Is a system of fermions in the crossover BCS-BEC regime a new type of superfluid?

Finite temperature properties of a Fermi gas in the unitary regime

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Also in Warsaw

Outline

- Some general remarks
- Path integral Monte Carlo for many fermions on the lattice at finite temperatures
- Thermodynamic properties of a Fermi gas in the unitary regime
- Conclusions

Superconductivity and superfluidity in Fermi systems

20 orders of magnitude over a century of (low temperature) physics

- ✓ Dilute atomic Fermi gases $T_c \approx 10^{-12} - 10^{-9}$ eV
- ✓ Liquid ^{3}He $T_c \approx 10^{-7}$ eV
- ✓ Metals, composite materials $T_c \approx 10^{-3} - 10^{-2}$ eV
- ✓ Nuclei, neutron stars $T_c \approx 10^{5} - 10^{6}$ eV
- QCD color superconductivity $T_c \approx 10^{7} - 10^{8}$ eV

units (1 eV $\approx 10^4$ K)

A little bit of history

Bertsch Many-Body X challenge, Seattle, 1999

What are the ground state properties of the many-body system composed of spin ½ 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 (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.**

- **Thomas' Duke group (2002) demonstrated experimentally that such systems are (meta)stable.**

Bertsch's regime is nowadays called *the unitary regime*

The system is very dilute, but strongly interacting!

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

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

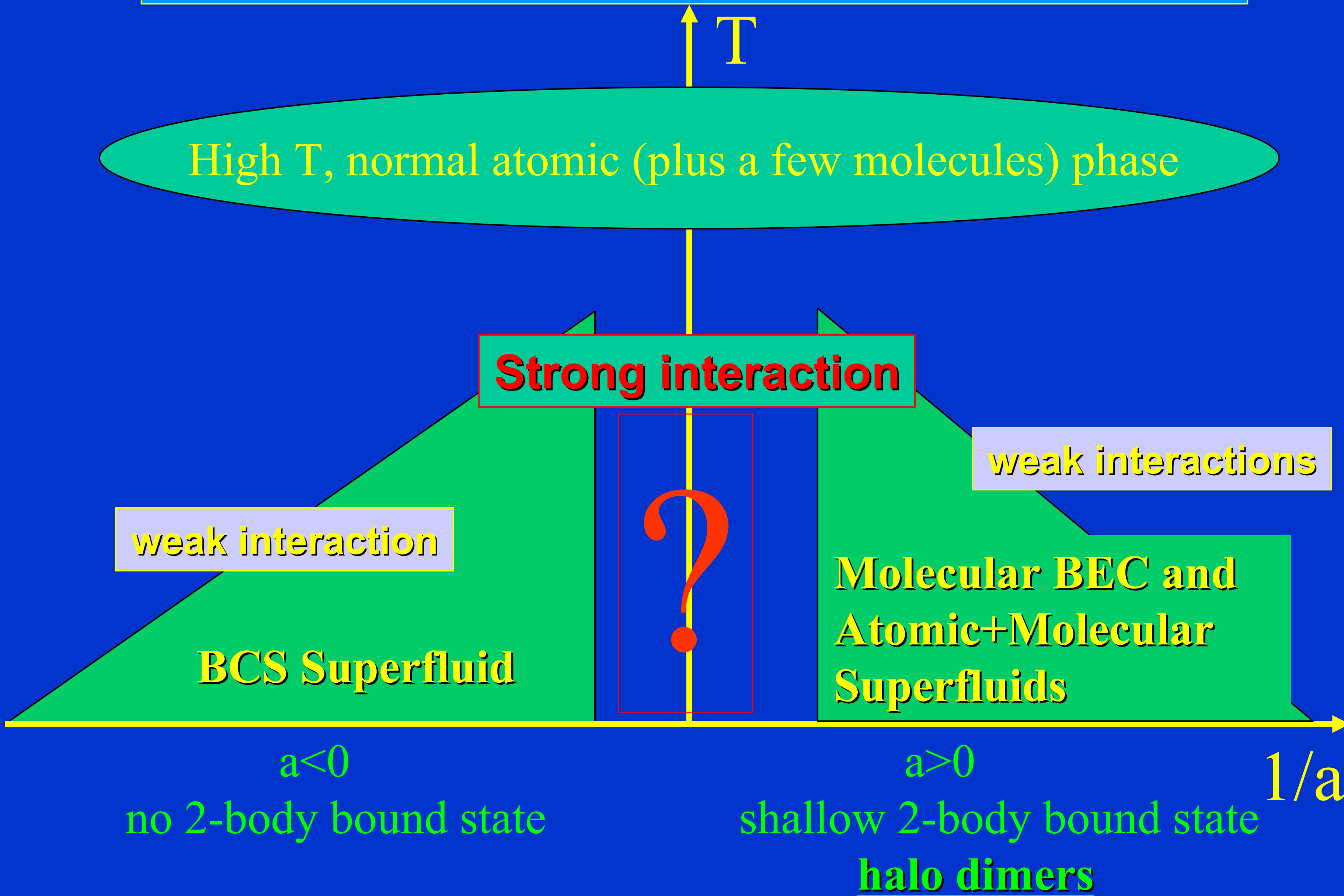
n - number density

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

r_0 - range of interaction

a - scattering length

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



Early theoretical approach to BCS-BEC crossover

Dyson (?), Eagles (1969), Leggett (1980) …

$$\left|gs\right\rangle = \prod_k \left(\mathrm{u}_k + \mathrm{v}_k a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow}\right)\left|vacuum\right\rangle$$ BCS wave function

$$\frac{m}{4\pi\hbar^2 a} = \sum_k \left(\frac{1}{2\varepsilon_k} - \frac{1}{2\mathrm{E}_k}\right)$$ gap equation

$$n = 2\sum_k \left(1 - \frac{\varepsilon_k - \mu}{\mathrm{E}_k}\right)$$ number density equation

$$\Delta \approx \frac{8}{\mathrm{e}^2}\varepsilon_F \exp\left(\frac{\pi}{2k_F a}\right)$$ pairing gap

$$\mathrm{E}_k = \sqrt{(\varepsilon_k - \mu)^2 + \Delta^2}$$ quasi-particle energy

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m}, \quad \mathrm{u}_k^2 + \mathrm{v}_k^2 = 1, \quad \mathrm{v}_k^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_k - \mu}{\mathrm{E}_k}\right)$$

$$\frac{\mathrm{E}_{\mathrm{total}}}{\mathrm{N}} = \frac{3}{5}\frac{\hbar^2 k_F^2}{2m} + \underline{\frac{\pi\hbar^2 a}{m}} n + \ldots - \frac{3\Delta^2}{8\mu}, \qquad n = \frac{k_F^3}{3\pi^2}$$

Neglected/overlooked

Exponentially suppressed in BCS

Consequences:

- Usual BCS solution for small and negative scattering lengths, with exponentially small pairing gap

- For small and positive scattering lengths this equations describe a gas a weakly repelling (weakly bound/shallow) molecules, essentially all at rest (almost pure BEC state)

$$\Psi\left(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4,\ldots\right)\approx \mathcal{A}\left[\varphi(\vec{r}_{12})\varphi(\vec{r}_{34})\ldots\right]$$

In BCS limit the particle projected many-body wave function has the same structure (BEC of spatially overlapping Cooper pairs)

- For both large positive and negative values of the scattering length these equations predict a smooth crossover from BCS to BEC, from a gas of spatially large Cooper pairs to a gas of small molecules

What is wrong with this approach:

• The BCS gap (a<0 and small) is overestimated, thus the critical temperature and the condensation energy are overestimated as well.

• In BEC limit (a>0 and small) the molecule repulsion is overestimated

• The approach neglects of the role of the "meanfield (HF) interaction," which is the bulk of the interaction energy in both BCS and unitary regime

• All pairs have zero center of mass momentum, which is reasonable in BCS and BEC limits, but incorrect in the unitary regime, where the interaction between pairs is strong !!!
(this situation is similar to superfluid ^{4}He)

$$\Psi\left(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4,\ldots\right) \approx \mathcal{A}\left[\varphi(\vec{r}_{12})\varphi(\vec{r}_{34})\ldots\right]$$

Fraction of non-condensed pairs (perturbative result)!?!

$$\frac{n_{ex}}{n_0} = \frac{8}{3\sqrt{\pi}}\sqrt{n_m a_{mm}^3}, \qquad n_m = \frac{n}{2}, \qquad a_{mm} \approx 0.6a$$

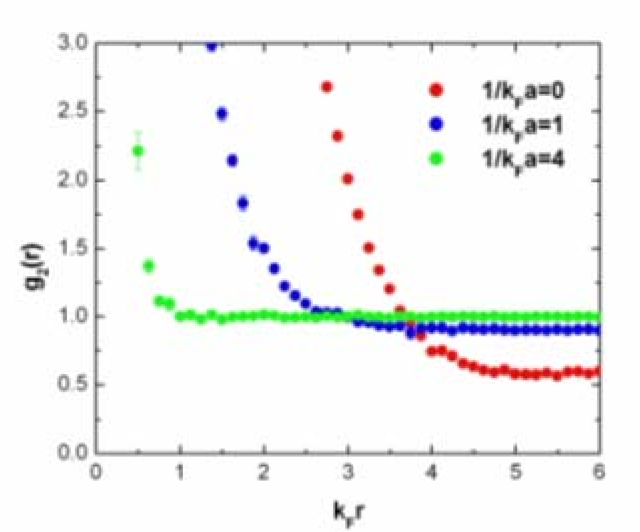
Two-body density matrix and condensate fraction

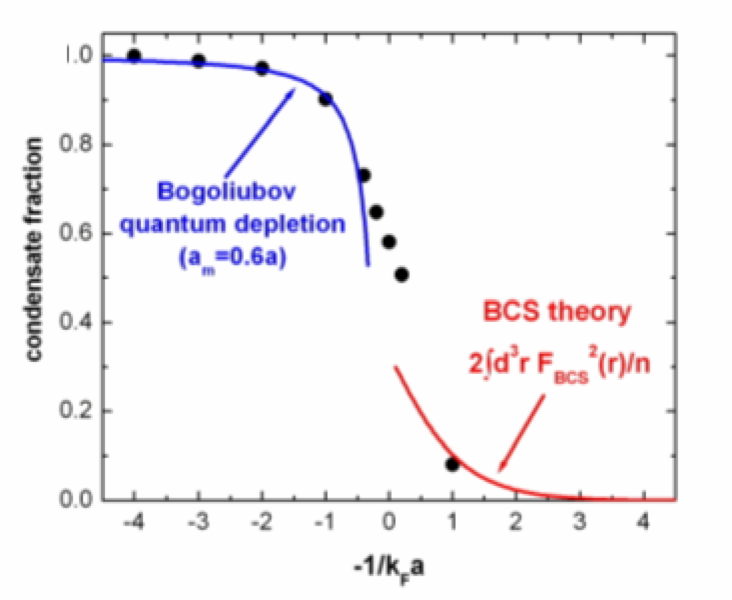
$$\langle \psi_\uparrow^+(\vec{r}_1+\vec{r})\psi_\downarrow^+(\vec{r}_2+\vec{r})\psi_\uparrow(\vec{r}_1)\psi_\downarrow(\vec{r}_2)\rangle \xrightarrow[r\to\infty]{} F^2(|\vec{r}_1-\vec{r}_2|)$$

where

$$F(|\vec{r}_1-\vec{r}_2|) = \langle \psi_\uparrow(\vec{r}_1)\psi_\downarrow(\vec{r}_2)\rangle$$ **order parameter**

$$g_2(r) = \frac{2}{N}\int d^3r_1 d^3r_2 \langle \psi_\uparrow^+(\vec{r}_1+\vec{r})\psi_\downarrow^+(\vec{r}_2+\vec{r})\psi_\uparrow(\vec{r}_1)\psi_\downarrow(\vec{r}_2)\rangle$$

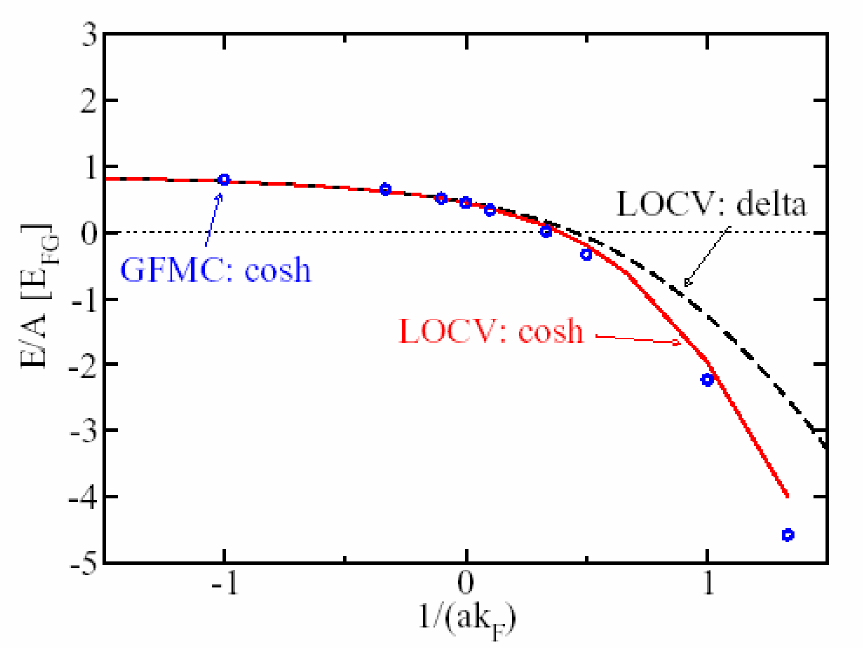


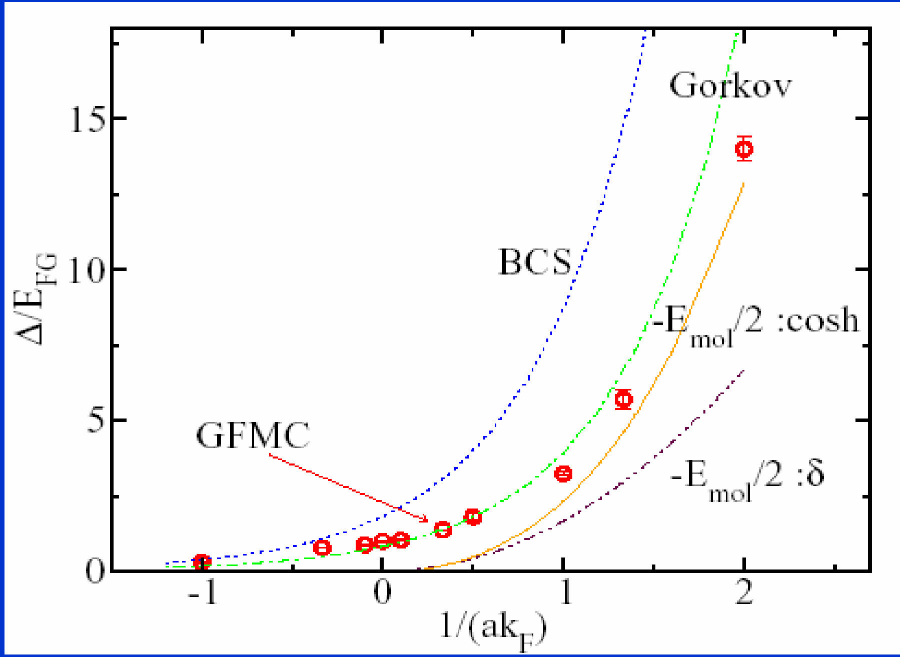


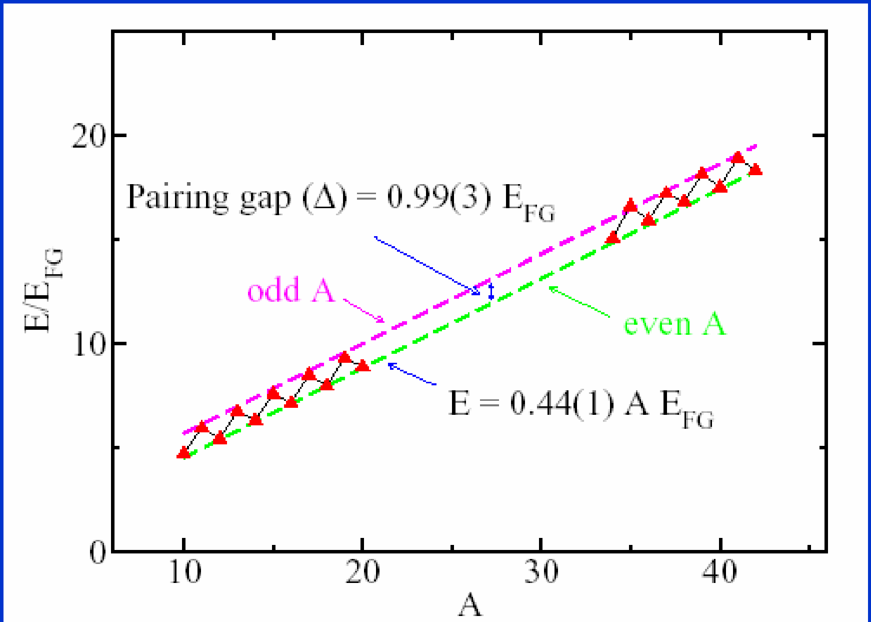
From a talk of Stefano Giorgini (Trento)

What is the best, the most accurate theory (so far) for the T=0 case?

Fixed-Node Green Function Monte Carlo approach at T=0







$$\Delta_{\mathrm{BCS}} \approx \frac{8}{\mathrm{e}^2}\varepsilon_F \exp\left(\frac{\pi}{2k_F a}\right)$$

$$\Delta_{\mathrm{Gorkov}} \approx \left(\frac{2}{e}\right)^{7/3}\varepsilon_F \exp\left(\frac{\pi}{2k_F a}\right)$$

Carlson *et al.* PRL 91, 050401 (2003)
Chang *et al.* PRA 70, 043602 (2004)
Astrakharchik *et al.* PRL 93, 200404(2004)

Theory for fermions at T >0 in the unitary regime

Put the system on a spatio-temporal lattice and use a path integral formulation of the problem

Grand Canonical Path-Integral Monte Carlo

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

$$\hat{N} = \int d^3x \; \left[\hat{n}_\uparrow(\vec{x}) + \hat{n}_\downarrow(\vec{x}) \right], \qquad \hat{n}_s(\vec{x}) = \psi_s^\dagger(\vec{x}) \psi_s(\vec{x}), \qquad s = \uparrow, \downarrow$$

Trotter expansion (*trotterization* of the propagator)

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

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

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

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 $L=N_s l$, with periodic boundary conditions

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

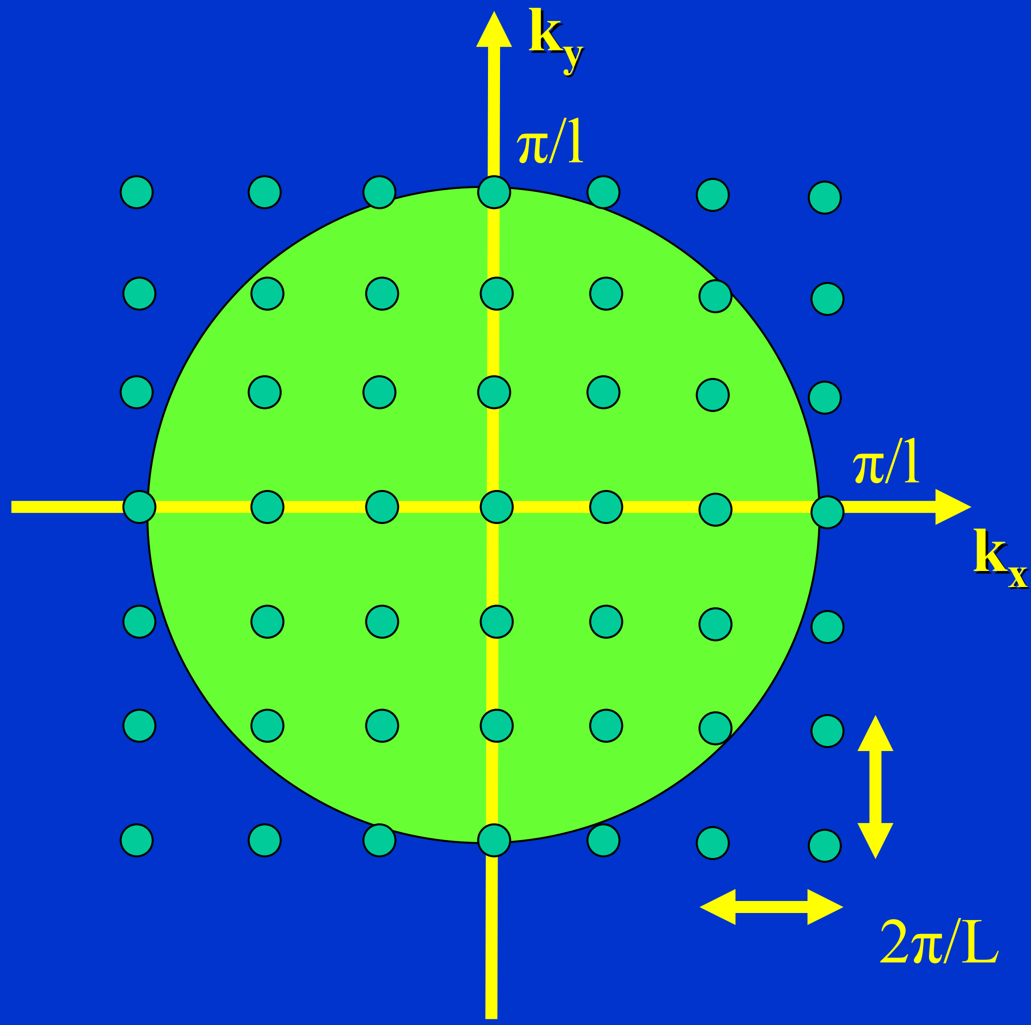
Discrete Hubbard-Stratonovich transformation

$$\exp(-\tau\hat{V})=\prod_{\vec{x}}\sum_{\sigma_\pm(\vec{x})=\pm1}\frac{1}{2}\left[1+\sigma_\pm(\vec{x})A\hat{n}_\uparrow(\vec{x})\right]\left[1+\sigma_\pm(\vec{x})A\hat{n}_\downarrow(\vec{x})\right],\qquad A=\sqrt{\exp(\tau g)-1}$$

σ-fields fluctuate both in space and imaginary time

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

Running coupling constant g defined by lattice



Momentum space

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

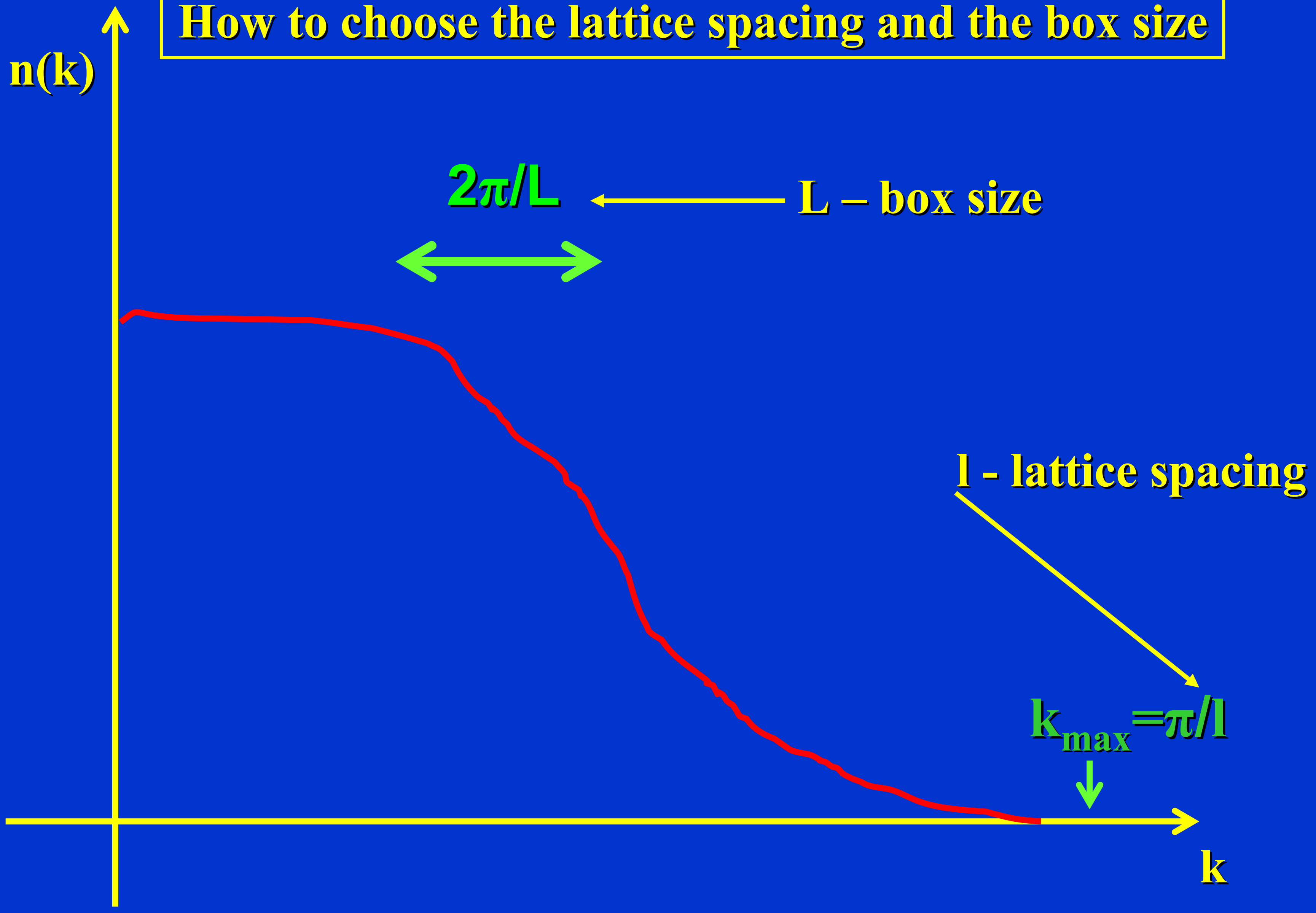
$$\delta\varepsilon > \frac{2\hbar^2\pi^2}{mL^2}$$

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

$$\xi \ll L = N_s l$$

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

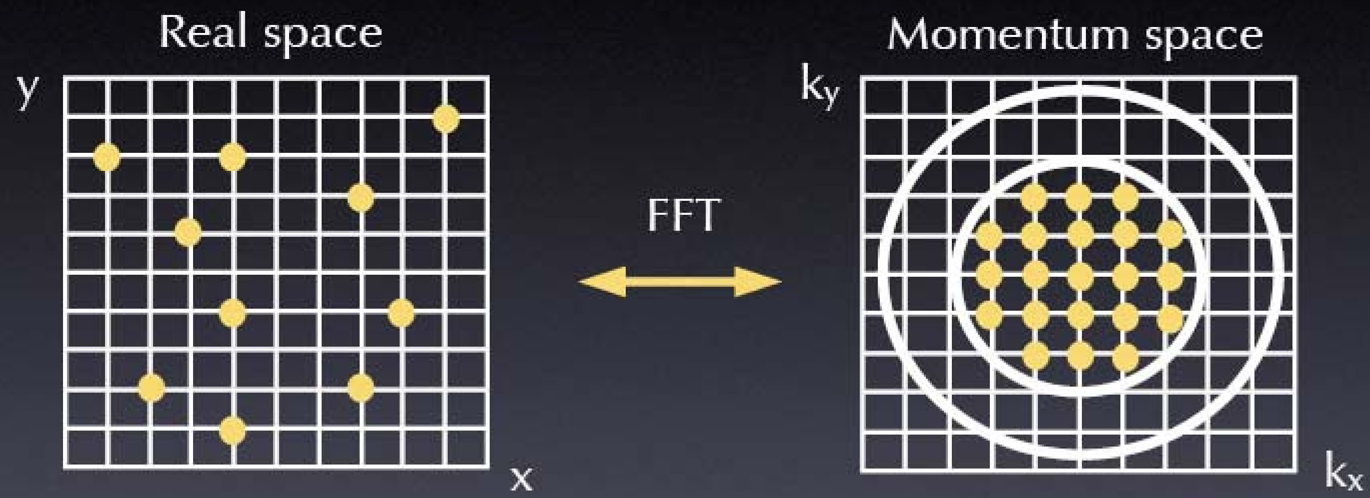
How to choose the lattice spacing and the box size



Fermions on a Lattice

How can we study fermions at finite temperature on a computer?

Path integrals on a 4D space-time lattice !



Lattice spacing: l

Finite volume: L^3

UV momentum cutoff: $\Lambda_{UV} = \dfrac{\pi}{l}$

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

$$\rightarrow \quad \boxed{\frac{\Lambda_{IR}^2}{2m} \ll \epsilon_F \ll \frac{\Lambda_{UV}^2}{2m} \qquad \frac{\delta p \, p_F}{m} \ll \Delta \ll \frac{\Lambda_{UV}^2}{2m}}$$

From a talk of J.E. Drut

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

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

One-body evolution operator in imaginary time

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

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

No sign problem!

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

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

More details of the calculations:

- Lattice sizes used from 6^3 x (300-1361), 8^3 x (250-1750) and 10^3

• 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 of about 0.5

• 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

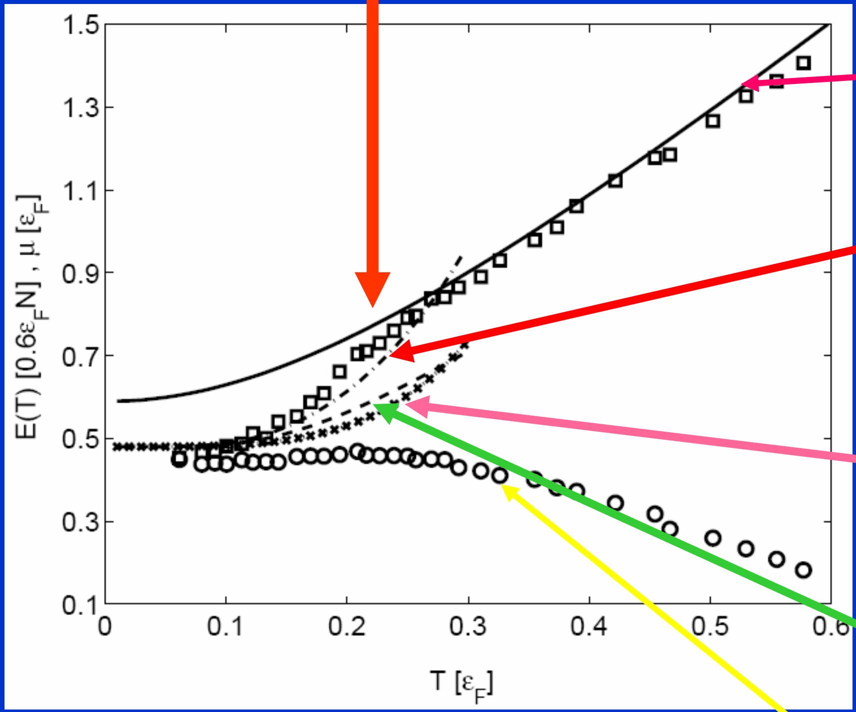
• At low temperatures use Singular Value Decomposition of the evolution operator $U(\{\sigma\})$ to stabilize the numerics

• Use 100,000-2,000,000 $\sigma(x,\tau)$- field configurations for calculations

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

$\mathbf{a = \pm\infty}$

Superfluid to Normal Fermi Liquid Transition



Normal Fermi Gas
(with vertical offset, solid line)

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

Bogoliubov-Anderson phonons contribution only (little crosses)
<u>People never consider this ???</u>

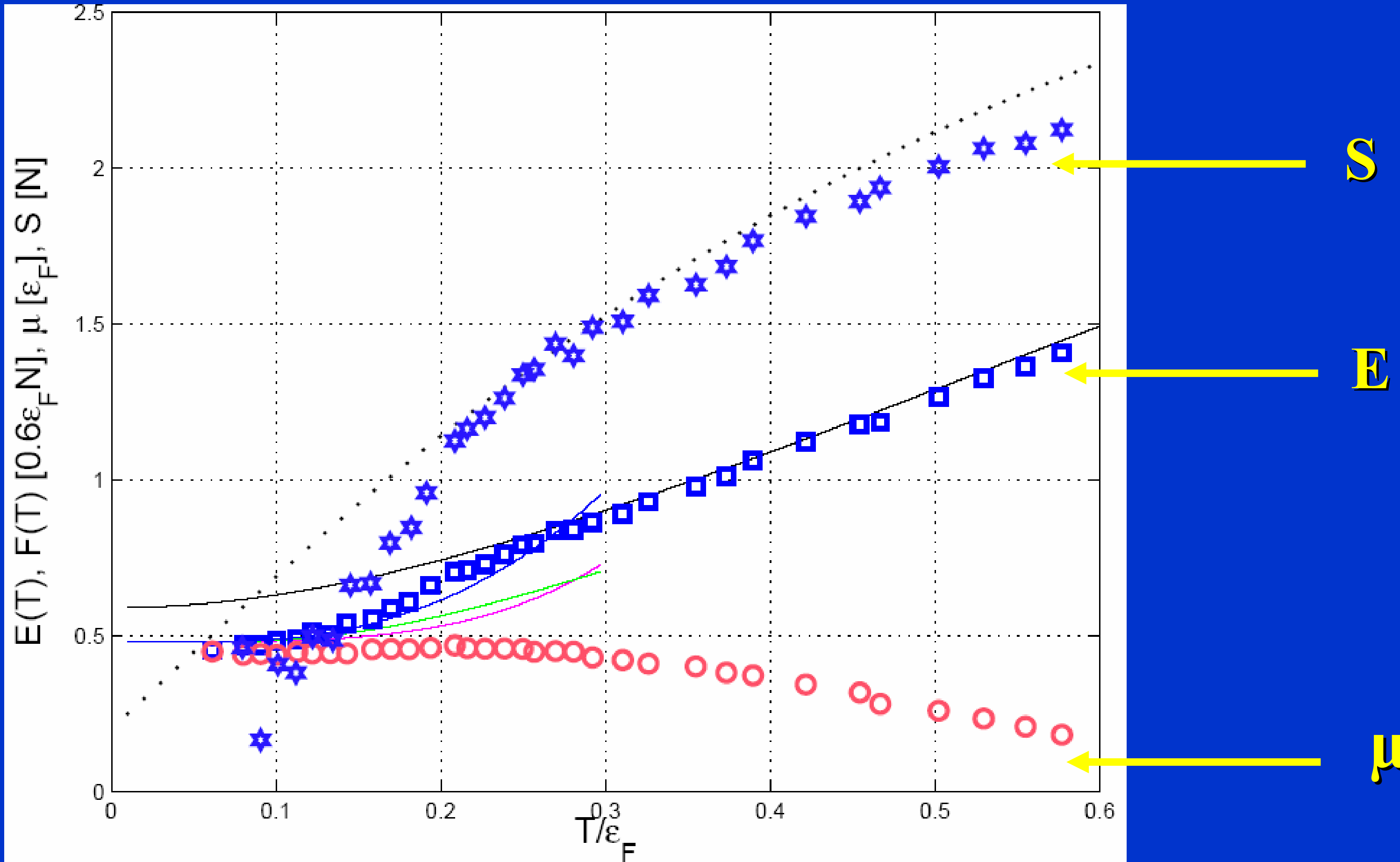
Quasi-particles contribution only (dashed line)

μ - chemical potential (circles)

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

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

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



$$E = \mu N - PV + TS = \frac{3}{5}\varepsilon_F(n)N \; e\left(\frac{T}{\varepsilon_F(n)}\right) = \varepsilon(n)nV$$

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

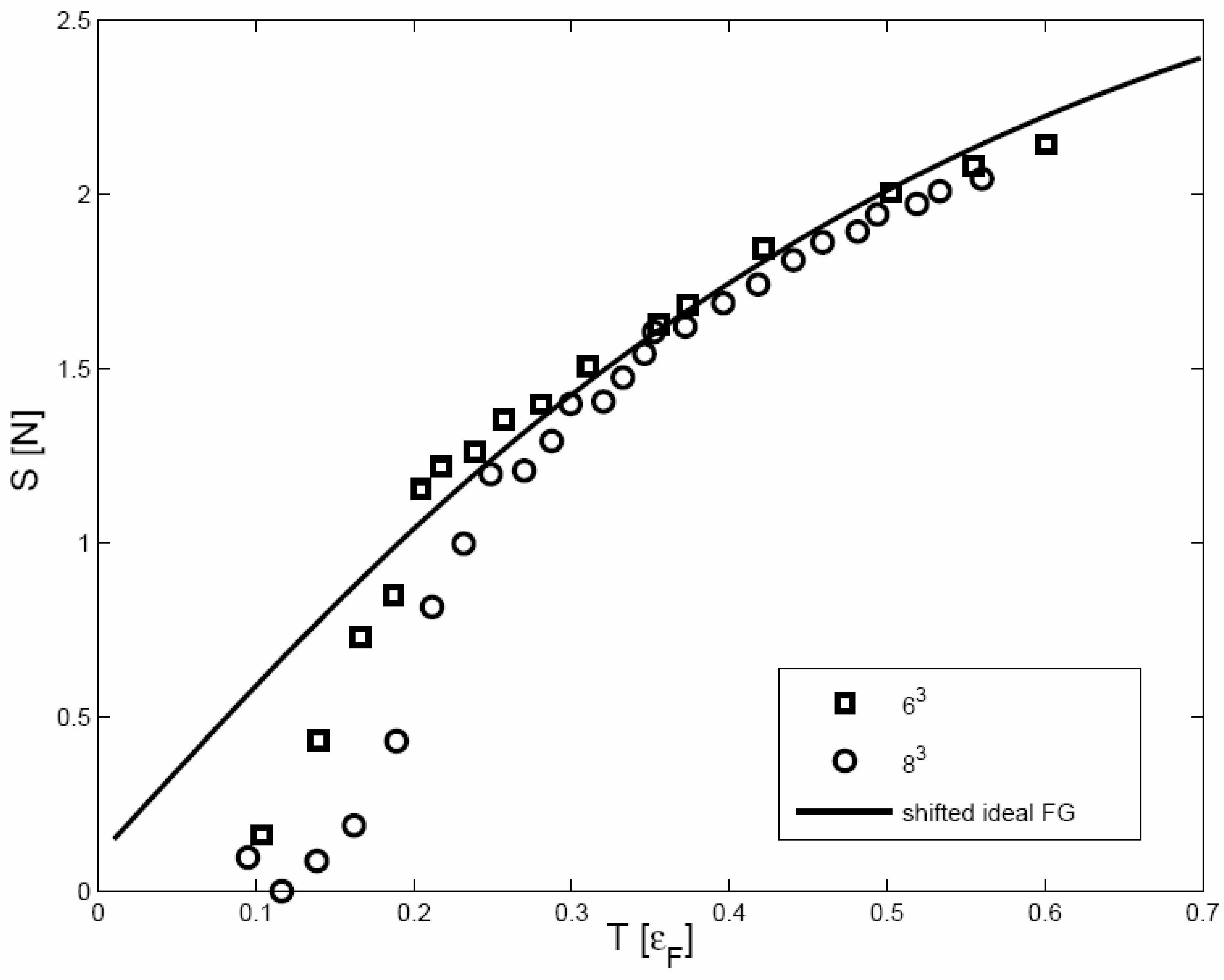
$$S = \frac{\frac{5}{3}e(n) - \mu}{T}N = N\sigma\left(\frac{T}{\varepsilon_F(n)}\right), \quad P = \frac{2}{3}e(n)n$$

The known dependence of the entropy on temperature at unitarity S(T) can be used to devise a *thermometer!*

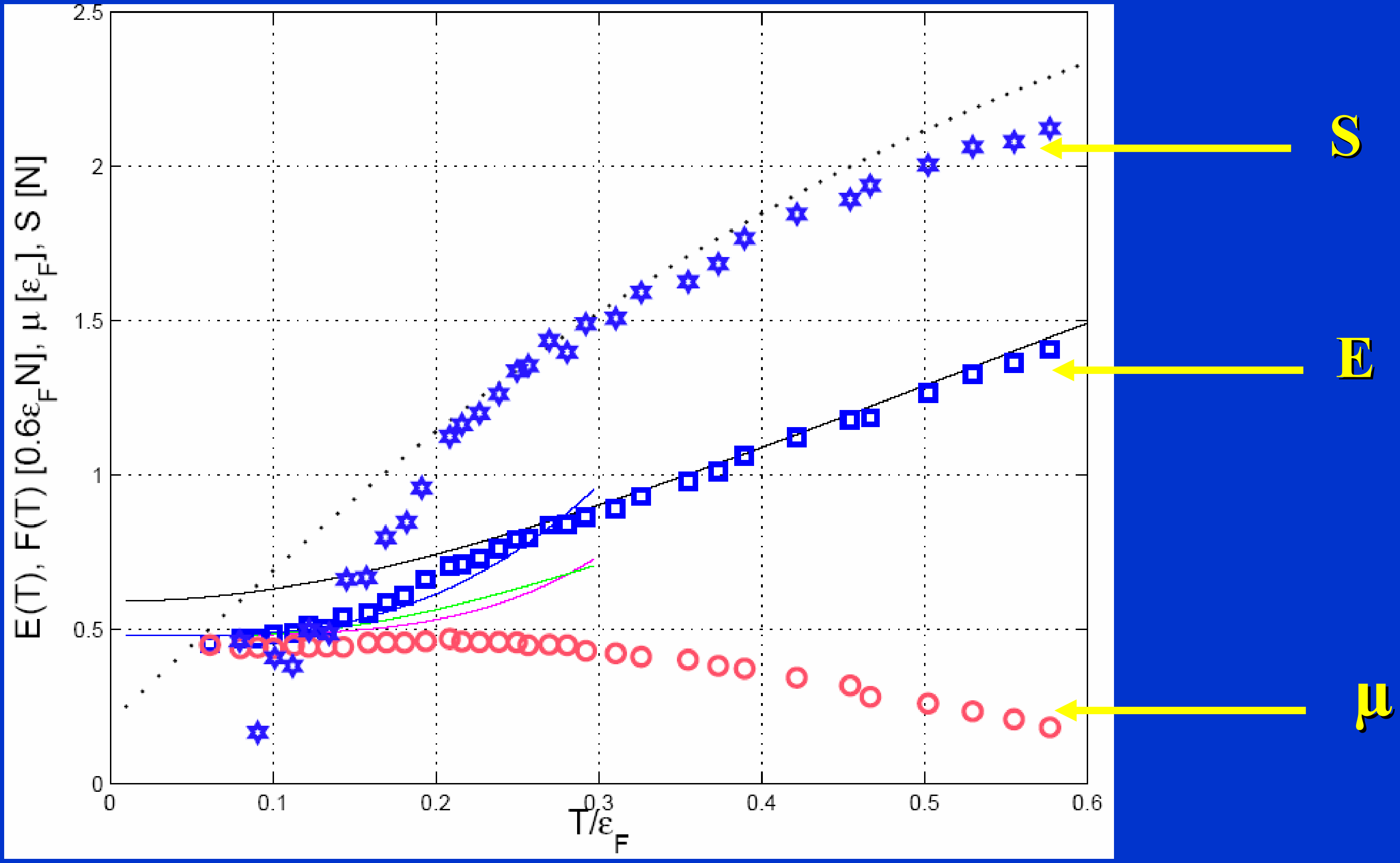
How?

- **The temperature can be measured either in the BCS or BEC limits, where interactions are weak, and easily be related to the entropy S(T)**

- **The system can then adiabatically (S= constant) be brought into the unitary regime and from the calculated S(T) one can *read* T**



S [N]
T [ε_F]
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.5
1
1.5
2
2.5
6^3
8^3
shifted ideal FG



NB The chemical potential is essentially constant below the critical temperature!

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

$$S(T) = N\frac{2}{5}\xi'\left(\frac{T}{\varepsilon_F}\right)$$

$$\mu(T) = \frac{dE(T)}{dN} = \varepsilon_F\left[\xi\left(\frac{T}{\varepsilon_F}\right) - \frac{2}{5}\frac{T}{\varepsilon_F}\xi'\left(\frac{T}{\varepsilon_F}\right)\right] \approx \xi_s\varepsilon_F \approx 0.44(2)\varepsilon_F$$

$$\Rightarrow \xi(x) = \xi_s + \varsigma_s x^{5/2}, \qquad \varsigma_s \approx 11(1)$$

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

assuming a Bogoliubov like spectrum $\varepsilon(p) = pc\sqrt{1+\frac{p^2}{4m_B^2c^2}}$

$$E(T) \approx \frac{3}{5}\varepsilon_F N\xi_s + \frac{\Gamma(3)\varsigma(3)}{4\pi^2\hbar^3c^3}T^4V, \quad \text{if} \quad T \ll m_Bc^2, \quad c^2 = \xi_s\frac{\mathrm{v}_F^2}{3}$$

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

$$\text{if} \quad T \gg m_Bc^2 \ \text{ for an ideal Bose gas}$$

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?**

Let us consider other power law behaviors

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

$$\mu(T) = \frac{dE(T)}{dN} = \varepsilon_F\left[\xi_s + \overline{\varsigma}_s\left(1 - \frac{2n}{5}\right)\left(\frac{T}{\varepsilon_F}\right)^n\right]$$

$$\frac{d\mu(T)}{dT} \le 0 \qquad \Rightarrow \qquad n \ge \frac{5}{2}$$

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

More Results...

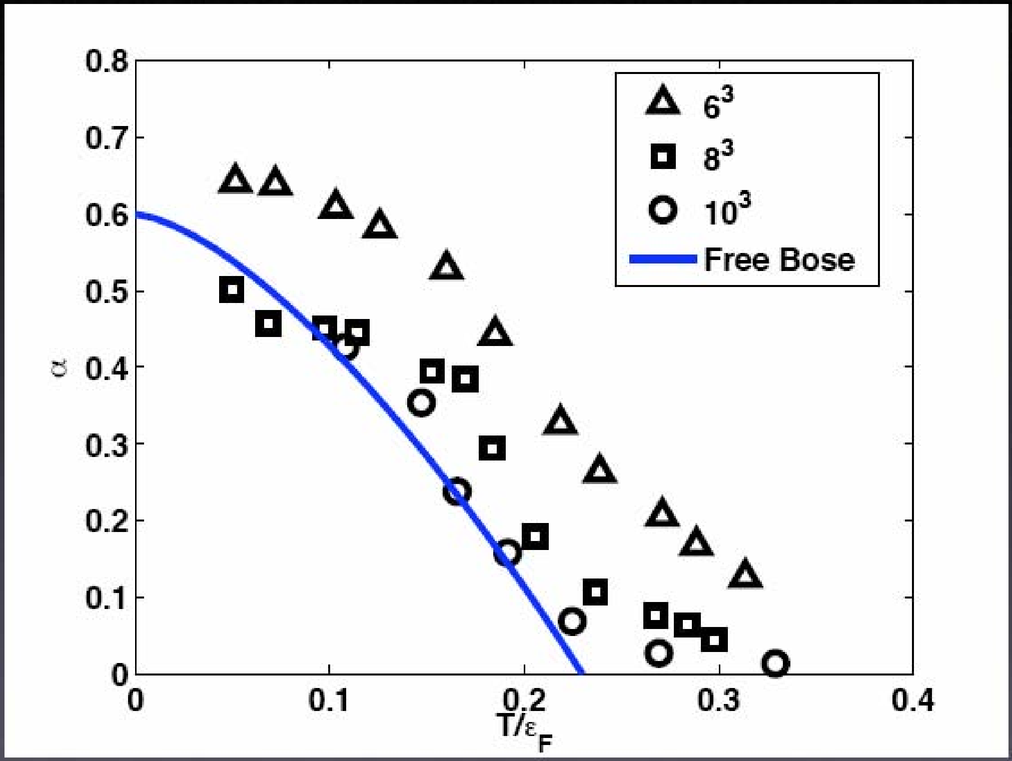
Condensate fraction α:
Order parameter for
Off Diagonal
Long Range Order
(C.N. Yang)

Free Bose gas-like:

$$\alpha(T) = \alpha(0)\left[1 - \left(\frac{T}{T_c}\right)^{3/2}\right]$$

Free : $\alpha(0) = 1$
Unitary: $\alpha(0) \cong 0.6$

$T_c = 0.23(2)$

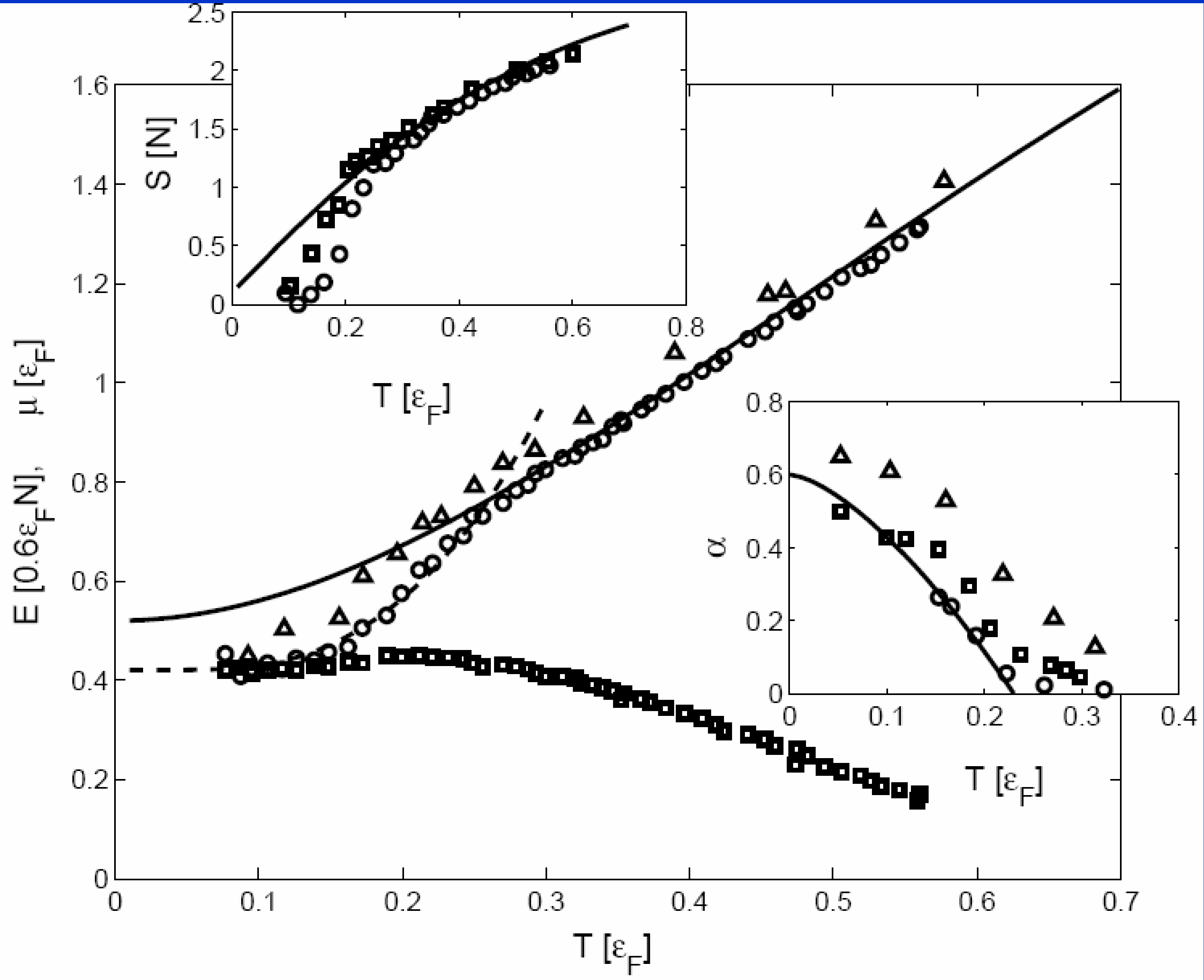


Functional form for an ideal Bose gas!

Two-body density matrix and condensate fraction

$$\left\langle \psi_\uparrow^\dagger(\vec{r}_1+\vec{r})\psi_\downarrow^\dagger(\vec{r}_2+\vec{r})\psi_\uparrow(\vec{r}_1)\psi_\downarrow(\vec{r}_2)\right\rangle \xrightarrow[r\to\infty]{} F^2(|\vec{r}_1-\vec{r}_2|)$$

From a talk of J.E. Drut



E [0.6ε_F N], μ [ε_F]
T [ε_F]
S [N]
T [ε_F]
α
T [ε_F]

Conclusions

✓ The present calculational scheme is free of the fermion sign problem (unlike the Quantum MC T=0 results). The T=0 limit of the present results confirms the QMC results.

✓ Fully non-perturbative calculations for a spin ½ many fermion system in the unitary regime at finite temperatures are feasible. This system undergoes a phase transition in the bulk at $T_c = 0.22\ (3)\ \varepsilon_F$

✓ The phase transition is observed in various thermodynamic potentials (total energy, entropy, chemical potential) as well as in the presence of off-diagonal long range order in the two-body density matrix. One can define also a thermometer.

✓ Below the transition temperature the system behaves as a free condensed Bose gas (!), which is superfluid at the same time! No thermodynamic hint of Fermionic degrees of freedom!
Above the critical temperature one observes the thermodynamic behavior of a free Fermi gas! No thermodynamic trace of bosonic degrees of freedom!

✓ New type of fermionic superfluid.