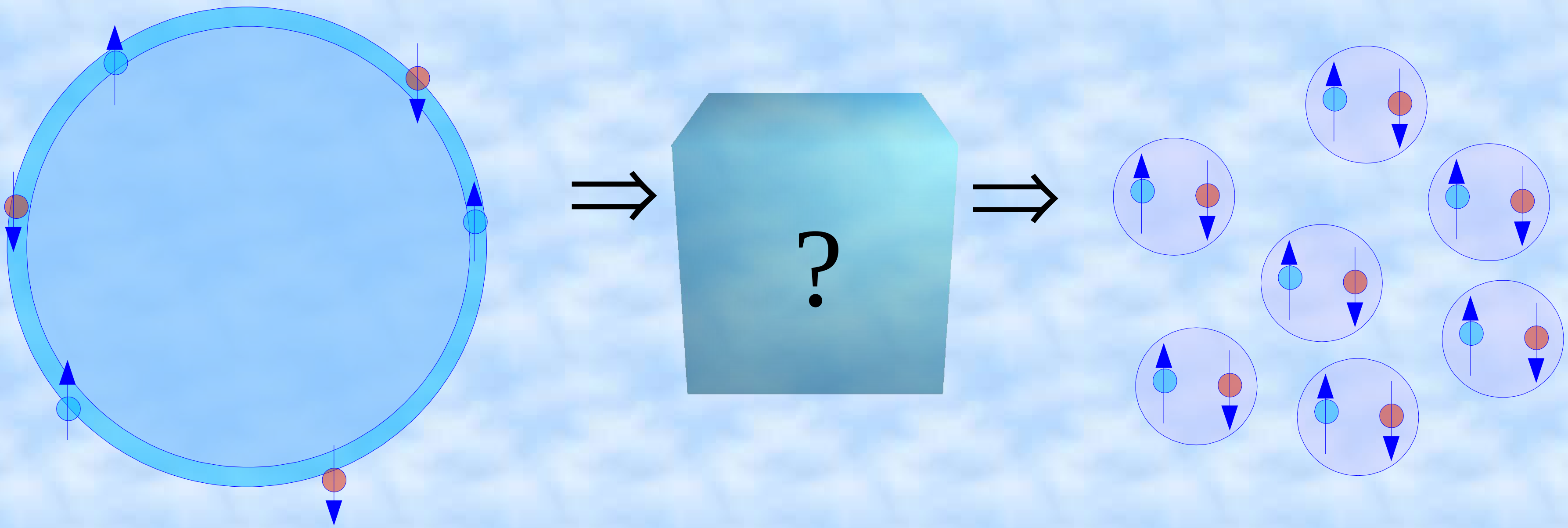
# Dilute Fermions: from Atoms to Neutron Matter

## Quantum Monte Carlo Studies

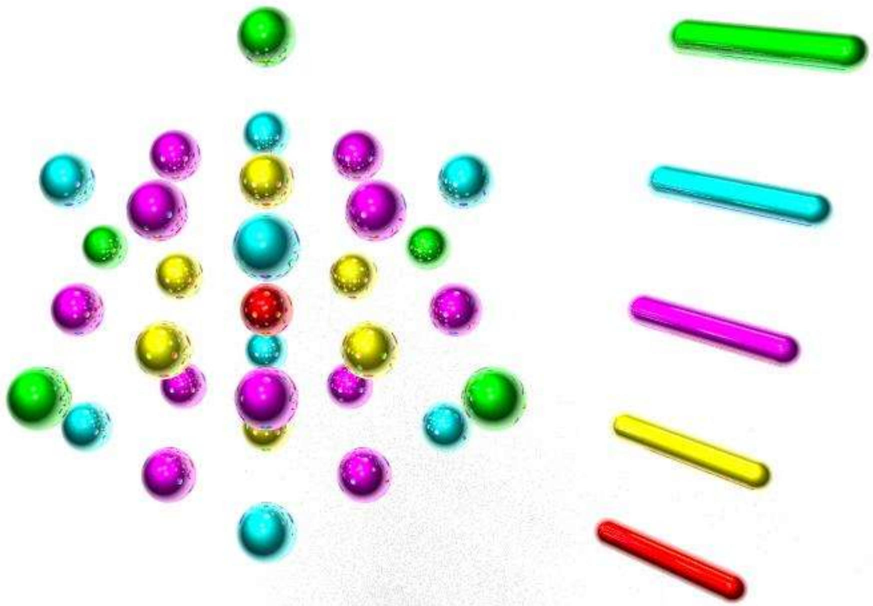
w/ K. Schmidt, V. Pandharipande, S.Y. Chang

- Methods for simple interactions
- What happens when we add a finite range?
- Methods for neutron matter
- Results for Neutron Matter : Energy, Gap, Pair Distributions,...



# Superfluids with QMC methods

Typically difficult, if $\Delta << \delta E$ (Fermi Surface)



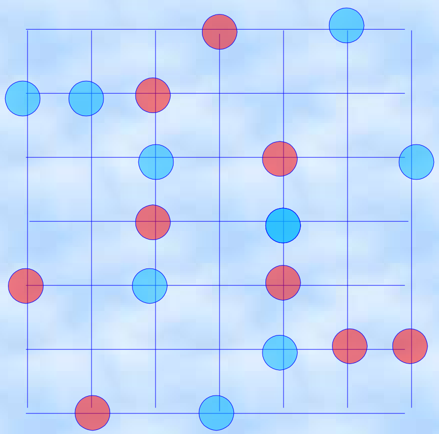
Crude depiction of the Fermi surface

# Infinite Scattering Length/Zero Range Limit

In the infinite scattering length limit, the fermi momentum is the only scale: $E = \xi\, E(FG) = \xi\, 3\, k_F^{\,2} / 10\, m$

Essentially a problem in 'geometry':
up/down pair equally likely to scatter to any momentum state;
damped by kinetic energy

From expansions in $(a\, k_F)$
$\xi = 0.326$ Heiselberg
$= 0.326,\ 0.568$ Baker



Expect strong BCS pairing

From BCS in terms of scattering length (Gorkov, Leggett):
Engelbrecht, Randeria and Sa de Melo
$\xi = 0.59$
They obtain both BCS and paired (Boson) limit

# Quantum Monte Carlo Methods:

Diffusion/ Green's function Monte Carlo: exp [ - $\beta$ H]
( Kalos, Ceperley, ...)

$H = T + V$

write down path integral in terms of particle paths:
V treated explicitly
Monte Carlo sampling used for T

Auxiliary Field Quantum Monte Carlo:
( Hirsch, Scalapino, Koonin, ...)

$H = V + T$

write down path integral in terms of particle orbitals:
T treated explicitly
Monte Carlo sampling used for V
Canonical/ Grand Canonical Ensemble & Finite SP basis

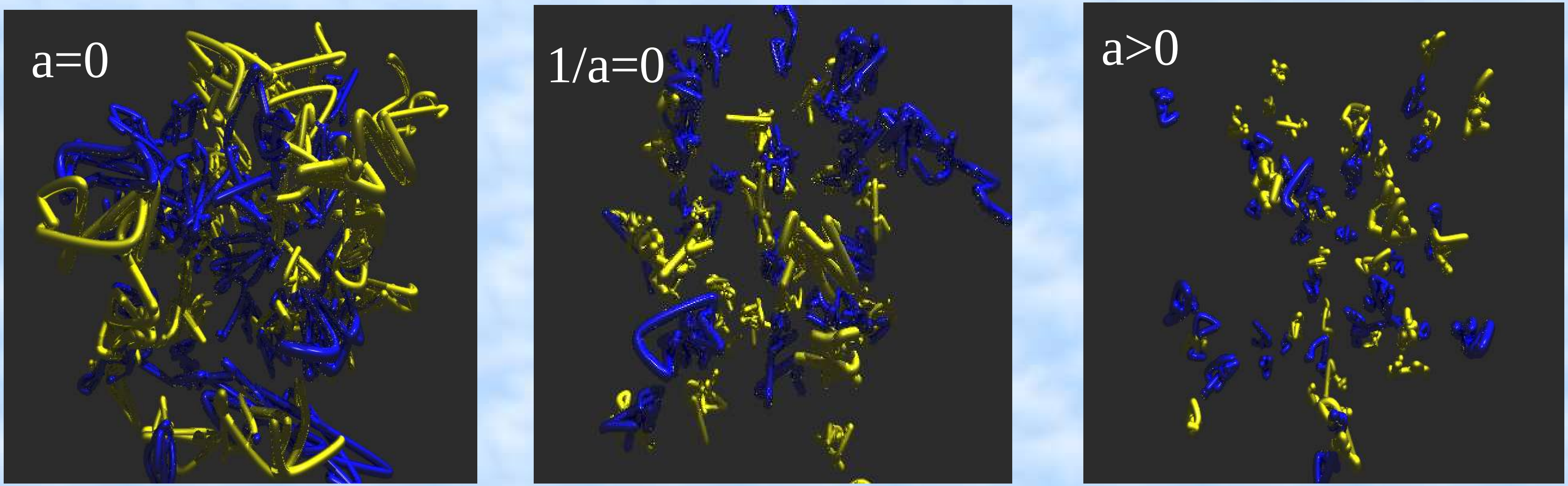
# DMC/ GFMC/ PIMC (finite T)

Applications: Liquid Helium (Ground State & Superfluid Phase Transition)
Electron Gas
Light Nuclei

$$\text{Exp} [ - H \tau ] = \exp [ - V \tau / 2 ] \exp [ - T \tau ] \exp [-V \tau/2 ]$$

Potential V: number (or spin-isospin matrix)

Kinetic Term sampled : $\exp [ - (R-R')^2 / ( 2 m \tau )$



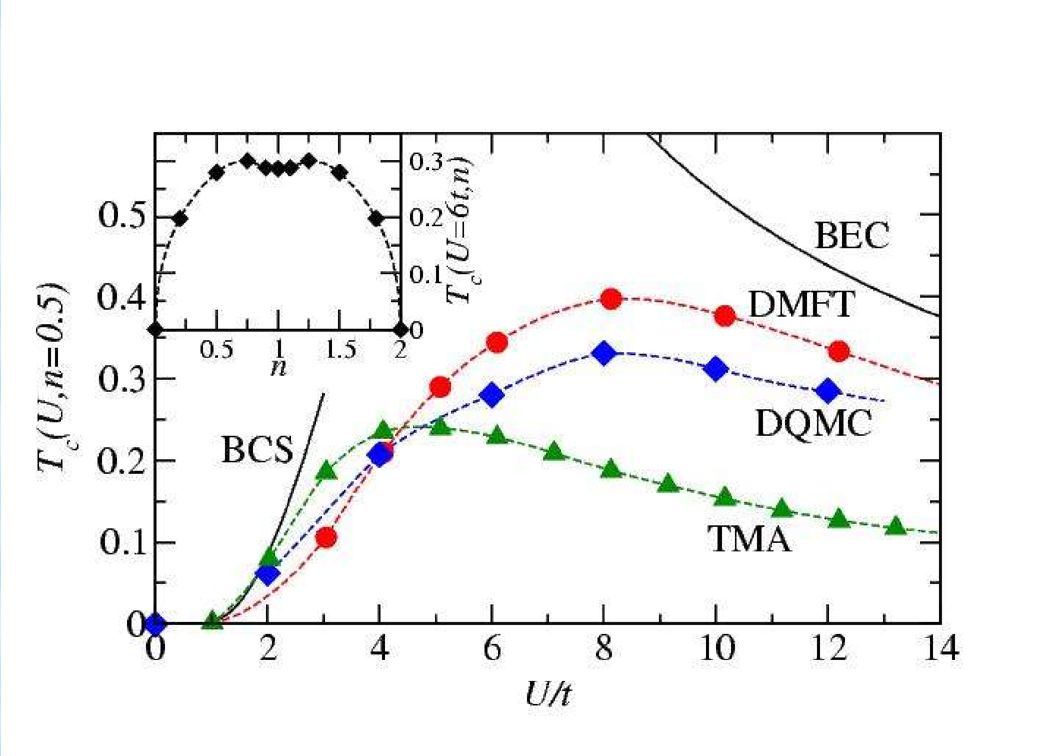

Direct connection between superfluidity and topological properties of the paths; original calc'n from Feynman; simulations see Ceperley RMP 67, 279, 1995.

Auxiliary Field QMC:

Hubbard Model, SMMC, ....

Exact Methods (no sign problem) possible in certain cases, eg:

Attractive Interactions (unpolarized)
Repulsive Interactions at half-filling,




¼ filling
Grand canonical

10x10x10

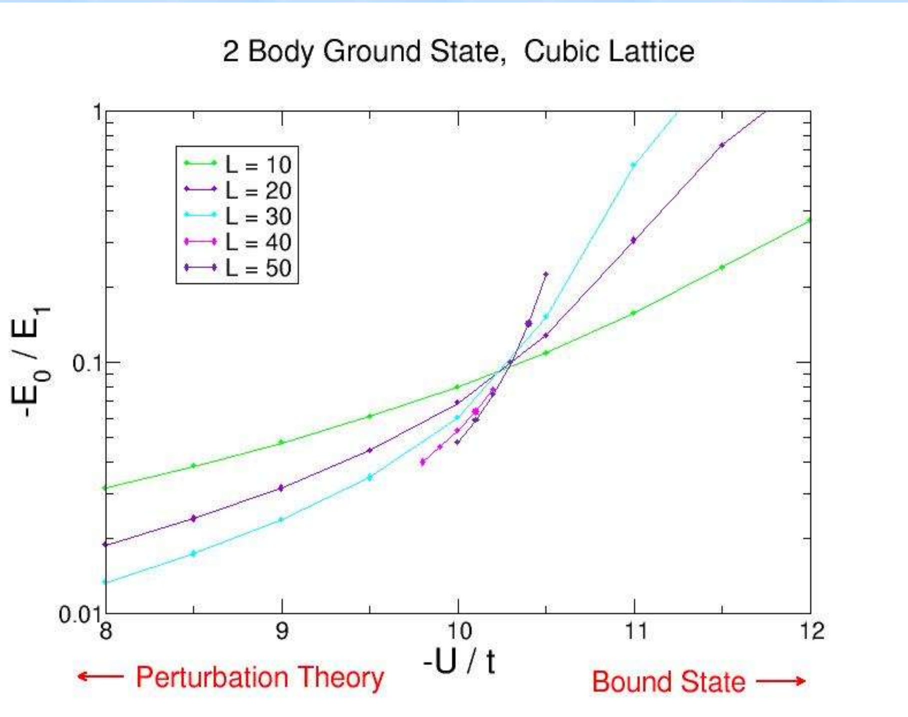
Sewer et al,
cond-mat/0204053

Must be extended to very low density regime

# Dilute Limit on the Lattice

Canonical Ensemble (Fixed Particle #)
Zero Temperature
Same as DMC/GFMC, but evolving single particle orbitals

Adjust coupling in 2-body system




Small Lattice Results

7 up, 7 dn: 5x5x5 - 5.6% filling

7x7x7 - 2% filling

U=-10 L=5 E/Ef = 0.48(1)
U=-10 L=7 E/Ef = 0.50(1)
U=-11 L=5 E/Ef = 0.35(1)
U=-11 L=7 E/Ef =

(VERY) PRELIMINARY

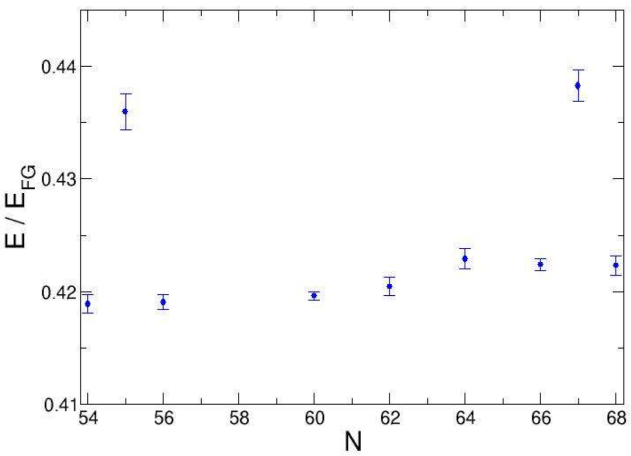
# QMC Treatment of 'Delta fn' Problem

Analytic Potential: $$v(r) = -\frac{2}{m}\frac{\mu^2}{\cosh^2(\mu r)}\ .$$

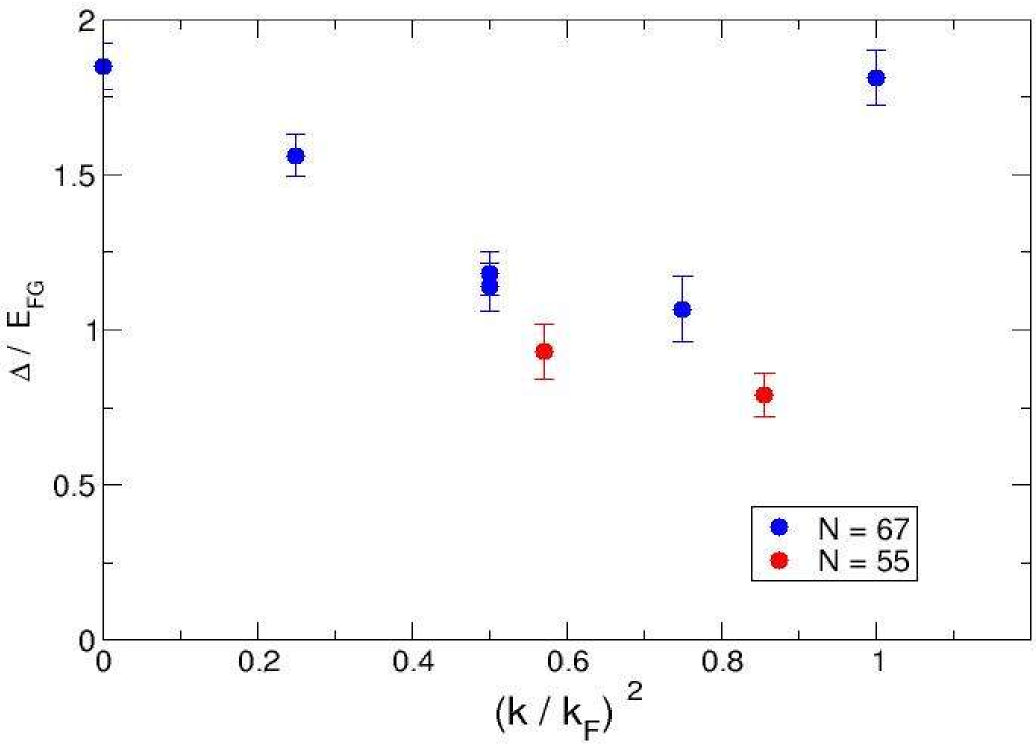
E=0 Solution: tanh(μr)/r

As μ ⇒ ∞, Volume integral of potential goes to zero
Potential, Kinetic Energies Diverge

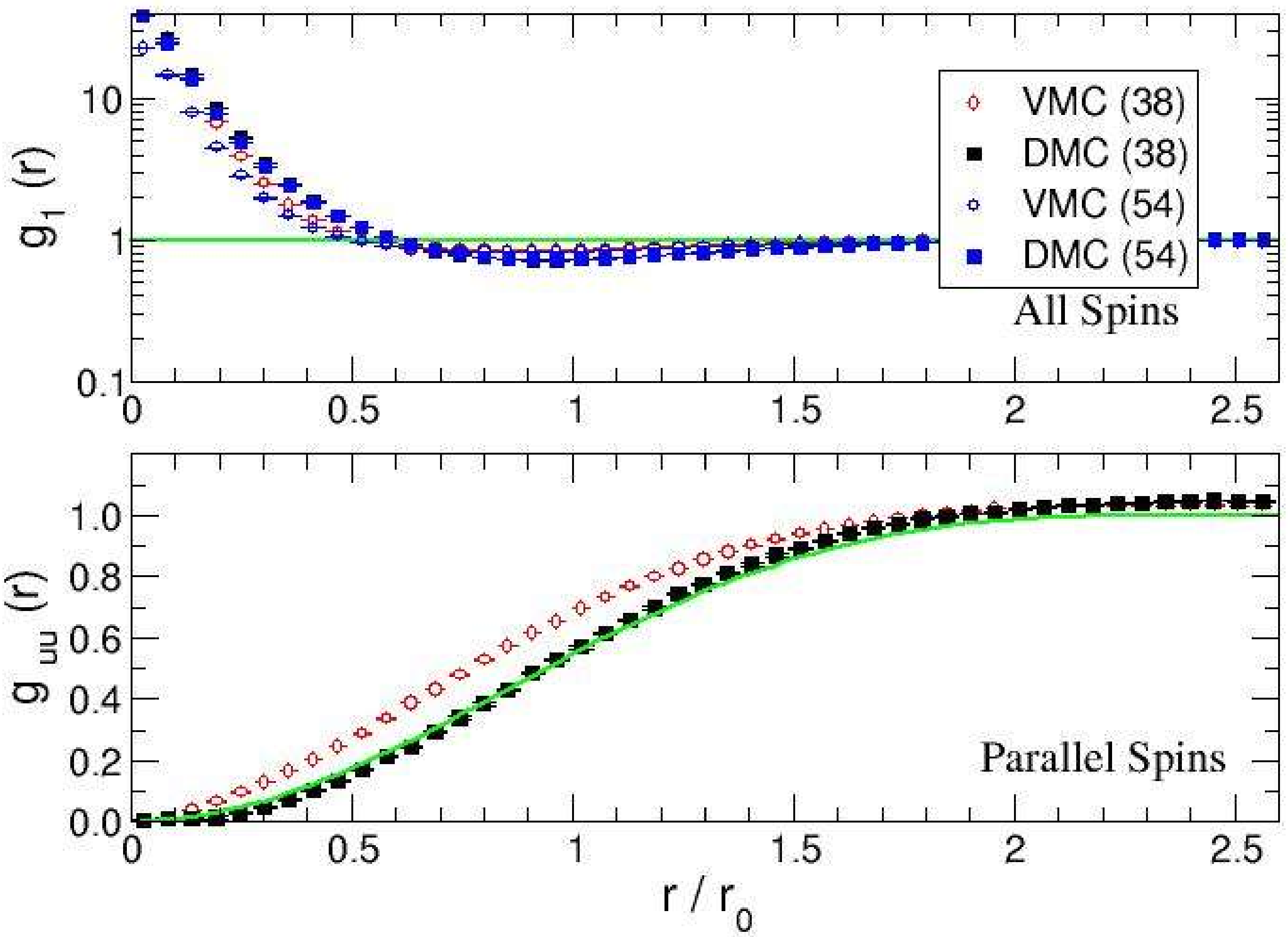
Energy / E (Fermi Gas)




Energy vs. k w/ unpaired fermion



# Pair Distribution



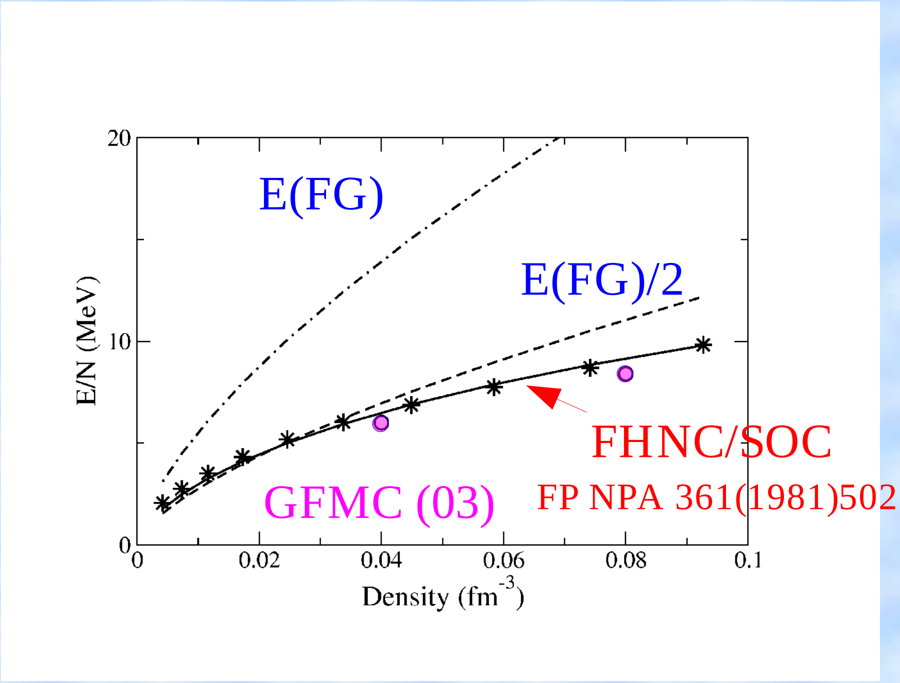
# Does this describe Neutron Matter, and at what densities?

Consider low-density ($< \rho_0$) neutron matter:

Scattering Length ~ -18 fm
Avg Pair Separation at $\rho_0$ ~ 1.5 fm
Effective Range ~ 2.8 fm
L.S interactions, ...

| $\rho(\mathrm{fm}^{-3})$ | $k_f\,a$ |
|---|---|
| 0.16 | - 30 |
| 0.01 | - 12 |
| 0.001 | - 5.5 |

T=0 Equation of State




Looks roughly like short-range attractive interaction

What are the global properties of the system?

- Equation of State
- Gap vs. Density
- Pair Distribution Functions
- Susceptibility (neutrinos)
- Superfluidity, ...

# BCS solution & the Gap

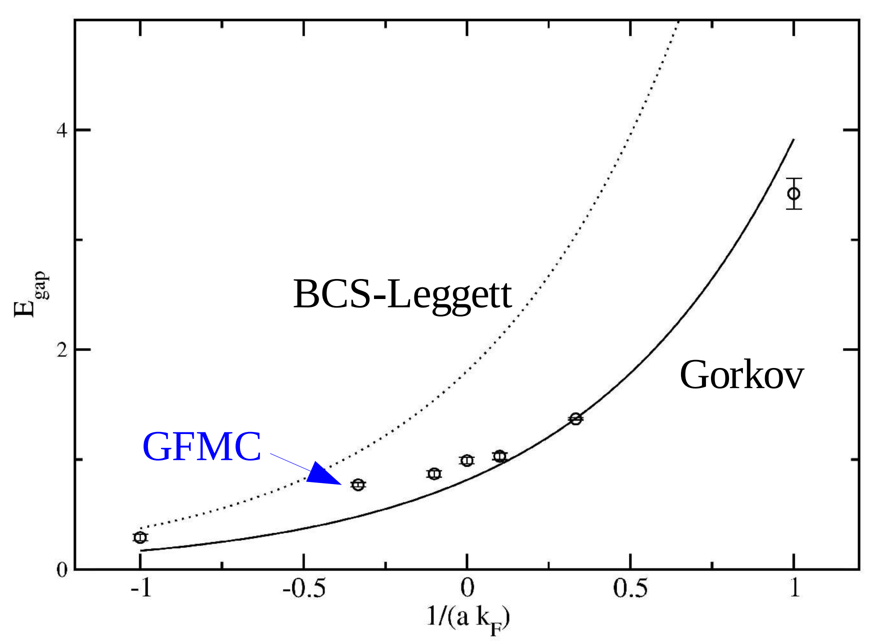
Superfluid Gap comparable to Fermi Energy.

Wavefunction:

$$\prod_i (u_i + v_i a^\dagger_{\mathbf{k}_i\uparrow} a^\dagger_{-\mathbf{k}_i\downarrow})|0\rangle \ .$$

$$\frac{\mathcal{N}_0}{k_F a_s} = \sum_{\mathbf{k}} \left[ \frac{1}{2\epsilon_{\mathbf{k}}} - \frac{\tanh(\beta E_{\mathbf{k}}/2)}{2E_{\mathbf{k}}} \right]$$

where $\mathcal{N}_0 = m k_F / 4\pi$.



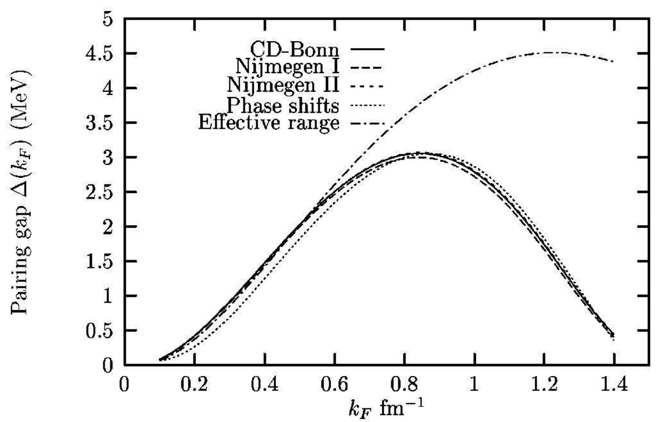



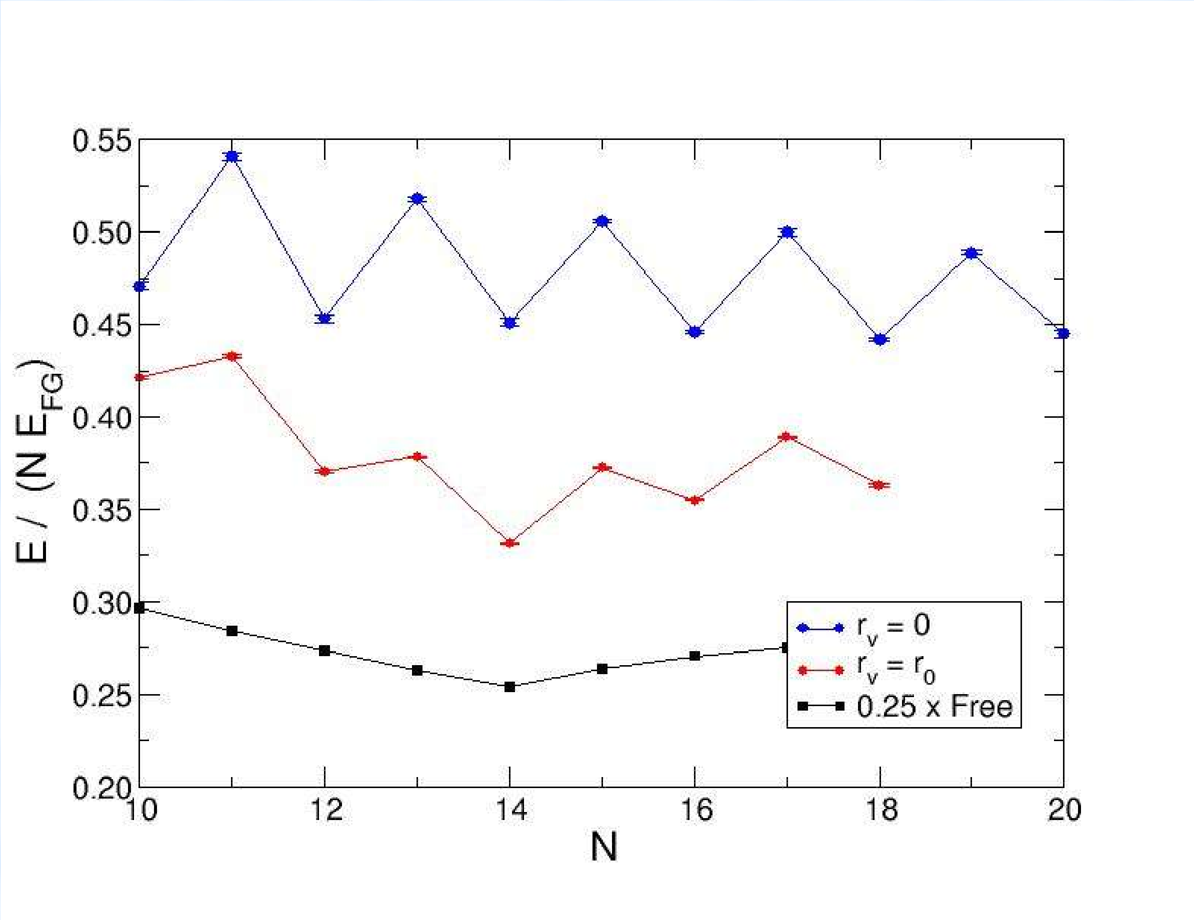

FIG. 6. $^1S_0$ energy gap in neutron matter with the CD-Bonn, Nijmegen I, and Nijmegen II potentials. In addition, we show the results obtained from phase shifts only, Eqs. (31)–(33), and the effective range approximation of Eq. (35). From Elgarøy and Hjorth-Jensen, 1998.

What happens with finite potential range?
In neutron matter $\Delta <<$ E(FG) ??

Dean and Hjorth-Jensen, RMP 75, 607 (2003)

# Simplest Case: Finite Range, Infinite Scattering Length

Set potential range $\mu$ : $r_0$ (effective range) = $r_e$ $1/\rho = (4\,\pi\,/\,3)\,r_e^{\,3}$

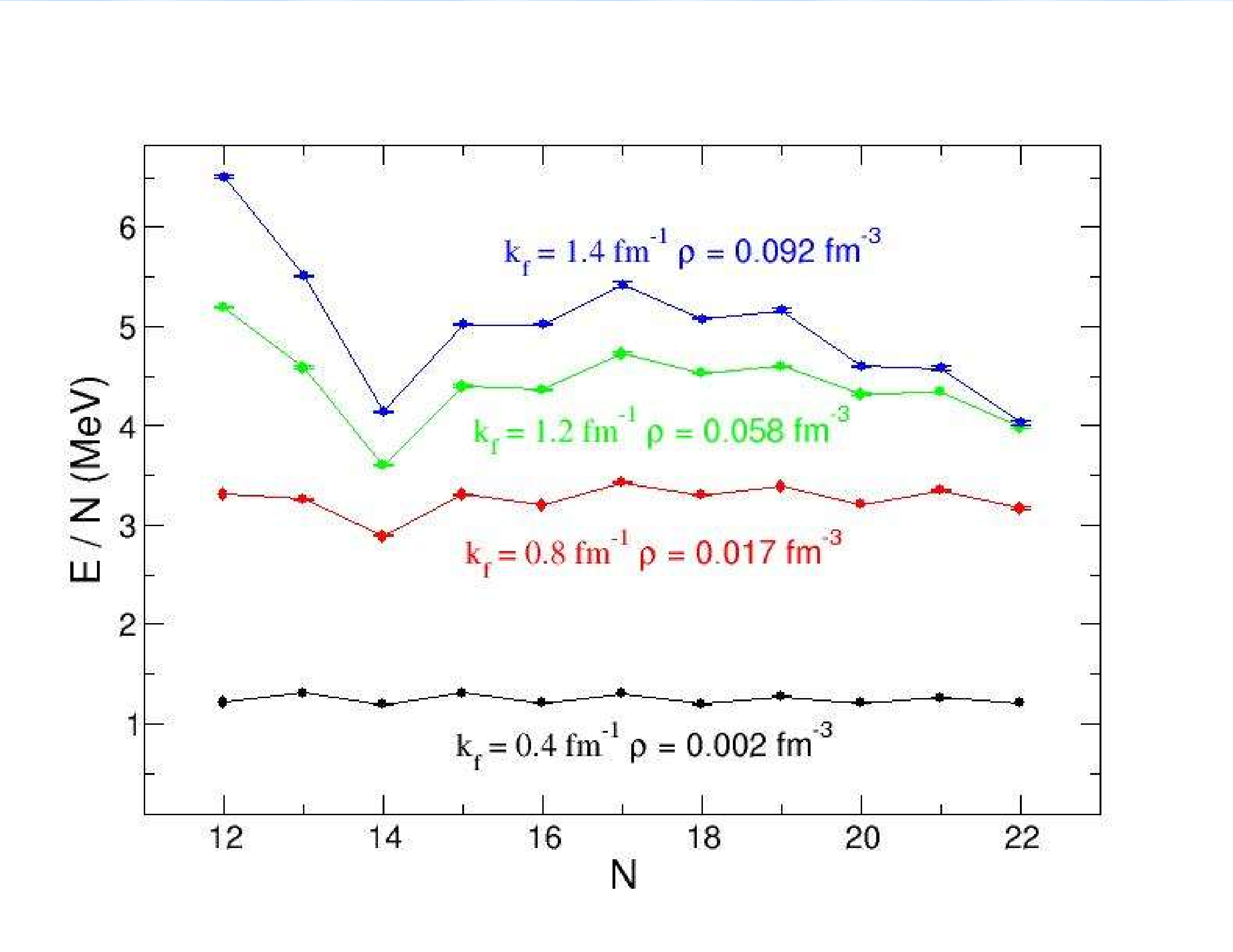



Energy decreases
Gap decreases (roughly a factor of 2)
Shell gaps appear

Caution: unstable for large N

# 'Quasi-Neutron' Matter

Adjust Strength of potential : $a = -18$ fm
Adjust Range of potential : $r_0 = 2.8$ fm



# Neutron Matter Calculations

Interaction: H = T + V

AV8' Interaction

$$v_{ij} = \sum_{p=1,4} v_p(r_{ij}) O^p_{ij} \ ,$$

$$O^{p=c,\sigma,t,b}_{ij} = 1, \ \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, \ S_{ij}, \ \mathbf{L} \cdot \mathbf{S} \ .$$

Variational
Wavefunction

$$\Psi_V = \left( \mathcal{S} \prod_{i<j} F_{ij} \right) \Phi \ ,$$

Fermi Gas / BCS

NN Correlations

GFMC w/ 14 neutrons

$2^{14}$ = 16384 wvfn components
<< 12C

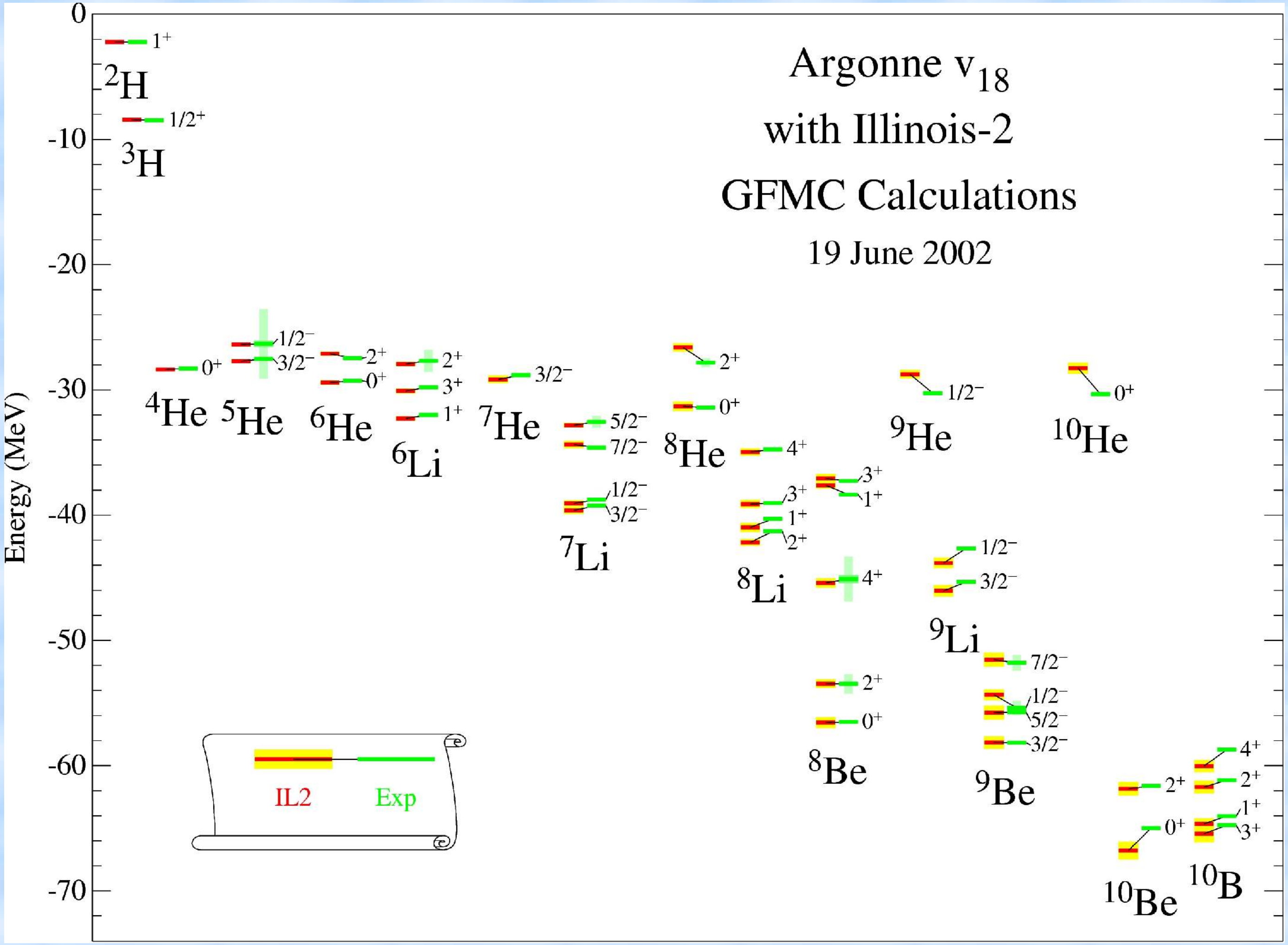
14 particles = 2*7
Fermi 'Sphere' w/
k= ( 0, 0, 0 )
( 0, 0, ±1)
( 0, ±1, 0 )
(±1, 0 ,0 )

# Light Nuclei

GFMC (DMC) for spatial coordinates
Explicit Sum over all spin-isospin components

Constraint on sum over all spin-isospin amplitudes.

Accurate but slows w/ A



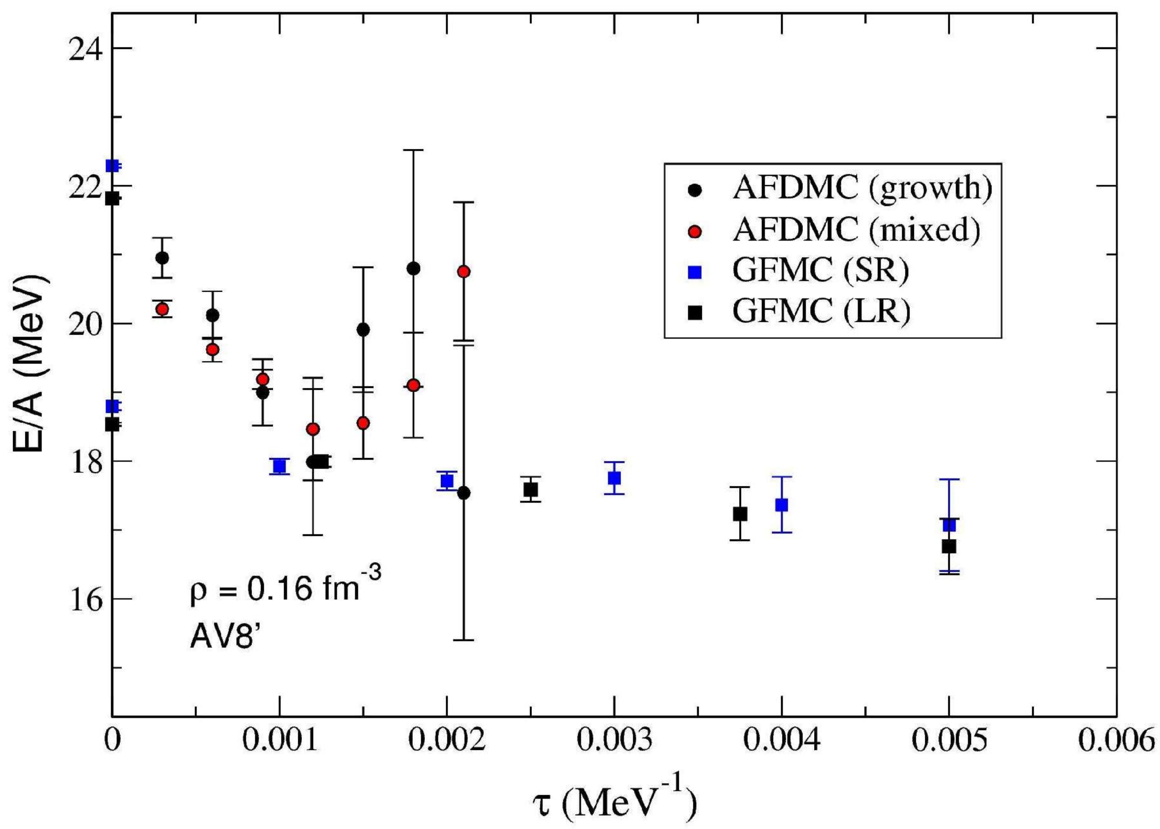
# AFDMC for Neutron Matter

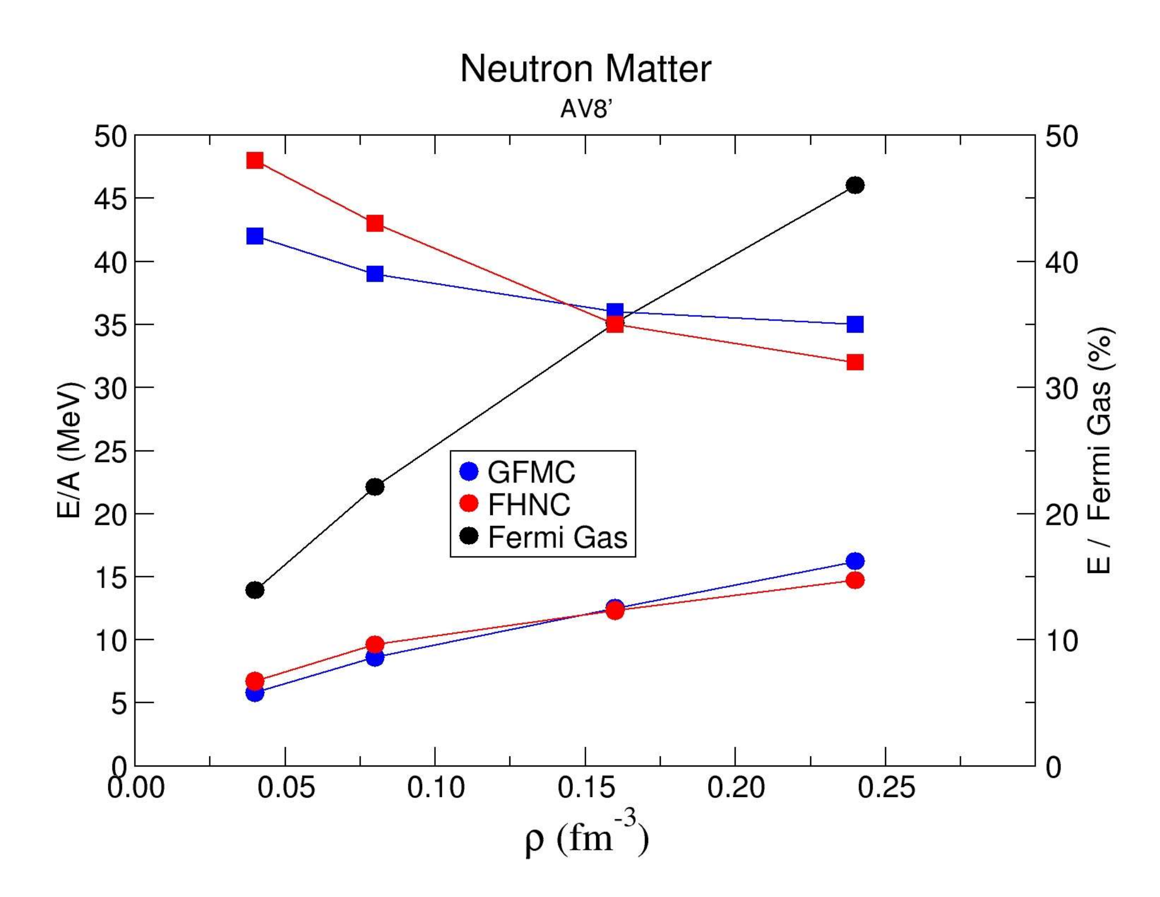
AFDMC
GFMC (DMC) for
spatial coordinates
Auxiliary Field for Spins

Constraint on Individual
Spin-Isospin State

Accuracy (constraint)
more difficult for nuclear matter

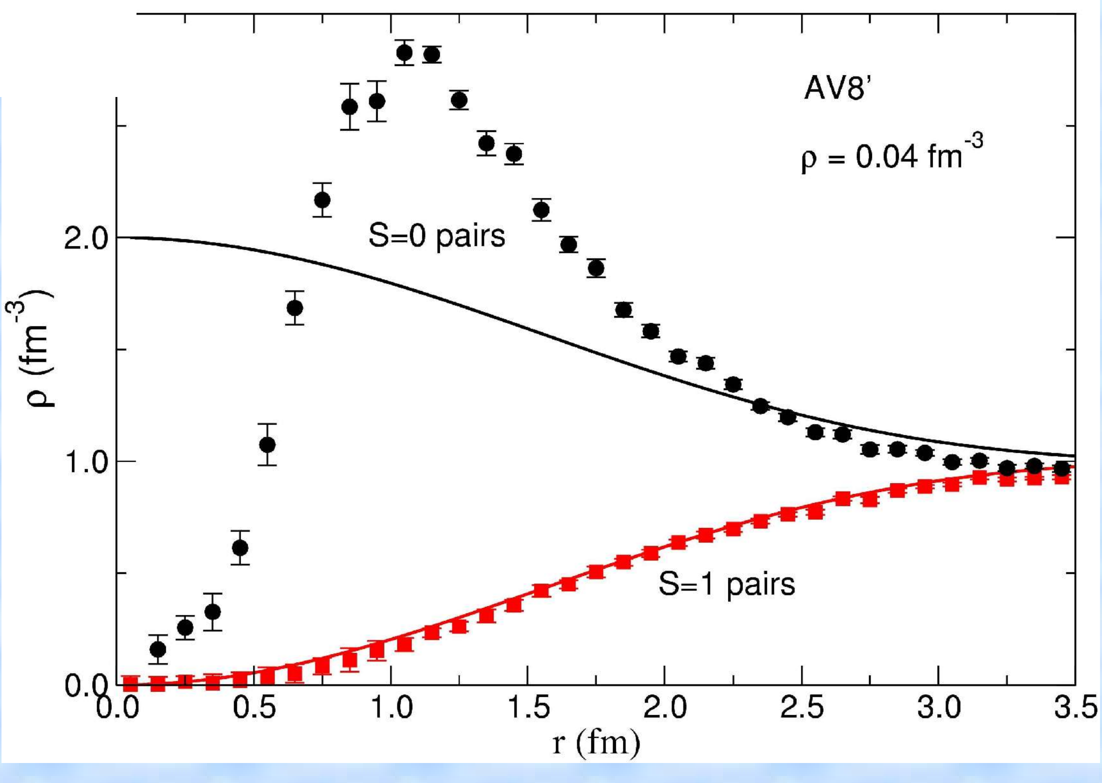
For neutron matter,
few (~4) % accuracy.





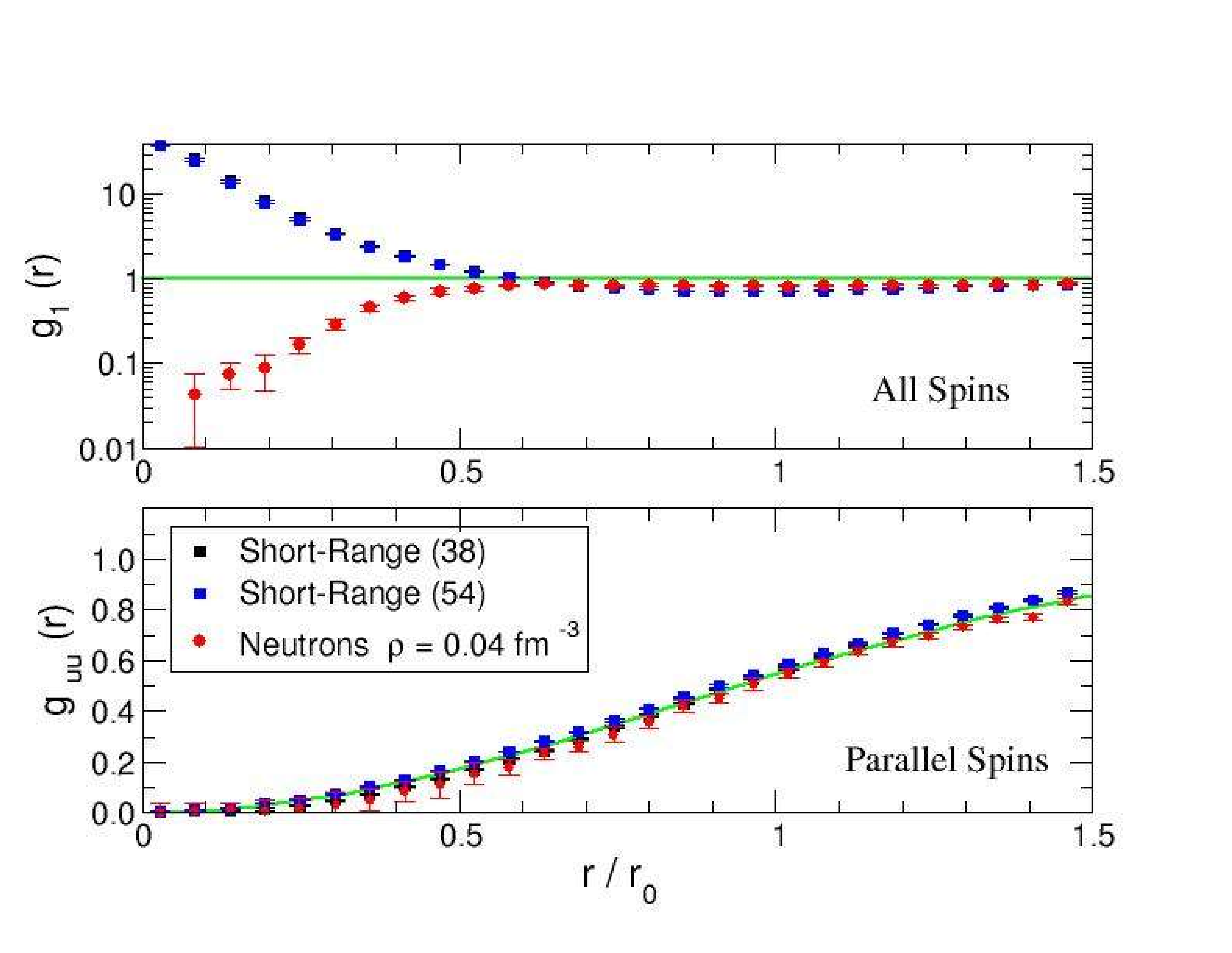

Energy vs. ρ

Comparison to Fermi Gas




Spin 0 & 1 Distributions
at $\rho = 0.04\ \mathrm{fm}^{-3}$
compared to Fermi Gas

# Pair Distributions: Delta Fn & Neutron Matter



# Gaps in Neutron Matter

Gaps: $\rho = 0.04\ \mathrm{fm}^{-3}$

| | GFMC | AFDMC |
|---|---|---|
| N=11 | 2.65(30) | |
| N=13 | 2.65(50) | 2.6(5) |
| N=15 | | 3.3(4) |

$\rho = 0.004\ \mathrm{fm}^{-3}$

| | GFMC |
|---|---|
| N=11 | 1.4(2) |
| N=13 | 1.0(2) |

VERY PRELIMINARY

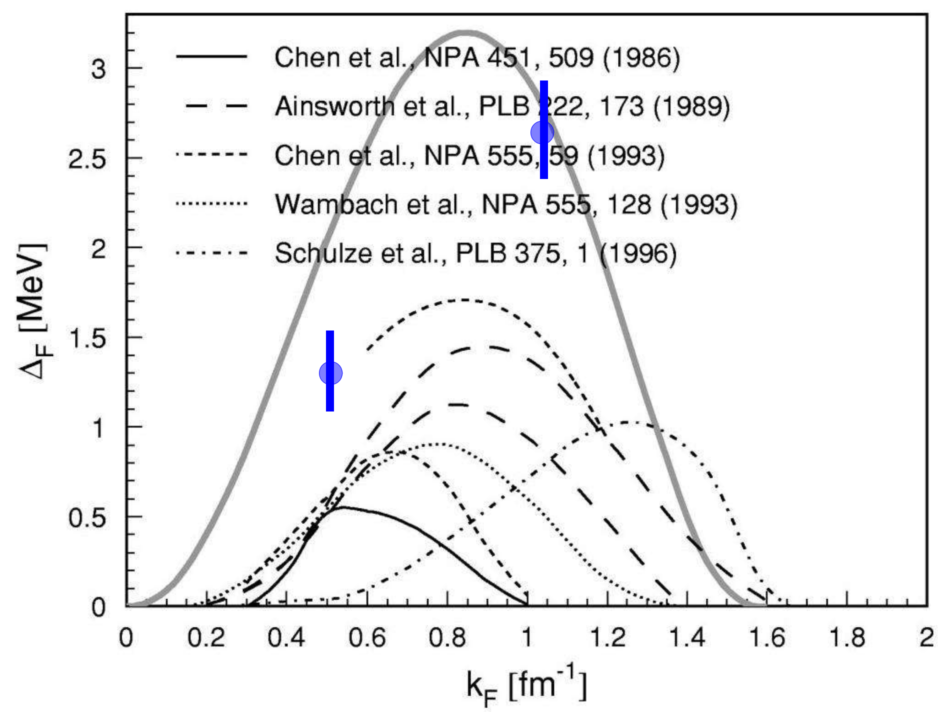
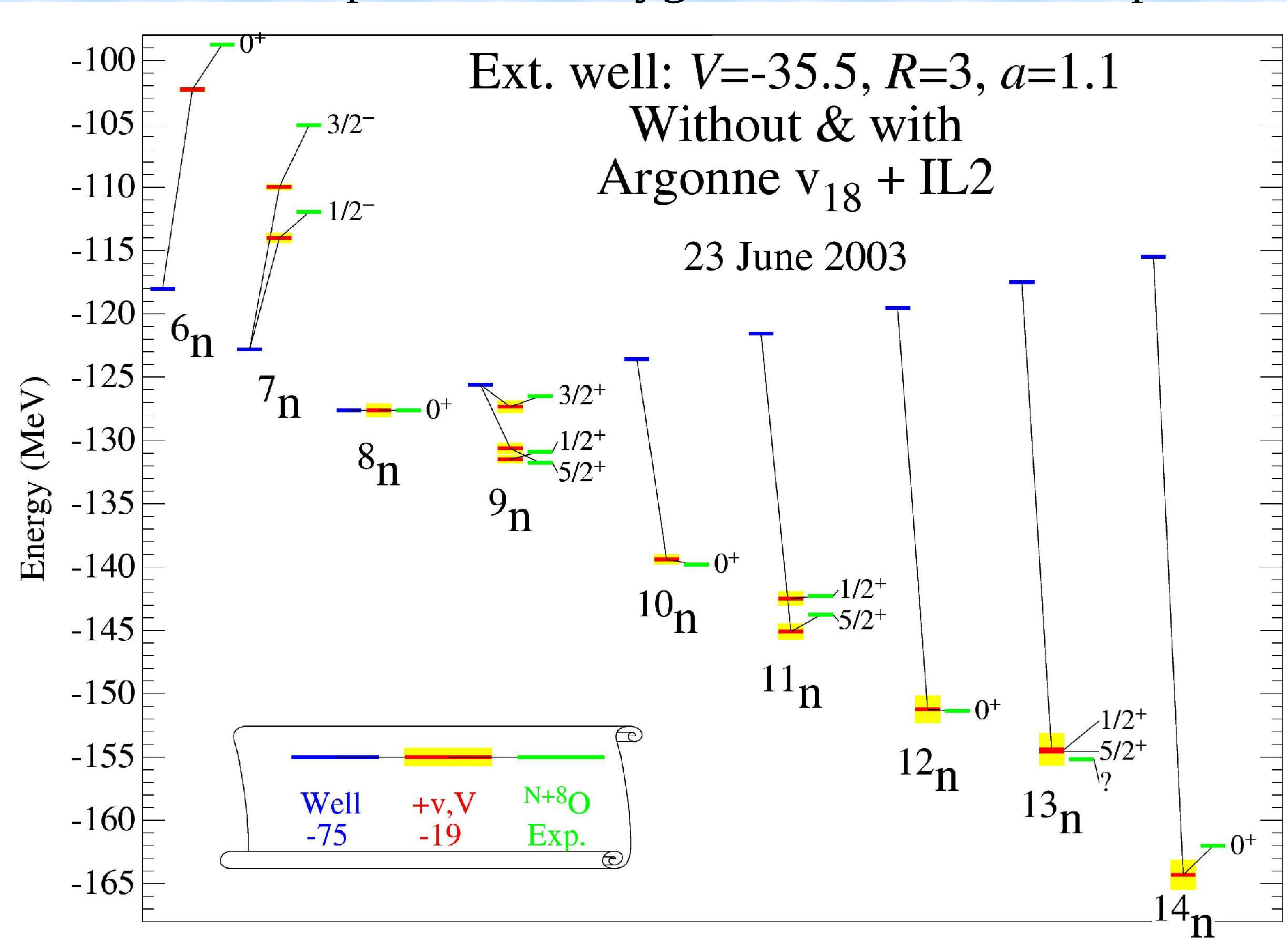



FIG. 14. The $^1S_0$ gap in pure neutron matter predicted in several publications taking account of polarization effects. From Lombardo and Schulze, 2001.

Shell Effects still to be investigated (AFDMC)

# Neutron Drops (aka Oxygen Isotopes)

Consider 6-14 neutrons in a well w/ realistic interactions
well simulates protons in Oxygen core; look at Isotopes




'Open shell'
BCS wvfns

# Immediate Future

- Finite Temperature / Superfluid Transition

  (1) estimate from Gap $\Delta$

  applicable in weakly attractive systems

  for $a=-\infty$ $\quad T \sim E(FG) = 0.60\,[\hbar^2/2m]\,k_f^2$

  (2) estimate from 'quasi-bosons' $m_B \sim 2\,m_F$; $\rho_B = \rho_F/2$

  applicable for deeply bound pairs

  thermal wavelength of bosons = boson interparticle spacing

  $$[\,2\,\beta\,/\,m\,]^{1/2} \cong [\,3\,/\,4\,\pi\,\rho_B\,]^{1/3} \Rightarrow T \sim (16/9\pi)^{2/3}\,[\hbar^2/2m]\,k_f^2$$

  $$\sim\; 0.68\,[\hbar^2/2m]\,k_f^2$$

- Spin Polarization; phase separation, etc.

- Dense Neutron Matter, neutrino response, ....

- Nuclei & finite shell gaps : IBM (?), ...