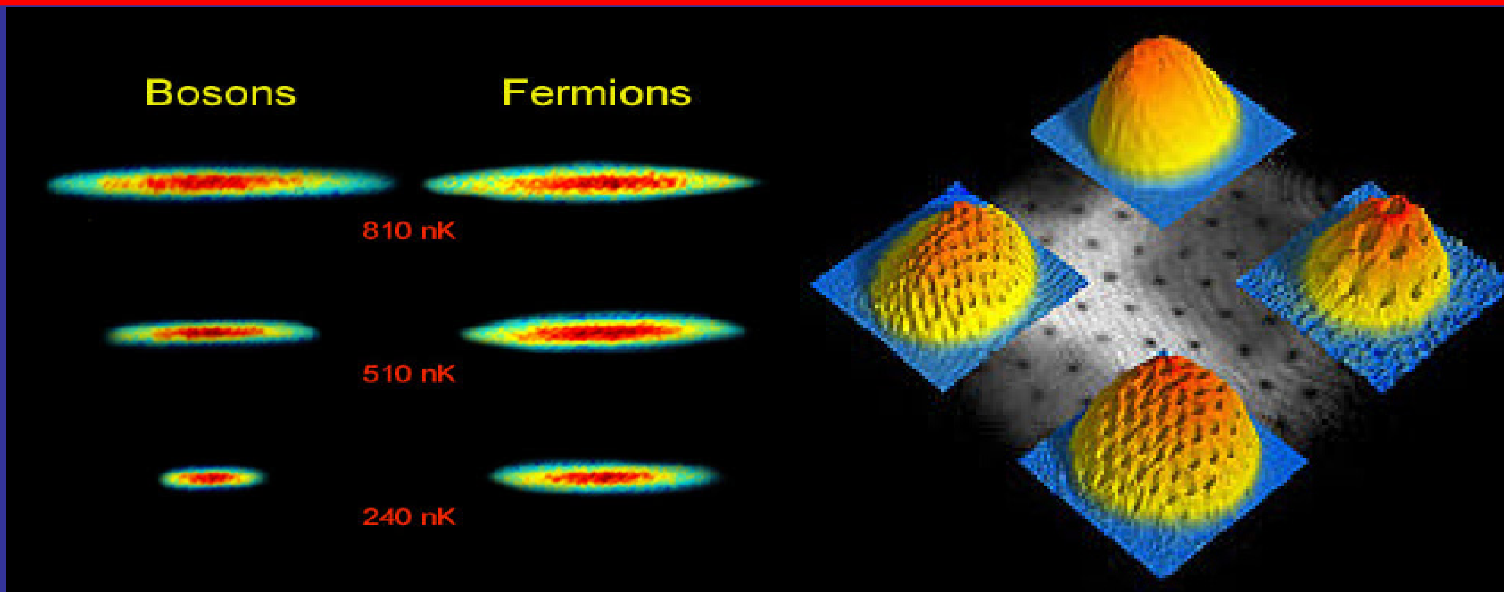
BCS-BEC crossover at finite temperature – Quantum Monte Carlo study



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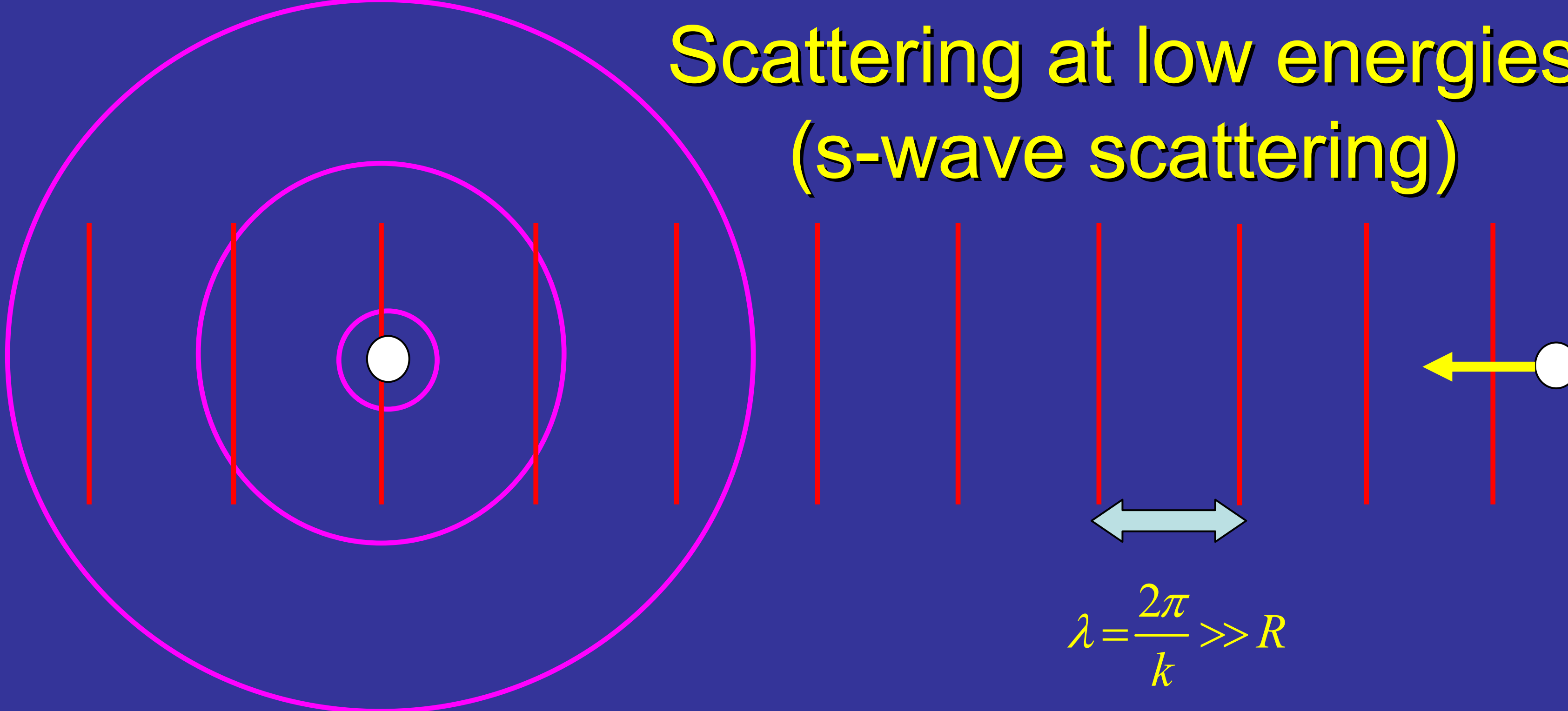
XXIV Max Born Symposium
Quantum Statistical Mechanics and Field Theory
25 - 27 September 2008

Scattering at low energies (s-wave scattering)



$$\lambda = \frac{2\pi}{k} >> R$$

R - radius of the interaction potential

$$\boxed{\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + f\frac{e^{ikr}}{r}; \quad f \text{ - scattering amplitude}}$$

$$f = \frac{1}{-ik - 1/a + \frac{1}{2} r_0 k^2}, \quad a \text{ - scattering length, } r_0 \text{ - effective range}$$

If $k \to 0$ then the interaction is determined by the scattering length alone.

$$E/E_{FG} = 1 + \frac{10}{9\pi}(k_F a)\left[1 + \frac{6}{35\pi}(k_F a)(11 - 2\ln 2) + \ldots\right] + \text{pairing}$$

Perturbation series

$$E_{FG} = \frac{3}{5}\varepsilon_F N$$ - Energy of the noninteracting Fermi gas

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.

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

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

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

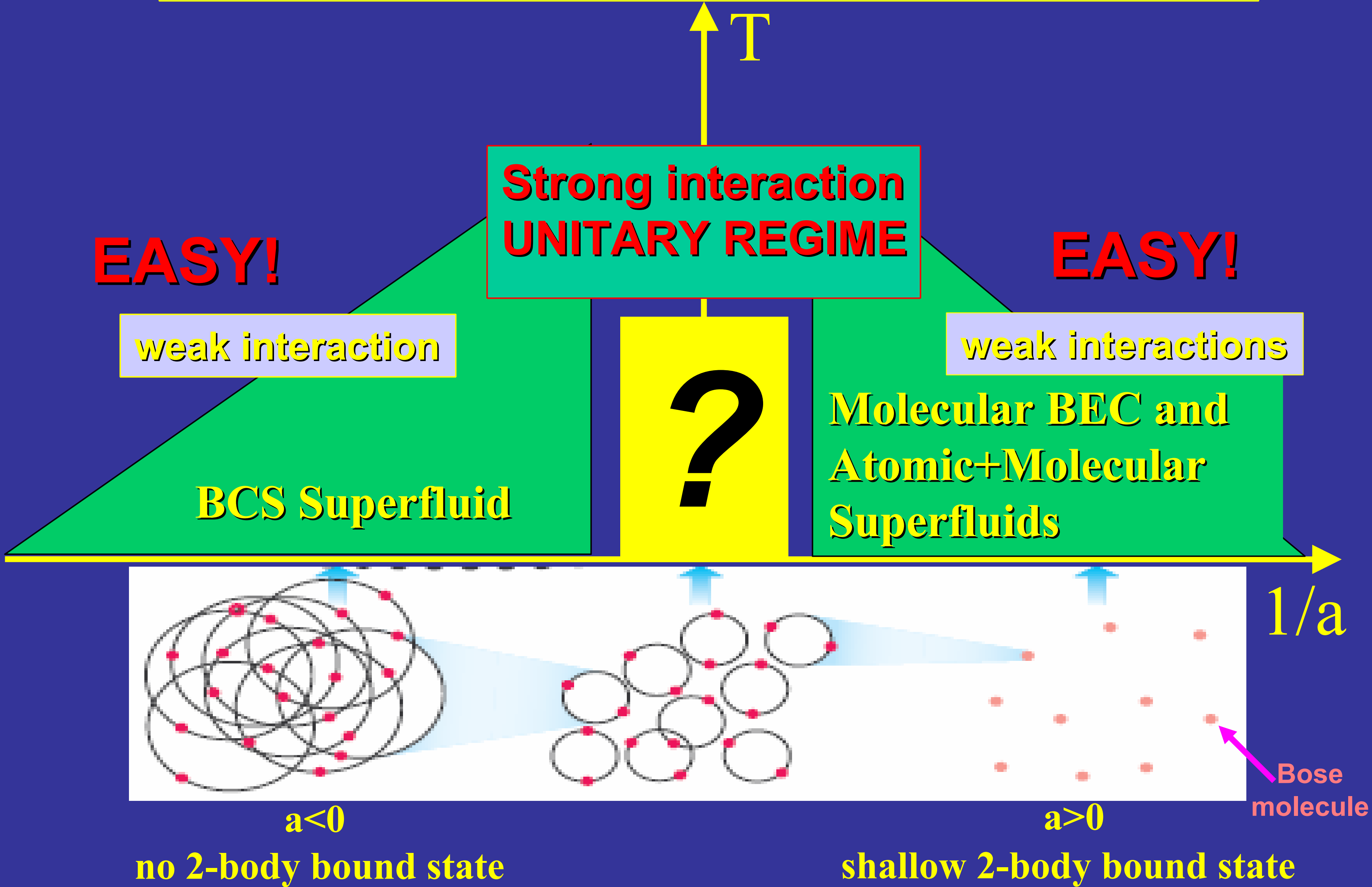
NONPERTURBATIVE REGIME

System is dilute but strongly interacting!

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

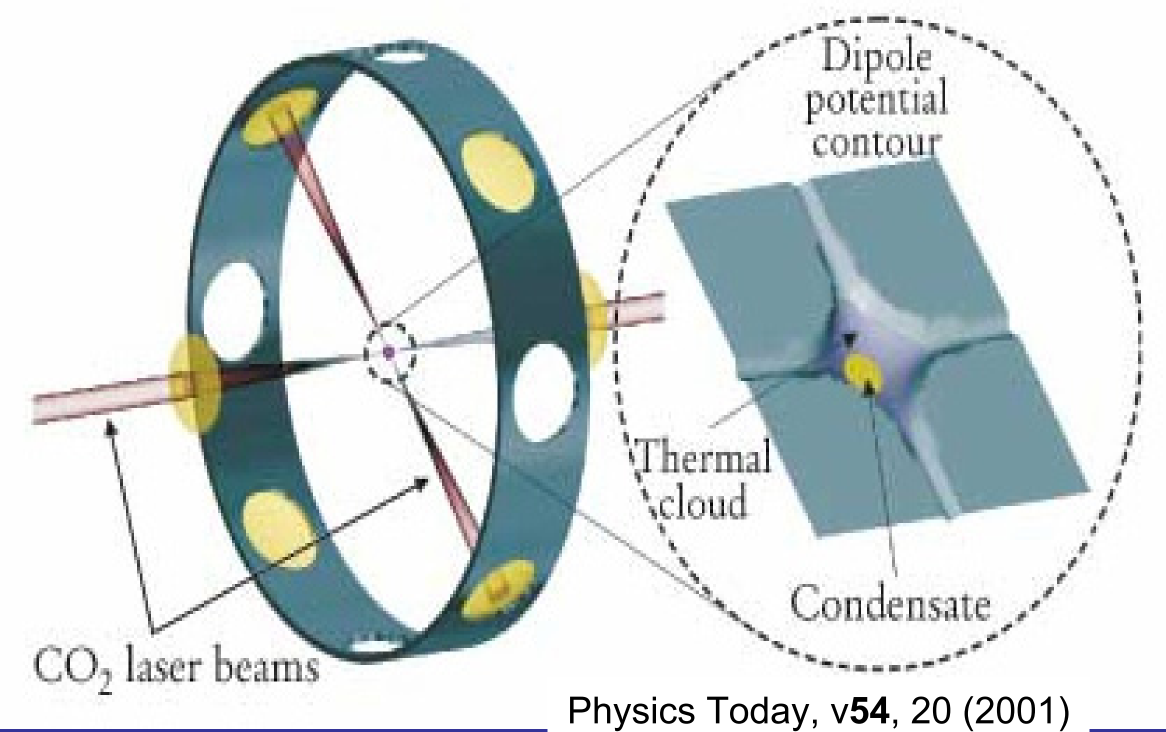
AT FINITE TEMPERATURE: $$\boxed{E(T) = \xi\left(\frac{T}{\varepsilon_F}\right) E_{FG},\quad \xi(0) = \xi_0}$$

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!**

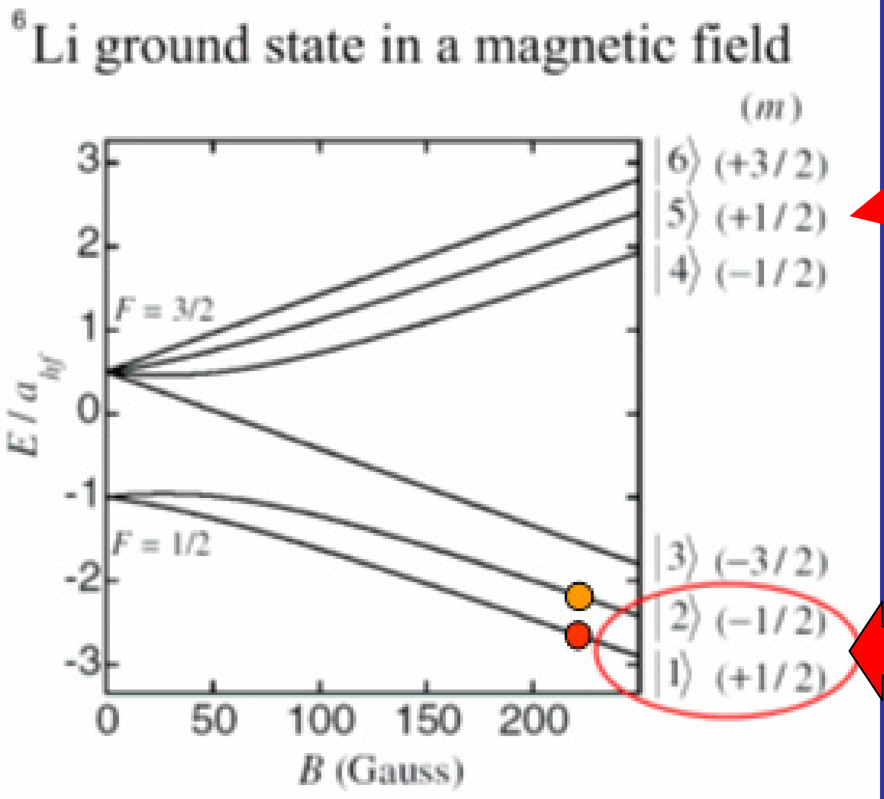


Physics Today, v**54**, 20 (2001)

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**

One fermionic atom in magnetic field



$$\left| F\, m_F \right\rangle$$

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

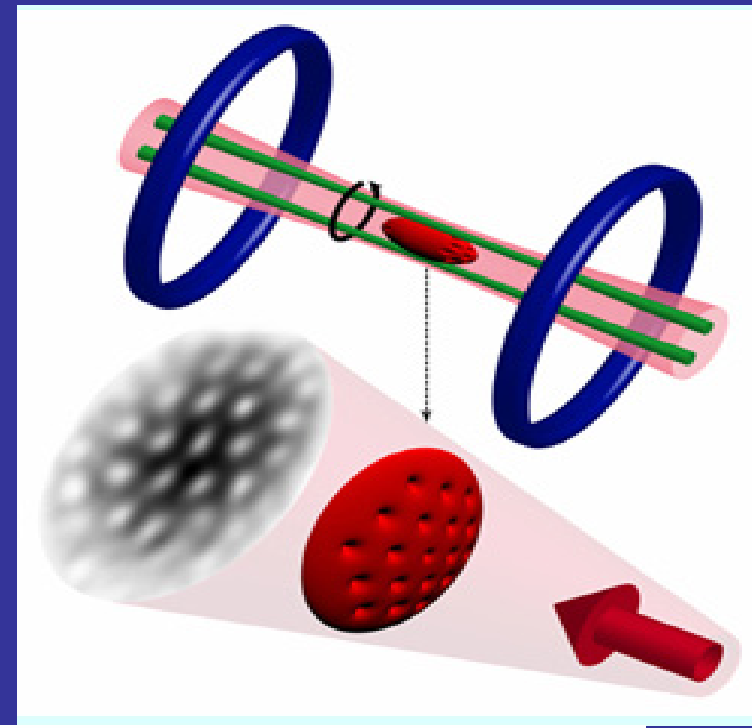
Nuclear spin   Electronic spin

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.
- Atoms in different hyperfine states experience interactions only in s-wave.

Evidence for fermionic superfluidity: vortices!

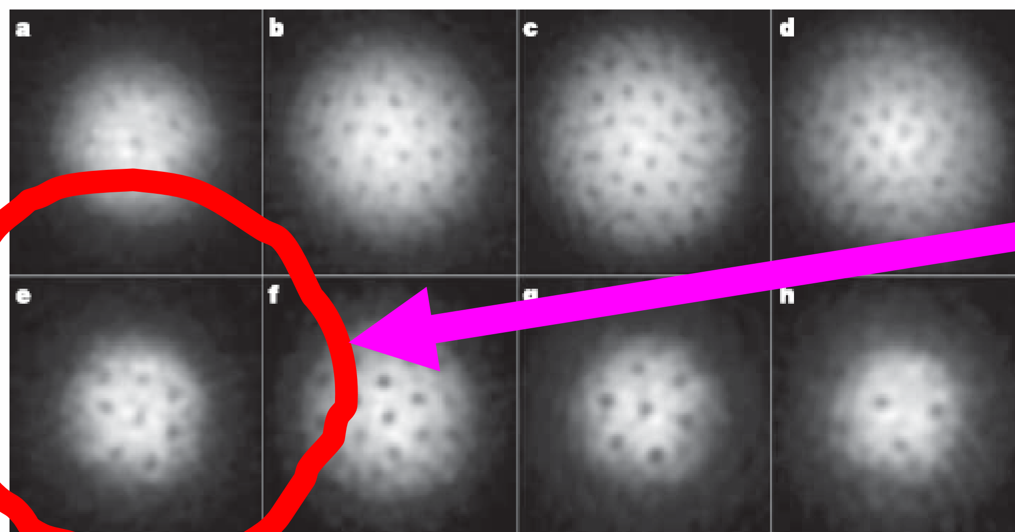


system of fermionic ^{6}Li atoms

Feshbach resonance: B=834G

BEC side: a>0

BCS side: a<0

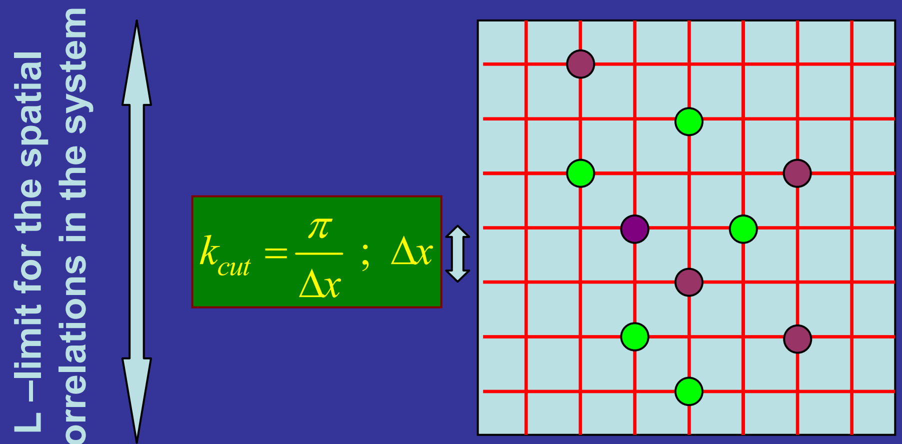


UNITARY REGIME

M.W. Zwierlein *et al*., Nature, 435, 1047 (2005)

Figure 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**) or 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 740 G (**a**), 766 G (**b**), 792 G (**c**), 812 G (**d**), 833 G (**e**), 843 G (**f**), 853 G (**g**) and 863 G (**h**). The field of view of each image is 880 μm × 880 μm.

Coordinate space



$Volume = L^3$

$lattice\ spacing = \Delta x$

- Spin up fermion

- Spin down fermion

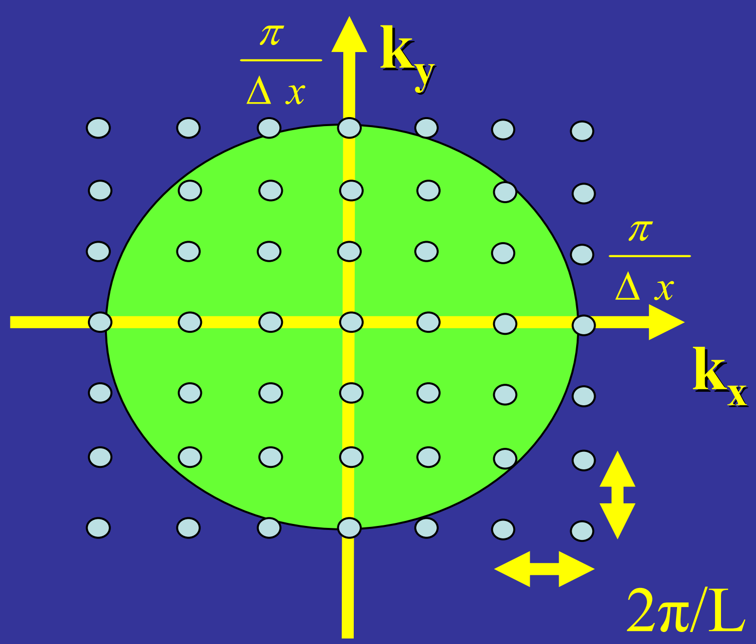
Periodic boundary conditions imposed

External conditions:

T - temperature

μ - chemical potential

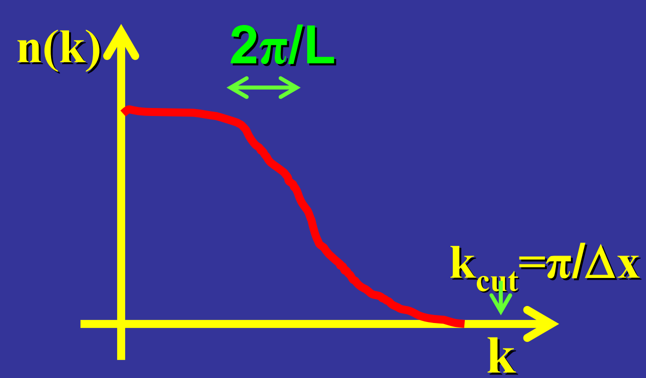
Momentum space



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

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

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



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

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

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

Running coupling constant g defined by lattice

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

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 for unpolarized system!

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

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: $\underline{8^3 \times 300}$ (high Ts) to $\underline{8^3 \times 1800}$ (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 .

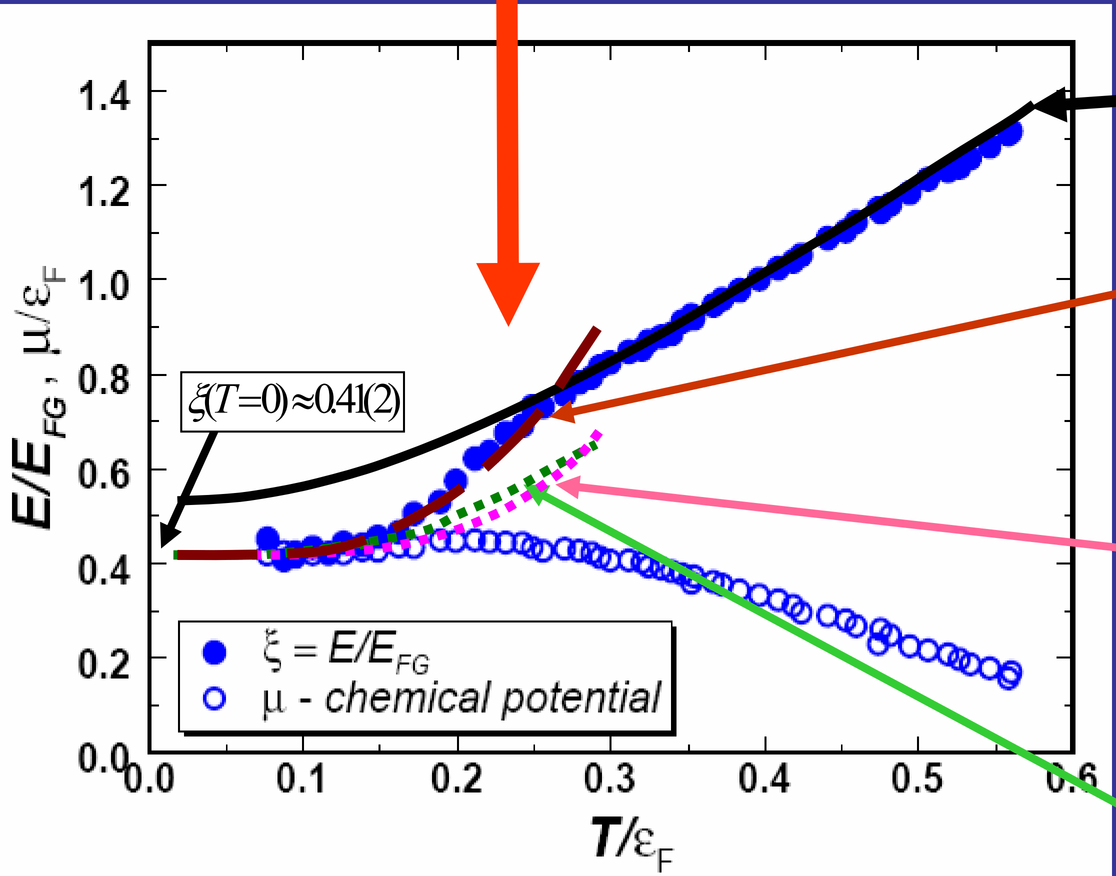
- Thermalize for 50,000 – 100,000 MC steps or/and use as a start-up field configuration a $\sigma(x,\tau)$-field configuration from a different T

- 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 = ±∞   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)

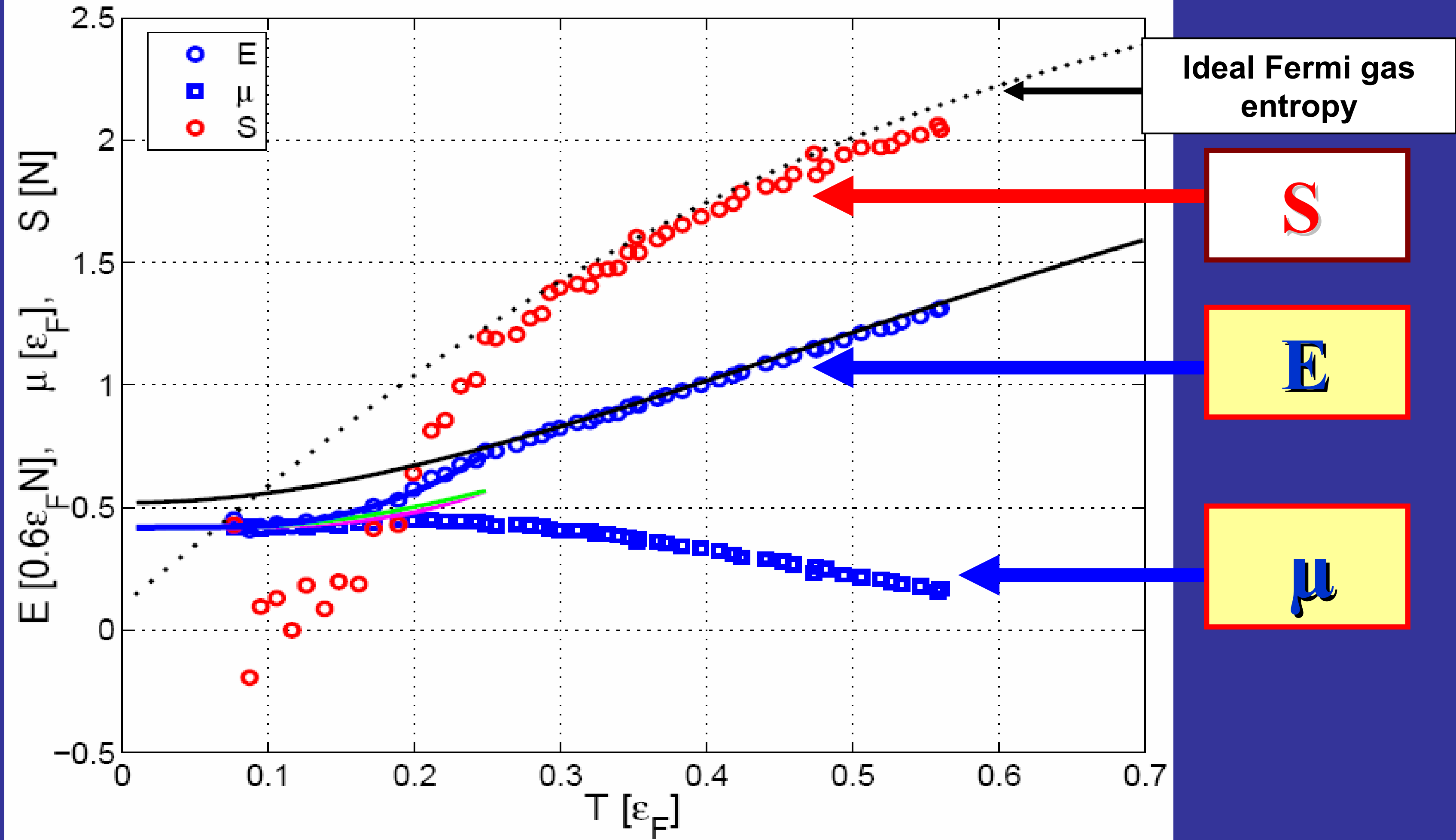
Quasi-particle contribution only
(dotted line)

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

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

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

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



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

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

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

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

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

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

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≥3 or n≤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.

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?

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

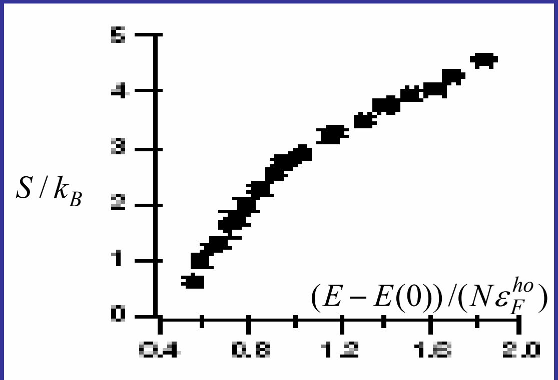
$n(\vec{r})$ - local density

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:

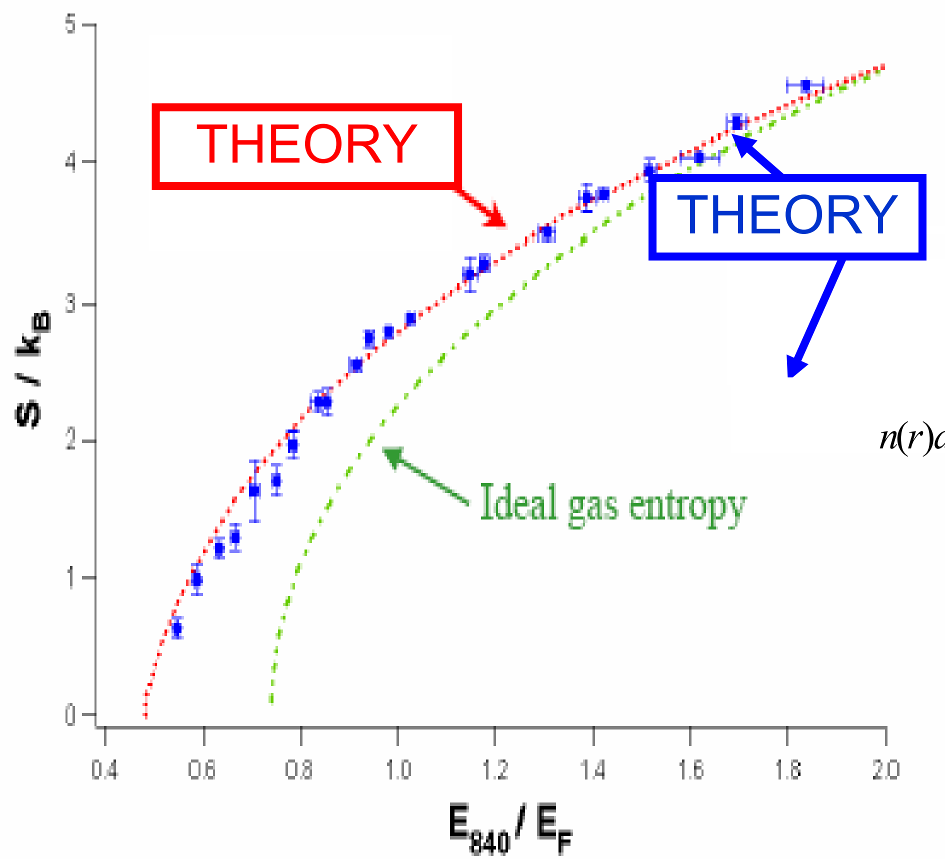
$$\frac{\delta\Omega}{\delta n(\vec{r})} = \frac{\delta(F - \lambda N)}{\delta n(\vec{r})} = \mu(x(\vec{r})) + U(r) - \lambda = 0$$

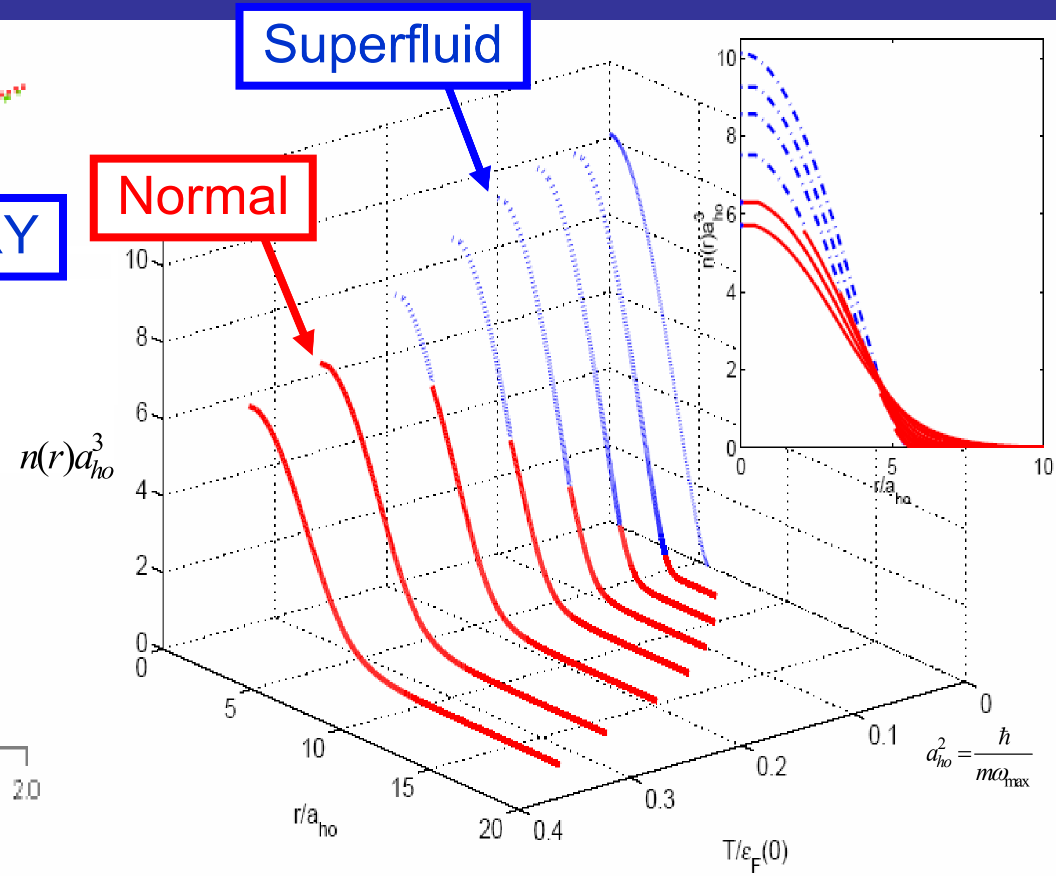
Using as an input the Monte Carlo results for the uniform system and experimental data (trapping potential, number of particles), we determine the density profiles.

Comparison with experiment

John Thomas' group at Duke University,

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



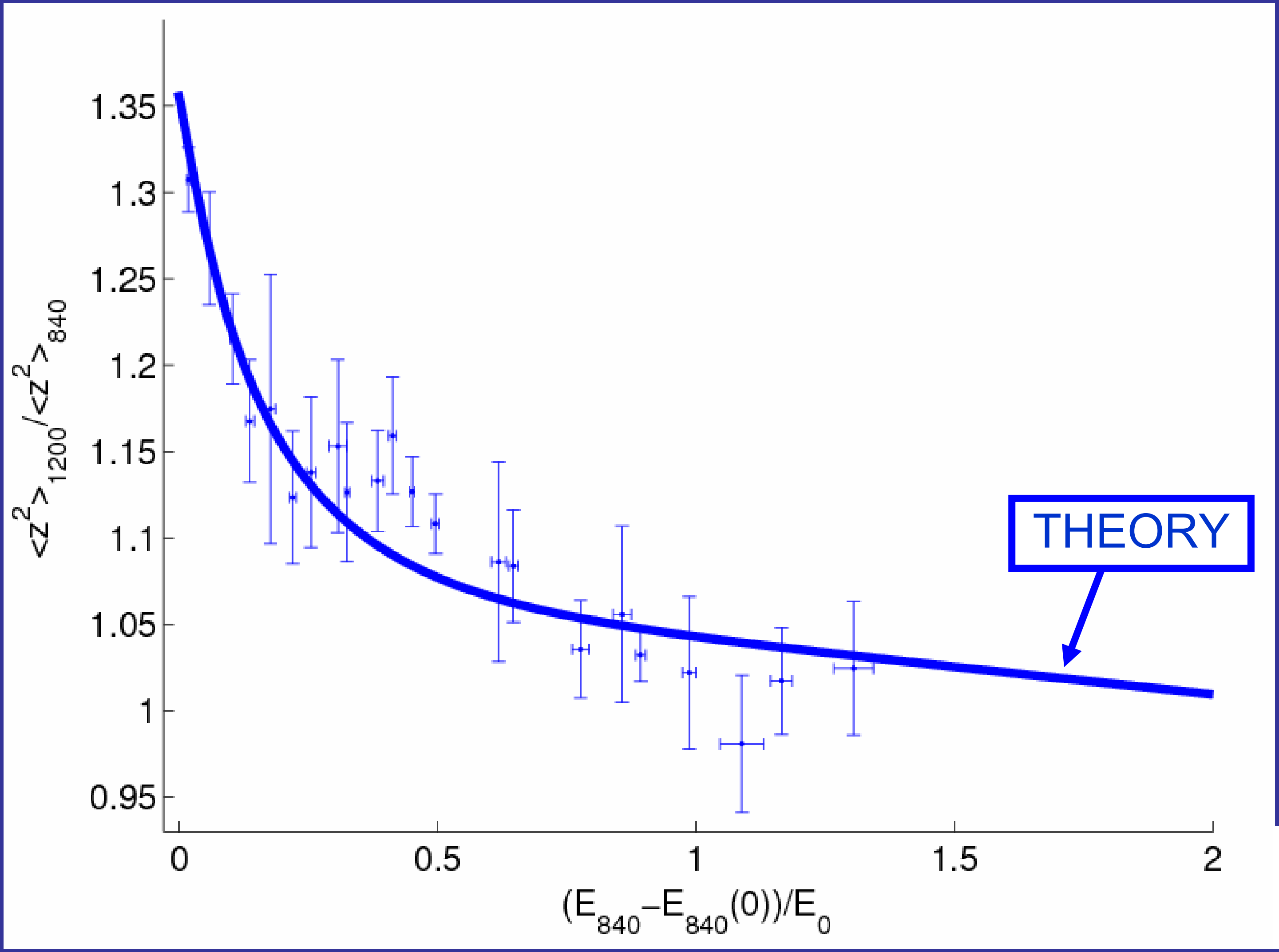


$\varepsilon_F(0)$ - Fermi energy at the center of the trap

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

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

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



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

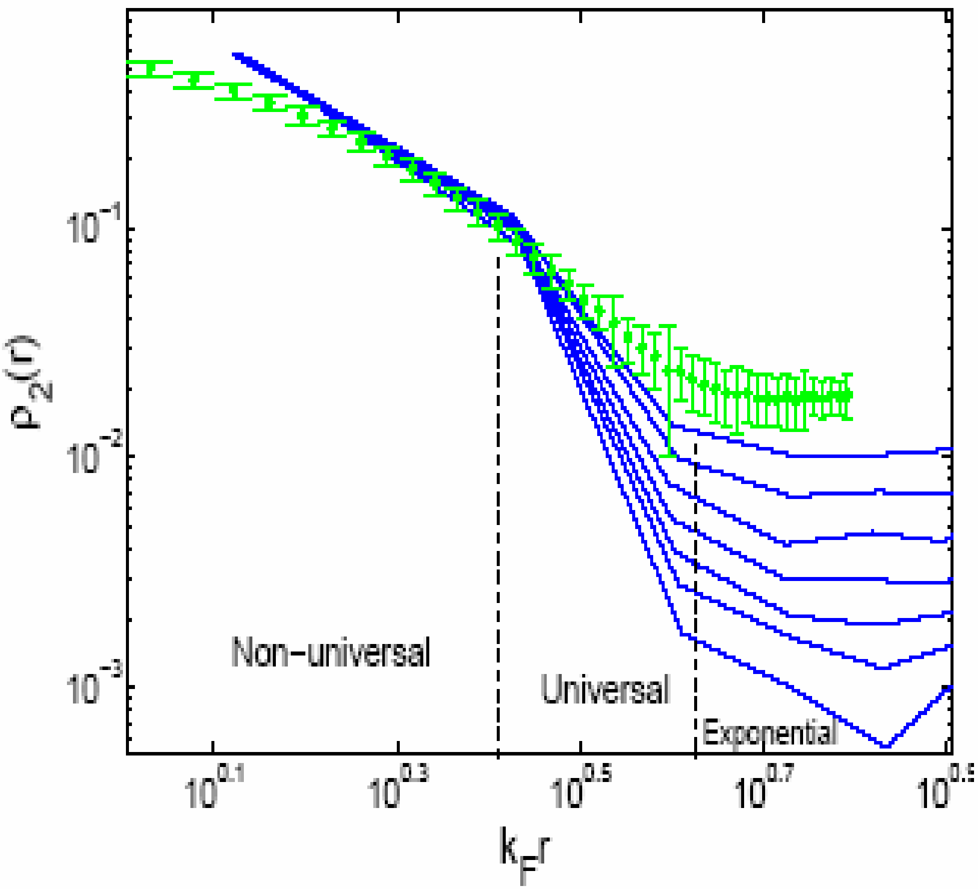
Ratio of the mean square cloud size at B=1200G to its value at unitarity (B=840G) as a function of the energy. Experimental data are denoted by point with error bars.

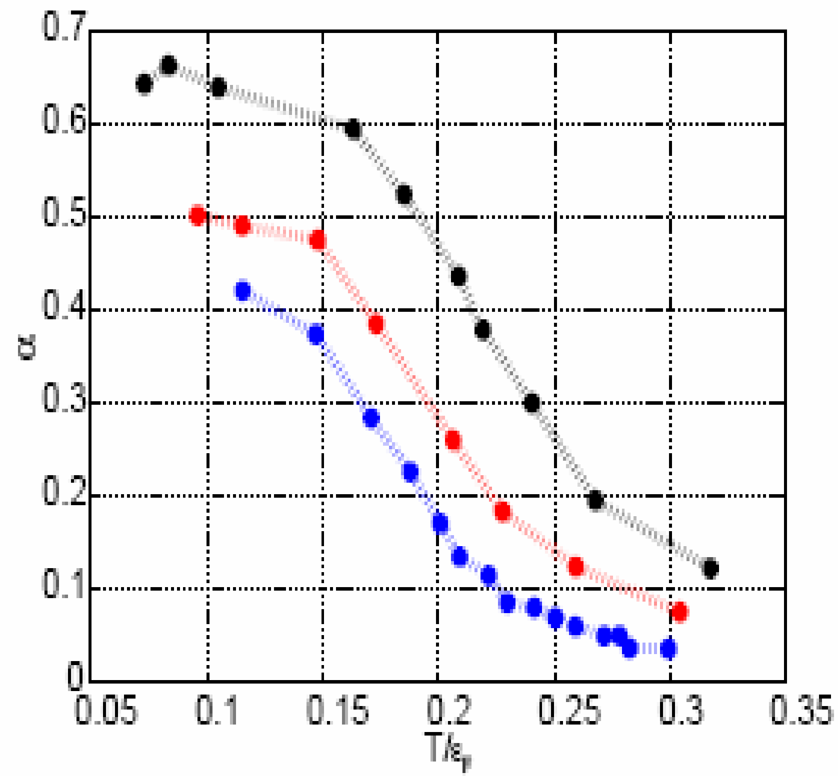
$$B = 1200G \Rightarrow 1/k_F a \approx -0.75 \qquad B = 840G \Rightarrow 1/k_F a \approx 0$$

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

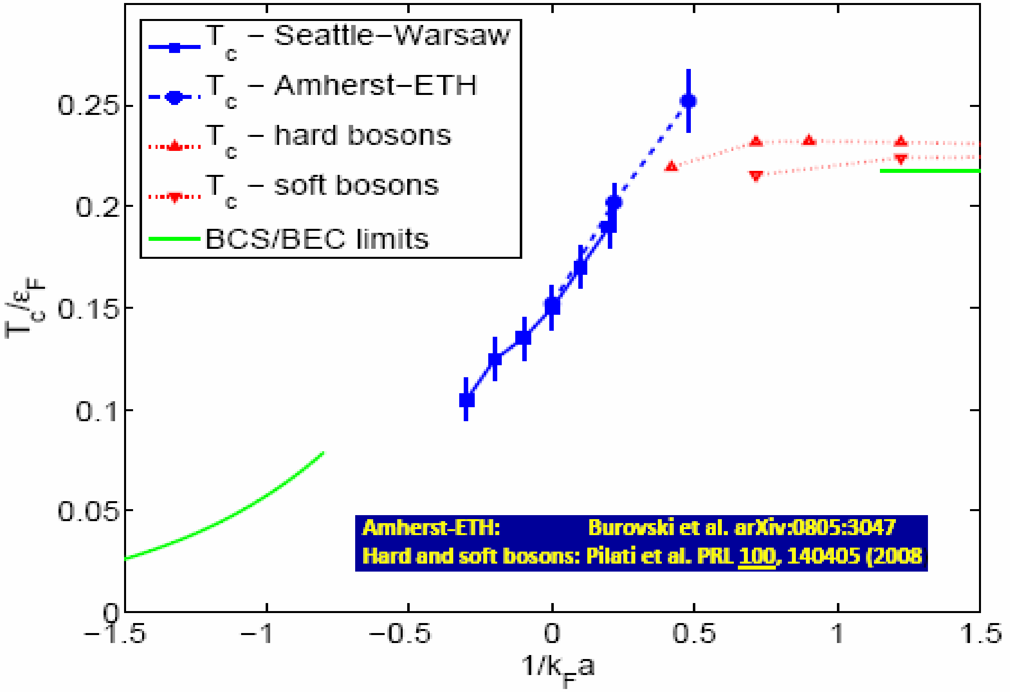
$$\rho_2^{\,P}(\vec{r}) = \frac{2}{N}\int d^3r_1 d^3r_2\, \rho_2(\vec{r}_1+\vec{r},\vec{r}_2+\vec{r},\vec{r}_1,\vec{r}_2)$$

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





Bulgac, Drut, and Magierski, arXiv:0803:3238



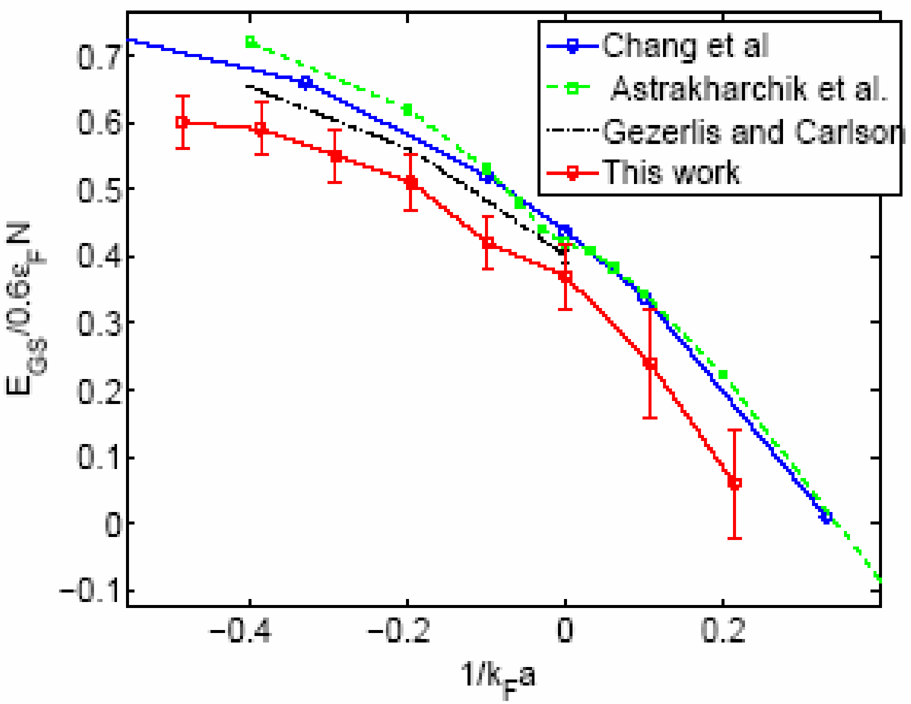
Results off unitary limit:

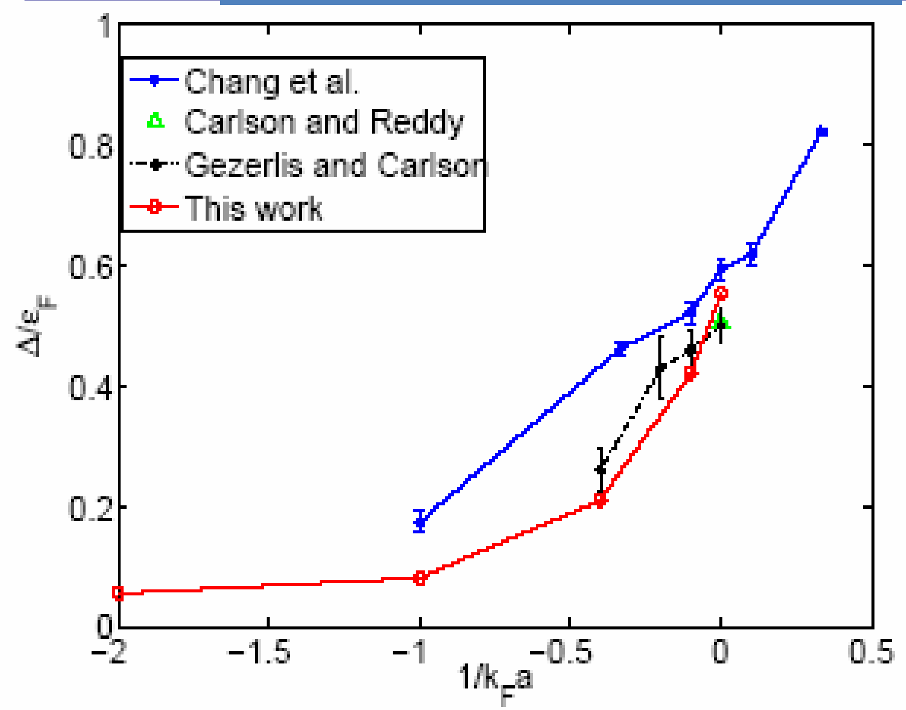
-Critical temperature

-Ground state energy

-Pairing gap

Bulgac, Drut, and Magierski, arXiv:0803:3238



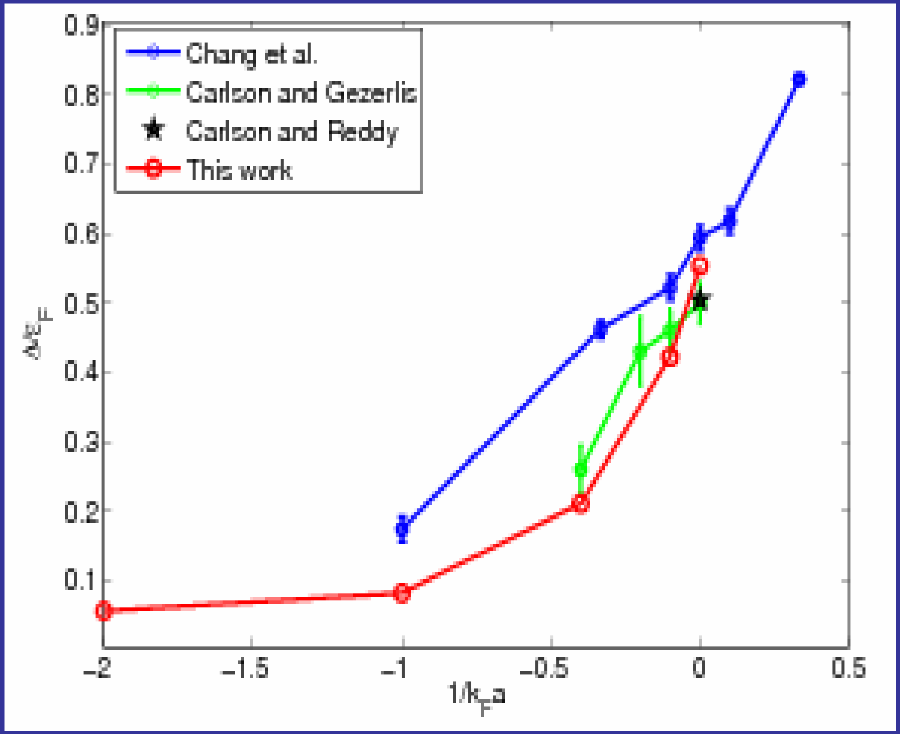


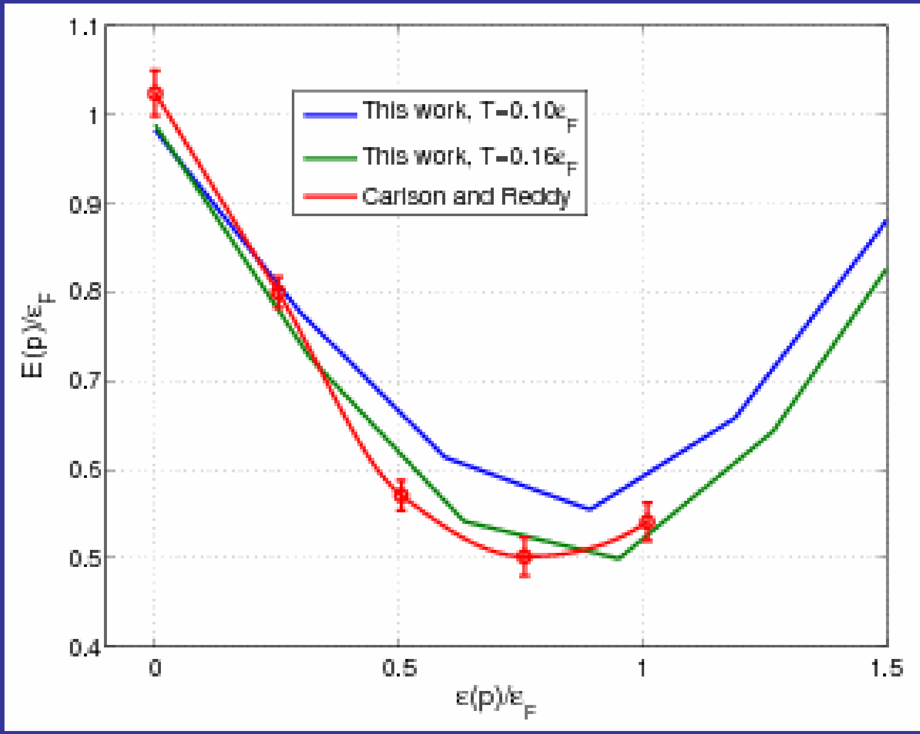
Pairing gap, pseudogap and quasi-particle spectrum

$$\chi(\mathbf{p}) = -\int_0^\beta d\tau \mathcal{G}_\beta(\mathbf{p},\tau)$$

$$\mathcal{G}_\beta(\mathbf{p},\tau) = \frac{\mathrm{Tr}[e^{-(\beta-\tau)(H-\mu N)}\psi_\uparrow(\mathbf{p})e^{-\tau(H-\mu N)}\psi_\uparrow^\dagger(\mathbf{p})]}{Z(\beta,\mu,V)}$$

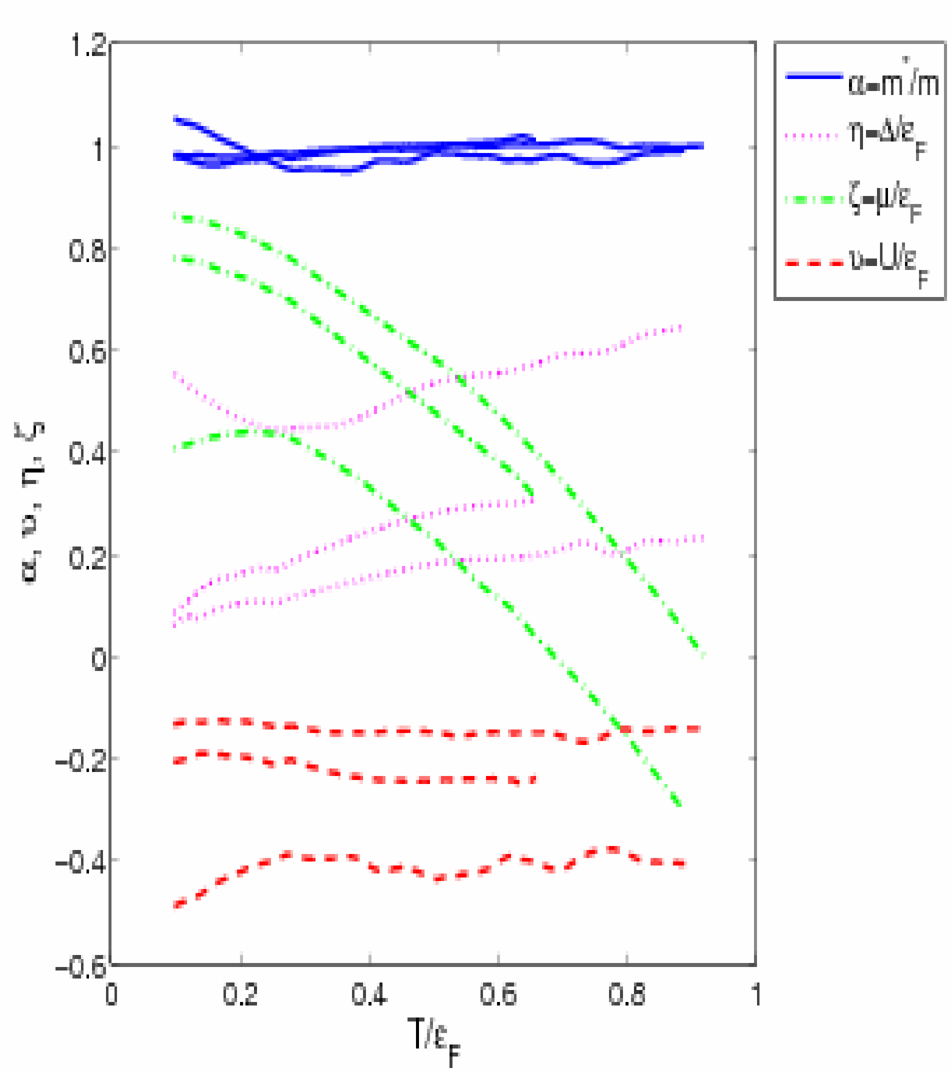
$$\chi(\mathbf{p}) = \frac{1}{E(\mathbf{p})}\frac{e^{\beta E(\mathbf{p})}-1}{e^{\beta E(\mathbf{p})}+1}$$

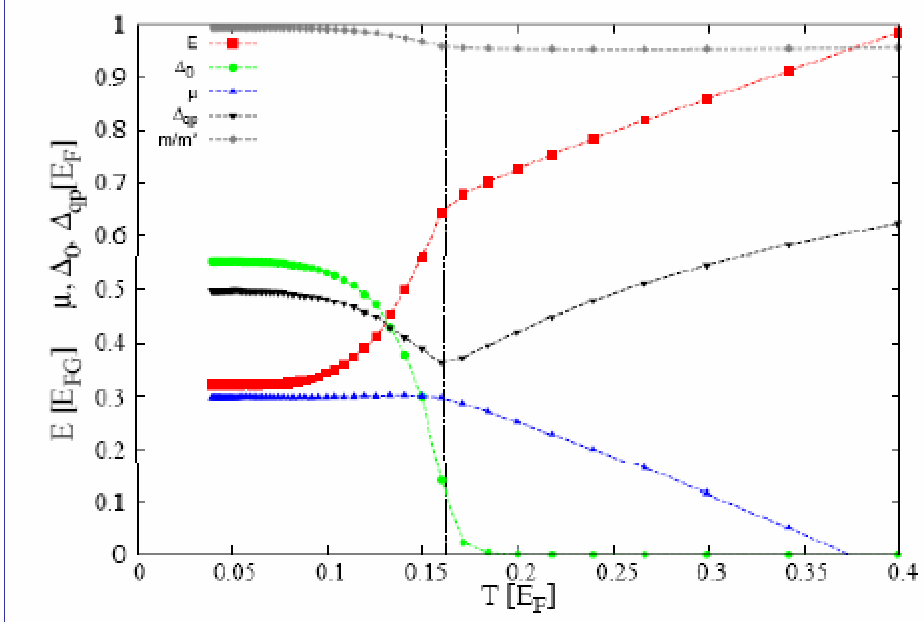


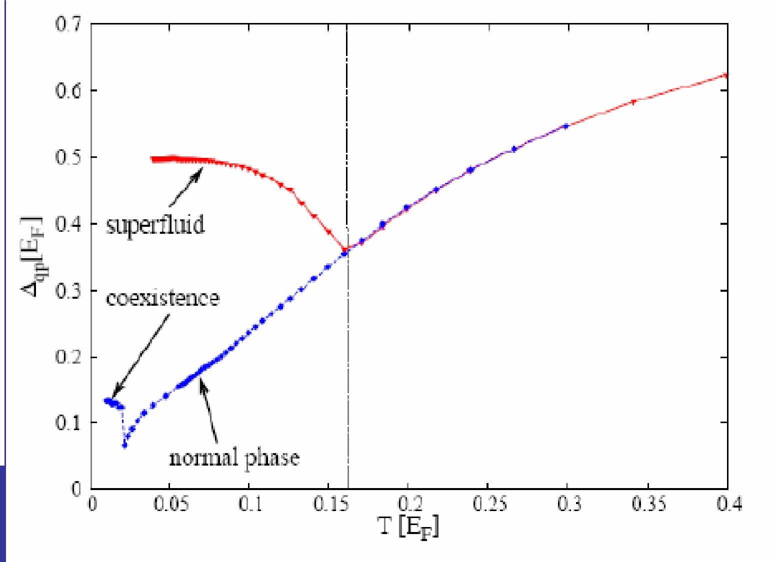


Quantum Monte Carlo

Dynamical Mean Field Theory (exact in infinite number of dimensions)







$$\frac{1}{k_F a} = -2, \; -1, \; 0$$

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

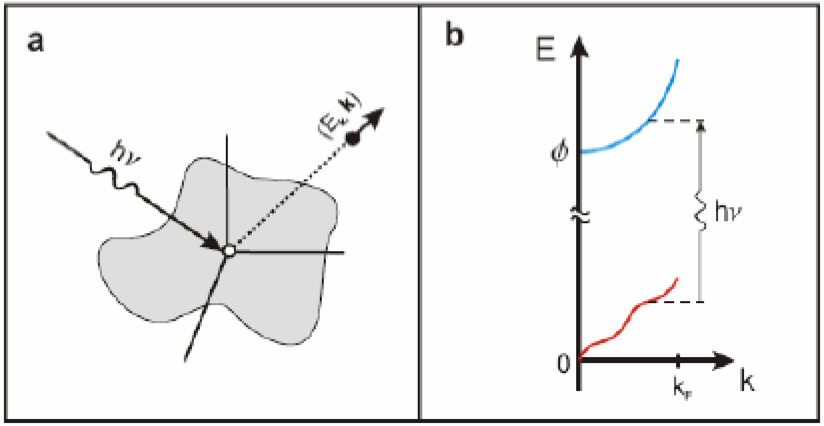
Bulgac, Drut, Magierski, and Wlazowski, arXiv:0801:1504

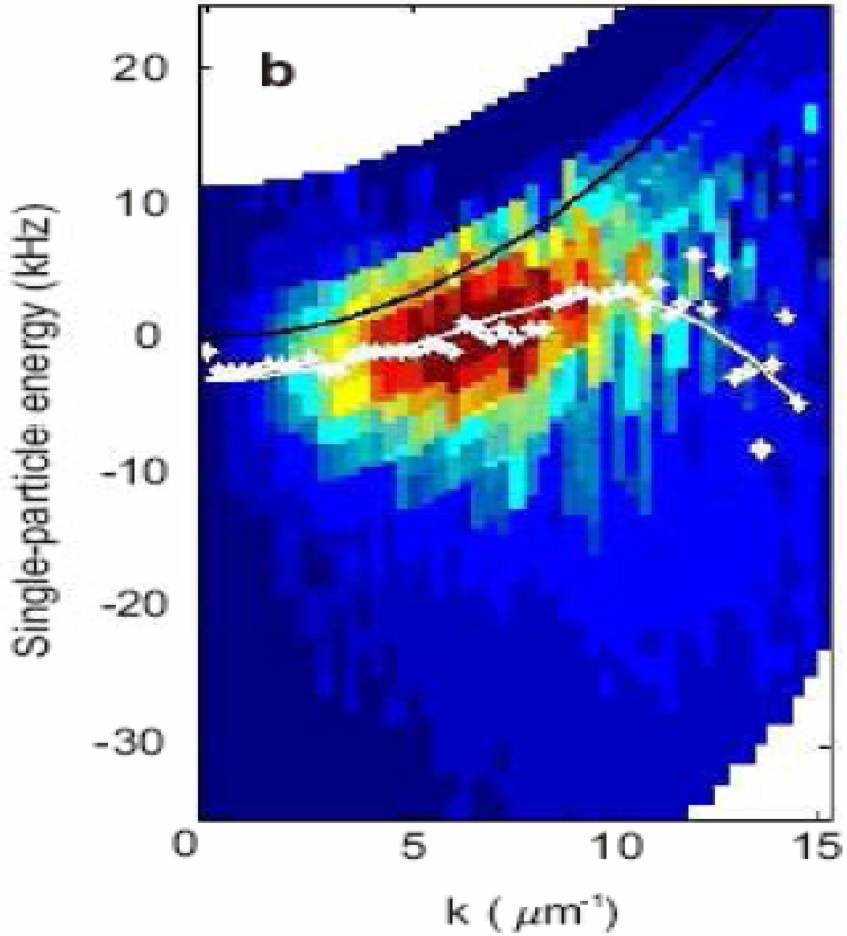
Superfluid to insulator phase transition in a unitary Fermi gas

Barnea, arXiv:0803:2293

Preliminary measurements of pseudogap in ultracold atomic gases

^{40}K at $T=T_c$





$$-E_s + h\nu = \frac{\hbar^2 k^2}{2m} + \phi$$

$$E(N) = E(N-1) + E_s$$

Using photoemission spectroscopy to probe a strongly interacting Fermi gas

Stewart, Gaebler and Jin, arXiv:0805:0026

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 $T_c = 0.15\ (1)\ \varepsilon_F$.

- ✓ Between T_c and $T_0 = 0.23(2)\ \varepsilon_F$ the system is neither superfluid nor follows the normal Fermi gas behavior. Possibly due to pairing effects.

- ✓ Chemical potential is constant up to the T_0 – 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.

- ✓ Results (energy, entropy vs temperature) agree with recent measurments: L. Luo et al., PRL 98, 080402 (2007)

- ✓ There is an evidence for the existence of *pseudogap* at unitarity.

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: $0.23(2)\varepsilon_F$