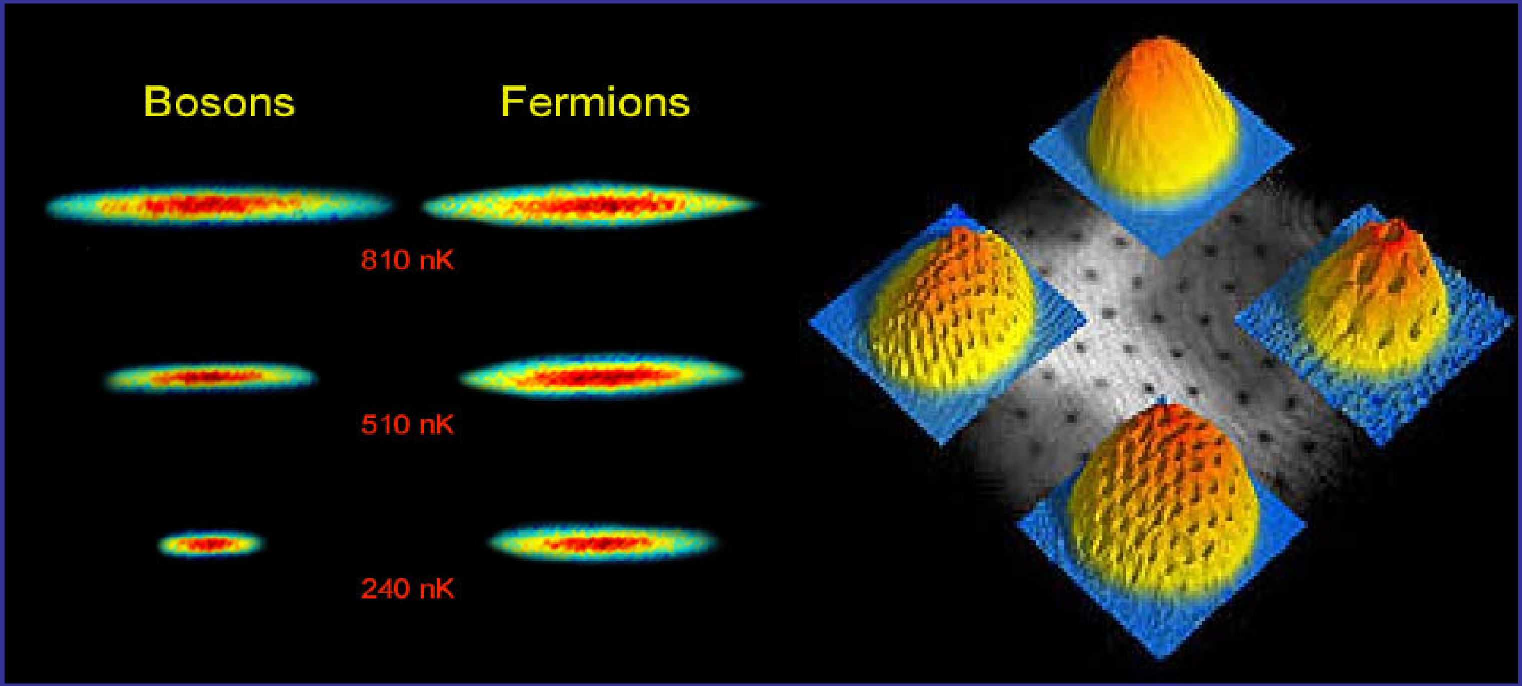
Uniform and nonuniform dilute and strongly interacting Fermi gas



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<u>In collaboration with:</u> Aurel Bulgac, Joaquin E. Drut (University of Washington, Seattle)

Outline

- BCS-BEC crossover. What is the unitary regime?
- Equation of state for the uniform Fermi gas in the unitary regime. Critical temperature.
- Thermodynamics of the unitary Fermi gas.
- Measurements of the entropy and the critical temperature in a harmonic trap.
- Local density approximation (LDA) for the unitary Fermi gas in a trap.

➢ What is the unitary regime?

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.

$\boxed{n\, r_0^3 \ll 1}$ $\boxed{n\, |a|^3 \gg 1}$

n - particle density
a - scattering length
r_0 - effective range

$$\boxed{i.e.\ \ r_0 \to 0,\ a \to \pm\infty}$$

NONPERTURBATIVE REGIME

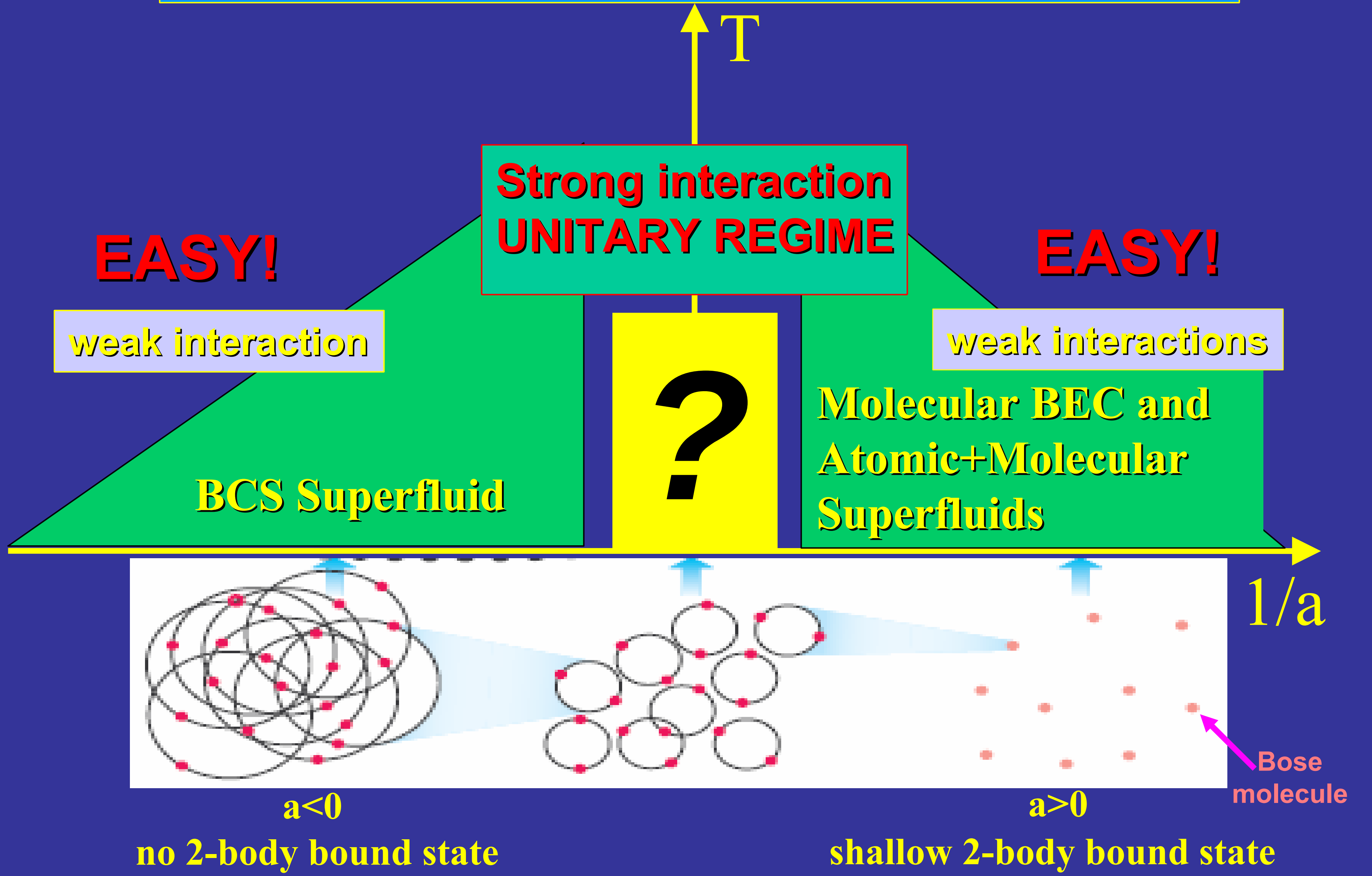
System is dilute but strongly interacting!

The only scale: $\boxed{E_{FG}/N = \frac{3}{5}\varepsilon_F}$

UNIVERSALITY: $\boxed{E(T) = \xi\left(\frac{T}{\varepsilon_F}\right) E_{FG}}$

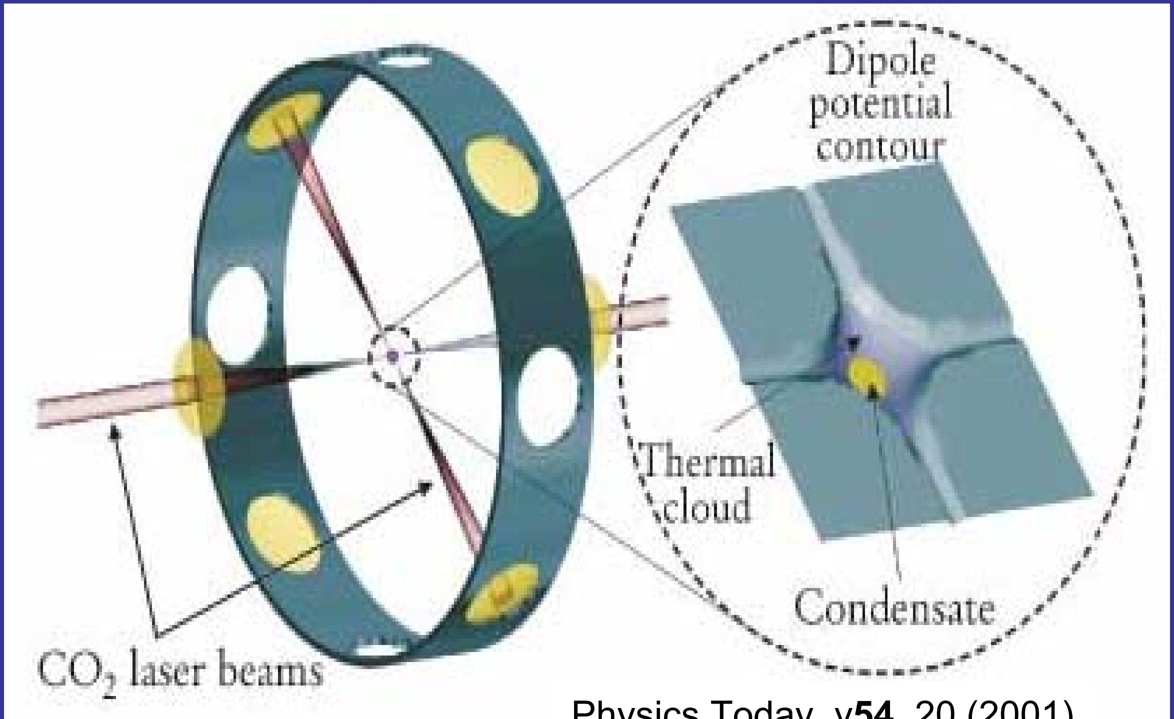
QUESTIONS: What is the shape of $\xi(T/\varepsilon_F)$?
What is the critical temperature for the superfluid-to-normal transition?
...

Expected phases of a two species dilute Fermi system
BCS-BEC crossover



In dilute atomic systems experimenters can control nowadays almost anything:

- The number of atoms in the trap: typically about 10^5-10^6 atoms divided 50-50 among the lowest two hyperfine states.
- The density of atoms
- Mixtures of various atoms
- The temperature of the atomic cloud
- **The strength of this interaction is fully tunable!**



Physics Today, v**54**, 20 (2001)

Who does experiments?

- **Jin's group at Boulder**
- **Grimm's group in Innsbruck**
- **Thomas' group at Duke**
- **Ketterle's group at MIT**
- **Salomon's group in Paris**
- **Hulet's group at Rice**

Neutron matter:

Effective range: $r_0 \approx 2.8$ fm

Scattering length: $a \approx -18.5$ fm

Density range

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

corresponds to

$n \approx 0.001 - 0.01\ \mathrm{fm}^{-3}$

$k_F \approx 0.3 - 0.7\ \mathrm{fm}^{-1}$

Hamiltonian

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

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

Theoretical approach: Fermions on 3D lattice

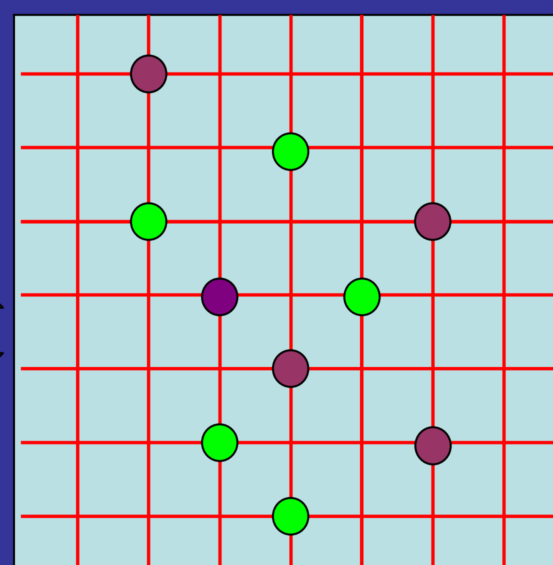
$$Volume = L^3$$

$$lattice\ spacing = \Delta x$$

Coordinate space

L –limit for the spatial correlations in the system

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



- Spin up fermion:

- Spin down fermion:

External conditions:

T - temperature

μ - chemical potential

Periodic boundary conditions imposed

Hamiltonian

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

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

Interaction:

$$\hat{T} = \hat{V} + \hat{V}\hat{G}^{(+)}(\varepsilon)\hat{T}$$

$$\left\langle \vec{k}\left|\hat{V}\right|\vec{k}'\right\rangle = \begin{cases} \dfrac{-g}{(2\pi)^3}; & k, k' < k_{cut} \\ 0; & \text{otherwise} \end{cases}$$

$$\left\langle \vec{k}\left|\hat{T}\right|\vec{k}'\right\rangle = \frac{-g}{(2\pi)^3}\sum_{n=0}^{\infty}\left[\int_{k_1<k_{cut}}\frac{d^3k_1}{(2\pi)^3}\frac{-g}{\varepsilon - \dfrac{\hbar^2k_1^2}{m} + i0^+}\right]^n$$

Interaction:

$$f(k) = -2\pi^2 \frac{m}{\hbar^2} \langle \vec{k} | \hat{T} | \vec{k}' \rangle \xrightarrow{k \to 0} \frac{1}{-ik + \frac{4\pi\hbar^2}{gm} - \frac{2k_{cut}}{\pi}}$$

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

Running coupling constant g defined by lattice

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

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

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

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

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

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

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

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

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

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 from 8^3 x 257 (high Ts) to 8^3 x 1732 (low Ts), <N>=50, and 6^3 x 257 (high Ts) to 6^3 x 1361 (low Ts), <N>=30.

- 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

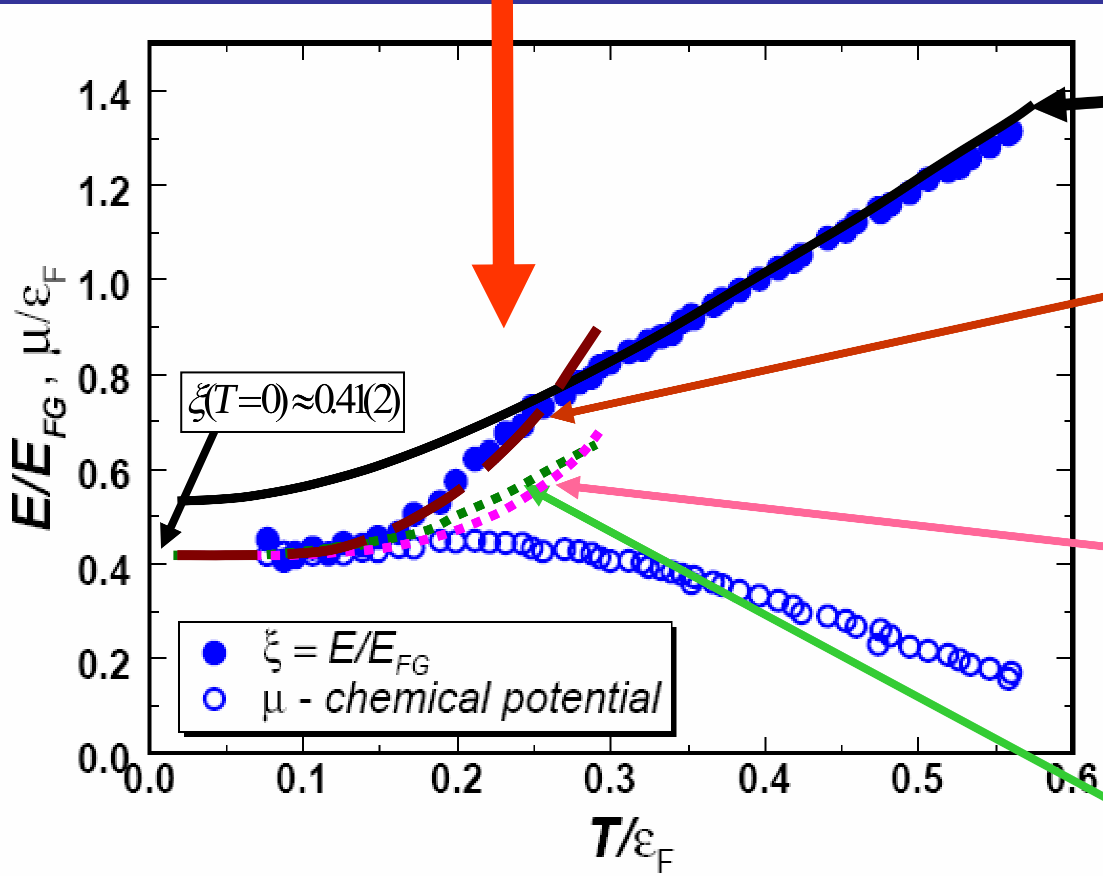
- At low temperatures use Singular Value Decomposition of the evolution operator $U(\{\sigma\})$ to stabilize the numerics.

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

- MC correlation "time" ≈ 150 – 200 time steps at $T \approx T_c$

$a = \pm\infty$

Superfluid to Normal Fermi Liquid Transition



Normal Fermi Gas
(with vertical offset, solid line)

Bogoliubov-Anderson phonons and quasiparticle contribution
(dashed line)

Bogoliubov-Anderson phonons contribution only (dotted line)

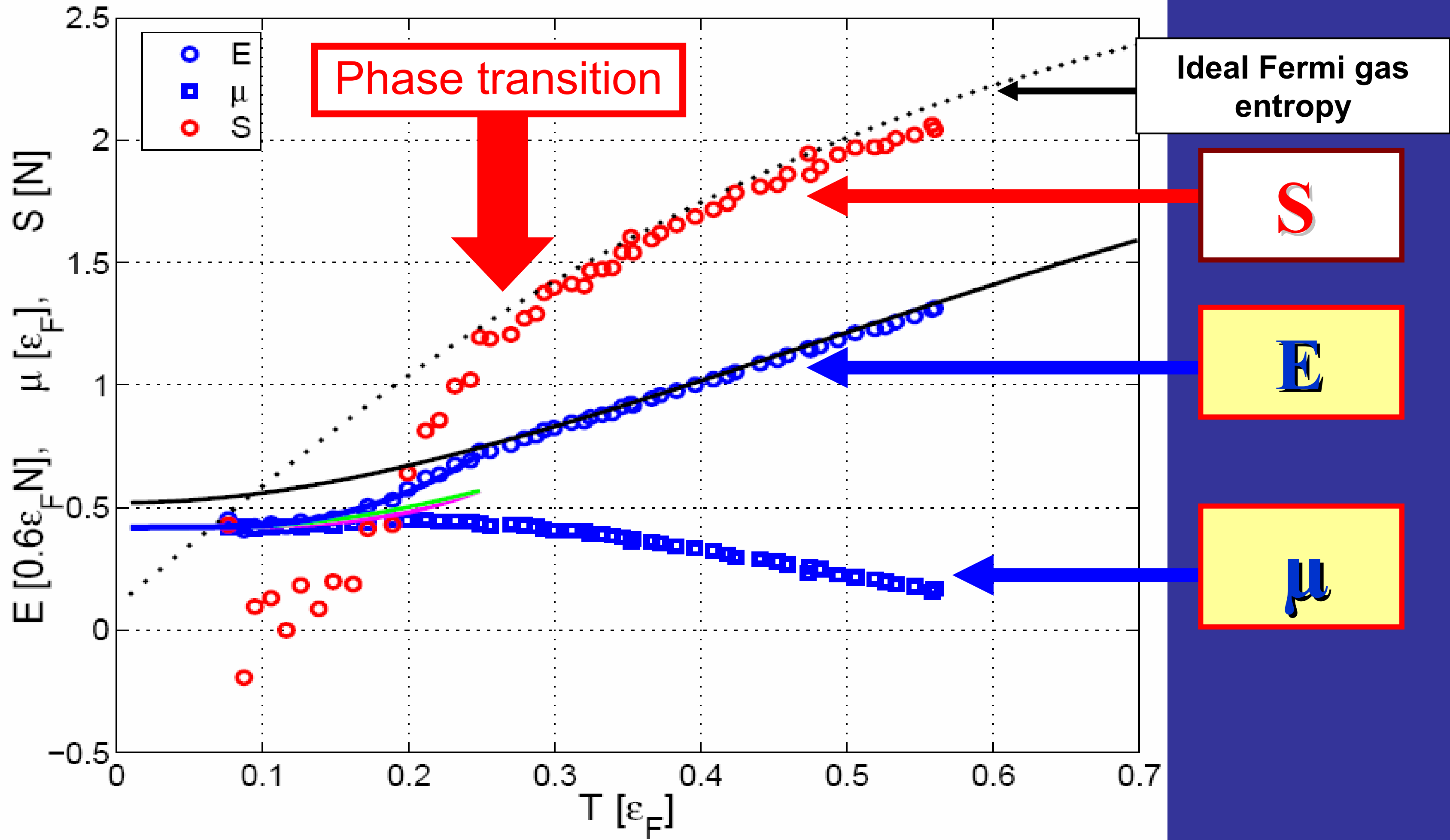
Quasi-particle contribution only
(dotted line)

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

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

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

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



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

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

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

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

Low temperature behaviour of a Fermi gas in the unitary regime

$$F(T) = \frac{3}{5}\varepsilon_F N \varphi\left(\frac{T}{\varepsilon_F}\right) = E - TS \quad \text{and} \quad \frac{\mu(T)}{\varepsilon_F} \approx \xi_s \approx 0.41(2) \text{ for } T < T_C$$

$$\mu(T) = \frac{dF(T)}{dN} = \varepsilon_F\left[\varphi\left(\frac{T}{\varepsilon_F}\right) - \frac{2}{5}\frac{T}{\varepsilon_F}\varphi'\left(\frac{T}{\varepsilon_F}\right)\right] \approx \varepsilon_F \xi_s$$

$$\varphi\left(\frac{T}{\varepsilon_F}\right) = \varphi_0 + \varphi_1\left(\frac{T}{\varepsilon_F}\right)^{5/2}$$

$$E(T) = \frac{3}{5}\varepsilon_F N\left[\xi_s + \varsigma_s\left(\frac{T}{\varepsilon_F}\right)^n\right]$$

Lattice results disfavor either $n \geq 3$ or $n \leq 2$ and suggest $n = 2.5(0.25)$

This is the same behavior as for a gas of <u>noninteracting</u> (!) bosons below the condensation temperature.

$$E(T) \approx \frac{3}{5}\varepsilon_F N \xi_s + \frac{m_B^{3/2}\Gamma\left(\frac{3}{2}\right)\varsigma\left(\frac{3}{2}\right)}{2^{1/2}\pi^2\hbar^3} T^{5/2} V, \quad \text{if} \quad T \gg m_B c^2$$

and fitting to lattice results $\Rightarrow \quad m_B \approx 3m$

- **Why this value for the bosonic mass?**
- **Why these bosons behave like noninteracting particles?**

Conclusions

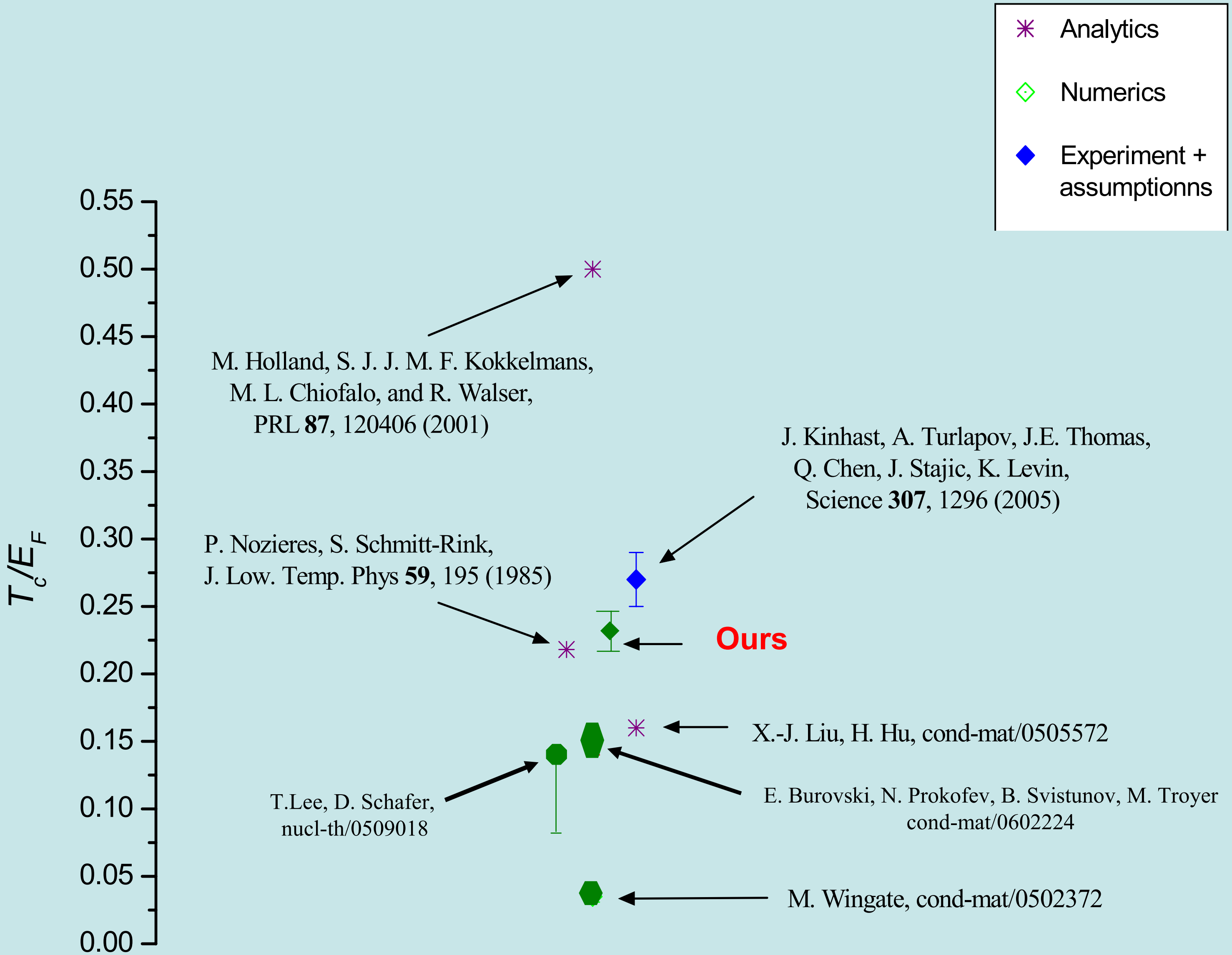
- ✓ Fully non-perturbative calculations for a spin ½ many fermion system in the unitary regime at finite temperatures are feasible and apparently the system undergoes a phase transition in the bulk at $T_c = 0.23\ (2)\ \varepsilon_F$
  (Exp: $T_c = 0.27(2)\ \varepsilon_F$, J. Kinast *et al.* Science, 307, 1296 (2005): Based on theoretical assumptions).

- ✓ Chemical potential is constant up to the critical temperature – note similarity with Bose systems!

- ✓ Below the transition temperature, both phonons and fermionic quasiparticles contribute almost equaly to the specific heat. In more than one way the system is at crossover between a Bose and Fermi systems.

There are reasons to believe that below the critical temperature this system is a new type of fermionic superfluid, with unusual properties.

Quest for unitary point critical temperature



Boris Svistunov’s talk (updated), Seattle 2005

Thermodynamics of the unitary Fermi gas

ENERGY: $E(x) = \frac{3}{5}\xi(x)\varepsilon_F N; \quad x = \frac{T}{\varepsilon_F}$

$$C_V = T\frac{\partial S}{\partial T} = \frac{\partial E}{\partial T} = \frac{3}{5}N\xi'(x) \Rightarrow S(x) = \frac{3}{5}N\int_0^x \frac{\xi'(y)}{y}dy$$

ENTROPY/PARTICLE: $\sigma(x) = \frac{S(x)}{N} = \frac{3}{5}\int_0^x \frac{\xi'(y)}{y}dy$

FREE ENERGY: $F = E - TS = \frac{3}{5}\varphi(x)\varepsilon_F N$

$$\varphi(x) = \xi(x) - x\sigma(x)$$

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

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

Note the similarity to the ideal Fermi gas

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

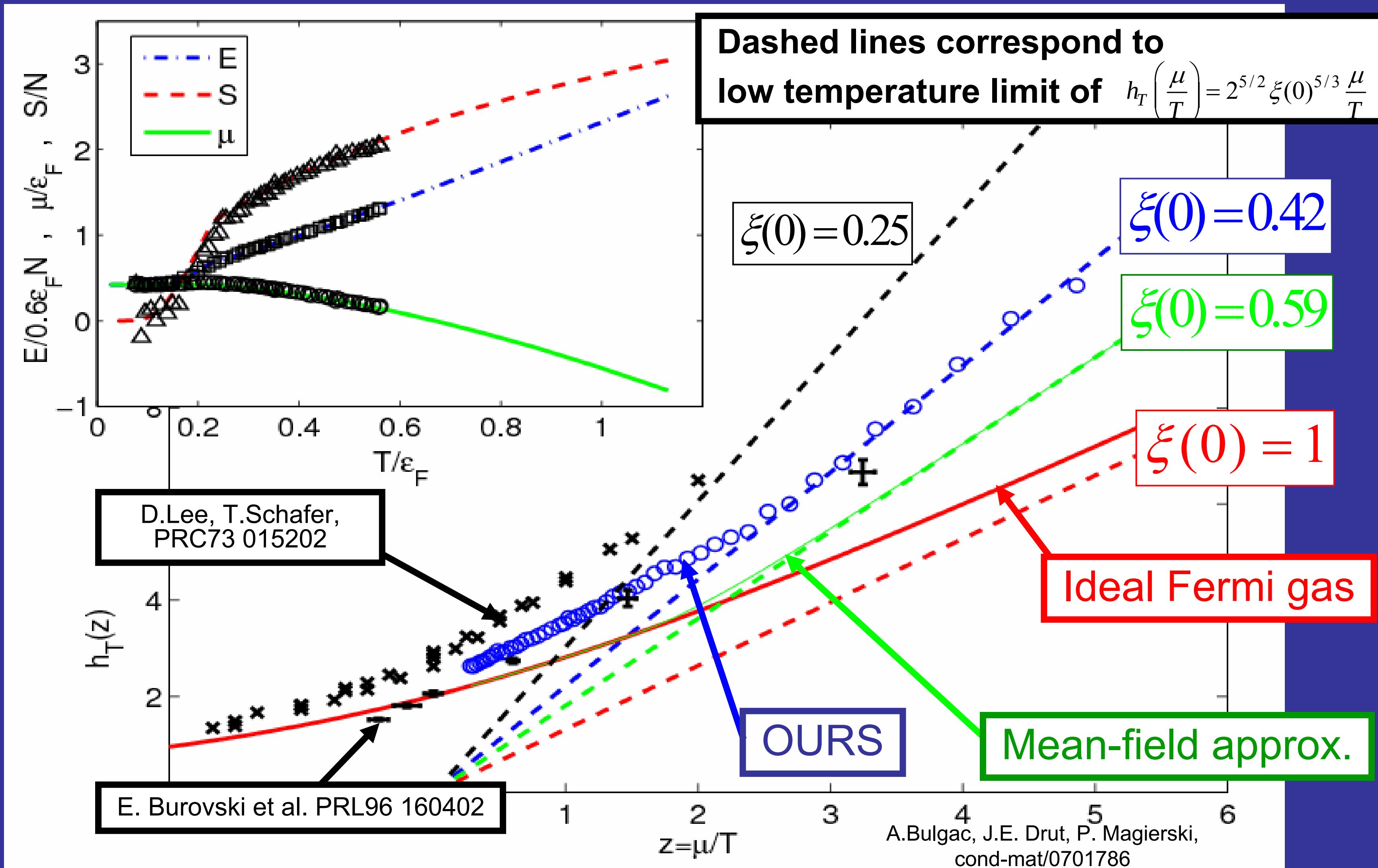
$$h_T\left(\frac{\mu}{T}\right) = \begin{cases} 2^{5/2}\xi(0)^{5/3}\frac{\mu}{T} & for \quad T \to 0 \\ \left(\frac{225\pi}{64}\right)^{1/5} e^{\frac{2}{5}\frac{\mu}{T}} & for \quad \mu \to -\infty \end{cases}$$

Thermodynamic stability condition implies:

$$\mathrm{Det}\begin{bmatrix} \frac{\partial^2 P}{\partial T^2} & \frac{\partial^2 P}{\partial T \partial \mu} \\ \frac{\partial^2 P}{\partial \mu \partial T} & \frac{\partial^2 P}{\partial \mu^2} \end{bmatrix} \ge 0 \Rightarrow \frac{3}{2}\beta^2\left(h_T\left(\frac{\mu}{T}\right)\right)^4 h''_T\left(\frac{\mu}{T}\right) \ge 0 \Rightarrow h''_T\left(\frac{\mu}{T}\right) - \text{convex function}$$

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 $P(T, \mu)$



Experiment

John Thomas' group at Duke University,

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

Dilute system of fermionic ^{6}Li atoms in a harmonic trap

- The number of atoms in the trap: N=1.3(0.2) x 10^5 atoms divided 50-50 among the lowest two hyperfine states.
- Fermi energy: $\varepsilon_F^{ho} = \hbar\Omega(3N)^{1/3}; \ \Omega = \left(\omega_x \omega_y \omega_z\right)^{1/3}$

$$\varepsilon_F^{ho} / k_B \approx 1\mu K$$

- Depth of the potential: $U_0 \approx 10\varepsilon_F^{ho}$
- How they measure: energy, entropy and temperature?

$$\left.\begin{array}{l} PV = \dfrac{2}{3}E \\ \vec{\nabla}P = -n(\vec{r})\vec{\nabla}U \end{array}\right\} \Rightarrow N\langle U \rangle = \frac{E}{2} \text{ - virial theorem}$$

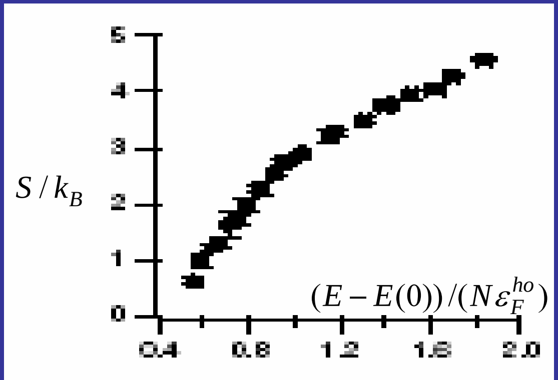
$n(\vec{r})$ - local density

Holds at unitarity and for noninteracting Fermi gas

- For the weakly interacting gas ($B=1200G \Rightarrow 1/k_F a \approx -0.75$) the energy and entropy is calculated. In this limit one can use Thomas-Fermi approach to relate the energy to the given density distribution. The entropy can be estimated as for the noninteracting system with 1% accuracy. In practice: $\left\langle z^2 \right\rangle_{B=1200} \Rightarrow E, S$
- The magnetic field is changed adiabatically (*S=const.*) to the value corresponding to the unitary limit: $B = 840G \Rightarrow 1/k_F a \approx 0$
- Relative energy in the unitary limit is calculated from virial theorem:

$$\boxed{\frac{E(T_1)}{E(T_2)} = \frac{\left\langle z^2 \right\rangle_{T_1}}{\left\langle z^2 \right\rangle_{T_2}}}$$

- Temperature is calculated from the identity: $\boxed{\frac{1}{T} = \frac{\partial S}{\partial E}}$
- The plot S(E) contains a cusp related to the phase transition:



$$\boxed{\begin{cases} E(T_c) - E(0) \approx 0.41(5) N \varepsilon_F^{ho}, \\ S_c / N \approx 2.7(2) k_B, \\ T_c \approx 0.29(3) \varepsilon_F^{ho} \end{cases}}$$

Theory: local density approximation (LDA)

Uniform system

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

Nonuniform system *(gradient corrections neglected)*

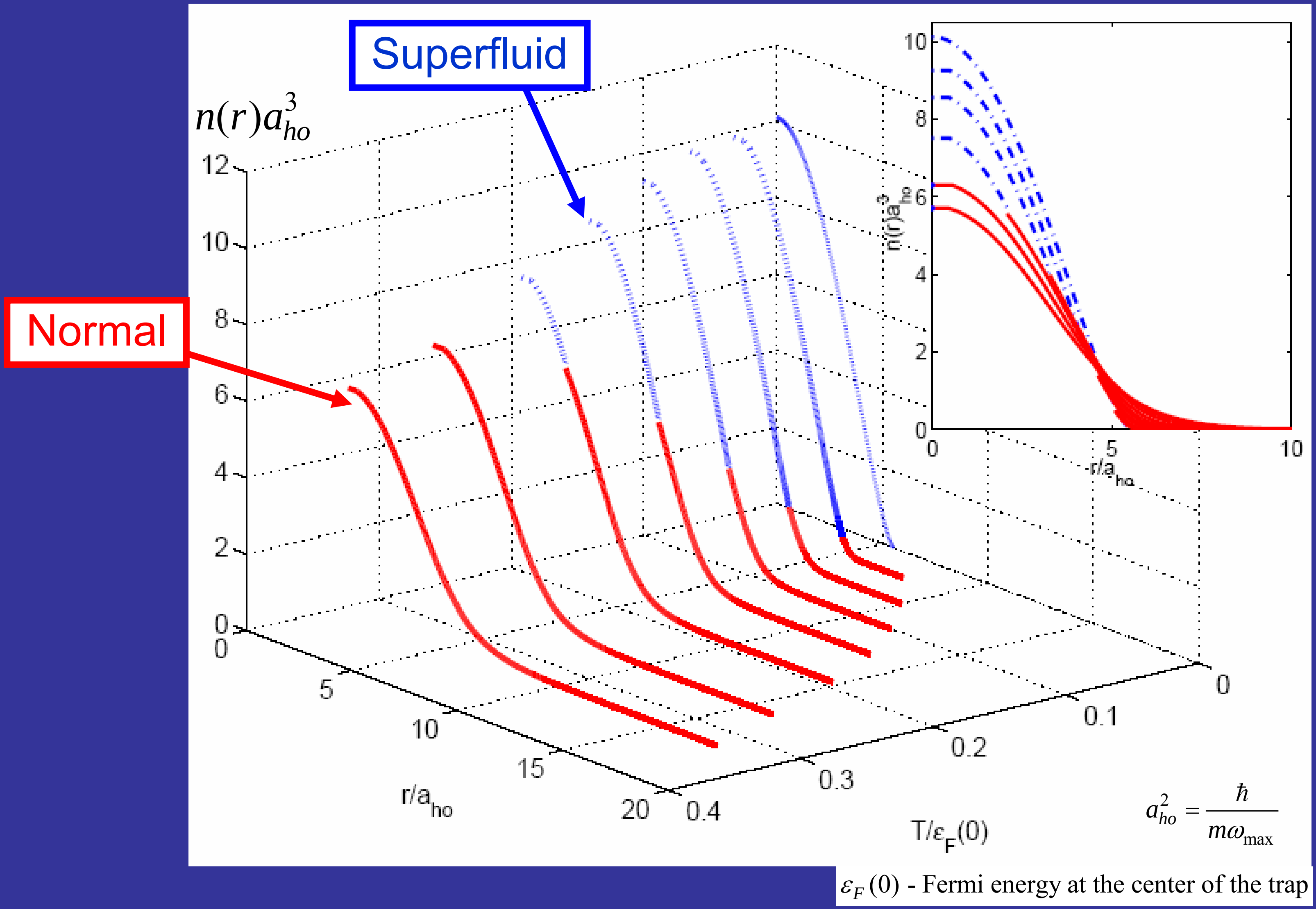
$$\Omega = \int d^3r \left[\frac{3}{5}\varepsilon_F(\vec{r})\varphi(x(\vec{r})) + U(\vec{r}) - \lambda\right] n(\vec{r})$$

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

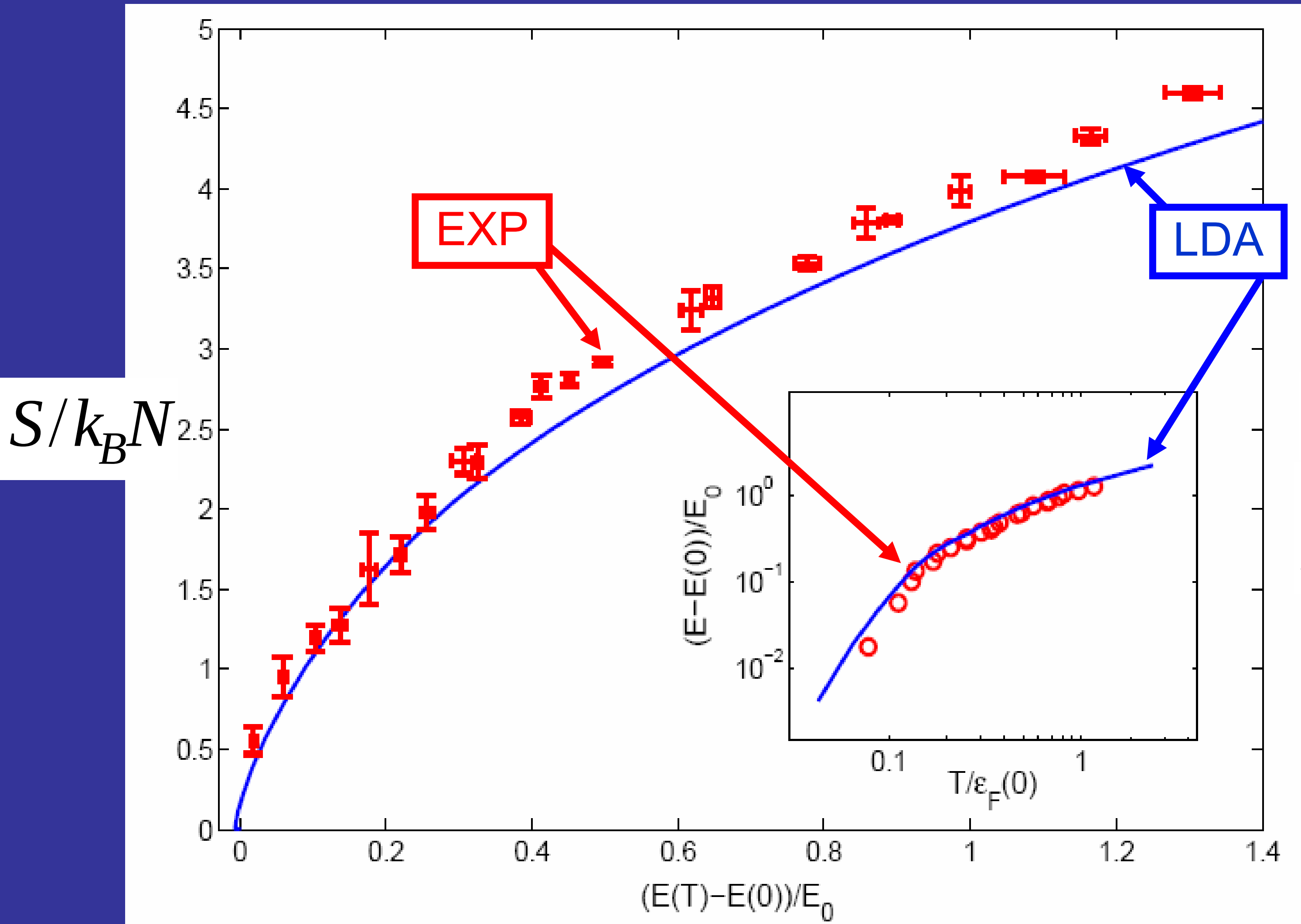
The overall chemical potential λ and the temperature T are constant throughout the system. The density profile will depend on the shape of the trap as dictated by:

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

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.



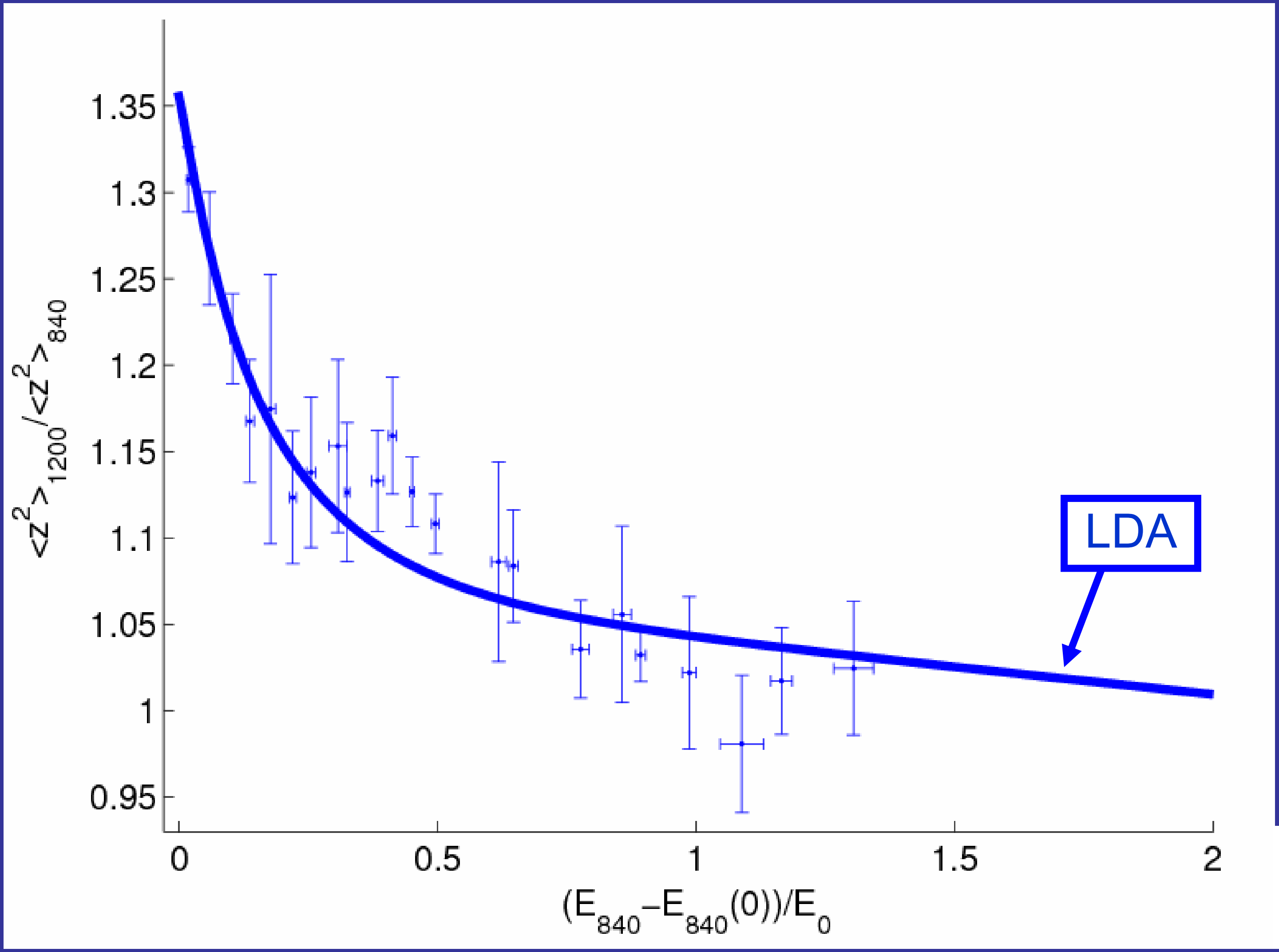
The radial (along shortest axis) density profiles of the atomic cloud in the Duke group experiment at various temperatures.



$$E_0 = N\varepsilon_F^{ho}$$

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

Entropy as a function of energy (relative to the ground state) for the unitary Fermi gas in the harmonic trap. Inset: log-log plot of energy as a function of temperature.



$$E_0 = N\varepsilon_F^{ho}$$

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.

$$B = 1200G \Rightarrow 1/k_F a \approx -0.75 \qquad B = 840G \Rightarrow 1/k_F a \approx 0$$

Summary

We presented the first model-independent comparison of recent measurements of the entropy and the critical temperature, performed by the Duke group: L.Luo, et al. Phys. Rev. Lett. 98, 080402, (2007), with our recent finite temperature Monte Carlo calculations.

EXP.

$$\begin{cases} E(T_c) - E(0) \approx 0.41(5) N\varepsilon_F^{ho}, \\ S_c / N \approx 2.7(2) k_B, \\ T_c \approx 0.29(3)\varepsilon_F^{ho} \end{cases}$$

THEORY

$$\begin{cases} E(T_c) - E(0) \approx 0.34(2) N\varepsilon_F^{ho}, \\ S_c / N \approx 2.4(3) k_B, \\ T_c \approx 0.27(3)\varepsilon_F^{ho} \end{cases}$$

A.Bulgac, J.E. Drut, P. Magierski, cond-mat/0701786

The results are consistent with the predicted value of the critical temperature for the uniform unitary Fermi gas: $0.23(2)\varepsilon_F$