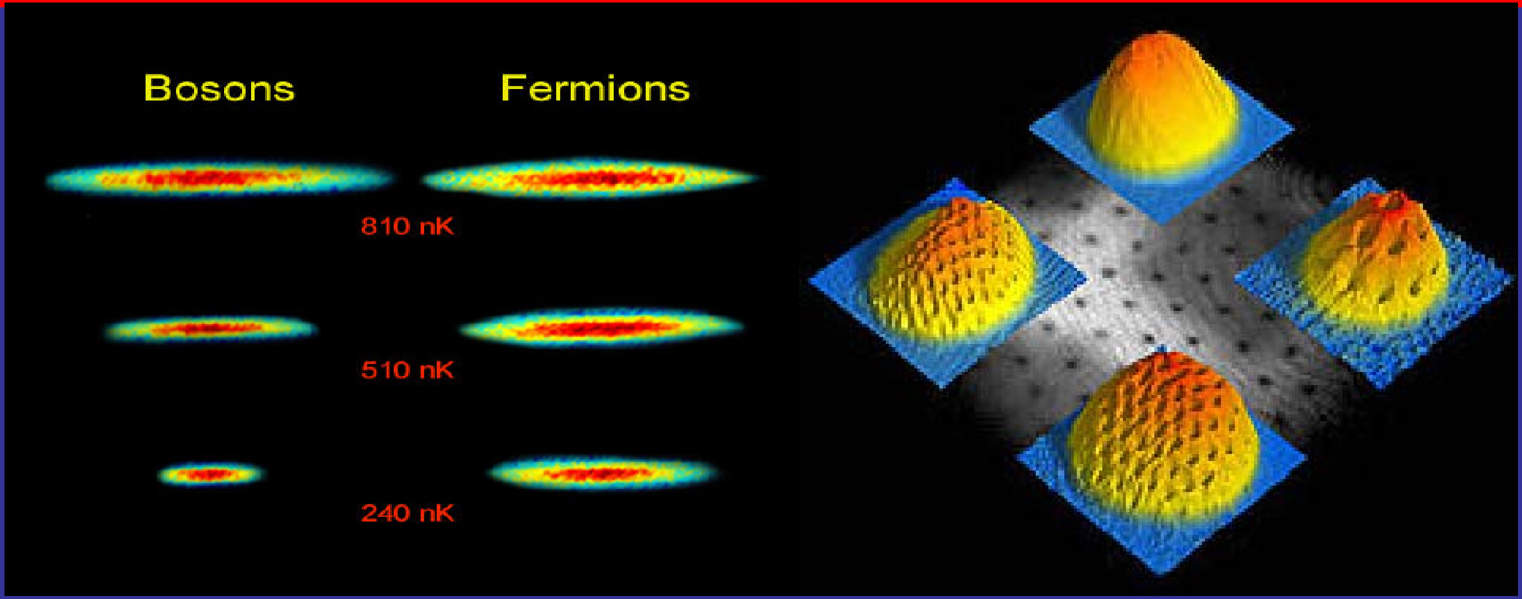
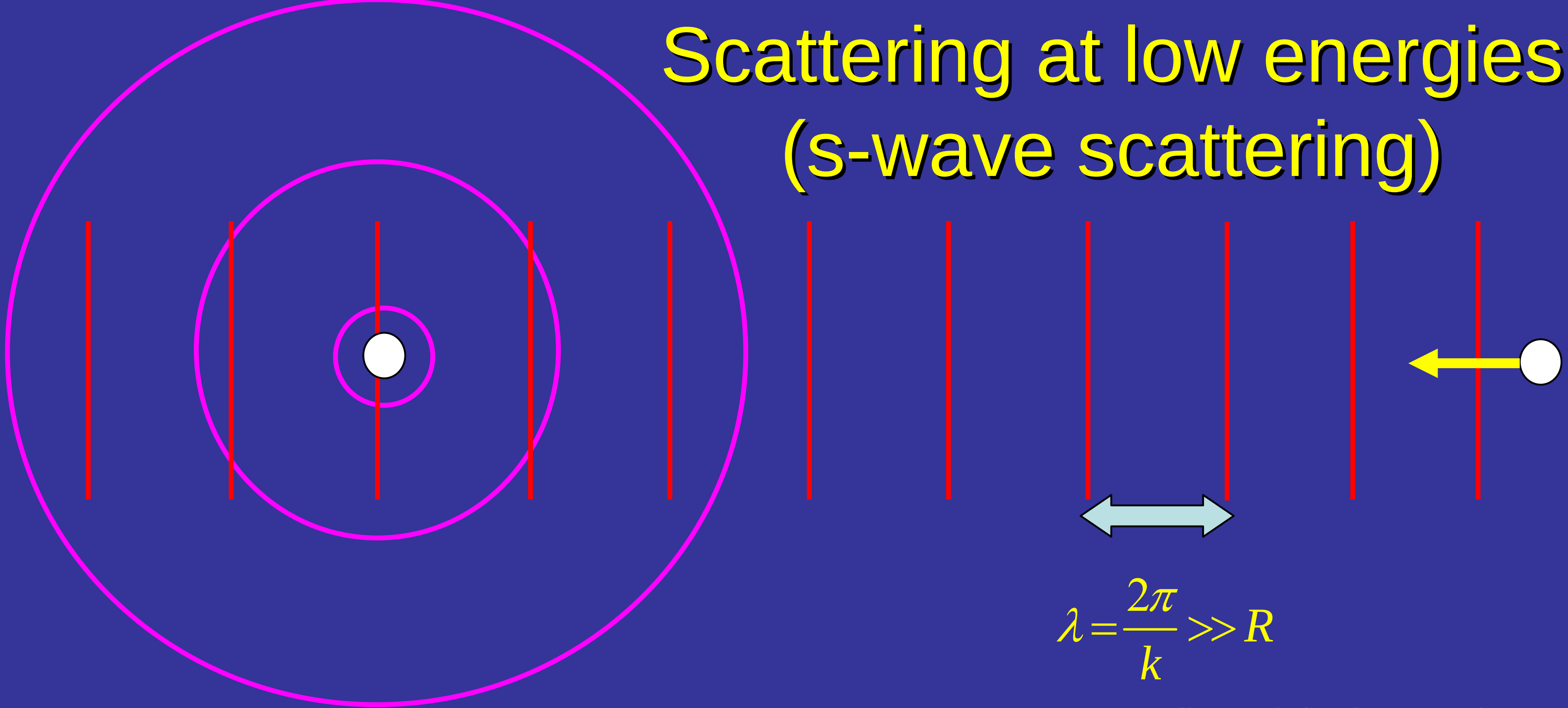
The Properties of the Unitary Fermi Gas at Finite Temperatures – Quantum Monte Carlo approach



Piotr Magierski
Warsaw University of Technology/University of Washington

<u>Collaborators:</u> Aurel Bulgac – University of Washington (Seattle),
Joaquin E. Drut – Ohio State University (Columbus),
Gabriel Wlazłowski (PhD student) – Warsaw University of Technology

Scattering at low energies (s-wave scattering)



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

R - radius of the interaction potential

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

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

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

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

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

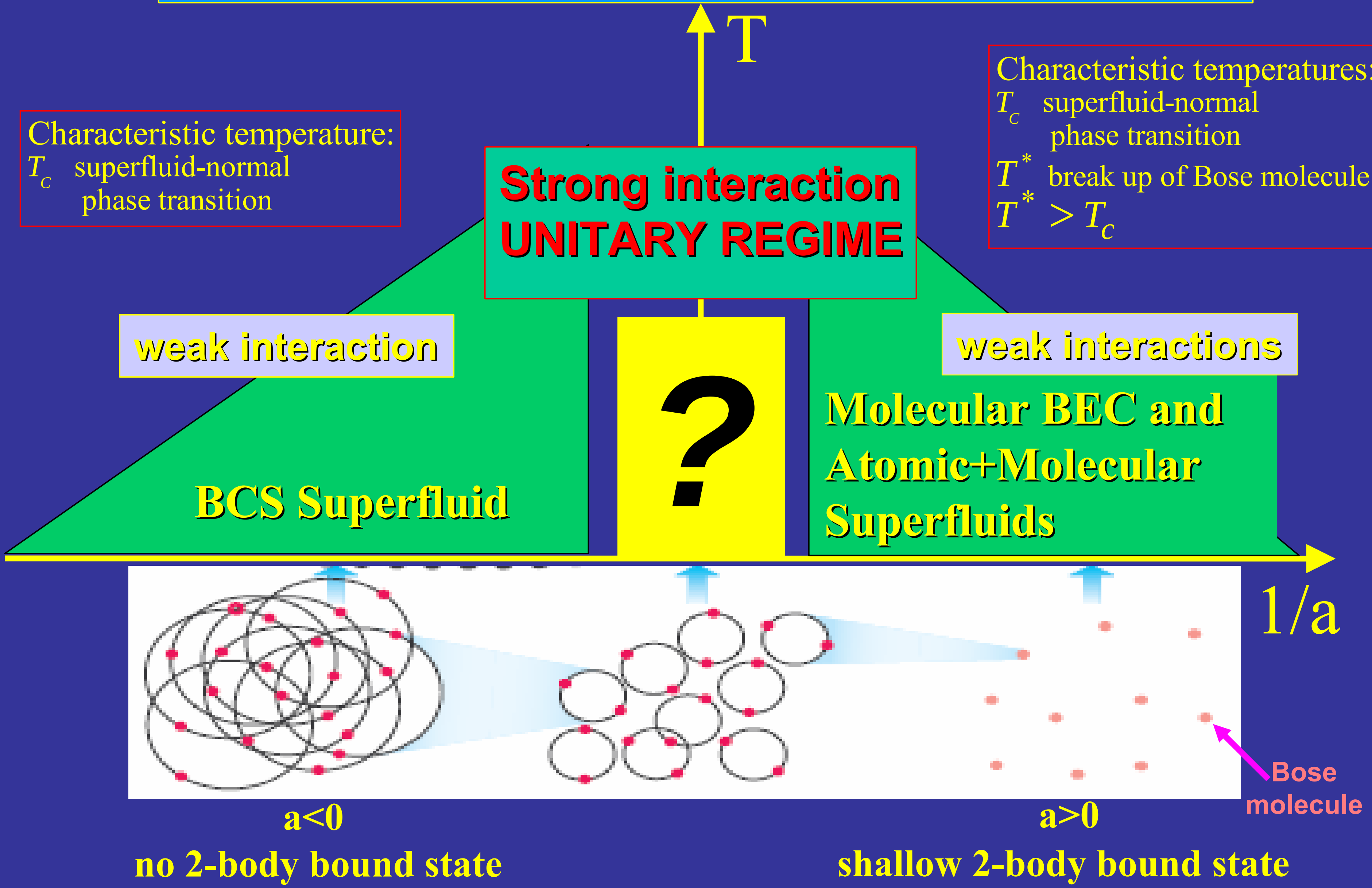
NONPERTURBATIVE REGIME

System is dilute but strongly interacting!

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

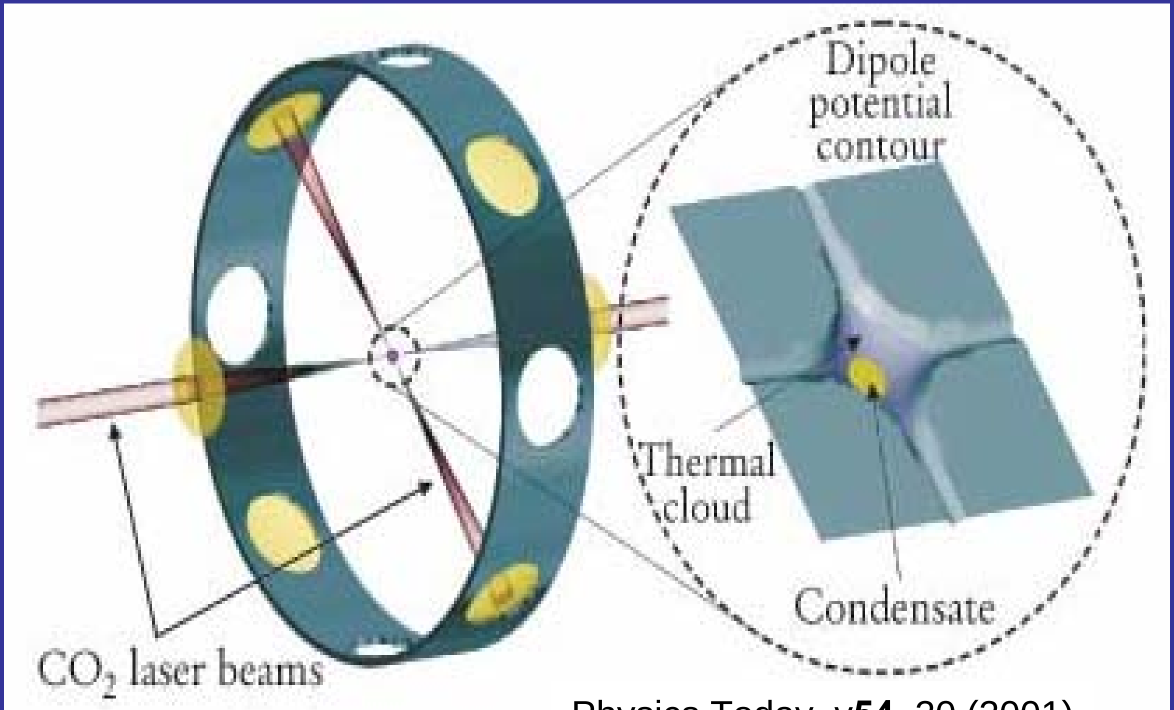
AT FINITE TEMPERATURE: $$E(T) = \xi\left(\frac{T}{\varepsilon_F}\right) E_{FG}, \quad \xi(0) = \xi_0$$

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!**

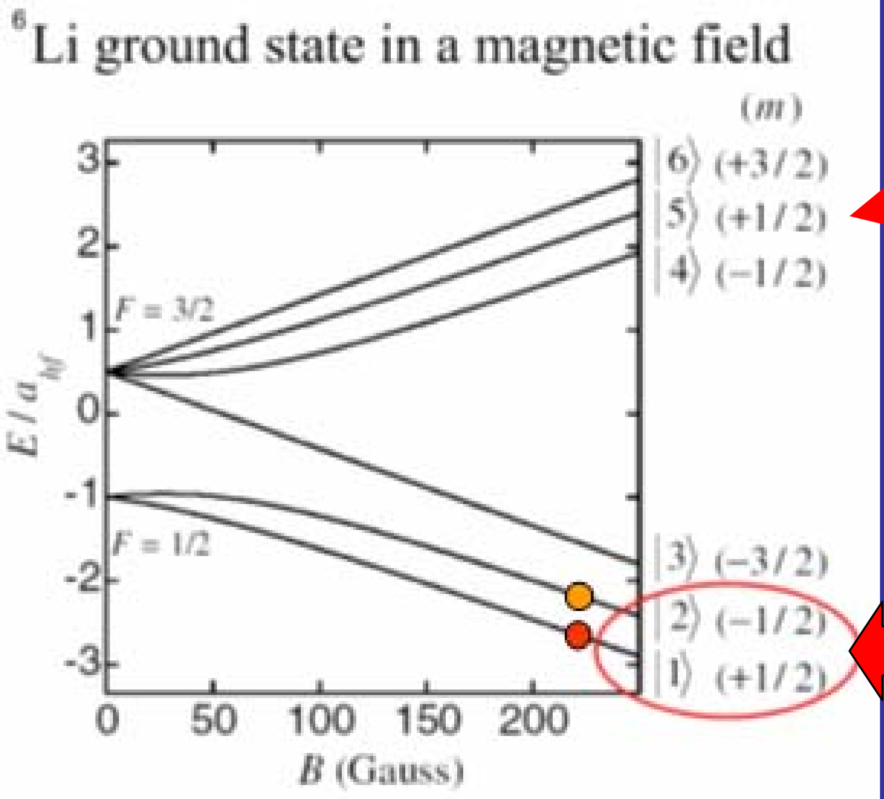


Physics Today, v**54**, 20 (2001)

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

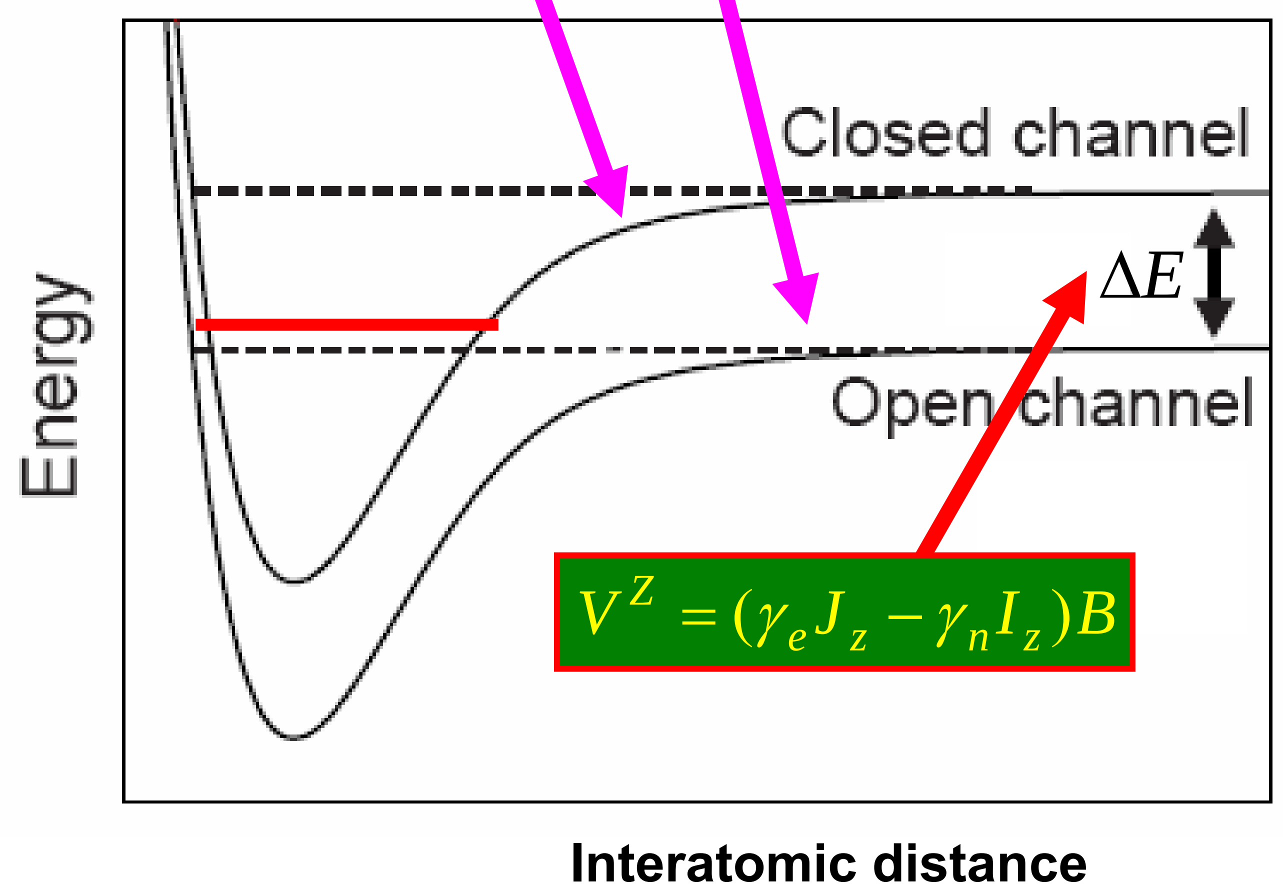
Effective Hamiltonian of an atom-atom system

$$H = \frac{\vec{p}^{\,2}}{2\mu} + \sum_{i=1}^{2} (V_i^{hf} + V_i^{Z}) + V_0(\vec{r})P_0 + V_1(\vec{r})P_1 + \ldots$$

$$V^{hf} = \frac{a_{hf}}{\hbar^2}\vec{I}\cdot\vec{J},\ V_i - \text{Coulomb term}$$

Tiesinga, Verhaar, Stoof, Phys. Rev. A47, 4114 (1993)

Channel coupling



$$V^{Z} = (\gamma_e J_z - \gamma_n I_z)B$$

One open channel with one resonant bound state (s-wave scattering)

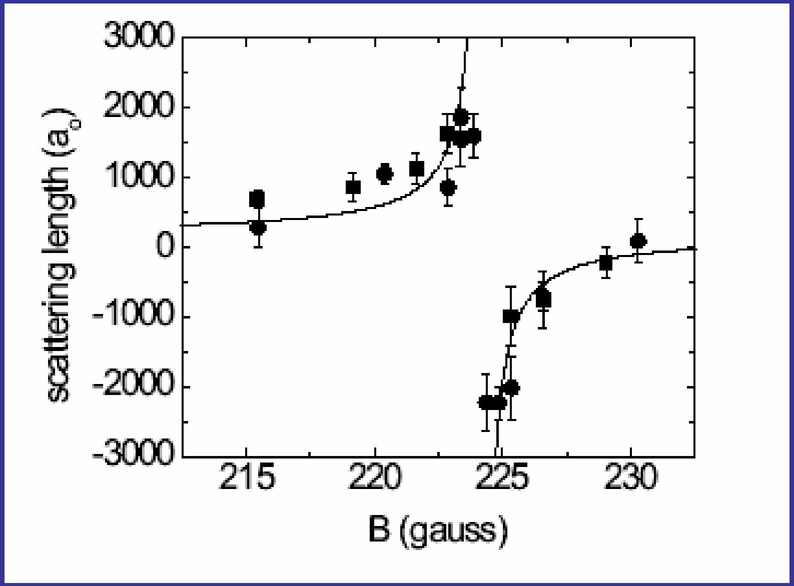
$$S(k) = S^{bg}(k)\left(1 - \frac{2ik|g|^2}{-\frac{4\pi\hbar^2}{m}\left(\nu - \frac{\hbar^2 k^2}{m}\right) + ik|g|^2}\right)$$

$$S^{bg}(k) = e^{-2ika_{bg}}, \quad \nu = \varepsilon_b - \varepsilon_0, \quad |g|^2 = \left|\left\langle \chi^+ \middle| V^{hf} \middle| \phi_b \right\rangle\right|^2 / k$$

A.J. Moerdijk et al.
Phys. Rev. A51 (1995)4852

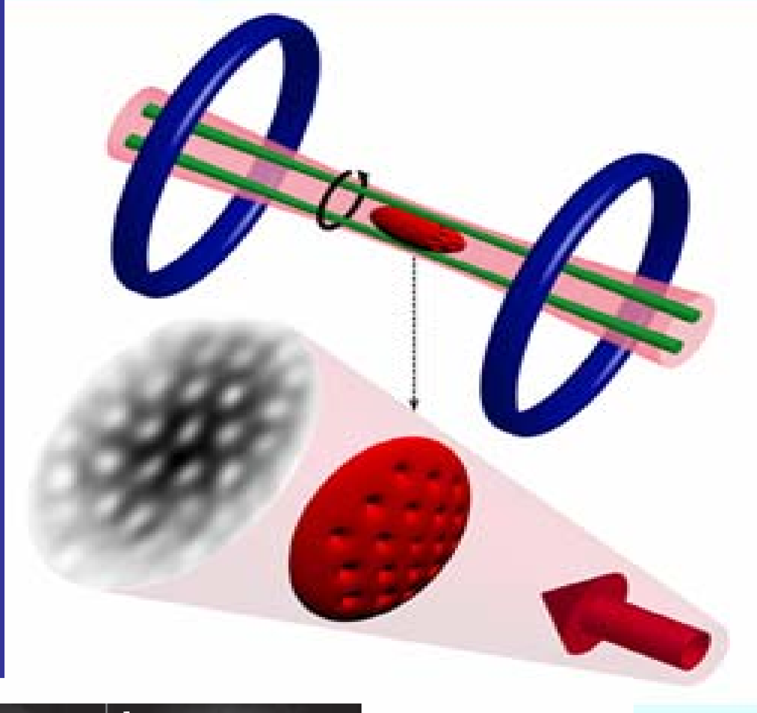
$$a = a_{bg} - \frac{m}{4\pi\hbar^2}\frac{|g|^2}{\nu}$$

$$\nu \sim B \Rightarrow a = a_{bg}\left(1 - \frac{\Delta B}{B - B_0}\right)$$



Regal and Jin, PRL 90, 230404 (2003)

Evidence for fermionic superfluidity: vortices!

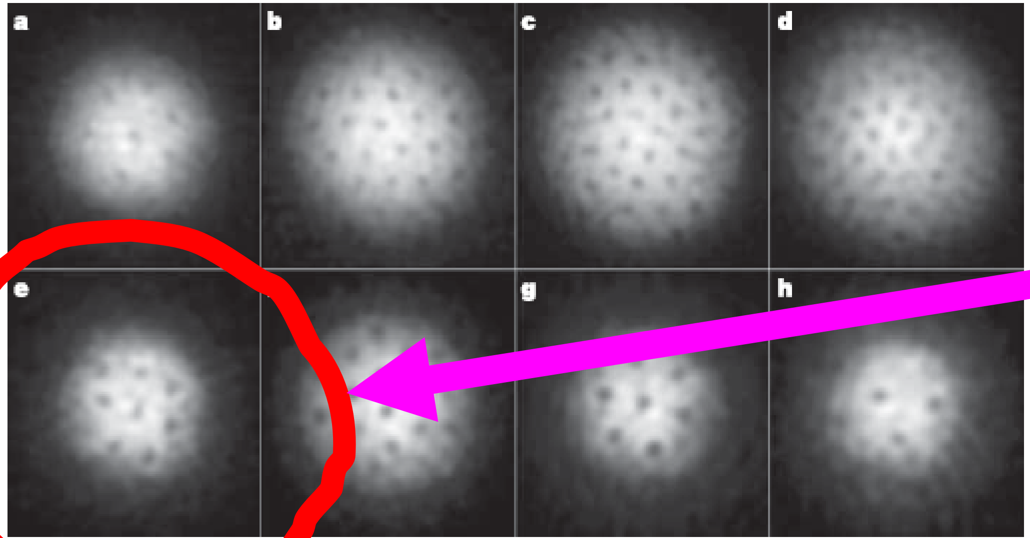


system of fermionic ^{6}Li atoms

Feshbach resonance: B=834G

BEC side: a>0

BCS side: a<0



UNITARY REGIME

Figure 2 | Vortices in a str[illegible]gly interacting gas of f[illegible]mionic atoms on the BEC- and the BCS-side of the Fe[illegible]. 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 [illegible] magnetic fields were 740 G (a), 766 G (b), 792 G [illegible] 843 G (f), 853 G (g) and 863 G (h). The field of view of each image is 880 μm × 880 μm.

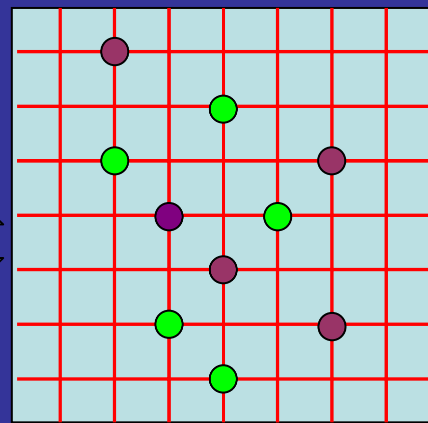
M.W. Zwierlein *et al*., Nature, 435, 1047 (2005)

Numerical simulations: see movies at www.phys.washington.edu/groups/qmbnt/vortices_movies.html

Coordinate space

L –limit for the spatial correlations in the system

$k_{cut} = \frac{\pi}{\Delta x}$; Δx



$Volume = L^3$

$lattice\ spacing = \Delta x$

- Spin up fermion

- Spin down fermion

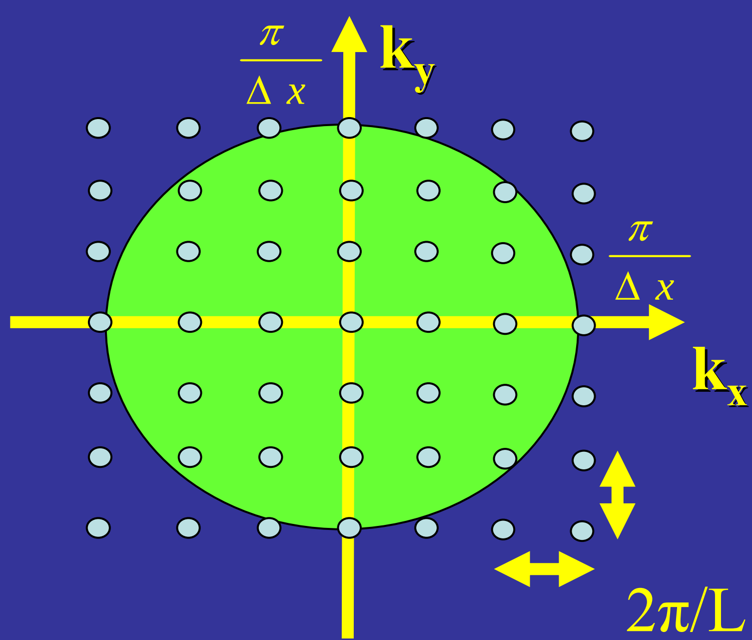
Periodic boundary conditions imposed

External conditions:

T - temperature

μ - chemical potential

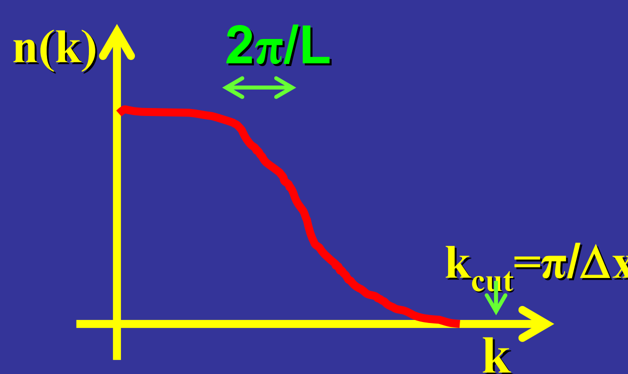
Momentum space



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

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

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



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

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

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

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)

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

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

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

More details of the calculations:

- Lattice sizes used: $6^3 - 10^3$.
  Imaginary time steps: $8^3 \times 300$ (high Ts) to $8^3 \times 1800$ (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

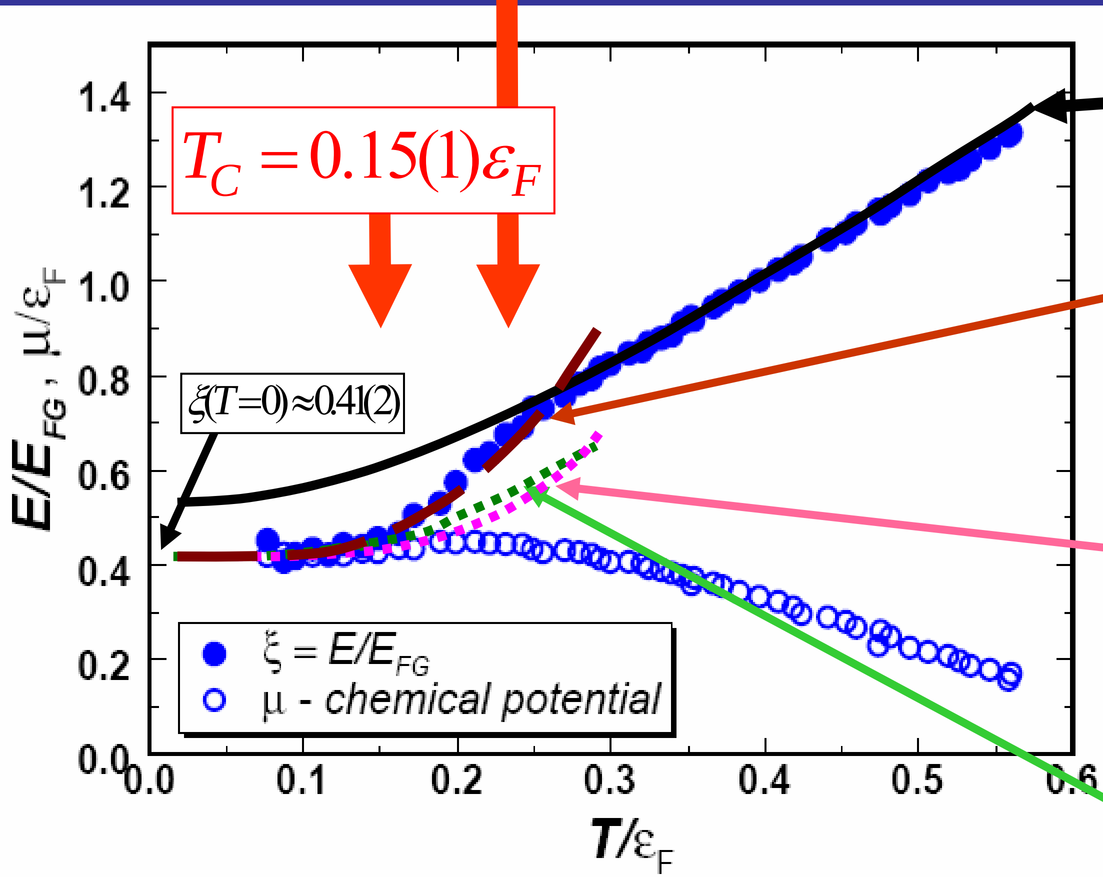
- At low temperatures use Singular Value Decomposition of the evolution operator $U(\{\sigma\})$ to stabilize the numerics.

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

- MC correlation "time" ≈ 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)

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

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

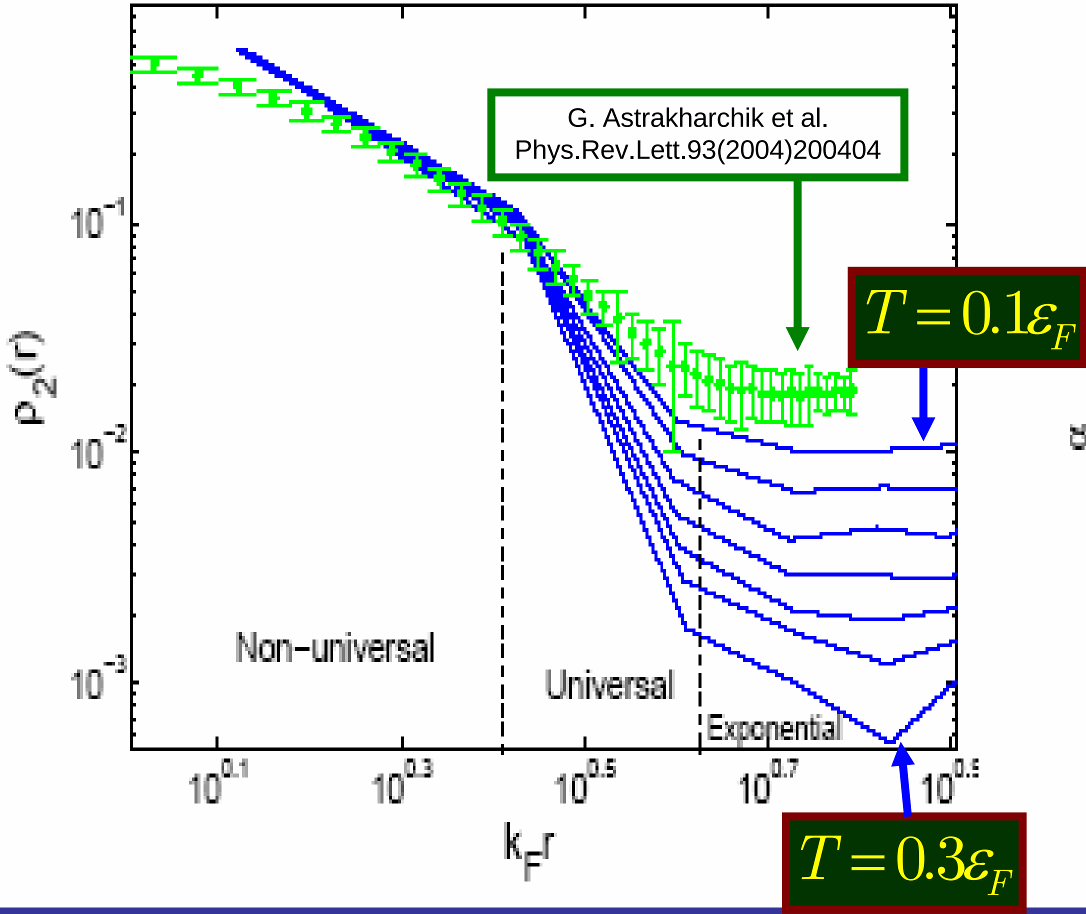
$$E_{\text{phonons}}(T) = \frac{3}{5}\varepsilon_F N \; \frac{\sqrt{3}\pi^4}{16\xi_s^{3/2}}\left(\frac{T}{\varepsilon_F}\right)^4, \qquad \xi_s \approx 0.41$$

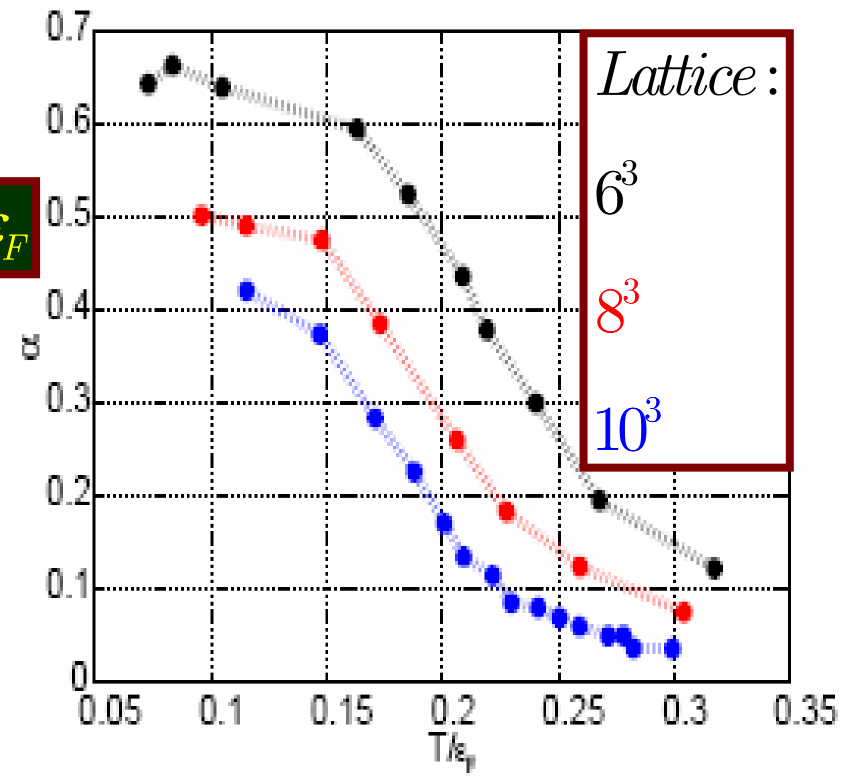
A. Bulgac, J.E. Drut, P. Magierski,PRL96,090404(2006)

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

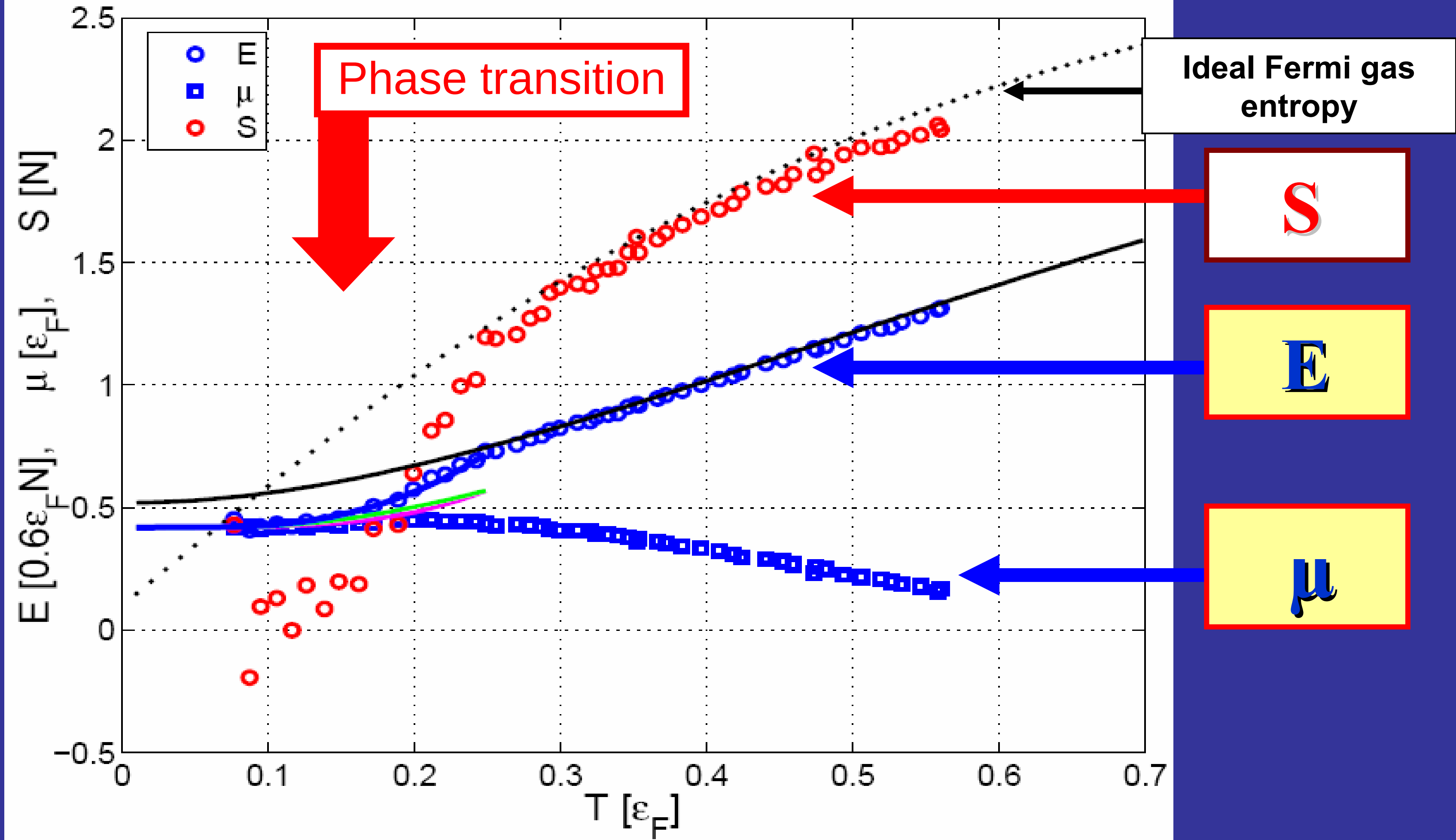
$$\rho_2^{\;P}(\vec{r}) = \frac{2}{N}\int d^3r_1 d^3r_2\, \rho_2(\vec{r}_1+\vec{r},\vec{r}_2+\vec{r},\vec{r}_1,\vec{r}_2)$$

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





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



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

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

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

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

Thermodynamics of the unitary Fermi gas

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

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

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

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

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

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

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

Note the similarity to the ideal Fermi gas

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?

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

$n(\vec{r})$ - 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:

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

- Temperature is calculated from the identity: $\frac{1}{T} = \frac{\partial S}{\partial E}$

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)*

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

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

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:

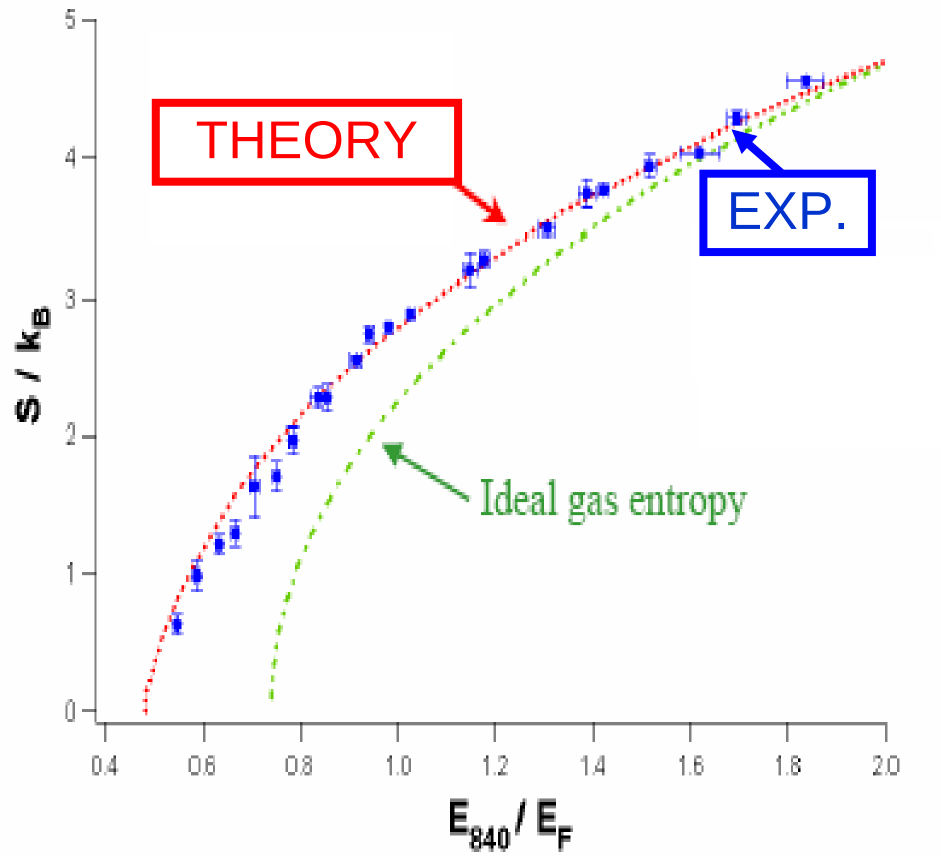
$$\frac{\delta\Omega}{\delta n(\vec{r})} = \frac{\delta(F - \lambda N)}{\delta n(\vec{r})} = \mu(x(\vec{r})) + U(r) - \lambda = 0$$

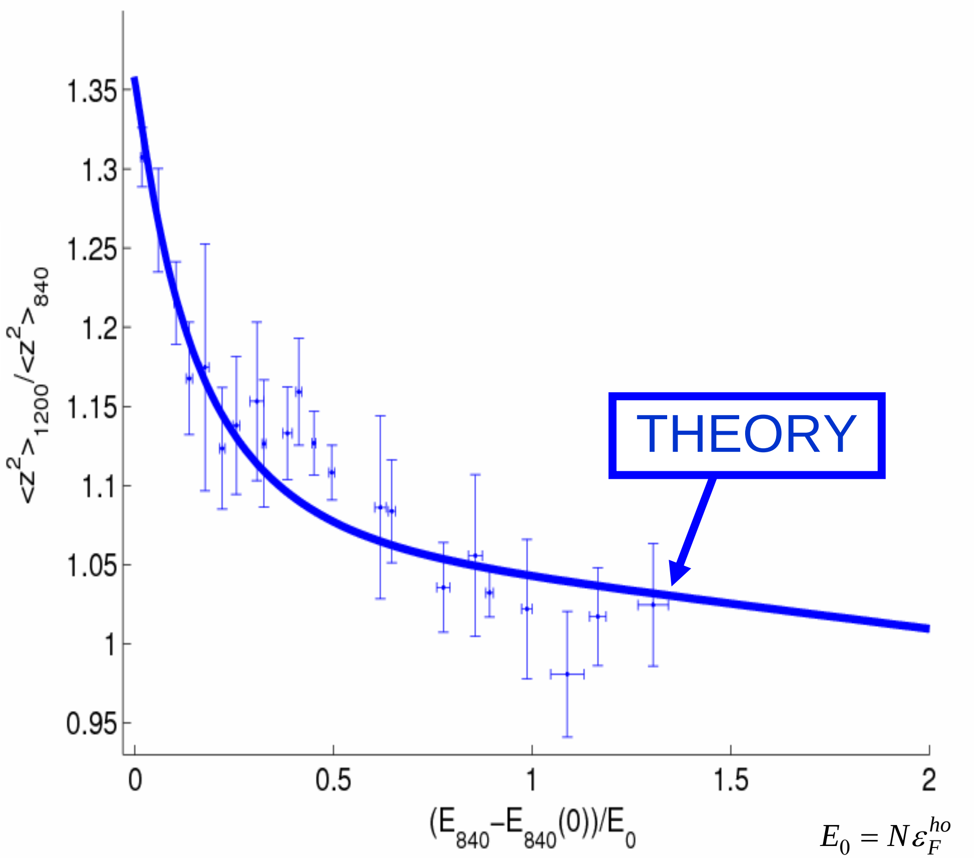
Using as an input the Monte Carlo results for the uniform system and experimental data (trapping potential, number of particles), we determine the density profiles.

Comparison with experiment

John Thomas' group at Duke University,

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





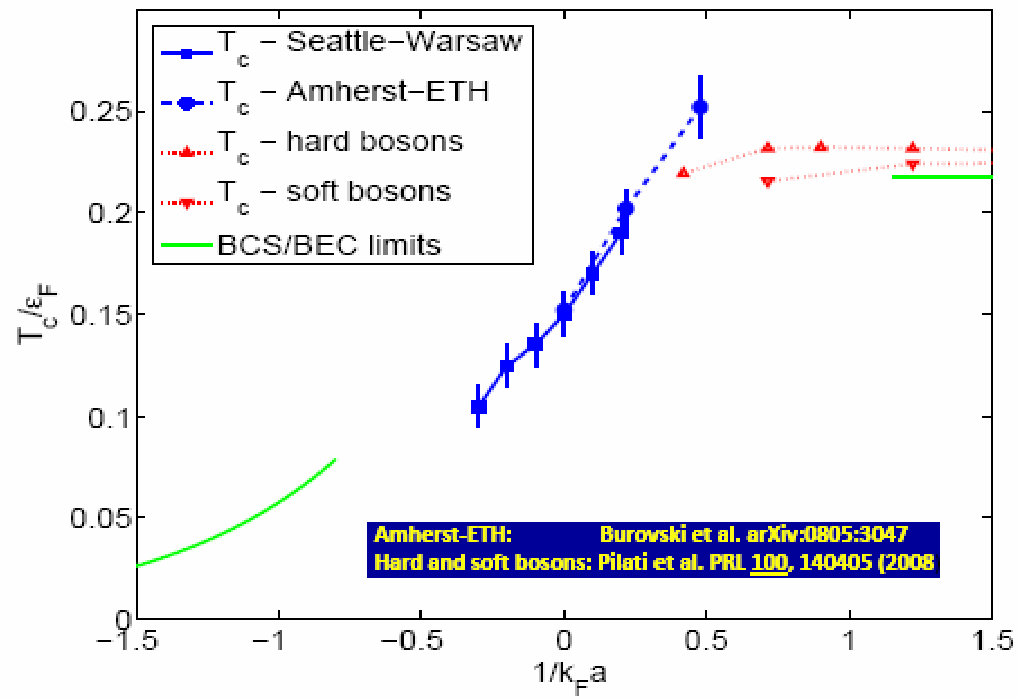
$E_0 = N\varepsilon_F^{ho}$

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.

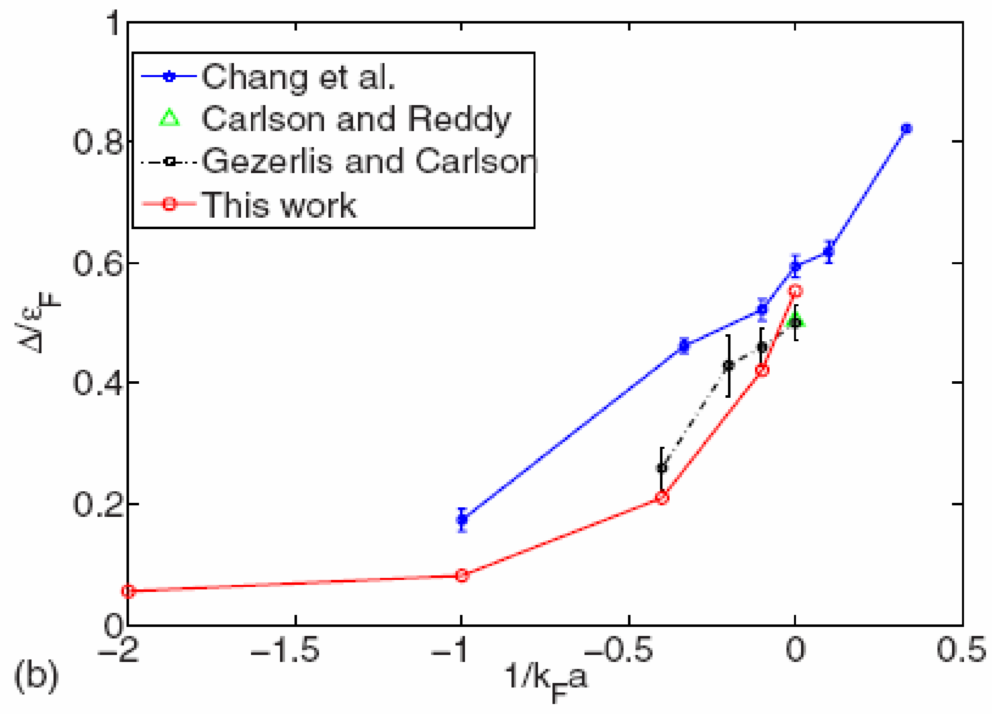
$B = 1200G \Rightarrow 1/k_F a \approx -0.75$

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



Results in the vicinity of the unitary limit:
- Critical temperature
- Pairing gap at T=0

Note that
- 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

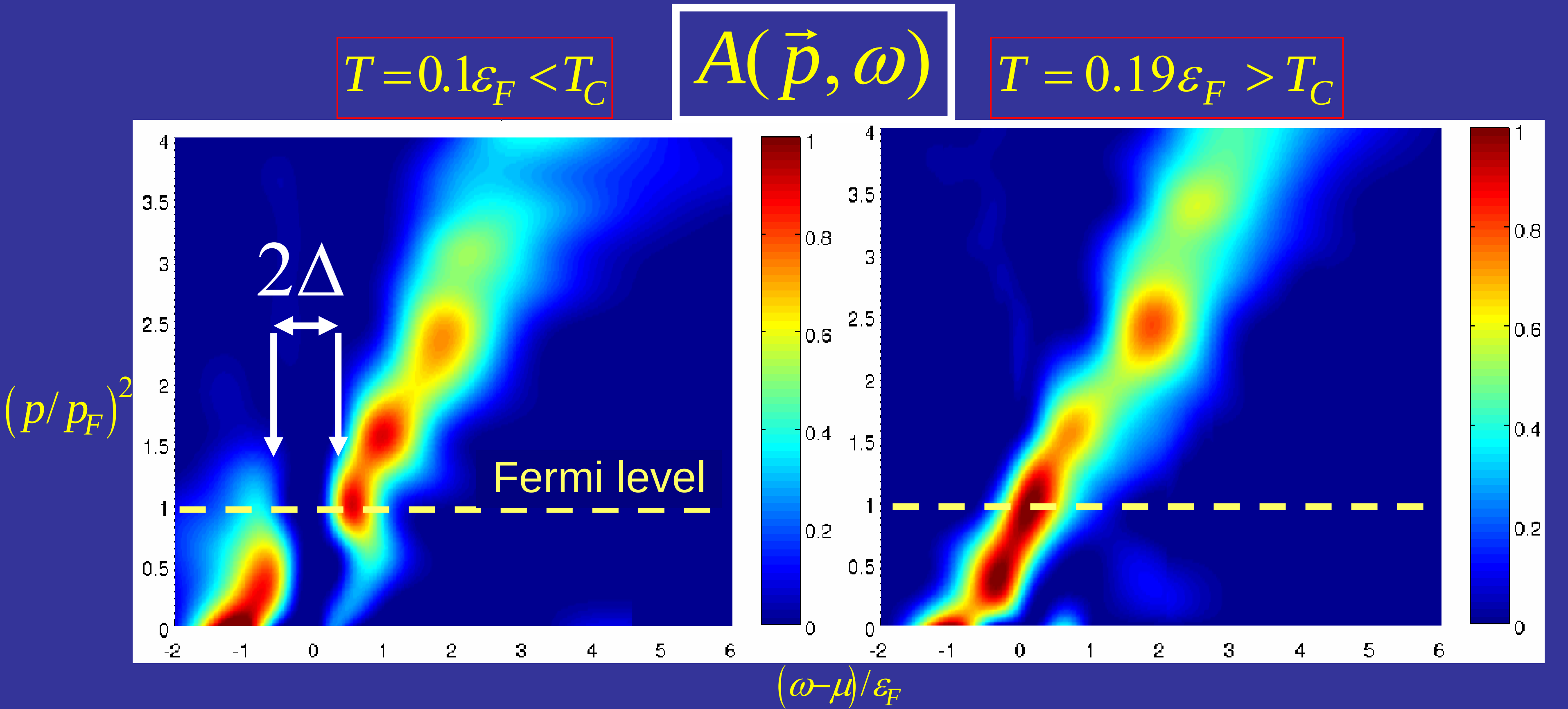
Spectral weight function: $A(\vec{p},\omega)$

$$G^{ret/adv}(\vec{p},\omega)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}d\omega'\frac{A(\vec{p},\omega')}{\omega-\omega'\pm i0^+}$$

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

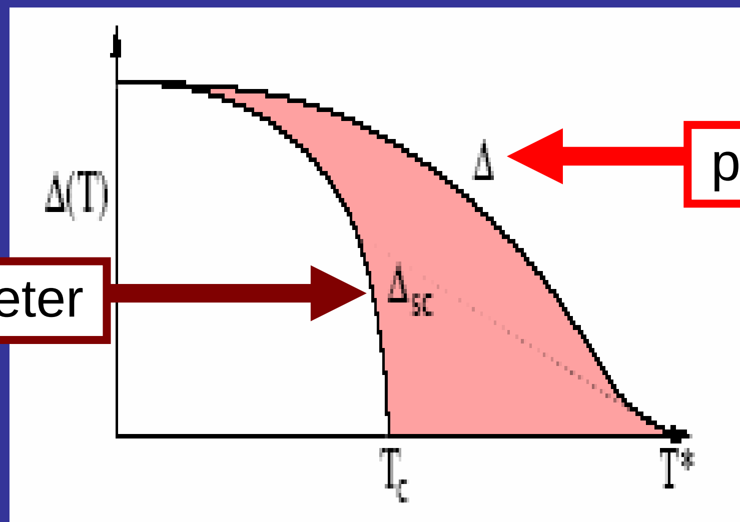
From Monte Carlo calcs.

In the limit of independent quasiparticles: $A(\vec{p},\omega)=2\pi\delta(\omega-E(p))$



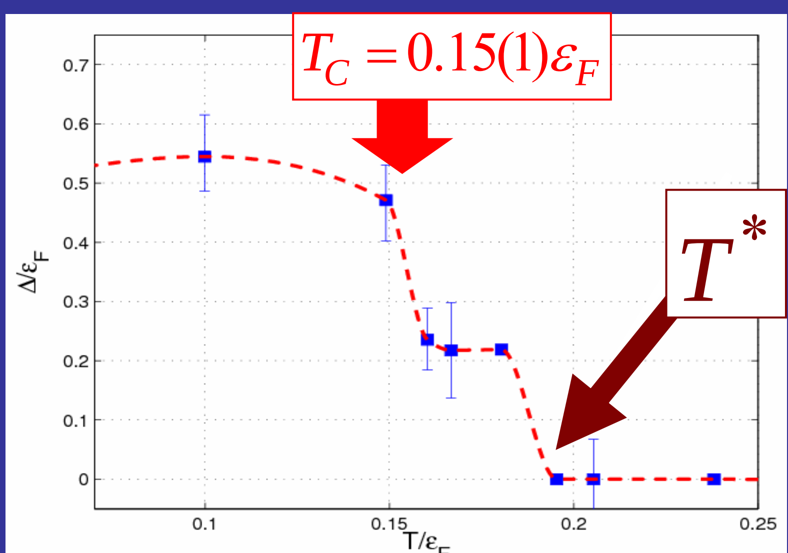
Pairing gap and pseudogap

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

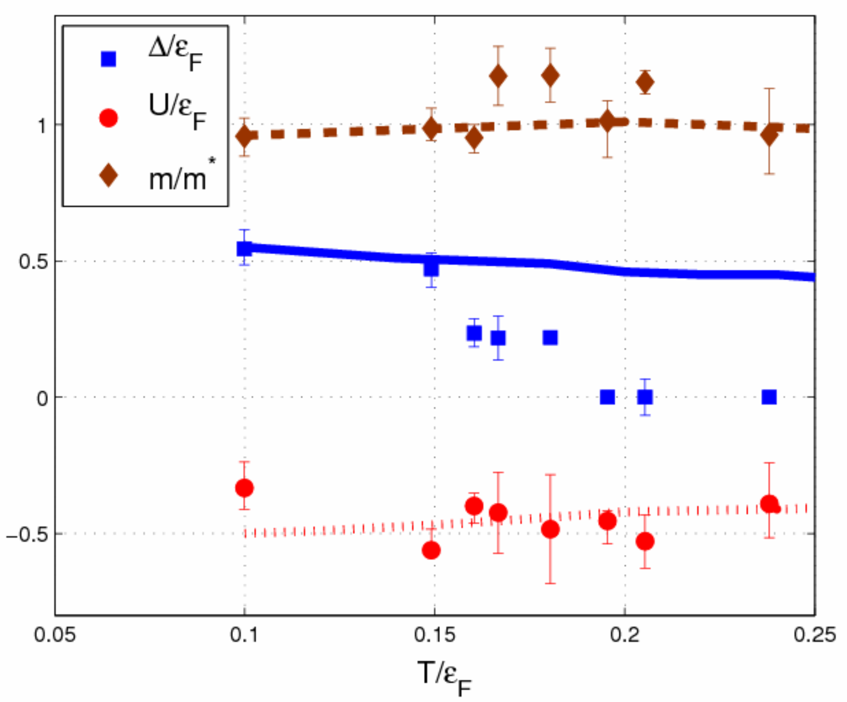
order parameter



Monte Carlo calculations

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

Single-particle properties

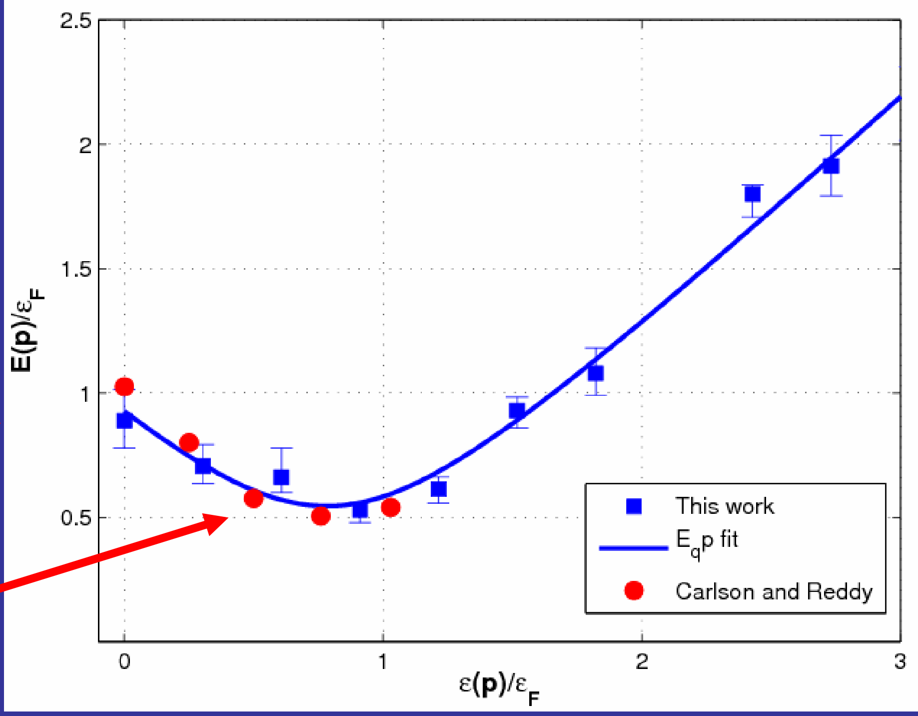


Effective mass: $m^* = (1.0 \pm 0.2) m$

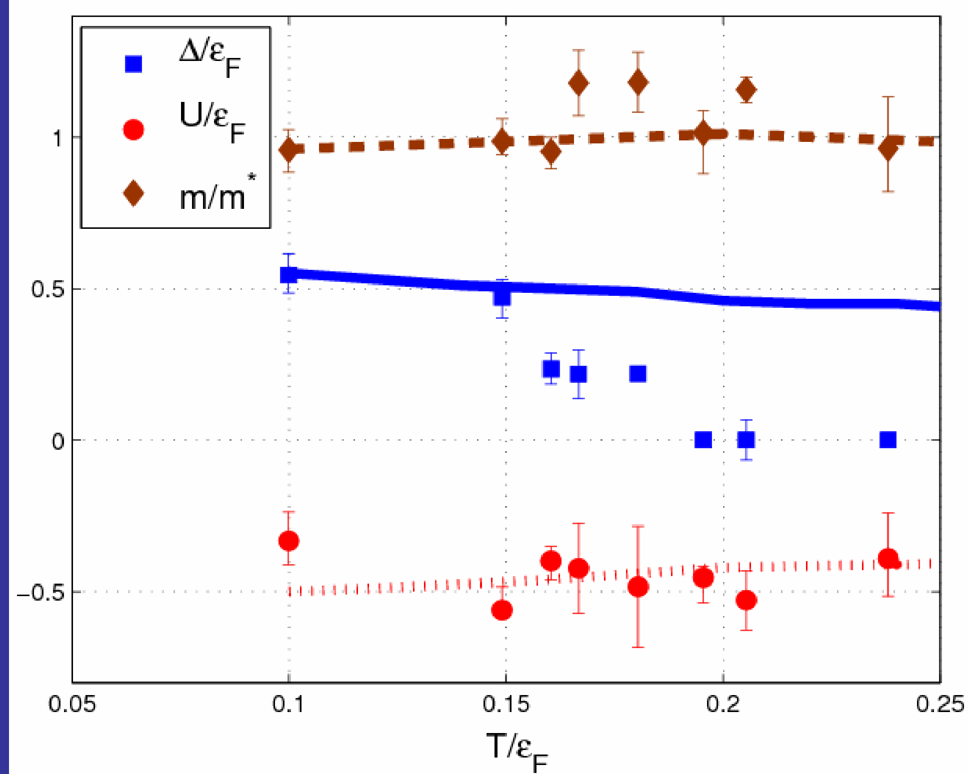
Mean-field potential: $U = (-0.5 \pm 0.2) \varepsilon_F$

Weak temperature dependence!

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



Fixed node MC calcs. at T=0



Dashed, dotted and solid lines

Susceptibility from the independent quasiparticle model

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

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

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

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

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 <u>neither superfluid nor follows the normal Fermi gas behavior</u>. Possibly due to pairing effects.

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

- ✓ The system at unitarity is NOT a BCS superfluid. There is an evidence for the existence of <u>*pseudogap*</u> at unitarity (similarity with high-Tc supeconductors).

- ✓ Description of the system at finite temperatures will pose a challenge for the density functional theory (two temperature scales are present).

- ✓ Surprisingly at low temperatures the gap extracted from the response function within the <u>independent quasiparticle model</u> accurately reproduce the one obtained from the spectral weight function.