Nuclear Talent course: Computational Many-body Methods for Nuclear Physics

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ECT*, June 25-July 13
Lecture slides with exercise for Tuesday July 2 2012

Nuclear Hamiltonian

The nuclear Hamiltonian is not well characterized.

- 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

$$v(r_{ij})\left[3\sigma_i \cdot \hat{\mathbf{r}}\sigma_j \cdot \hat{\mathbf{r}} - \sigma_i \cdot \sigma_j\right]$$

- 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.

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,
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  - 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 (and experiment) give a pseudoscalar coupling to the pion field. The dirac operator is $i\gamma^5$. We want the nonrelativistic limit. In the standard representation we have the Dirac equation with

$$\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad i\beta\gamma^5 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \quad (1)$$

One-pion exchange continued

The coupling to a classical pseudoscalar field $\phi_c(\mathbf{r})$ gives the Dirac Hamiltonian

$$H_D = \alpha \cdot \mathbf{p} + \beta m + ig\beta\gamma^5\phi_c(\mathbf{r})$$

g a coupling constant.
In terms of upper and lower components $H|\psi\rangle = E|\psi\rangle$ with $E = \varepsilon + m$,

$$\sigma \cdot \mathbf{p}|\psi_-\rangle + m|\psi_+\rangle + ig\phi_c(\mathbf{r})|\psi_-\rangle = (\varepsilon + m)|\psi_+\rangle$$
$$\sigma \cdot \mathbf{p}|\psi_+\rangle - m|\psi_-\rangle - ig\phi_c(\mathbf{r})|\psi_+\rangle = (\varepsilon + m)|\psi_-\rangle$$

Nonrelativistic $\rightarrow |\varepsilon| \ll m$. Ignore ε compared to $2m$.

$$\frac{\sigma \cdot \mathbf{p} - ig\phi_c(\mathbf{r})}{2m}|\psi_+\rangle = |\psi_-\rangle + \ldots$$

Substitute into $|\psi_+\rangle$ equation:

$$\frac{(\sigma \cdot \mathbf{p} + ig\phi_c)(\sigma \cdot \mathbf{p} - ig\phi_c)}{2m} = \varepsilon|\psi_+\rangle \qquad (2)$$

One pion exchange continued

Use Pauli identity

$$\sigma \cdot A \sigma \cdot B = \mathbf{A} \cdot \mathbf{B} + i \sigma \cdot (\mathbf{A} \times \mathbf{B})$$

$$\begin{aligned} H_{nr} &= \frac{p^2}{2m} - i \frac{g}{2m} [\sigma \cdot p, \phi_c(\mathbf{r})] + O(g^2) \\ &= \frac{p^2}{2m} - \frac{g}{2m} \sigma \cdot \nabla \phi_c(\mathbf{r}) \end{aligned}$$

The effective pion coupling to a nucleon labeled i in the nonrelativistic limit is

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

where the pion field is

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

$$\pi = \pi_1 + i\pi_2$$

One-pion exchange continued

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

$$\begin{aligned}\Delta H &= \sum_{m\neq n}\frac{\langle n'|V|m\rangle\langle m|V|n\rangle}{E_n-E_m}\\ &= -g_\pi^2\tau_1\cdot\tau_2\sum_k\frac{\langle \mathbf{r}_1 s_1'\mathbf{r}_2 s_2'|\sigma_1\cdot\nabla_1 e^{i\mathbf{k}\cdot\mathbf{r}_1}\sigma_2\cdot\nabla_2 e^{-i\mathbf{k}\cdot\mathbf{r}_2}|\mathbf{r}_1 s_1\mathbf{r}_2 s_2\rangle}{\omega_k^2}\end{aligned}$$

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

$$\begin{aligned}V_{1-\pi} &= -g_\pi^2\tau_1\cdot\tau_2\sum_k\sigma_1\cdot\nabla\sigma_2\cdot\nabla\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{k^2+m_\pi^2} = -\frac{g_\pi^2}{4\pi}\tau_1\cdot\tau_2\sigma_1\cdot\nabla\sigma_2\cdot\nabla\frac{e^{-m_\pi r}}{r}\\ &= -\frac{g_\pi^2}{4\pi}\tau_1\cdot\tau_2\left[t_{12}\left(\frac{m_\pi}{r^2}+\frac{1}{r^3}+\frac{m_\pi^2}{3r}\right)+\sigma_1\cdot\sigma_2\left(\frac{m_\pi^2}{3r}-4\pi\delta^3(\mathbf{r})\right)\right]\frac{e^{-m_\pi r}}{r}\\ t_{12} &= 3\sigma_1\cdot\hat{\mathbf{r}}\sigma_2\cdot\hat{\mathbf{r}}-\sigma_1\cdot\sigma_2\end{aligned}$$

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).[1] (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.

[1] 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[1], 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:

$$V = \sum_{p=1}^{N_{\rm op}} v_p(r_{ij}) O_{ij}^p \tag{3}$$

- The first 14 operators are $(1,\ \sigma_i \cdot \sigma_j,\ t_{ij},\ \mathbf{L}_{ij} \cdot \mathbf{S}_{ij},\ L^2,\ L^2(\sigma_i \cdot \sigma_j),\ (\mathbf{L}_{ij} \cdot \mathbf{S}_{ij})^2$ and these multiplied by $\tau_i \cdot \tau_j$. The last 4 operators break isospin invariance. Defining $T_{ij} \equiv 3\tau_{iz}\tau_{jz} - \tau_i \cdot \tau_j$, they are $T_{ij},\ T_{ij}\sigma_i \cdot \sigma_j,\ T_{ij}t_{ij}, \tau_{iz} + \tau_{jz}$. $\mathbf{L} \cdot \mathbf{S}$ is the spin orbit operator $\mathbf{L}_{ij} = \frac{1}{2}\mathbf{r}_{ij} \times (\nabla_i - \nabla_j)$, $\mathbf{S}_{ij} = \frac{1}{2}(\sigma_i + \sigma_j)$.

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

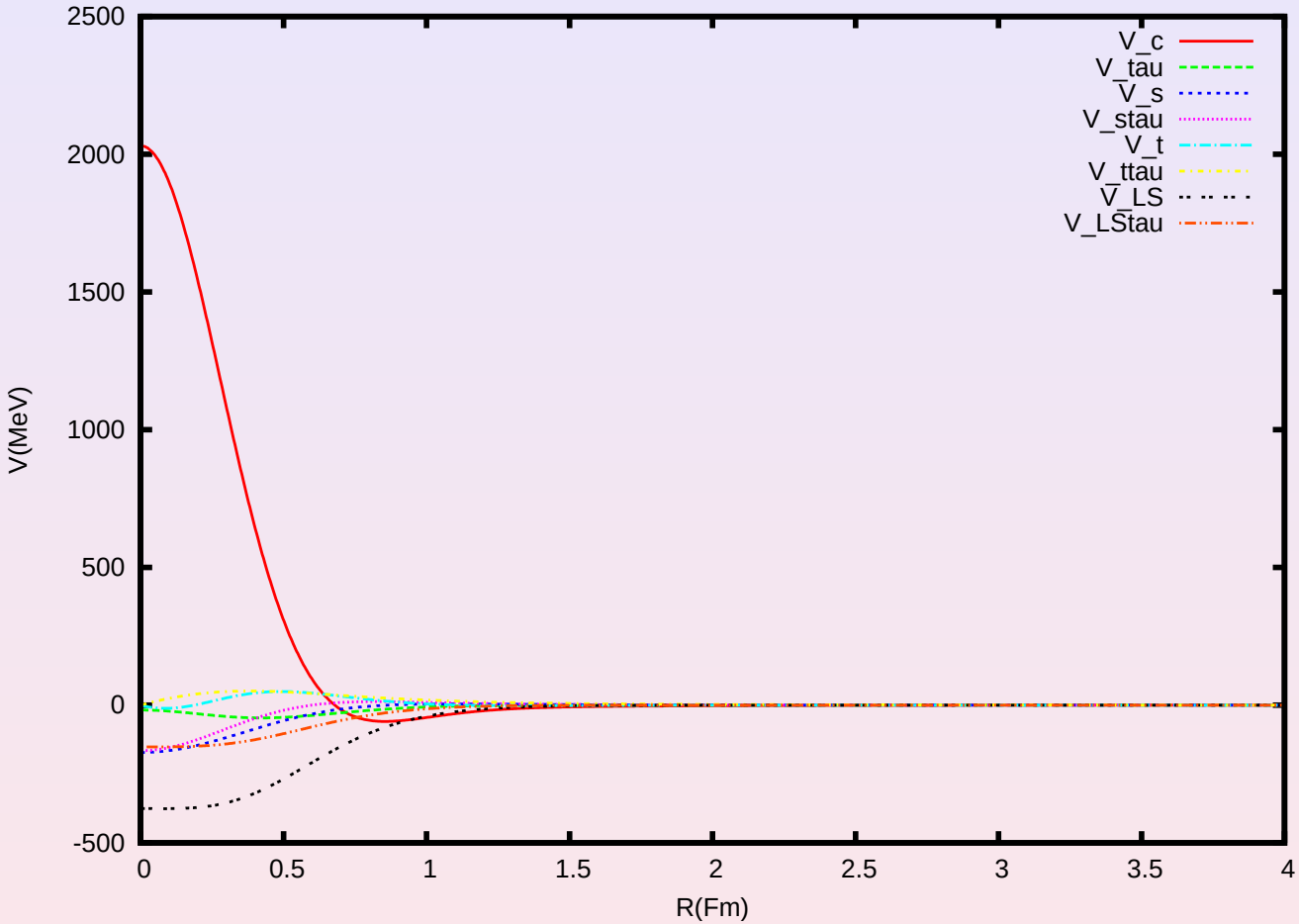
Argonne v_{18} terms

Physics:

- 1 (central) potential
- $(\sigma_i \cdot \sigma_j)$ 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.
- $\mathbf{L}\cdot\mathbf{S}$, couples spin and orbital angular momentum – interaction conserves total $\mathbf{J} = \mathbf{L} + \mathbf{S}$. This term is momentum dependent.
- $(\tau_i \cdot \tau_j)$ acts like $(\sigma_i \cdot \sigma_j)$ 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 that nuclear Monte Carlo uses contains:

- Nonrelativistic kinetic energy

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

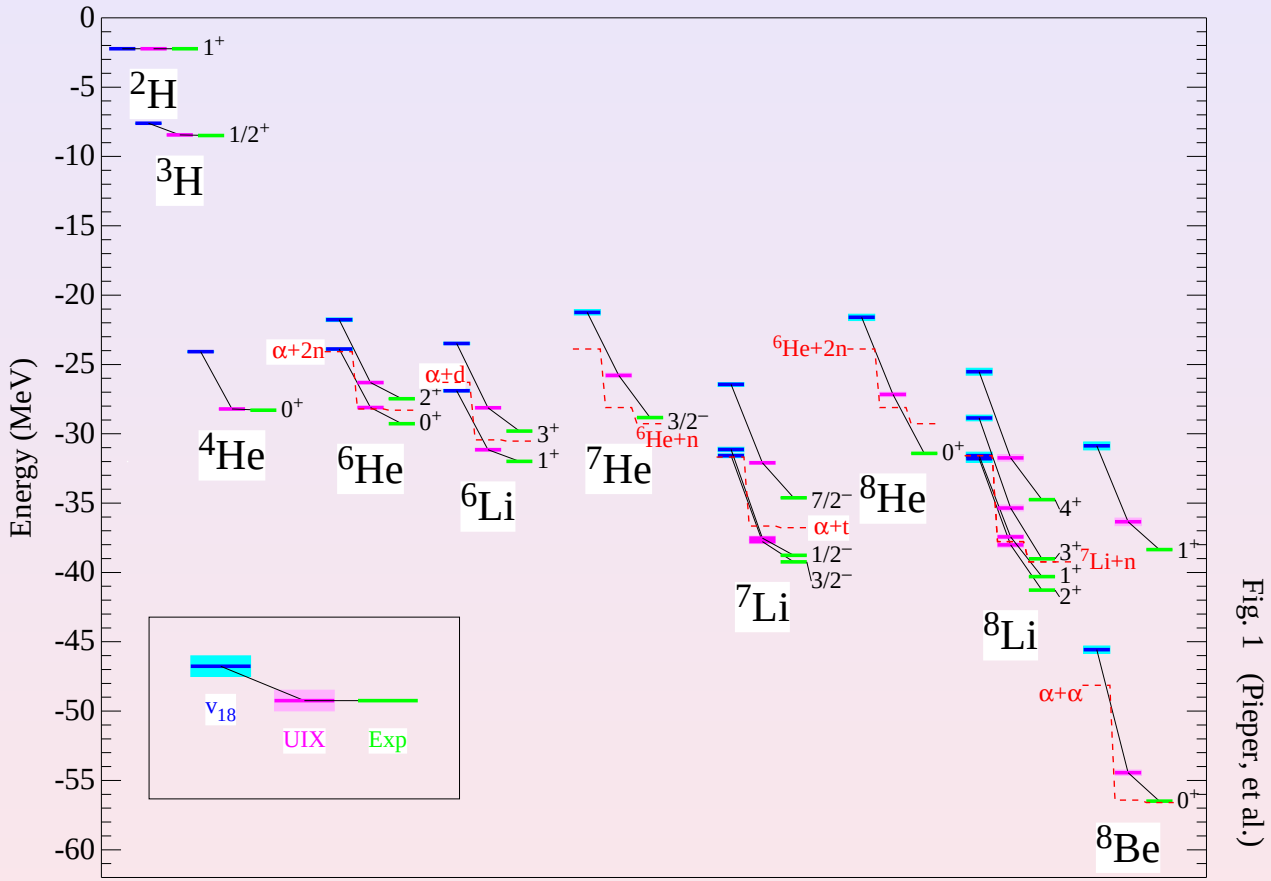
  or if the mass difference is ignored (1 part out of 500),

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

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

GFMC light nuclei comparison

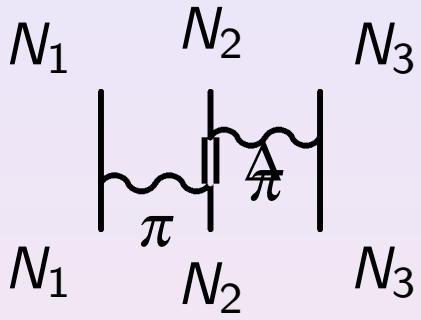
GFMC calculations give[1]



[1] 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
  $\tau \longrightarrow \mathbf{T}$ 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.

Fujita-Miyazawa continued

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

$$A\sum_{\text{cyc}}\left(\{X_{ij},X_{jk}\}\{\tau_i\cdot\tau_j,\tau_i\cdot\tau_k\}+\frac{1}{4}[X_{ij},X_{jk}][\tau_i\cdot\tau_j,\tau_i\cdot\tau_k]\right)$$

where

$$X_{ij}=T(r_{ij})t_{ij}+Y(r_{ij})\sigma_i\cdot\sigma_j$$

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 $R = \{\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_A\}$ 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

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

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

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

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

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

Isospin symmetry continued

- 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/T 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$\uparrow$, p$\downarrow$, n$\uparrow$, n$\downarrow$ basis.
  $R \equiv 3A$ x, y, z coordinates for the nucleons
  $S \equiv A$ discrete values selecting one of p$\uparrow$, p$\downarrow$, n$\uparrow$, n$\downarrow$
  $\Psi_T(R, S) =$ 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)

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

Constructing a good trial function

- The model state $\langle RS|\Phi\rangle$ is one or a small linear combination of Slater determinants of single particle orbitals $\phi(\mathbf{r}, s)$. These are usually calculated from a shell-model or mean field calculation.
- When a pair of particles is close together, their pair potential dominates. The pair correlations approximately solve a two-body Schrödinger equation.

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

Good trial functions continued

- 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.
- Additional forms and parameters can be added to include important additional physics.

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.

Additional Implementation notes

- The symmetrized product requires $N!$ operations. Its effect is small. Instead of summing, the order of the Jastrow operators is sampled.
- Calculating the derivatives is costly when spin-isospin sums are done. The Los Alamos/Argonne/Illinois collaboration uses numerical derivatives rather than direct calculation as we showed for the central potential.
  E.G.

$$\partial_{j\alpha}\Psi_T(R,S) = \frac{\Psi_T(R+h\hat{\mathbf{x}}_{j\alpha},S) - \Psi_T(R-h\hat{\mathbf{x}}_{j\alpha},S)}{2h}$$

- Energy calculation is about $6A$ times more expensive than wave function evaluation. Energies are calculated when the walkers are uncorrelated.

VMC/GFMC results 1

J. Carlson, "Green's function Monte Carlo study of light nuclei," Phys. Rev. C **36**, 2026 (1987).

TABLE III. Triton with $AV6$ interaction.

Method	Time Step (MeV^{-1})	Energy (MeV)	$\langle V_{ij} \rangle$ (MeV)	$\langle r_i^2 \rangle^{1/2}$ (fm)
Variational		-6.33 ± 0.05	-43.7 ± 1.0	1.95 ± 0.03
Faddeev (5 channels)		-6.46		
Faddeev (34 channels)		-7.15		
GFMC	4.0×10^{-4}	-7.23 ± 0.08	-49 ± 1	1.88 ± 0.04
GFMC	2.0×10^{-4}	-7.20 ± 0.08	-50 ± 1	1.83 ± 0.03
GFMC	1.0×10^{-4}	-7.23 ± 0.08	-49 ± 1	1.85 ± 0.03
Extrapolation		-7.22 ± 0.12	-52 ± 3	1.75 ± 0.10

VMC/GFMC results 2

TABLE IV. Alpha particle with $AV6$ interaction.

Method	Time Step (MeV^{-1})	Energy (MeV)	$\langle V_{ij} \rangle$ (MeV)	$\langle r_i^2 \rangle^{1/2}$ (fm)
Variational		-22.75 ± 0.10	-122 ± 1	1.50 ± 0.01
GFMC	1.0×10^{-4}	-24.89 ± 0.12	-126 ± 1	1.49 ± 0.02
GFMC	5.0×10^{-5}	-24.84 ± 0.09	-124 ± 2	1.50 ± 0.02
Extrapolation		-24.79 ± 0.20	-122 ± 30	1.50 ± 0.04

VMC/GFMC results 3

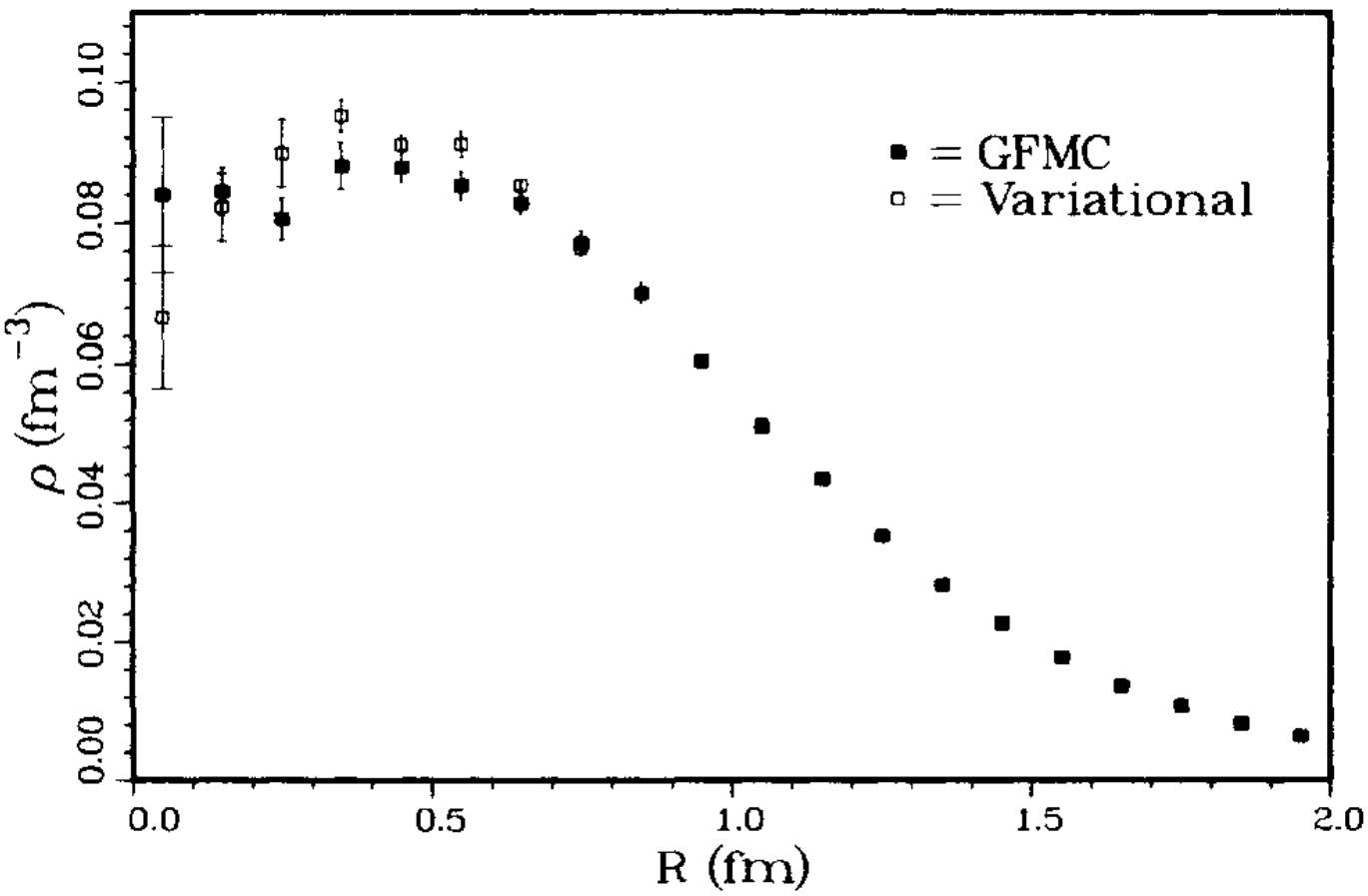


FIG. 2. Point nucleon distribution for the alpha particle with the $AV6$ interaction. The curve labeled "GFMC" is the mixed estimate for the smallest time step used (see text).

GFMC 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.

Importance sampling and Path Constraint

- Importance sampling goes through exactly as for spin-independent interactions. The problem for GFMC is that calculating derivatives and local energy is expensive.
- Instead GFMC calculations usually use the unsimplified form:

$$|\Psi_I \Psi(t+\Delta t)\rangle = \sum_{i=1}^{N_w} w_i \int dX P(X) \frac{\langle \Psi_I | T(X) | R_i \rangle}{\langle \Psi_I | R_i \rangle} \frac{T(X)}{W(X,R_i)} |R_i\rangle$$

  and sample from the undrifted gaussian for all coordinates. An equally good sample would have been with all samples with opposite sign.
- Evaluate

$$P_\pm = \frac{\langle \Psi_I | T(X_\pm) | R_i \rangle}{\langle \Psi_I | R_i \rangle}$$

  for each choice. Pick $X_\pm$ with probability

$$\frac{P_\pm}{P_+ + P_-}$$

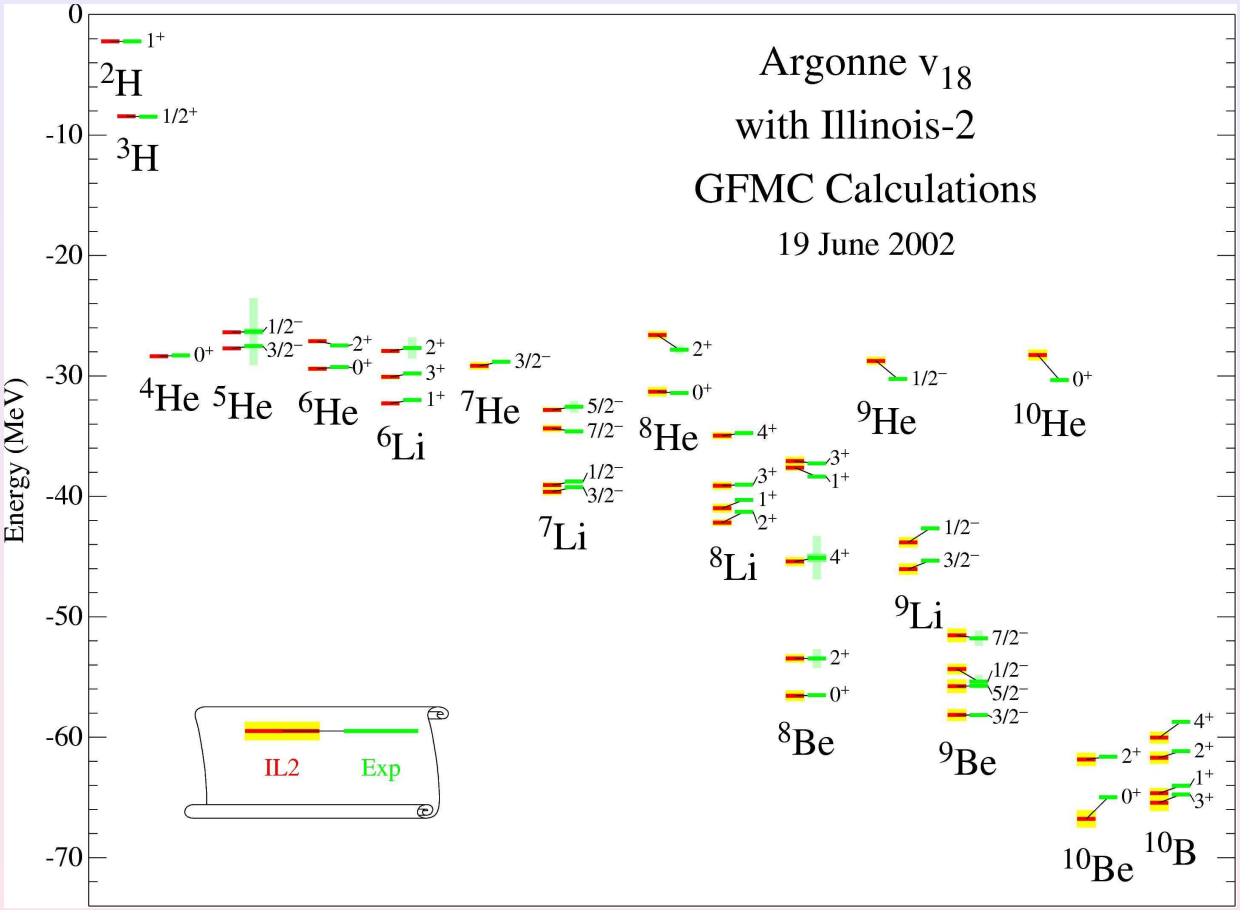
  and include a weight of $P_+ + P_-$.

Importance sampling path constraint

- 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 using a fixed phase/fixed node approximation. (Not an upper bound).
- A small number of forward walking steps are used to partially correct the energy.

Results for GFMC

Energies:[1]



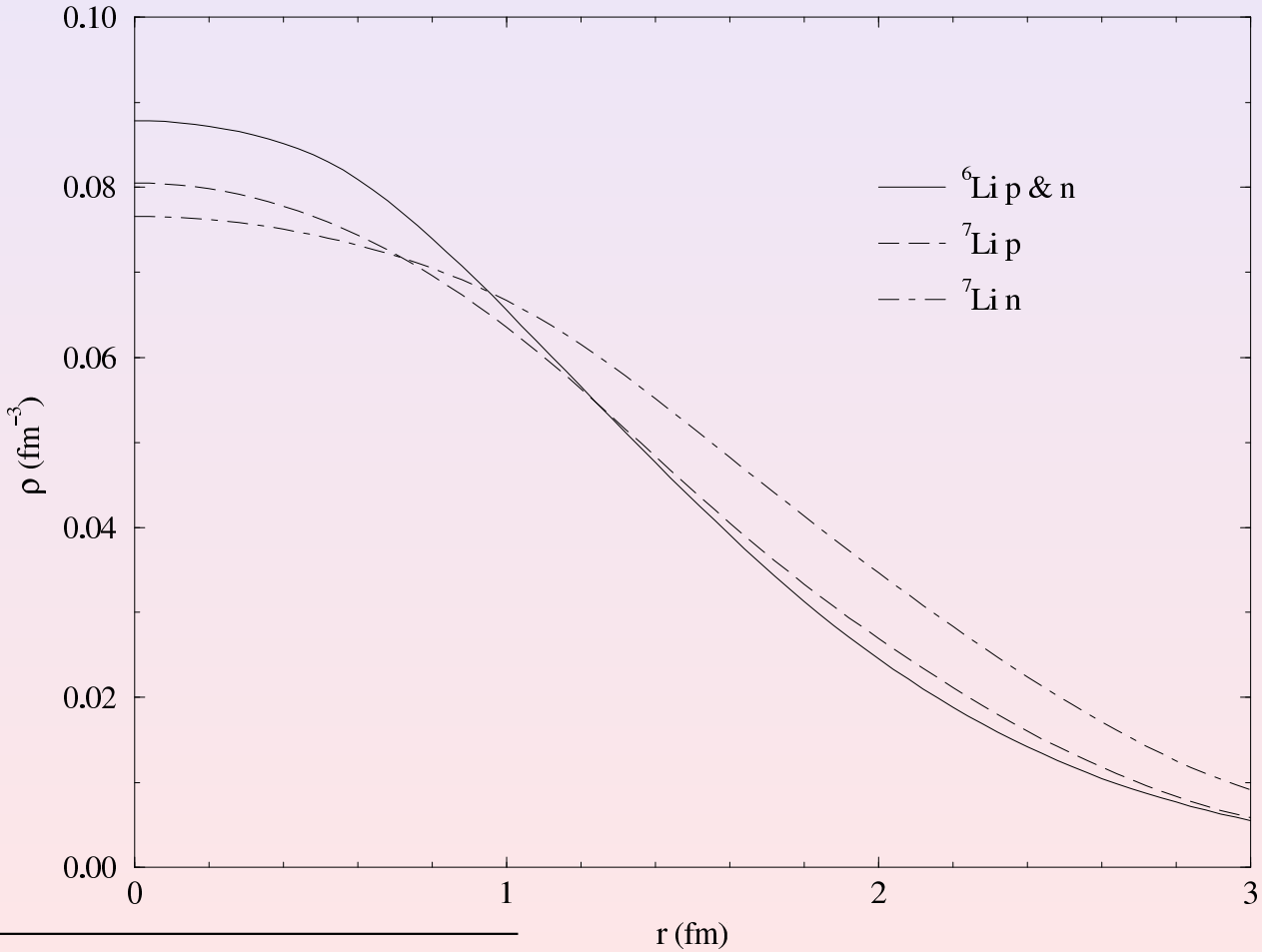
Pieper, Wiringa, & Varga

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

Other expectations

Other expectation values typically use extrapolations from mixed and variational estimates. For example proton and neutron densities:[1]

Fig. 16 (Pudliner, et al.)



[1] B. S. Pudliner, V. R. Pandharipande, J. Carlson, Steven C. Pieper, and R. B. Wiringa, *Quantum Monte Carlo calculations of nuclei with $A < 7$*, Phys.Rev.

^{8}Be two alpha particle structure

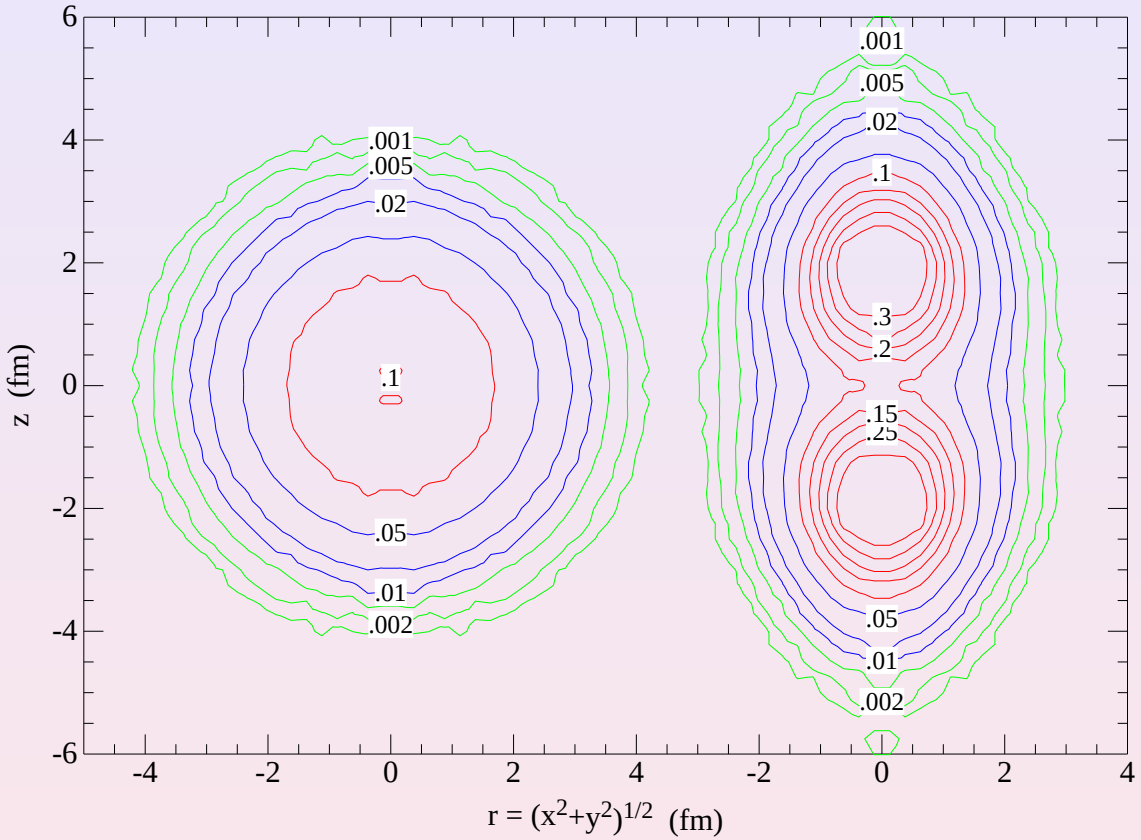


Fig. 15 (Wiringa, et al.)

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.) If Moore's law holds $\rightarrow$ all nuclei in about 600 years.
- 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).

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

- 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 as described earlier

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

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

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

Breakup continued

- 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

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

Breakup continued

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

$$
\begin{aligned}
V_{nc} &= \frac{1}{2}\sum_{i,j,n} \sigma_i \cdot \psi_n^{(\sigma)}(i)\lambda_n^{(\sigma)}\psi_n^{(\sigma)}(j)\cdot\sigma_j \\
&+ \frac{1}{2}\sum_{i,j,n} \sigma_i \cdot \psi_n^{(\sigma\tau)}(i)\lambda_n^{(\sigma\tau)}\psi_n^{(\sigma\tau)}(j)\cdot\sigma_j\tau_i\cdot\tau_j \\
&+ \frac{1}{2}\sum_{i,j,n} \tau_i \cdot \tau_j \psi_n^{(\tau)}(i)\lambda_n^{(\tau)}\psi_n^{(\tau)}(j)
\end{aligned}
$$

Breakup continued

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

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

Breakup continued

- The Hubbard-Stratonovich transformation is

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

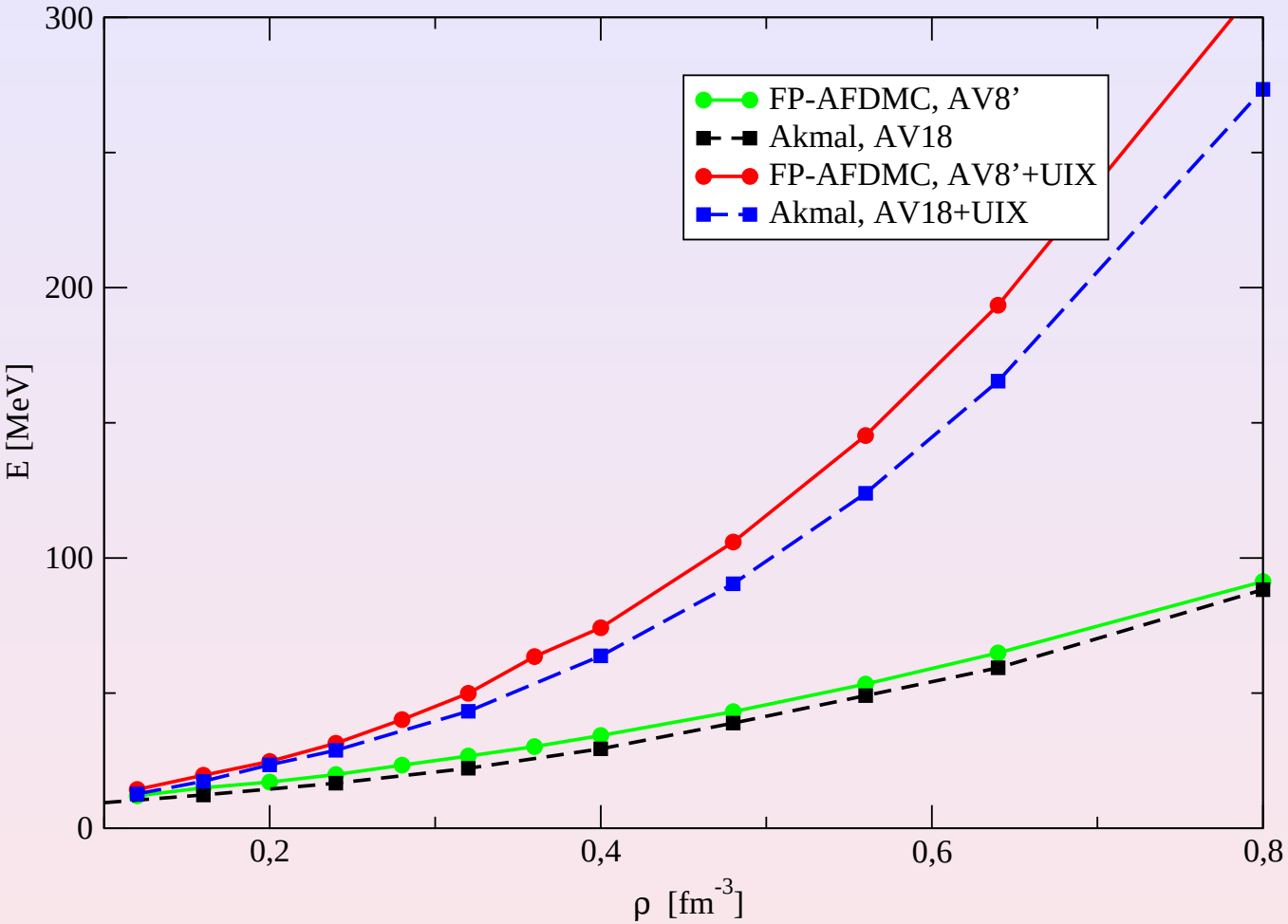
- Our O_n don't commute, so we need to keep the time steps small so that the commutator terms can be ignored. Each of the O_n is a sum of 1-body operators as required above.
- We require 3A Hubbard-Stratonovich variables for the σ terms, $9A$ variables for the $\sigma\tau$ terms, and $3A$ variables for 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[1].
- 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 yet.

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

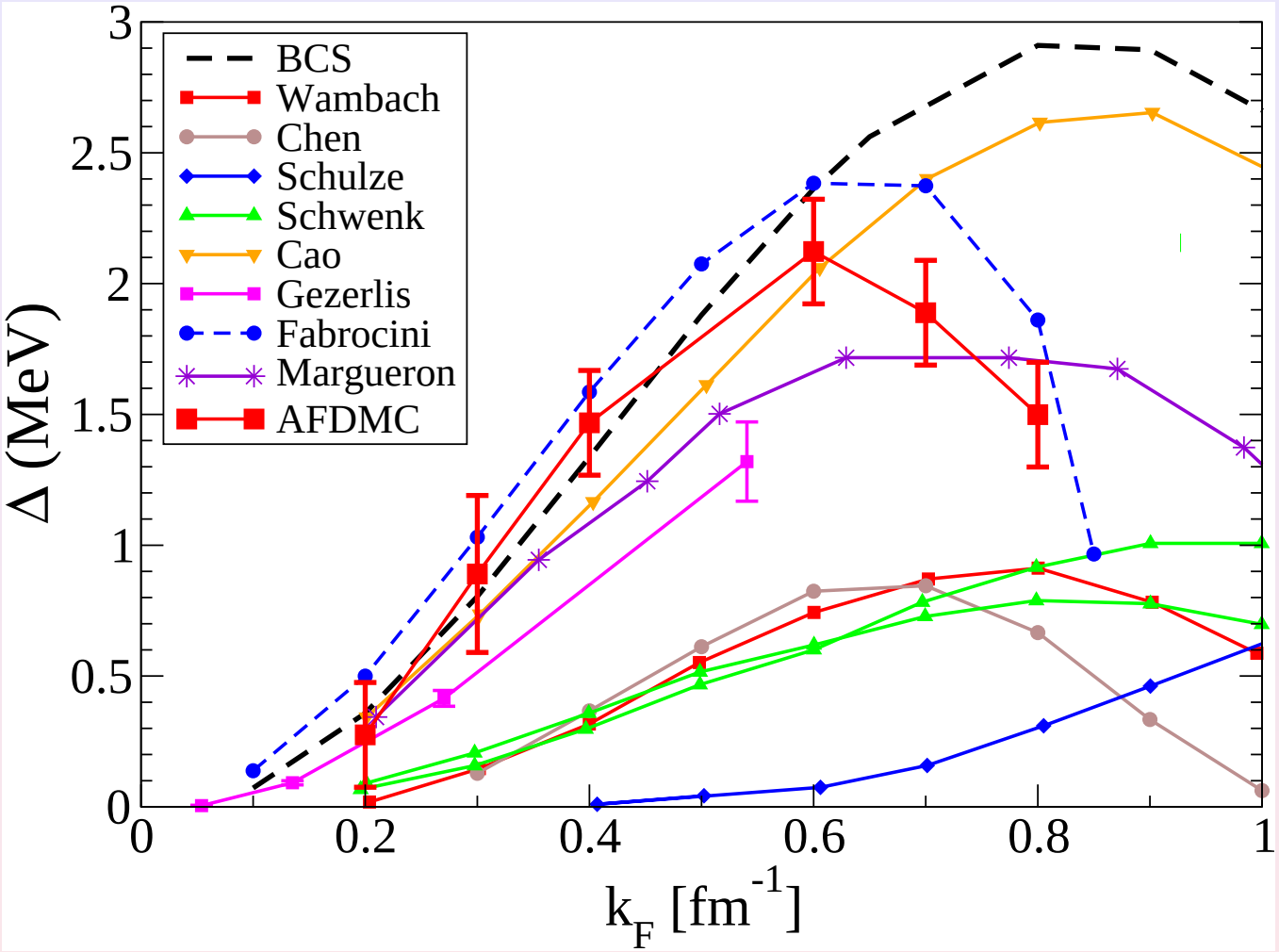
Neutron matter equation of state



Akmal refers to the FHNC calculation[1]

[1] 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).

Neutron matter energy gaps



Calculated energies gap (AFDMC) compared to other calculations.