Spin 1/2 Fermions on a 3D-Lattice in the Unitary Regime at Finite Temperatures

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Also in Warsaw

Outline

- Some general remarks

- Path integral Monte Carlo for many fermions on the lattice at finite temperatures and bulk finite T properties

- 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)

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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!

<u>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.</u>

- *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!

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

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

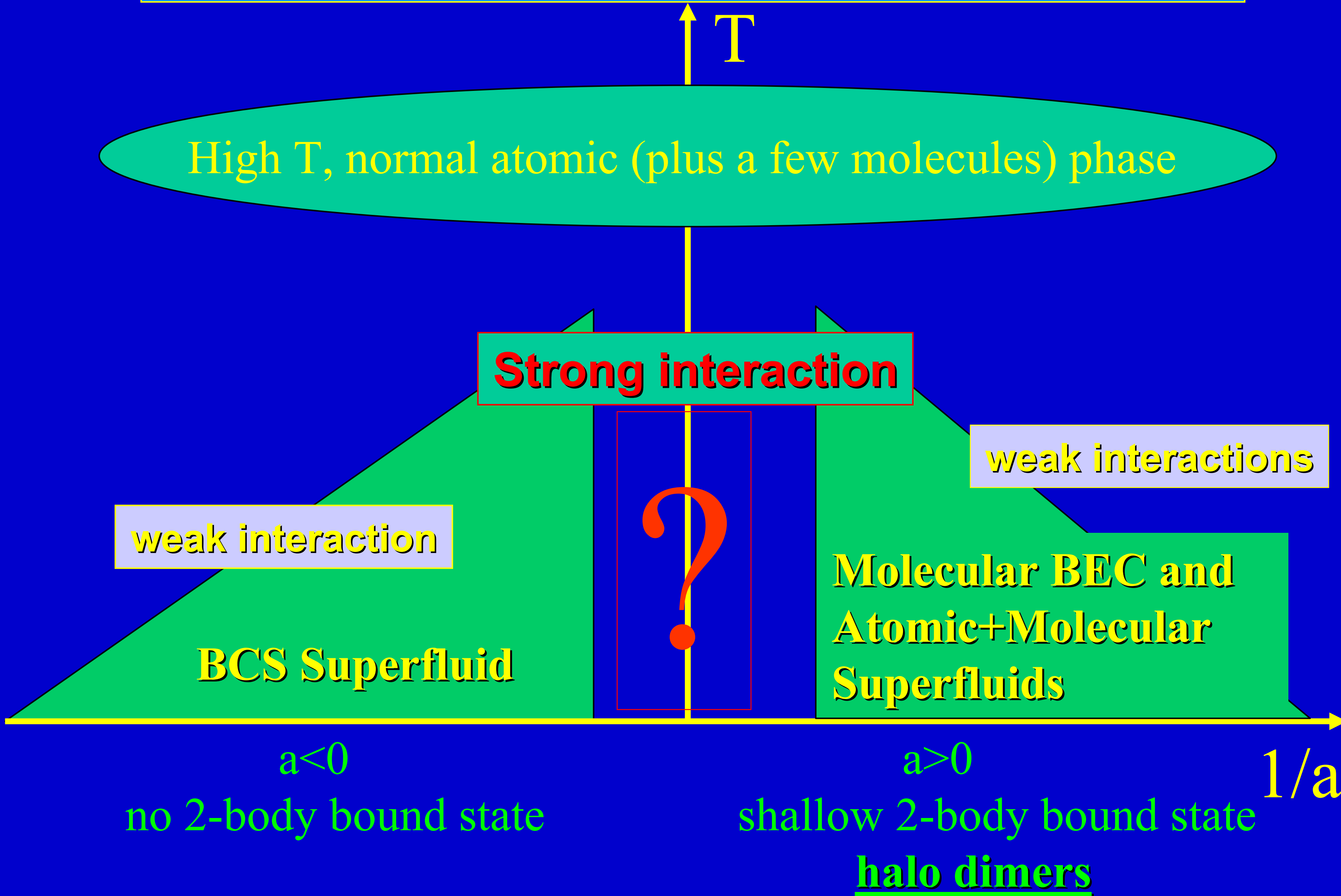
n - number density

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

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) …

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

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

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

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

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

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m}, \quad u_k^2 + v_k^2 = 1, \quad v_k^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_k - \mu}{E_k} \right)$$

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

Neglected/overlooked

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 <u>in the unitary regime</u>, where <u>the interaction between pairs is strong !!!</u> (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)!?!

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

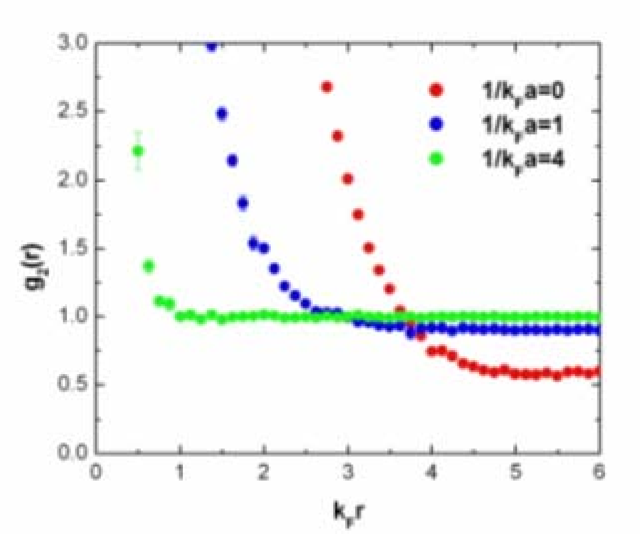
Two-body density matrix and condensate fraction

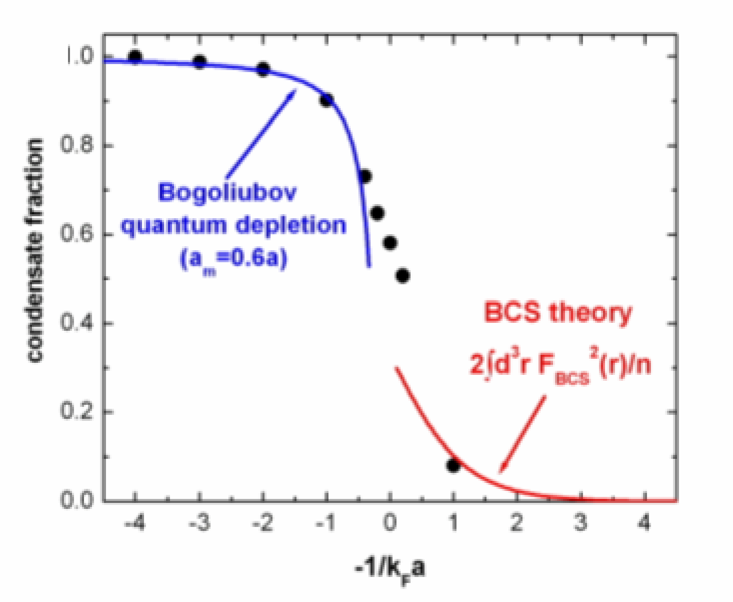
$$\left\langle \psi_\uparrow^+(\vec{r}_1+\vec{r})\psi_\downarrow^+(\vec{r}_2+\vec{r})\psi_\uparrow(\vec{r}_1)\psi_\downarrow(\vec{r}_2)\right\rangle \xrightarrow[r\to\infty]{} F^2(|\vec{r}_1-\vec{r}_2|)$$

where

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

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

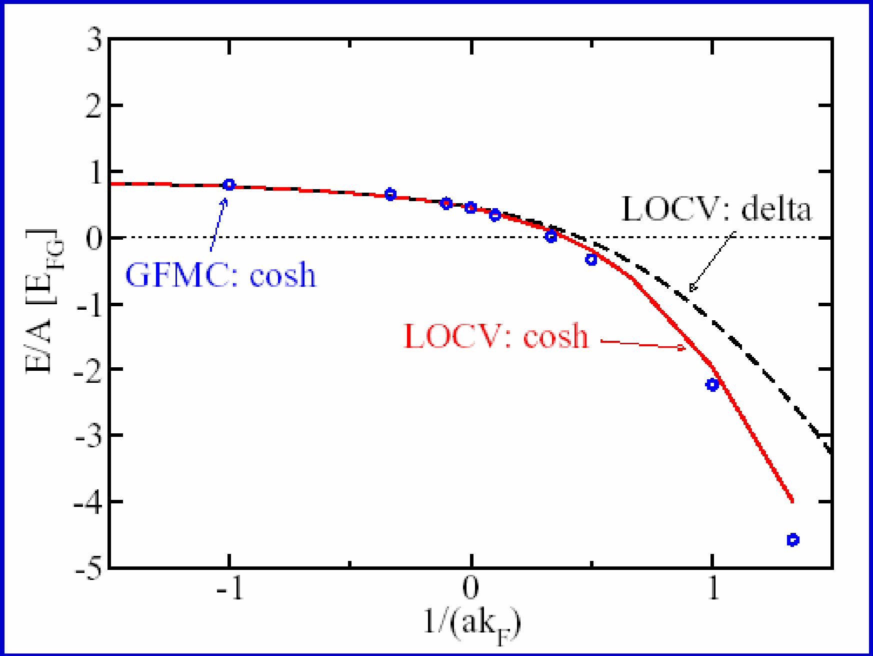


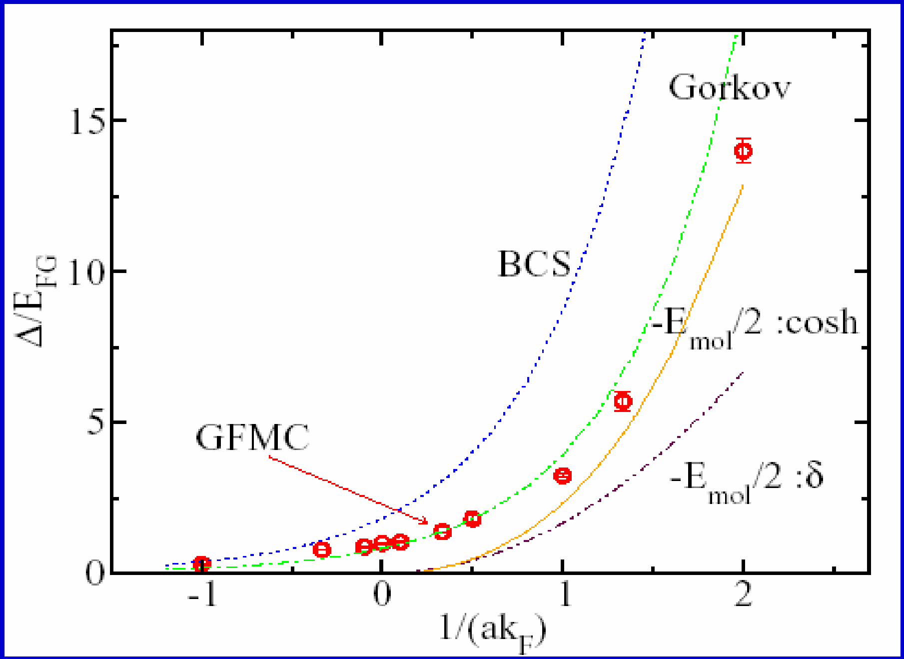


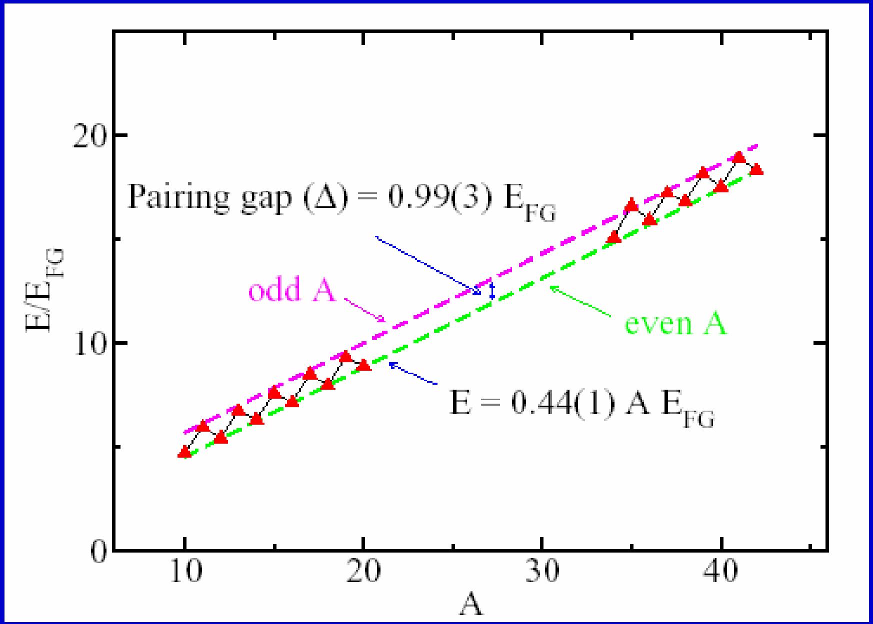
From a talk of Stefano Giorgini (Trento)

What is the best theory for the T=0 case?

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







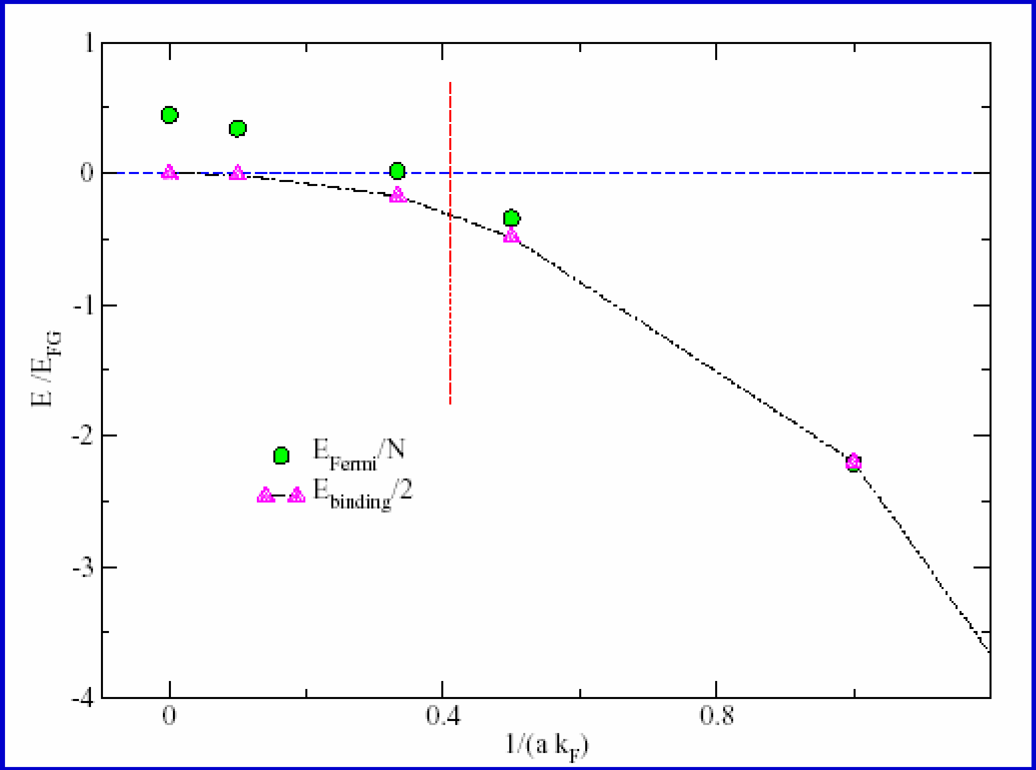
$$\Delta_{\mathrm{BCS}} \approx \frac{8}{\mathrm{e}^2}\varepsilon_F \exp\left(\frac{\pi}{2k_F a}\right)$$

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

Carlson *et al.* PRL 91, 050401 (2003)

Chang *et al.* PRA 70, 043602 (2004)

Astrakharchik *et al.* PRL 93, 200404(2004)



Even though two atoms can bind, there is no binding among dimers!

Fixed node GFMC results, J. Carlson *et al.* (2003)

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

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

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

A short detour

Let us consider the following one-dimensional Hilbert subspace
(*the generalization to more dimensions is straightforward*)

$P^2 = P$ projector in this Hilbert subspace

$$\langle x|P|y\rangle = \int_{-\frac{\pi}{l}}^{\frac{\pi}{l}} \frac{dk}{2\pi} \exp[ik(x-y)] = \frac{\sin\left[\frac{\pi}{l}(x-y)\right]}{\pi(x-y)},$$

$$\Delta_\alpha(x) = P\left[\delta\left(x - x_\alpha\right)\right], \qquad \left\langle \Delta_\alpha \mid \Delta_\beta \right\rangle = \Delta_\alpha(x_\beta) = \Delta_\beta(x_\alpha) = K_\alpha \delta_{\alpha\beta}$$

$$\psi(x) = \sum_{\alpha=1}^{N} c_\alpha \Delta_\alpha(x) + O(\exp(-cN)) \approx \sum_n \psi(nl) \frac{\sin\left[\frac{\pi}{l}(x-nl)\right]}{\frac{\pi}{l}(x-nl)}$$

$$c_\alpha = \int dx \frac{1}{K_\alpha} \Delta_\alpha(x)\psi(x) = \frac{1}{K_\alpha}\psi(x_\alpha), \qquad x_\alpha = nl$$

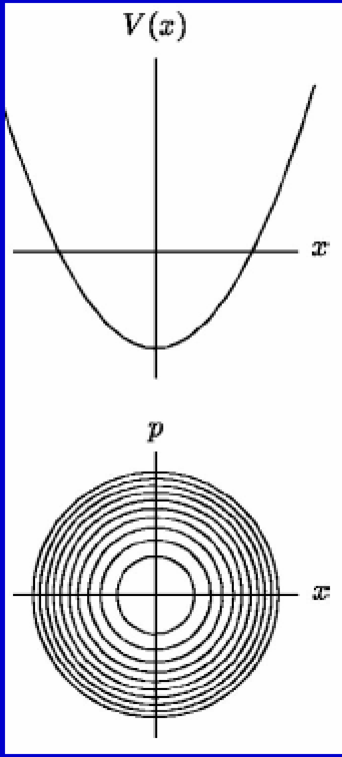
Littlejohn *et al*. J. Chem. Phys. **116**, 8691 (2002)

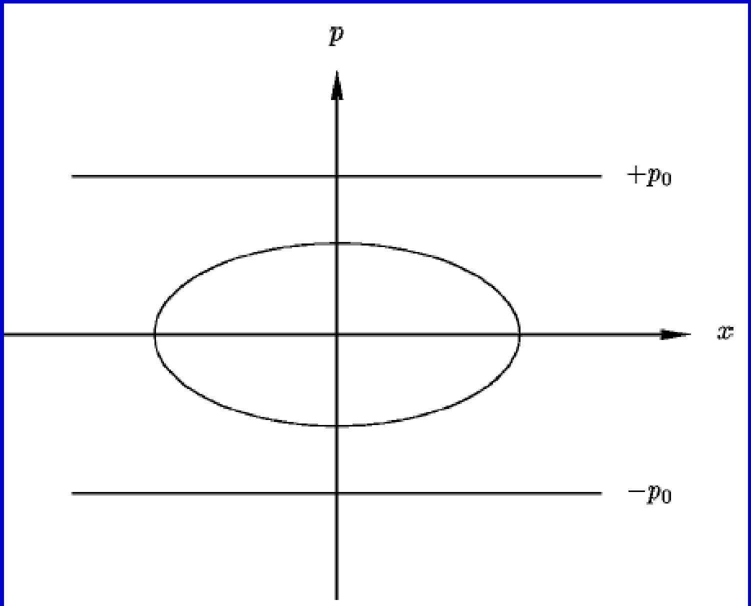
Schroedinger equation

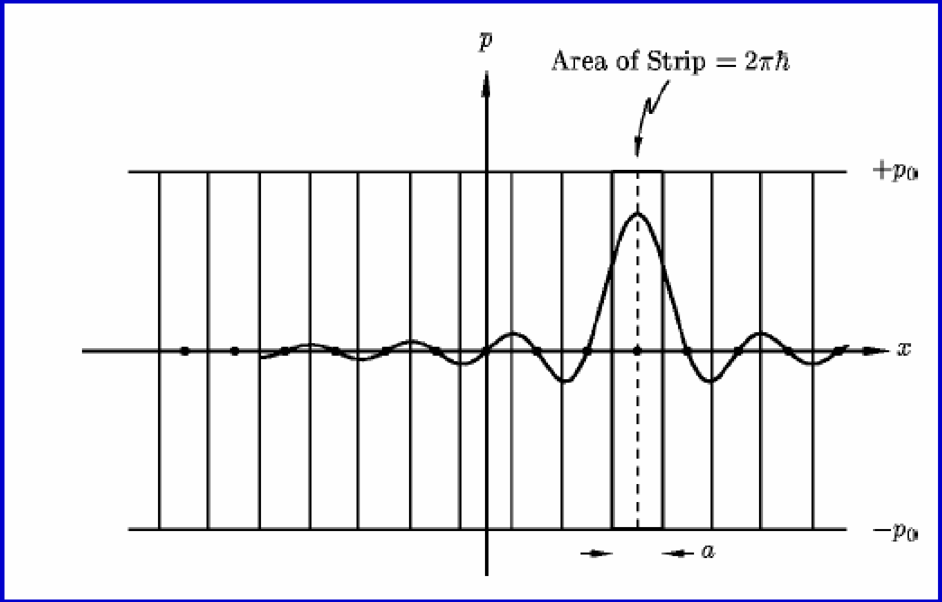
$$\psi(x) = \sum_{\alpha=1}^{N} d_\alpha F_\alpha(x) + O(\exp(-cN))$$

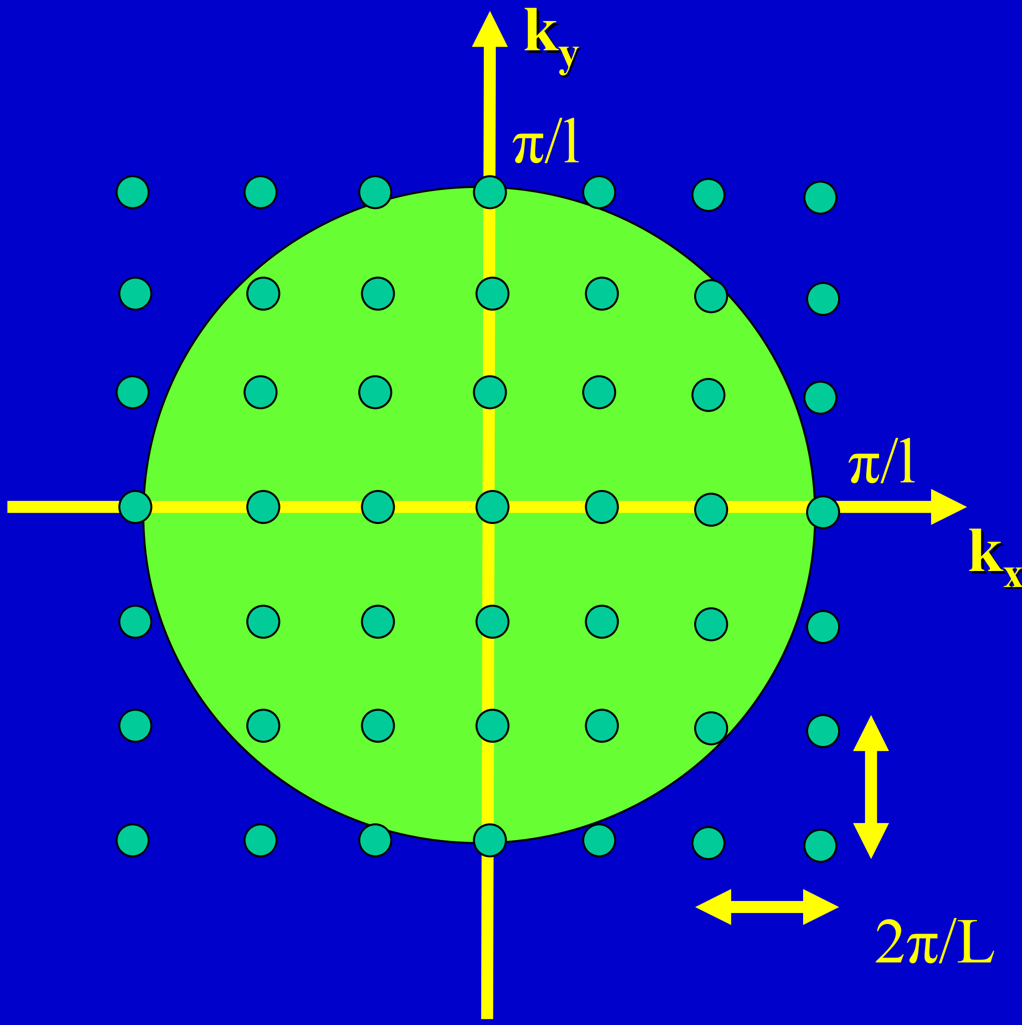
$$F_\alpha(x) = \frac{1}{\sqrt{K_\alpha}} \Delta_\alpha(x), \quad x_\alpha = nl, \qquad \langle F_\alpha \mid F_\beta \rangle = \delta_{\alpha\beta}$$

$$\sum_\beta \left[\langle F_\alpha \mid T \mid F_\beta \rangle + V(x_\alpha)\delta_{\alpha\beta} \right] d_\beta = E d_\alpha$$









Momentum space

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

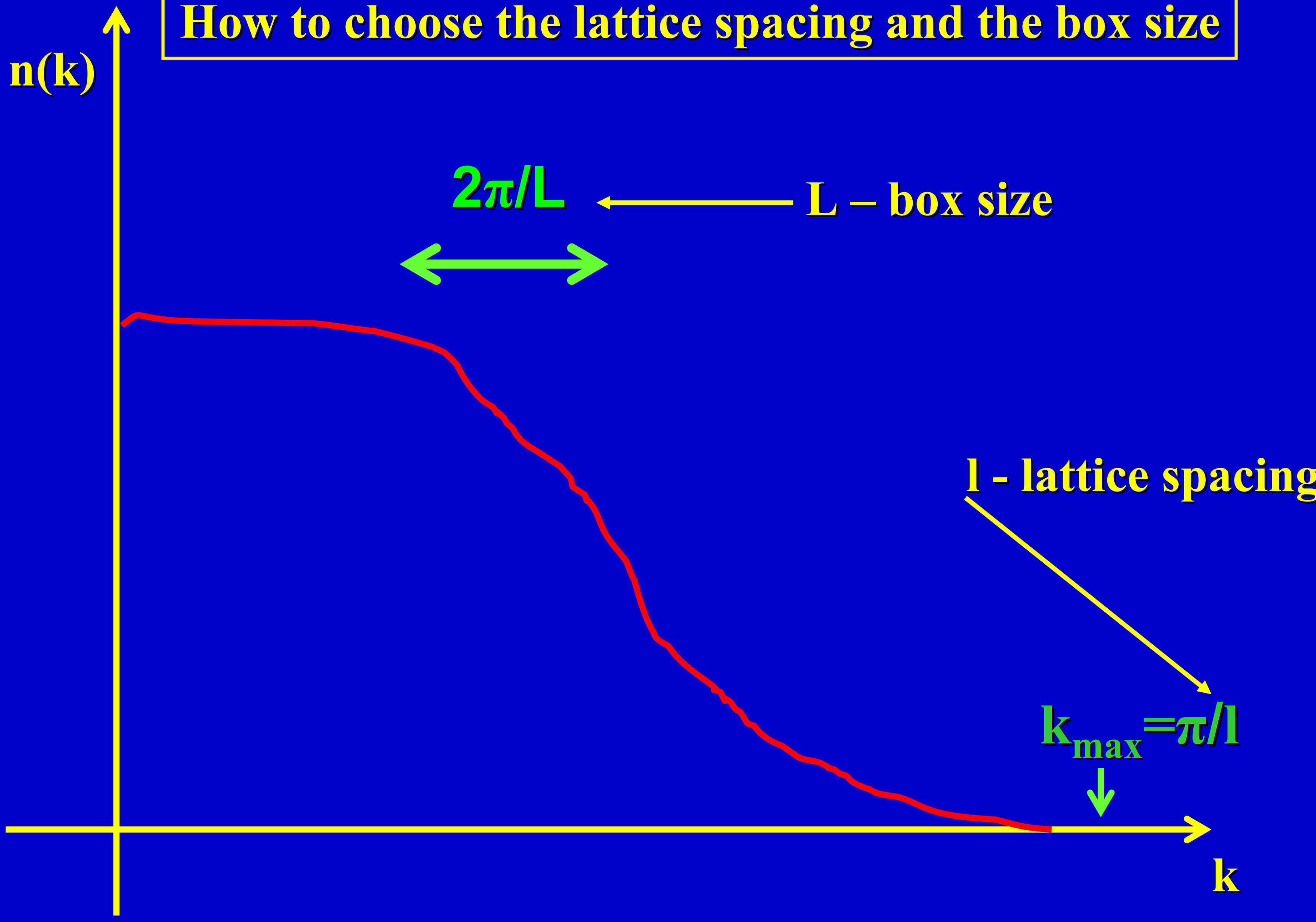
$$\delta\varepsilon > \frac{2\hbar^2\pi^2}{mL^2}$$

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

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

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

How to choose the lattice spacing and the box size



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

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

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!

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

<u>All traces can be expressed through these single-particle density matrices</u>

More details of the calculations:

- Lattice sizes used from 6^3 x 300 (high Ts) to 6^3 x 1361 (low Ts)

8^3 running (incomplete, but so far no surprises) and larger sizes to come

• 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 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

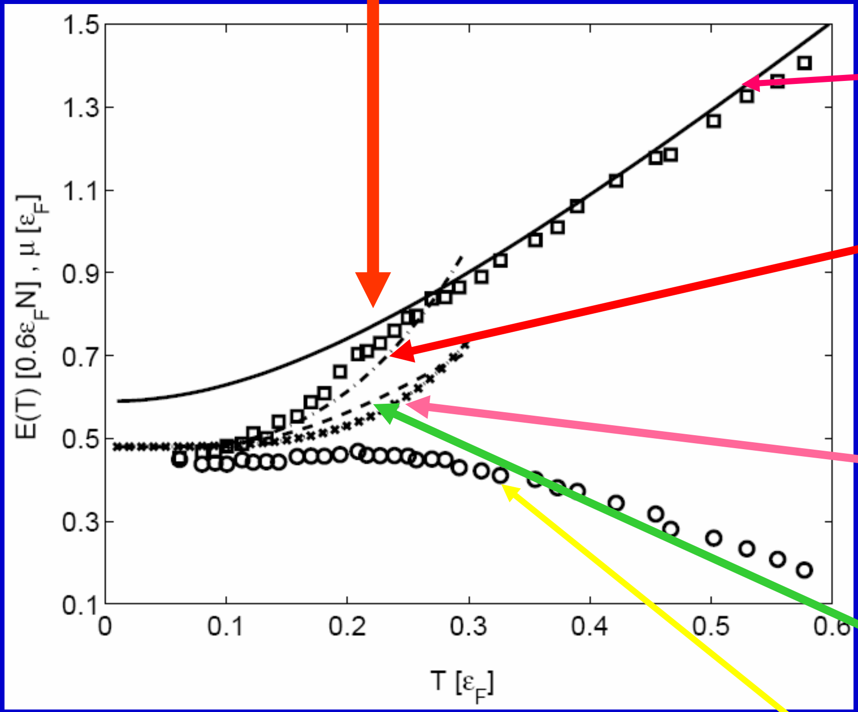
• At low temperatures use Singular Value Decomposition of the evolution operator $U(\{\sigma\})$ to stabilize the numerics

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

• MC correlation "time" ≈ 250 – 300 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
(dot-dashed lien)

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

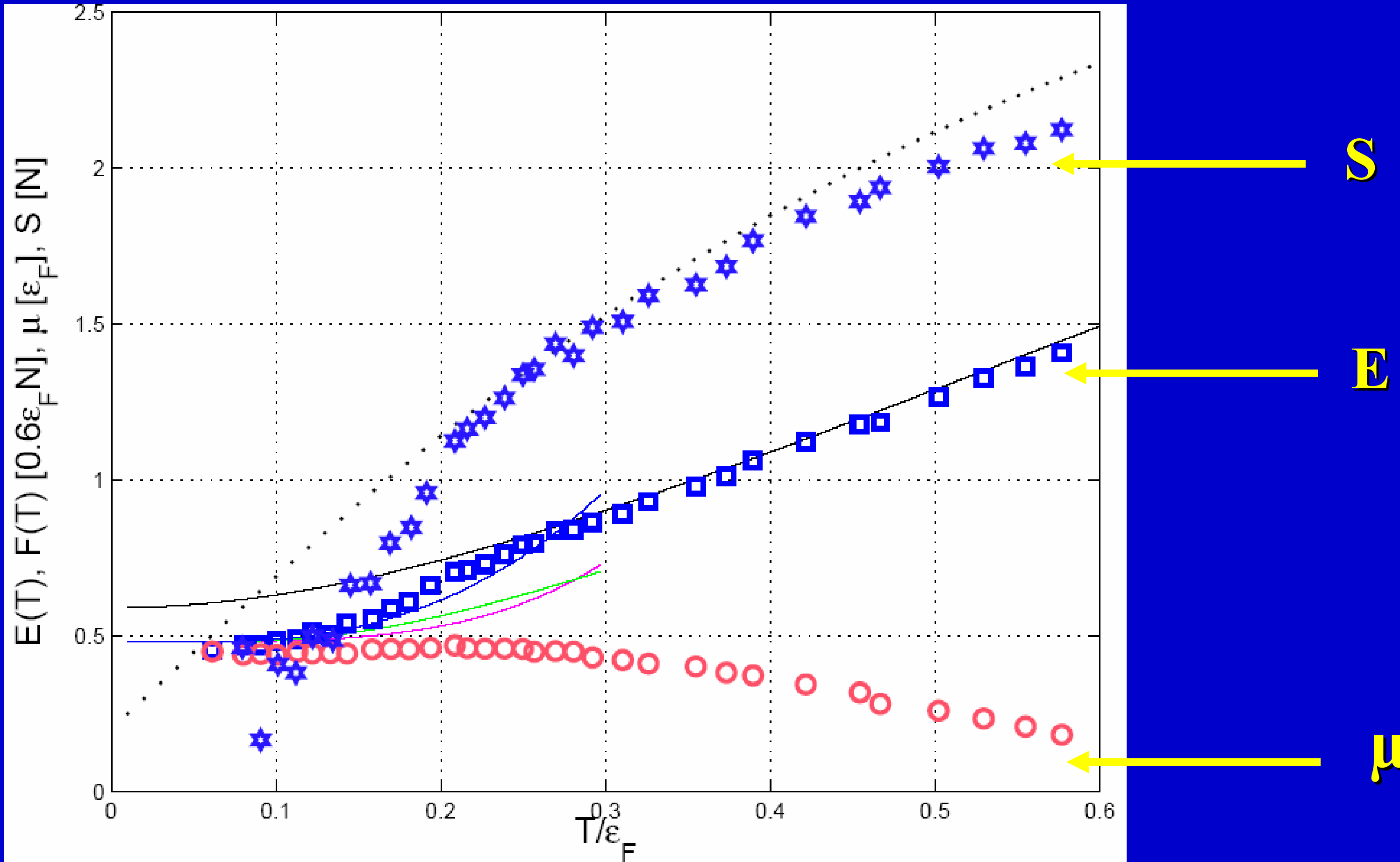
Quasi-particles contribution only
(dashed line)

μ - chemical potential
(circles)

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

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

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



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

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

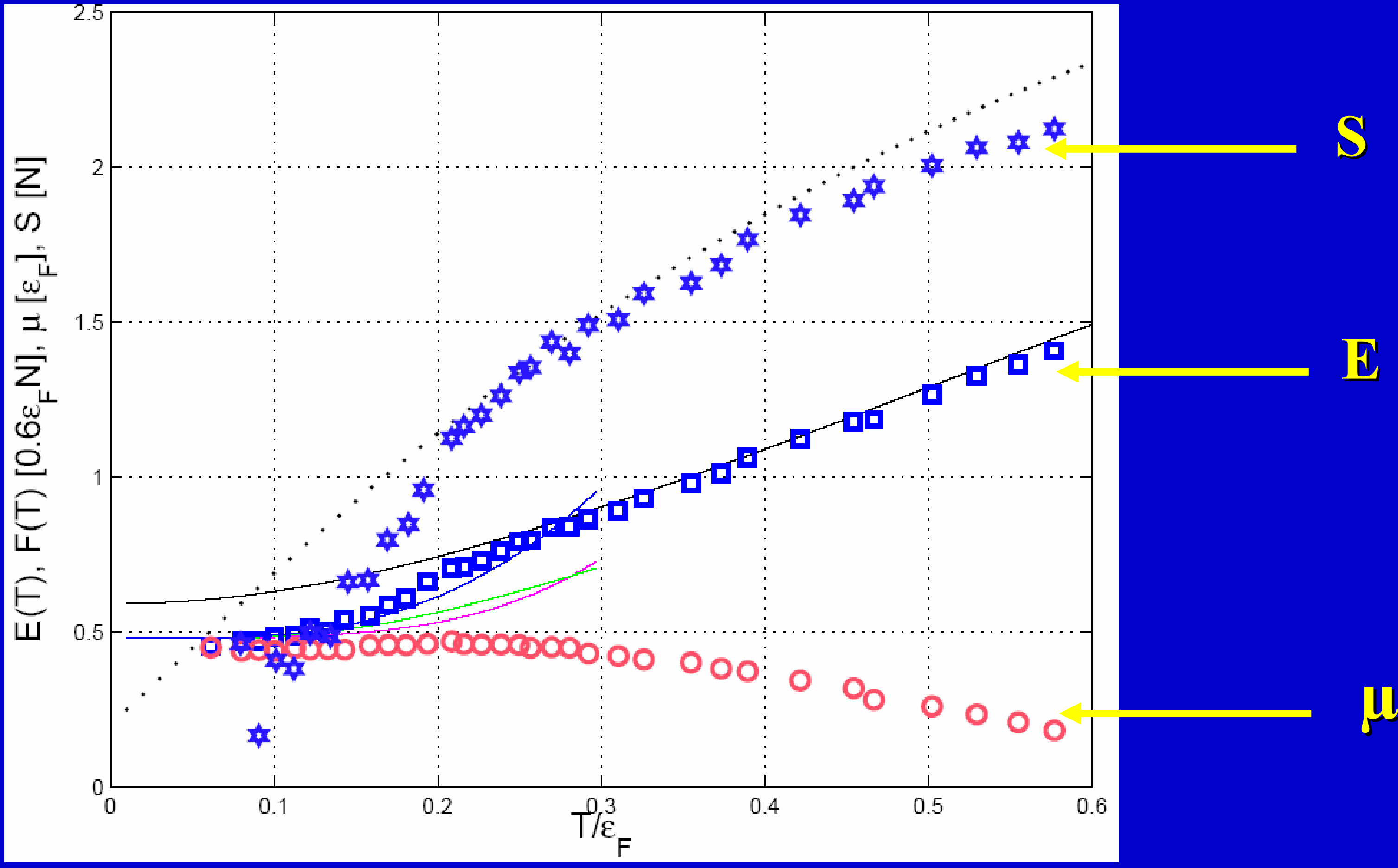
$$S = \frac{\frac{5}{3}e(n) - \mu}{T}N = N\sigma\left(\frac{T}{\varepsilon_F(n)}\right), \quad P = \frac{2}{3}e(n)n$$

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**



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

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

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

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

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

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

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

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

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

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?**

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 $n=2.5(0.25)$

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 $T_c = 0.22\ (3)\ \varepsilon_F$**

(One variant of the fortran 90 program, version in matlab, has about 500 lines, and it can be shortened also. This is about as long as a PRL!**)**

✓ **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.**