Fermions in the unitary regime at finite temperatures from path integral auxiliary field Monte Carlo simulations

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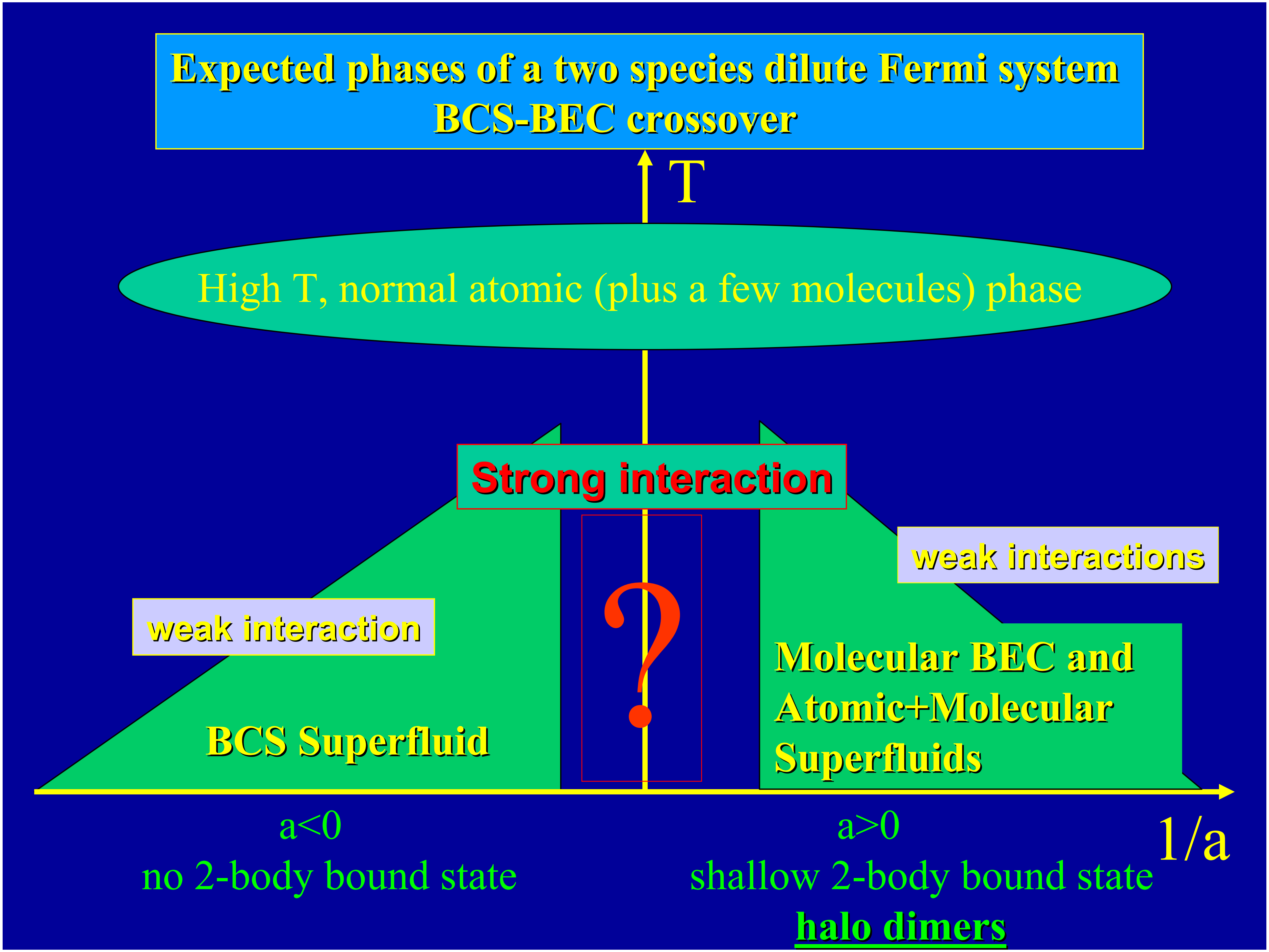
Also in Warsaw


Expected phases of a two species dilute Fermi system
BCS-BEC crossover
T
High T, normal atomic (plus a few molecules) phase
Strong interaction
weak interactions
weak interaction
?
Molecular BEC and
Atomic+Molecular
Superfluids
BCS Superfluid
a<0
no 2-body bound state
a>0
shallow 2-body bound state
halo dimers
1/a

Early theoretical approach

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

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

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

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 <u>in the unitary regime</u>, where <u>the interaction between pairs is strong !!!</u>
(this situation is similar to superfluid ^{4}He)

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

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

What people use a lot ?

Basically this is Eagles' and Leggett's model, somewhat improved.

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Rarified Liquid Properties of Hybrid Atomic-Molecular Bose-Einstein Condensates

Eddy Timmermans,[1] Paolo Tommasini,[2] Robin Côté,[2,*] Mahir Hussein,[2,3] and Arthur Kerman[4]

$$\begin{aligned}\hat H = &\int d^3r\, \hat\psi_a^\dagger\left[-\frac{\hbar^2\nabla^2}{2m} + \frac{\lambda_a}{2}\hat\psi_a^\dagger\hat\psi_a + \lambda\hat\psi_m^\dagger\hat\psi_m\right]\hat\psi_a \\ &+ \int d^3r\, \hat\psi_m^\dagger\left[-\frac{\hbar^2\nabla^2}{4m} + \frac{\lambda_m}{2}\hat\psi_m^\dagger\hat\psi_m + \epsilon\right]\hat\psi_m \\ &+ \frac{\alpha}{\sqrt{2}}\int d^3r\,\{\hat\psi_m^\dagger\hat\psi_a\hat\psi_a + \hat\psi_m\hat\psi_a^\dagger\hat\psi_a^\dagger\}, \qquad (2)\end{aligned}$$

$$\Psi\left(\vec r_1,\vec r_2,\vec r_3,\vec r_4,\ldots\right) \approx \mathcal{A}\left[\varphi(\vec r_{12})\varphi(\vec r_{34})\ldots\right]$$

$$\varphi(\vec r_{12}) \;\Rightarrow\; \varphi_{\downarrow\downarrow}(X_{12}) + \psi_{\uparrow\downarrow}(X_{12})$$

closed channel wave function (frozen)
electron spins are antiparallel

open channel wave function
electron spins are parallel

only one state included (effective boson) and only the amplitude is varied

Why?

✓ **Meanfield calculations (even with fluctuations added on top) are easy**

✓ **It was unclear how to treat the unitary regime**

Timmermans *et al.* realized that a contact interaction proportional to either a very large or infinite scattering length makes no sense in meanfield approximation.

$$U(\vec{r}_1 - \vec{r}_2) = \frac{4\pi\hbar^2 a}{m}\delta(\vec{r}_1 - \vec{r}_2)$$

The two-channel approach, which they introduced initially for bosons, does not seem, superficially at least, to share this difficulty.

However, it is known (for a long time) that corrections to such a meanfield approach will be governed by the parameter **na^3** anyway, so, the problem has not been really solved.

Is there a better way?

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

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

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

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

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

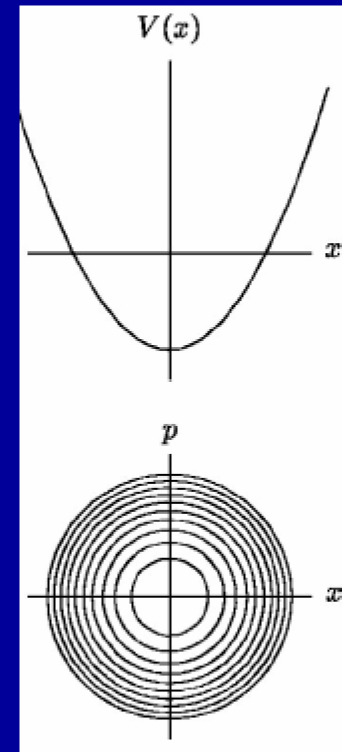
Littlejohn *et al.* J. Chem. Phys. **116**, 8691 (2002)

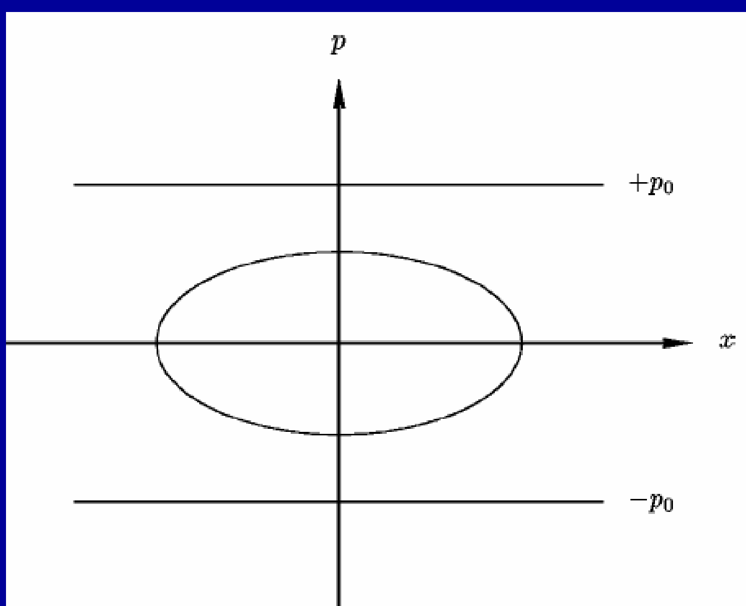
Schroedinger equation

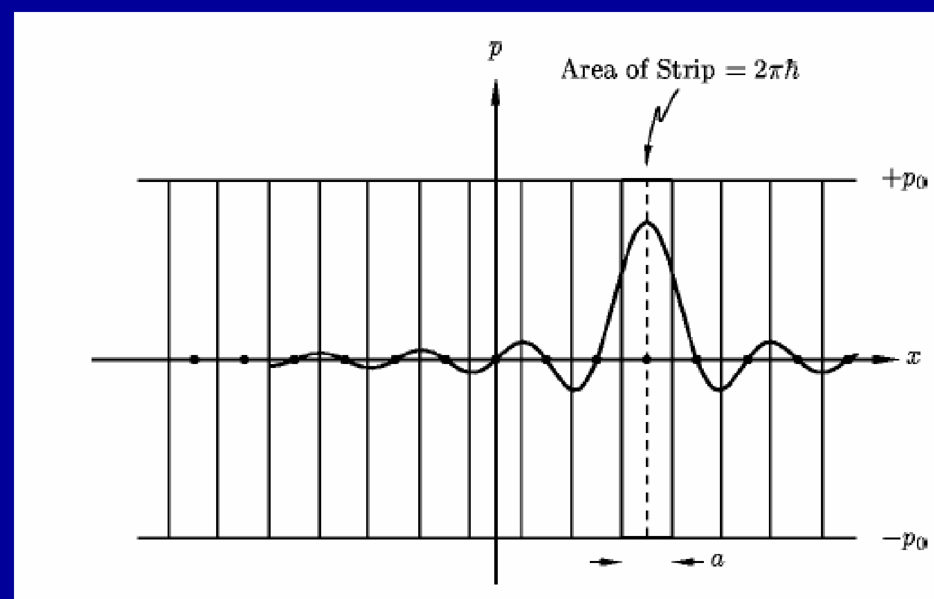
$$\psi(x) = \sum_{\alpha=1}^{N} d_\alpha F_\alpha(x) + O(\exp(-cN))$$

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

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







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

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

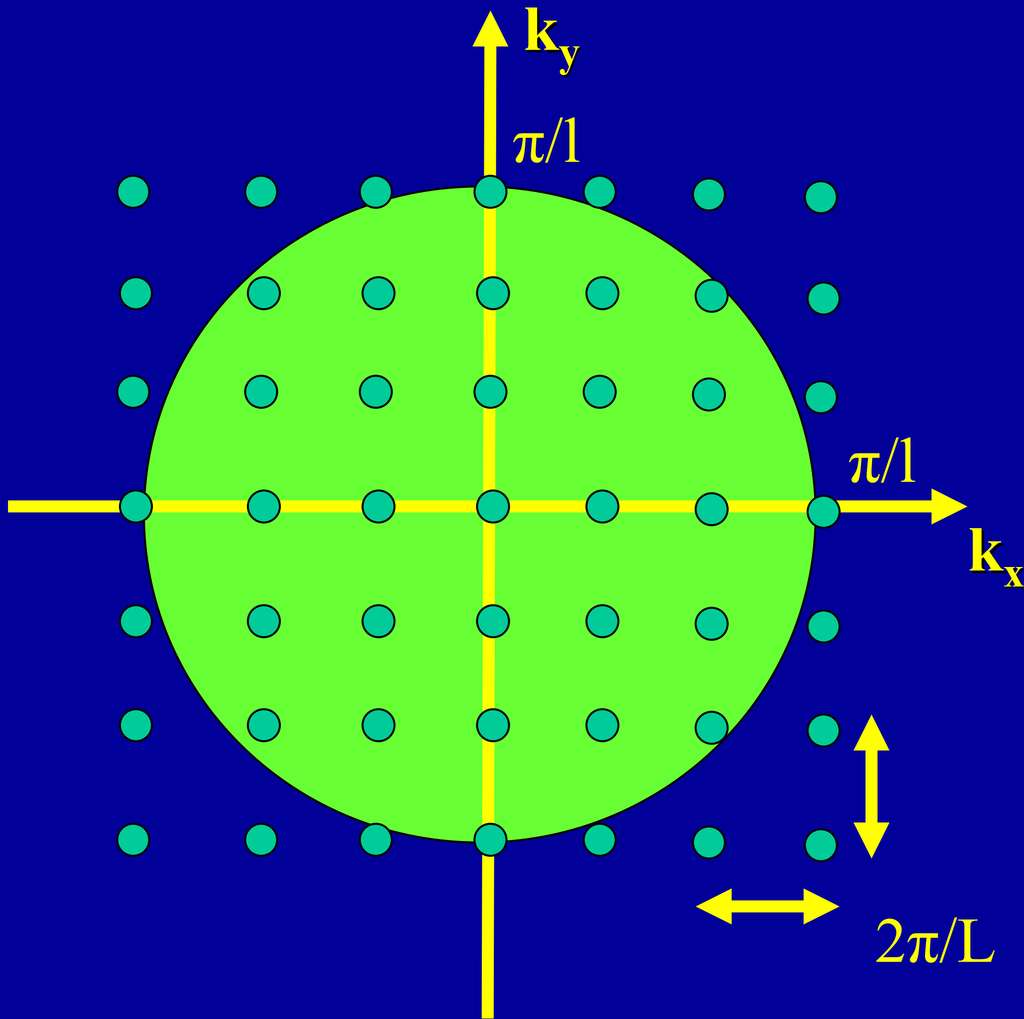
Discrete Hubbard-Stratonovich transformation

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

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

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

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

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

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

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

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

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

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 6^3x30 (high Ts) to 6^3x120 (low Ts)

(runs with ten times smaller time steps, up to 800 time steps, also performed)
8^3 running and larger sizes to come

• Effective use of FFT 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 100,000-1,000,000 $\sigma(x,\tau)$- field configurations for calculations

What we know so far from other approaches?

(at resonance)

$$T_{BEC} = 0.218\ \varepsilon_F \quad \text{at } a = +0$$

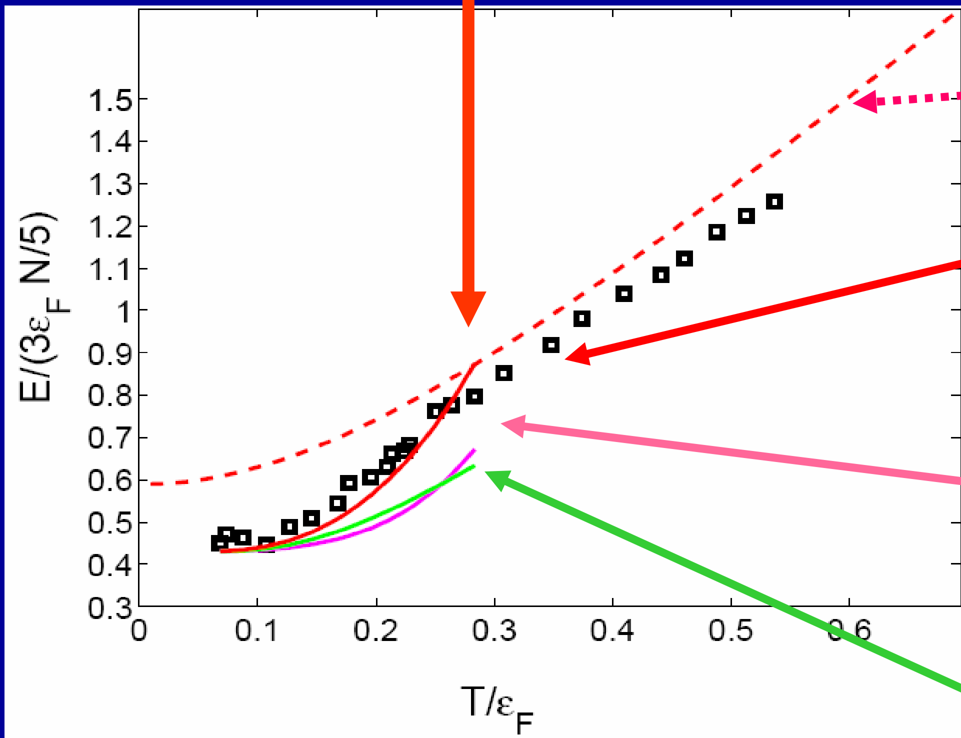
$$T_{Eagles} = 0.277\ \varepsilon_F \quad \text{at } a = \pm\infty$$

$$T_{MF+Fluct} = 0.23\ \varepsilon_F \quad \text{at } a = \pm\infty$$

$$\frac{C_s(T_c)}{C_n(T_c)} = 2.43 \quad \text{in the BCS limit}$$

$a = \pm\infty$

Superfluid to Normal Fermi Liquid Transition



Normal Fermi Gas

Bogoliubov-Anderson phonons and quasiparticle contribution (red line)

Bogoliubov-Anderson phonons contribution only (magenta line)
People never consider this ???

Quasi-particles contribution only (green line)

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

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

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

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

Conclusions

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

(One variant of the fortran 90 program, also 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 $T_c = 0.24\ (3)\ \varepsilon_F$**

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