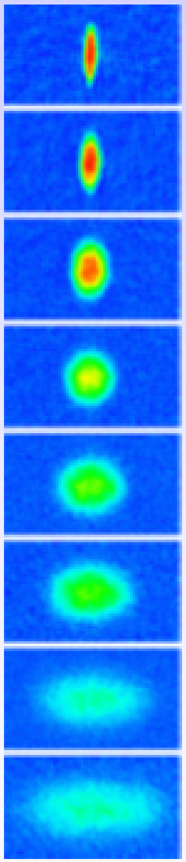
Fermions on a Lattice in the Unitary Regime at Finite Temperatures

Aurel Bulgac, Joaquin E. Drut and Piotr Magierski
University of Washington, Seattle, WA

Also in Warsaw

Why Study Fermi Gases ?

Duke Physics
Atom Cooling and Trapping



- Fermions are the building blocks of matter
- Strongly-interacting Fermi gases are stable
- Link to other interacting Fermi systems:
  - High-T_C superconductors – Neutron stars
  - Lattice field theory
  - Quark-gluon plasma of Big Bang
  - String theory!

O'Hara et al., Science 2002

From a talk of J.E. Thomas (Duke)

Outline

- What is the unitary regime?

- The two-body problem, how one can manipulate the two-body interaction? Feshbach resonance

- Brief overview of existing theoretical understanding

- Path integral Monte Carlo for many fermions on the lattice at finite temperatures

- Conclusions

What is the *Holy Grail* of this field?

Fermionic superfluidity!

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)

➢ 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.

The system is very dilute, but strongly interacting!

$$n\, r_0^3 \ll 1$$

$$n\, |a|^3 \gg 1$$

n - number density

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

r_0 - range of interaction

a - scattering length

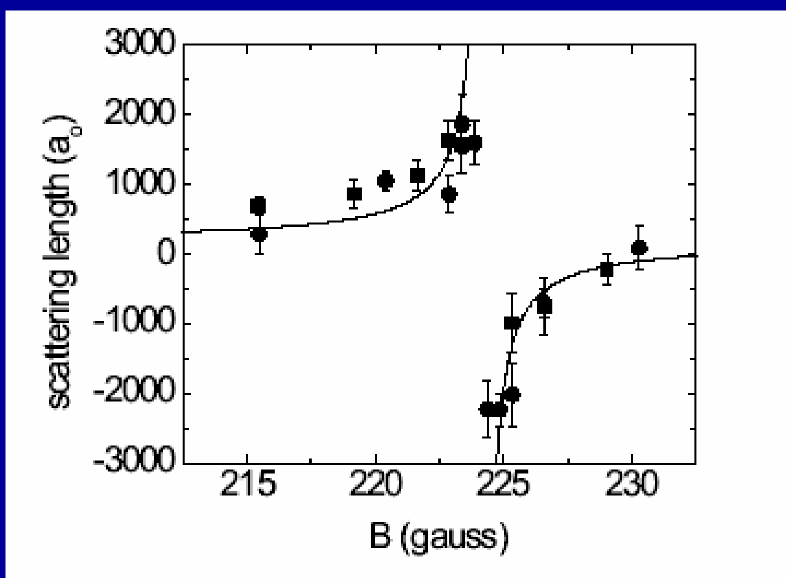
Feshbach resonance

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

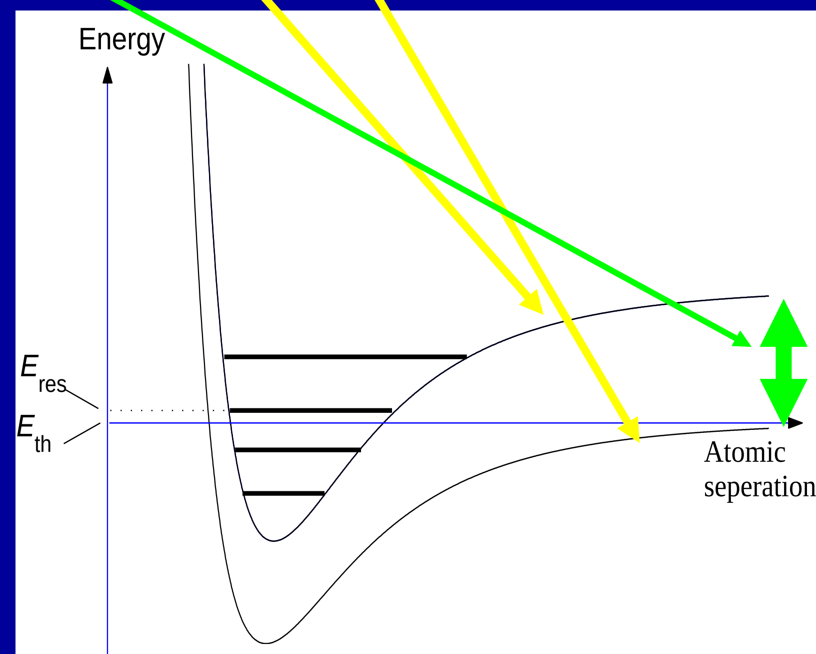
$$V^{hf} = \frac{a_{hf}}{\hbar^2}\vec{S}^{e}\cdot\vec{S}^{n},\; V^{Z} = (\gamma_e S_z^e - \gamma_n S_z^n)B$$

Channel coupling

Tiesinga, Verhaar, Stoof
Phys. Rev. A**47**, 4114 (1993)



Regal and Jin
Phys. Rev. Lett. **90**, 230404 (2003)



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>

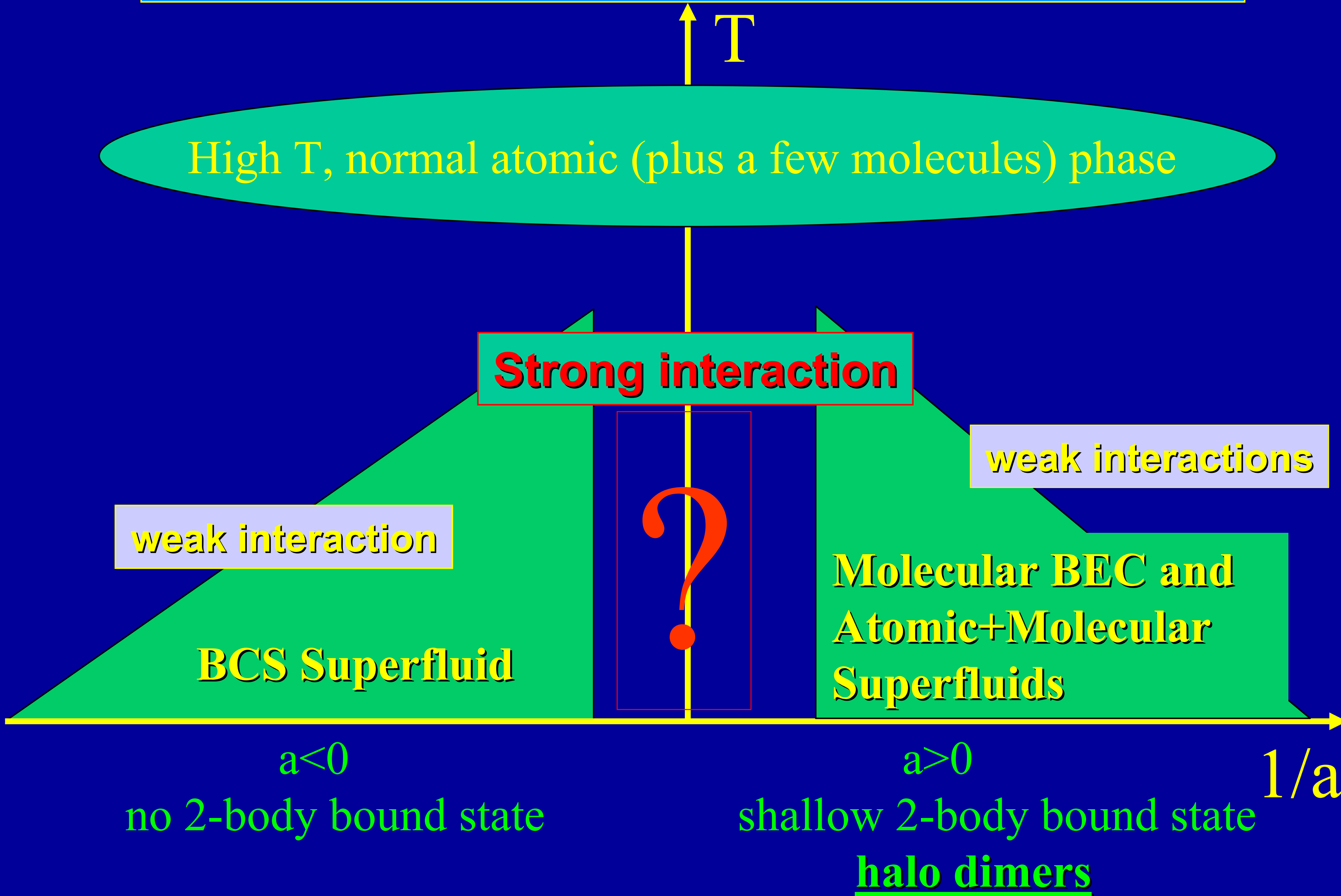
- ***systems of bosons are unstable (Efimov effect)***
- ***systems of three or more fermion species are unstable (Efimov effect)***

- **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.**

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



Early theoretical approach

Eagles (1969), Leggett (1980) …

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

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

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

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

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)

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

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

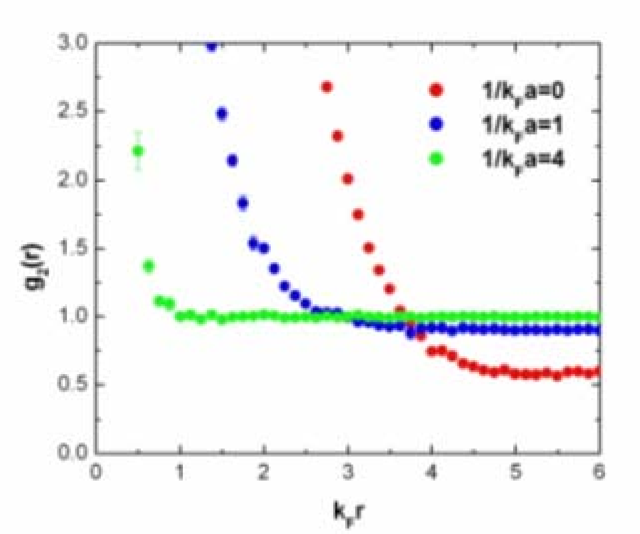
Two-body density matrix and condensate fraction

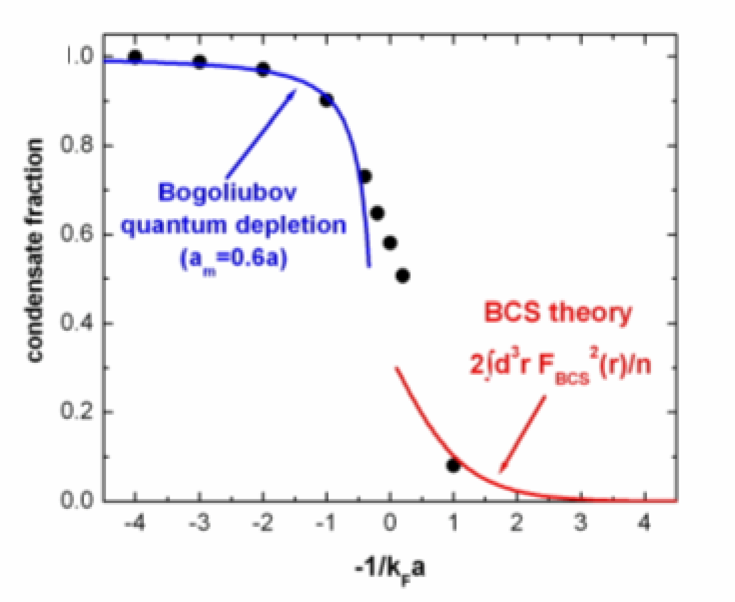
$$\left\langle \psi_{\uparrow}^{+}(\vec{r}_1+\vec{r})\psi_{\downarrow}^{+}(\vec{r}_2+\vec{r})\psi_{\uparrow}(\vec{r}_1)\psi_{\downarrow}(\vec{r}_2)\right\rangle \xrightarrow[r\to\infty]{} F^2(|\vec{r}_1-\vec{r}_2|)$$

where

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

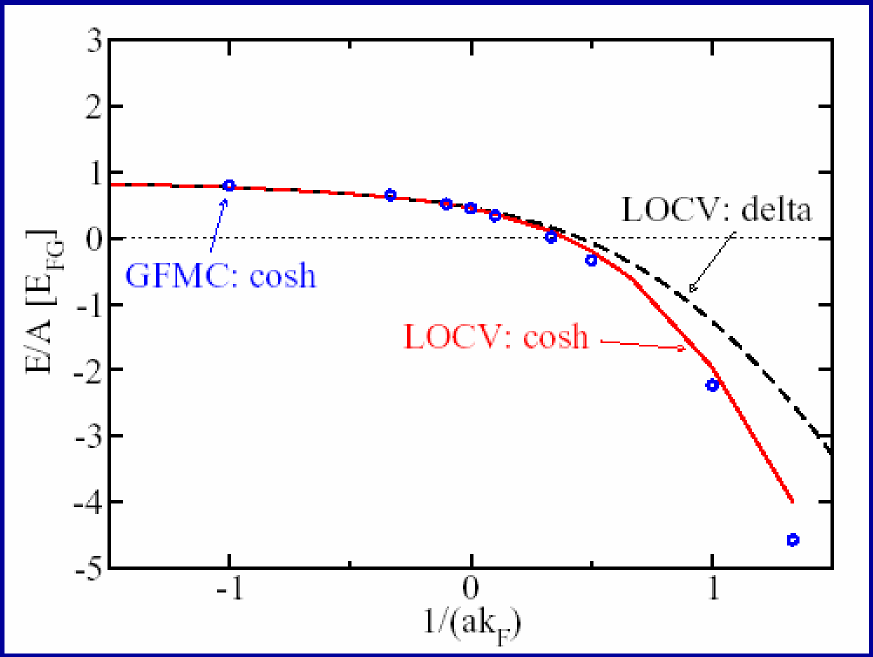
$$g_2(r)=\frac{2}{N}\int d^3r_1 d^3r_2 \left\langle \psi_{\uparrow}^{+}(\vec{r}_1+\vec{r})\psi_{\downarrow}^{+}(\vec{r}_2+\vec{r})\psi_{\uparrow}(\vec{r}_1)\psi_{\downarrow}(\vec{r}_2)\right\rangle$$

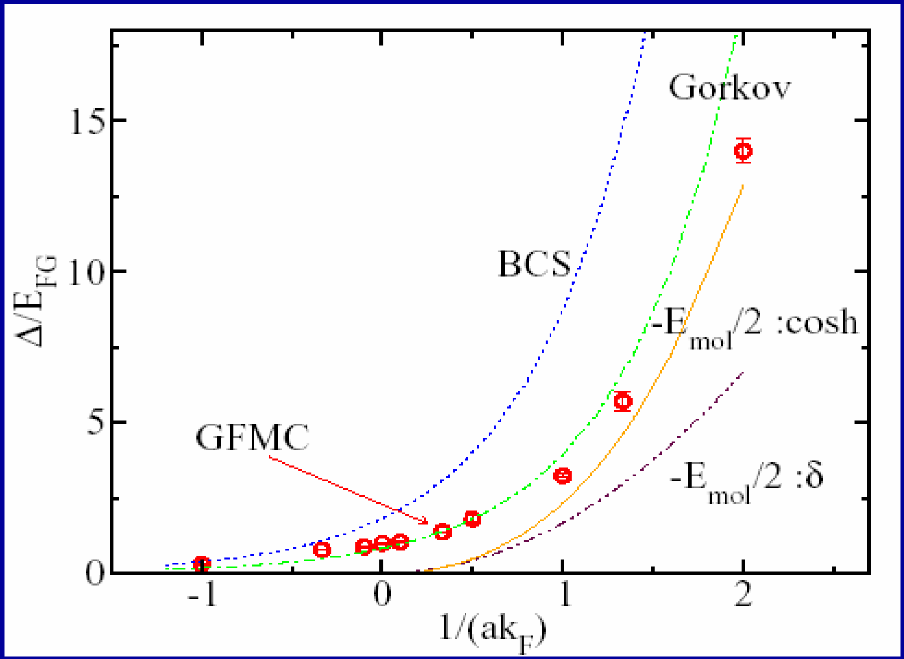


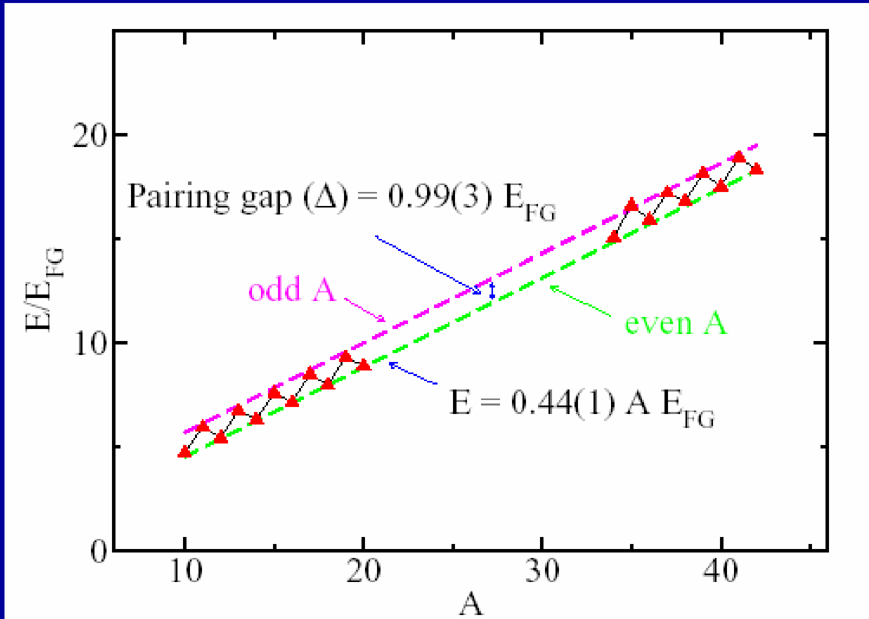


From a talk of Stefano Giorgini (Trento)

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







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

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

$$E_{\rm FG} = \frac{3}{5}\varepsilon_F$$

Carlson *et al.* PRL <u>91</u>, 050401 (2003)
Chang *et al.* PRA <u>70</u>, 043602 (2004)

Finite Temperatures

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!

How to implement the path integral?

Put the system on a spatio-temporal 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

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

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

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

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

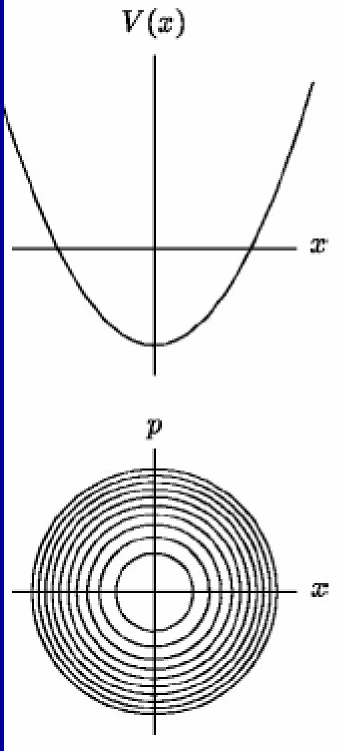
Littlejohn *et al*. J. Chem. Phys. **116**, 8691 (2002)

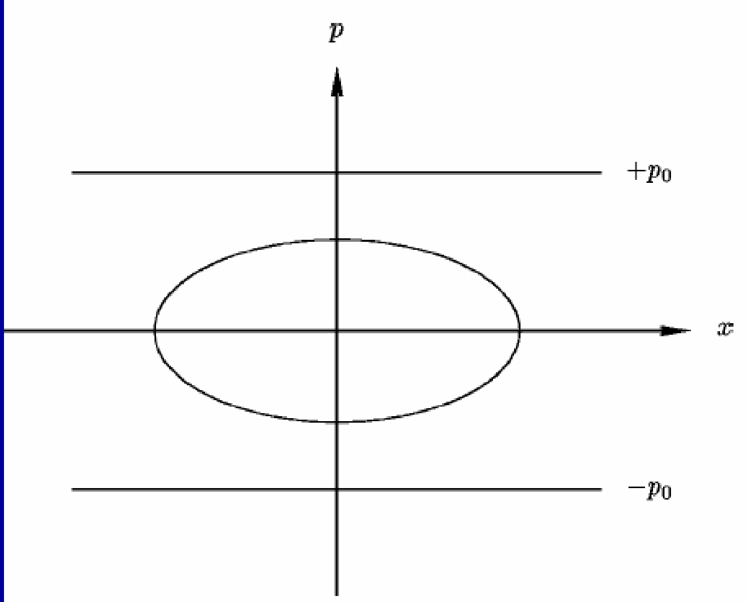
Schroedinger equation

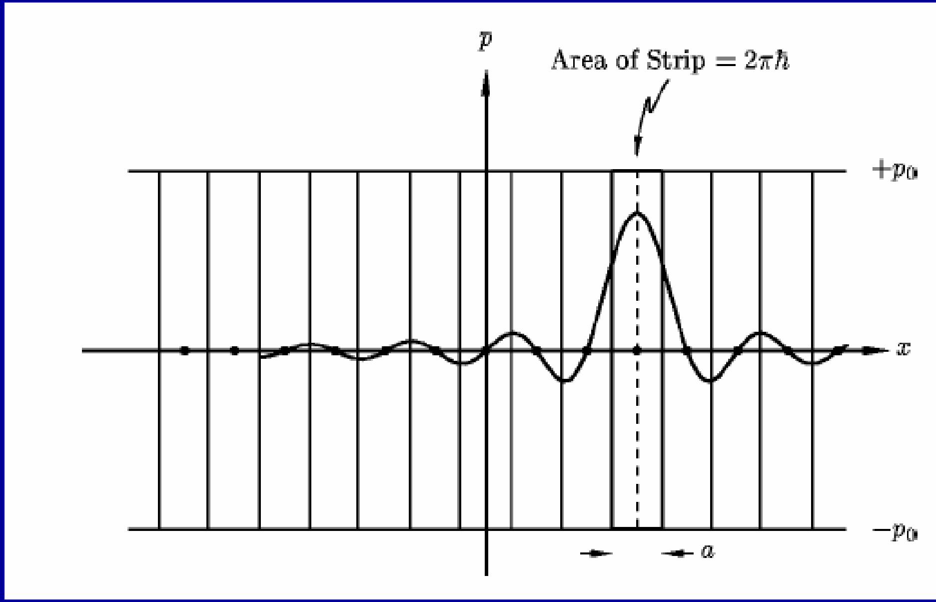
$$\psi(x) = \sum_{\alpha=1}^{N} d_\alpha F_\alpha(x) + O(\exp(-cN))$$

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

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







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

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

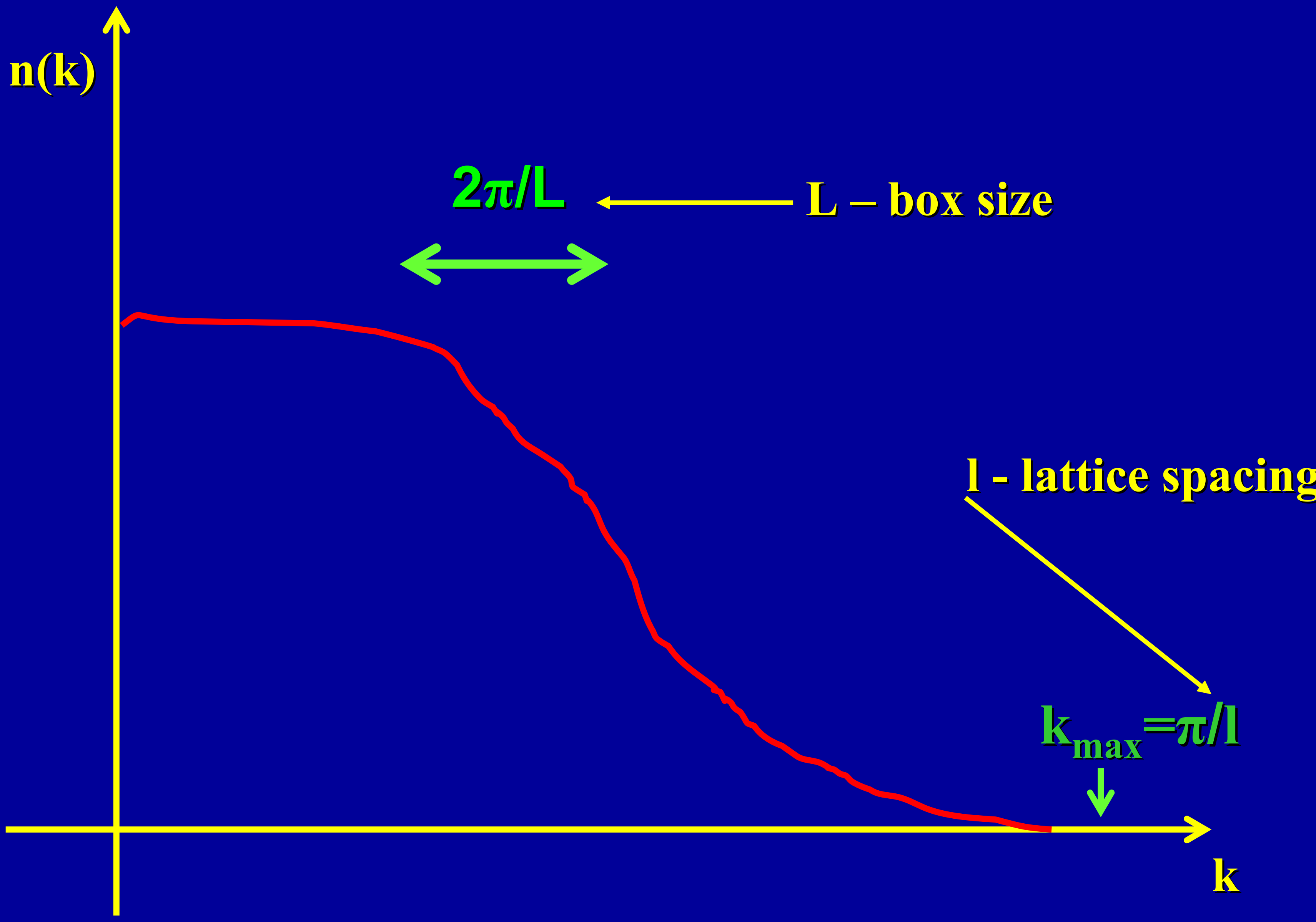
Discrete Hubbard-Stratonovich transformation

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

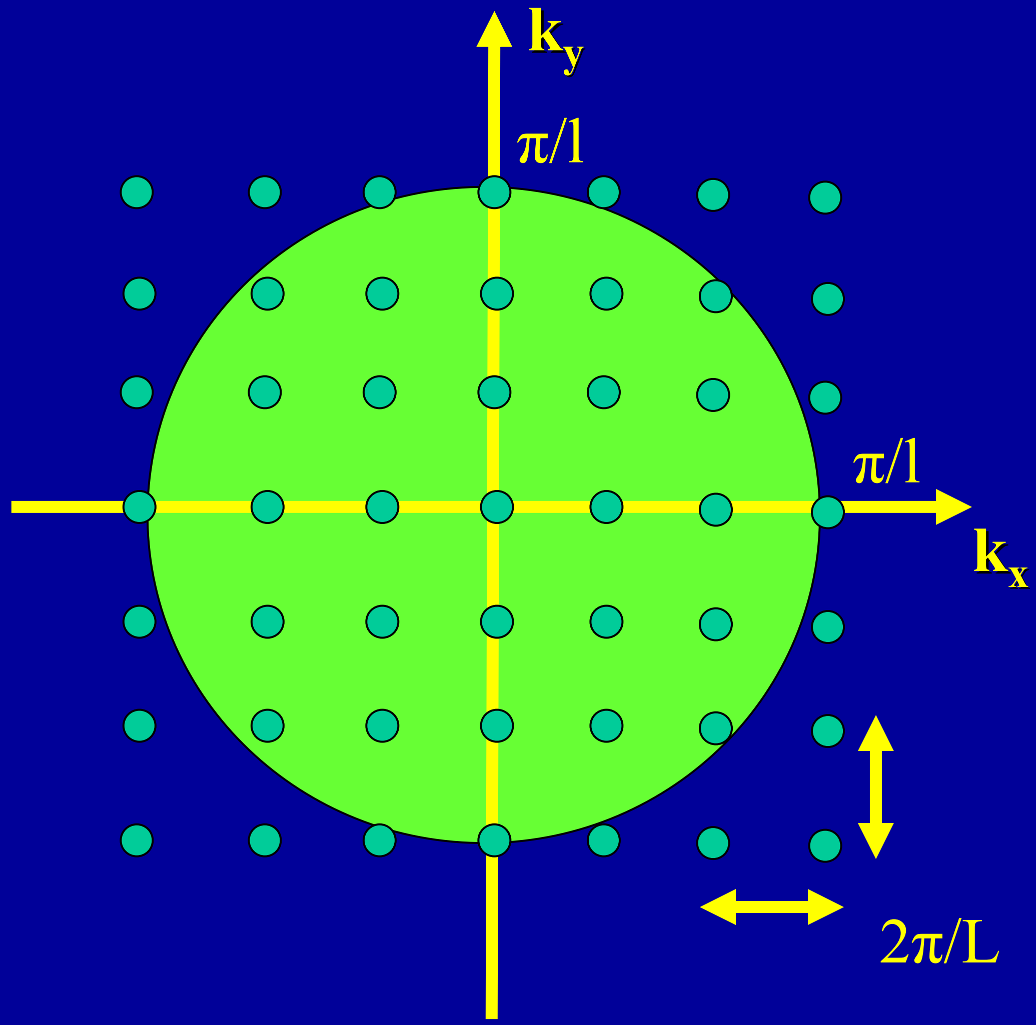
σ-fields fluctuate both in space and imaginary time

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

Running coupling constant g defined by lattice



How to choose the lattice spacing and the box size



Momentum space

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

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

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

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

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

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

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

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!

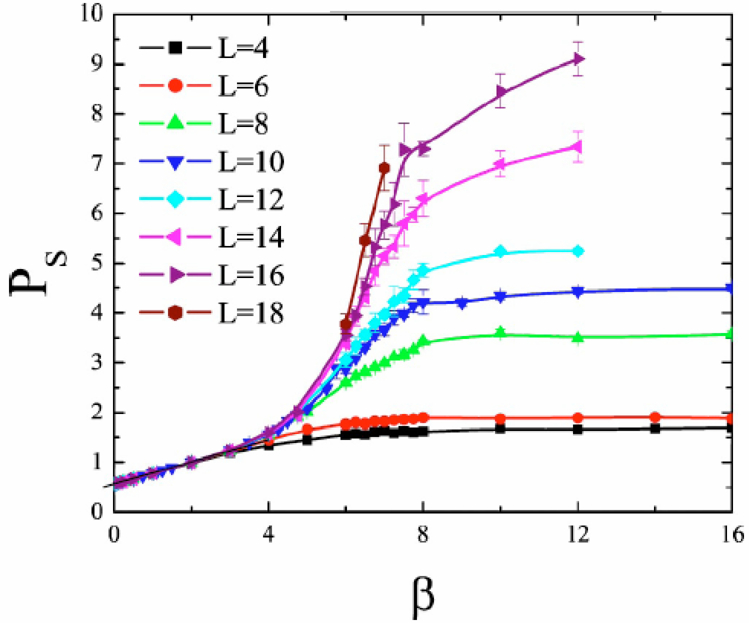
$$n_\uparrow(\vec{x},\vec{y})=n_\downarrow(\vec{x},\vec{y})=\sum_{k,l<k_c}\varphi_{\vec{k}}(\vec{x})\left[\frac{\hat{U}(\{\sigma\})}{1+\hat{U}(\{\sigma\})}\right]_{\vec{k}\ \vec{l}}\varphi^*_{\vec{l}}(\vec{y}),\qquad \varphi_{\vec{k}}(\vec{x})=\frac{\exp(i\vec{k}\cdot\vec{x})}{\sqrt{V}}$$

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

PHYSICAL REVIEW B **69**, 184501 (2004)

Critical temperature for the two-dimensional attractive Hubbard model

Thereza Paiva,[1] Raimundo R. dos Santos,[1] R. T. Scalettar,[2] and P. J. H. Denteneer[3]



$$P_s = \langle \Delta^\dagger \Delta + \Delta \Delta^\dagger \rangle \tag{2}$$

with

$$\Delta^\dagger = \frac{1}{\sqrt{N}} \sum_i c^\dagger_{\mathbf{i}\uparrow} c^\dagger_{\mathbf{i}\downarrow} . \tag{3}$$

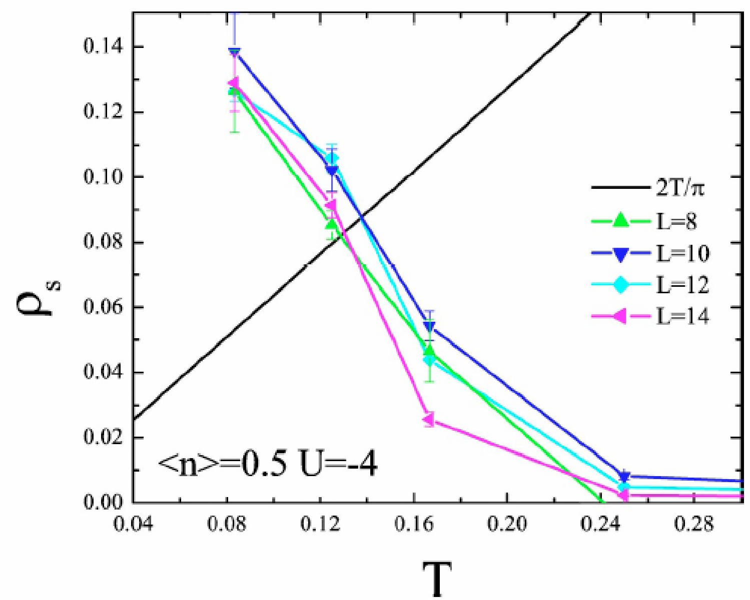


FIG. 4. (Color online) Helicity modulus as a function of temperature for $\langle n \rangle = 0.5$ and different lattice sizes L. The straight line corresponds to $2T/\pi$.

$$T_c = \frac{\pi}{2} \rho_s^- , \tag{14}$$

PHYSICAL REVIEW B **66**, 140504(R) (2002)

Quantum Monte Carlo study of the three-dimensional attractive Hubbard model

Alain Sewer,[1,2] Xenophon Zotos,[1] and Hans Beck[2]

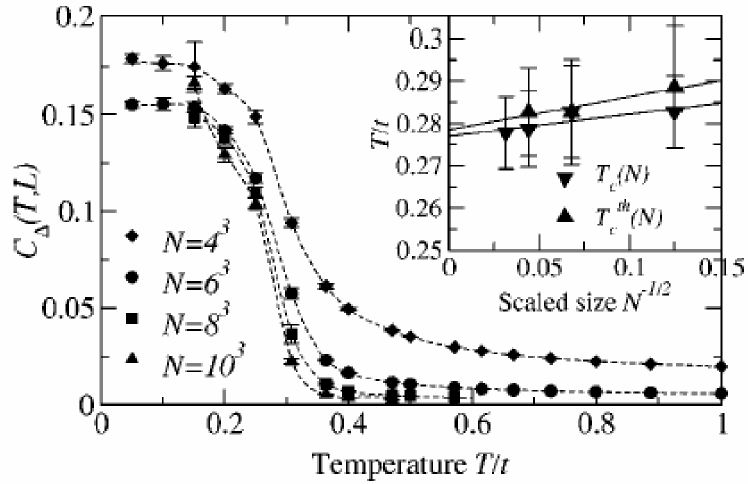


FIG. 1. *Main*, temperature and size dependences of the pair-pair correlation function (2) for the case $U=6t$ and $n=0.5$. *Inset*, linear extrapolation to the thermodynamic limit of the size-dependent critical temperatures $T_c(N)$ and $T_c^{\mathrm{th}}(N)$, same U and n.

$$C_\Delta(T,N)=\frac{1}{N}\sum_{i,j}\langle \Delta_i\Delta_j^\dagger+\Delta_j\Delta_i^\dagger\rangle, \tag{2}$$

$$\chi_P(T,N)=\frac{1}{T}\frac{1}{N}\sum_{i,j}\langle \mathbf{S}_i\cdot\mathbf{S}_j\rangle. \tag{3}$$

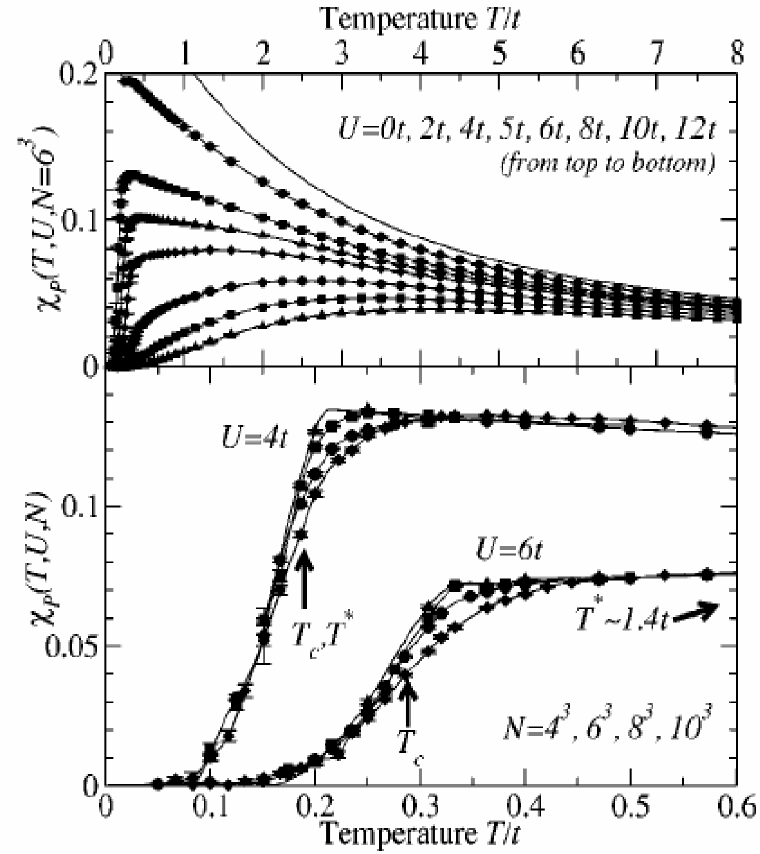


FIG. 3. Pauli susceptibility χ_P. *Top*, T dependence for various values of U (size $N=6^3$). *Bottom*, T and N dependence close to the transition temperature and separation of T_c and T^*, same symbols as in Fig. 1 ($n=0.5$ for both cases).

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

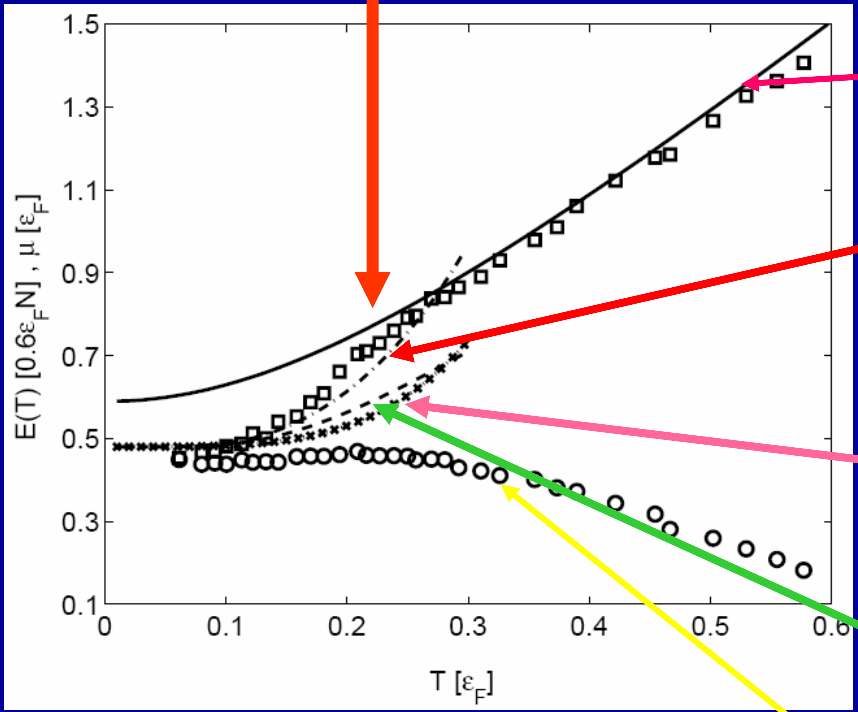
- At low temperatures use Singular Value Decomposition of the evolution operator $U(\{\sigma\})$ to stabilize the numerics

- 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)
People never consider this ???

Quasi-particles contribution only
(dashed line)

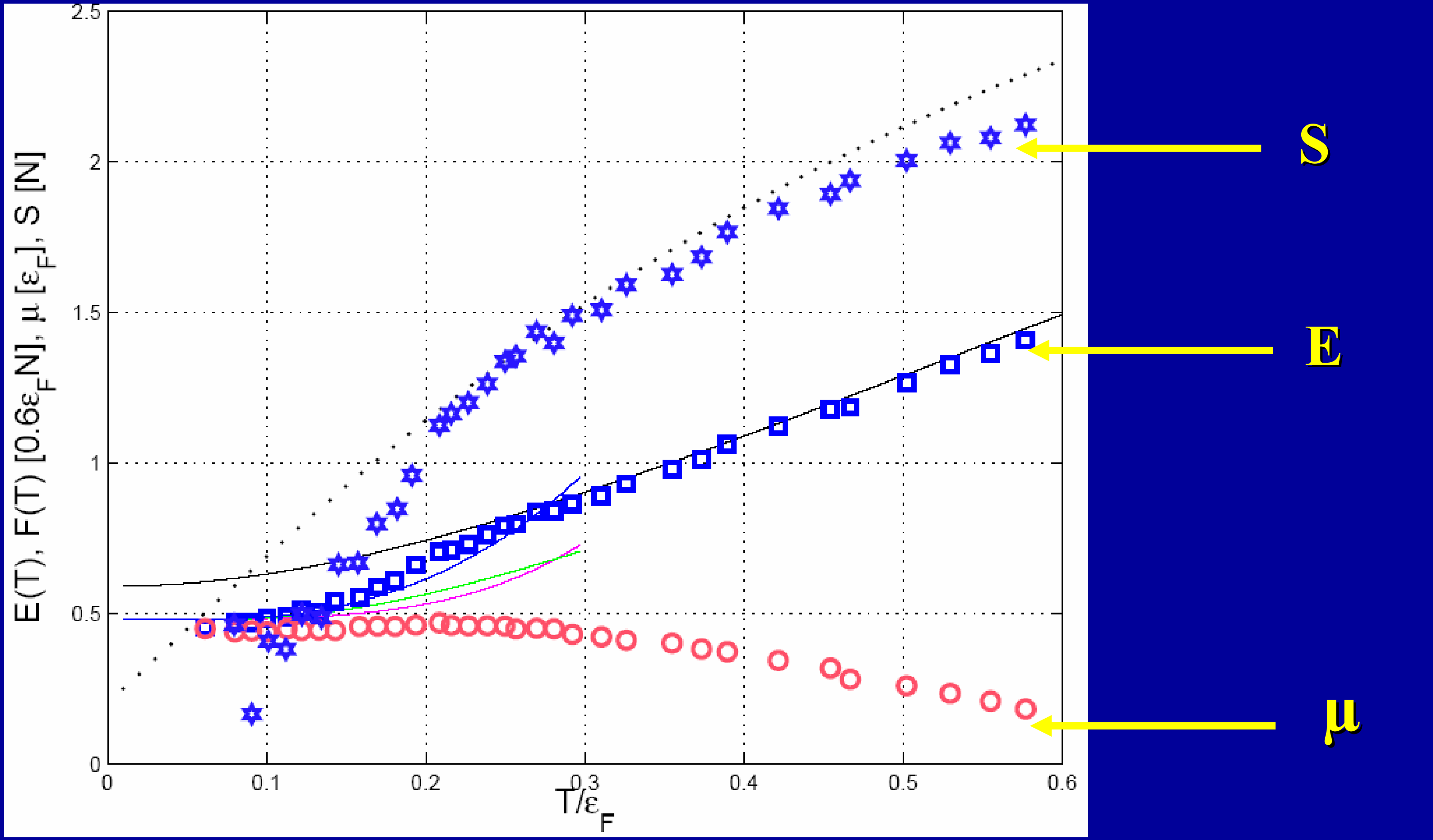
μ - chemical potential
(circles)

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

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

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

$$\frac{C_s(T_c)}{C_n(T_c)} \approx 2 \qquad (2.43 \text{ in BCS})$$



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

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

$$S = N\sigma\left(\frac{T}{\varepsilon_F(n)}\right), \qquad P = \frac{2}{3}\varepsilon(n)n$$

Conclusions

✓ **Fully non-perturbative calculations for a spin ½ many fermion system in the unitary regime at finite temperatures are feasible**

(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!)

✓ **Apparently the system undergoes a phase transition at $T_c = 0.22\ (3)\ \varepsilon_F$**

✓ **Below the transition temperature both phonons and (fermionic) quasiparticles contribute almost equally to the specific heat**