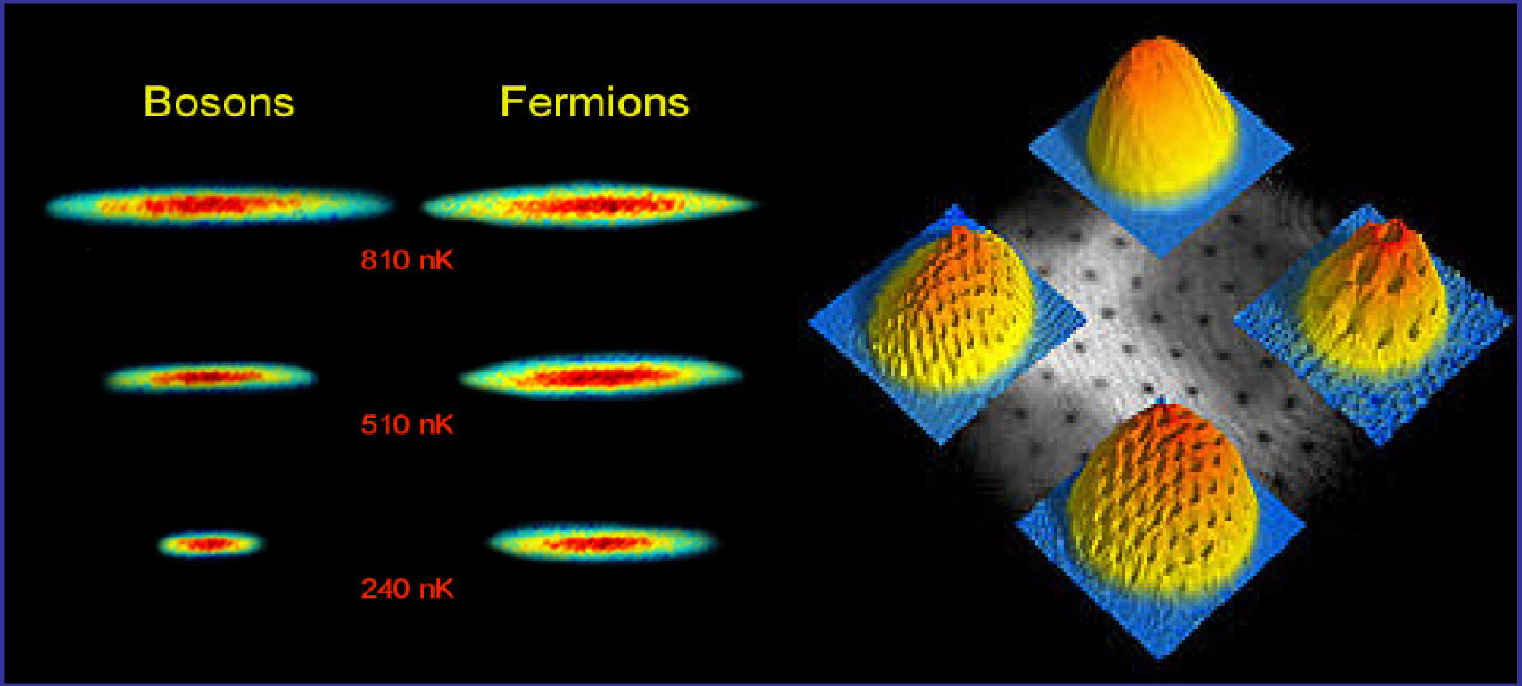
Equation of state for dilute and strongly interacting Fermi gas



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Outline

- General remarks
- Path integral Monte Carlo description of strongly interacting Fermi gases.
- Equation of state for the Fermi gas in the unitary regime. Thermodynamic properties. Critical temperature.
- 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)

Fermi gas: n - number density, a - scattering length

What is the energy of the dilute Fermi gas? $E(k_F a) = ?$

$(k_F r_0 << 1)$

$\varepsilon_F = \frac{\hbar^2 k_F^{\ 2}}{2m}; \quad n = \frac{k_F^{\ 3}}{3\pi^2}$ **- particle density**

$$E/E_{FG} = 1 + \frac{10}{9\pi}(k_F a)\left[1 + \frac{6}{35\pi}(k_F a)(11 - 2\ln 2) + \ldots\right] + \text{pairing}$$

$E_{FG} = \frac{3}{5}\varepsilon_F N$ - Energy of the noninteracting Fermi gas

BCS pairing gap

$$\Delta_{BCS} = \frac{8}{e^2}\frac{\hbar^2 k_F^2}{2m}\exp\left(\frac{\pi}{2k_F a}\right),$$ iff $k_F |a| << 1$ and $\frac{1}{k_F} << \eta = \frac{1}{k_F}\frac{\varepsilon_F}{\Delta}$ - size of the Cooper pair

$$\frac{E_{HF+BCS}}{E_{FG}} = 1 + \frac{10}{9\pi}(k_F a) + \ldots - \frac{5}{8}\left(\frac{\Delta_{BCS}}{\varepsilon_F}\right)^2 = 1 + \frac{10}{9\pi}(k_F a) + \ldots - \frac{40}{e^4}\exp\left(\frac{\pi}{k_F a}\right)$$

Mean-field term **BCS term**

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

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

NONPERTURBATIVE REGIME

System is dilute but strongly interacting!

The only scale: $E_{FG}/N = \frac{3}{5}\varepsilon_F$

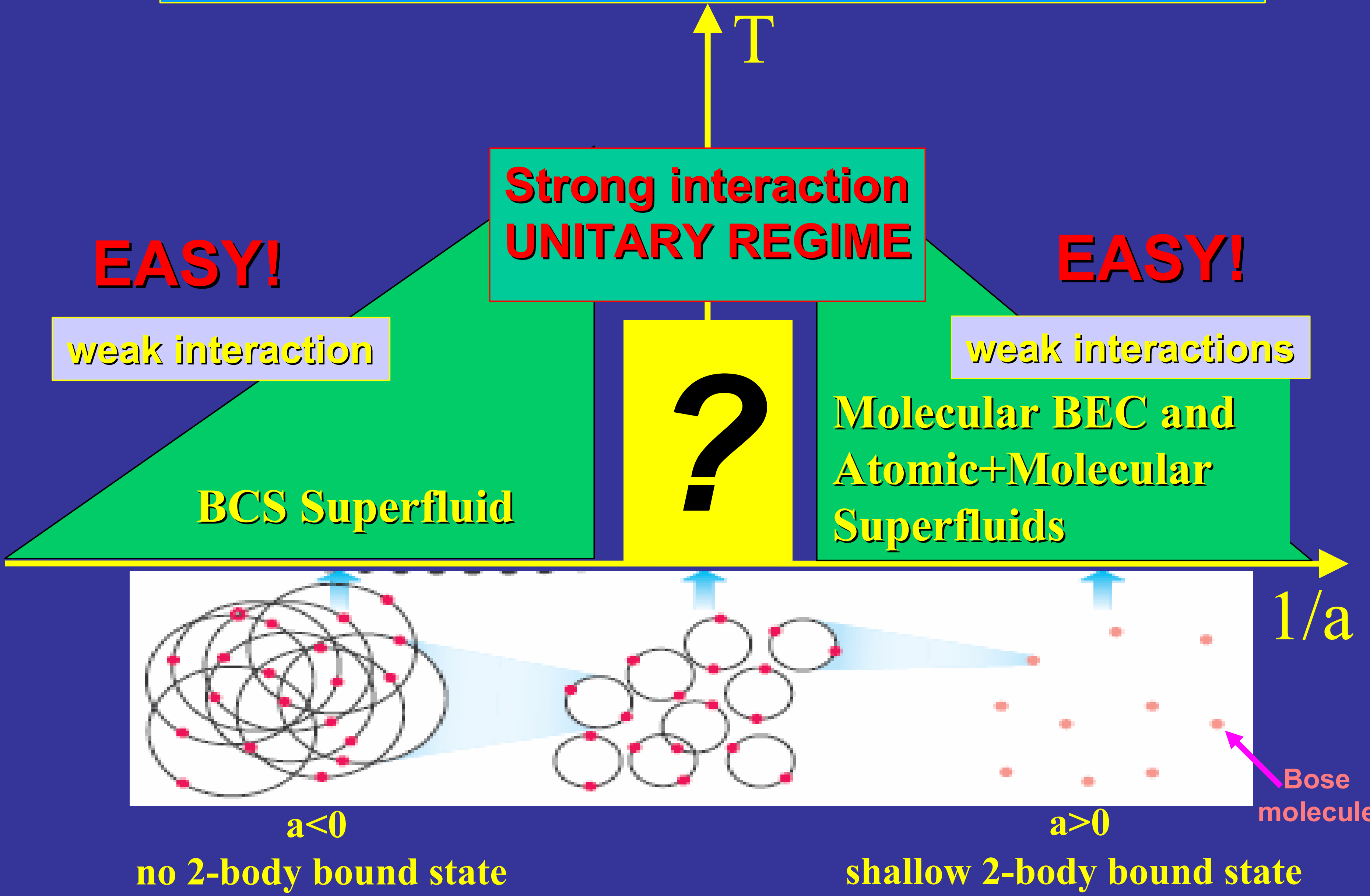
UNIVERSALITY: $E(T) = \xi\left(\frac{T}{\varepsilon_F}\right) E_{FG}$

QUESTIONS: **What is the shape of** $\xi(T/\varepsilon_F)$ **?**

What is the critical temperature for the superfluid-to-normal transition?

...

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



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:** $\boxed{\xi(T=0) \approx 0.44}$

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

Neutron matter:

Effective range: $r_0 \approx 2.8$ fm

Scattering length: $a \approx -18.5$ fm

Density range

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

corresponds to

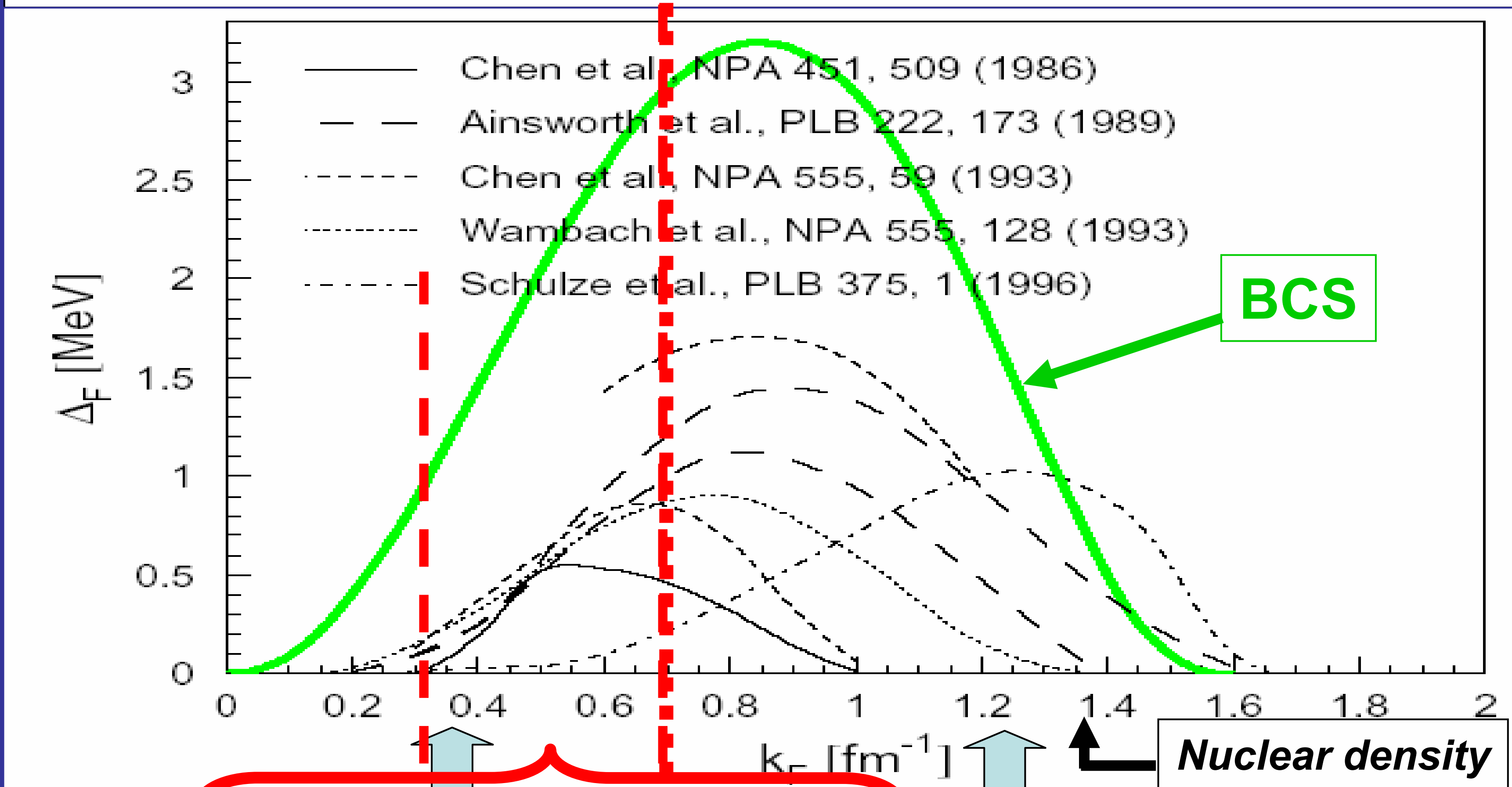
$n \approx 0.001 - 0.01\ \text{fm}^{-3}$

$k_F \approx 0.3 - 0.7\ \text{fm}^{-1}$

Neutron matter

Neutron-neutron scattering
Scattering length: $a \approx -18.5\ fm$
Effective range: $r_0 \approx 2.8\ fm$

s-wave pairing gap in infinite neutron matter with realistic NN-interactions



Dilute matter: only a, r_0 matter

Details of the n

$n \approx 0.001 - 0.01\ fm^{-3}$

$k_F \approx 0.3 - 0.7\ fm^{-1}$

Close to the unitary limit

Hamiltonian

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

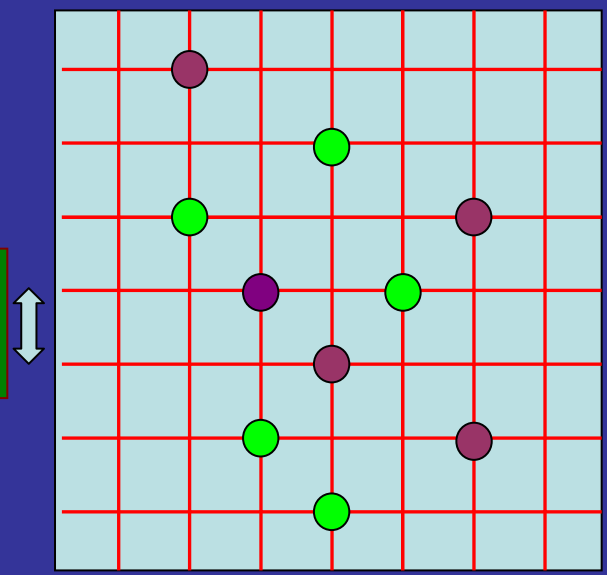
$$\hat{N} = \int d^3r \; \left(\hat{n}_\uparrow(\vec{r}) + \hat{n}_\downarrow(\vec{r}) \right); \;\; \hat{n}_s(\vec{r}) = \hat{\psi}_s^\dagger(\vec{r}) \hat{\psi}_s(\vec{r})$$

Theoretical approach: Fermions on 3D lattice

Coordinate space

L –limit for the spatial correlations in the system

$$k_{cut} = \frac{\pi}{\Delta x} \; ; \;\; \Delta x$$



$$Volume = L^3$$

$$lattice\ spacing = \Delta x$$

- Spin up fermion: ↑

- Spin down fermion: ↓

External conditions:

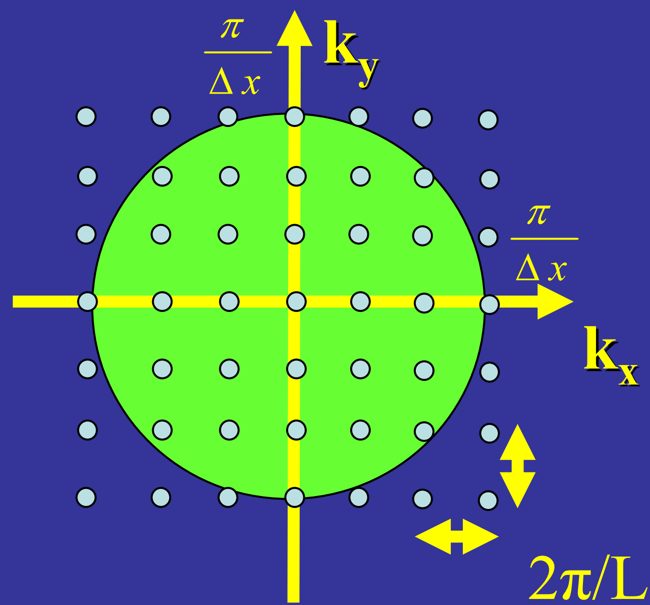
T - temperature

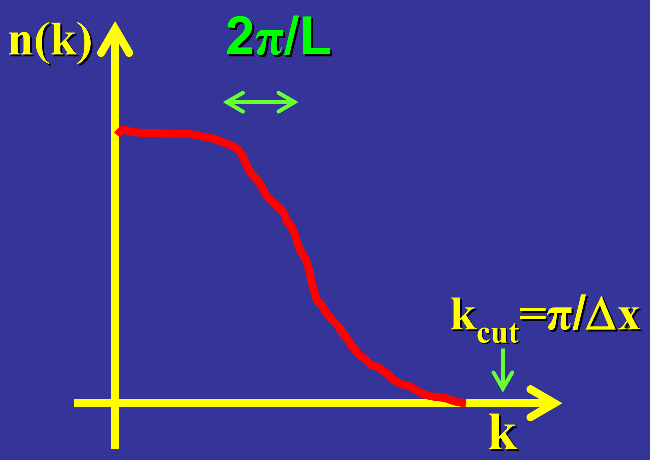
μ - chemical potential

Periodic boundary conditions imposed

Theoretical approach: Fermions on 3D lattice

Momentum space





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

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

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

REAL SPACE $\overset{FFT}{\Longleftrightarrow}$ **MOMENTUM SPACE**

Grand Canonical Path-Integral Monte Carlo

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

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

Trotter expansion

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

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

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

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

Discrete Hubbard-Stratonovich transformation

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

σ-fields fluctuate both in space and imaginary time

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

Running coupling constant g defined by lattice

$$\frac{1}{g}=\frac{m}{2\pi\hbar^2\Delta x}$$ - UNITARY LIMIT

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

$$\int D\sigma(\vec{r},\tau) \equiv \sum_{\{\sigma(\vec{r},1)=\pm 1\}} \sum_{\{\sigma(\vec{r},2)=\pm 1\}} \cdots \sum_{\{\sigma(\vec{r},N_\tau)=\pm 1\}} \quad ; \quad N_\tau \tau = \frac{1}{T}$$

$$\hat{U}(\{\sigma\}) = T_\tau \exp\{-\int_0^\beta d\tau[\hat{h}(\{\sigma\}) - \mu]\}$$

One-body evolution operator in imaginary time

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

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

No sign problem!

$$n_\uparrow(\vec{x},\vec{y}) = n_\downarrow(\vec{x},\vec{y}) = \sum_{k,l<k_c} \psi_{\vec{k}}(\vec{x}) \left[\frac{U(\{\sigma\})}{1+U(\{\sigma\})}\right]_{\vec{k}\,\vec{l}} \psi^*_{\vec{l}}(\vec{y}), \qquad \psi_{\vec{k}}(\vec{x}) = \frac{\exp(i\vec{k}\cdot\vec{x})}{\sqrt{L^3}}$$

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

$$\hat{U}(\{\sigma\}) = T_\tau \exp\{-\int_0^\beta d\tau[\hat{h}(\{\sigma\}) - \mu]\}; \;\; \hat{h}(\{\sigma\}) - \text{one-body operator}$$

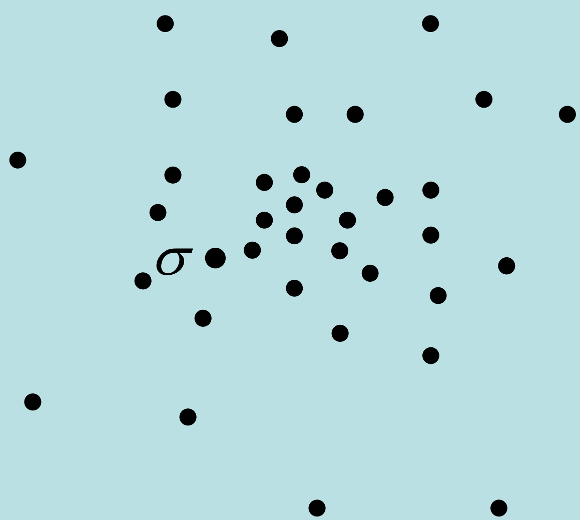
$$U(\{\sigma\})_{kl} = \left\langle \psi_k \middle| \hat{U}(\{\sigma\}) \middle| \psi_l \right\rangle; \quad \left|\psi_l\right\rangle \text{- single-particle wave function}$$

$$E(T) = \left\langle \hat{H} \right\rangle = \int \frac{D[\sigma(\vec{r},\tau)]e^{-S[\sigma]}}{Z(T)} \, E[U(\{\sigma\})]$$

$E[U(\{\sigma\})]$- energy associated with a given sigma field

Quantum Monte-Carlo:

Sigma space sampling



$$P(\sigma) \propto e^{-S[\sigma]}$$

$$\bar{E}(T) = \frac{1}{N_\sigma} \sum_{k=1}^{N_\sigma} E\left(U(\{\sigma_k\})\right)$$

$\bar{E}(T)$ - stochastic variable

$\left\langle \bar{E}(T) \right\rangle = E(T)$

$$\sqrt{\left\langle \bar{E}(T)^2 \right\rangle - \left\langle \bar{E}(T) \right\rangle^2} \propto 1 \big/ \sqrt{N_\sigma}$$

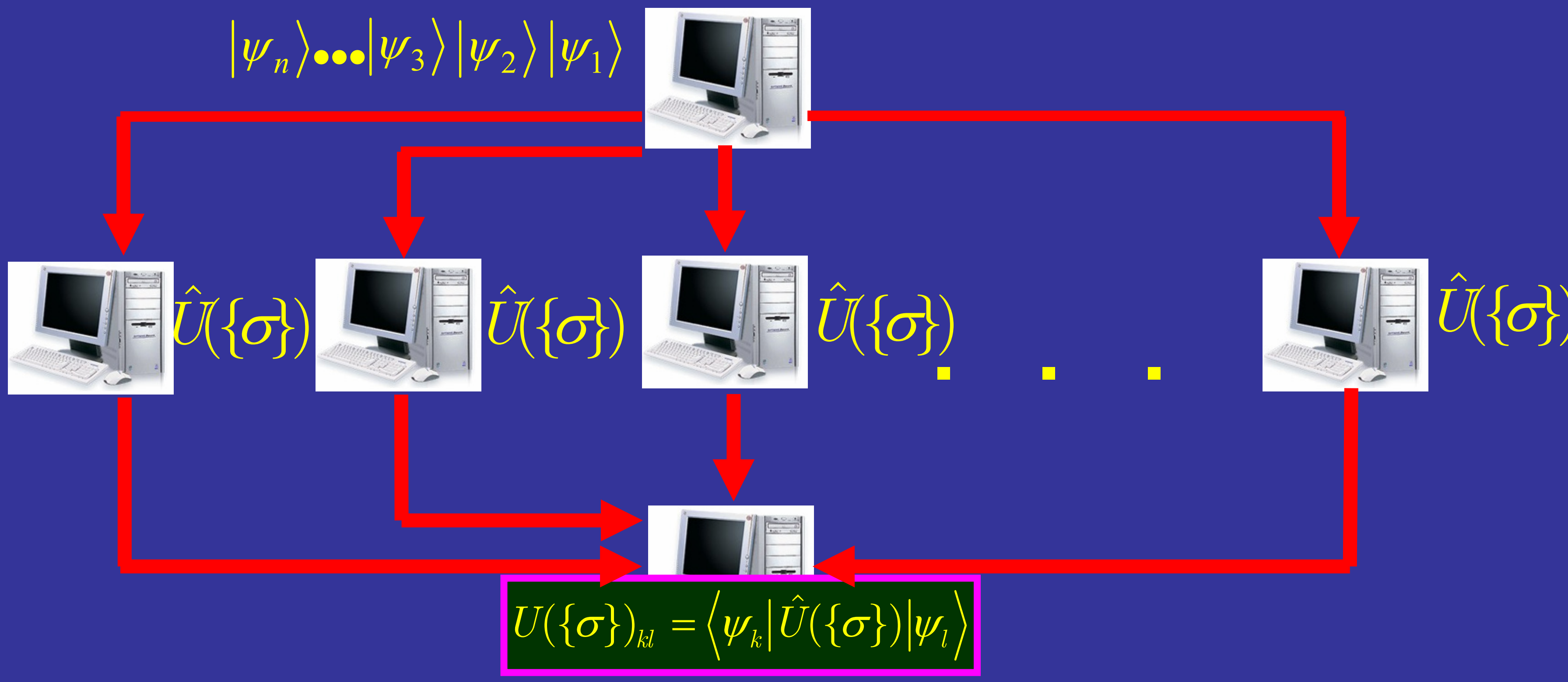
N_σ - number of uncorrelated samples

Quantum Monte-Carlo: parallel computing

$$\hat{U}(\{\sigma\}) = T_\tau \exp\{-\int_0^\beta d\tau[\hat{h}(\{\sigma\}) - \mu]\}; \ \hat{h}(\{\sigma\}) - \text{one-body operator}$$

$$U(\{\sigma\})_{kl} = \langle \psi_k | \hat{U}(\{\sigma\}) | \psi_l \rangle; \quad |\psi_l\rangle \text{- single-particle wave function}$$

For each sigma *n* single particle states have to be evolved.



More details of the calculations:

- Lattice sizes used from 8^3 x 257 (high Ts) to 8^3 x 1732 (low Ts), <N>=50, and 6^3 x 257 (high Ts) to 6^3 x 1361 (low Ts), <N>=30.

- 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

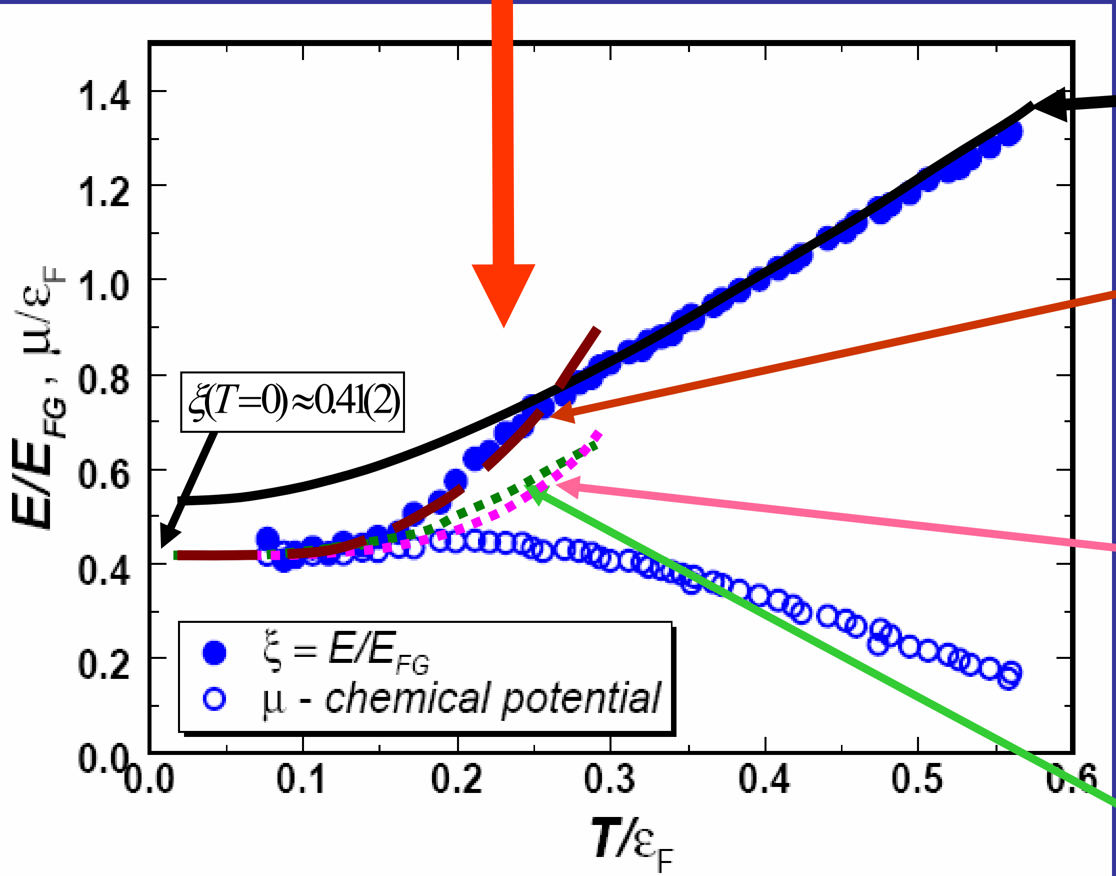
- At low temperatures use Singular Value Decomposition of the evolution operator $U(\{\sigma\})$ to stabilize the numerics.

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

- MC correlation "time" $\approx$ 150 – 200 time steps at $T \approx T_c$

a = ±∞

Superfluid to Normal Fermi Liquid Transition



Normal Fermi Gas
(with vertical offset, solid line)

Bogoliubov-Anderson phonons and quasiparticle contribution
(dashed line)

Bogoliubov-Anderson phonons contribution only (dotted line)

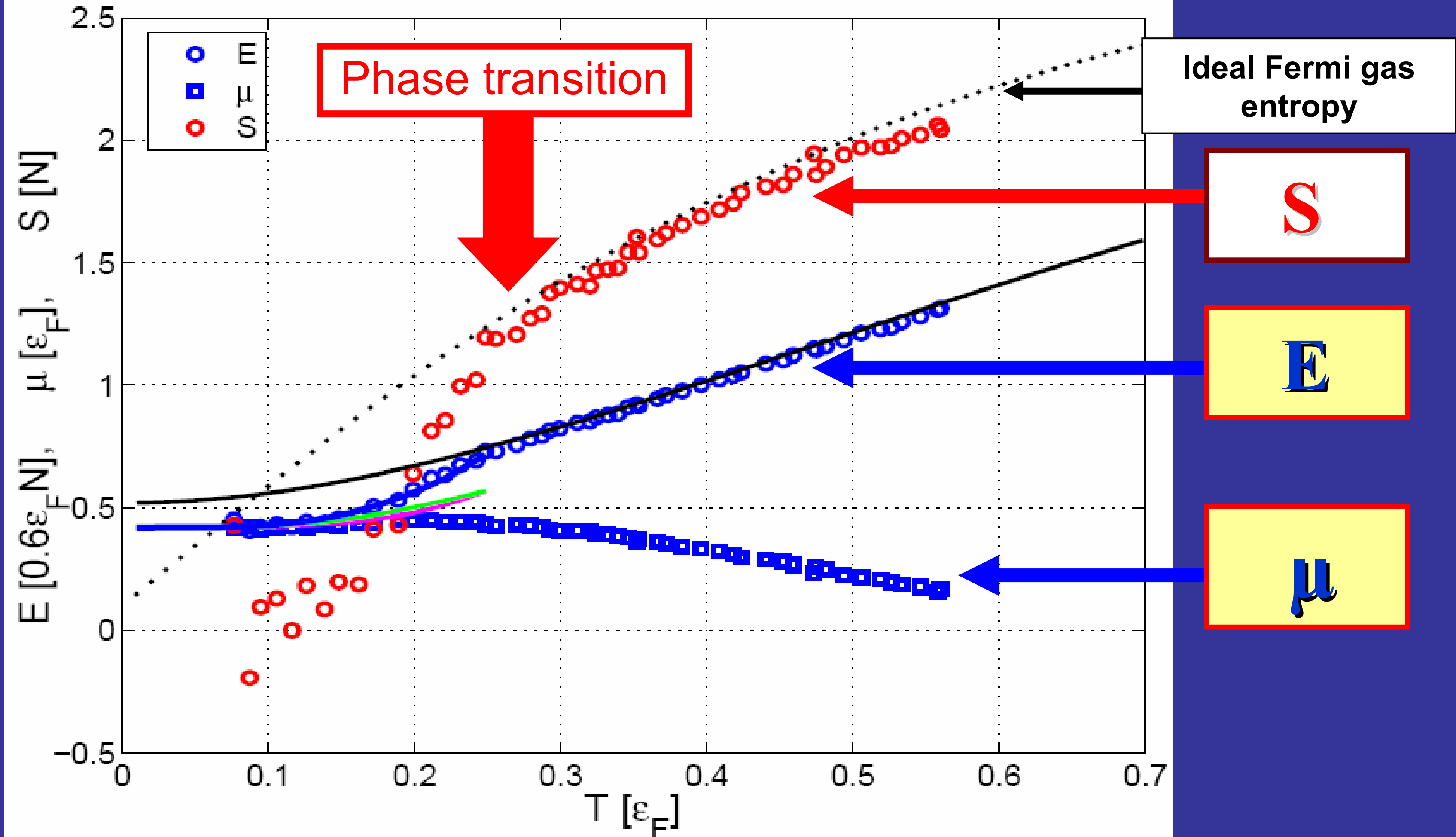
Quasi-particle contribution only
(dotted line)

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

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

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

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



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

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

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

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

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

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

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

More Results...

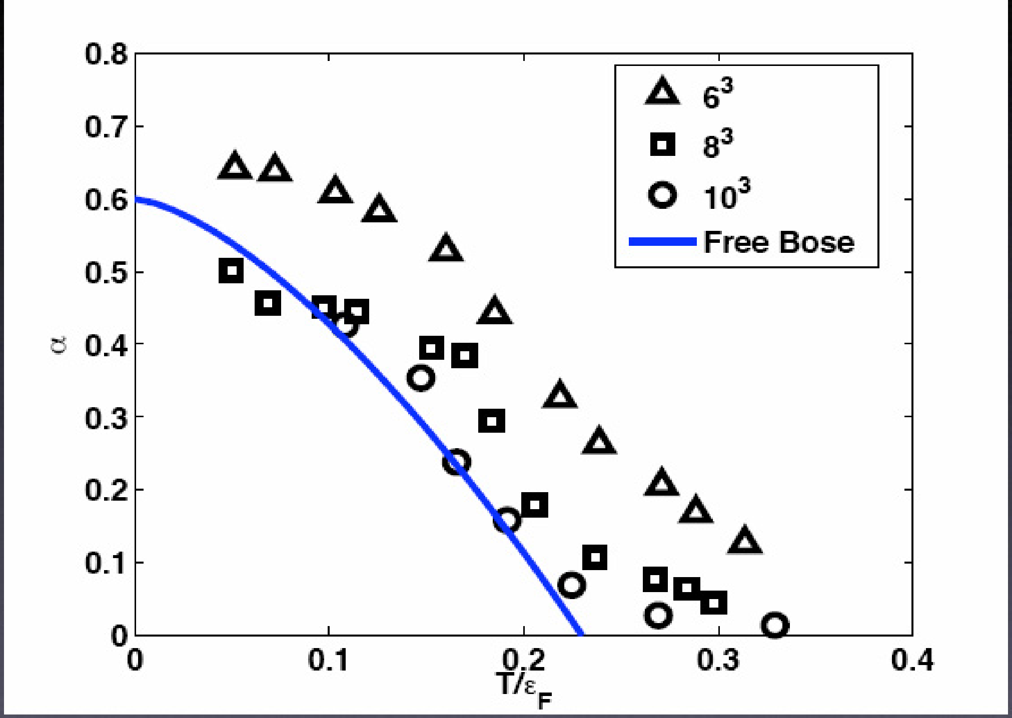
Condensate fraction α:
Order parameter for
Off Diagonal
Long Range Order
(C.N. Yang)

Free Bose gas-like:

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

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

$T_c = 0.23(2)$



From a talk of J.E. Drut

Low temperature behaviour of a Fermi gas in the unitary regime

$$E(T) = \frac{3}{5}\varepsilon_F N \xi\left(\frac{T}{\varepsilon_F}\right) \quad \text{and} \quad \frac{\mu(T)}{\varepsilon_F} \approx \xi_s \approx 0.41(2) \text{ for } T < T_C$$

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

$$\xi\left(\frac{T}{\varepsilon_F}\right) = \xi_s + \varsigma_s\left(\frac{T}{\varepsilon_F}\right)^{5/2}, \qquad \varsigma_s \approx 11(1)$$

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

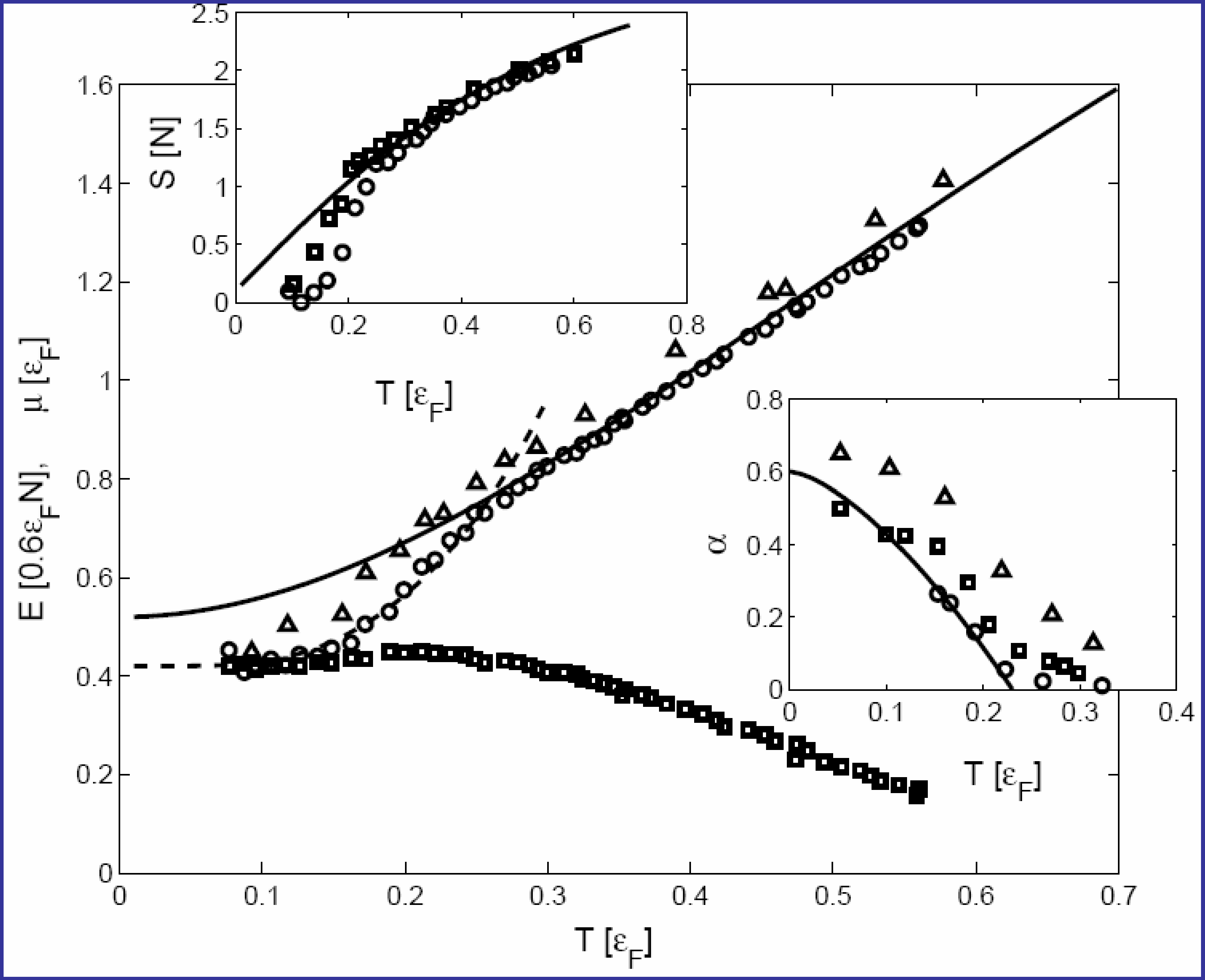
Lattice results disfavor either n≥3 or n≤2 and suggest n=2.5(0.25)

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

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

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?**



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

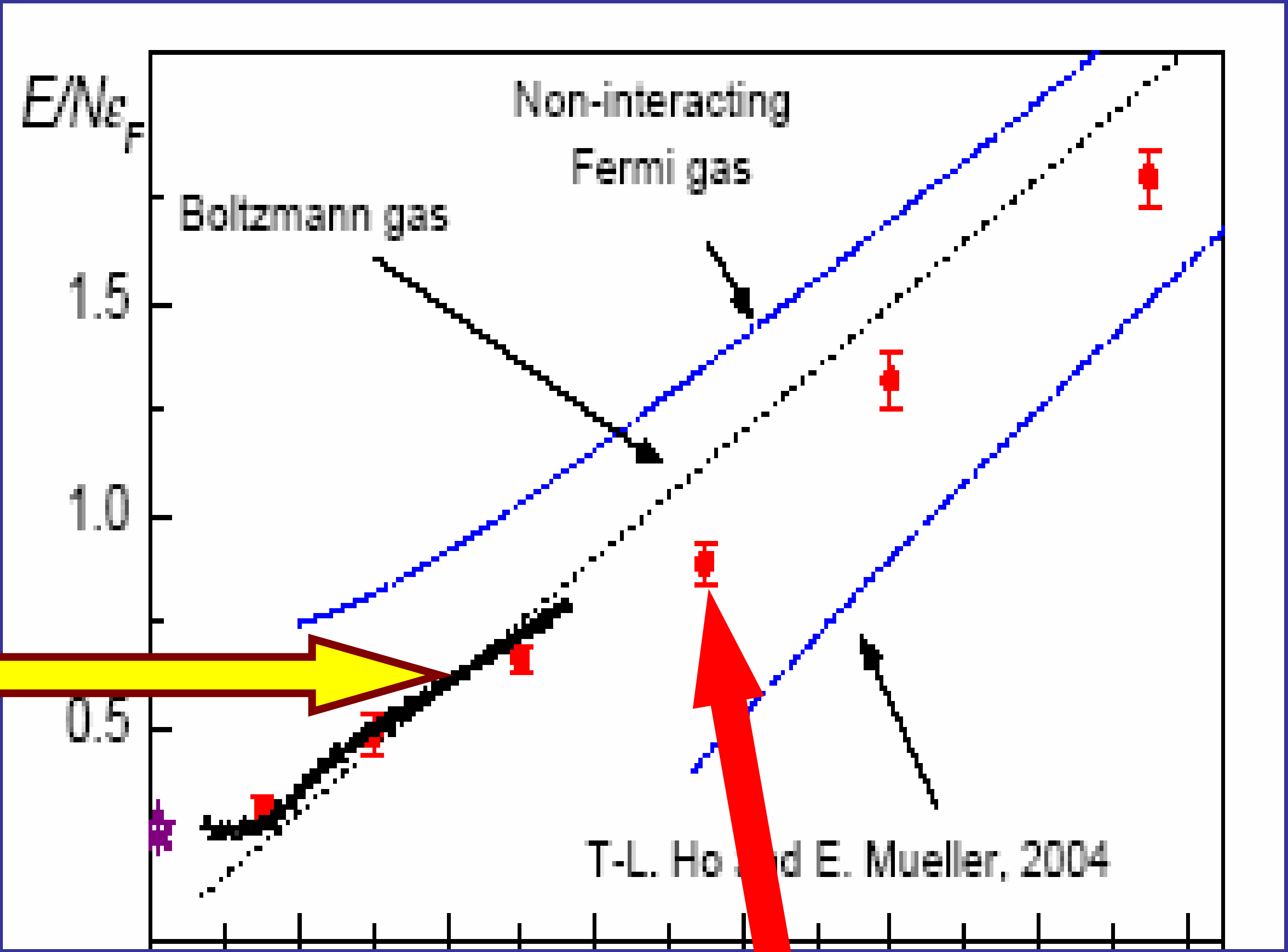
Conclusions

- ✓ 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 $T_c = 0.23\ (2)\ \varepsilon_F$
  (Exp: $T_c = 0.27(2)\ \varepsilon_F$, J. Kinast *et al.* Science, 307, 1296 (2005): Based on theoretical assumptions).

- ✓ Chemical potential is constant up to the critical temperature – note similarity with Bose systems!

- ✓ 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.

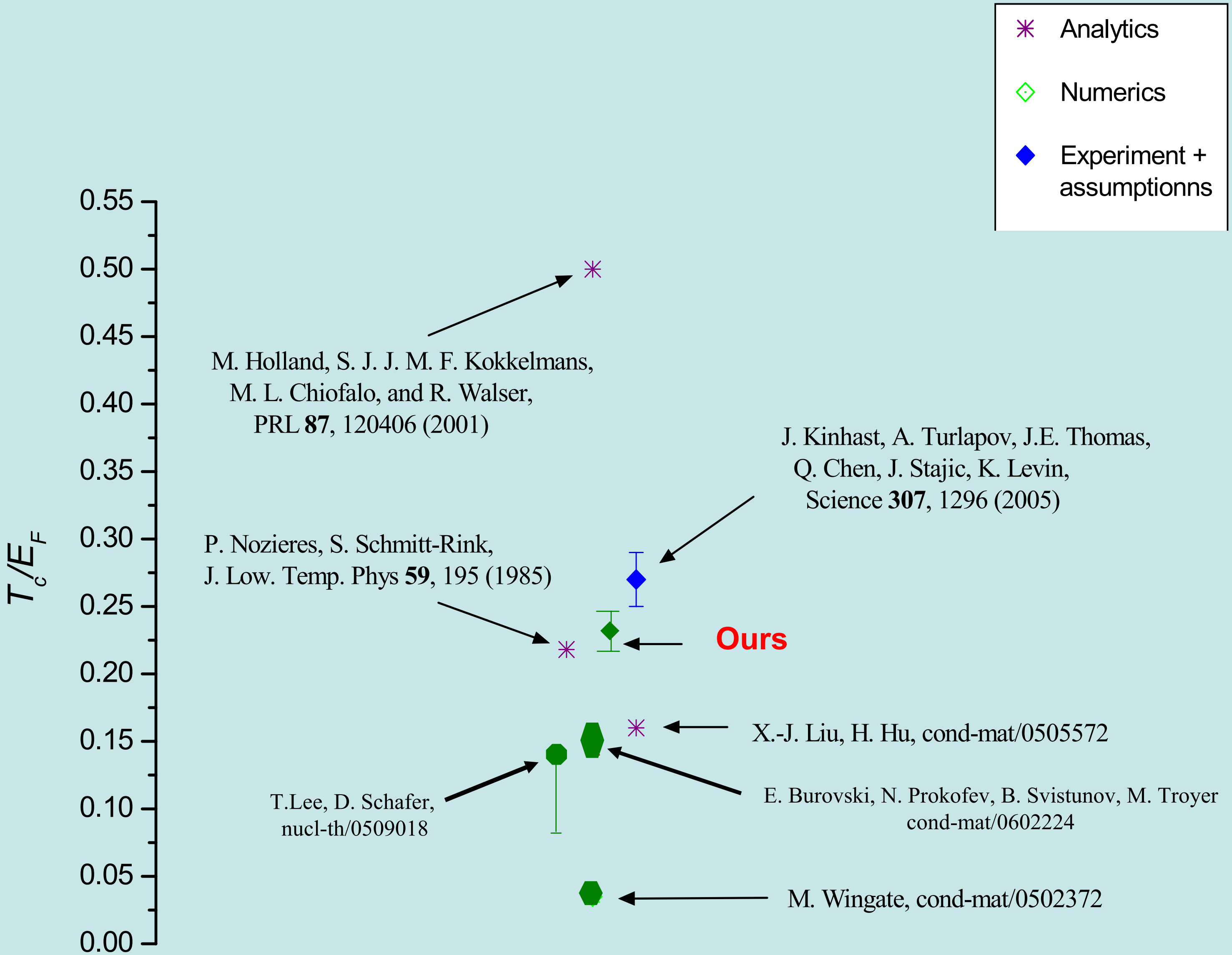
There are reasons to believe that below the critical temperature this system is a new type of fermionic superfluid, with unusual properties.



OURS

From: E.Burovski, N.Prokof'ev, B.Svistunov, M.Troyer, cond-mat/0602224

Quest for unitary point critical temperature



Boris Svistunov’s talk (updated), Seattle 2005