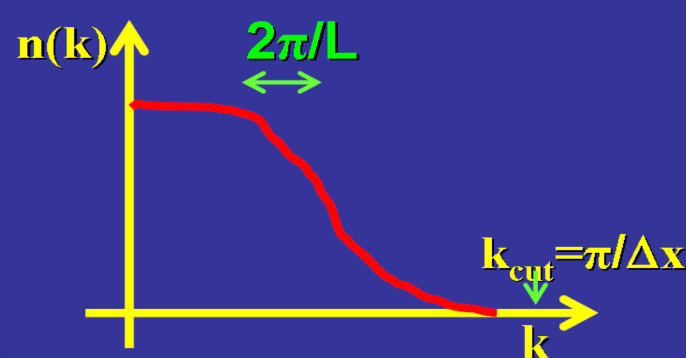
# Momentum space




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

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

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



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

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

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

Running coupling constant g defined by lattice

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

Trotter expansion (*trotterization* of the propagator)

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

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

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

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

$$+O(\tau^3)$$

Discrete Hubbard-Stratonovich transformation

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

σ-fields fluctuate both in space and imaginary time

$$\hat{U}(\sigma)=\prod_{j=1}^{N_\tau}\hat{W}_j(\sigma);$$

$$\hat{W}_j(\sigma)=\exp\left[-\tau\left(\hat{T}-\mu\hat{N}\right)/2\right]\prod_{\vec{r}}\left[1+\sigma(\vec{r})A\hat{n}_{\uparrow}(\vec{r})\right]\left[1+\sigma(\vec{r})A\hat{n}_{\downarrow}(\vec{r})\right]\exp\left[-\tau\left(\hat{T}-\mu\hat{N}\right)/2\right]$$

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

$$\int D\sigma(\vec{r},\tau) \equiv \sum_{\{\sigma(\vec{r},1)=\pm 1\}} \sum_{\{\sigma(\vec{r},2)=\pm 1\}} \cdots \sum_{\{\sigma(\vec{r},N_\tau)=\pm 1\}} \quad ; \quad N_\tau \tau = \frac{1}{T}$$

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

**One-body evolution operator in imaginary time**

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

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

**No sign problem!**

$$n_\uparrow(\vec{x},\vec{y}) = n_\downarrow(\vec{x},\vec{y}) = \sum_{k,l<k_c} \psi_{\vec{k}}(\vec{x}) \left[\frac{U(\{\sigma\})}{1 + U(\{\sigma\})}\right]_{\vec{k}\vec{l}} \psi^*_{\vec{l}}(\vec{y}), \qquad \psi_{\vec{k}}(\vec{x}) = \frac{\exp(i\vec{k}\cdot\vec{x})}{\sqrt{L^3}}$$

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

# More details of the calculations:

Lattice sizes used: $6^3$ – $10^3$. Imaginary time steps:$8^3$ x 300 (high Ts) to $8^3$ x 1800 (low Ts)

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 $\sigma(r,\tau)$ 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.

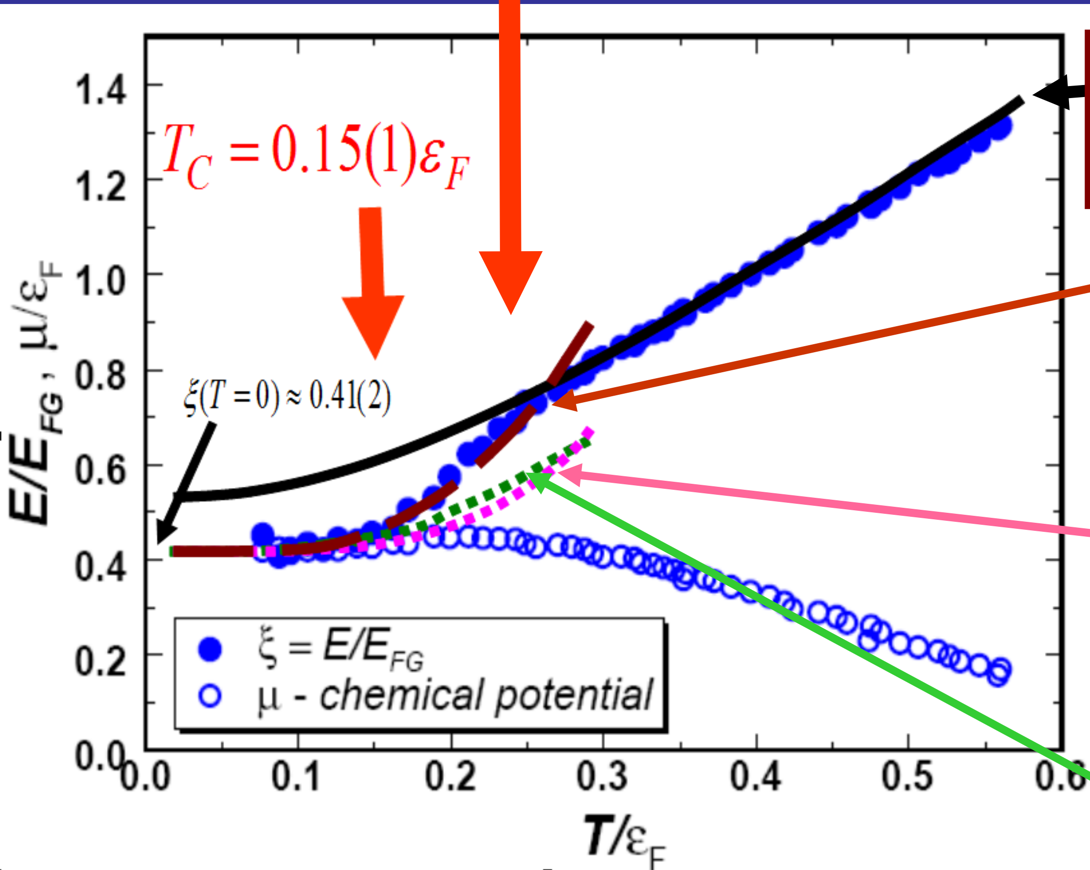
At low temperatures use Singular Value Decomposition of the evolution operator $U(\{\sigma\})$ to stabilize the numerics.

Use 200,000-2,000,000 $\sigma(x,\tau)$- field configurations for calculations

MC correlation "time" $\approx$ 250 – 300 time steps at $T \approx T_c$

## $a = \pm\infty$

# Deviation from Normal Fermi Gas




**Normal Fermi Gas**
(with vertical offset, solid line)

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

Bogoliubov-Anderson phonons contribution only (dotted line)

**Quasi-particle contribution only**
(dotted line)

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

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

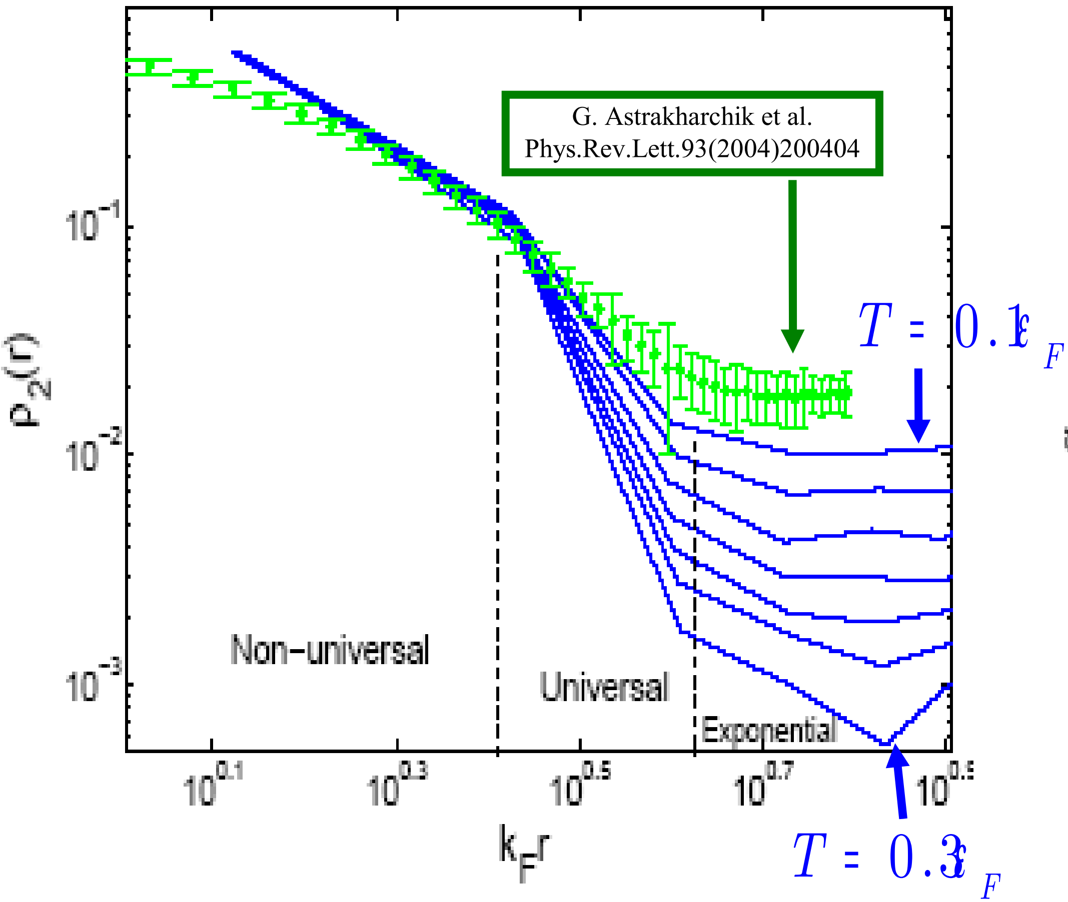
$$E_{\text{phonons}}(T) = \frac{3}{5}\varepsilon_F N \frac{\sqrt{3}\pi^4}{16\xi_s^{3/2}}\left(\frac{T}{\varepsilon_F}\right)^4, \qquad \xi_s \approx 0.41$$

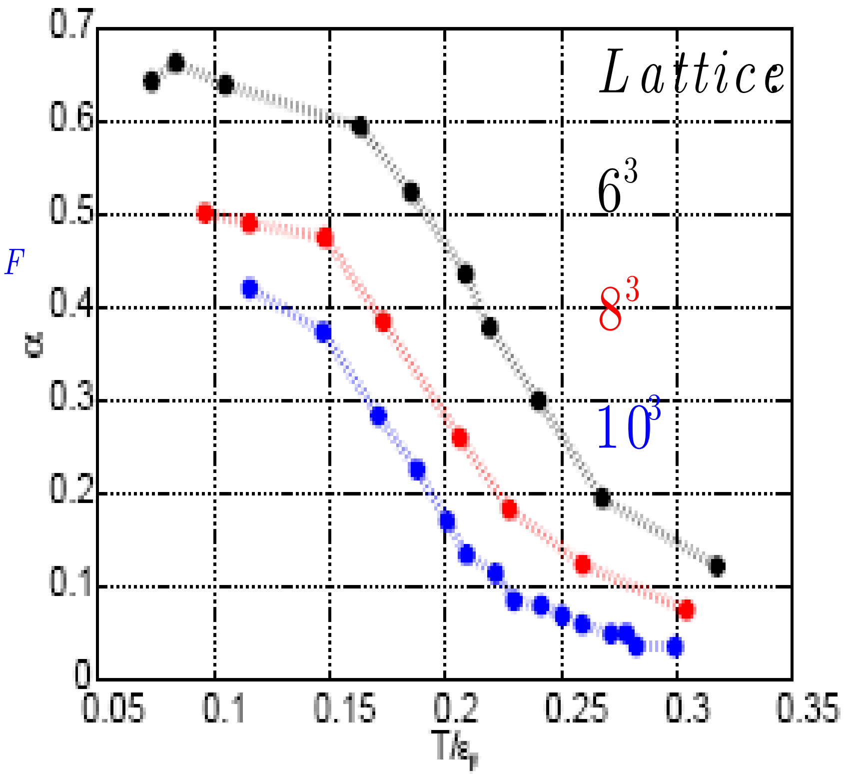
A. Bulgac, J.E. Drut, P. Magierski, PRL96, 090404(2006)

$$\rho_2(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4) = \left\langle \hat{\psi}^\dagger_\uparrow(\vec{r}_1)\hat{\psi}^\dagger_\downarrow(\vec{r}_2)\hat{\psi}_\downarrow(\vec{r}_4)\hat{\psi}_\uparrow(\vec{r}_3)\right\rangle$$

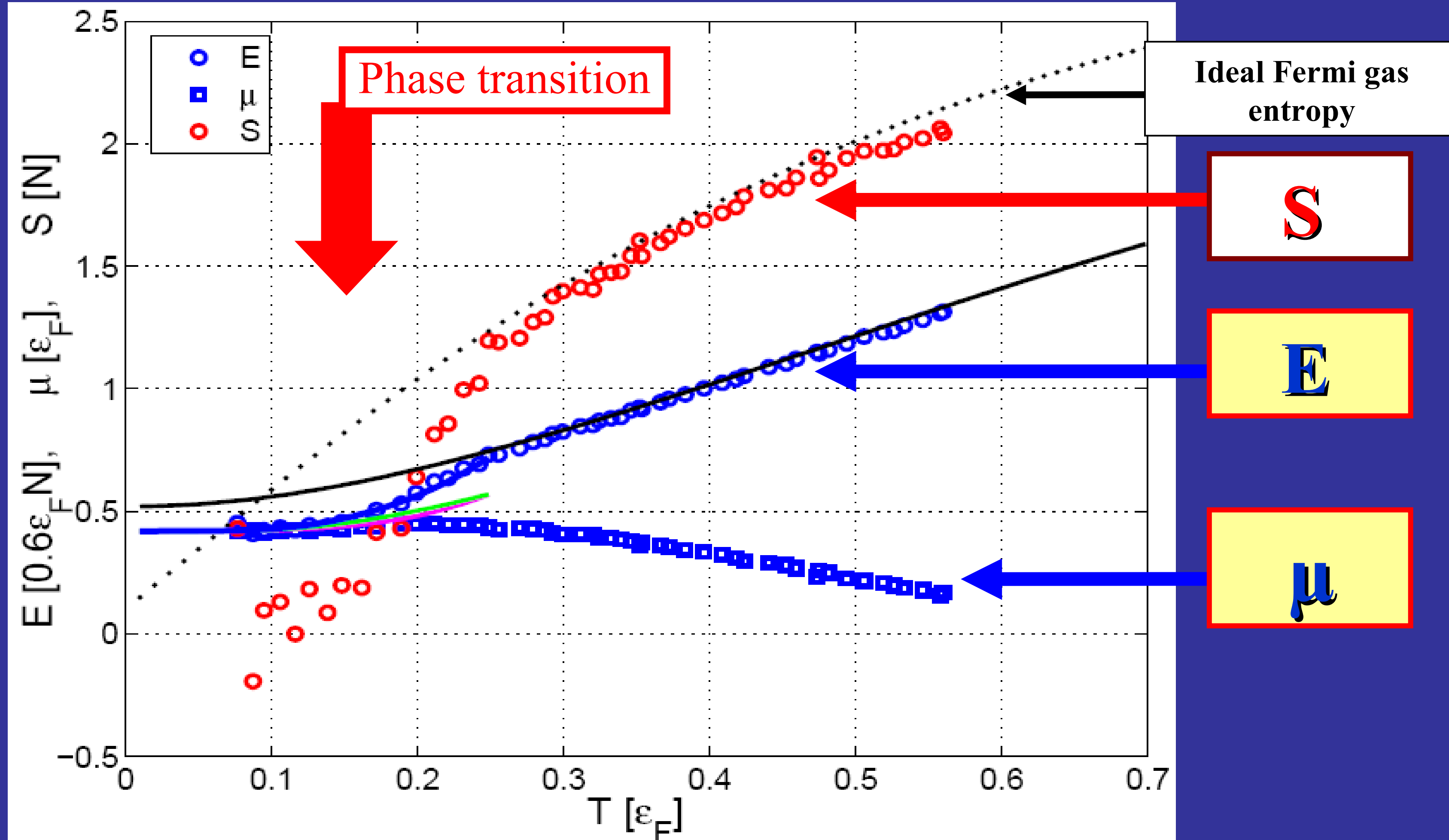
$$\rho_2{}^P(\vec{r}) = \frac{2}{N}\int d^3r_1 d^3r_2 \rho_2(\vec{r}_1+\vec{r},\vec{r}_2+\vec{r},\vec{r}_1,\vec{r}_2)$$

$$\lim_{r\to\infty}\rho_2{}^P(\vec{r}) = \alpha \text{ - condensate fraction}$$




A. Bulgac, J.E. Drut, P. Magierski, Phys. Rev. A78:023625,2008




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

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

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

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

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

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

$$P(T,\mu) = \frac{2}{5}\beta\left(T h_T\left(\frac{\mu}{T}\right)\right)^{5/2} \quad ; \quad \beta = \frac{1}{6\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}$$

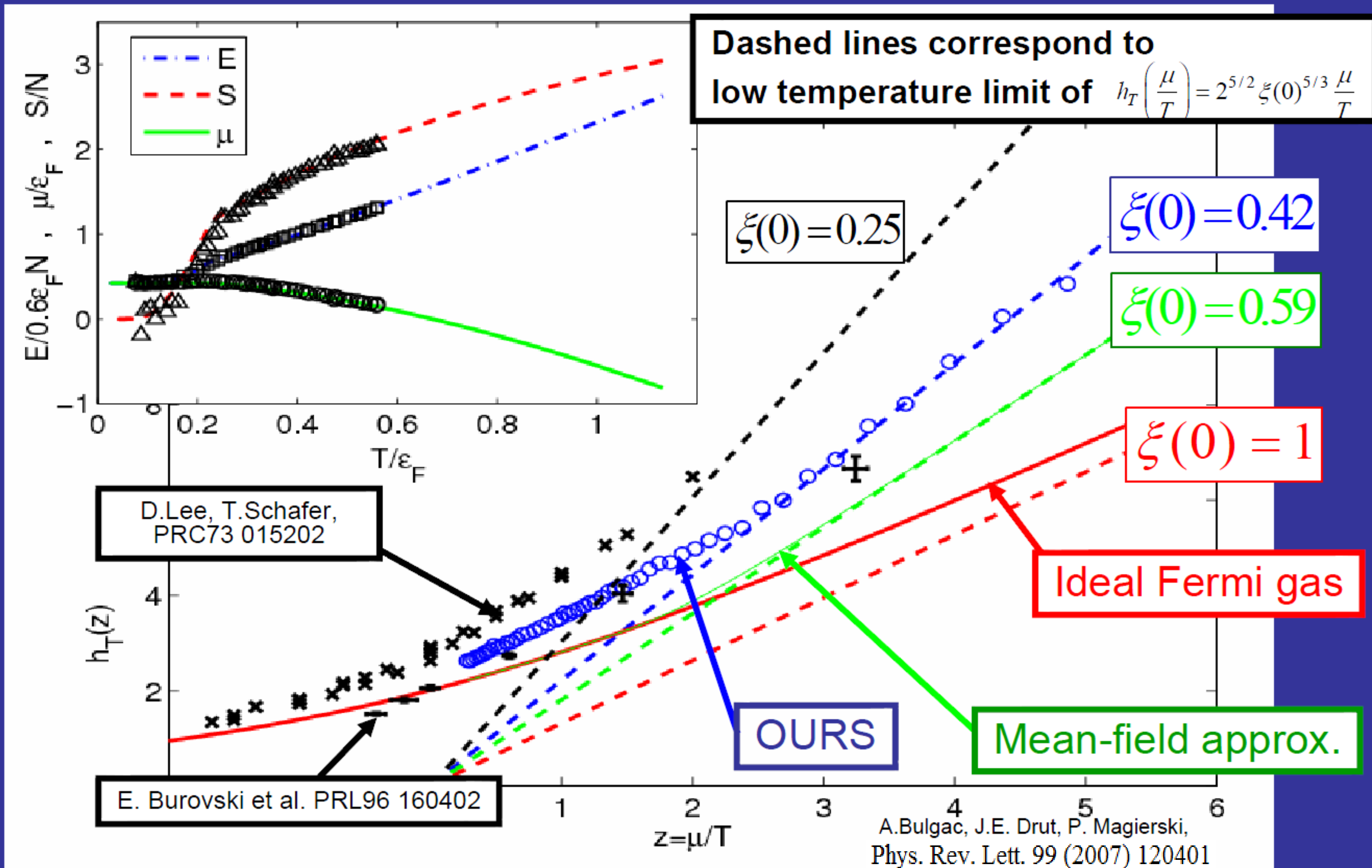
$$h_T\left(\frac{\mu}{T}\right) = \begin{cases} 2^{5/2}\xi(0)^{5/3}\frac{\mu}{T} & for \quad T \to 0 \\ \left(\frac{225\pi}{64}\right)^{1/5} e^{\frac{2}{5}\frac{\mu}{T}} & for \quad \mu \to -\infty \end{cases}$$

Thermodynamic stability condition implies:

$$Det\begin{bmatrix} \frac{\partial^2 P}{\partial T^2} & \frac{\partial^2 P}{\partial T \partial \mu} \\ \frac{\partial^2 P}{\partial \mu \partial T} & \frac{\partial^2 P}{\partial \mu^2} \end{bmatrix} \geq 0 \Rightarrow h_T''\left(\frac{\mu}{T}\right) \geq 0 \Rightarrow h_T\left(\frac{\mu}{T}\right) \text{ - convex function}$$

Since: $\Omega(V,T,\mu) = -VP(T,\mu)$

at all temperatures the pressure calculated in the BCS/meanfield approximation will give variational estimate from below of $P(T,\mu)$



# Local density approximation (LDA)

Nonuniform system

*(gradient corrections neglected)*

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

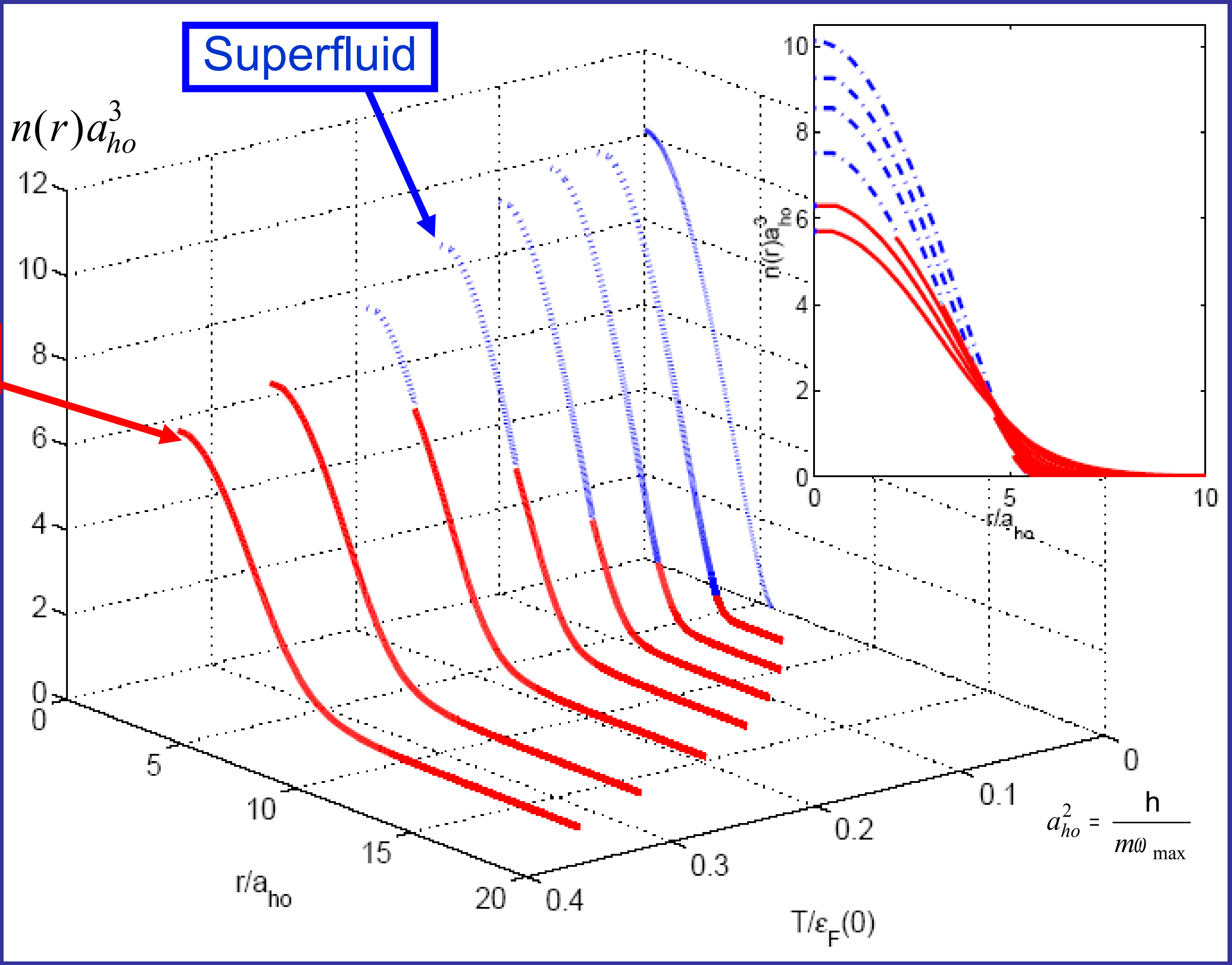
$$x(\vec{r}) = \frac{T}{\varepsilon_F(\vec{r})}; \quad \varepsilon_F(\vec{r}) = \frac{\hbar^2}{2m}\left[3\pi^2 n(\vec{r})\right]^{2/3}$$

$$F = E - TS = \tfrac{3}{5}\varphi(x)\varepsilon_F N$$

$$\varphi(x) = \xi(x) - x\sigma(x); \; \sigma(x) = S/N$$

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

**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.**



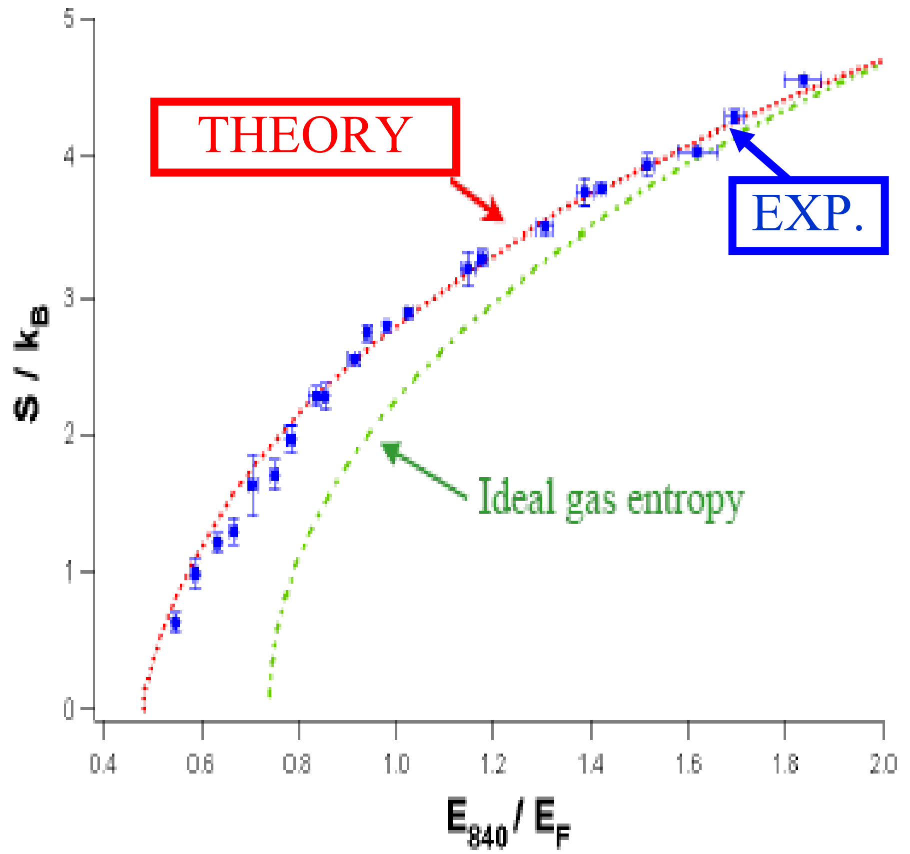

$\varepsilon_F(0)$ - Fermi energy at the center of the trap

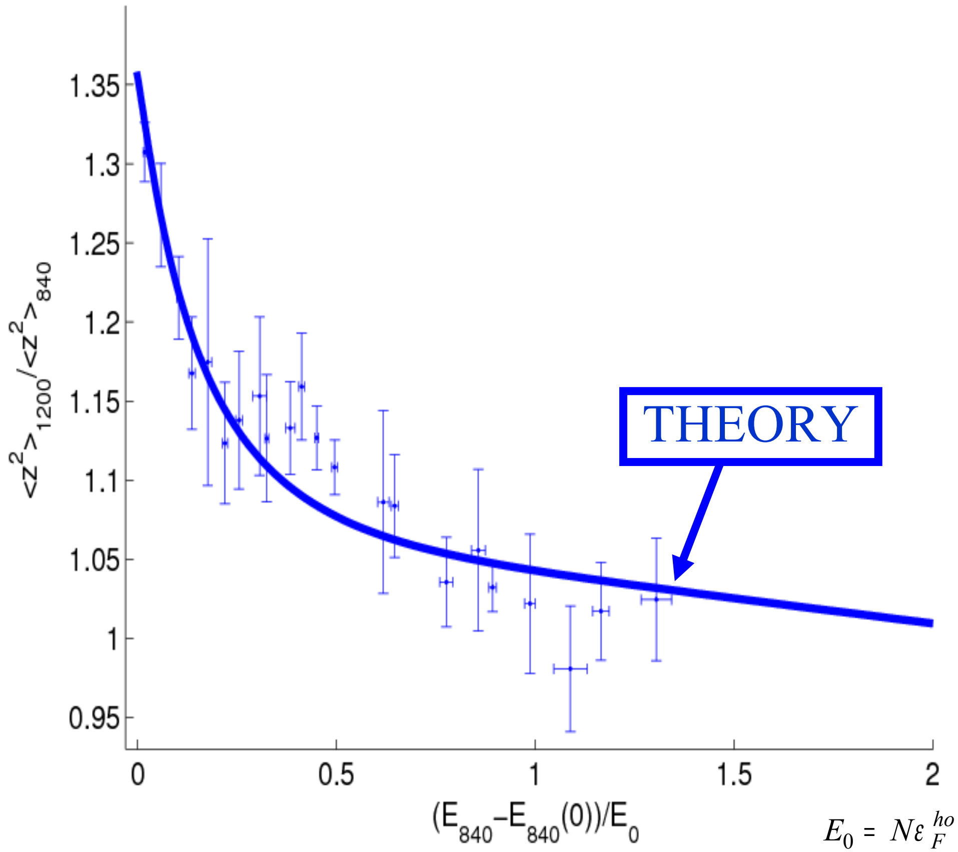
The radial (along shortest axis) density profiles of the atomic cloud in the Duke group experiment at various temperatures.

# Comparison with experiment

John Thomas' group at Duke University,

**L.Luo, et al. Phys. Rev. Lett. 98, 080402, (2007)**



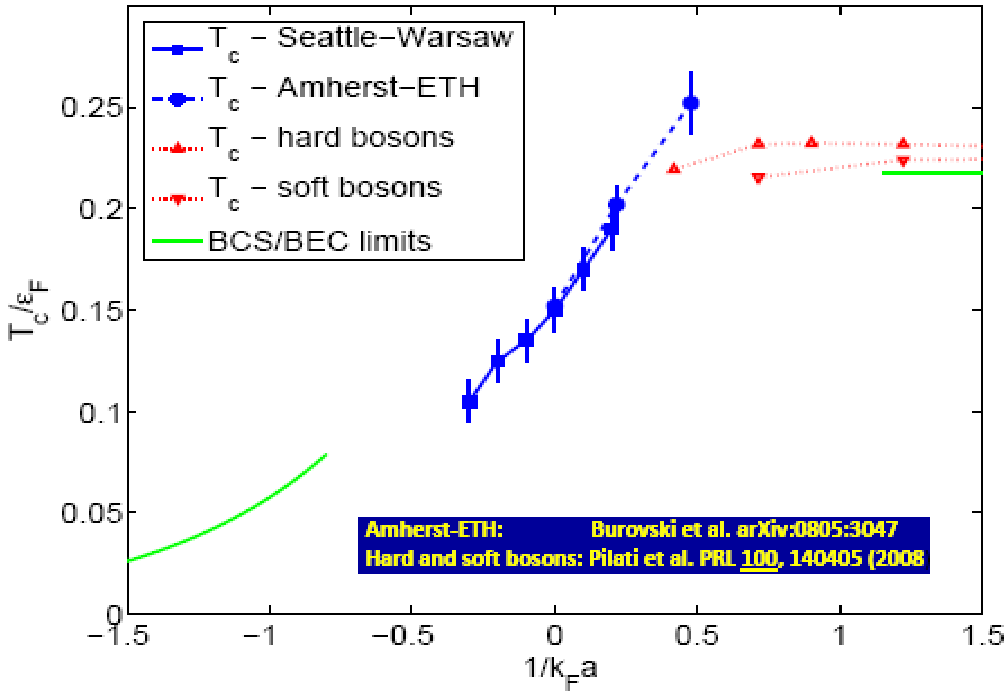

$E_0 = N\varepsilon_F^{ho}$

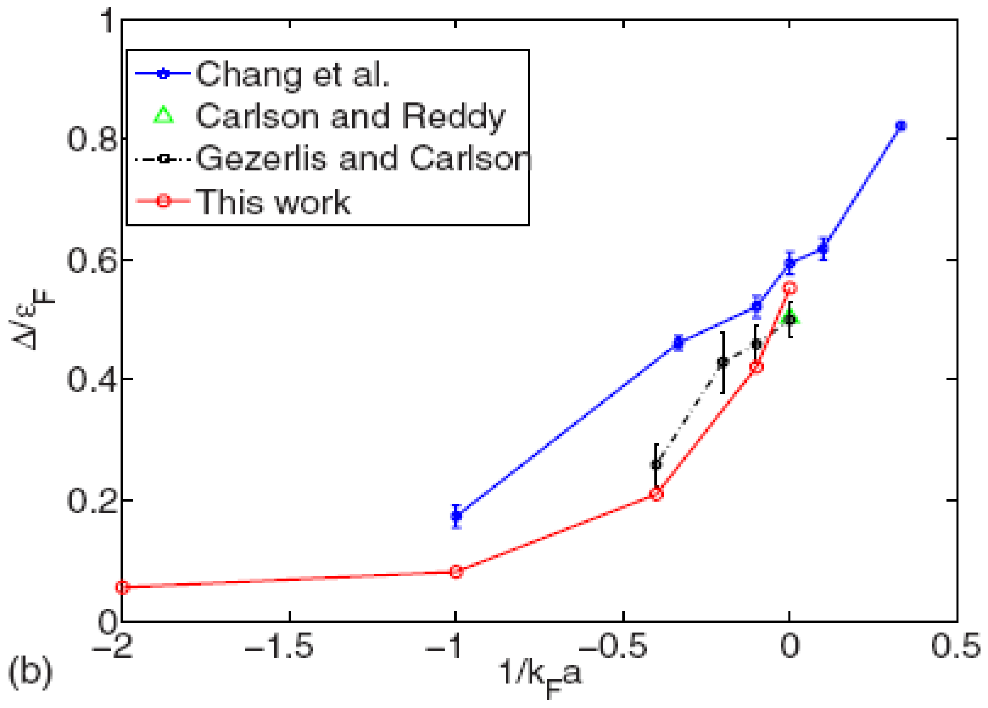
**Entropy as a function of energy (relative to the ground state) for the unitary Fermi gas in the harmonic trap.**

**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.**

$B = 1200G \quad 1/k_F a \approx -0.75$

Theory: **Bulgac, Drut, and Magierski PRL 99, 120401 (2007)**




**Results in the vicinity of the unitary limit:**

-Critical temperature

-Pairing gap at T=0

<u>Note that</u>

- at unitarity: $\Delta/\varepsilon_F \approx 0.5$
- for atomic nucleus: $\Delta/\varepsilon_F \approx 0.03$

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

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:** $A(\vec{p},\omega) = 2\pi\delta(\omega - E(p))$

## Maximum entropy method

From Bayes' theorem: $P(A|G) \propto P(G|A)P(A)$

A priori probability: $P(A) \propto \exp(\alpha S)$

Relative entropy: $$S(\mathcal{M}) = \sum_{k=1}^{n_A} \Delta\omega \left[ A(\omega_k) - \mathcal{M}(\omega_k) - A(\omega_k) \ln \left( \frac{A(\omega_k)}{\mathcal{M}(\omega_k)} \right) \right].$$

Likelihood function: $P(G|A) \propto \exp\left(-\frac{1}{2}\chi^2\right)$ $\quad \chi^2 = \sum_{i=1}^{n_\tau} \left( \frac{\tilde{\mathcal{G}}_{\tau_i} - \mathcal{G}(\tau_i)}{\sigma_{\tau_i}} \right)^2$ $\quad \mathcal{G}(\tau_i) = \sum_{k=1}^{n_A} \frac{e^{-\omega_k \tau_i}}{1 + e^{-\omega_k \beta}} A_k \Delta\omega.$

Maximum entropy method: $\min_{A(\omega)} \left( \frac{1}{2}\chi^2 - \alpha S \right)$

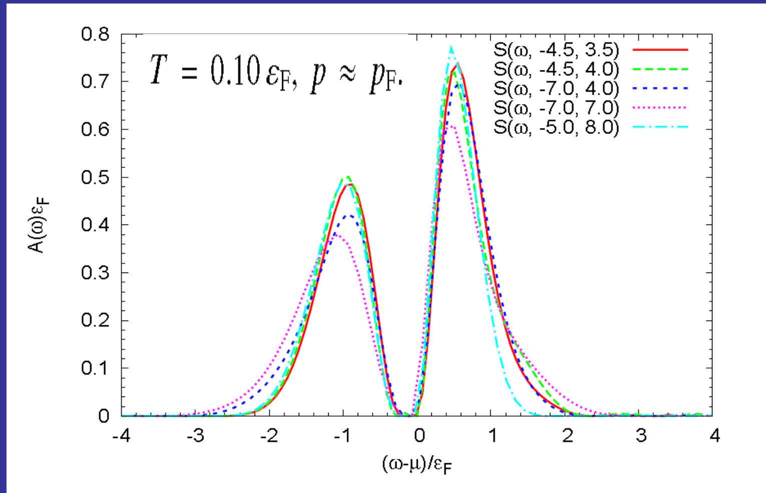
## SVD method

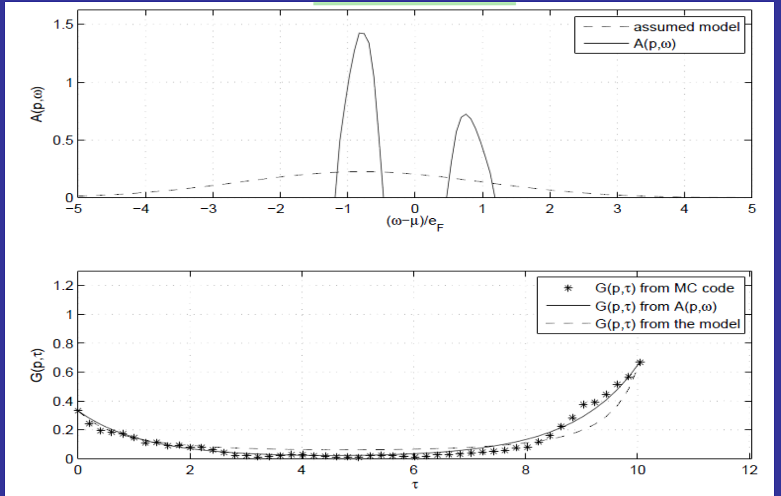
$$\mathcal{G}(\boldsymbol{p}, \tau_i) = (\mathcal{K}A)(\boldsymbol{p}, \tau_i).$$

$$\mathcal{K}u_i = \lambda_i \vec{v}_i, \quad \mathcal{K}^* \vec{v}_i = \lambda_i u_i,$$

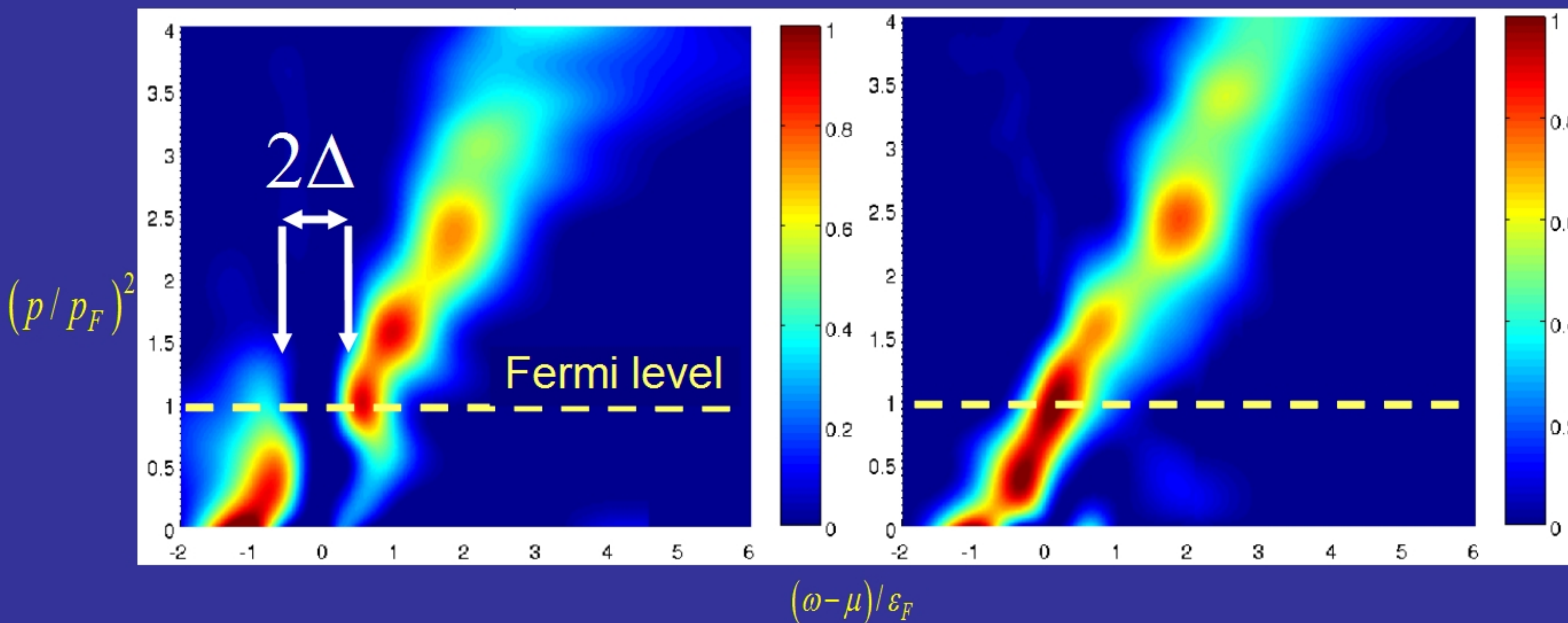
$$u_i(\omega) = \frac{1}{\sigma_i} \sum_{k=1}^{n_\tau} (\vec{v}_i)_k \phi_{\tau_k}(\omega) = -\frac{1}{2\pi\sigma_i} \sum_{k=1}^{n_\tau} (\vec{v}_i)_k \frac{e^{-\omega\tau_k}}{1 + e^{-\omega\beta}}.$$

$$A(\boldsymbol{p}, \omega) = \sum_{i=1}^{r} b_i(\boldsymbol{p}) u_i(\omega), \quad b_i(\boldsymbol{p}) = \frac{1}{\lambda_i} (\vec{\mathcal{G}}(\boldsymbol{p}) \cdot \vec{v}_i),$$



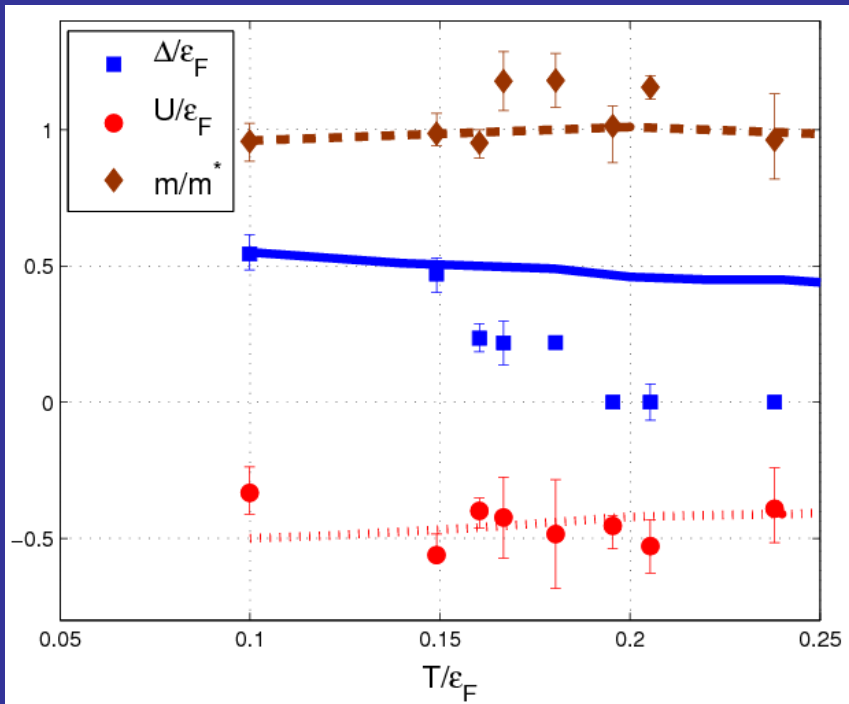




$T = 0.1\varepsilon_F < T_C$ $A(p,\omega)$ $T = 0.2\varepsilon_F > T_C$




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

# Single-particle properties



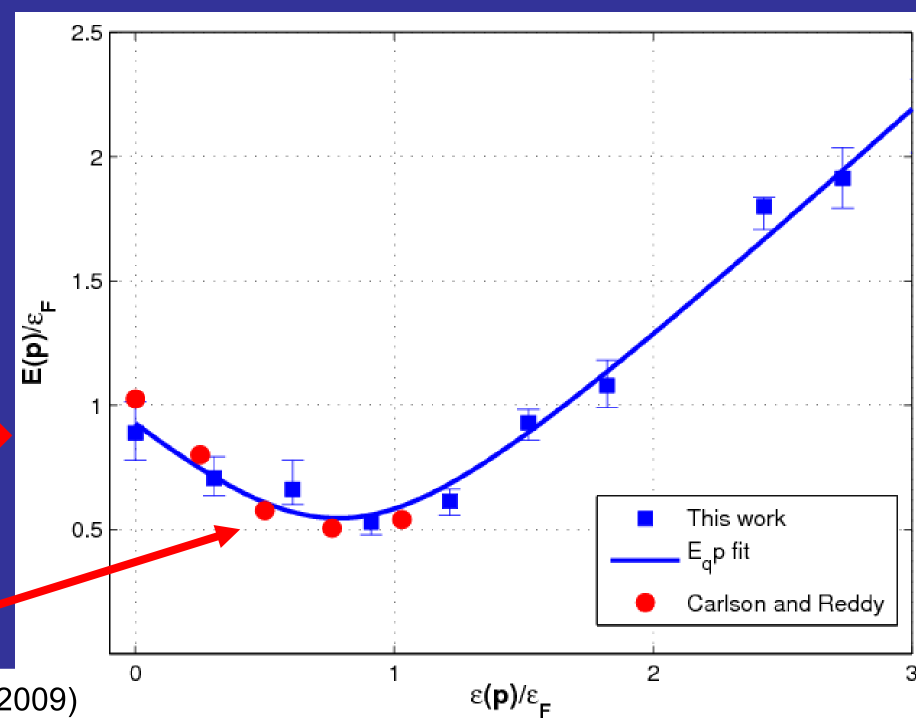

Effective mass: $m^* = (1.0 \pm 0.2)m$

Mean-field potential: $U = (-0.5 \pm 0.2)\varepsilon_F$

Weak temperature dependence!

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

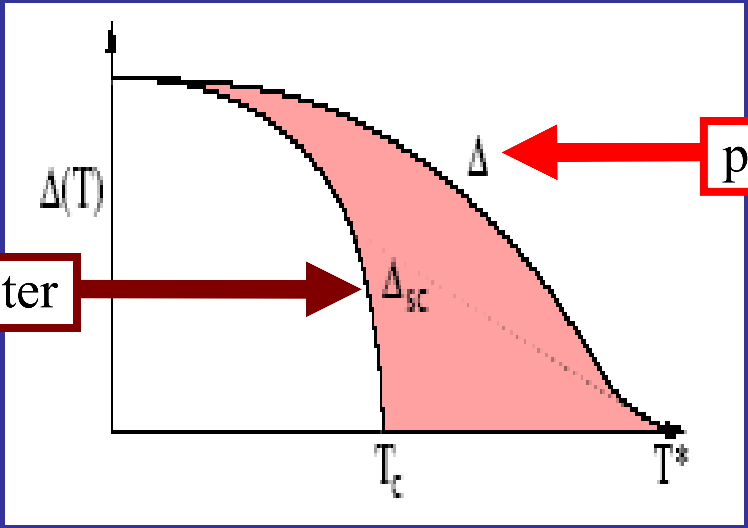
Fixed node MC calcs. at T=0




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

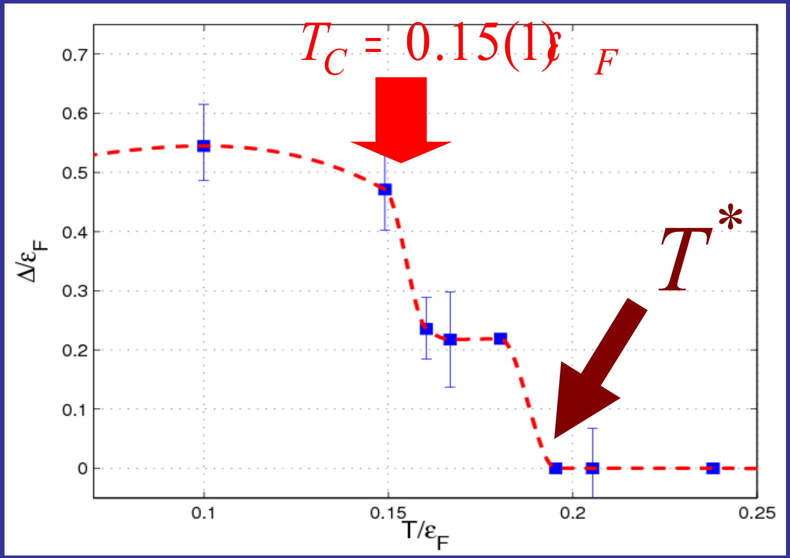
# Pairing gap and pseudogap

Outside the BCS regime close to the unitary limit, but still before BEC, superconductivity/superfluidity emerge out of a very exotic, non-Fermi liquid normal state



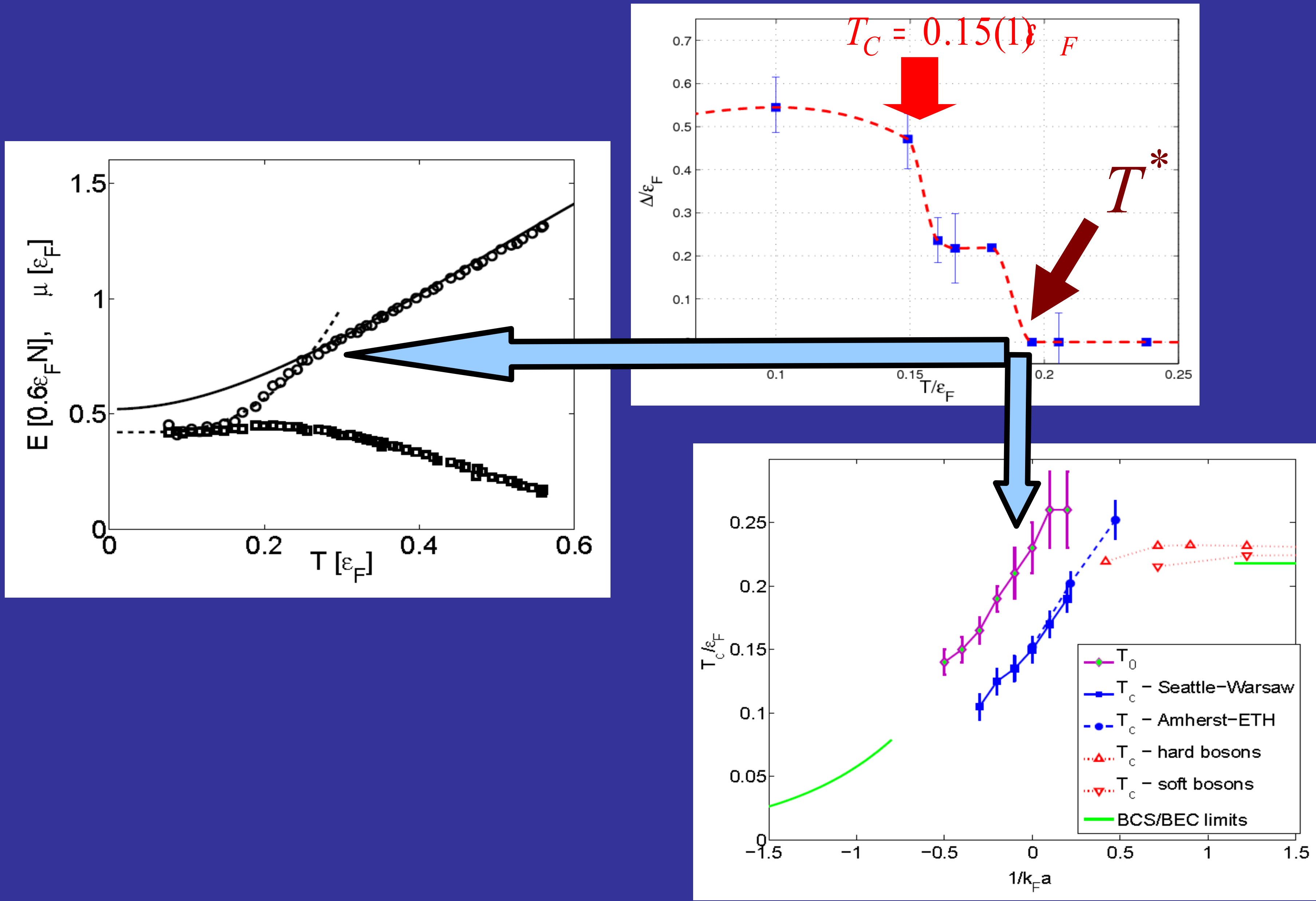

pseudogap

order parameter

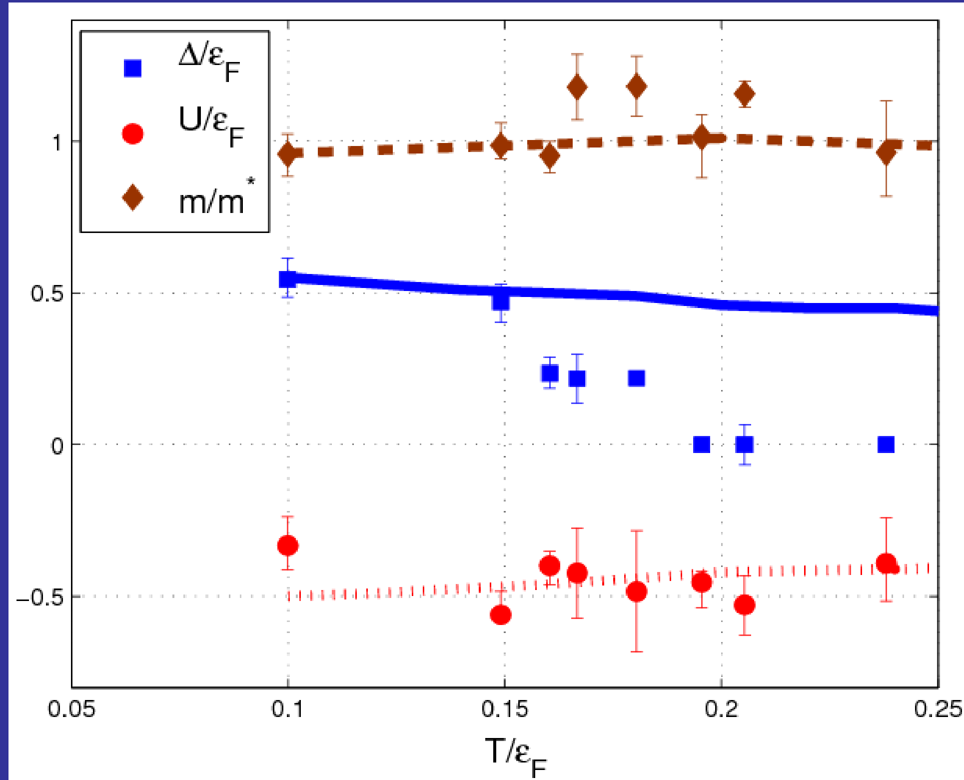



Monte Carlo calculations

*The onset of superconductivity occurs in the presence of fermionic pairs!*



$T_C = 0.15(1)\varepsilon_F$
$T^*$
Δ/ε_F
T/ε_F
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.1
0.15
0.2
0.25
E [0.6ε_F N], μ [ε_F]
T [ε_F]
1.5
1
0.5
0
0
0.2
0.4
0.6
T_c/ε_F
1/k_F a
0.25
0.2
0.15
0.1
0.05
0
−1.5
−1
−0.5
0
0.5
1
1.5
T_0
T_c − Seattle−Warsaw
T_c − Amherst−ETH
T_c − hard bosons
T_c − soft bosons
BCS/BEC limits




Dashed, dotted and solid lines

Susceptibility from the independent quasiparticle model

$$\chi(\boldsymbol{p}) = -\int_0^\beta d\tau \mathcal{G}(\boldsymbol{p},\tau) = \frac{1}{E(\boldsymbol{p})}\frac{e^{\beta E(\boldsymbol{p})}-1}{e^{\beta E(\boldsymbol{p})}+1}.$$

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

$\alpha = m/m^*, U, \quad \Delta$

**Parameters (effective mass, mean-field potential, pairing gap) extracted from the response function within the <u>independent quasiparticle model</u> accurately reproduce results obtained directly from the spectral weight function below the critical temperature!**

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

# Preliminary measurements of pseudogap in ultracold atomic gases

$^{40}K$

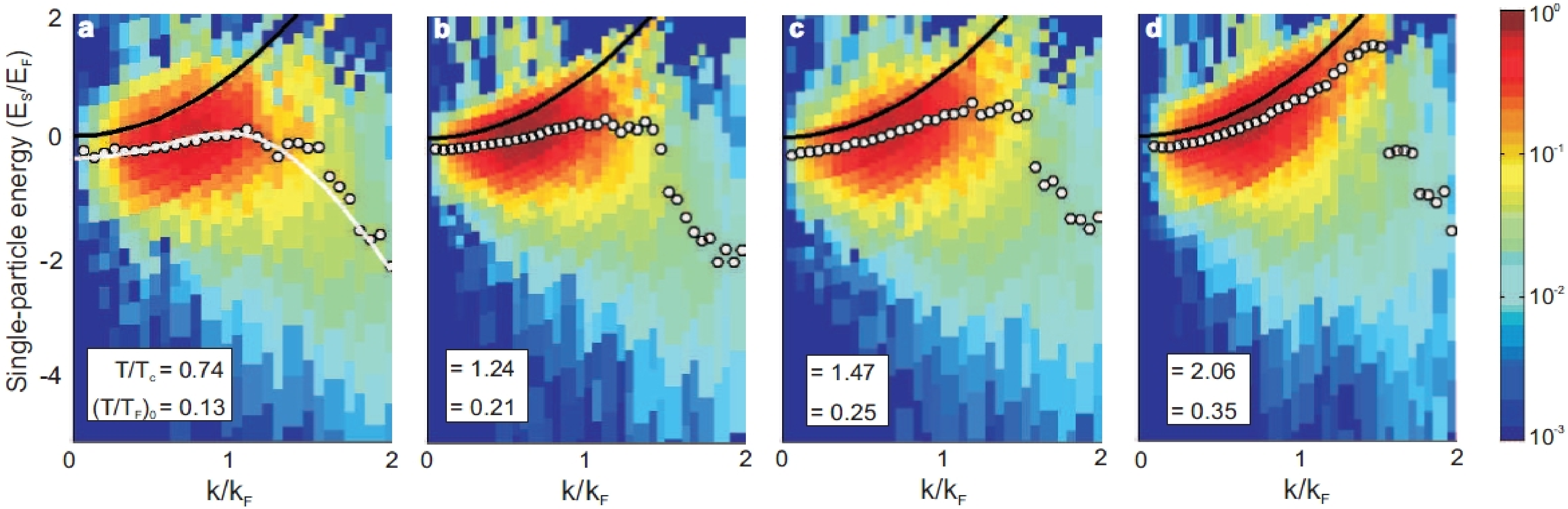



FIG. 1: **Photoemission spectra throughout the pseudogap regime.** Spectra are shown for Fermi gases at four different temperatures, each with an interaction strength characterized by $(k_F a)^{-1} \approx 0.15$. The intensity plots show the fraction of out-coupled atoms as a function of their single-particle energy (normalized to $E_F$) and momentum (normalized to $k_F$), where $E = 0$ corresponds to a non-interacting particle at rest. The spectra are normalized so that integrating them over momentum and energy gives unity. White dots indicate the centers extracted from gaussian fits to individual energy distribution curves (traces through the data at fixed momentum). The black curve is the quadratic dispersion expected for a free particle. **a** At $T = 0.74\,T_c$, we observe a BCS-like dispersion with back-bending, consistent with previous measurements [6]. The white curve is a fit to a BCS-like dispersion, Eqn. 1. **b,c** At $T = 1.24\,T_c$ and $T = 1.47\,T_c$, respectively, the dispersion with back-bending persists even though there is no longer any superfluidity. **d** At $T = 2.06\,T_c$, the dispersion does not display back-bending in the range of $0 < k < 1.5\,k_F$. In all the plots there is a negative dispersion for $k/k_F > 1.5$. We attribute this weak feature (note the log scale) to a $1/k^4$ tail and not to the gap.


J. P. Gaebler, J. T. Stewart, T. E. Drake, D. S. Jin, A. Perali, P. Pieri, G. C. Strinati, arXiv:1003.1147