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Advanced School on Quantum Monte Carlo Methods in Physics and Chemistry

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Spin/isospin 1 & 2

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Quantum Monte Carlo with spin and isospin

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The nuclear Hamiltonian

The nuclear Hamiltonian is not well characterized.

Compare to electronic structure:

- $V = \frac{q_i q_j}{r_{ij}}$ to a very good approximation.
- Corrections like spin-orbit, hyperfine structure, retardation, etc. usually can either be ignored or use perturbation theory.
- Interaction cannot flip spins – spins can be assigned to particles.
- Relativistic effects are $O[(v/c)^2]$ and $v/c \simeq \frac{e^2}{\hbar c} \simeq \frac{1}{137}$

In nuclear physics

- There are many proposed Hamiltonians – often fits to experimental data with theoretical constraints.
- The most important interaction term, the one-pion exchange potential, looks like the hyperfine interaction

$$v(r_{ij})\left[3\vec{\sigma}_i \cdot \hat{r}\vec{\sigma}_j \cdot \hat{r} - \vec{\sigma}_i \cdot \vec{\sigma}_j\right]$$

- Spin-orbit forces are important.
- Three-body forces are important.
- $v/c \simeq \frac{1}{10}$
- The interaction can both flip spins and exchange charge (a proton can emit a virtual π^+ becoming a neutron and a neutron can absorb the π^+ becoming a proton.

Ab initio thoughts

- If we could solve QCD for low energy quarks, gluons and photons, we would obtain nuclear physics.

- Lattice QCD calculations of single nucleons (3 valence quarks) are difficult.

- Lattice QCD calculations of two nucleon interactions (6 valence quarks) has only just begun. It requires 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.

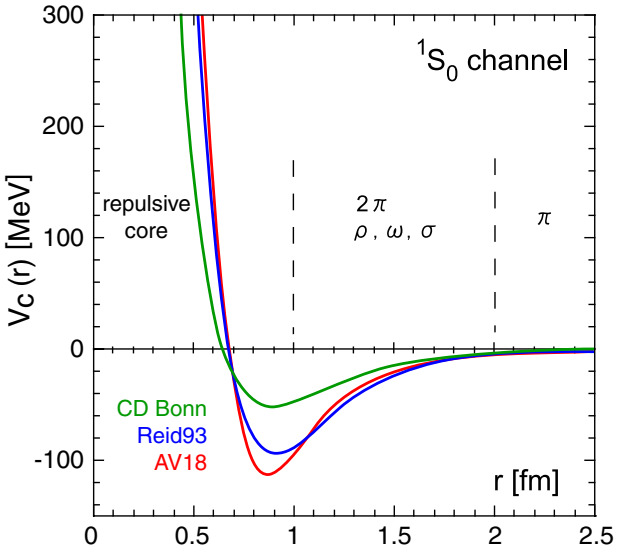
  They looked at just the ${}^1S_0$ and ${}^3S_1$ channels.

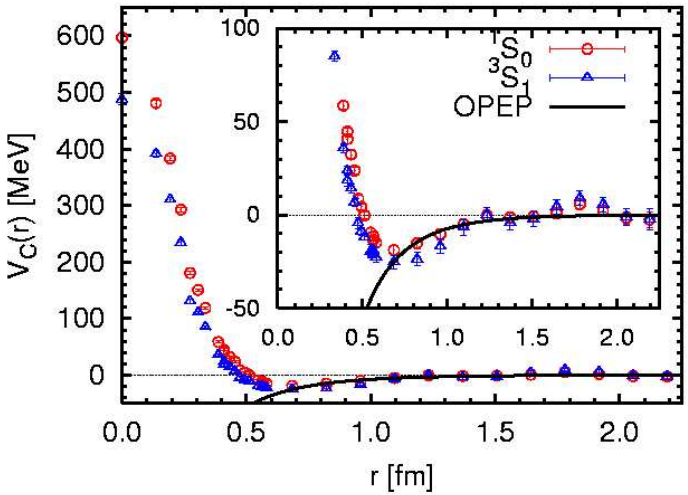
  Quenched approximation (no quark sea!) They used a π mass of 530 MeV (about 4 times the physical mass)

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

Crude Lattice QCD results

A realistic force would require a lattice at least 10 times larger in each direction to get get a reasonable pion mass and nuclei spacing. This would mean 10^4 times more lattice points. The quenched approximation would need to be removed. This makes the calculations much more expensive since a this means ratios of determinants with dimension of the lattice size must be calculated (and introduces a fermion sign problem).





Fits to data

Since ab initio calculations of the nuclear force are out of reach, phenomenological approaches are used.

- Effective field theories either from QCD or phenomenological [proton uud, neutron udd, Δ uuu etc., mesons π^+ $u\bar{d}$, π^0 $u\bar{u} - d\bar{d}$, π^- $d\bar{u}$, ρ, ω etc.

- Phenomenological potentials

Generally use a combination of theoretical forms from field theory with parameters chosen to fit experimental scattering data.

Isospin

We often initially ignore electromagnetism (electromagnetic effects are small on the nuclear scale) $\hbar c = 197.3$ MeV-Fm, so $e^2 = \frac{e^2}{\hbar c}\hbar c \simeq 1.4 MeV/Fm$. So electromagnetic effects change the particle masses by a few MeV, change nuclear binding energies somewhat, and make high mass nuclei have a neutron excess.

If the u and d quark masses are taken equal and electromagnetism is neglected, QCD is isospin invariant. For our purposes, that means that the proton and neutron are viewed as a single kind of particle, the nucleon, with two isospin states. Conventionally,

proton $=$ isospin up.

neutron $=$ isospin down.

Even if the Hamiltonian does not commute with isospin rotations, we can use the isospin formalism. So we continue to use it when we reintroduce electromagnetic effects.

Pauli matrices for nucleons

The nuclear spin is described by an up spin amplitude and a down spin amplitude. All spin operators can be expressed as linear combinations of the identity and the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The same Pauli operators are used for the nucleon isospin. Conventionally the symbols τ_x, τ_y, τ_z are used for the isospin degrees of freedom.

A nucleon spin-isospin state is then expressed as a linear combination of the four states $|p\uparrow\rangle$, $|p\downarrow\rangle$, $|n\uparrow\rangle$, $|n\downarrow\rangle$. A general Hermitian operator in this space is a real linear combination of the identity, 1, and σ_α, τ_β, $\sigma_\alpha\tau_\beta$. Which gives the 16 independent real numbers that specify a Hermitian 4×4 matrix.

One pion exchange example

The three kinds of pions π^+, π^0, π^- form an isospin one particle if electromagnetism is ignored. (Here $\hbar = c = 1$)

QCD dictates that the effective pion coupling to a nucleon labeled i in the nonrelativistic limit is

$$V = \sum_i g_\pi \vec{\sigma}_i \cdot \vec{\nabla}_i \left[\tau_x \pi_x(\vec{r}_i) + \tau_y \pi_y(\vec{r}_i) + \tau_z \pi_z(\vec{r}_i)\right]$$

where the pion field is

$$\begin{aligned} \pi_\alpha &= \sum_{\vec{k}} \frac{1}{\sqrt{2\omega_k}} \left[a_{\vec{k}\alpha} e^{i\vec{k}\cdot\vec{r}} + a^+_{\vec{k}\alpha} e^{-i\vec{k}\cdot\vec{r}}\right] \\ \omega_k^2 &= k^2 + m_\pi^2 \end{aligned}$$

$$\pi^\pm = \frac{\pi_x \pm i\pi_y}{\sqrt{2}} \quad \pi_z = \pi^0$$

In the static limit (large nucleon mass compared to pion energy), second order perturbation theory then gives for the interaction

$$\begin{aligned}\Delta E_n &= \sum_{m\neq n} \frac{\langle n|V|m\rangle\langle m|V|n\rangle}{E_n - E_m} \\ &= -g_\pi^2 \tau_1\cdot\tau_2 \sum_k \frac{\langle \vec{r}_1 s_1 \vec{r}_2 s_2|\vec{\sigma}_1\cdot\vec{\nabla}_1 e^{i\vec{k}\cdot\vec{r}_1}\vec{\sigma}_2\cdot\vec{\nabla}_2 e^{-i\vec{k}\cdot\vec{r}_2}|\vec{r}_1 s_1 \vec{r}_2 s_2\rangle}{\omega_k^2}\end{aligned}$$

The effective potential between the nucleons separated by $\vec{r} = \vec{r}_1 - \vec{r}_2$ is

$$\begin{aligned}V_{1-\pi} &= -g_\pi^2 \tau_1\cdot\tau_2 \sum_k \vec{\sigma}_1\cdot\vec{\nabla}\vec{\sigma}_2\cdot\vec{\nabla}\frac{e^{i\vec{k}\cdot\vec{r}}}{k^2+m_\pi^2} = -\frac{g_\pi^2}{4\pi}\tau_1\cdot\tau_2\vec{\sigma}_1\cdot\vec{\nabla}\vec{\sigma}_2\cdot\vec{\nabla}\frac{e^{-m_\pi r}}{r} \\ &= -\frac{g_\pi^2}{4\pi}\tau_1\cdot\tau_2\left[t_{12}\left(\frac{m_\pi}{r^2}+\frac{1}{r^3}+\frac{m_\pi^2}{3r}\right)+\vec{\sigma}_1\cdot\vec{\sigma}_2\left(\frac{m_\pi^2}{3r}-4\pi\delta^3(\vec{r})\right)\right]\frac{e^{-m_\pi r}}{r} \\ t_{12} &= 3\vec{\sigma}_1\cdot\hat{r}\vec{\sigma}_2\cdot\hat{r}-\vec{\sigma}_1\cdot\vec{\sigma}_2\end{aligned}$$

Realistic Potentials

All realistic two-body potentials have a one pion exchange term, other terms that have the form of other types of physical processes, and purely phenomenological terms that are used to fit experimental scattering data and the deuteron properties.

The Nijmegen group has tabulated the world's published N-N scattering data below 350 MeV (Below the pion production threshold).[†]

(4301 data points)

Realistic potentials fit this data at a confidence level of $\chi^2/N_{data} \sim 1$.

These potentials to a large extent give equivalent results for several nuclear and neutron matter properties.

[†] V. G. J. Stoks, R. A. M. Klomp, M. C. M. Rentmeester, J. J. de Swart, *Partial-wave analysis of all nucleon-nucleon scattering data below 350 MeV*, Phys. Rev C **48**, 792-815 (1993).

Scattering data

- proton-proton scattering – proton beam – hydrogen target – clean.
- proton-neutron scattering – proton beam – deuterium target – must subtract proton-proton and neutron-proton correlation.
- neutron-neutron scattering – usually not done – deuterium beam –deuterium target subtract proton-proton, neutron-proton and correlation effects.
- Extracting three-body and higher potentials is very difficult since it is hard to control and measure the relative momenta of the constituents.

Two-body potential choices

Different kinds of calculations are simpler with different forms of the potential.

Basis set calculations like shell-model (i.e. configuration interaction) and coupled-cluster converge faster with soft potentials – hard cores require many basis states. Nonlocality is not a problem.

Monte Carlo needs to sample the nonlocal parts (e.g. the momentum dependent parts like $\frac{p^2}{2m}$) and works best if these components give a positive Green's function. Hard-cores are no problem for Monte Carlo methods working in position space.

Variational methods based on position space integrals are harder with nonlocal interactions.

Argonne v_{18} family

The Argonne[†], and the previous Urbana potentials, were developed for integral equation methods. They have weak nonlocality and substantially more local repulsion at short distances than other potentials. This makes them popular for integral equations and Monte Carlo calculations, but less popular for shell model and coupled-cluster calculations.

They have the form:

$$V = \sum_{p=1}^{N_{\rm op}} v_p(r_{ij}) O_{ij}^p \tag{1}$$

The first 14 operators are
$(1,\ \vec{\sigma}_i \cdot \vec{\sigma}_j,\ t_{ij},\ \vec{L}_{ij} \cdot \vec{S}_{ij},\ L^2,\ L^2(\vec{\sigma}_i \cdot \vec{\sigma}_j),\ (\vec{L}_{ij} \cdot \vec{S}_{ij})^2$ and these multiplied by $\tau_i \cdot \tau_j$. The final 4 operators break isospin invariance. Defining $T_{ij} \equiv 3\tau_{iz}\tau_{jz} - \vec{\tau}_i \cdot \vec{\tau}_j$, they are $T_{ij},\ T_{ij}\vec{\sigma}_i \cdot \vec{\sigma}_j,\ T_{ij}t_{ij}, \tau_{iz} + \tau_{jz}$.

$\vec{L} \cdot \vec{S}$ is the spin orbit operator $\vec{L}_{ij} = \frac{1}{2}\vec{r}_{ij} \times (\nabla_i - \nabla_j)$, $\vec{S}_{ij} = \frac{1}{2}(\vec{\sigma}_i + \vec{\sigma}_j)$.

[†] R. B. Wiringa, V. G. J. Stoks, R. Schiavilla, *Accurate nucleon-nucleon potential with charge-independence breaking*, Phys. Rev C **51**, 38-51, (1995).

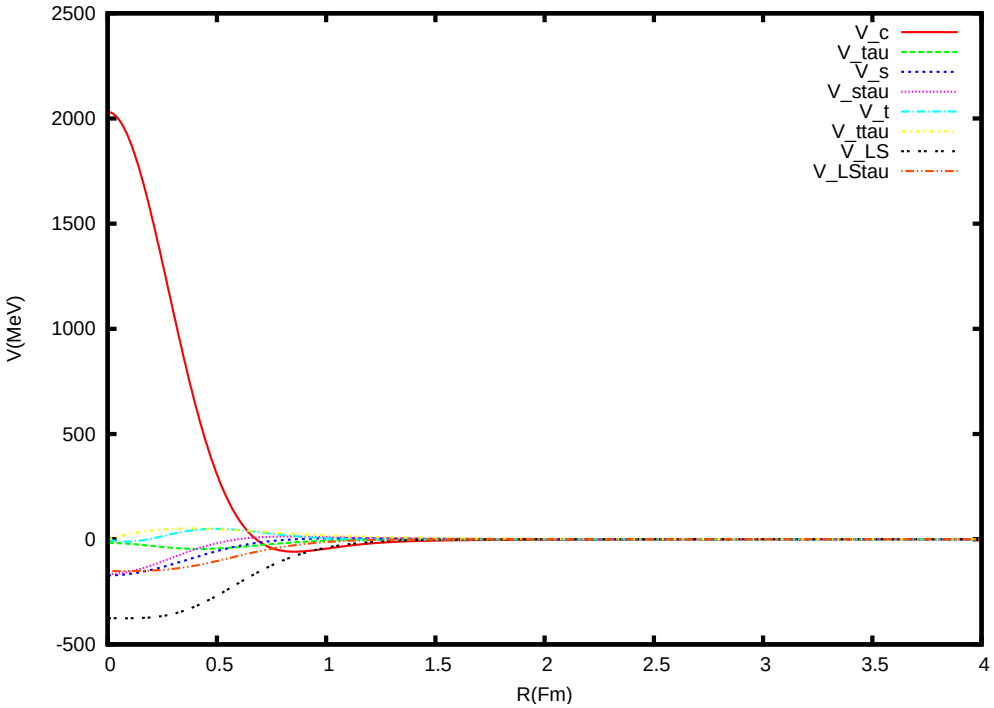
Argonne v_{18} terms

Physics:

- 1 (central) potential
- $(\vec{\sigma}_i \cdot \vec{\sigma}_j)$ is 1 in spin triplet $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$ states, -3 in spin singlet $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$ states.
- t_{ij} tensor (spin dipole-dipole) operator as in one pion exchange.
- $\vec{L} \cdot \vec{S}$, couples spin and orbital angular momentum – interaction conserves total $\vec{J} = \vec{L} + \vec{S}$. This term is momentum dependent.
- $(\vec{\tau}_i \cdot \vec{\tau}_j)$ acts like $(\vec{\sigma}_i \cdot \vec{\sigma}_j)$ except on proton-neutron states.

Other terms are weaker and can often be included with perturbation theory.

Potential graph



The first 8 operators of Argonne v_{18}.

Electromagnetism

Electromagnetic terms are added which have the same spin operators as those in the first 14 and have different strengths between neutron-neutron, neutron-proton and proton-proton pairs corresponding to the different charge densities of the different nucleons.

Basic Hamiltonian

The Hamiltonian we will use contains:

- Nonrelativistic kinetic energy

$$\sum_i p_i^2 \left[\frac{1}{4m_p} + \frac{1}{4m_n} + \tau_{iz} \left(\frac{1}{4m_p} - \frac{1}{4m_n} \right) \right]$$

  or if the mass difference is ignored (1 part out of 500),

$$\sum_i p_i^2 \left[\frac{1}{4m_p} + \frac{1}{4m_n} \right] .$$

- Sum over pairs of a two-body potential such as Argonne v_{18}
- Sum over triplets of a three-body potential ...

Light nuclei and two-body potential

The Schrödinger equation for two-particles is readily integrated. All realistic potentials reproduce the measured deuteron properties within experimental errors.

There are a variety of methods for 3- and 4-body calculations. Monte Carlo, Fadeev, Fadeev-Yakubovsky, Hyperspherical variational, no-core shell model, etc.

All show the inadequacy of using only two-body pair potentials.

For example, ^{3}He and ^{4}He are underbound.

GFMC light nuclei comparison

GFMC calculations give[†]

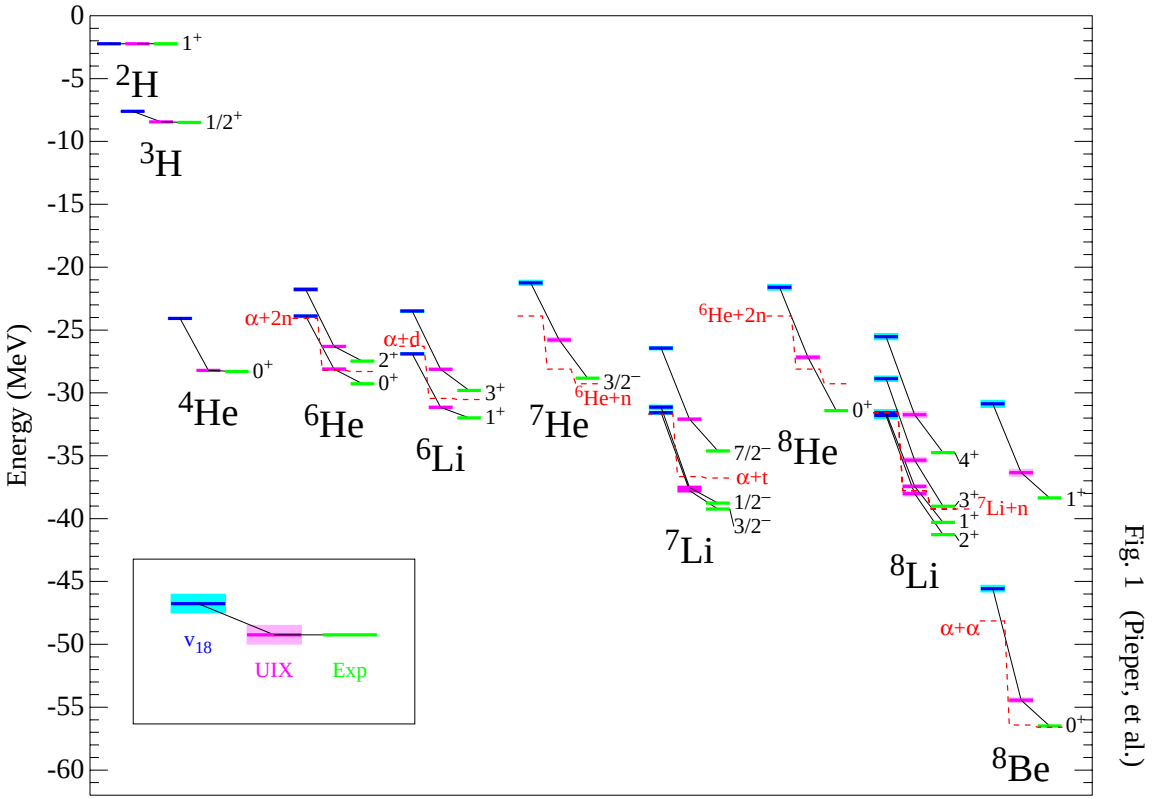


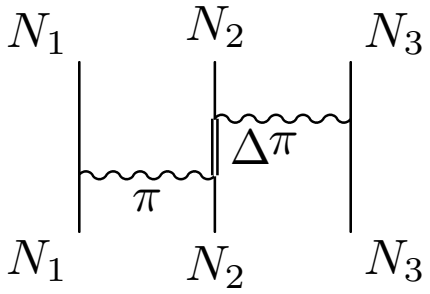
Fig. 1 (Pieper, et al.)

[†] 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).

Three-body interactions

- The form of the 3-body interactions in nuclei are principally from the Δ resonance.

- Largest is Fujita-Miyazawa



- Integrating out the pions assuming large nucleon and Δ masses gives a static transition potential $v_{NN\leftrightarrow N\Delta}$ which has the same form as one-pion exchange except

  $\vec{\tau} \longrightarrow \vec{T}$ where $\langle\frac{1}{2}|\tau|\frac{1}{2}\rangle$ becomes $\langle\frac{1}{2}|T|\frac{3}{2}\rangle$

  and similarly for spin.

  Can use Wigner-Eckart theorem to calculate the matrix elements.

- Integrating out the Δ and assuming a large Δ mass gives the Fujita-Miyazawa form in the Urbana and Illinois 3-body potentials

$$A \sum_{\text{cyc}} \left(\{X_{ij}, X_{jk}\}\{\vec{\tau}_i \cdot \vec{\tau}_j, \vec{\tau}_i \cdot \vec{\tau}_k\} + \frac{1}{4}[X_{ij}, X_{jk}][\vec{\tau}_i \cdot \vec{\tau}_j, \vec{\tau}_i \cdot \vec{\tau}_k] \right)$$

  where

$$X_{ij} = T(r_{ij})t_{ij} + Y(r_{ij})\vec{\sigma}_i \cdot \vec{\sigma}_j$$

  is the 1-pion exchange potential with a gaussian cut off at short distances.

  This is the same form and cutoff that is used in the Argonne v_{18} potential.

- A purely phenomenological central three-body repulsion is added to keep neutron rich systems from being overbound.

A nuclear state

- We can specify the nuclear wave function $\Psi(R,S)$ by giving the positions $R = \{\vec{r}_1, \vec{r}_2, ..., \vec{r}_A\}$ of the A nucleons, and their spin isospin state $S = \{s_1, s_2, ..., s_N\}$ where $s_i = p\uparrow, p\downarrow, n\uparrow, n\downarrow$.

- For given positions of the A nucleons for a nucleus with charge of Ze, the number of spin states is 2^A. The number of charge Z states is the number of ways of assigning Z protons and $A-Z$ neutrons to A nucleons, or $A!/((A-Z)!Z!)$.

- $$\text{Number of Spin} - \text{Isospin states} = 2^A \frac{A!}{(A-Z)!Z!}$$

- For light nuclei Variational and Green's function Monte Carlo Calculations sample the spatial positions as in central diffusion Monte Carlo and perform full numerical summations over the spin-isospin states.

Time Reversal

Since we ignore weak interactions for nuclear structure, the Hamiltonian is time-reversal invariant.

The time-reversal operator is

$$\mathcal{T} = \left[\prod_{i=1}^{N} \sigma_{xi}\sigma_{zi}\right] K$$

K takes the complex conjugate of the wave function on the right.

Think of coupling the spin to a magnetic field – time reversing the currents flips the magnetic field, so it must flip the spin too.

The time reversal operator flips all of the spins. For nondegenerate states, the time reversed state is proportional to the original state.

We only need to calculate the amplitude of half the spin states – the amplitudes for all spins flipped is given by time reversal.

Isospin Symmetry

If we solve the isoscalar part of the Hamiltonian and include the electromagnetic and other isospin breaking terms as perturbations, isospin becomes a good quantum number.

For example the number of states with $T = 0$ can be calculated:

- The number of $T_z = 1$ states is

$$\frac{A!}{(A/2+1)!(A/2-1)!}$$

  These must have $T > 0$, and operating with T^- will give the same number of $T > 0$, $T_z = 0$ states.

- The number of $T_z = 0$ states is

$$\frac{A!}{(A/2+1)!(A/2-1)!}$$

so the number of $T = 0$ states is the difference

$$\frac{A!}{(A/2)!(A/2)!}\frac{2}{A+2}$$

This reduces the number of spin-isospin states by a factor of $2/(A+2)$.

Stirling's approximation says $N! \simeq \sqrt{2\pi N}\left(\frac{N}{e}\right)$ or $\frac{A!}{(A/2)!(A/2)!} \simeq \sqrt{\frac{2}{\pi A}}2^A$, so all of these tricks cannot get rid of the exponential behavior.

The number of states for some representative nuclei:

Nucleus	Spin	Isospin	Total	Good Isospin/Time Reversal
^{4}He	16	6	96	16
^{8}Be	256	70	17920	1792
^{12}C	4096	924	3784704	270336
^{16}O	65536	12870	8.4×10^8	4.7×10^7

Monte Carlo Spin Sampling

We sample the spatial degrees of freedom exactly as for central potentials (i.e. Metropolis for variational or diffusion with drift and branching for DMC/GFMC.)

We want to sample the spin and isospin.

In the usual p↑, p↓, n↑, n↓ basis.

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

$S \equiv A$ discrete values selecting one of p↑, p↓, n↑, n↓

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

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

Variational Calculation

Spin-isospin sums

$$\begin{aligned}
\langle H \rangle &= \int dR E_L(R) P(R) \,, \\
P(R) &= \frac{\sum_S |\Psi_T(R,S)|^2}{\int dR \sum_S |\Psi_T(R,S)|^2} \,, \\
E_L(R) &= \frac{\sum_{S,S'} \Psi_T^*(R,S') H_{S',S} \Psi_T(R,S)}{\sum_S |\Psi_T(R,S)|^2} \,,
\end{aligned}$$

or spin-isospin samples

$$\begin{aligned}
\langle H \rangle &= \int dR \sum_S E_L(R,S) P(R,S) \,, \\
P(R,S) &= \frac{|\Psi_T(R,S)|^2}{\int dR \sum_S |\Psi_T(R,S)|^2} \,, \\
E_L(R,S) &= \frac{\sum_{S'} \Psi_T^*(R,S') H_{S',S} \Psi_T(R,S)}{|\Psi_T(R,S)|^2} \,.
\end{aligned}$$

Good trial functions

We could sample the spin-isospin states with low variance if we could calculate $\Psi_T(R,S)$ efficiently.

All known nontrivial trial functions require order 4^A operations to calculate either 1 or all the spin states. This is why the full spin sums are done for light nuclei GFMC calculations.

Example of a good but exponentially hard to evaluate trial function (Jastrow correlation operator)

$$\Psi_T(R,S) = \langle RS|\mathcal{S}\prod_{i<j}\left[\sum_{p=1}^{M} f_p(r_{ij})O^{(p)}(i,j)\right]|\Phi\rangle$$

Constructing a good trial function

Constructed in the same general way as electronic structure.

The model state $\langle RS|\Phi\rangle$ is one or a small linear combination of Slater determinants of single particle orbitals $\phi(\vec{r}, s)$. These are usually calculated from a shell-model or mean field calculation [analogous to using Hartree-Fock or local-density orbitals in electronic structure].

When a pair of particles is close together, their pair potential dominates. The pair correlations approximately solve a two-body Schrödinger equation.

$$\left[-\frac{\hbar^2\nabla_{ij}^2}{m} + \sum_{p=1}^{M} v_p(r_{ij})O^{(p)}(i,j)\right]\left[\sum_{p=1}^{M} f_p(r_{ij})O^{(p)}(i,j)\right]$$

$$\simeq \lambda\left[\sum_{p=1}^{M} f_p(r_{ij})O^{(p)}(i,j)\right]$$

- Expanded in angular momentum eigenstates
- A "healing" constraint where the correlation operator goes to the identity at some distance d. d is a variational parameter.
- The "eigenvalue" is calculated in each angular momentum channel to satisfy the constraint.
- As in electronic structure, additional forms and parameters can be added to include important additional physics. (For example, The $J = 0$ excited state of ^{12}C looks more like 3 ^{4}He particles than a single determinant of orbitals).

Why exponential scaling

- We have the positions and spin-isospin of each particle.
- To evaluate the wave function, we pick a pair, and operate with the pair correlation operator $\sum_{p=1}^{M} f_p(r_{ij}) O^{(p)}(i,j)$.
- The tensor operator can flip the spins into any of the 4 states $\uparrow\uparrow$, $\uparrow\downarrow$, $\downarrow\uparrow$, and $\downarrow\downarrow$.
- The τ operators can exchange the isospins, so if we have a pn pair it can become an np pair.
- The correlation for a pair can produce 4 or 8 states from the starting state.
- The next pair operator can produce 4 or 8 states from each of these.
- It takes just $A/2$ pair operators to produce all of the approximately 4^A states. There are $A(A-1)/2$ pair operators.

Full Spin-Isospin Sum Variational

Evaluating these wave functions for one spin-isospin state takes essentially the same amount of work as evaluating the wave function for all of the spin-isospin states.

The variance is lowered if the full spin-isospin sum is done:

$$\begin{aligned}
\langle H \rangle &= \int dR E_L(R) P(R) \,, \\
P(R) &= \frac{\sum_S |\Psi_T(R,S)|^2}{\int dR \sum_S |\Psi_T(R,S)|^2} \,, \\
E_L(R) &= \frac{\sum_{S,S'} \Psi_T^*(R,S') H_{S',S} \Psi_T(R,S)}{\sum_S |\Psi_T(R,S)|^2} \,,
\end{aligned}$$

Notice that the Hamiltonian only couples 4 or 8 spin states per pair potential term, so its evaluation is not expensive.

Three-body potential – v_8'

The three-body potential is more expensive, but still polynomial.

Many of the nonlocal terms are small. The GFMC calculations are done with a simplified potential Argonne v_8'. It contains just the first 8 operators of the v_{18} potential and is an isoscalar projection (so isospin is conserved).

Corrections to get the v_{18} results are done using first order perturbation theory.

Spin-Isospin Sum propagator

To implement a GFMC method, we sample

$$|\Psi(t)\rangle = e^{-(H-E_T)t}|\Psi(0)\rangle$$

- The simplest short time approximation $e^{-Ht} \simeq e^{-Tt}e^{-Vt}$ can be implemented by sampling the kinetic energy terms exactly as for potentials without spin-isospin dependence.

- Potential is usually factored into pair (or triplet) products:

$$e^{-\sum_{ij} v_{ij}t} \simeq \prod_{i<j} e^{-v_{ij}t}$$

- Each term can be written as a sparse matrix in spin-isospin space.

- In fact that first 6 terms of the v_8 potential form a group and the spin-orbit terms are small so

$$\exp(-[v_c + v_\sigma \vec{\sigma}_1 \cdot \vec{\sigma}_2 + v_t t_{12} + v_\tau \vec{\tau}_1 \cdot \vec{\tau}_2 + v_{\sigma\tau} \vec{\tau}_1 \cdot \vec{\tau}_2 \vec{\sigma}_1 \cdot \vec{\sigma}_2 + v_{t\tau} t_{12} \vec{\tau}_1 \cdot \vec{\tau}_2]\Delta t)$$
$$= p_c + p_\sigma \vec{\sigma}_1 \cdot \vec{\sigma}_2 + p_t t_{12} + p_\tau \vec{\tau}_1 \cdot \vec{\tau}_2 + p_{\sigma\tau} \vec{\tau}_1 \cdot \vec{\tau}_2 \vec{\sigma}_1 \cdot \vec{\sigma}_2 + p_{t\tau} t_{12} \vec{\tau}_1 \cdot \vec{\tau}_2$$

$$\begin{aligned}
e_1 &= e^{-(v_c+v_\sigma+2v_t+v_\tau+v_{\sigma\tau}+2v_{t\tau})\Delta t} \\
e_2 &= e^{-(v_c+v_\sigma-4v_t+v_\tau+v_{\sigma\tau}-4v_{t\tau})\Delta t} \\
e_3 &= e^{-(v_c+v_\sigma+2v_t-3v_\tau-3v_{\sigma\tau}-6v_{t\tau})\Delta t} \\
e_4 &= e^{-(v_c+v_\sigma-4v_t-3v_\tau-3v_{\sigma\tau}+12v_{t\tau})\Delta t} \\
e_5 &= e^{-(v_c-3v_\sigma+v_\tau-3v_{\sigma\tau})\Delta t} \\
e_6 &= e^{-(v_c-3v_\sigma-3v_\tau+9v_{\sigma\tau})\Delta t}
\end{aligned}$$

$$\begin{aligned}
p_c &= (6e_1 + 3e_2 + 2e_3 + e_4 + 3e_5 + e_6)/16 \\
p_\sigma &= (6e_1 + 3e_2 + 2e_3 + e_4 - 9e_5 - 3e_6)/48
\end{aligned}$$

$$
\begin{aligned}
p_t &= (3e_1 - 3e_2 + e_3 - e_4)/24 \\
p_\tau &= (2e_1 + e_2 - 2e_3 - e_4 + e_5 - e_6)/16 \\
p_{\sigma\tau} &= (2e_1 + e_2 - 2e_3 - e_4 - 3e_5 + 3e_6)/48 \\
p_{t\tau} &= (e_1 - e_2 - e_3 + e_4)/24\,.
\end{aligned}
$$

Pair product propagator

A pair product propagator can be used by solving the two-body propagator equation in the J, L, S channels The $L = J + 1$ and $L = J - 1$ are coupled. The true propagator cannot be written in terms of the product of the pair propagators since the spin-orbit terms do not then take the correct derivatives of the other terms in the propagator. (See more later.)

However, with appropriate counter terms a pair propagator can be used. The form of the relative coordinate propagator is the same as the potential for v_8' interaction – in each isospin channel:

$$\begin{aligned} G(\vec{r}\,'_{12}, \vec{r}_{12}) &= A(\vec{r}\,'_{12}, \vec{r}_{12}) + \vec{B}_1(\vec{r}\,'_{12}, \vec{r}_{12}) \cdot \vec{\sigma}_1 \vec{B}_2(\vec{r}\,'_{12}, \vec{r}_{12}) \cdot \vec{\sigma}_2 \\ &\quad + \sum_{\alpha\beta} C_{\alpha\beta}(\vec{r}\,'_{12}, \vec{r}_{12}) \sigma_{1\alpha} \sigma_{2\beta} \end{aligned}$$

Importance sampling and Path Constraint

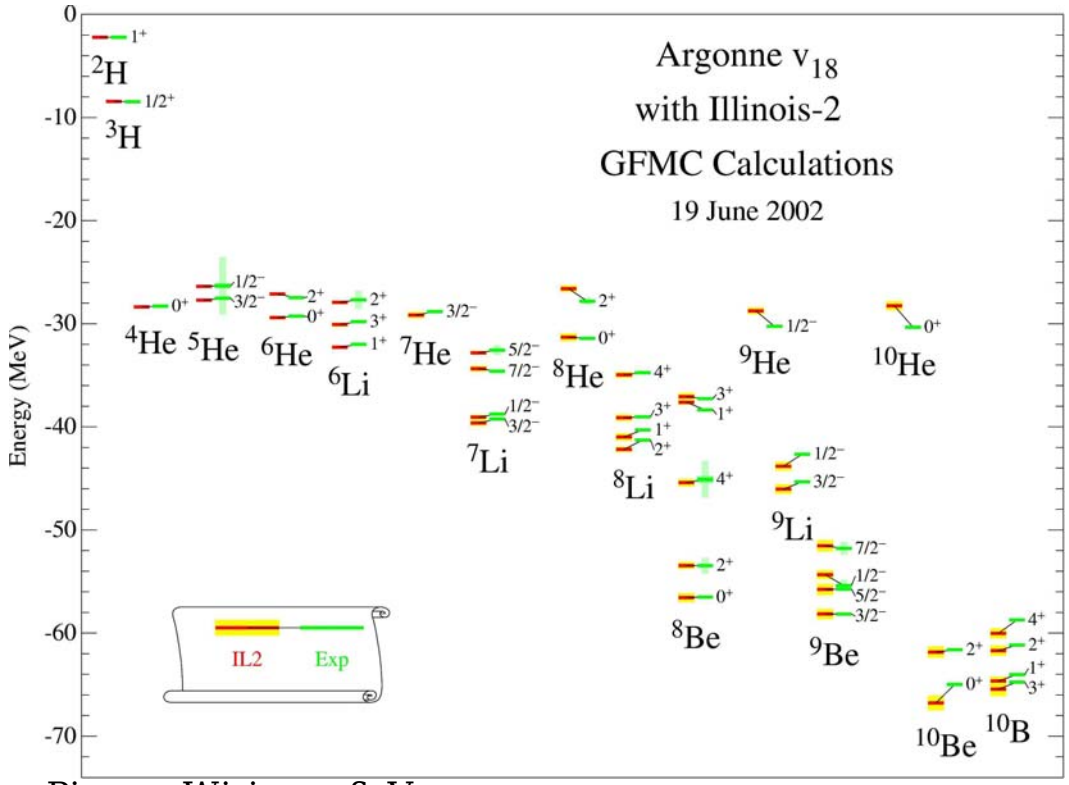
Importance sampling goes through exactly as for spin-independent interactions. The importance function is calculated by summing over all the spin states of the walker with a good trial function. It then is just a function of R.

Fermion sign problem is usually dealt with by restricting the real part of the importance function to be positive. (Not an upper bound).

A small number of forward walking steps are used to partially correct the energy.

Results for GFMC

Energies:[†]

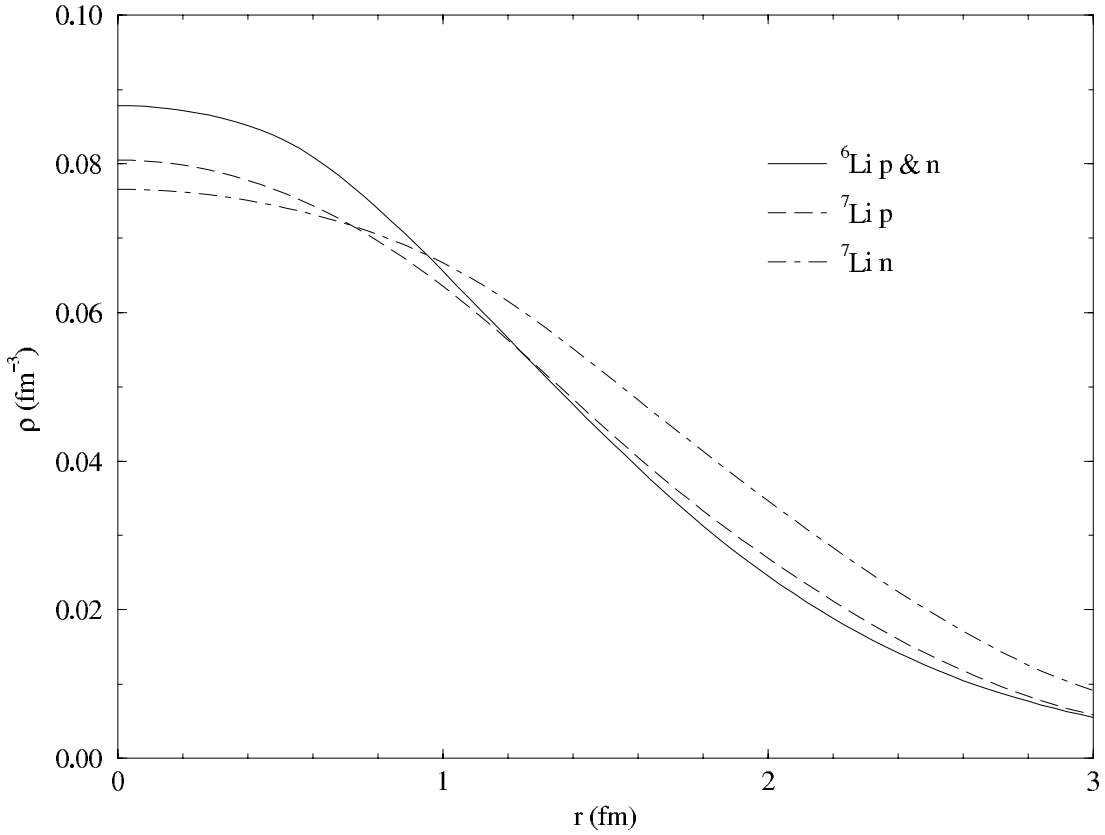


Pieper, Wiringa, & Varga

[†] S.C. Pieper, K. Varga, R.B. Wiringa, *Quantum Monte Carlo calculations of* $A = 9, 10$ *nuclei*, Phys. Rev. C **66**, 044310 (2002).

Other expectation values typically use extrapolations from mixed and variational estimates. For example proton and neutron densities:[†]

Fig. 16 (Pudliner, et al.)



[†] B. S. Pudliner, V. R. Pandharipande, J. Carlson, Steven C. Pieper, and R. B. Wiringa, *Quantum Monte Carlo calculations of nuclei with* $A \leq 7$, Phys.Rev. C **56** 1720-1750, (1997).

^{8}Be two alpha particle structure

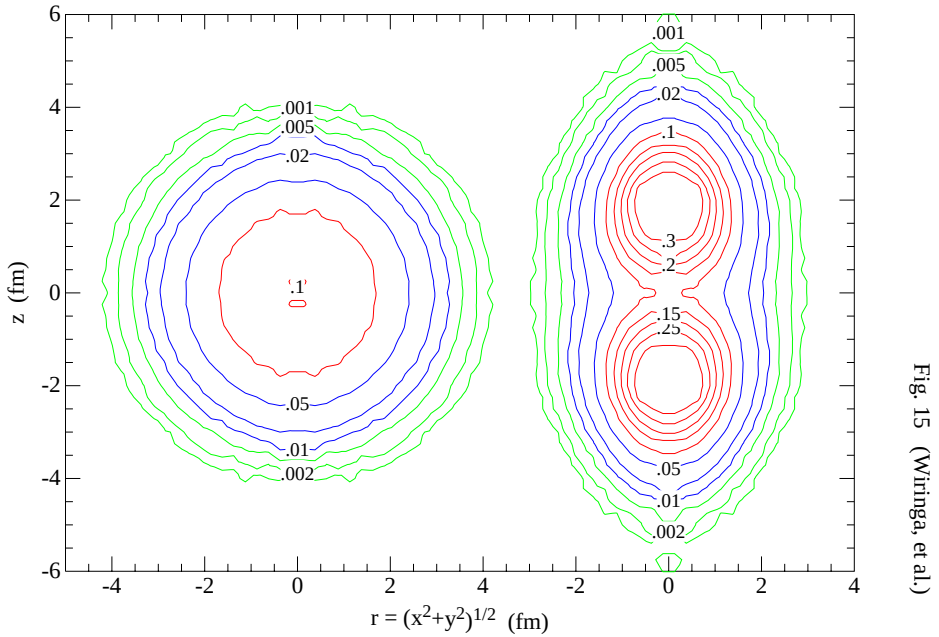


Fig. 15 (Wiringa, et al.)

The left side is in the laboratory frame.

The right side is in a frame defined by the principal axes of the moment of inertia tensor.

Spin-Isospin Sampling

- The exponential growth of the spin-isospin states with number of particles means that full spin-isospin sums are limited by Moore's law. About 1 new nucleon every 2 years. (^{4}He 20 years ago, ^{12}C now.)

- The exponential growth of spatial coordinates with number of particles just meant we needed to use Monte Carlo sampling.

- The solution for the spin-isospin problem is the same.

- Sampling the spin-isospin was hindered by the lack of trial wave functions that can be evaluated efficiently.

Auxiliary Field Diffusion Monte Carlo Philosophy

- We abandon (at least to start) the good trial function forms that we do not know how to evaluate efficiently.
- For a particular sample of the particle positions, the potential problem corresponds to sampling a spin Hamiltonian on a lattice (the current particle positions). We can use methods developed for sampling these problems.
- We use the method developed by Shiwei Zhang and coworkers for the spin-isospin part introducing complex auxiliary fields and a path constraint.

Trial wave function

Since the operator product form requires exponential operations to evaluate, we take a simple Slater-Jastrow trial function (or a Pfaffian-Jastrow wave function).

$$\begin{aligned}\Psi_T(R,S) &= \langle RS|\Psi_T\rangle \\ &= \prod_{i<j} f(r_{ij}) \det \begin{pmatrix} \phi_1(\vec{r}_1,s_1) & \phi_1(\vec{r}_2,s_2) & \dots & \phi_1(r_A,s_a) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_A(\vec{r}_1,s_1) & \phi_A(\vec{r}_2,s_2) & \dots & \phi_A(r_A,s_a) \end{pmatrix}.\end{aligned}$$

A walker consists of a position and a spinor $(a_{p\uparrow}, a_{p\downarrow}, a_{n\uparrow}, a_{n\downarrow})$ for each particle.

The ϕ_n are typically good $J = L + S$ orbitals for nuclei, and plane waves times spinors for matter in a periodic simulation cell.

Auxiliary Field Propagator

- We look at the short time propagator split into kinetic and potential parts.
- The particle positions are sampled from the importance sampled kinetic energy gaussian just as in diffusion Monte Carlo.
- Given a set of spinors for the particles, we want to sample a new set of spinors according to the potential energy.
- One way to keep this form is to sample the propagator so that it is a sum of terms like

$$\prod_{i=1}^{A} e^{A+B_\alpha \sigma_{i\alpha}+C_\beta \tau_{i\beta}+D_{\alpha\beta}\sigma_{i\alpha}\tau_{i\beta}}$$

  Each spinor is rotated and multiplied by a weight.

Sampling with an Auxiliary Field

We use the Hubbard-Stratonovich transformation

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

We must write the spin-isospin dependent interaction as a sum of squares of the spin-isospin operators. We sample the x variables and the linear O_n then rotate the spinors.

Auxiliary field sampling Details

We diagonalize the interaction in spinor space.

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

For A particles, the v_6 interaction can be written as

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

- Our A matrices are zero when $i = j$ and symmetric.
- All the A matrices are real and symmetric and have 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

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

We want the squares of operators so we write

$$
\begin{aligned}
V_{nc} &= \frac{1}{2}\sum_{n=1}^{3A}(O_n^{(\sigma)})^2\lambda_n^{(\sigma)} \\
&+ \frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{3A}(O_{n\alpha}^{(\sigma\tau)})^2\lambda_n^{(\sigma\tau)} \\
&+ \frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{A}(O_{n\alpha}^{(\tau)})^2\lambda_n^{(\tau)}
\end{aligned}
$$

with

$$
\begin{aligned}
O_n^{(\sigma)} &= \sum_i \vec{\sigma}_i \cdot \vec{\psi}_n^{(\tau)}(i) \\
O_{n\alpha}^{(\sigma\tau)} &= \sum_i \tau_{i\alpha}\vec{\sigma}_i \cdot \vec{\psi}_n^{(\sigma\tau)}(i) \\
O_{n\alpha}^{(\tau)} &= \sum_i \tau_{i\alpha}\psi_n^{(\tau)}(i)
\end{aligned}
$$

- 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 two $3A$ by $3A$ matrices and one A by A 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).

Spin-Orbit Interaction

- The spin-orbit contains the momentum in the $\vec{L} = \vec{r} \times \vec{p}$ part. This makes the propagator for spin-orbit nonlocal.

- We can operate the derivative in the $\vec{L}_{jk} \cdot \vec{S}_{jk}$ operator on the free propagator G_0 (the gaussian).

$$(\vec{\nabla}_j - \vec{\nabla}_k) G_0(R, R') = -\frac{m}{\hbar^2 \Delta t} (\Delta \vec{r}_j - \Delta \vec{r}_k) G_0(R, R') \ ,$$

- Our first attempt is spin-orbit part P_{LS}

$$P_{LS} \quad = \quad \exp\left(\sum_{j \neq k} \frac{m v_{LS}(r_{jk})}{4\imath\hbar^2} [\vec{r}_{jk} \times (\Delta \vec{r})_{jk}] \cdot \vec{\sigma}_j \right)$$

where $(\Delta \vec{r})_{jk} = \Delta \vec{r}_j - \Delta \vec{r}_k$.

Spin-Orbit Problem

- Unfortunately this is not quite right – it includes some spurious contributions linear in Δt.

- Look at the Green's function equation,

$$\begin{aligned}\Psi(R) &= \Delta t \left[\frac{1}{2m}\sum_j \nabla_j^2 - V + E_0\right]\Psi(R) \\ &+ \int dR' G_0(R,R') P_{LS}[\Psi(R) - \sum_p \Delta\vec{r}_p \cdot \vec{\nabla}_p \Psi(R)] + \ldots\end{aligned}$$

- The Δr terms in P_{LS} integrated with the Δr terms in the expansion of Ψ give the spin-orbit interaction correctly.

- Pairs of Δr terms in P_{LS} give additional spurious terms which have the form of additional two- and three-body potentials.

- We must subtract those terms off.

Three-body interaction for neutrons

The spin-independent part is trivial for Monte Carlo. You know where the particles are so it just gives an extra spin-independent potential.

The Fujita-Miyazawa part is

$$A\sum_{\rm cyc}\left(\{X_{ij},X_{jk}\}\{\vec{\tau}_i\cdot\vec{\tau}_j,\vec{\tau}_i\cdot\vec{\tau}_k\}+\frac{1}{4}[X_{ij},X_{jk}][\vec{\tau}_i\cdot\vec{\tau}_j,\vec{\tau}_i\cdot\vec{\tau}_k]\right)$$

where

$$X_{ij}=T(r_{ij})t_{ij}+Y(r_{ij})\vec{\sigma}_i\cdot\vec{\sigma}_j$$

For neutrons $\vec{\tau}_i\cdot\vec{\tau}_j=1$, so only the anticommutator terms contribute, and the spin operator that appears twice drops out. The three-body potential looks like a two-body spin potential whose strength is modified by the position of the third particle.

Results for neutron systems

- Neutron Matter Equation of State[†].
- Neutron Matter Spin Susceptibility[‡].
- Model Neutron Drops (Unambiguous comparison to GFMC)[§].
- Even odd energy gaps using Pfaffian trial functions for $^1S_0$ BCS pairing in low density neutron matter[¶].

[†] S. Gandolfi, et al., Quantum Monte Carlo calculation of the equation of state of neutron matter , in preparation. M. Bouadani, et al., Pion condensation in high density neutron matter, in preparation. A. Sarsa, S. Fantoni, K. E. Schmidt and F. Pederiva, *Neutron matter at zero temperature with auxiliary field diffusion Monte Carlo method*, Phys. Rev. C **68**, 024308 (2003).

[‡] S. Fantoni, A. Sarsa, K.E. Schmidt, *Spin Susceptibility of Neutron Matter at Zero Temperature*, Phys. Rev. Lett. **87**, 181101 (2001).

[§] S. Gandolfi, K.E. Schmidt, F. Pederiva, and S. Fantoni, Three nucleon interaction role in neutron drops, in preparation. F. Pederiva, A. Sarsa, K. E. Schmidt and S. Fantoni, Auxiliary field diffusion Monte Carlo calculation of ground state properties of neutron drops, Nucl. Phys. A **742**, 255 (2004).

[¶] A. Fabrocini, S. Fantoni, A. Yu Illarionov, and K.E. Schmidt, $^1S_0$ *superfluid phase transition in neutron matter with realistic nuclear potentials and modern many-body theories*, Phys. Rev. Lett. **95**, 192501 (2005).

Results for neutron and proton systems

- Symmetric nuclear matter.[†]
- Selected nuclei.[‡]

[†] S. Gandolfi, F. Pederiva, S. Fantoni, and K. E. Schmidt Quantum Monte Carlo Calculations of Symmetric Nuclear Matter Phys. Rev. Lett. **98**, 102503 (2007).

[‡] S. Gandolfi, F. Pederiva, S. Fantoni, and K. E. Schmidt, Auxiliary Field Diffusion Monte Carlo Calculation of Nuclei with A40 with Tensor Interactions, Phys. Rev. Lett. **99**, 022507 (2007).

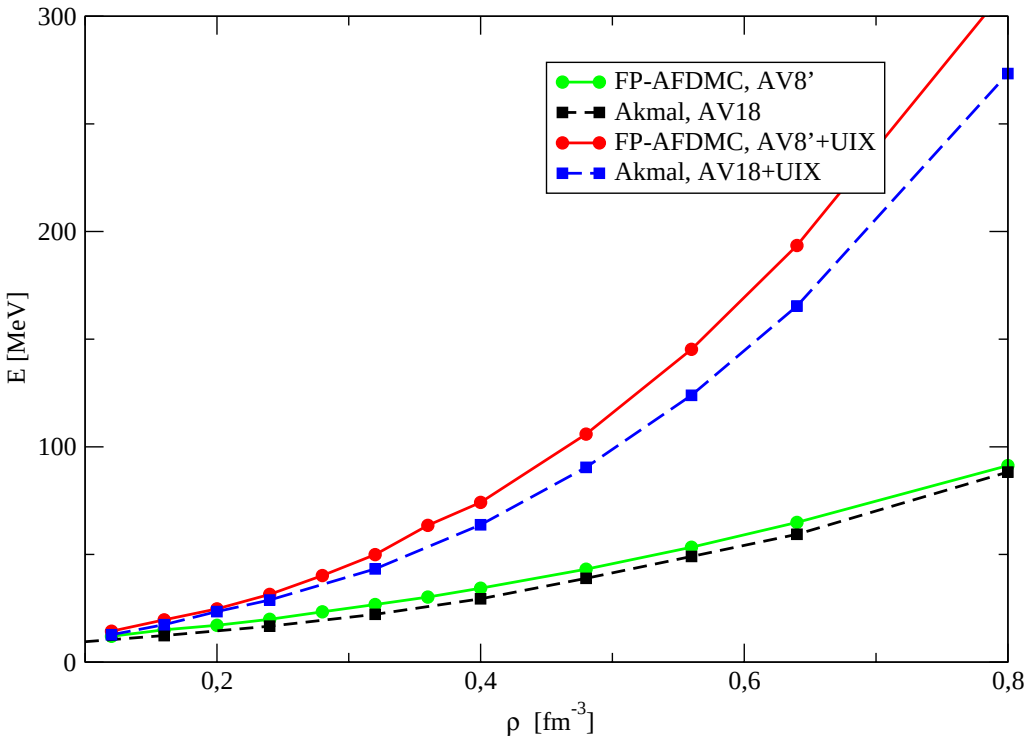
GFMC Model neutron drop comparison

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).

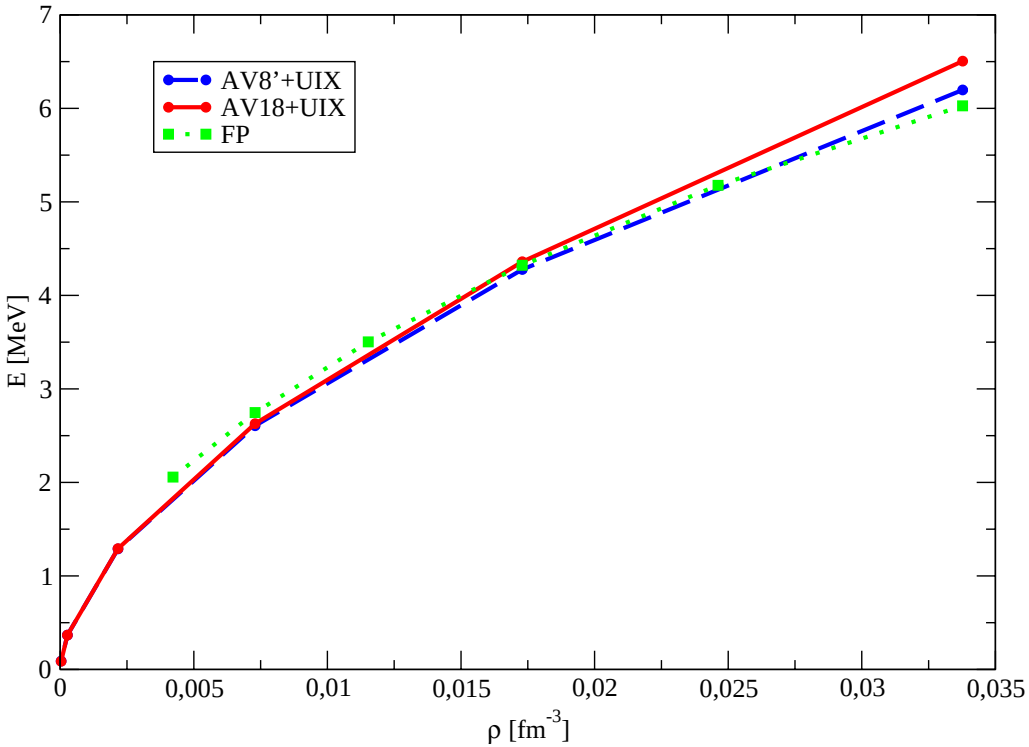
Neutron matter equation of state



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).

Spin Susceptibility of neutron matter

The spin susceptibility and corresponding response functions can be related to the neutrino cross sections in neutron matter. These cross sections have important implications for the dynamics of supernovae.

The long wave length static response can be calculated from the energy. Adding a magnetic field, the spin response is described by

$$\begin{aligned} H &= H_0 - \sum_i \vec{\sigma}_i \cdot \vec{b} \\ \vec{b} &= \mu \vec{B} \\ \mu &= 6.03 \times 10^{-18}\ \mathrm{MeV/Gauss} \end{aligned}$$

The spin susceptibility is

$$\chi = -n\mu^2 \left. \frac{\partial^2 E_0(b)}{\partial b^2} \right|_{b=0}$$

where $E_0(b)$ is the ground state energy in the field b.

The spin polarization with the field along $\hat{z}$ is $p = \langle \sigma_z \rangle$. Using AFDMC we can calculate $E_0(J_z, b)$ within the constrained path approximation. Using the chain rule, we can write

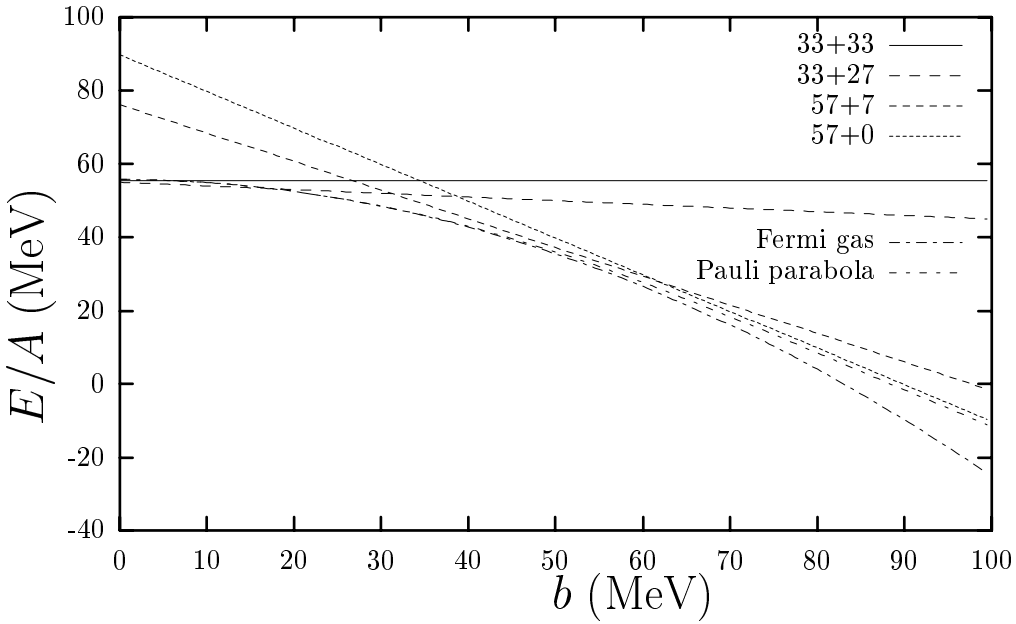
$$\frac{\chi}{\chi_{\text{Pauli}}} = \frac{\hbar^2 k_f^2 \left(\frac{\partial p}{\partial b}\right)^2}{3m \frac{\partial E}{\partial J_z^2}}$$

and

$$p(J_z) = -\left.\frac{\partial E_0(b, J_z)}{\partial b}\right|_{b=0}$$

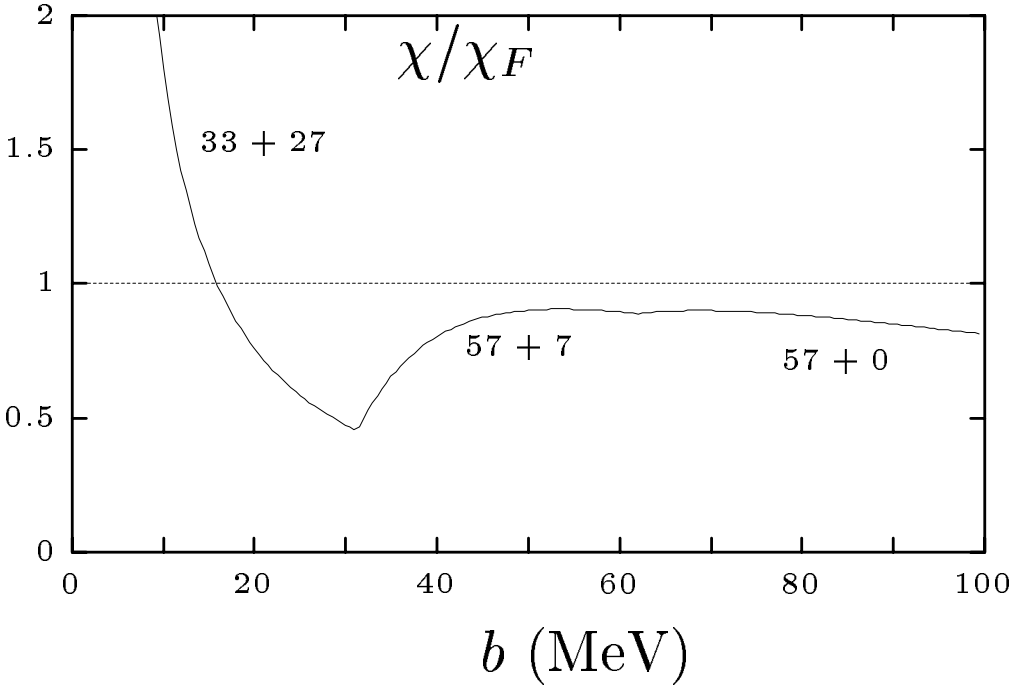
Noninteracting Energy with magnetic field

The energy of noninteracting neutrons as a function of magnetic field at $\rho = 0.32\ \mathrm{fm}^{-3}$ for various finite sized close shell trial functions with spin up and down values shown. Also plotted is the correct infinite system energy and the parabolic Pauli estimate.



NonInteracting Susceptibility

The susceptibility χ of non–interacting fermions obtained by assuming that the energies are quadratic in b, and normalized to the exact Fermi free gas value χ_F.



Calculation of Susceptibility

Assuming:

$E_0(J_z)$ is quadratic in J_z even at $57\uparrow + 7\downarrow$,

$p(J_z)$ is linear in J_z even at $57\uparrow + 7\downarrow$,

Energy is linear in b even at 50 MeV.

Compressibility

ρ/ρ_0	Reid[†]	Reid6[‡]	AU18[§]	AU6-CBF[¶]	AU6'
0.75	0.91	2.06	1.10	0.85	0.89(3)
1.25	0.70	1.35	0.71	0.45	0.47(3)
2.0	0.49	0.77	0.26	0.23	0.21(3)
2.5	0.42	0.60	0.15	0.17	0.14(3)

Compressibility ratio $\mathcal{K}/\mathcal{K}_F$ of neutron matter. The AFDMC results for the AU6' interaction are compared with other calculations. The statistical error is given in parentheses.

[†] Brueckner calculations by S. O. Bäckmann and C. G. Källman, Phys. Lett. B **43** (1973) 263.

[‡] CBF calculations by A. D. Jackson, E. Krotscheck, D. E. Meltzer and R. A. Smith, Nucl. Phys. A **386** (1992) 125.

[§] FHNC calculations of A. Akmal,V. R. Pandharipande and D. G. Ravenhall, Phys. Rev. C **58** (1998) 1804.

[¶] CBF calculations of A. Fabricini, private communication.

Spin Susceptibility

ρ/ρ_0	Reid[†]	Reid6[‡]	AU6'	AU8'	Reid6
0.75	0.45	0.53	0.40(1)		
1.25	0.42	0.50	0.37(1)	0.39(1)	0.36(1)
2.0	0.39	0.47	0.33(1)	0.35(1)	
2.5	0.38	0.44	0.30(1)		

Spin susceptibility ratio χ/χ_F of neutron matter. The AFDMC results for the interactions AU6', AU8' and Reid6 are compared with those obtained from the Landau parameters calculated from FHNC and CBF theories. The statistical error is given in parentheses.

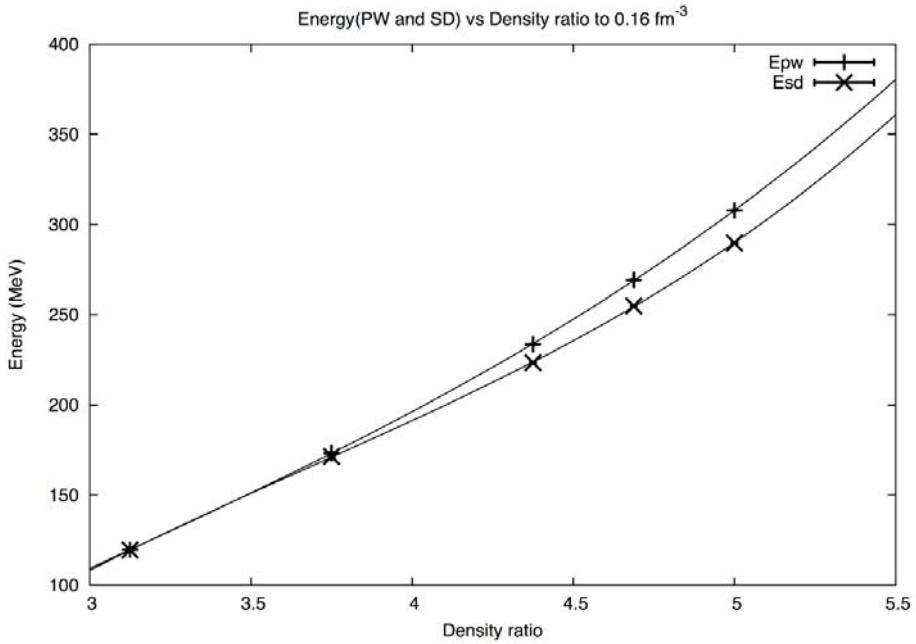
[†] Brueckner calculations by S. O. Bäckmann and C. G. Källman, Phys. Lett. B **43** (1973) 263.

[‡] CBF calculations by A. D. Jackson, E. Krotscheck, D. E. Meltzer and R. A. Smith, Nucl. Phys. A **386** (1992) 125.

Pion Condensate in neutron matter

- It has been conjectured that a "pion condensate" occurs in neutron stars
- This refers to a spin-density wave in neutron matter at high densities.
- The $\vec{\sigma} \cdot \vec{\nabla}\pi$ coupling to the pion field indicates that such a wave would be accompanied by a pion field with a nonzero ground-state expectation – sort of a condensate.
- Salt, NaCl, has a separation of charge which gives a ground-state expectation of the electric field – maybe we should call this a photon condensate.

Pion Condensate Results



PW = Plane wave model state

SD = Spin density wave model state

He Isotopes

^{4}He

AFDMC v_6' -27.13(10) MeV
Hyperspherical v_6' -26.93(1) MeV[†]
GFMC v_6' -26.93(1) MeV [-26.23(1) -0.7 MeV Coulomb][‡]
Expt -28.296 MeV

^{8}He

AFDMC v_6' -23.6(5) MeV (Unstable to breakup into ^{4}He+2n)
GFMC v_6' -23.55(8) MeV [-22.85(8) -0.7 MeV Coulomb]
Expt -31.408 MeV

[†] G. Orlandini, private communication

[‡] R.B. Wiringa and S.C. Pieper, *Evolution of Nuclear Spectra with Nuclear Forces*, Phys. Rev. Lett. **89**, 182501 (2002).

Oxygen

^{16}O

AFDMC v_6' -100.7(4) MeV (Unstable to breakup to 4 ^{4}He)
Expt -127.619 MeV

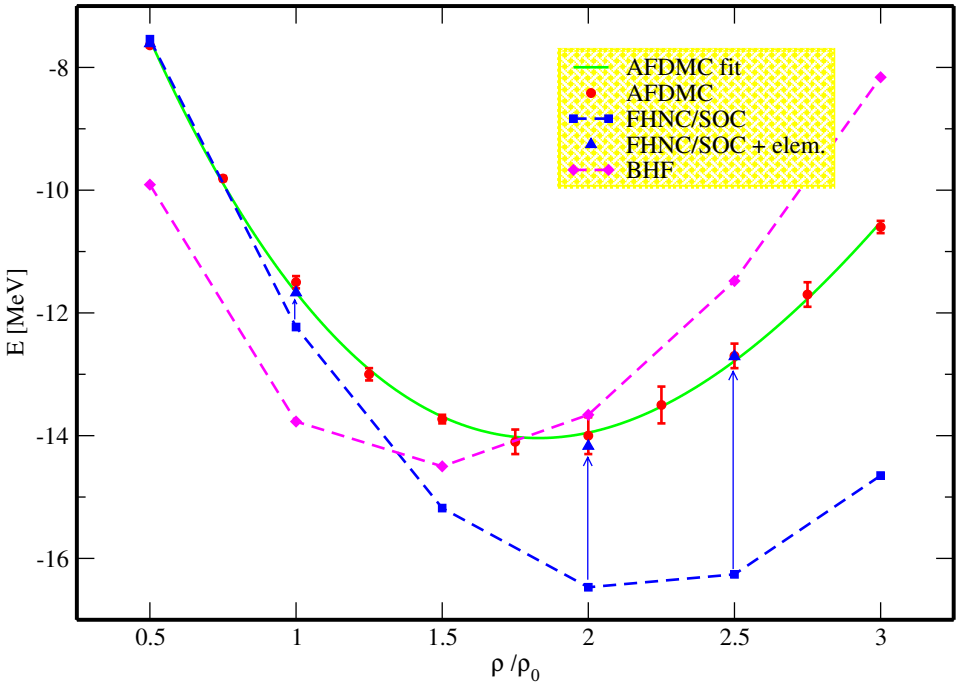
AFDMC Urbana v_{14} truncated to 6 operators -90.8(1) MeV
Cluster Monte Carlo give for the 6 operator part of v_{14} (optimized for 14 operators), -83.2 MeV[†]

[†] S. C. Pieper, R. B. Wiringa, and V. R. Pandharipande, *Variational Calculation of the Ground-State of* ^{16}O, Phys. Rev. C **46**, 1741-1756 (1992).

Calcium

^{40}C AFDMC v_6' -272(2) MeV (Equal to 10 ^{4}He)
Expt -342.051 MeV

Nuclear matter Energy, 28 particles



Dashed lines correspond to calculations performed with other methods† (blue line with squares: FHNC/SOC; magenta with diamonds: BHF). Blue triangles are FHNC/SOC results corrected with elementary diagrams.

† I. Bombaci, A. Fabrocini, A. Polls, I. Vidaña, *Spin-orbit tensor interactions in homogeneous matter of nucleons: accurancy of modern many-body theories*, Phys. Lett. B, **609**, 232 (2005).

The AFDMC equation of state is fit to

$$\frac{E}{A} = \frac{E_0}{A} + \alpha(x-\bar{x})^2 + \beta(x-\bar{x})^3,$$

$x = \rho/\rho_0$ $\rho_0 = 0.16$ fm$^-3$.

$E_0/A =$ -14.04(4) MeV
$\alpha =$ 3.09(6) MeV
$\beta =$ -0.44(8) MeV
$\bar{x} =$ 1.83(1)
The compressibility
$K = 9\bar{x}^2 \left(\partial^2 \left(E/A\right)/\partial x^2\right)_{\bar{x}}$ at saturation density $\bar{x}$ is $\sim$ 190 MeV.

Results with 76 and 108 particles are within 3 percent of those for 28 particles.

Conclusions and Future

- The auxiliary field Diffusion Monte Carlo calculations can give accurate results for nuclei, neutron and nuclear matter.
- They have polynomial scaling with system size
- The three-body and spin-orbit potentials need to be included for the neutron-proton case.
- Asymmetric matter can be calculated.
- Physics of neutron rich nuclei can be studied – these are difficult to produce in laboratories, but important for R-process reactions.
- Temperature > 0 is possible.