Pairing in neutron matter with auxiliary field diffusion Monte Carlo

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Outline of Talk

- Introduction
- The nuclear Hamiltonian.
- Diffusion Monte Carlo.
- Spin sampling with auxiliary field diffusion Monte Carlo method.
- Fixed Phase Approximation
- Trial wave functions with general BCS pairing using pfaffians
- Results

Introduction

Properties of superfluid neutron matter have important consequences in neutron star cooling and dynamics.

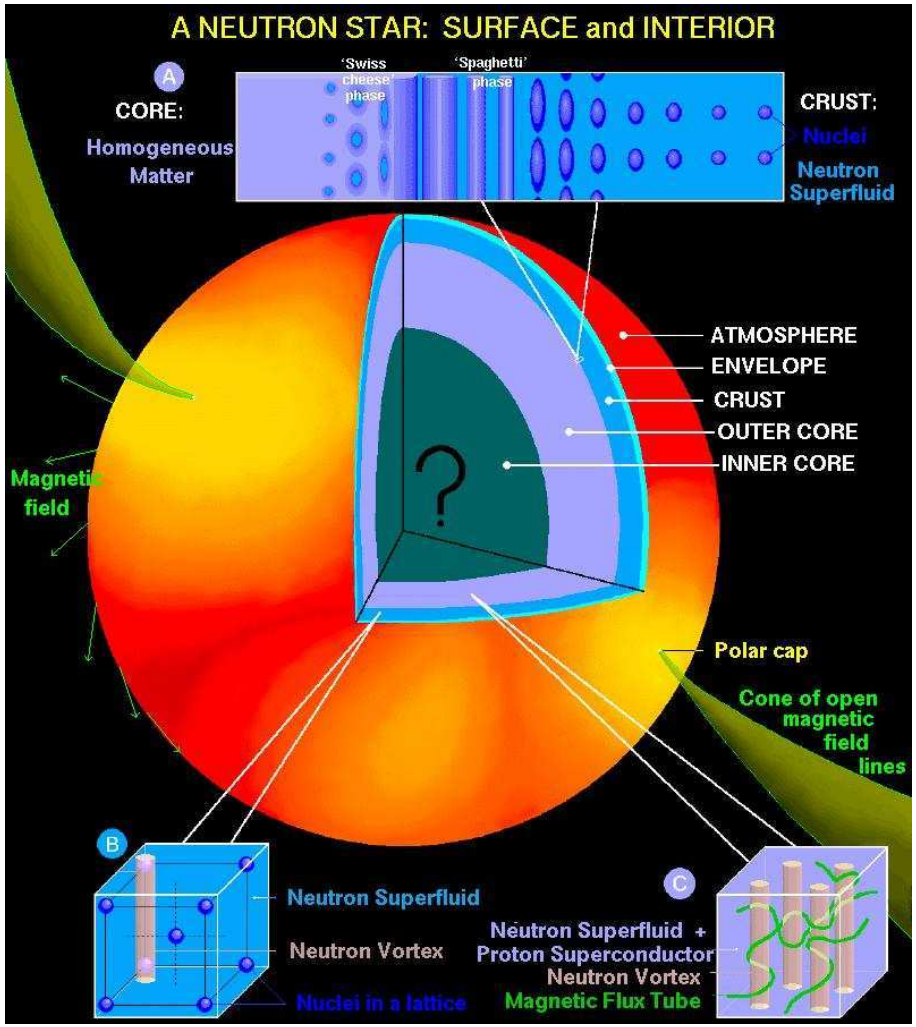
Part of a larger program to calculate the structure of nuclei (which also have pairing correlations).

Here I will talk only about ground states.

The Hamiltonian will be for nonrelativistic protons and neutrons interacting with a potential (mostly local).

Monte Carlo calculations need to be able to sample the nonlocal parts of the propagator.

Neutron Star Structure



Schematic neutron star structure from J.M.Lattimer and M. Prakash, *The physics of neutorn stars*, Science **304**, 536 (2004).

QCD?

We use phenomenological interactions fit to experiment.

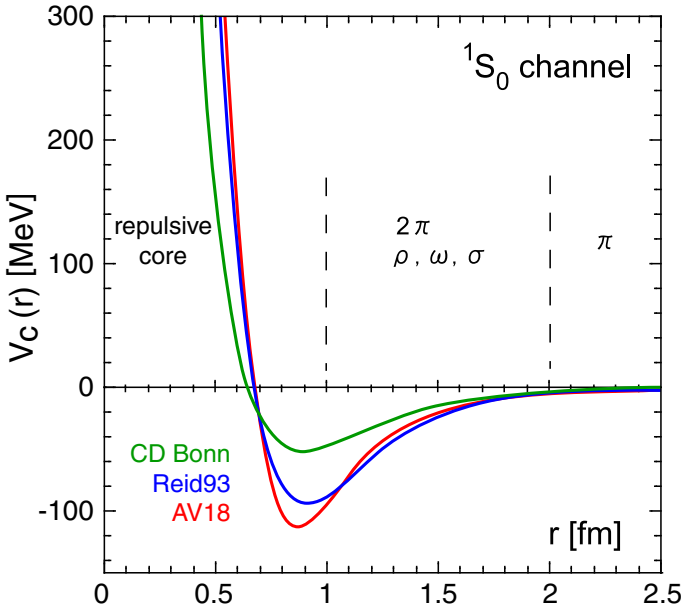
Lattice QCD calculations of two-nucleon interactions have only just begun. Large extrapolations and approximations

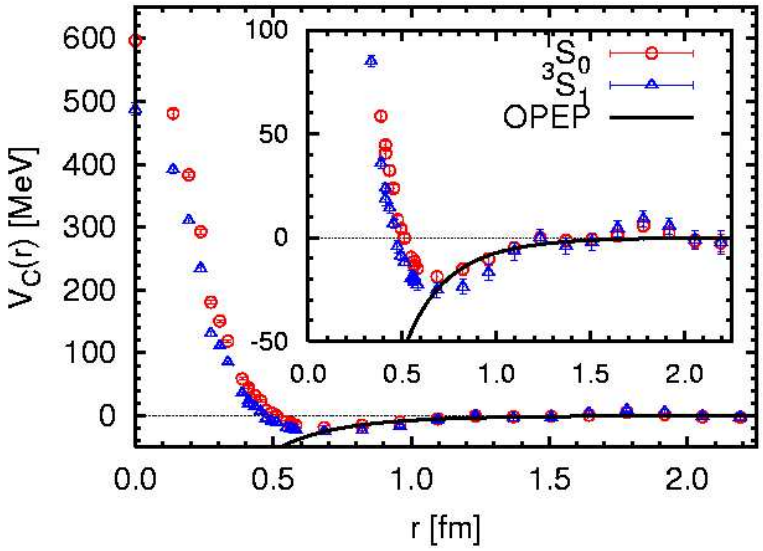
For example, Ishii et al.[†] use a 32^4 lattice with a simulation cell of 4.4 Fm on a side.

They looked at just the ${}^1S_0$ and ${}^3S_1$ channels.

Quenched approximation. They used a π mass of 530 MeV.

[†] N. Ishii, S. Aoki, and T.Hatsuda, *Nuclear Force from Lattice QCD*, Phys. Rev. Lett. **99** 022001 (2007).


$^1S_0$ channel
repulsive core
2π
ρ , ω , σ
π
CD Bonn
Reid93
AV18
V_C (r) [MeV]
r [fm]
300
200
100
0
-100
0
0.5
1
1.5
2
2.5


$^1S_0$
$^3S_1$
OPEP
V_C(r) [MeV]
r [fm]
600
500
400
300
200
100
0
0.0
0.5
1.0
1.5
2.0
100
50
0
-50

Hamiltonian

The Hamiltonian is

$$H = \sum_i \frac{p_i^2}{2m_i} + \sum_{i<j} \sum_{p=1}^{M} v_p(r_{ij}) O^{(p)}(i,j) + V_3$$

- i and j label the two nucleons
- r_{ij} is the distance separating the two nucleons
- $O^{(p)}$ include central, spin, isospin, and spin orbit operators, and M is the maximum number of operators (i.e. 18 in Argonne v_{18} model).

For our calculations we use:

For purely neutron systems the Argonne v_8' and the Urbana or Illinois three-body potentials

The operator terms in Argonne v_8' are

$$\begin{aligned}\sum_p v(r_{ij})O_{ij}^{(p)} &= v_c(r_{ij}) + v_\tau(r_{ij})\vec{\tau}_i\cdot\vec{\tau}_j \\ &+v_\sigma(r_{ij})\vec{\sigma}_i\cdot\vec{\sigma}_j + v_{\sigma\tau}(r_{ij})\vec{\sigma}_i\cdot\vec{\sigma}_j\vec{\tau}_i\cdot\vec{\tau}_j \\ &+v_t(r_{ij})t_{ij} + v_{t\tau}(r_{ij})t_{ij}\vec{\tau}_i\cdot\vec{\tau}_j \\ &+v_{LS}(r_{ij})(\vec{L}_i-\vec{L}_j)\cdot(\vec{S}_i+\vec{S}_j) \\ &+v_{LS\tau}(r_{ij})(\vec{L}_i-\vec{L}_j)\cdot(\vec{S}_i+\vec{S}_j)\vec{\tau}_i\cdot\vec{\tau}_j\end{aligned}$$

The central Part can be handled using standard GFMC or DMC.

The most successful method for light nuclei uses Monte Carlo for the spatial variables and complete summation over the spin-isospin states.

The number neutron spin states for A neutrons is 2^A.

The exponential growth of these states limits this brute force method to less than 20 neutrons. (For nuclei ^{12}C is the largest).

Diffusion Monte Carlo for Central Potentials

Schrödinger equation in imaginary time (measured in units of energy^{-1}) is the diffusion equation

$$\begin{aligned}(H - E_T)\Psi(R,t) &= \\ \left[-\frac{\hbar^2}{2m}\nabla^2 + V(R) - E_T\right]\Psi(R,t) &= -\frac{\partial}{\partial t}\Psi(R,t)\end{aligned}$$

Formal solution

$$\begin{aligned}\Psi(R,t) &= e^{-(H-E_T)t}\Psi(R,0) \\ H\Psi_n(R) &= E_n\Psi_n(R) \\ \Psi(R,0) &= \sum_n a_n\Psi_n(R) \\ \Psi(R,t) &= e^{-(E_0-E_T)t}a_0\Psi_0(R) + \sum_{n\neq 0} e^{-(E_n-E_0)t}a_n\Psi_n(R)\end{aligned}$$

Result converges to the lowest energy eigenstate not orthogonal to $\Psi(R,0)$.

Schematic Implementation

$$\Psi(R, t + \Delta t) = \int dR' e^{-(V(R)-E_T)\Delta t} \langle R | e^{-\frac{P^2}{2m}\Delta t} | R' \rangle \Psi(R', t)$$

- A particles (in a periodic box for matter).
- Use a short time approximation for the Green's function.
- Sample gaussian for the kinetic energy term, evaluate the diagonal potential terms as a weight.
- Use branching to control population.
- Use importance sampling to improve variance.
- For Fermions the wave function changes sign. Use fixed node or transient estimation.

Monte Carlo Spin Sampling

We want to sample the spin.

In the usual $\uparrow$, $\downarrow$ basis.

$R \equiv 3N$ x, y, z coordinates for the nucleons

$S \equiv N$ discrete values selecting one of $\uparrow$, $\downarrow$

$\Psi_T(R, S) =$ Trial wavefunction - a complex number for given R and S.

$H_{S,S'}(R) =$ the Hamiltonian

There are roughly 2^A spin-isospin states. We could sample them with low variance if we could calculate $\Psi_T(R, S)$ efficiently.

All known nontrivial trial functions require order 2^N operations to calculate either 1 or all the spin states.

We use trial functions with no spin-isospin operator correlations.

Sampling with an Auxiliary Field

We diagonalize the interaction in spinor space.

This requires Order(N^3) operations – same complexity as determinant.

For N neutrons, the v_6 interaction can be written as

$$\begin{aligned} V &= \sum_{i<j}[\sum_{p=1}^{6} v_p(r_{ij})O^{(p)}(i,j)] = V_c + V_{nc} \\ &= V_c + \frac{1}{2}\sum_{i,\alpha,j,\beta} \sigma_{i,\alpha} A^{(\sigma)}_{i,\alpha,j,\beta} \sigma_{j,\beta} \end{aligned}$$

- Our A matrix is zero when $i = j$ and symmetric.

- the A matrix is real and symmetric and has real eigenvalues and eigenvectors.

- The eigenvectors and eigenvalues are defined by

$$\sum_{j,\beta} A^{(\sigma)}_{i,\alpha,j,\beta} \vec{\psi}^{\sigma}_{n}(j) \cdot \hat{x}_{\beta} = \lambda^{(\sigma)}_{n} \vec{\psi}^{\sigma}_{n}(i) \cdot \hat{x}_{\alpha}$$

The matrices can be written in terms of their eigenvectors and eigenvalues to give the noncentral potential

$$V_{nc} = \frac{1}{2} \sum_{i,j,n} \vec{\sigma}_i \cdot \vec{\psi}^{(\sigma)}_{n}(i) \lambda^{(\sigma)}_{n} \vec{\psi}^{(\sigma)}_{n}(j) \cdot \vec{\sigma}_j$$

We want the squares of operators so we write

$$V_{nc} = \frac{1}{2}\sum_{n=1}^{3A}(O_n^{(\sigma)})^2\lambda_n^{(\sigma)}$$

with

$$O_n^{(\sigma)} = \sum_i \vec{\sigma}_i \cdot \vec{\psi}_n^{(\tau)}(i)$$

- The Hubbard-Stratonovich transformation is

$$e^{-\frac{1}{2}\lambda_n O_n^2 \Delta t} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx e^{-\frac{1}{2}x^2 + x\sqrt{-\lambda_n \Delta t}O_n}$$

- Our O_n don't commute, so we need to keep the time steps small so that the commutator terms can be ignored. Each of the O_n is a sum of 1-body operators as required above.

- We require 3A Hubbard-Stratonovich variables for the σ terms, $9A$ variables for the $\sigma\tau$ terms, and $3A$ variables for the τ terms. Each time step requires the diagonalization of a $3A$ by $3A$ matrix.

- Many other breakups are possible.

Constrained Path

- We still have the usual fermi sign problem, in this case the overlap of our walkers with the trial function will be complex.

- We constrain the path so that the walker has the same phase as the trial function, and deform the path of the auxiliary field integration so that the auxiliary variables are complex[†].

- For spin independent potentials this reduces to the fixed-node or fixed phase approximation.

- There is a variational principle for the mixed energy but not an upper bound principle. Expectation values of H have an upper bound principle but are not implemented here.

[†] S. Zhang and H. Krakauer, *Quantum Monte Carlo method using phase-free random walks with Slater determinants*, Phys. Rev. Lett. **90**, 136401 (2003).

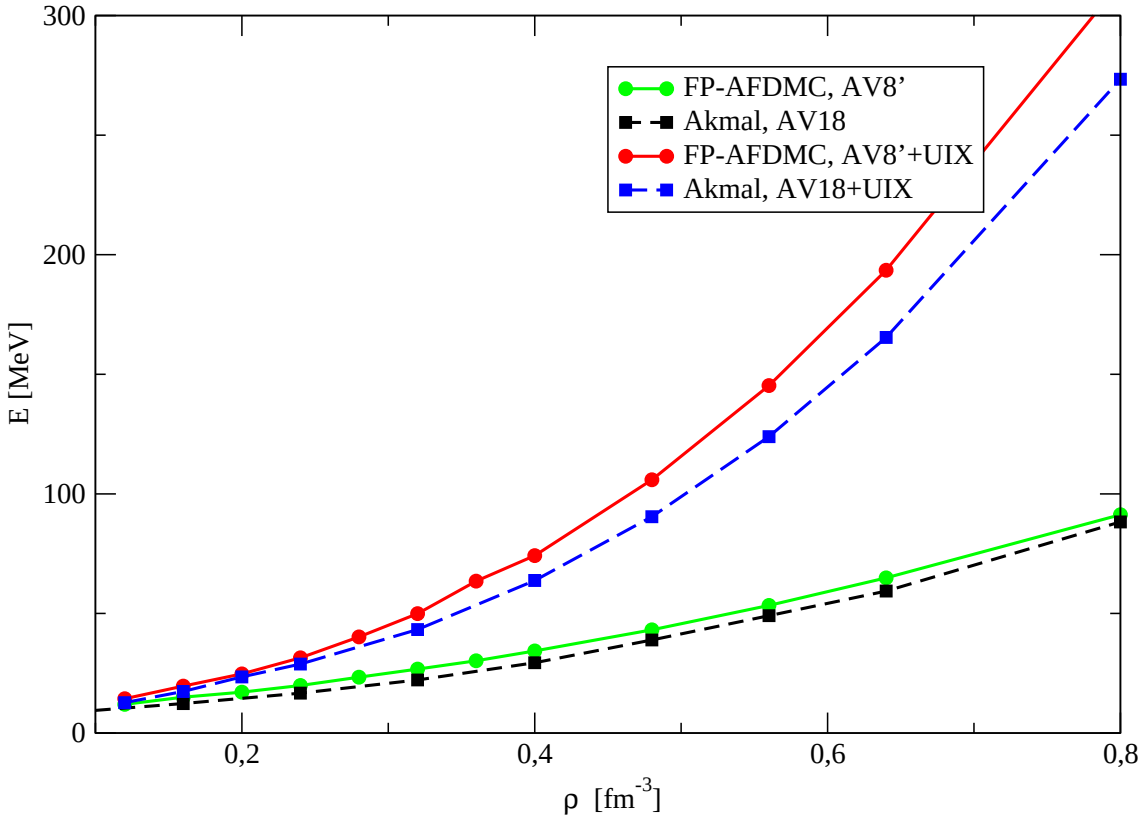
GFMC Model neutron drop comparison

Table 1: Ground state AFDMC energies of $^8n(0^+)$, $^7n(\frac{1}{2}^+)$ and $^7n(\frac{3}{2}^+)$ droplets for $V_0 = 20$MeV and the AU8' and AU6' interactions. The cluster variational Monte Carlo (CVMC) and GFMC results[†] for the AU8' and the full AU18 (Argonne v_{18} plus Urbana IX) are also reported for comparison. The last column reports the spin–orbit splittings (SOS) in MeV of ^7n, given by the energy difference between the $^7n(\frac{3}{2}^+)$ and $^7n(\frac{1}{2}^+)$ states.

	$^8n(0^+)$	$^7n(\frac{1}{2}^+)$	$^7n(\frac{3}{2}^+)$	SOS
GFMC(AU18)	-37.8(1)	-33.2(1)	-31.7(1)	1.5(2)
CVMC(AU18)	-35.5(1)	-31.2(1)	-29.7(1)	1.5(2)
GFMC(AU8')	-38.3(1)	-34.0(1)	-32.4(1)	1.6(2)
AFDMC(AU8')	-37.55(2)	-33.06(3)	-31.51(2)	1.55(5)

[†] S. C. Pieper, V. R. Pandharipande, R. B. Wiringa, and J. Carlson, *Realistic models of pion-exchange three-nucleon interactions*, Phys. Rev. C **64**, 14001 (2001).

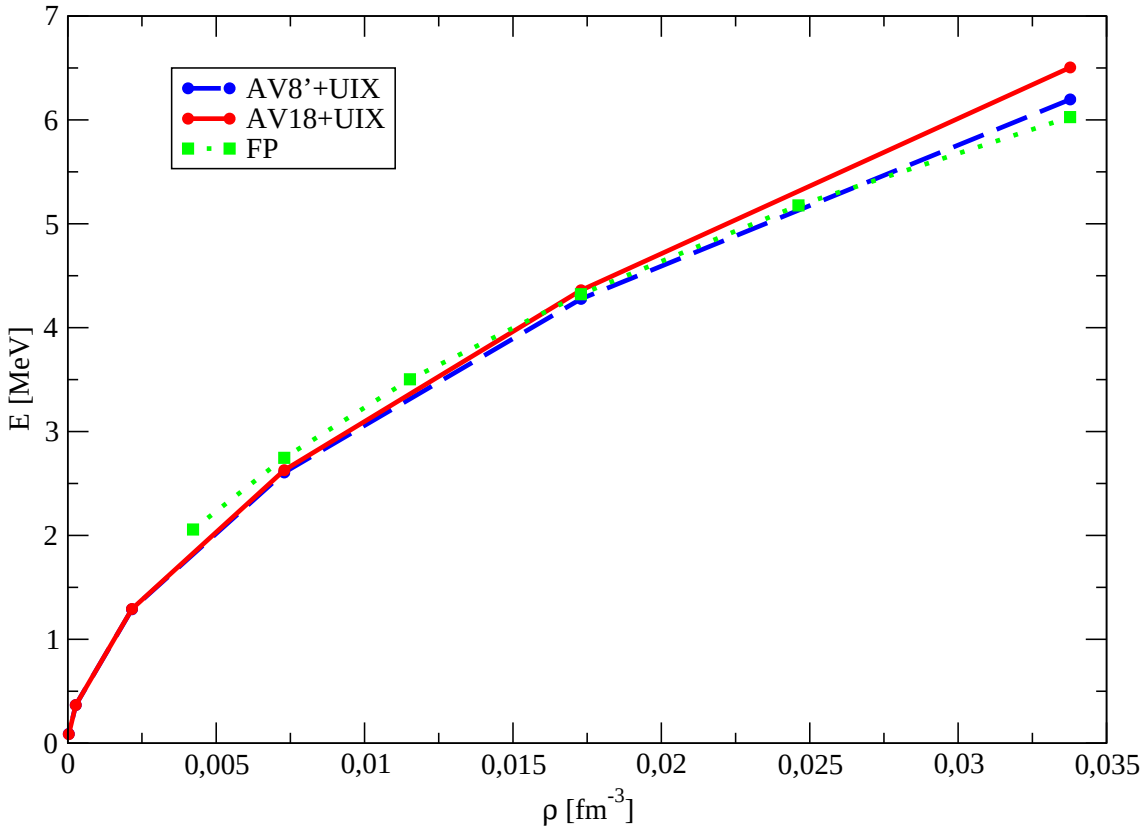
Neutron matter equation of state



Akmal refers to the FHNC calculation[†]

[†] A. Akmal, V.R. Pandharipande, and D.G. Ravenhall, Equation of state of nucleon matter and neutron star structure, Phys. Rev. C **58** 1804 (1998).

Low density neutron matter with Argonne v_{18}



FP is the calculation of Friedman and Pandharipande (not v_{18}, but the low energy channels are not very different).†

† B. Friedman and V.R. Pandharipande, Hot and cold, nuclear and neutron matter, Nucl. Phys. A **361**, 502 (1981).

Wave Functions

- Most Fermion trial wave functions are built out of Slater determinants of single-particle orbitals.

$$\Psi_T = \mathcal{A}[\psi_1(\vec{r}_1, s_1)\psi_2(\vec{r}_2, s_2)...\psi_N(\vec{r}_N, s_N)]$$

  - Linear combinations.
  - Backflow correlations $\Rightarrow \vec{r}_i \longrightarrow \vec{r}_i + \sum_{j \neq i} \xi_{ij}\vec{r}_{ij}$.

- Fermion superfluids and superconductors are more efficiently described by BCS pairing wave functions,

$$\begin{aligned} \Psi_T &= \mathcal{A}[\phi(\vec{r}_1, s_1; \vec{r}_2, s_2)...\phi(\vec{r}_{N-1}, s_{N-1}; \vec{r}_N, s_N)] \\ &= \mathcal{A}[\phi_{12}\phi_{34}...\phi_{N-1\,N}] \,. \end{aligned}$$

- For spin independent Hamiltonians, and equal numbers of fermions, the slater determinant can be written in the BCS form.

- An arbitrary BCS form corresponds to a large linear combination of slater determinants.

- Nodal Structure of the BCS form and Slater determinants can be quite different. The BCS form allows pair exchange without node crossing.

Relationship to Standard BCS

The BCS form used here is the standard BCS form projected onto N particles.

For a bulk system of spin singlet pairs,

$$
\begin{aligned}
|BCS\rangle &= \prod_{\vec{k}} \left[u_k + v_k c^+_{\vec{k}\uparrow} c^+_{-\vec{k}\downarrow} \right] |0\rangle \\
\phi(\vec{r}_1, s_1; \vec{r}_2, s_2) &\propto \sum_{\vec{k}} \frac{v_k}{u_k} \cos\left(\vec{k} \cdot [\vec{r}_1 - \vec{r}_2] \right) \left[\langle s_1 s_2 | \uparrow\downarrow\rangle - \langle s_1 s_2 | \downarrow\uparrow\rangle \right]
\end{aligned}
$$

In general

$$
\begin{aligned}
|BCS\rangle &= \prod_{n} \left[u_n + v_n c^+_n c^+_{n'} \right] |0\rangle \\
\phi(\vec{r}_1, s_1; \vec{r}_2, s_2) &\propto \sum_{n} \frac{v_n}{u_n} \left[\psi_n(\vec{r}_1, s_1) \psi_{n'}(\vec{r}_2, s_2) - \psi_n(\vec{r}_2, s_2) \psi_{n'}(\vec{r}_1, s_1) \right]
\end{aligned}
$$

Combinations of paired and unpaired orbitals

A general state with n paired and o unpaired orbitals for a total of $N = 2n + o$ particles can be written as

$$\mathcal{A}[\phi_{12}\phi_{34}...\phi_{2n-1,2n}...\psi_1(2n+1)...\psi_o(N)]$$

which is the Pfaffian of the $(N+o) \times (N+o)$ matrix

$$\begin{pmatrix}
0 & \phi_{12} & \phi_{13} & \dots & \phi_{1N} & \psi_1(1) & \dots & \psi_o(1) \\
-\phi_{12} & 0 & \phi_{23} & \dots & \phi_{2N} & \psi_1(2) & \dots & \psi_o(2) \\
-\phi_{13} & \phi_{23} & 0 & \dots & \phi_{3N} & \psi_1(3) & \dots & \psi_o(3) \\
\vdots & \vdots & \vdots & \vdots\vdots & \vdots & \vdots & \vdots\vdots & \vdots \\
-\phi_{1N} & -\phi_{2N} & -\phi_{3N} & \dots & 0 & \psi_1(N) & \dots & \psi_o(N) \\
-\psi_1(1) & -\psi_1(2) & -\psi_1(3) & \dots & -\psi_1(N) & 0 & \dots & 0 \\
\vdots & \vdots & \vdots & \vdots\vdots & \vdots & \vdots & \vdots\vdots & \vdots \\
-\psi_o(1) & -\psi_o(2) & -\psi_o(3) & \dots & -\psi_o(N) & 0 & \dots & 0
\end{pmatrix},$$

where the lower $o \times o$ section is all zeroes.

Spin singlet pairing reduces to a determinant.

Calculations of Pfaffians – $O(N^3)$ operations[†]

[†] M. Bajdich, L. Mitas, L. K. Wagner and K. E. Schmidt, *Pfaffian Pairing and backflow wave functions for electronic-Structure Quantum Monte Carlo methods*, Phys. Rev. B" **77**, 115112 (2008).

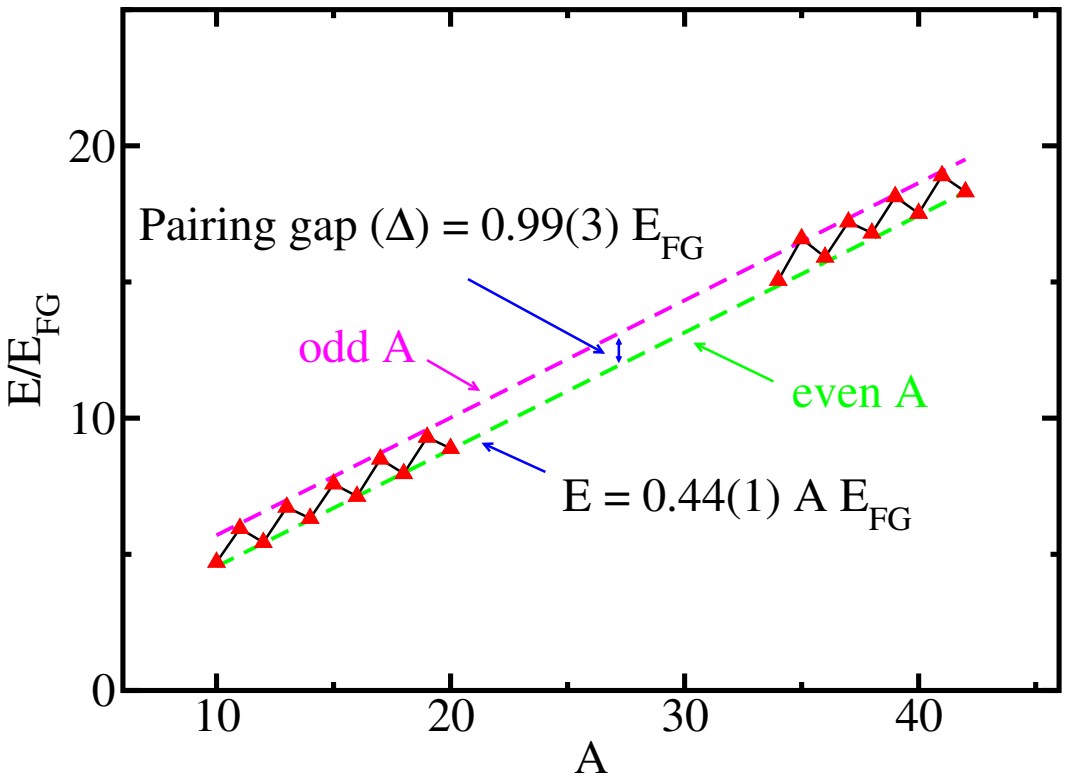
Central Spin Singlet Application

Dilute $\equiv$ range R of the interaction $\ll$ than interparticle spacing r_0, or $k_F R \ll 1$, $\rho = \frac{3}{4\pi r_0^3} = \frac{k_F^3}{3\pi^2}$

If the scattering length a is large – short range interactions can strongly modify the dilute gas properties, $k_F|a| \gg 1$.

Low density neutron matter (in inner crust of neutron stars) $R \sim 2$ fm, $a = -18$ fm.

Energy and even-odd energy gap for $\mathbf{a} = -\infty$ [†]



Energy as a function of particle number A.

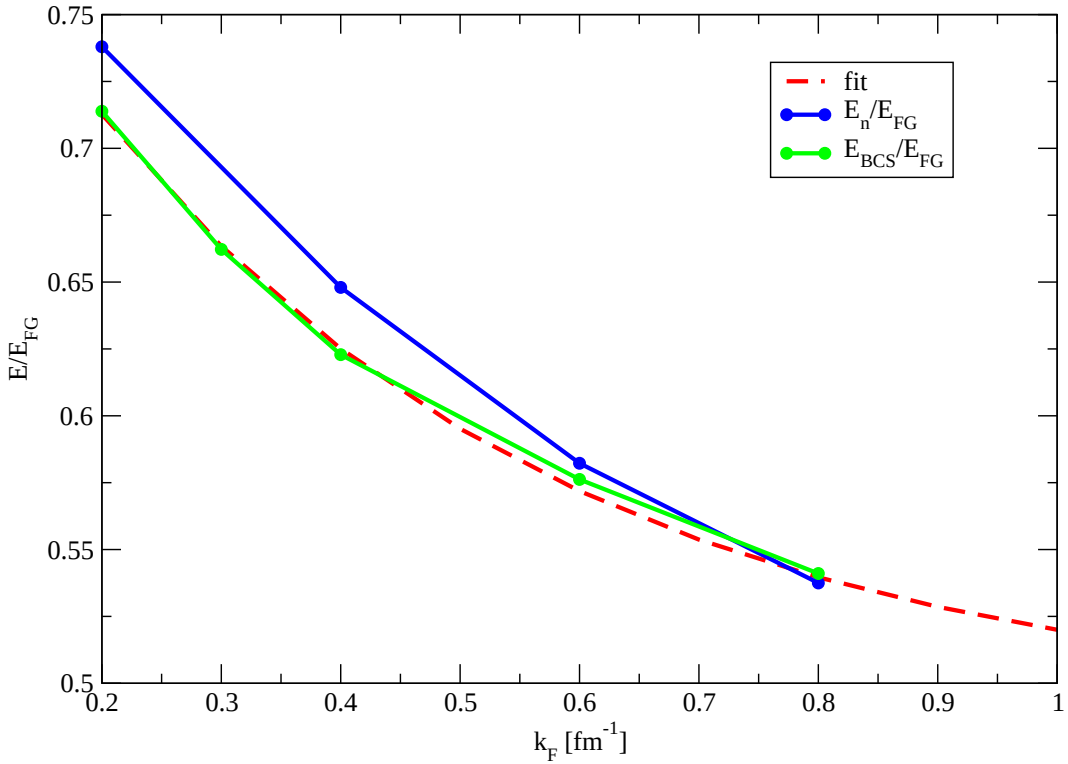
Slater determinant nodes give an energy of $E/A = 0.54 E_{FG}$.

[†] J.Carlson, S-Y Chang, V.R. Pandharipande, and K.E. Schmidt, "Superfluid Fermi Gases with Large Scattering Length", Phys. Rev. Lett. **91**, 050401 (2003).

Neutron Matter Calculations

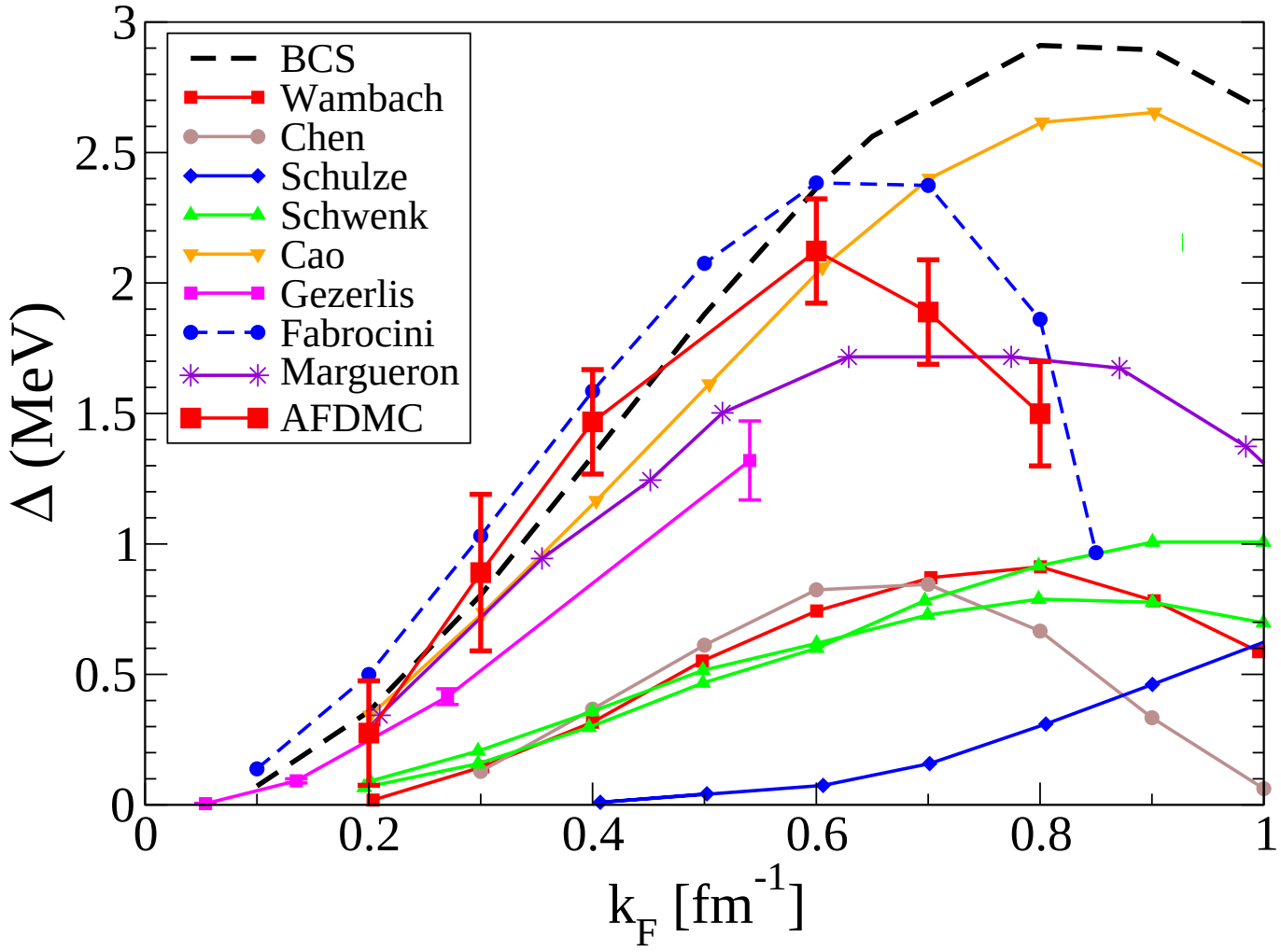
We begin with Fermi-hypernetted chain correlated basis function method to produce the trial wave function for the constraint.

Even though the dominant low density pairing is spin singlet, since the particles' spin can be flipped by the potential, the Pfaffian is needed.



Calculated BCS versus normal equation of state

Neutron matter energy gaps



Calculated energies gap (AFDMC) compared to other calculations.

Conclusions and Future

- Monte Carlo calculations can give enough precision to extract energy gaps for neutron matter.
- Using correlated basis function (CBF) pairing amplitudes as a constraint give gaps close to CBF and BCS.
- A direct Monte Carlo search for the pairing amplitudes is computationally difficult for nucleon systems.
- Pairing in other channels can be investigated.
- Asymmetric matter – addition of protons