Thermodynamic properties and phase transitions in dilute fermion matter

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Slides will be posted on my webpage

Why would one want to study this system?

One reason:

**(for the nerds, I mean the hard-core theorists,
not for the phenomenologists)**

Bertsch's 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.

Let me consider as an example the hydrogen atom.

The ground state energy could only be a function of:

- ✓ Electron charge
- ✓ Electron mass
- ✓ Planck's constant

and then trivial dimensional arguments lead to

$$E_{gs} = \frac{e^4 m}{\hbar^2} \times \frac{1}{2}$$

Only the factor ½ requires some hard work.

Let me now turn to dilute fermion matter

The ground state energy is given by such a function:

$$E_{gs} = f(N, V, \hbar, m, a, r_0)$$

Taking the scattering length to infinity and the range of the interaction to zero, we are left with:

$$E_{gs} = F(N, V, \hbar, m) = \frac{3}{5}\varepsilon_F N \times \xi$$

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

Pure number

Part of what George Bertsch essentially asked in 1999 is: ***Tell me the value of ξ !***

But he wished to know the properties of the system as well: ***The system turned out to be superfluid !***

$$E_{gs} = \frac{3}{5}\varepsilon_F N \times \xi \qquad \Delta = \varepsilon_F \times \varsigma$$

$$\xi = 0.40(1), \qquad \zeta = 0.50(1)$$

Now these results are a bit unexpected.

✓ **The energy looks almost like that of *a non-interacting system*!** **(no other dimensional parameters in the problem)**

✓ **The system has *a huge pairing gap*!**

✓ **This system is a very strongly interacting one, since the *elementary cross section is infinite*!**

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!

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.

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

• Baker (LANL, 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.

Carlson et al (2003) have also shown that the system has <u>a huge pairing gap</u> !

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

The initial Bertsch's Many Body challenge has evolved over time and became the problem of *Fermions in the Unitary Regime*.

The system is very dilute, but strongly interacting!

$$\boxed{n\, r_0^3 \ll 1} \qquad \boxed{n\, |a|^3 \gg 1}$$

n - number density

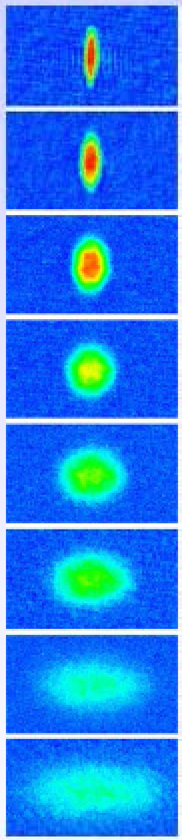
$$\boxed{r_0 \ll n^{-1/3} \approx \lambda_F/2 \ll |a|}$$

r_0 - range of interaction

a - scattering length

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)

Superconductivity and Superfluidity in Fermi Systems

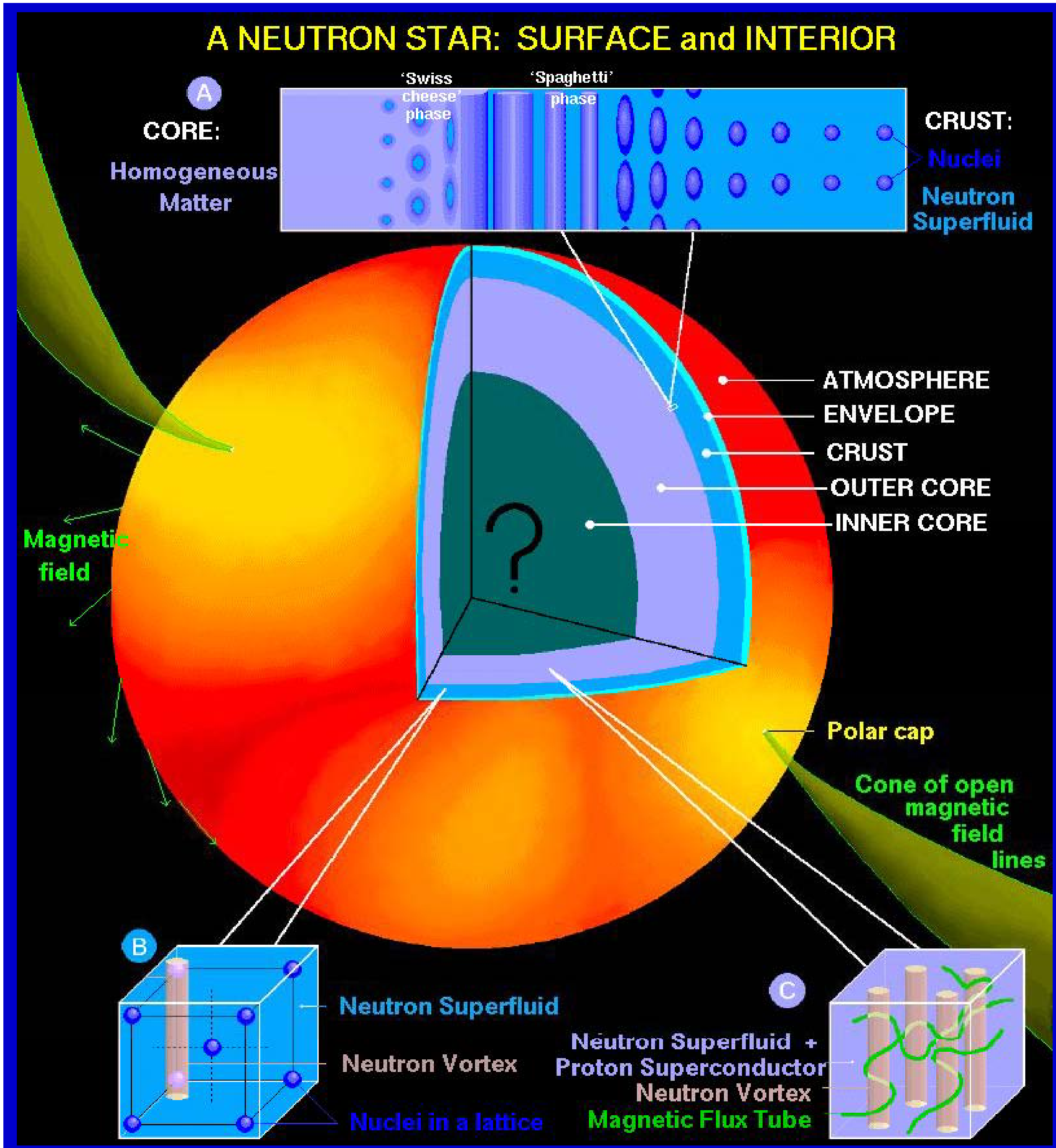
20 orders of magnitude over a century of (low temperature) physics

- ✓ **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)

Let's see how good we are at what we are doing after about ¾ of century of nuclear physics.

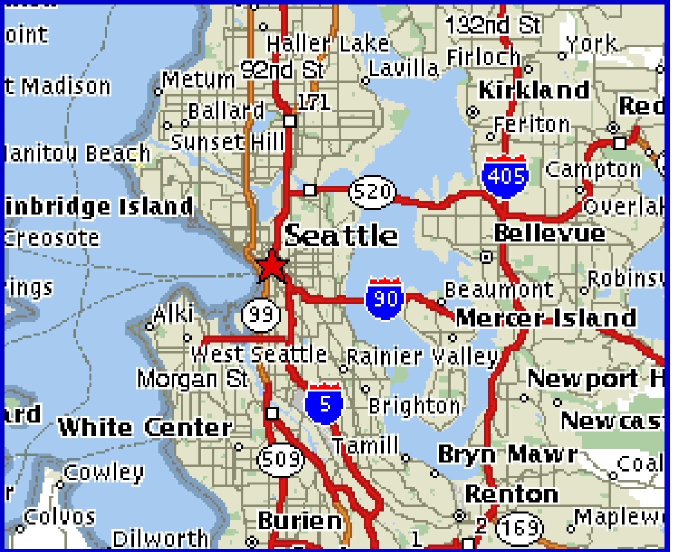
Let us look at the properties of a neutron star?



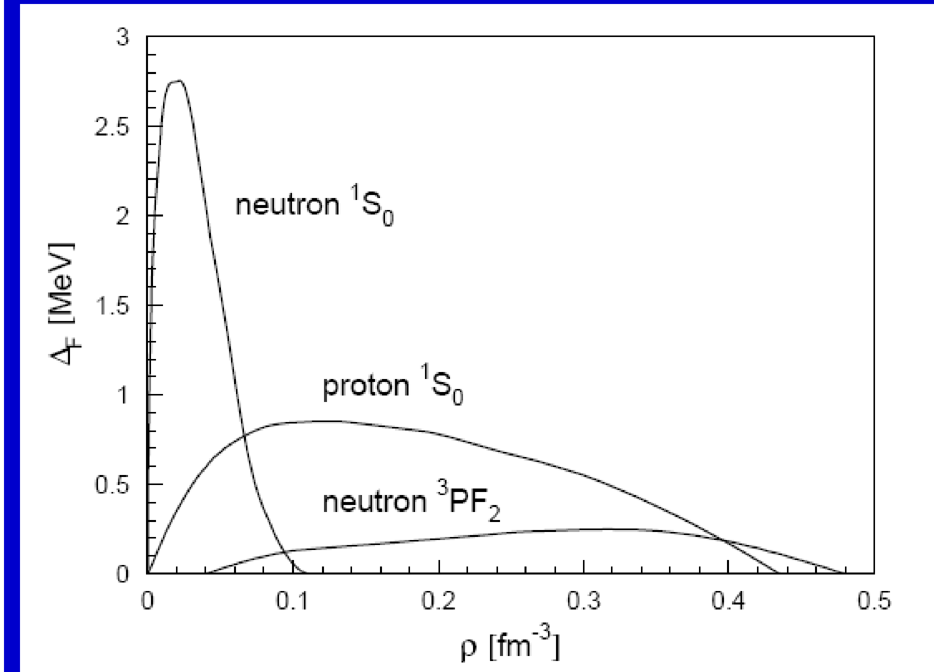
• **A neutron star will cover the map at the bottom**

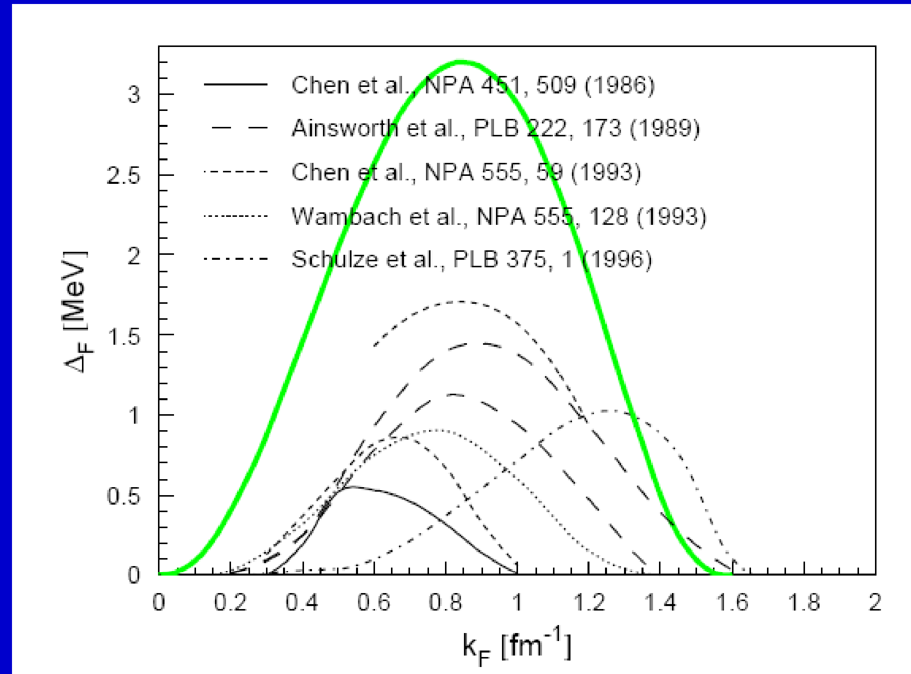
• **The mass is about 1.5 solar masses**

• **Density ≈ 10^{14} g/cm^3**



Author: Dany Page (UNAM)





These are "simple BCS" results.

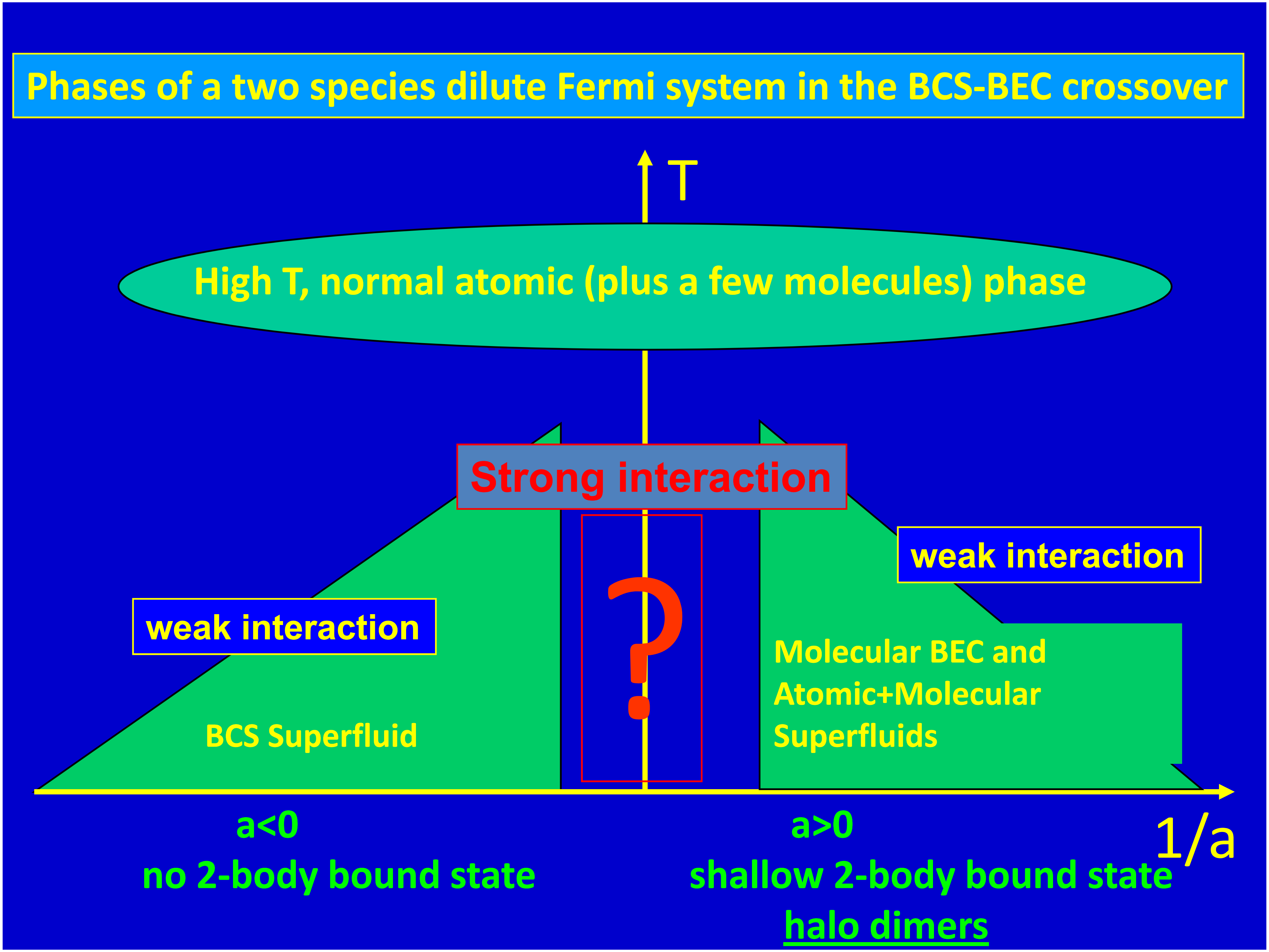
These are "beyond BCS" results for the $^1S_0$ neutron pairing gap only, except the green curve.

a neutron star. We have seen that most of the results that can be found in the literature, are obtained within the BCS approximation.

Unfortunately, as has also been pointed out, this approximation cannot be considered reliable in any region of density, since neutron matter is a strongly correlated Fermi system: The same nucleons that participate to the pairing cou-

Lombardo and Schultze, Lect. Notes Phys. 578, 30 (2001)

Clearly we have some serious problems here!


Phases of a two species dilute Fermi system in the BCS-BEC crossover
T
High T, normal atomic (plus a few molecules) phase
Strong interaction
weak interaction
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

Theoretical tools and features:

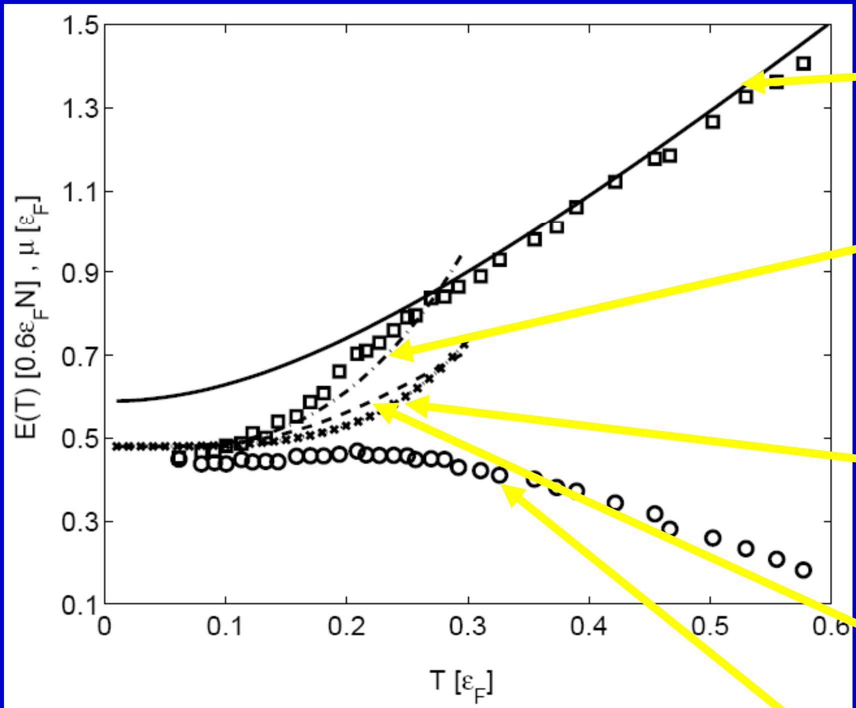
- Canonical and Grand Canonical Ensembles
- Hubbard-Stratonovich transformation
- Auxiliary Field Quantum Monte-Carlo
- Absence of Fermion sign problem
- Markov process, Metropolis importance sampling, decorrelation, …
- Renormalization of the two-body interaction
- Spatio- (imaginary) temporal lattice formulation of the problem
- One-particle temperature (Matsubara) propagator
- Extension of Density Functional Theory to superfluid systems
- Superfluid to Normal phase transition (second order)
- Off-diagonal long range order, condensate fraction, finite size scaling and extraction of critical temperature
- S- and P-wave superfluidity, induced interactions
  (NB - bare interaction in s-wave only)
- Larkin-Ovchinnikov-Fulde-Ferrell superfluidity (LOFF/FFLO)
- Quantum phase transitions (T=0, first and second order)
- Phase separation
- Pairing gap and pseudo-gap
- Supersolid

I will not talk about:

- Pairing Gap and Pseudo-Gap
- Vortices and their structure
- Collective oscillations, sound modes
- Time-dependent phenomena
- Large amplitude collective motion
- Small systems in traps within GFMC/DMC and building of ASLDA functional (superfluid DFT)
- Detailed comparison of theory and experiment

$a = \pm\infty$

Bulgac, Drut, and Magierski
Phys. Rev. Lett. 96, 090404 (2006)



Normal Fermi Gas
(with vertical offset, solid line)

Bogoliubov-Anderson phonons and quasiparticle contribution (dot-dashed line)

Bogoliubov-Anderson phonons contribution only

Quasi-particles contribution only (dashed line)

μ - chemical potential (circles)

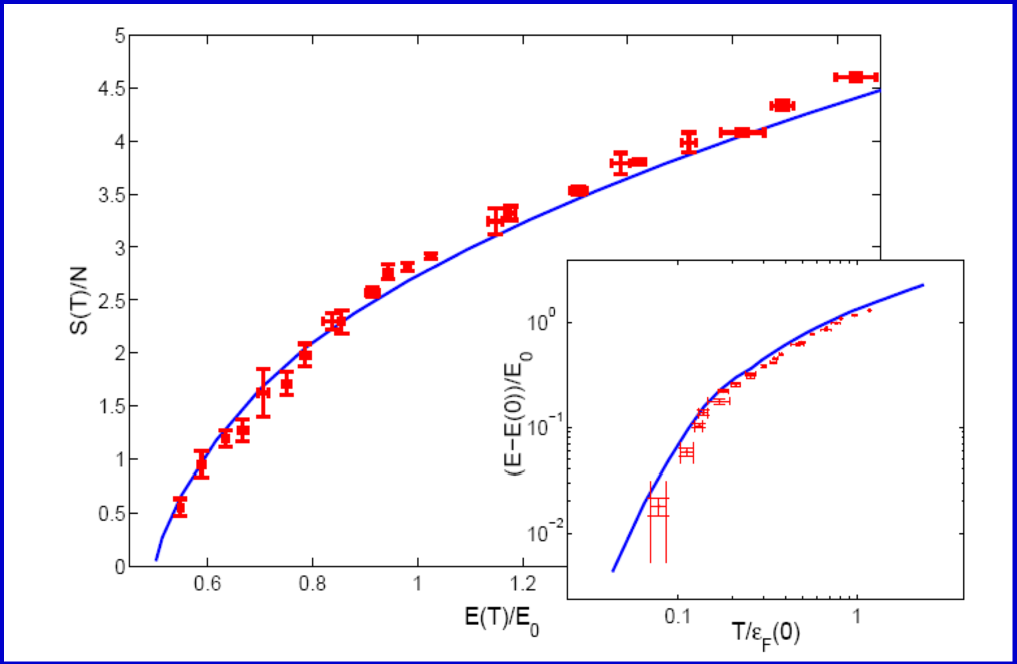
$$E_{\text{phonons}}(T) = \frac{3}{5}\varepsilon_F N \frac{\sqrt{3}\pi^4}{16\xi_s^{3/2}}\left(\frac{T}{\varepsilon_F}\right)^4, \qquad \xi_s \approx 0.44$$

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

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

Experiment (about 100,000 atoms in a trap):

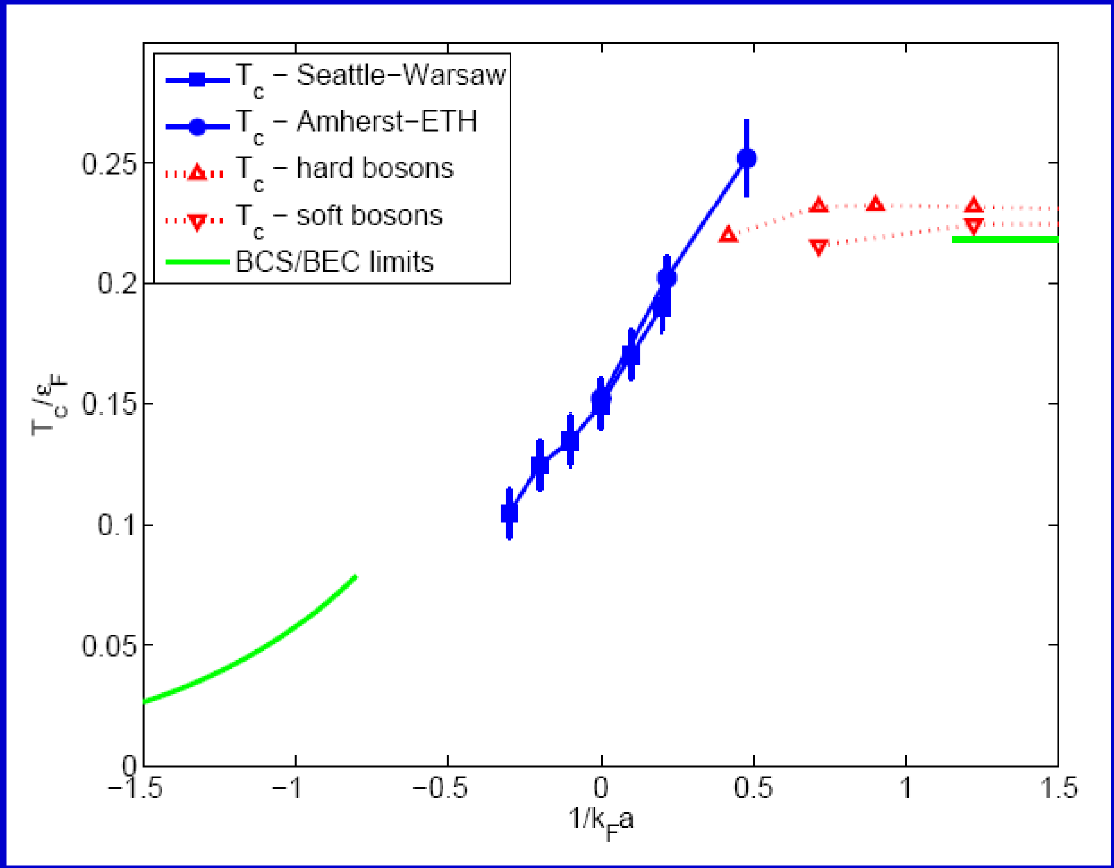
Measurement of the Entropy and Critical Temperature of a Strongly Interacting Fermi Gas, Luo, Clancy, Joseph, Kinast, and Thomas, Phys. Rev. Lett. 98, 080402 (2007)



Ab initio theory (no free parameters)

Bulgac, Drut, and Magierski, Phys. Rev. Lett. 99, 120401 (2007)

Critical temperature for superfluid to normal transition



Bulgac, Drut, and Magierski, Phys. Rev. A 78, 023625 (2008)

Amherst-ETH: Burovski et al. Phys. Rev. Lett. 101, 090402 (2008)

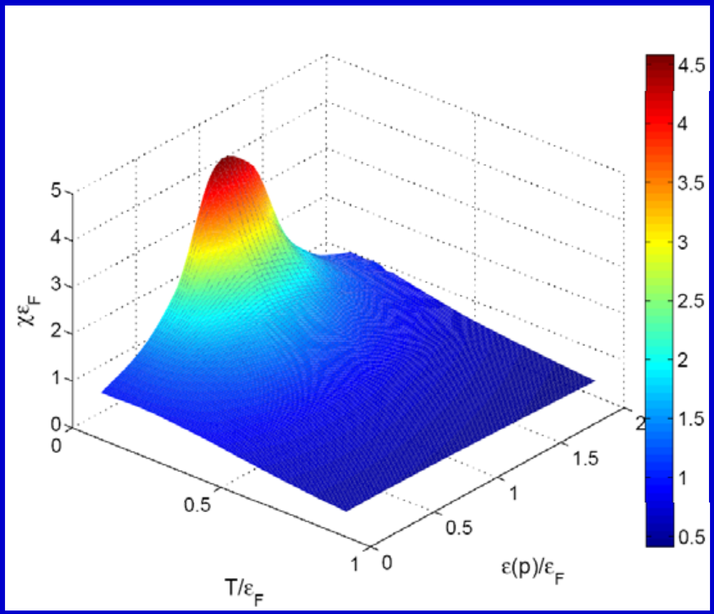
Hard and soft bosons: Pilati et al. PRL 100, 140405 (2008)

Response of the two-component Fermi gas in the unitary regime

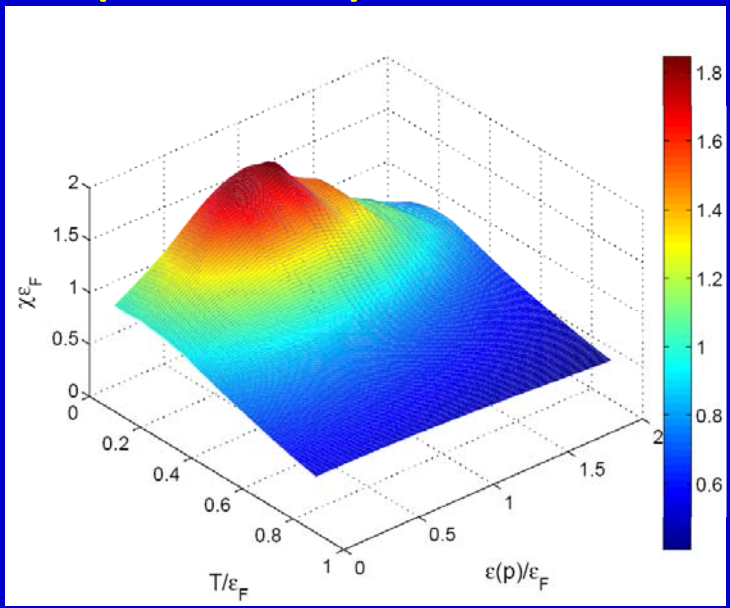
Bulgac, Drut, and Magierski, arXiv:0801:1504

$$\chi(\vec{p}) = -T\frac{d}{dg}\frac{\mathrm{Tr}\{\exp[-\beta(\mathrm{H}-\mu\mathrm{N}+\mathrm{g}\,\psi(\vec{\mathrm{p}}))]\,\psi^{\dagger}(\vec{\mathrm{p}})\}}{\mathrm{Tr}\{\exp[-\beta(\mathrm{H}-\mu\mathrm{N}+\mathrm{g}\,\psi(\vec{\mathrm{p}}))]\}}\Bigg|_{g=0} = -\int_0^{\beta} d\tau\,\mathrm{G}(\vec{p},\tau)$$

One-body temperature (Matsubara) Green's function

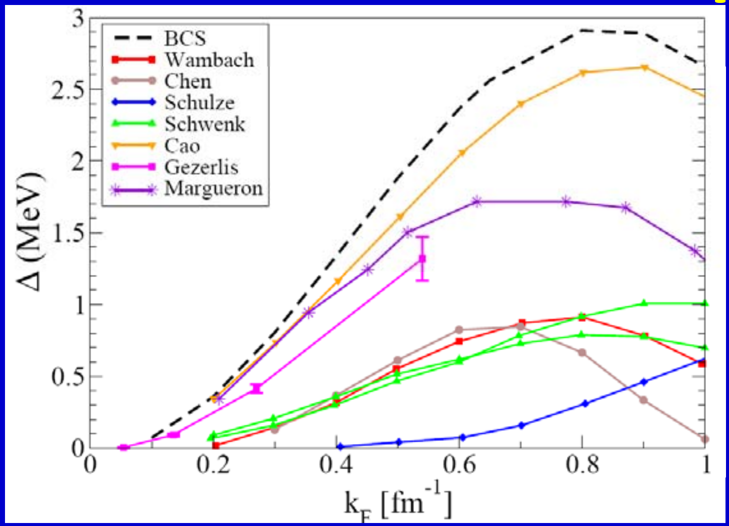


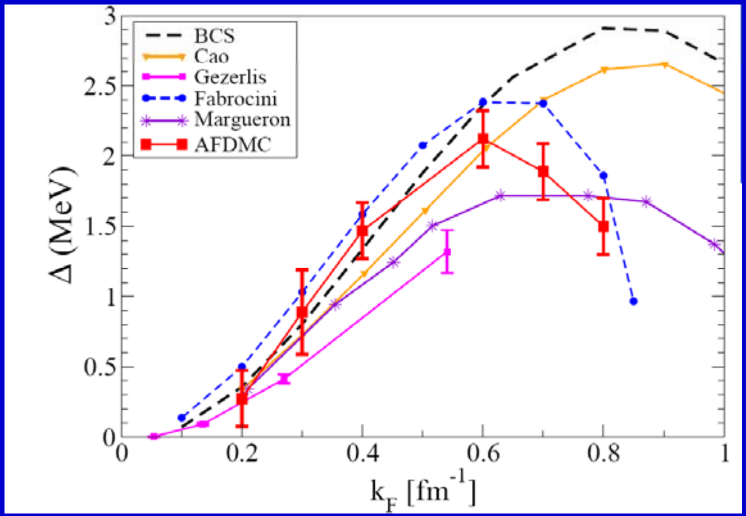
$$\frac{1}{k_F a} = -2$$



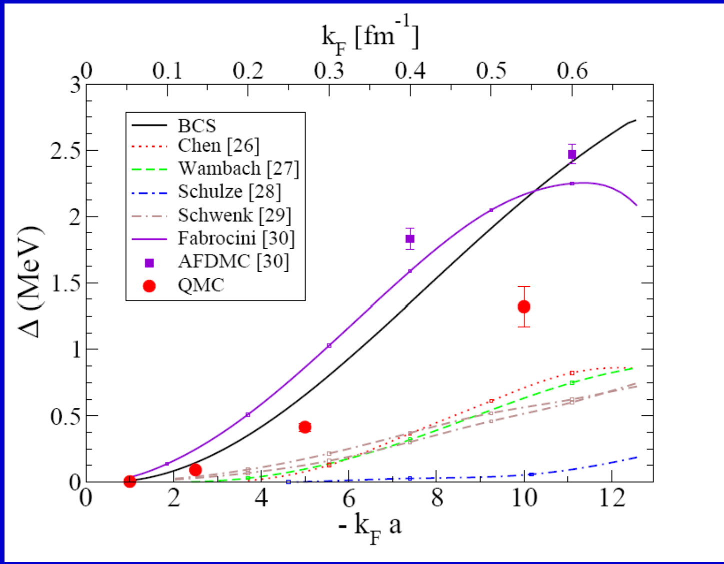
$$\frac{1}{k_F a} = 0$$

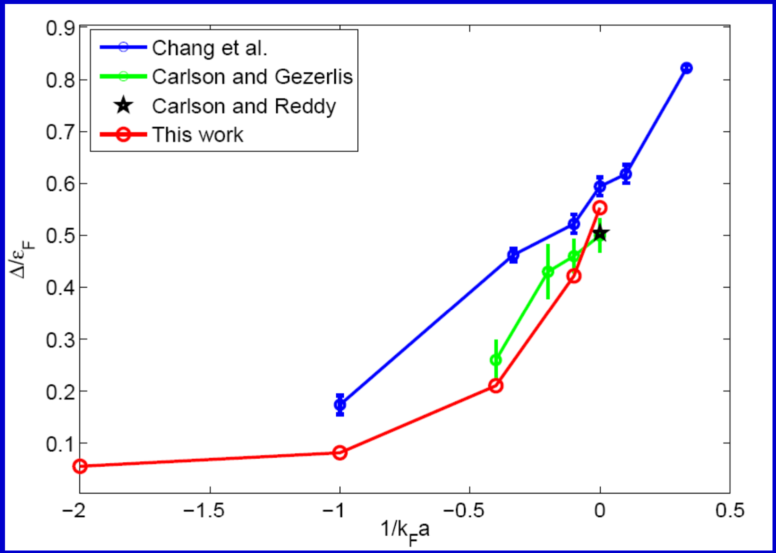
Ab initio calculation of pairing gap in neutron matter





Gandolfi et al. arXiv:0805.2513





Gezerlis and Carlson
PRC 77, 032801 (2008)

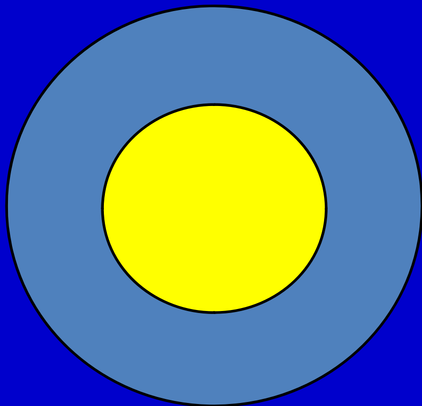
Bulgac, Drut and Magierski,
arXiv:0801.1504, PRA 78, 023625 (2008)

Until now we kept the numbers of spin-up
and spin-down equal.

What happens when there are not enough partners for everyone to pair with?

(In particular this is what one expects to happen in color superconductivity, due to the heavier strange quark)

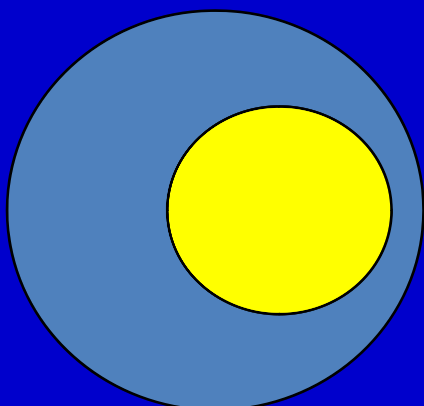
What theory tells us?



Green – Fermi sphere of spin-up fermions

Yellow – Fermi sphere of spin-down fermions

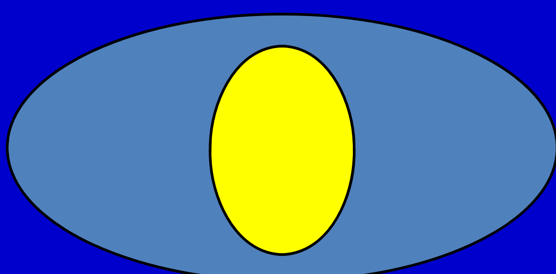
$$\text{If} \quad \left|\mu_\uparrow - \mu_\downarrow\right| < \frac{\Delta}{\sqrt{2}} \quad \text{the same solution as for } \mu_\uparrow = \mu_\downarrow$$



LOFF/FFLO solution (1964)

Pairing gap becomes a spatially varying function

Translational invariance broken



Muether and Sedrakian (2002)

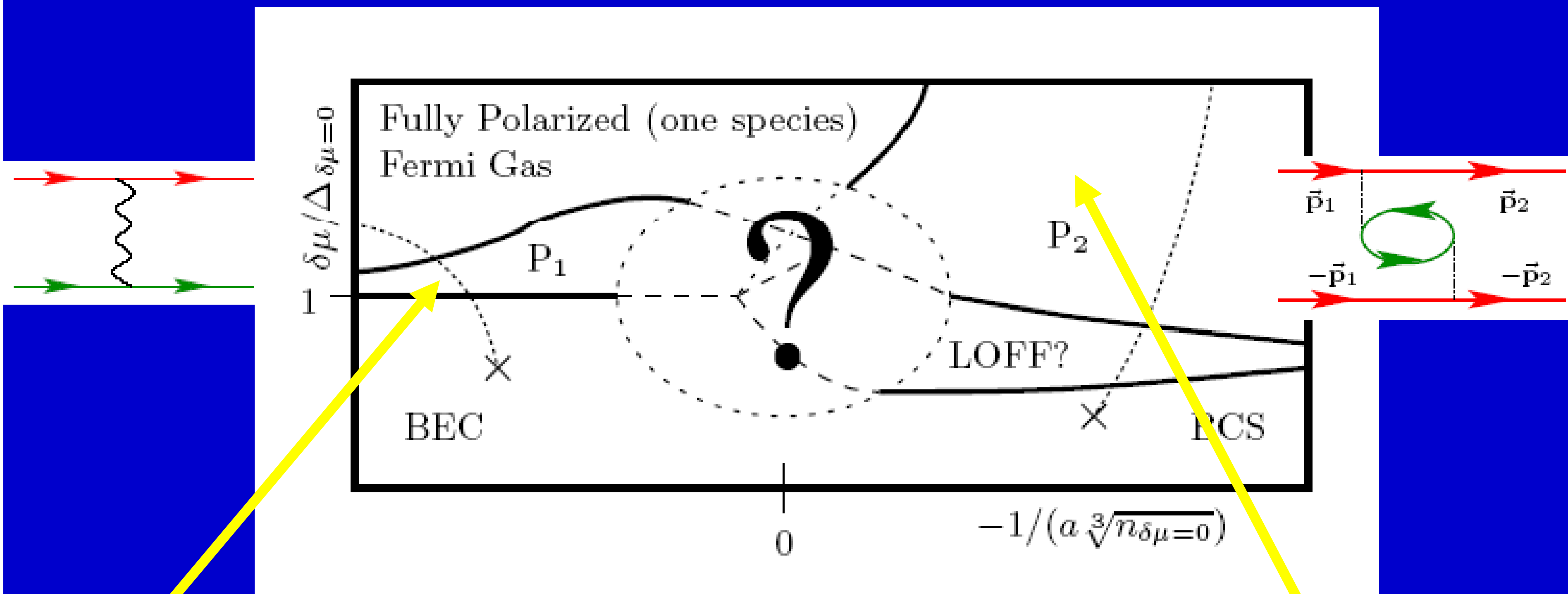
Translational invariant solution

Rotational invariance broken

What we think is happening in spin imbalanced systems?

Induced P-wave superfluidity

Two new superfluid phases where before they were not expected

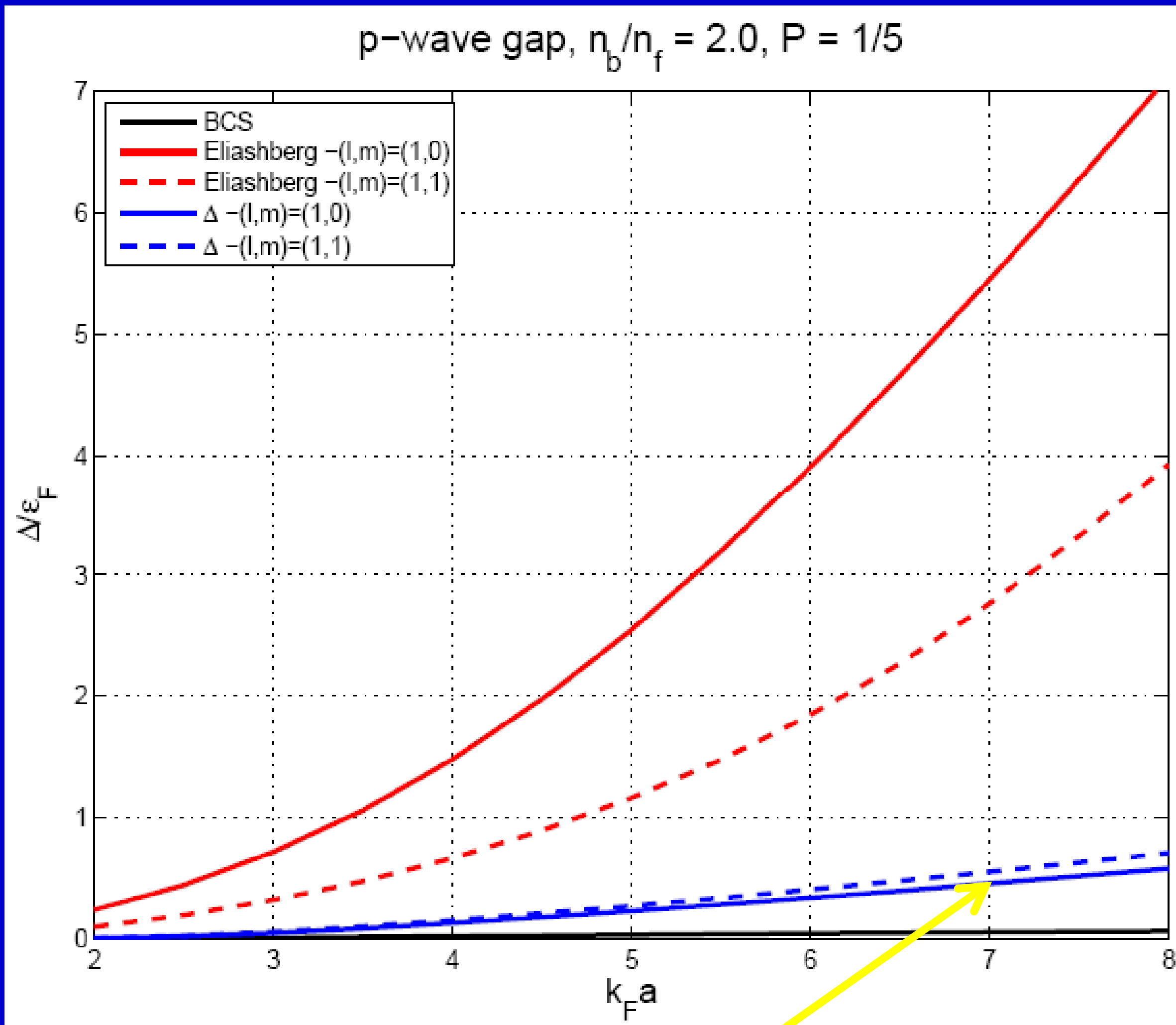


One Bose superfluid coexisting with one P-wave Fermi superfluid

Two coexisting P-wave Fermi superfluids

Bulgac, Forbes, Schwenk, Phys. Rev. Lett. 97, 020402 (2006)

Going beyond the naïve BCS approximation



Eliashberg approx. (red)

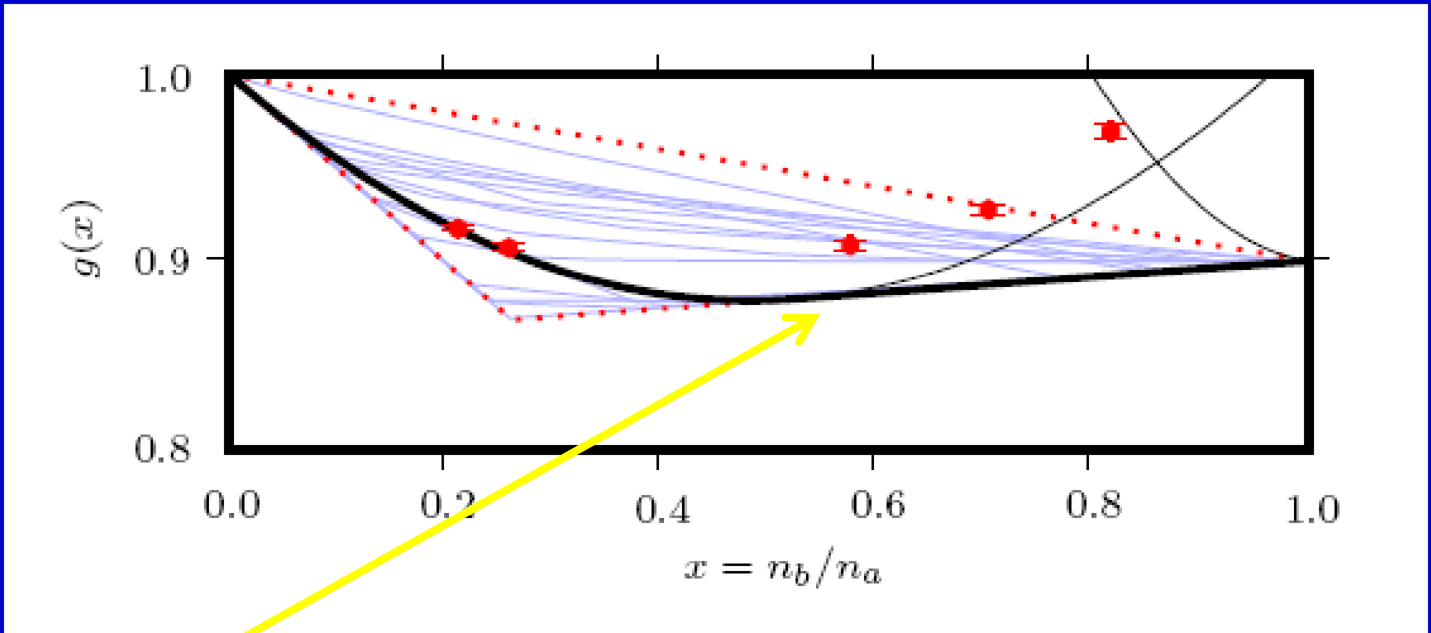
BCS approx. (black)

<u>Full momentum and frequency dependence of the self-consistent equations (blue)</u>

Bulgac and Yoon, unpublished (2007)

What happens at unitarity?

Bulgac and Forbes, PRA 75, 031605(R) (2007)

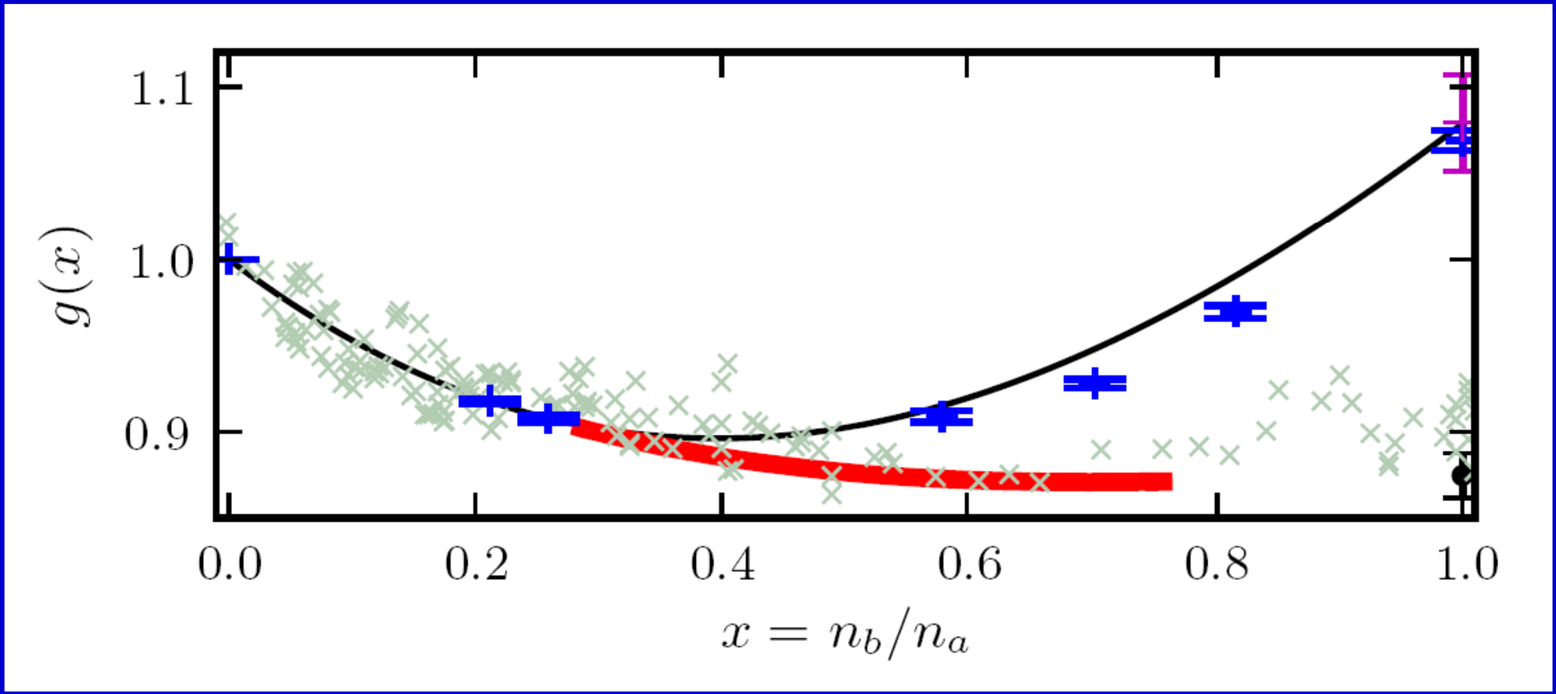


Predicted quantum first phase order transition, subsequently observed in MIT experiment , Shin *et al*. Nature, 451, 689 (2008)

Red points with error bars – subsequent DMC calculations for normal state due to Lobo et al, PRL 97, 200403 (2006)

$$E(n_a, n_b) = \frac{3}{5}\frac{(6\pi^2)^{2/3}\hbar^2}{2m}\left[n_a g\left(\frac{n_b}{n_a}\right)\right]^{5/3}, \qquad n_a \geq n_b$$

A refined EOS for spin unbalanced systems



<u>Red line: Larkin-Ovchinnikov phase</u>

Bulgac and Forbes, arXiv:0804:3364
Phys. Rev. Lett. accepted

Black line: normal part of the energy density

Blue points: DMC calculations for normal state, Lobo et al, PRL <u>97</u>, 200403 (2006)

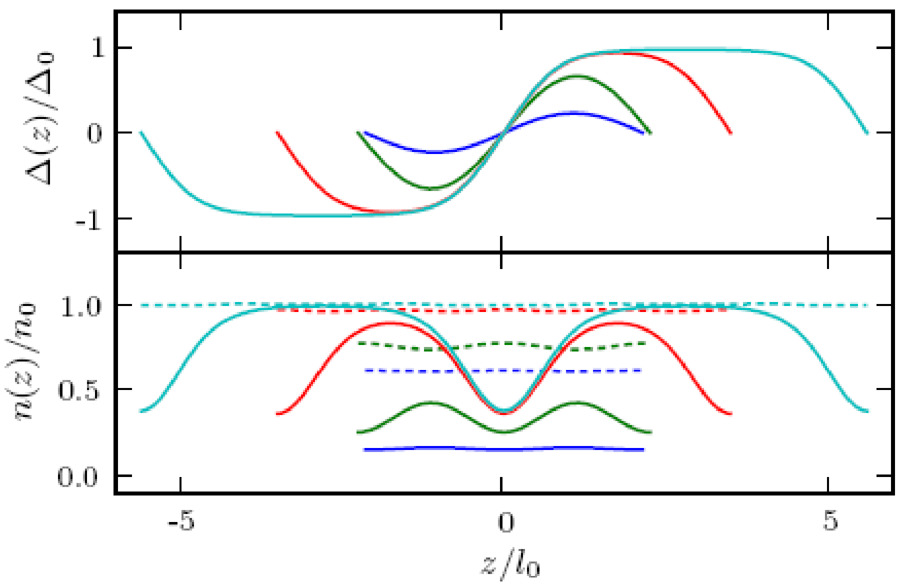
Gray crosses: experimental EOS due to Shin, Phys. Rev. A 77, 041603(R) (2008)

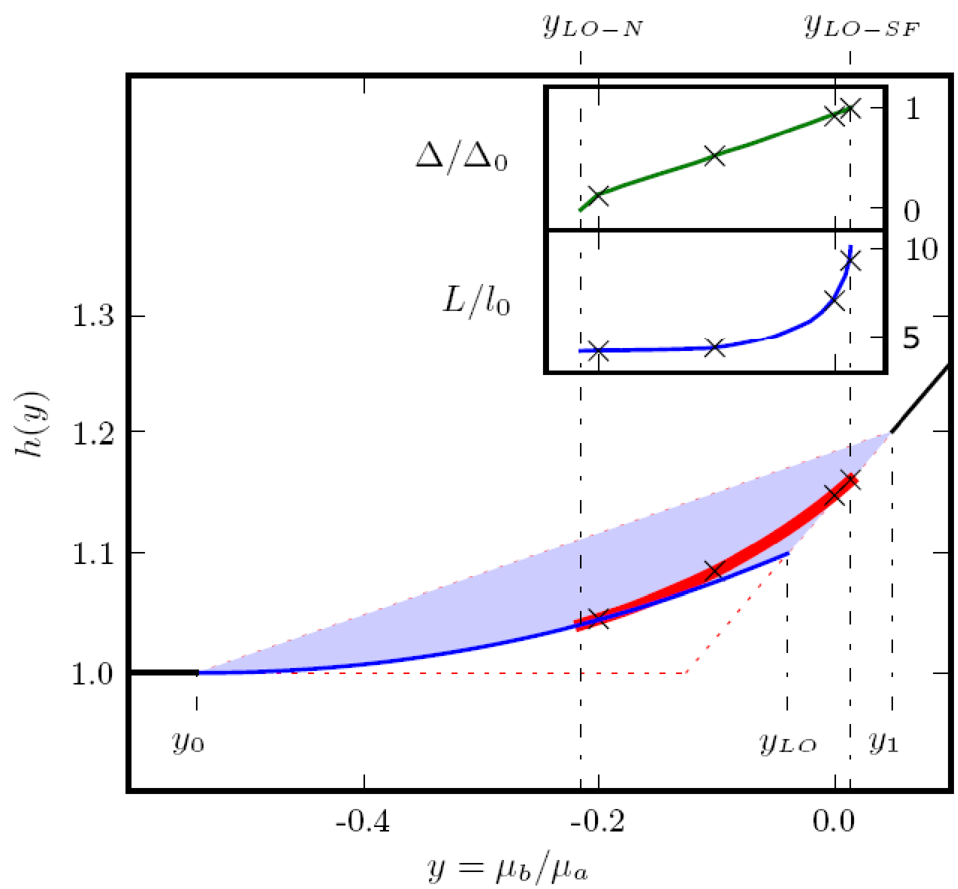
$$E(n_a, n_b) = \frac{3}{5}\frac{(6\pi^2)^{2/3}\hbar^2}{2m}\left[n_a g\left(\frac{n_b}{n_a}\right)\right]^{5/3}$$

How this new refined EOS for spin imbalanced systems was obtained?

Through the use of the (A)SLDA , which is an extension of the Kohn-Sham LDA to superfluid systems

A Unitary Fermi Supersolid: the Larkin-Ovchinnikov phase





Bulgac and Forbes, arXiv:0804:3364
PRL accepted

$$P[\mu_a, \mu_b] = \frac{2}{30\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\left[\mu_a h\left(\frac{\mu_b}{\mu_a}\right)\right]^{5/2}$$

Some of the lessons learned so far:

We have (finally) control over the calculation of the pairing gap in dilute fermion/neutron matter (second order phase transition superfluid to normal)

There are strong indications that the pseudo-gap (spectral gap above the critical temperature) is present in these systems

At moderate spin imbalance the system turns into a supersolid with pairing of the LOFF type (first and second order quantum phase transitions)

At large spin imbalance two *simbiotic* superfluids appear (p-wave superfluidity)

There is a controlled way to construct an energy density functional for superfluid systems, relevant for UNEDF