Właściwości rozrzedzonych, silnie skorelowanych gazów fermionowych

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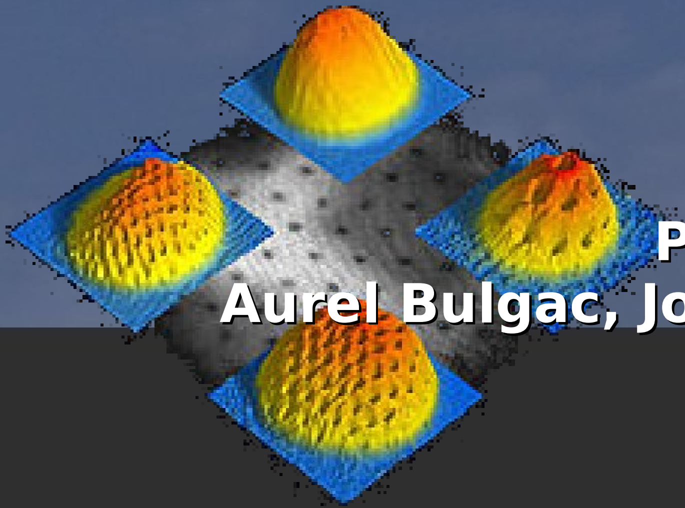
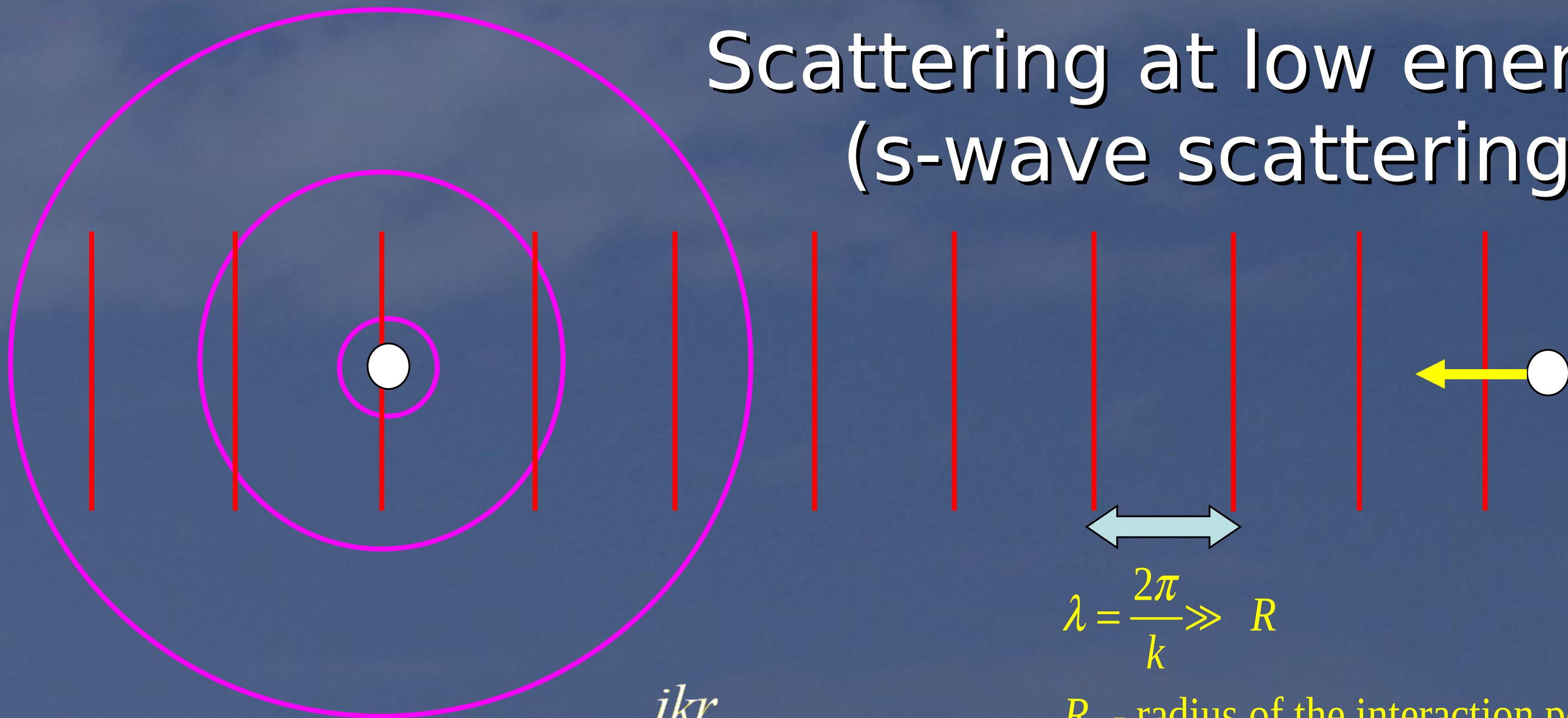


Współpraca:
Piotr Magierski (Warsaw University of Technology)
Aurel Bulgac, Joaquin E. Drut (University of Washington, Seattle)

Plan

- Rozrzedzone gazy fermionowe – definicja, oddziaływanie, reżim unitarny
- Możliwości eksperymentalne
- Kwantowe Monte Carlo
- Szczelina energetyczna dla reżimu unitarnego
- Obliczenia dla rozrzedzonej materii neutronowej – równanie stanu, szczelina energetyczna

Scattering at low energies (s-wave scattering)



$$\lambda = \frac{2\pi}{k} \gg R$$

R - radius of the interaction potential

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + f(k)\frac{e^{ikr}}{r};$$

$f(k)$ - scattering amplitude

$$f(k) \overset{k\to 0}{=} \frac{1}{-ik - \frac{1}{a} + \frac{1}{2}r_0 k^2},$$

Interaction between neutrons is determined by the scattering length and effective range, if k → 0

Interaction II

Leading term of Skyrme force
Suitable for dilute fermionic gases

$$V(\vec{r}-\vec{r}\,')=-g\,\delta(\vec{r}-\vec{r}\,')$$

$$\hat{V}=-g\int d^3\vec{r}\; n_\uparrow(\vec{r})\,n_\downarrow(\vec{r})$$

$$n_\lambda(\vec{r})=a_\lambda^\dagger(\vec{r})\,a_\lambda(\vec{r})$$

Momentum cut-off

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

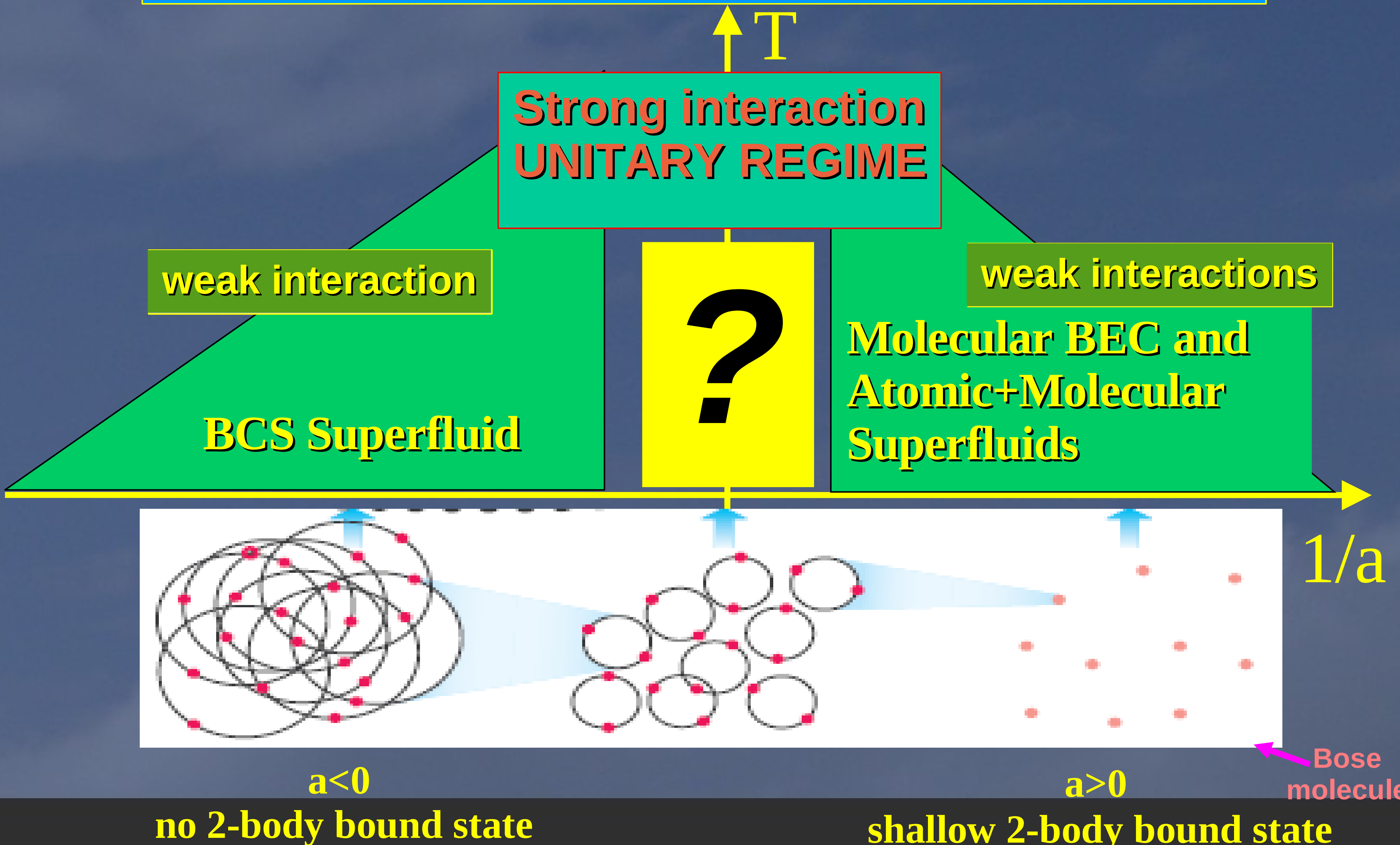
Relation between coupling constant and scattering length

For neutron matter:
scattering length: a=-18.5 fm
effective range: r_0=2.8 fm

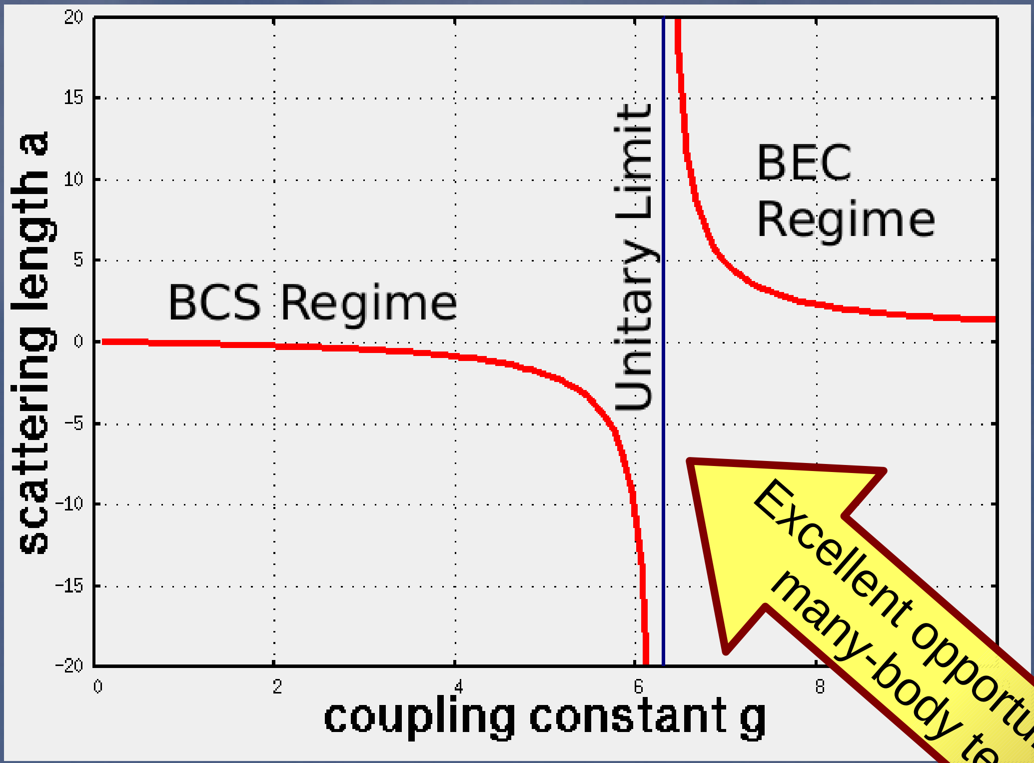
$$V(\vec{r}-\vec{r}\,')=-g_0\,\delta(\vec{r}-\vec{r}\,')+g_1\left[\nabla^2\delta(\vec{r}-\vec{r}\,')+\delta(\vec{r}-\vec{r}\,')\nabla^2\right]$$

Unitary limit I

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



Theory and experiment



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

Experimentally scattering length can be tuned by changing external magnetic field (via so called Fano-Feshbach resonance)

Excellent opportunity to tests many-body techniques

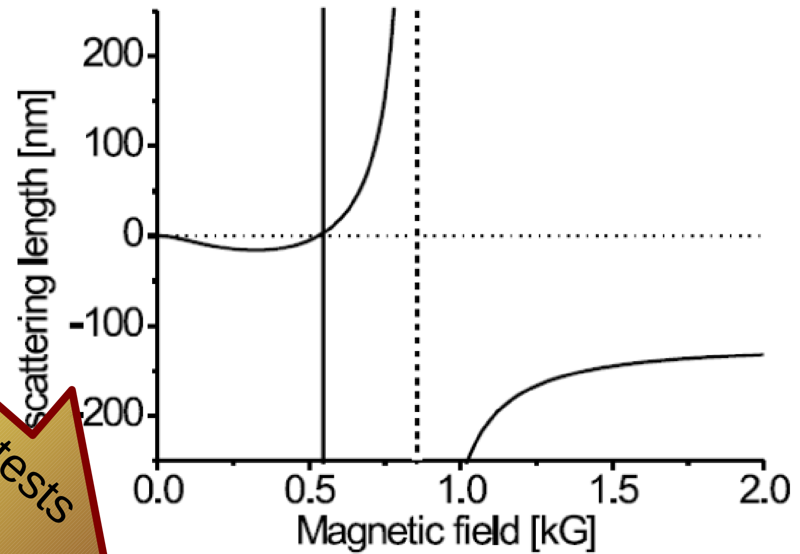


FIG. 4: Magnetic field dependence of the scattering length in ^{6}Li, showing a broad Feshbach resonance at $B_0 \simeq 834$ G and a narrow Feshbach resonance at $B_0 \simeq 543$ G (can not be resolved on this scale). From Bourdel *et al.* (2003).

Experiments with atomic gases

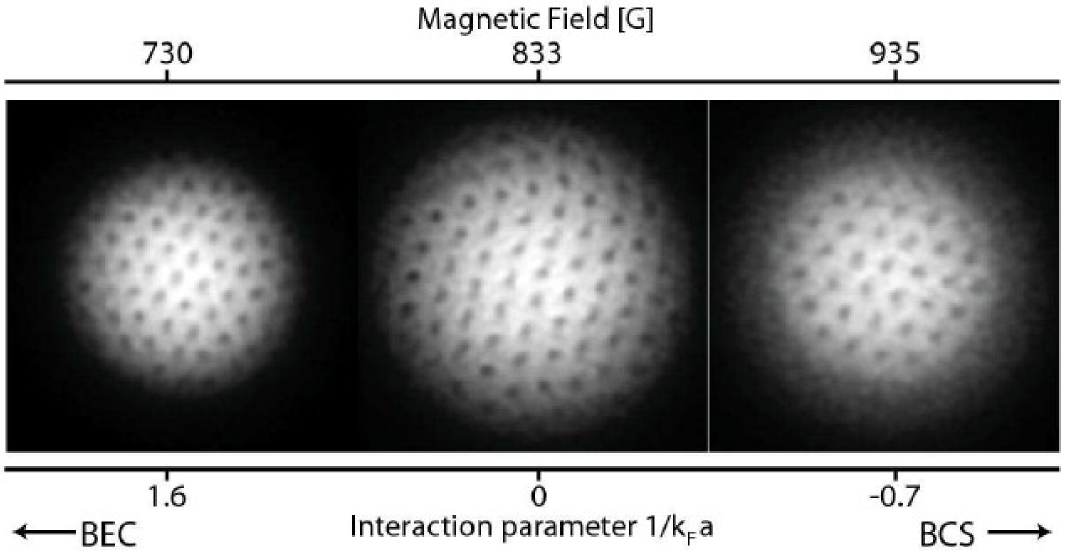
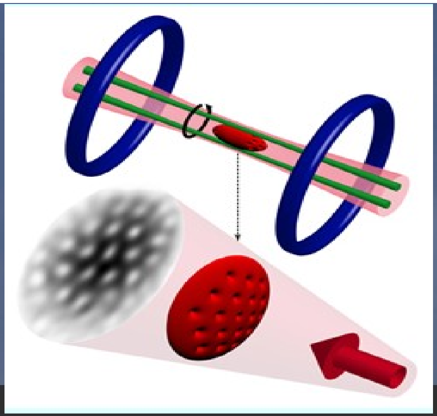


FIG. 36 Vortex lattice in a rotating gas of ^{6}Li precisely at the Feshbach resonance and on the BEC and BCS side. Reprinted with permission from Zwierlein *et al.* (2005).



Evidence for fermionic superfluidity – vortices!

Control parameters of experiments:

- The number of atoms in the trap
- The density of atoms
- Mixtures of various atoms
- The temperature of the atomic cloud
- The strength of interaction

Universality of unitary regime I

$$a \to \pm\infty, \quad r_0 \to 0$$

$$f(k) \overset{k\to 0}{=} \frac{1}{-ik}$$

The only relevant length scales remain the inverse of the Fermi wavevector.

All thermodynamic quantities should be universal function of the Fermi energy E_F and of the ratio T/T_F

Example: $E(T) = \xi(T/T_F)\, E_{FG}$

Energy of noninteracting Fermi gas

Dimensionless universal function

Universality of unitary regime II

$$P=-\frac{\partial E}{\partial V}=\frac{2}{5}\xi\,\varepsilon_F\frac{N}{V}\quad\Rightarrow\quad PV=\frac{2}{3}E$$

Holds at **unitarity**
and
for **noninteracting** Fermi gas

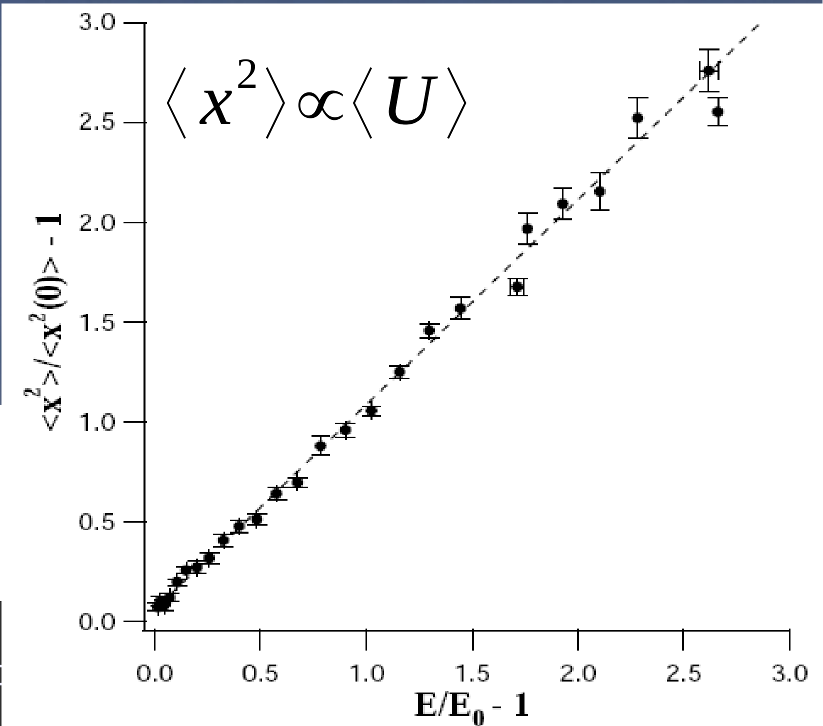
$$\left.\begin{aligned}PV&=\frac{2}{3}E\\ \vec{\nabla}P&=-n(\vec{r})\vec{\nabla}U\end{aligned}\right\}\quad\Rightarrow\quad N\langle U\rangle=\frac{E}{2}\quad\Rightarrow\quad\frac{E(T_1)}{E(T_2)}=\frac{\langle U\rangle_{T_1}}{\langle U\rangle_{T_2}}$$

The mechanical equilibrium

Universality requires
a unitarity Fermi gas to
obey the virial theorem for
an ideal gas

arXiv:cond-mat/0503620

Fig. 1 shows $\langle x^2\rangle$ as a function E. The dashed line shows the fit, $\langle x^2\rangle/\langle x^2(0)\rangle = 1.03\,(0.02)\,E/E_0$, which is in close agreement with the virial theorem prediction of



Quantum Monte Carlo I

Definition of the problem

$$Z(\beta,\mu)=Tr\{e^{-\beta(\hat{H}-\mu\hat{N})}\}$$

$$O(\beta,\mu)=\frac{1}{Z}Tr\{\hat{O}e^{-\beta(\hat{H}-\mu\hat{N})}\}$$

Idea of Hubbard-Stratonovich transformation

Where

$$\hat{H}=\hat{T}+\hat{V}$$

$$\underbrace{e^{-\tau\hat{V}}}_{\text{2 Body Op.}}=\int d\vec{\sigma}\ \underbrace{e^{\hat{w}(\vec{\sigma})}}_{\text{1 Body Op.}}$$

All of the difficulty arises from the two-body interaction.

Monte Carlo quadrature

Quantum Monte Carlo II

General form for expectation value of operator takes form

$$O(\beta,\mu) = \frac{Tr\{\hat{O}e^{-\beta(\hat{H}-\mu\hat{N})}\}}{Tr\{e^{-\beta(\hat{H}-\mu\hat{N})}\}} = \frac{\int D\vec{\sigma}\,W(\vec{\sigma})O(\vec{\sigma})}{\int D\vec{\sigma}\,W(\vec{\sigma})}$$

Needed algorithm for performing multidimensional integrals

$$D\vec{\sigma} = \prod_{j=1}^{N_\tau} d\vec{\sigma}_j$$

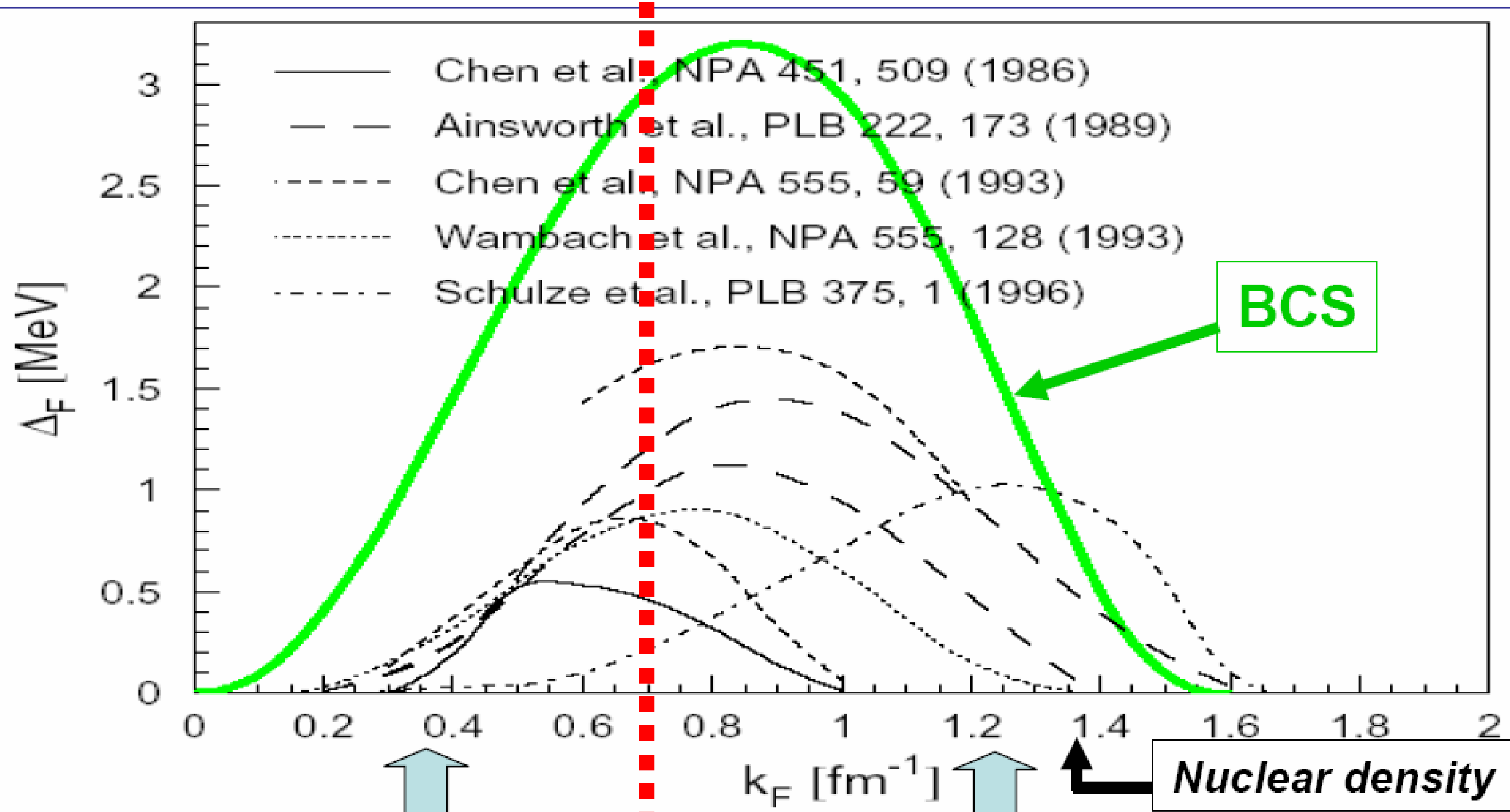
If W is real and non-negative for all domain of integration we can use Monte Carlo techniques

Unfortunately, **many of the hamiltonians of physical interest suffer from a sign problem**

(Origin of sign problem antisymmetry of wave function)

Current challenge I – energy gap

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



Dilute matter: only a, r_0 matter

Details of the n-n potential matter

Summary on superfluidity and heat capacity

Neutrons, protons and other baryons in neutron star interiors can be in superfluid state

Superfluidity is very model dependent (too many different microscopic models)

Superfluidity is a Fermi surface phenomena which affects thermodynamics and kinetics of neutron star matter

In particular, superfluidity can strongly affect heat capacity of neutron star interiors

What are the effects of superfluidity on neutrino emission and neutron star cooling?

→ *Next le*

Slide from:
Dima Yakovlev (St. Petersburg, Russia)
Cooling of Compact Stars
Ladek Zdroj, Poland, 18-29 February 2008
http://www.ift.uni.wroc.pl/~karp44/lectures/lectures_yakovlev

Quasi-particle spectrum

For quasi-particle approach

$$E(\vec{p}) = \sqrt{\left(\frac{\vec{p}^{\,2}}{2m^*} + U - \mu\right)^2 + \Delta^2}$$

"pairing" gap

m*, U, Δ are temperature dependent parameters

Effective mass

single-particle potential

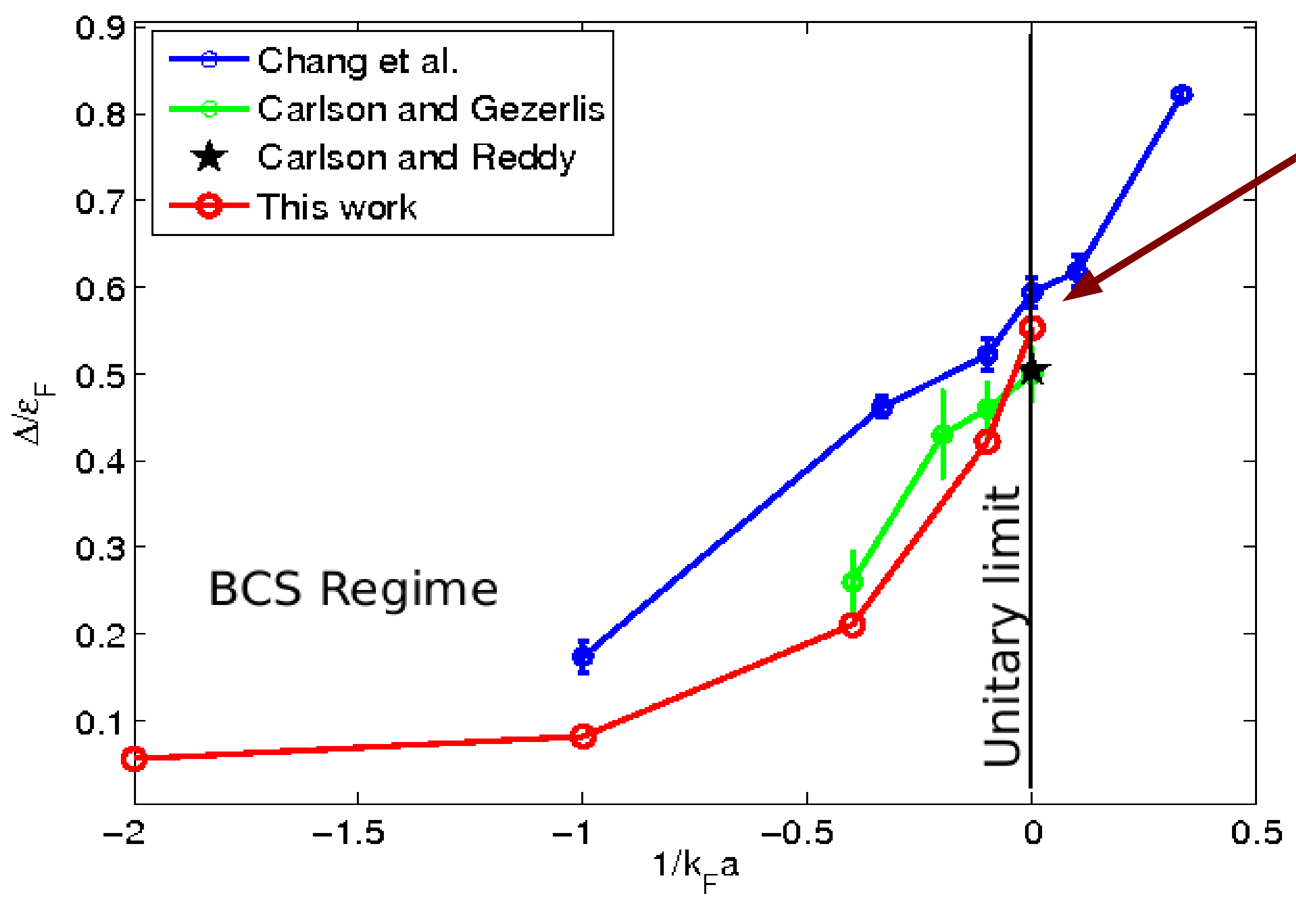
Our algorithm

Uncontrolled approximation

Compute exactly response function χ(p) as a function of T

Fit parameters m*, U, Δ to reproduce χ(p)

Unitary limit – energy gap I



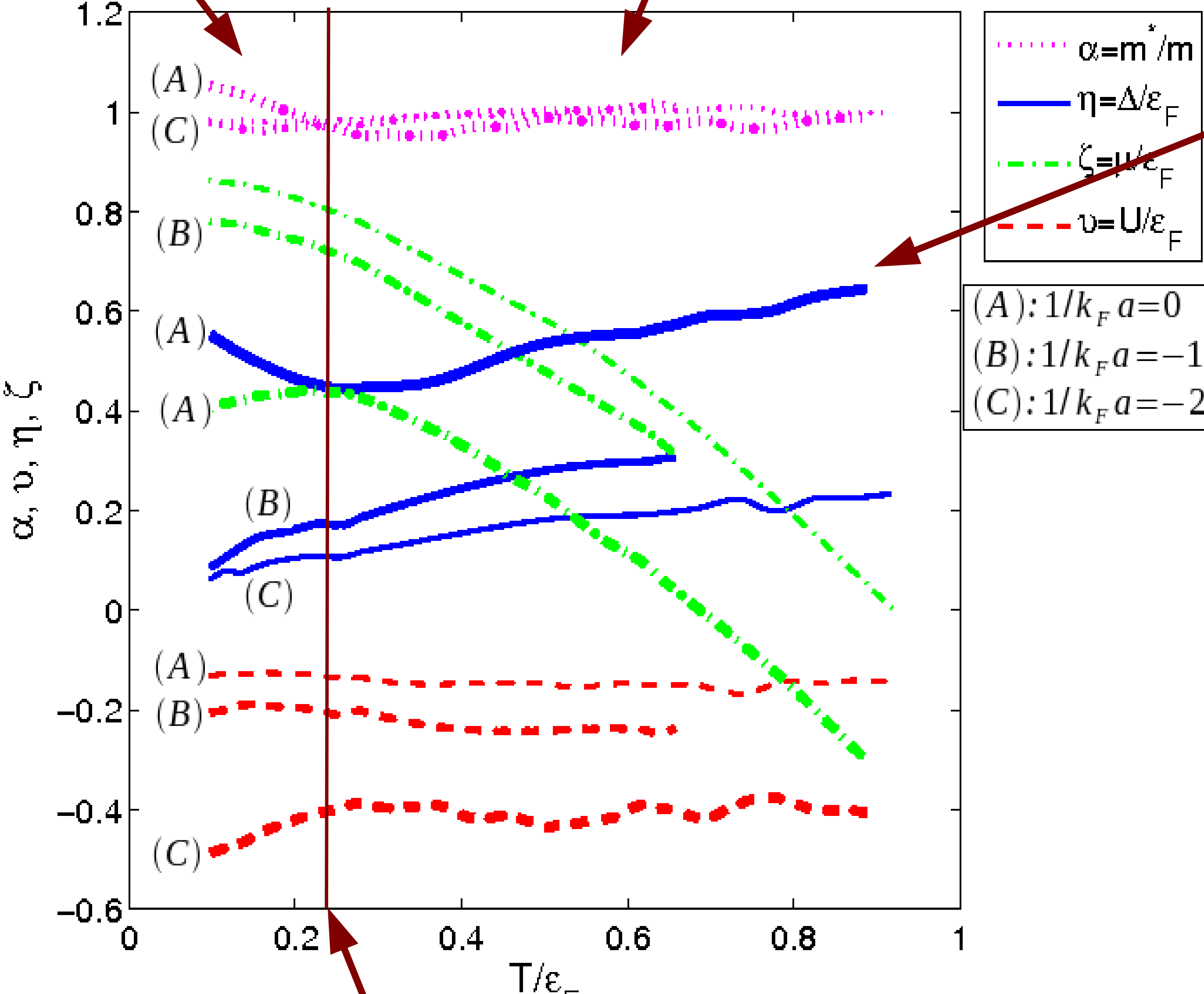
For unitary limit $\Delta/e_F=0.5$!
System is strongly correlated!

The pairing gap extracted from the response function at the lowest temperature (T=0.1eF) compared to the values for T=0

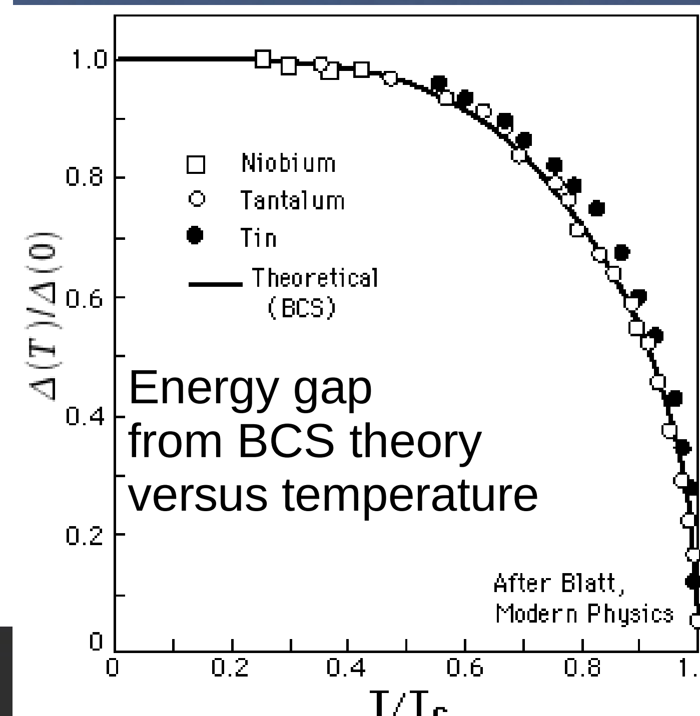
Superfluid phase

Normal phase

Unitary limit – energy gap II



The “pairing” gap extracted using the procedure described above demonstrates a rather unexpected behavior as function of temperature.



Energy gap from BCS theory versus temperature

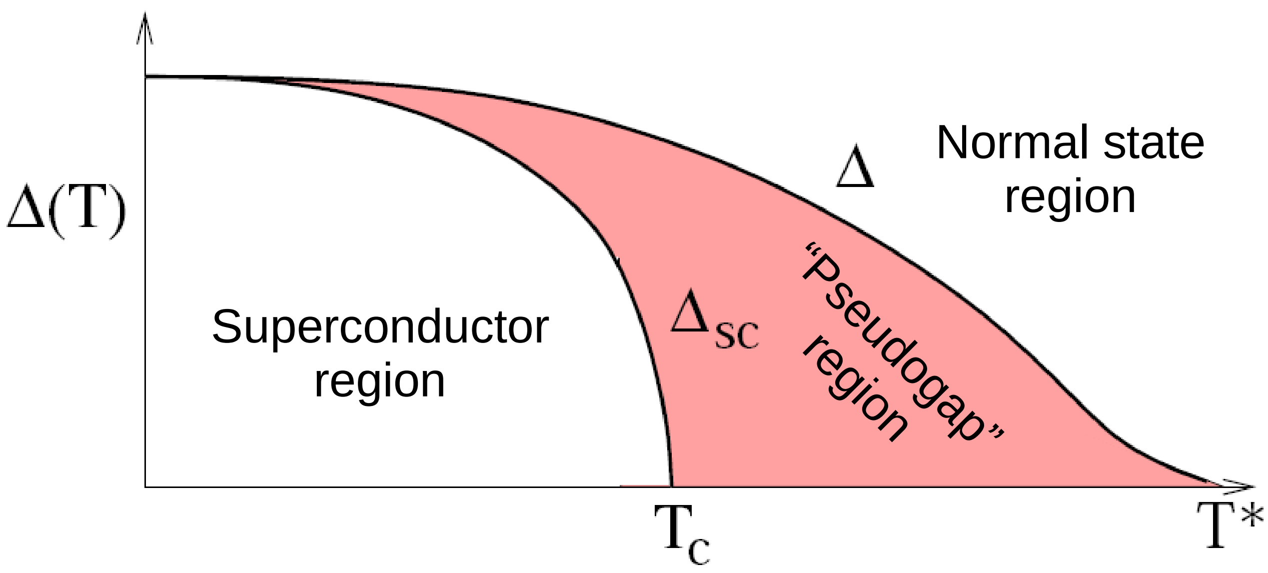
Critical temperature for unitarity: **T_c=0.23e_F**

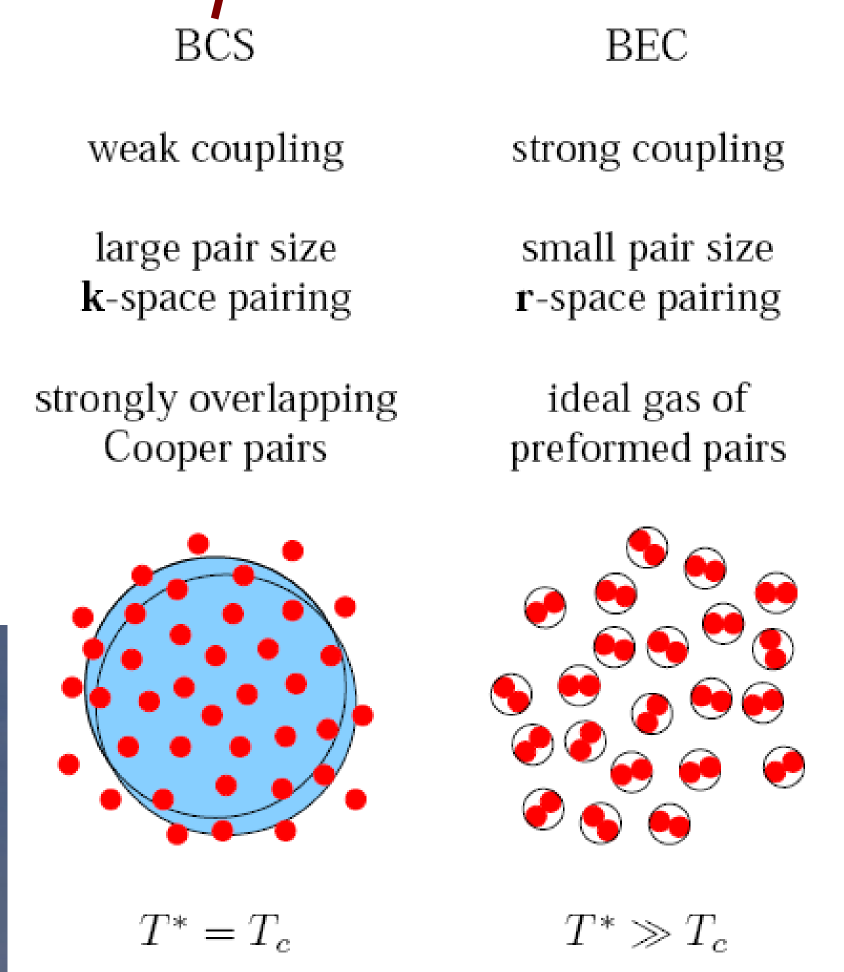
A. Bulgac, J.E. Drut, P. Magierski, Phys. Rev. Lett. 96 (2006) 090404

High temperature superconductors I

The excitations of the system must smoothly evolve from fermionic in the BCS regime to bosonic in the BEC regime

BCS assumes $\Delta_{sc} = \Delta$

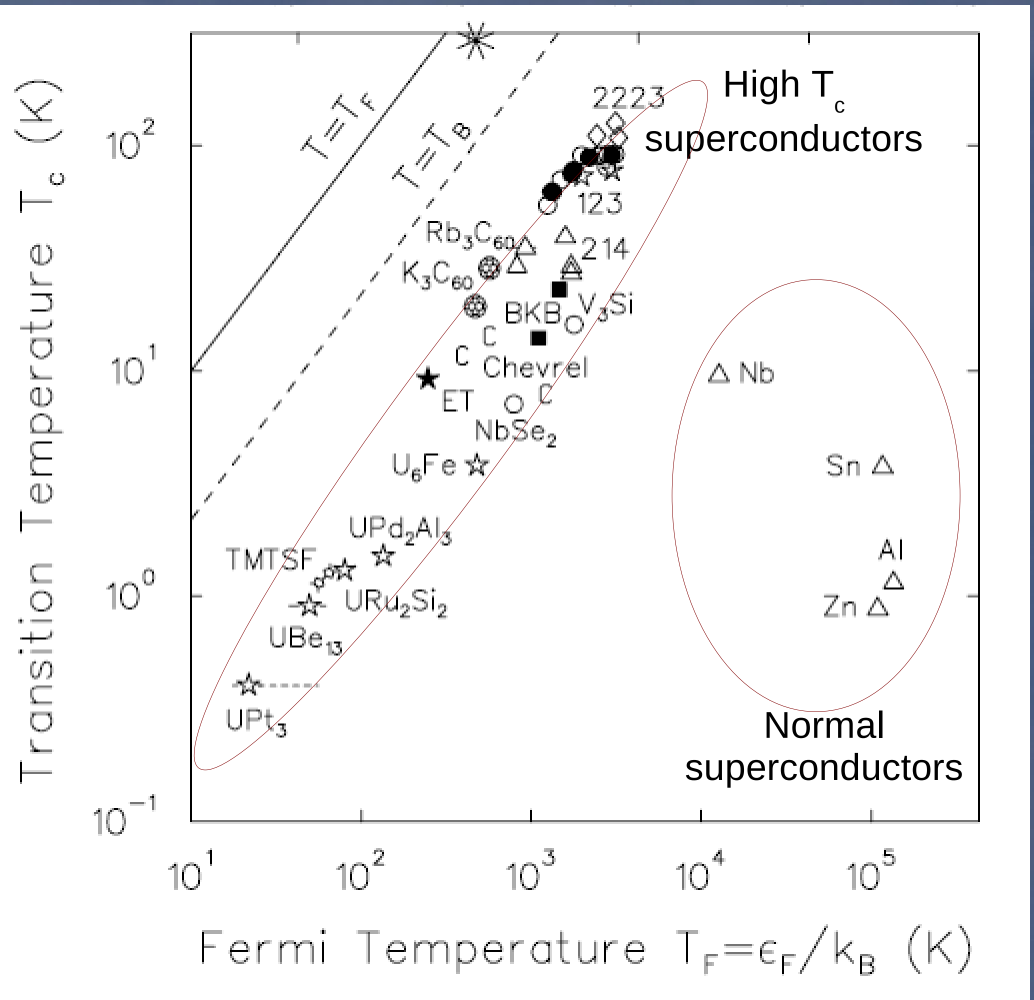




T_c - temperature at which pairs condensate

T* - temperature at which pairs form

High temperature superconductors II



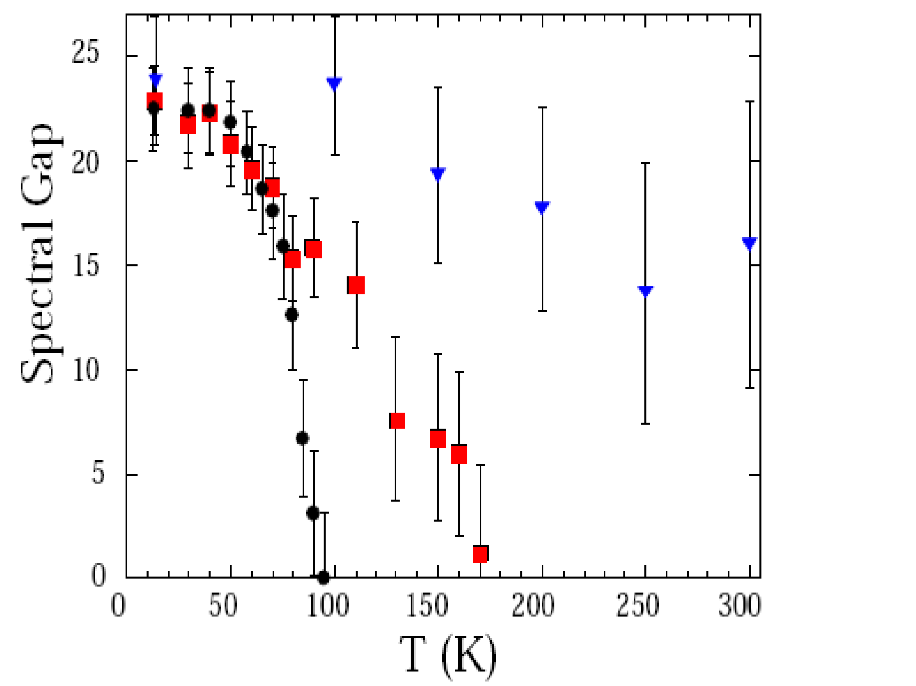


FIG. 9 (Color) Temperature dependence of the excitation gap from ARPES measurements for optimally doped (filled black circles), underdoped (red squares) and highly underdoped (blue inverted triangles) single-crystal BSCCO samples (taken from Ding *et al.*, 1996). There exists a pseudogap phase above T_c in the underdoped regime.

Pictures from:
Physics Reports 412, 1-88 (2005)

Energy gap – experiments

Determination of the Superfluid Gap in Atomic Fermi Gases by Quasiparticle Spectroscopy

André Schirotzek, Yong-il Shin, Christian H. Schunck and Wolfgang Ketterle
Department of Physics, MIT-Harvard Center for Ultracold Atoms, and Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts, 02139
(Dated: August 13, 2008)

TABLE I: Superfluid gap Δ, Hartree term U and final state interaction E_{final} in terms of the Fermi energy $\epsilon_{F\uparrow}$ for various interaction strengths $1/k_F a$.

$1/k_F a$	Δ	U	E_{final}
-0.25	0.22	-0.22	0.22
0	**0.44**	**-0.43**	**0.16**
0.38	0.7	-0.59	0.14
0.68	0.99	-0.87	0.12

But BCS model is assumed

Using photoemission spectroscopy to probe a strongly interacting Fermi gas

J. T. Stewart, J. P. Gaebler, and D. S. Jin*
JILA, Quantum Physics Division, National Institute of Standards and Technology and Department of Physics, University of Colorado, Boulder, CO 80309-0440, USA

Current challenge II – dilute neutron matter

Strongly interacting fermi gases
(unitary limit)

SIGN PROBLEM!

Generalization to finite
effective range
(suitable for dilute neutron matter)

Extension to dense
nuclear matter

Neutron star crust
(EoS, specific heat,
neutrino scattering)

Constraints for parameters
of nuclear energy
density functional

Interaction with effective range I

$$\hat{V} = \frac{1}{2}\sum_{i\neq j} g(\vec{r},\vec{r}\,')n_{\lambda}(\vec{r})n_{\lambda'}(\vec{r}\,')$$

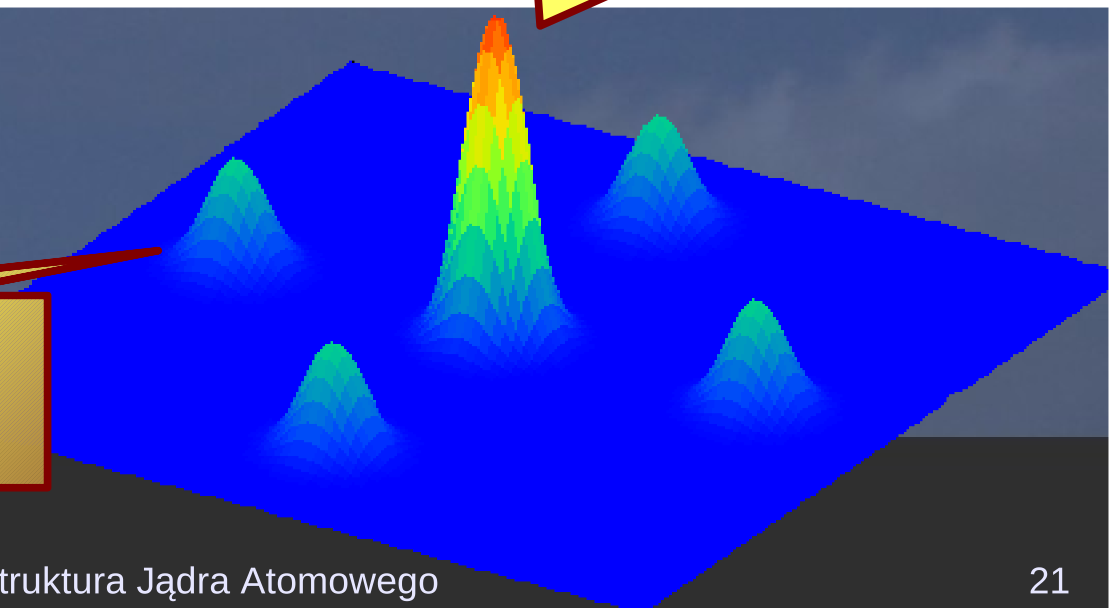
where $n_i = a_i^{\dagger}a_i$ is occupation operator, $i = (\vec{r},\lambda)$ and

$$g(\vec{r},\vec{r}\,') = \begin{cases} 6g, & |\vec{r}-\vec{r}\,'| = 0 \\ g, & |\vec{r}-\vec{r}\,'| = b \\ 0, & otherwise. \end{cases}$$

Contact interaction - 6g

We choose values of g and b to reproduce correctly
- **scattering length (a_s=-18.5 fm)**
- **effective range (r_{eff}=2.8 fm)**

Nearest neighborhood interaction - g



Interaction with effective range II

Contains the same physics:

$$V(\vec{r}-\vec{r}\,')=-g_0\,\delta(\vec{r}-\vec{r}\,')+g_1[\nabla^2\delta(\vec{r}-\vec{r}\,')+\delta(\vec{r}-\vec{r}\,')\nabla^2]$$

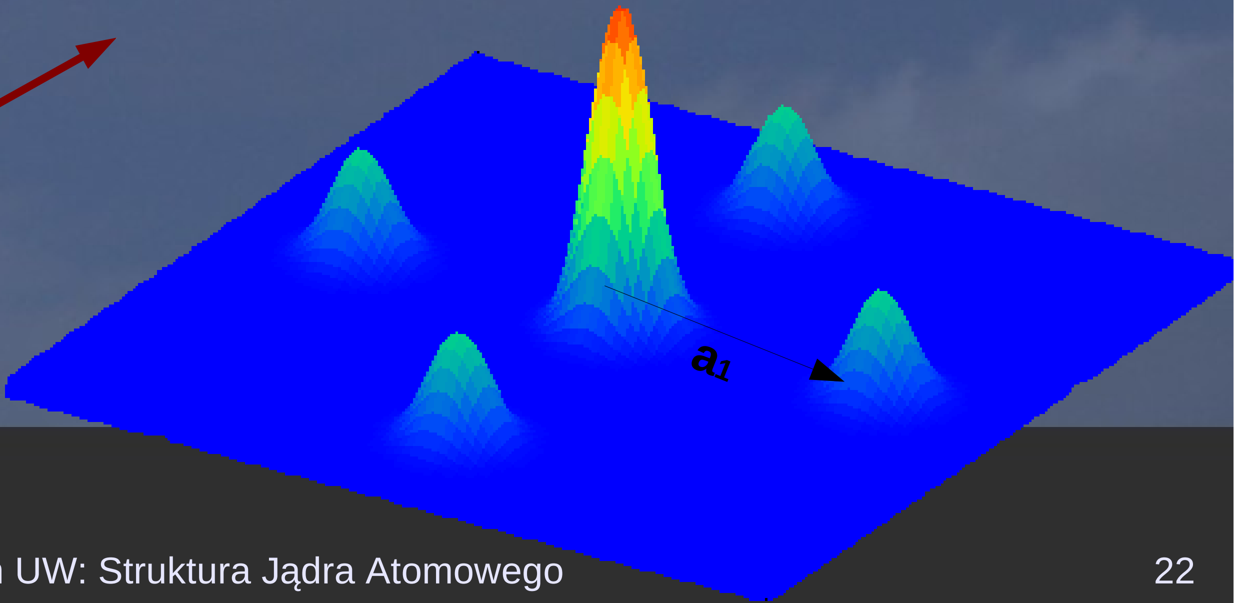
Lattice => discretization

Three point difference formula

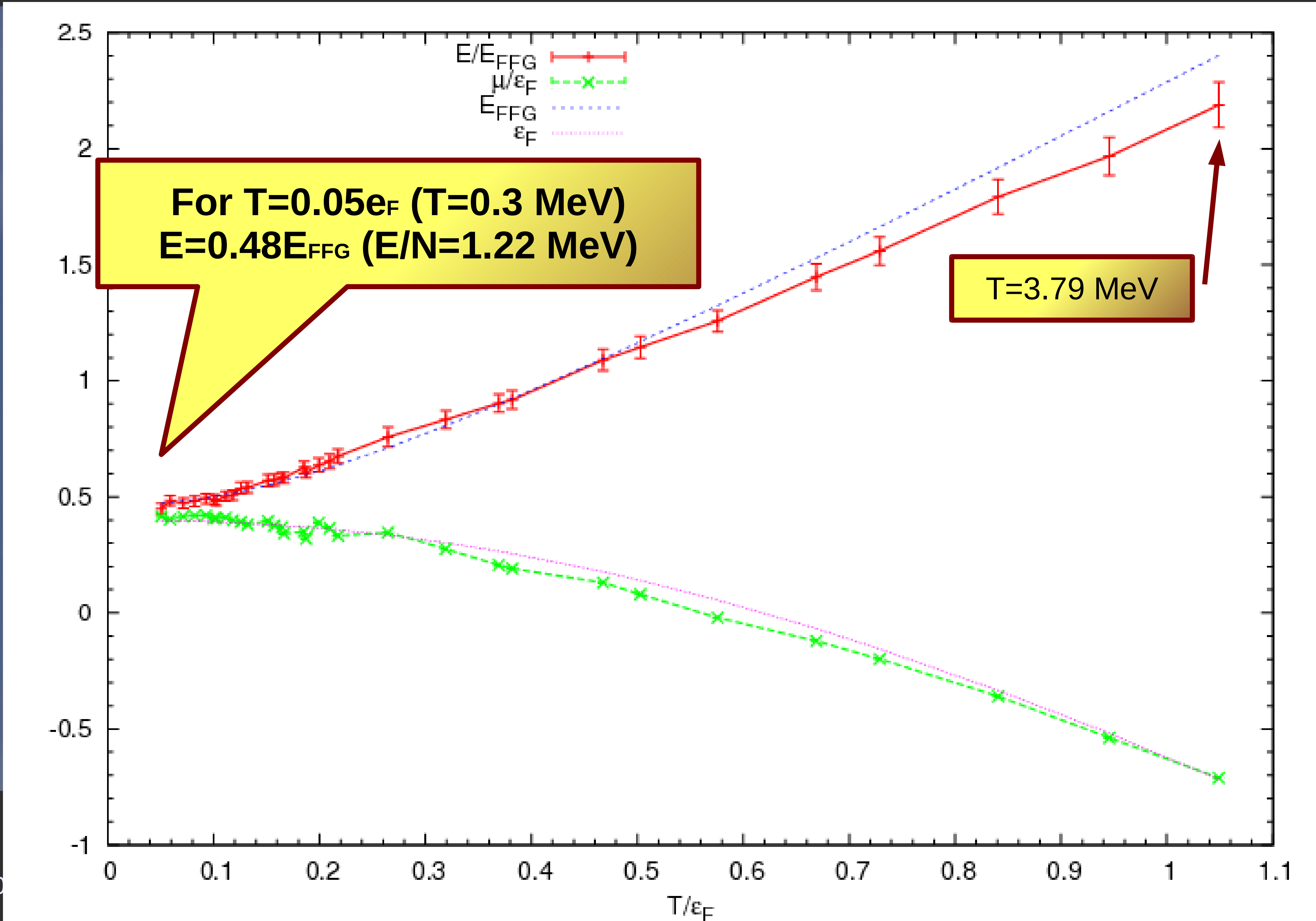
$$\nabla^2\psi(\vec{r})=\sum_{i=1}^{3}\frac{1}{\vec{a}_i^{\,2}}[\psi(\vec{r}-\vec{a}_i)+\psi(\vec{r}+\vec{a}_i)-2\psi(\vec{r})]$$

Contact interaction contribution

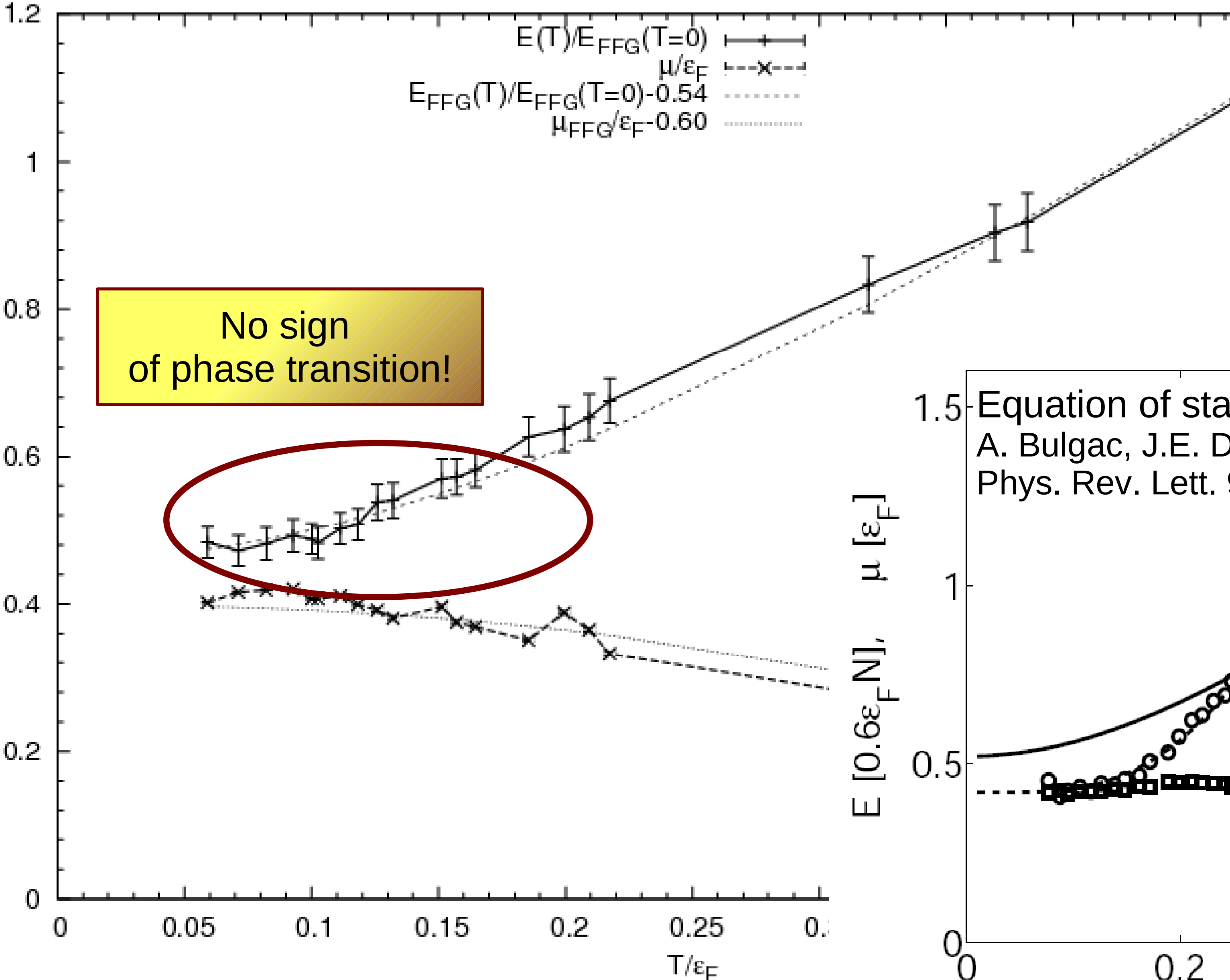
Nearest neighborhood contribution



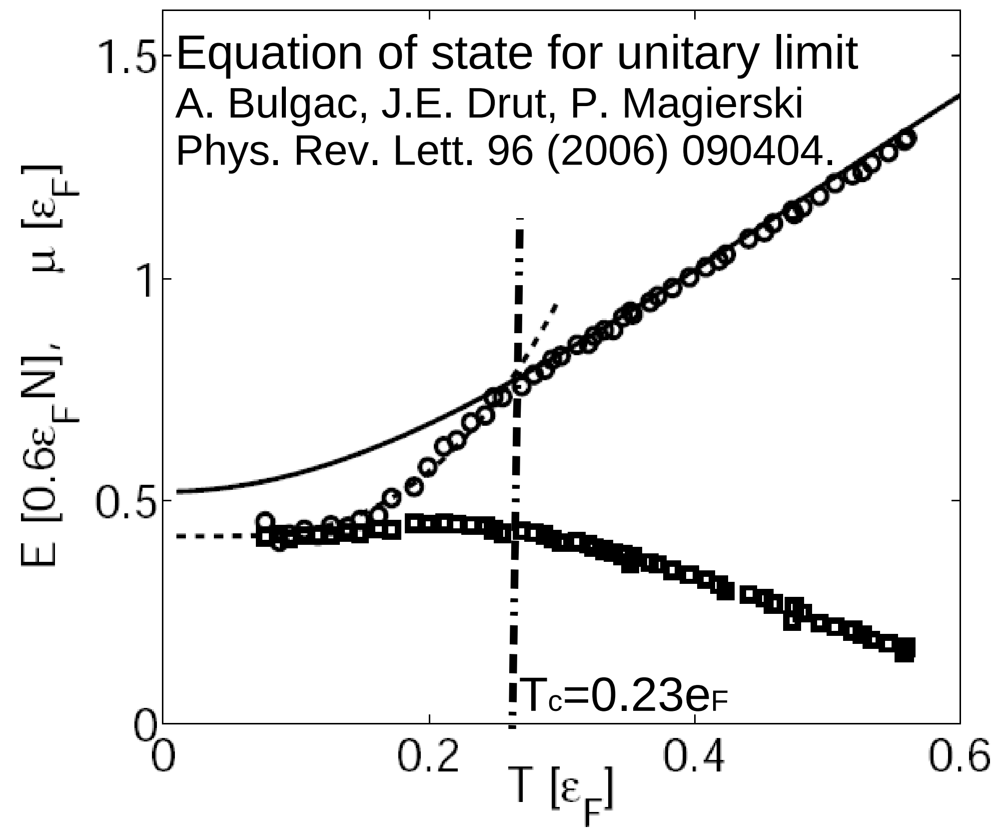
Equation of State for $\rho=0.02\rho_0$



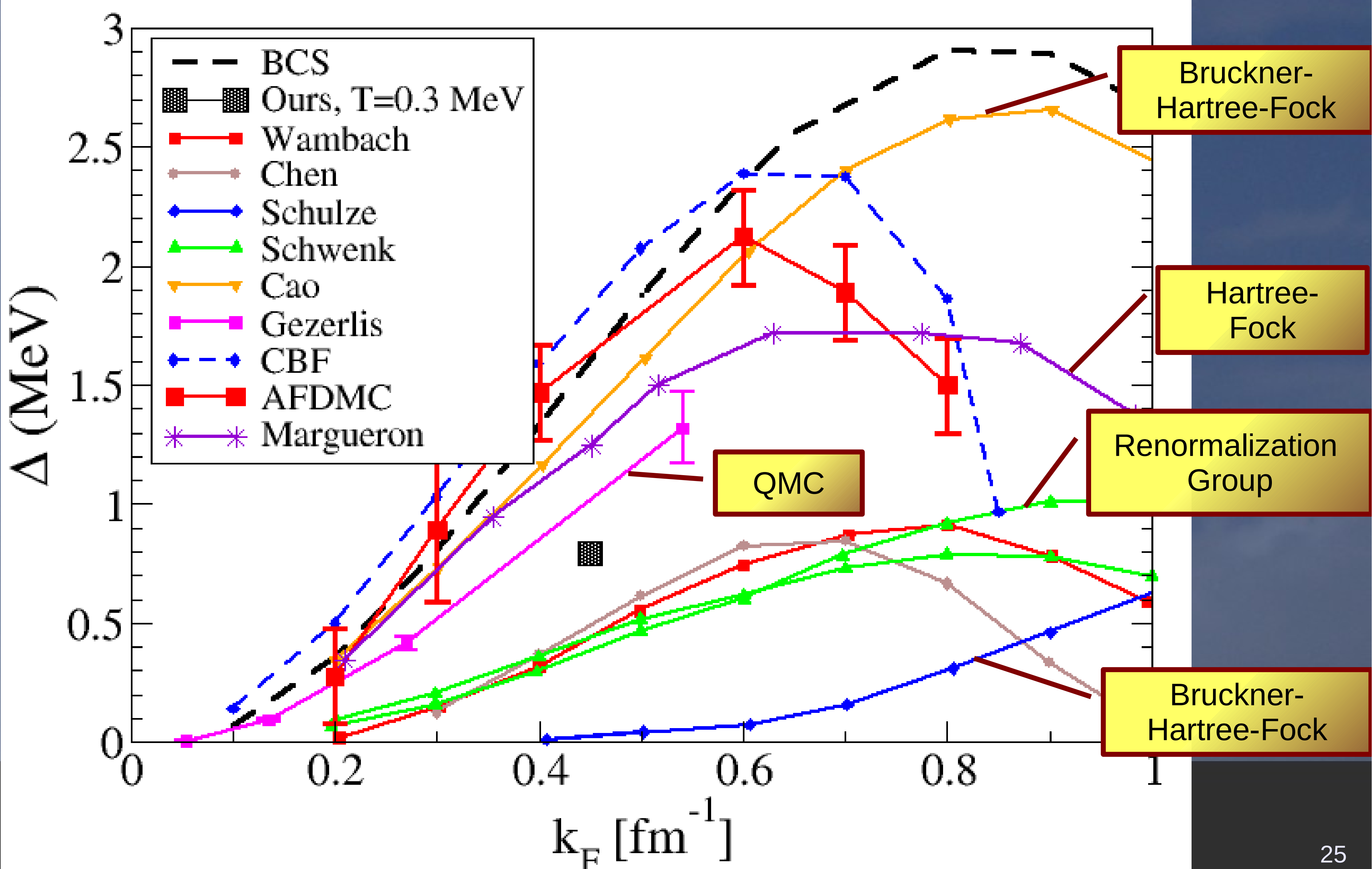
Equation of State for $\rho=0.02\rho_0$



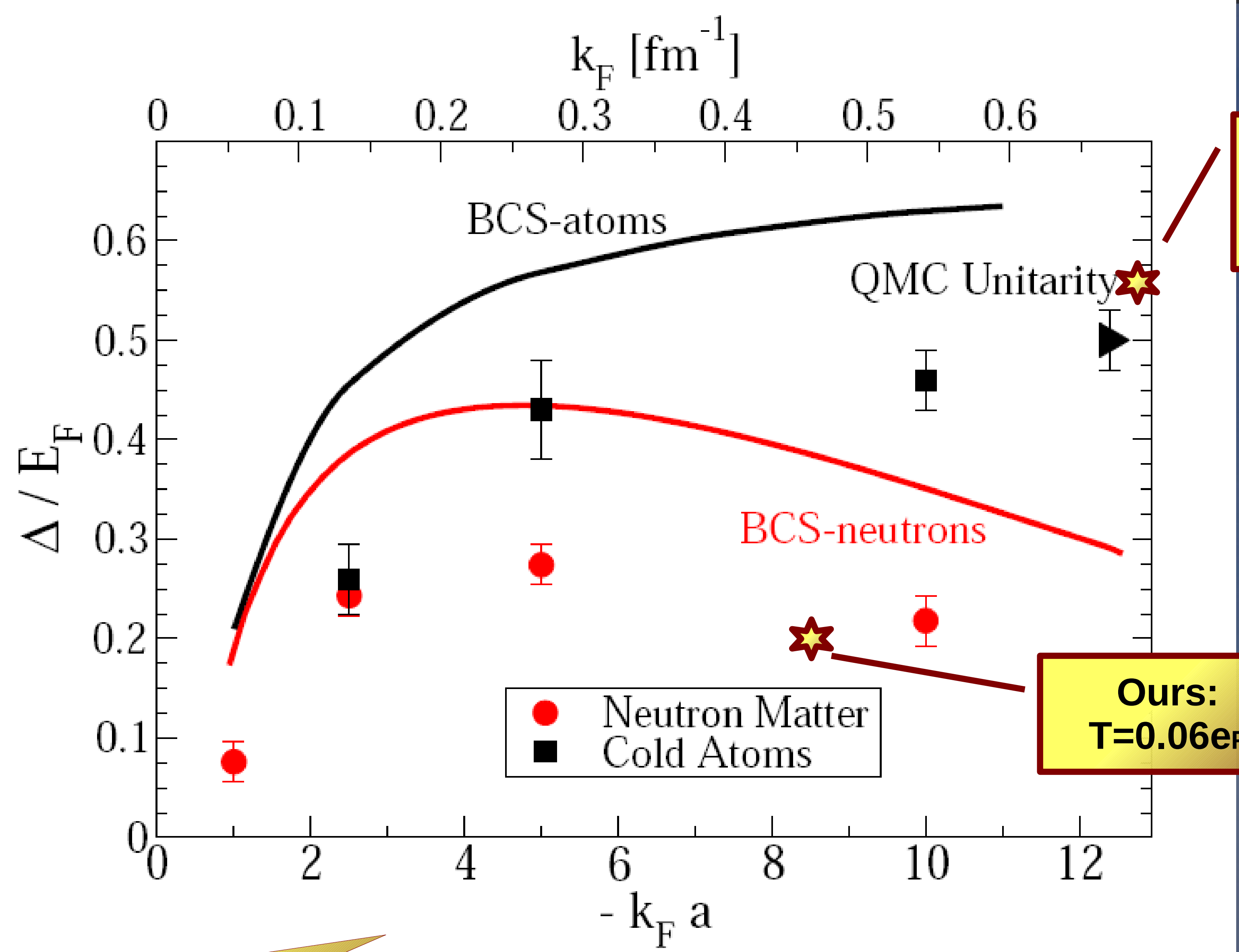
No sign
of phase transition!



Energy gap for $\rho=0.02\rho_0$



Energy gap for $\rho=0.02\rho_0$



Ours: unitarity $T=0.1e_F$

Ours: $T=0.06e_F$

Picture from:
A. Gezerlis, J. Carlson
Phys. Rev. C 77, 032801 (2008)

Dziękuję za uwagę

Quantum Monte Carlo I

Definition of the problem

$$Z(\beta,\mu)=Tr\{e^{-\beta(\hat{H}-\mu\hat{N})}\}$$

$$O(\beta,\mu)=\frac{1}{Z}Tr\{\hat{O}e^{-\beta(\hat{H}-\mu\hat{N})}\}$$

Trotter expansion

$$e^{-\beta(\hat{H}-\mu\hat{N})}=\prod_{j=1}^{N_\tau}e^{-\tau(\hat{H}-\mu\hat{N})}$$

$$=\prod_{j=1}^{N_\tau}\underbrace{e^{-\frac{\tau}{2}(\hat{T}-\mu\hat{N})}}_{\text{1 Body Op.}}\overbrace{e^{-\tau\hat{V}}}\underbrace{e^{-\frac{\tau}{2}(\hat{T}-\mu\hat{N})}}_{\text{1 Body Op.}}+0(\tau^3)$$

All of the difficulty arises from the two-body interaction.

What can we do?

Approximate by one-body operator
(idea of mean field calculations)

Another approach

$$\underbrace{e^{-\tau\hat{V}}}_{\text{2 Body Op.}} = \int d\vec{\sigma}\; \underbrace{e^{\hat{w}(\vec{\sigma})}}_{\text{1 Body Op.}}$$

Hubbard-Stratonovich transformation

In our case:

$$\hat{V} = -g\int d^3\vec{r}\; n_{\uparrow}(\vec{r})\, n_{\downarrow}(\vec{r})$$

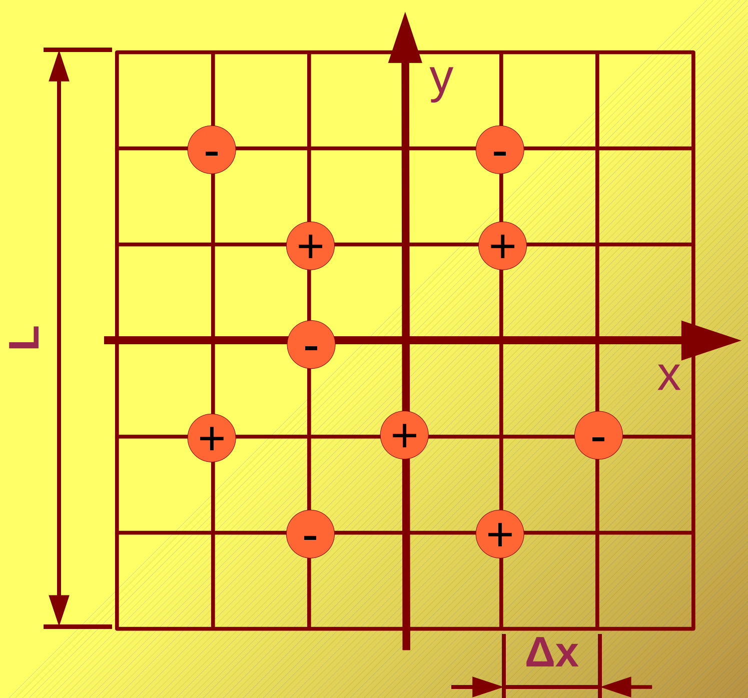
$$e^{-\tau\hat{V}} = \sum_{\sigma(\vec{r})\pm 1} e^{\sum_{\vec{r},\lambda} \ln(1+A\sigma(\vec{r}))\, n_{\lambda}(\vec{r})}, \quad A = \sqrt{e^{\tau g} - 1}$$

Discrete Hubbard-Stratonovich transformation

Lattice calculations I

External conditions:
T – temperature
μ – chemical potential

Coordinate representation: **r**, spin



$$e^{-\tau\hat{V}}\psi \sim e^{f(\sigma)n_\lambda(\vec{r})}\psi$$

One particle basis
wave functions of coordinate operator

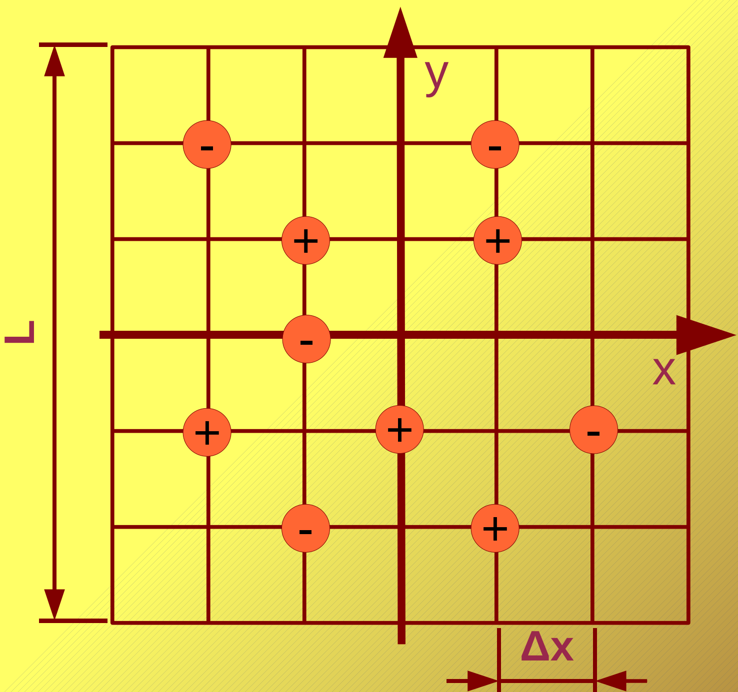
$$\phi_{\vec{r}\,'} = \delta(\vec{r} - \vec{r}\,')$$

The error generated by space discretization decreases exponentially as a function of lattice dimension

Lattice calculations II

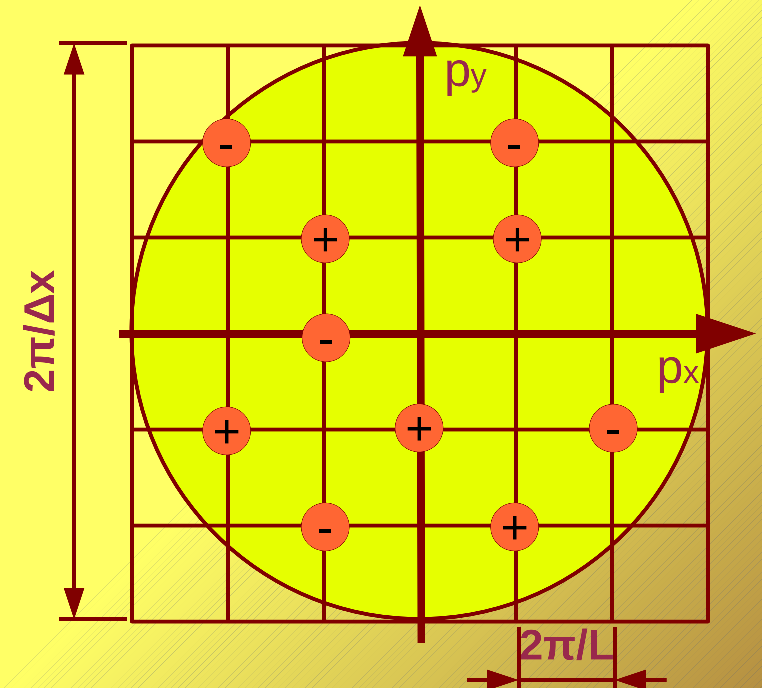
External conditions:
T – temperature
μ – chemical potential

Coordinate representation: **r**, spin



$$e^{-\tau \hat{V}} \psi \sim e^{f(\sigma) n_\lambda(\vec{r})} \psi$$

Momentum representation: **p**, spin

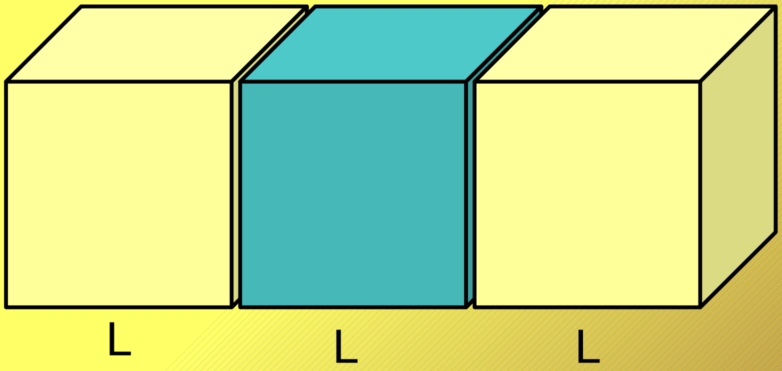


$$e^{\frac{-\tau}{2}\hat{T}} \psi \sim e^{\frac{p^2}{2\mathrm{m}} n_\lambda(\vec{p})} \psi$$

Periodic boundary conditions imposed

Lattice calculations III

L – limit of the spacial correlations in the system

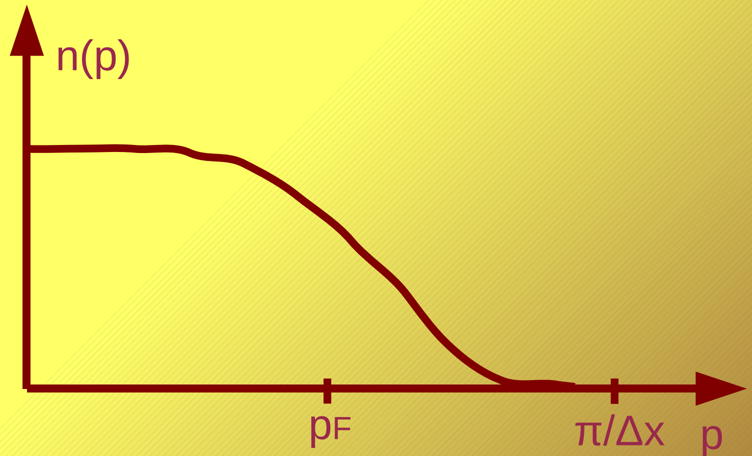


$$\xi \sim \varepsilon^{-\nu}, \quad \varepsilon = \frac{|T - T_0|}{T_0}$$

$$T \to T_0 \Rightarrow \xi \to \infty$$

Momentum cut-off

$$p_{cut} = \pi / \Delta x$$



Quasi-particle spectrum I

Definition of the static response function:

$$\chi_{AB}=\frac{1}{Z}\int_0^{\beta} d\lambda\; Tr\left\{e^{-(\beta-\lambda)(\hat{H}-\mu\hat{N})}\Delta\hat{A}\,e^{-\lambda(\hat{H}-\mu\hat{N})}\Delta\hat{B}\right\}$$

$$\Delta\hat{O}=\hat{O}-\langle\hat{O}\rangle,\quad \langle\hat{O}\rangle=\frac{1}{Z}Tr\left\{\hat{O}\,e^{-\beta(\hat{H}-\mu\hat{N})}\right\}$$

The static response function
measures the susceptibility of the observable B
with respect to the perturbation A.

$\langle\hat{B}\rangle_X-\langle\hat{B}\rangle_0=\chi_{AB}X$ where $\hat{H}(X)=\hat{H}-X\hat{A}$

Quasi-particle spectrum I

Let us define the static response function as

$$\chi(\vec{p}) = -\int_0^\beta d\tau\, G(\vec{p},\tau)$$

temperature Green's function

This response can be easily evaluated in the case of an independent-(quasi)particle model

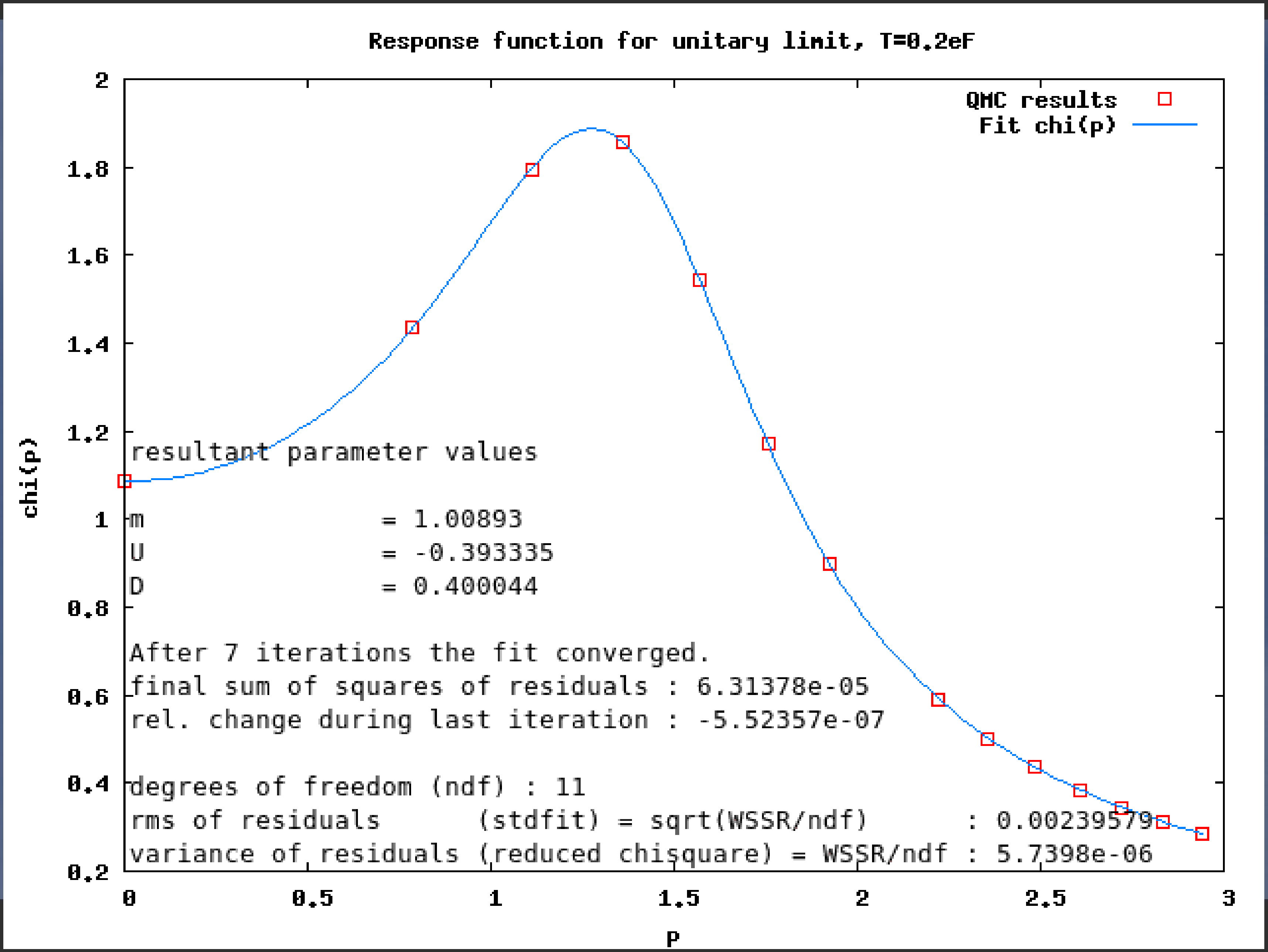
$$\chi(\vec{p}) = \frac{1}{E(\vec{p})} \frac{e^{\beta E(\vec{p})}-1}{e^{\beta E(\vec{p})}+1}$$

E(p) are the single-(quasi)particle excitation energies

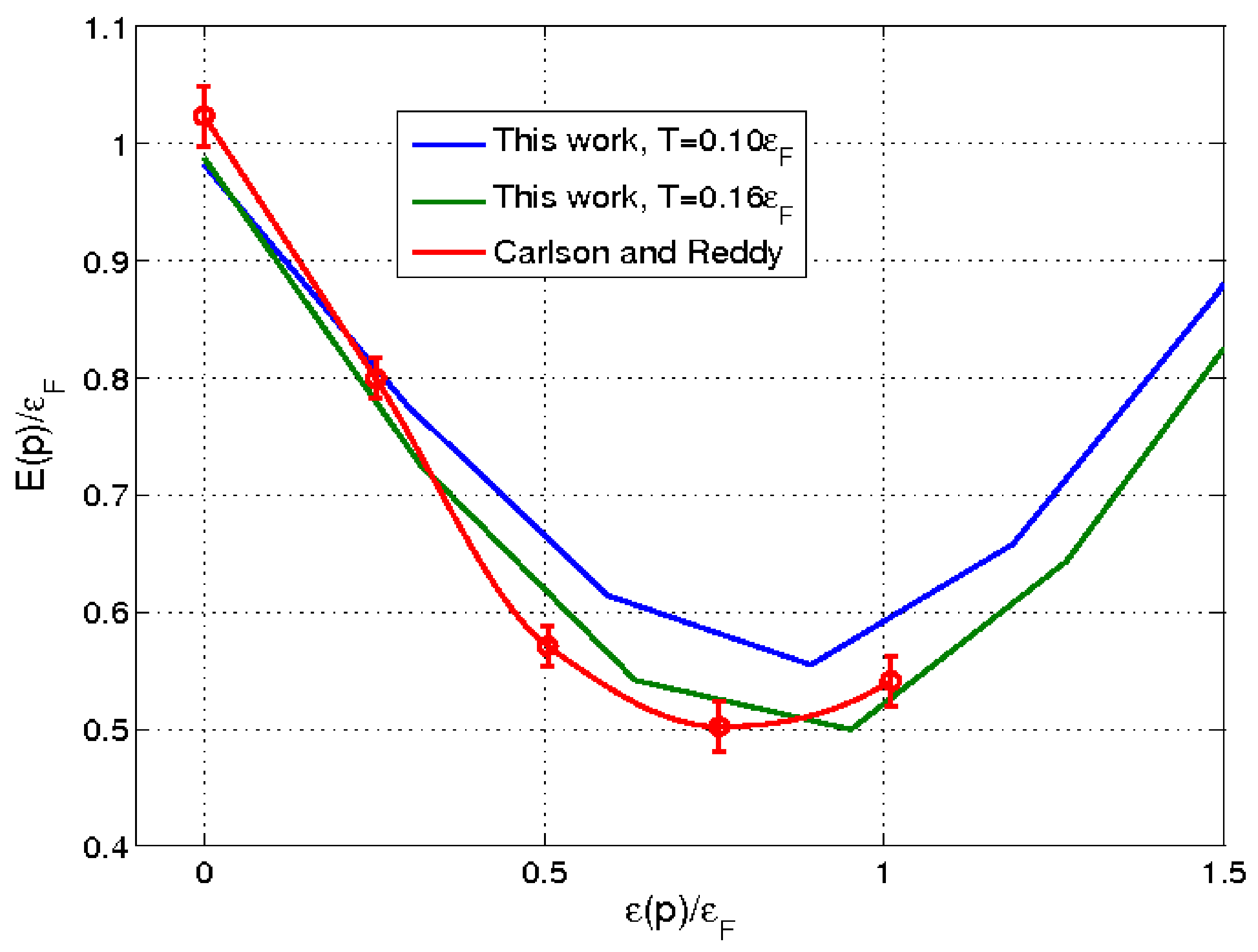
In case of noninteracting gas:

$$E(\vec{p}) = \frac{\vec{p}^{\,2}}{2\mathrm{m}} - \mu$$

Unitary limit – energy gap I

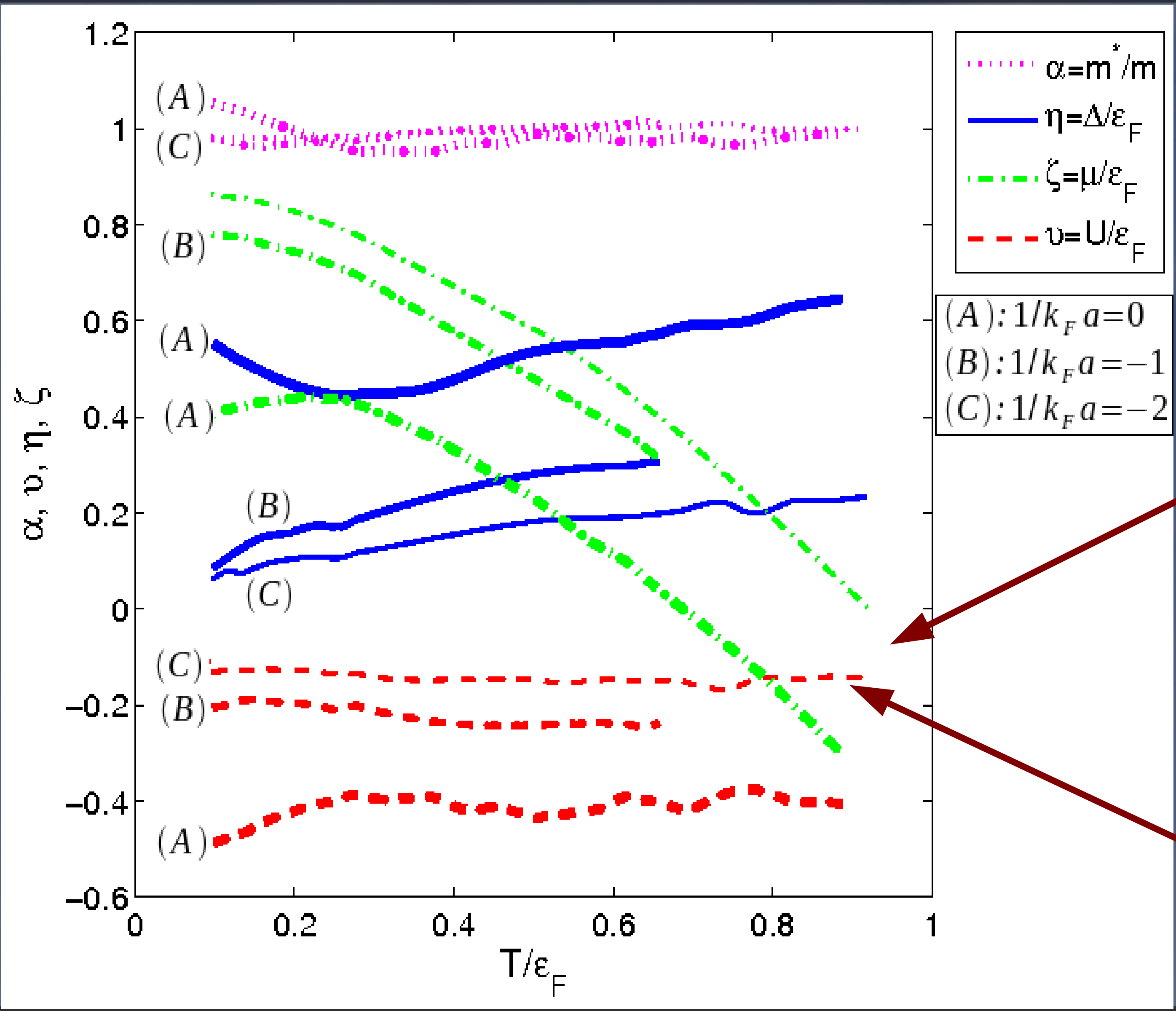


Unitary limit – energy gap III



The two lowest temperatures quasi-particle spectra compared to the one calculated for T=0

Unitary limit – energy gap IV



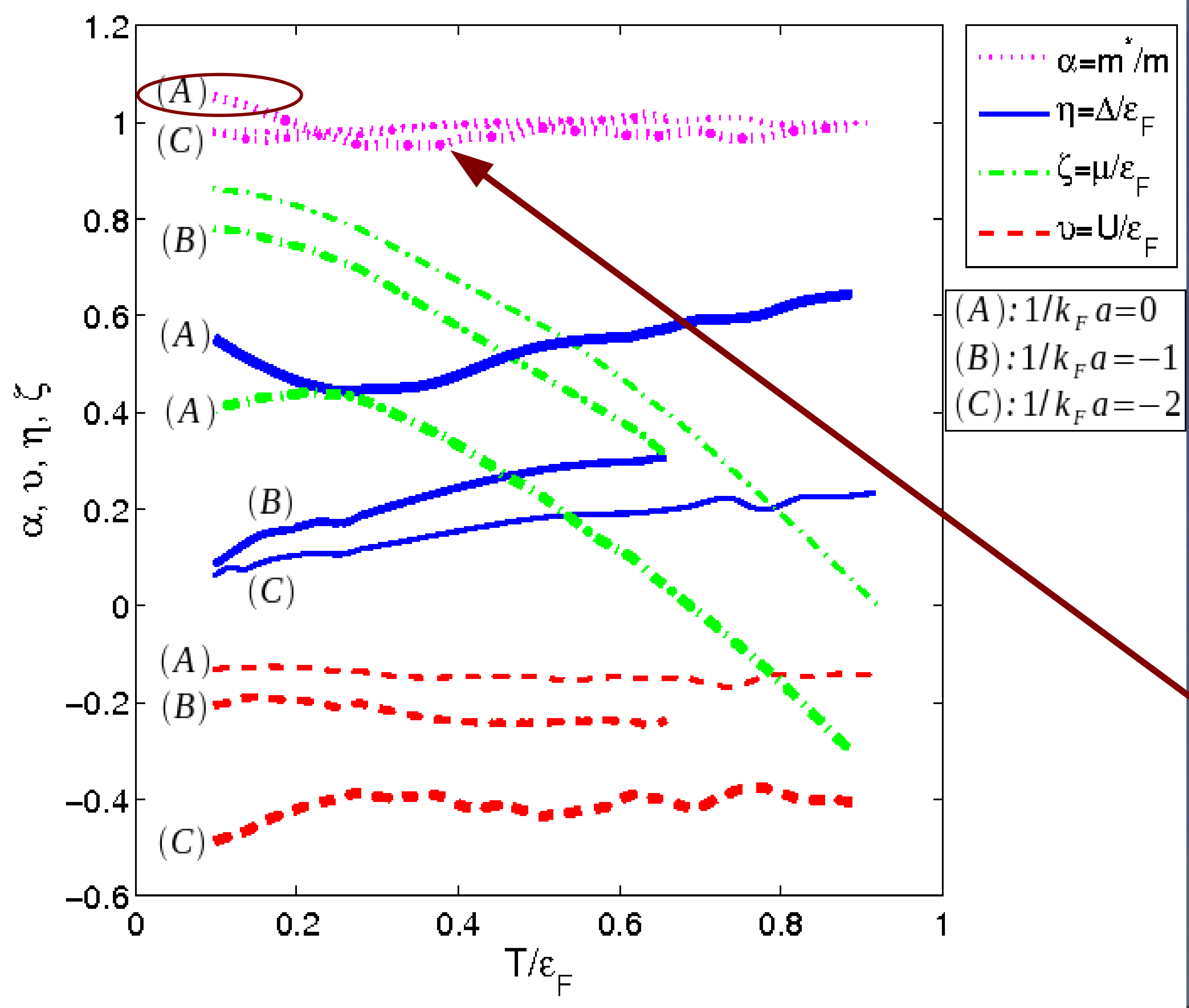
The value of the single-particle potential U shows essentially no temperature dependence in the range investigated by us.

Away from unitarity in the BCS regime the value of the potential U is very close to its Hartree-Fock value estimated as:

$$U = 4\pi a n / (1 - 2 p_{cut} a/\pi)$$

$$n = k_F^3 / 3\pi^2$$

Unitary limit – energy gap V

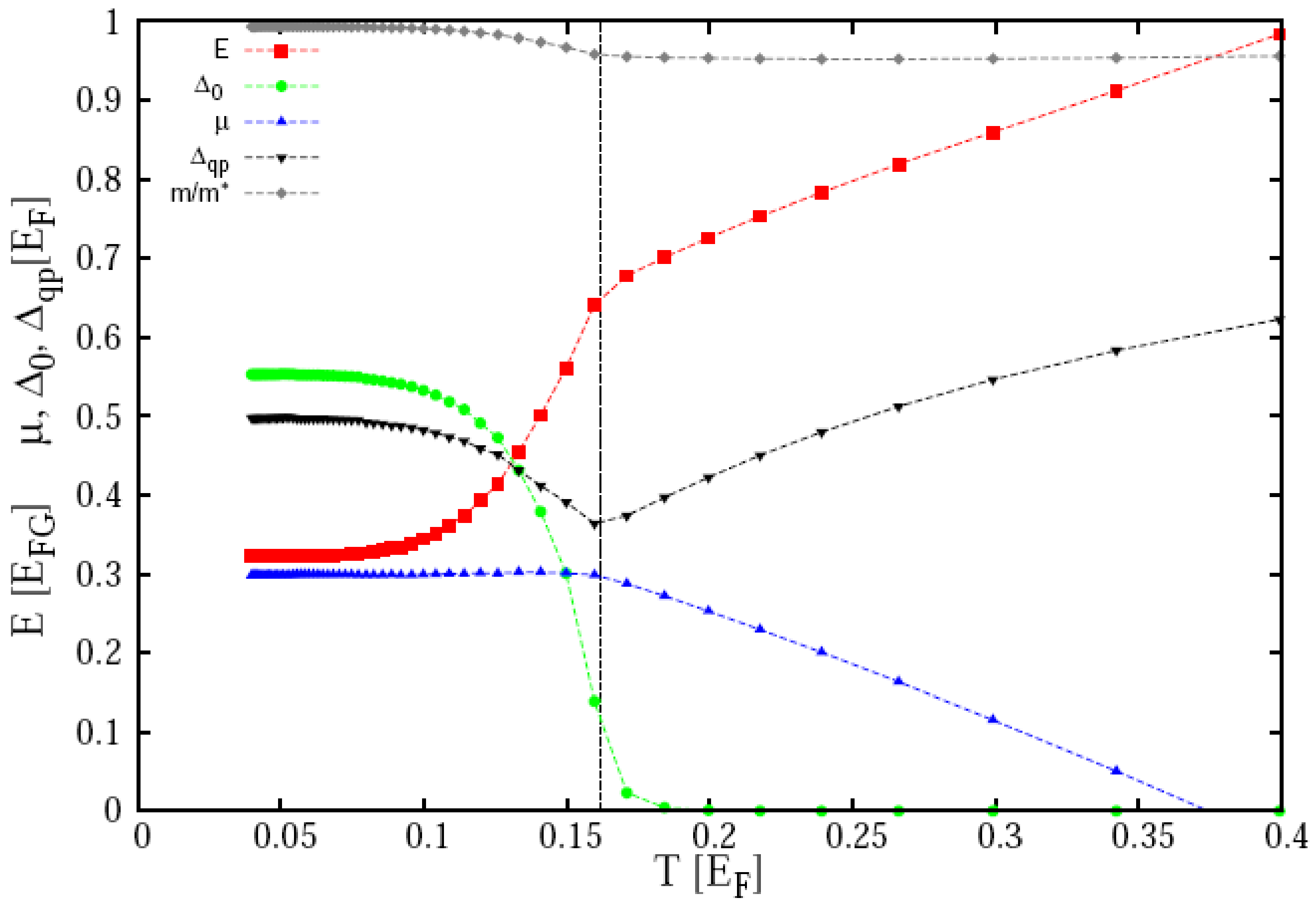


The value of the effective mass shows a little of temperature dependence only at unitarity

Away from unitarity the effective mass m* is essentially always equal to the bare mass

Superfluid to insulator phase transition in a unitary Fermi gas

Nir Barnea*
The Racah Institute of Physics, The Hebrew University, 91904 Jerusalem, Israel.
Institute for Nuclear Theory, University of Washington, 98195 Seattle, Washington, USA
(Dated: March 15, 2008)
arXiv:0803.2293



Δ_{qp} – energy gap in the single particle excitation spectrum

Δ_0 – order parameter

$$\Delta_0 = U \langle T c_\uparrow(0^+) c_\downarrow(0) \rangle$$

For weakly interacting fermions, in the BCS regime:

$$\Delta_{qp} = \Delta_0$$

H-S Transformation with effective range

Another approach

$$\underbrace{e^{-\tau \hat{V}}}_{\text{2 Body Op.}} = \int d\vec{\sigma}\; \underbrace{e^{\hat{w}(\vec{\sigma})}}_{\text{1 Body Op.}}$$

Hubbard-Stratonovich transformation

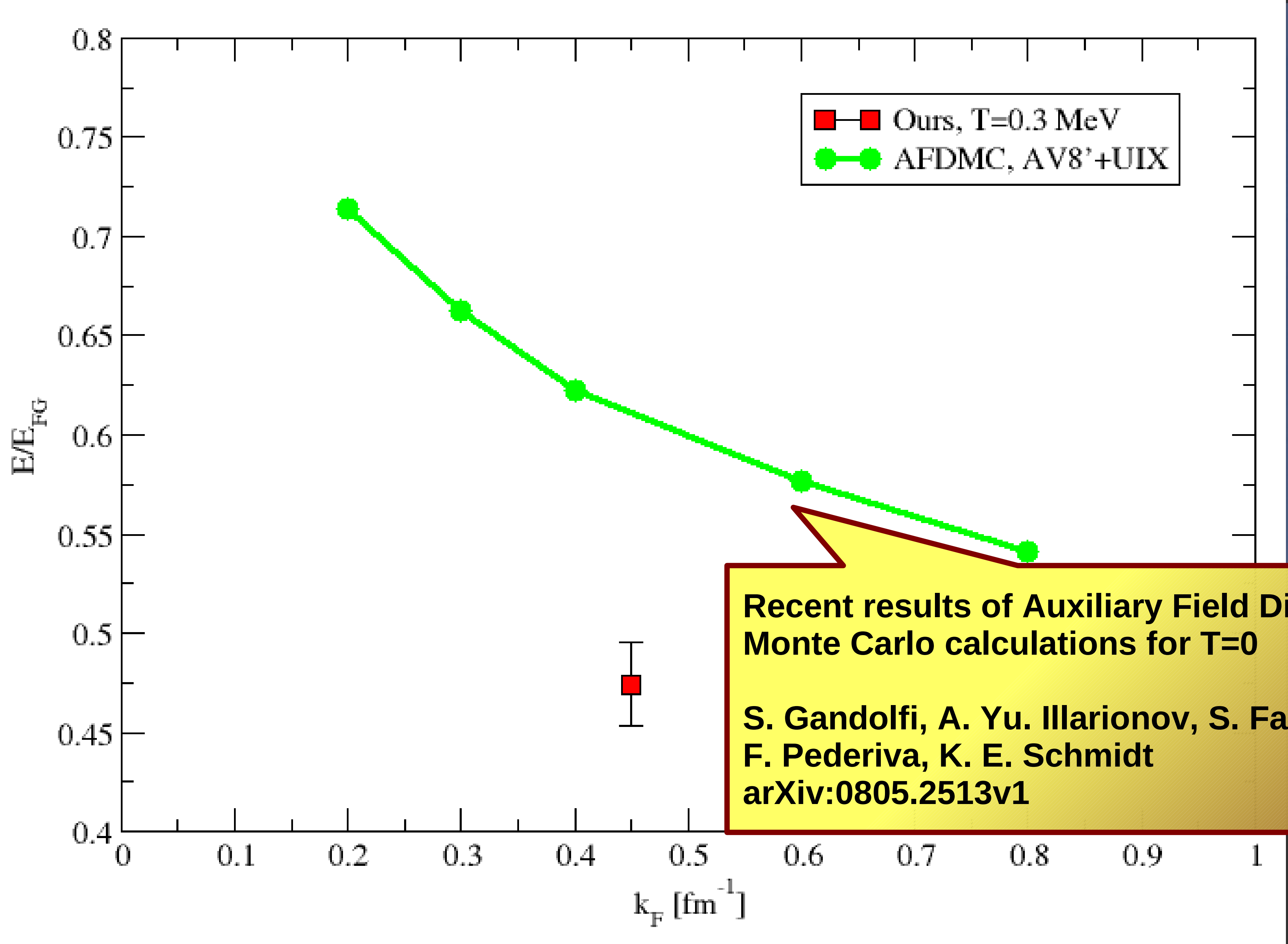
In our case:

$$e^{-\tau \hat{V}} = \prod_{|\vec{r}-\vec{r}\,'|=b} \frac{1}{k} \sum_{i=1}^{k} e^{\sigma_i(\vec{r},\vec{r}\,')(n_\uparrow(\vec{r})+n_\downarrow(\vec{r})+n_\uparrow(\vec{r}\,')+n_\downarrow(\vec{r}\,'))}$$

Real numbers

Discrete Hubbard-Stratonovich transformation

Equation of State for $\rho=0.02\rho_0$



Recent results of Auxiliary Field Diffusion Monte Carlo calculations for T=0

S. Gandolfi, A. Yu. Illarionov, S. Fantoni, F. Pederiva, K. E. Schmidt arXiv:0805.2513v1