Quantum Monte Carlo calculations of nuclei and nuclear matter

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Outline of Talk

- Introduction
- The nuclear Hamiltonian.
- Formulating diffusion Monte Carlo with auxiliary fields
- Dealing with the Fermion Problem
- Results
- Future

Introduction

We want to be able to predict the structure of nuclei and nuclear and neutron matter.

I will talk only about ground states.

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

Monte Carlo calculations must choose a basis and sample the nonlocal parts of the propagator.

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 either Urbana or Illinois three-body potentials or density dependence.

For nuclei and nuclear matter, we have used the Argonne v_6' potential. Three-body effects with density dependence. Spin-orbit is still a problem, but we recent progress indicates it can now be included.

The operator terms in Argonne v_8' are

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

Diffusion Monte Carlo Projection

Project to lowest state not orthogonal to the starting function
$|\psi(0)\rangle = \sum_n a_n |\Psi_n\rangle$

$$
\begin{aligned}
|\psi(t)\rangle &= e^{-(H-E_T)t}|\psi(0)\rangle \\
&= e^{-(E_0-E_T)t}\left[a_0|\Psi_0\rangle + \sum_{n>0} e^{-(E_n-E_0)t}|\Psi_n\rangle\right]
\end{aligned}
$$

Choose E_T to keep normalization approximately constant.

Choosing the sampled basis

We need a complete or overcomplete basis – Walkers. We choose $|RS\rangle$, where R represents the positions of the particles, and S are the spin states.

GFMC – S is a linear combination of all spin isospin states $\sim \frac{A!}{Z!(A-Z)!}2^A$ complex coefficients.

AFDMC – S is an outer product of spinors $p\uparrow$, $p\downarrow$, $n\uparrow$, $n\downarrow$, $\sim 4A$ complex coefficients

We write the initial state as a linear combination of sampled walkers.

We must be able to write the propagator as

$$e^{-(H-E_T)\Delta t} = \int dX \quad \underbrace{P(X)}_{\text{Probability density}} \quad \underbrace{T(X)}_{\text{basis change operator}}$$

$$T(X)|RS\rangle = \underbrace{W(X,R,S)}_{\text{weight}} \quad \underbrace{|R'S'\rangle}_{\text{new walker}}$$

The set of X play the role of auxiliary fields.

Auxiliary fields with the Hubbard-Stratonovich Transformation

For the GFMC basis, the $T(X)$ can be a product of the space translation operator $e^{-\frac{i}{\hbar}P\cdot A}$ and any spin operators multiplied by spatial functions.

The v_8' Hamiltonian is a quadratic form in these operators.

For AFDMC, $T(X)$ can be a product of the space translation operator $e^{-\frac{i}{\hbar}P\cdot A}$ and products of single particle spin operators multiplied by spatial functions.

The v_6' Hamiltonian is a quadratic form in these operators. (For neutrons the v_8' Hamiltonian + three-body interaction too)

Hubbard-Stratonovich transformation linearizes quadratic forms.

$$e^{\frac{O^2}{2}} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-\frac{x^2}{2}} e^{xO}$$

For example

$$e^{-\frac{p^2}{2m}\Delta t} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-\frac{x^2}{2}} e^{-\frac{i}{\hbar}px\sqrt{\frac{\hbar^2\Delta t}{m}}}$$

is diffusion Monte Carlo.

Spin Sampling with an Auxiliary Field

We diagonalize the interaction in spinor space to get operator squares.

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.

Importance sampling and path Constraint

In order to minimize the variance of the computed expectation values, include importance sampling.

Walker positions and spins are sampled from a new state

$$|\Psi_I \Psi(t)\rangle = \sum_{i=1}^{N_w} w_i |R_i S_i\rangle$$

where

$$\langle RS|\Psi_I \Psi(t)\rangle = \langle \Psi_I|RS\rangle \langle RS|\Psi(t)\rangle$$

Propagation becomes

$$
\begin{aligned}
|\Psi_I \Psi(t+\Delta t)\rangle &= \sum_{i=1}^{N_w} w_i \int dX P(X) \frac{\langle \Psi_I | R_i' S_i' \rangle}{\langle \Psi_I | R_i S_i \rangle} T(X) | R_i S_i \rangle \\
&= \sum_{i=1}^{N_w} w_i \int dX \underbrace{P(X) \frac{\langle \Psi_I | T(X) | R_i S_i \rangle}{\langle \Psi_I | R_i S_i \rangle}}_{\text{Drifted Gaussian} - \text{Local energy weight}} \cdot \\
&\quad \cdot \underbrace{\frac{T(X)}{W(X, R_i, S_i)} | R_i S_i \rangle}_{\text{Normalized walker}} \qquad (1)
\end{aligned}
$$

Local energy

$$
E_L(R,S) = \frac{\langle \Psi_I | H | RS \rangle}{\langle \Psi_I | Rs \rangle}
$$

Weight becomes $e^{-(E_L(R,S)-E_T)\Delta t}$ - Low variance

- 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).

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, A. Yu. Illarionov, K.E. Schmidt, F. Pederiva, and S. Fantoni, "Quantum Monte Carlo calculation of the equation of state of neuton matter" Phys. Rev. C **79**, 054005 (2009).

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

[§] 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); and S. Gandolfi, F. Pederiva, A. Illarionov, S. Fantoni, and K.E. Schmidt, in press (2008).

Results for neutron and proton systems

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

[†] 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 A $\leq$ 40 with Tensor Interactions, Phys. Rev. Lett. **99**, 022507 (2007).

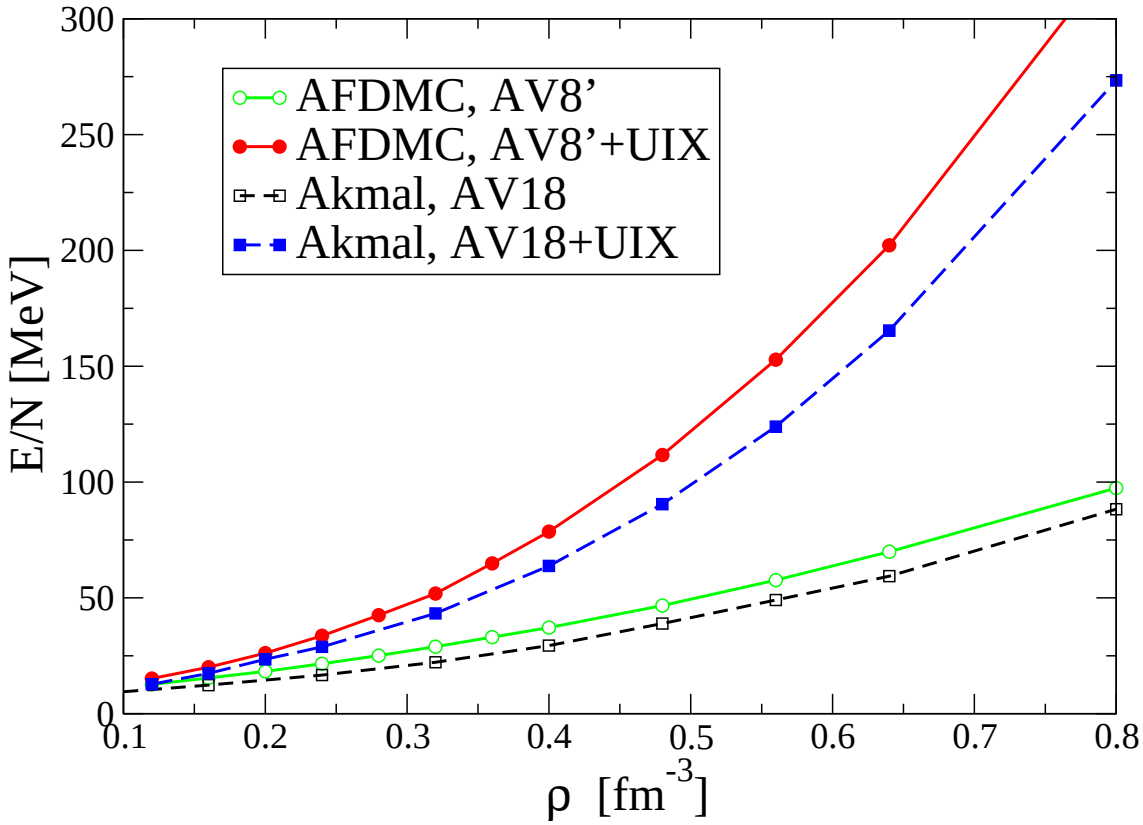
GFMC Model neutron drop comparison

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).

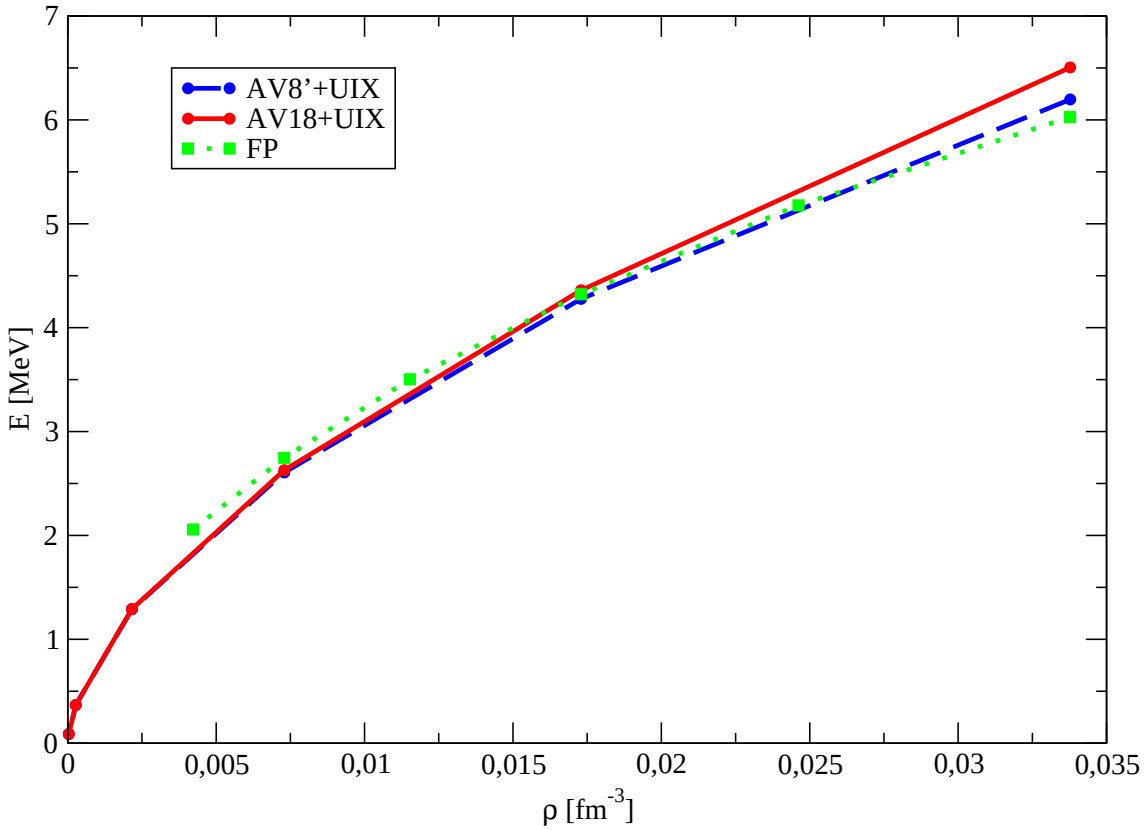
Neutron matter equation of state



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).

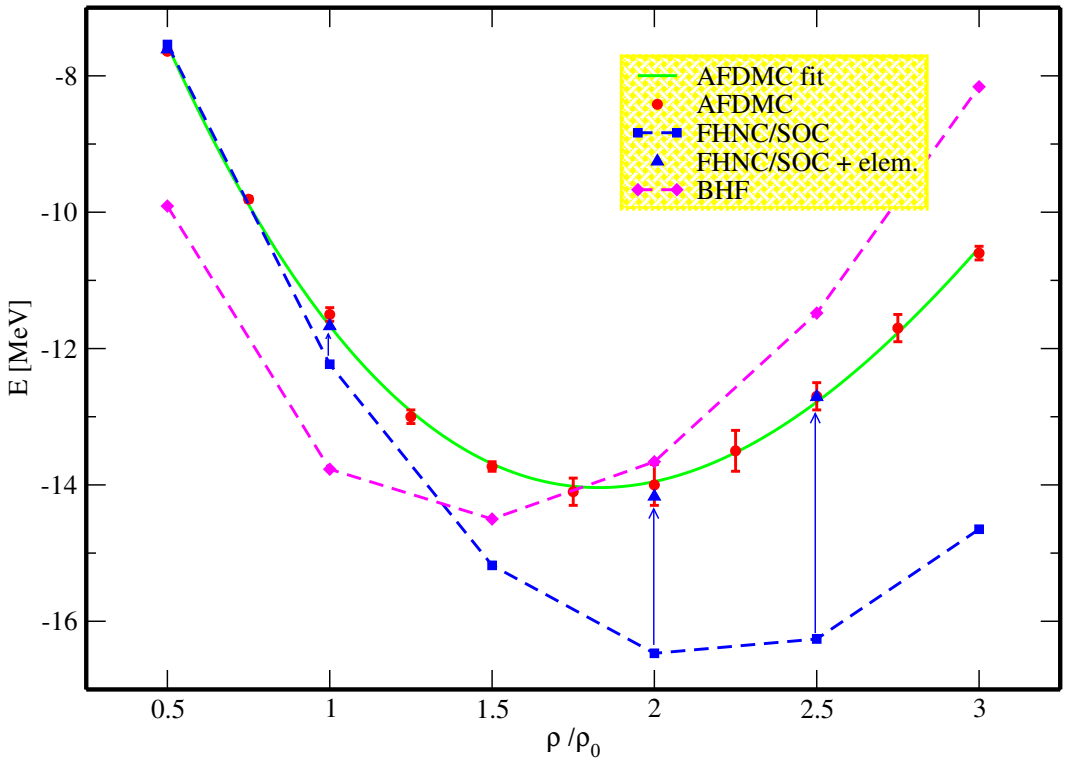
Low density neutron matter with Argonne v_{18}



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).

Nuclear matter Energy, 28 particles, v_8' truncated to v_6



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
α = 3.09(6) MeV
β = -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.

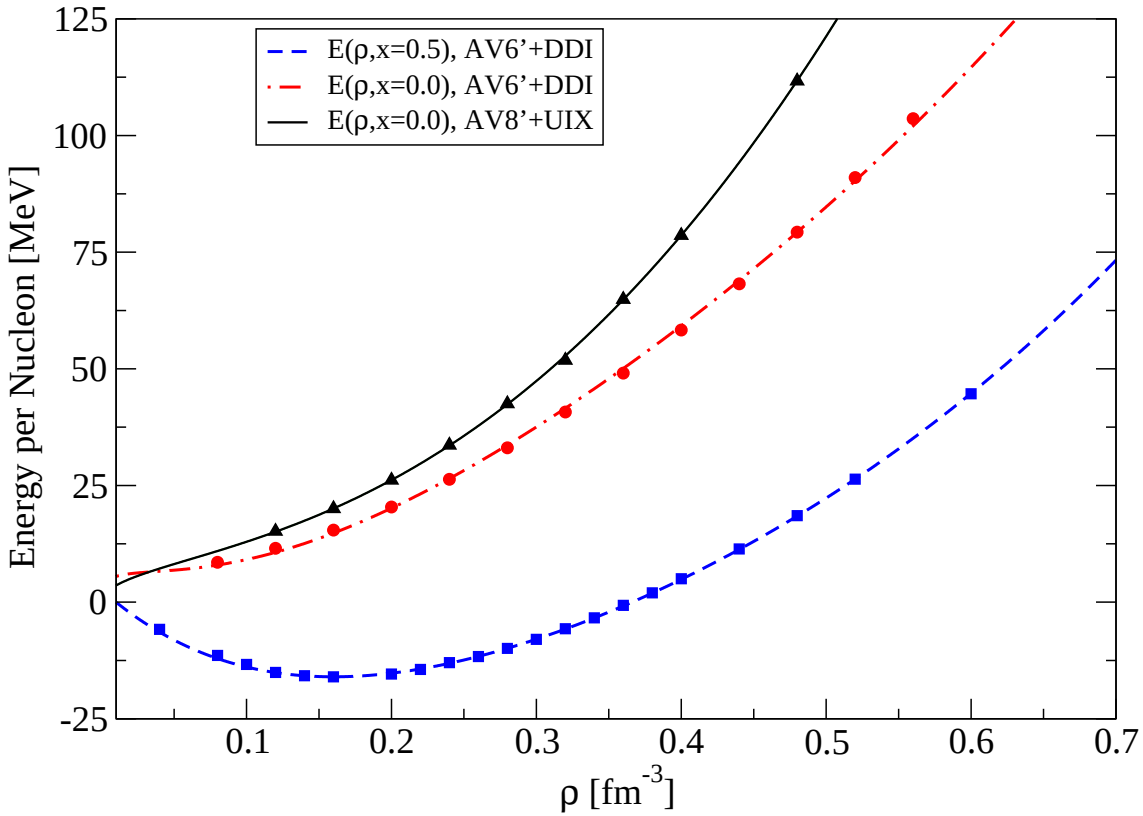
Results with 76 and 108 particles are within 3 percent of those for 28 particles.

Neutron and nuclear matter with three-nucleon interaction from density dependence

(Friedman-Lagaris-Pandharipande form)

$$V_3(\rho) = 3\gamma_2\rho^2 e^{-\gamma_3\rho}\left[1 - \frac{2}{3}\left(\frac{\rho_n - \rho_p}{\rho_n + \rho_p}\right)^2\right]$$

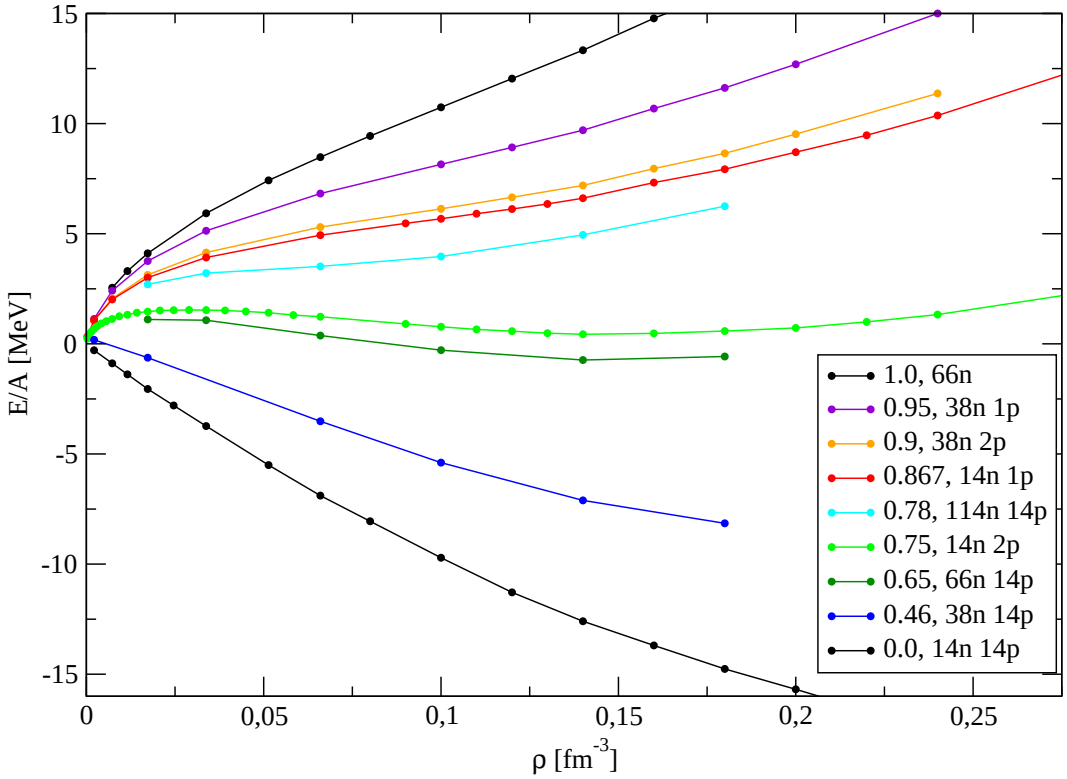
Adjust NN AV6' to reproduce symmetric nuclear matter equilibrium, $\rho_0 = 0.16$ fm^{-3}, $E(\rho_0) = -16$ MeV, compressibility $K \simeq 240$MeV.


E(ρ,x=0.5), AV6'+DDI
E(ρ,x=0.0), AV6'+DDI
E(ρ,x=0.0), AV8'+UIX
Energy per Nucleon [MeV]
125
100
75
50
25
0
-25
0.1
0.2
0.3
0.4
0.5
0.6
0.7
ρ [fm^-3]

Asymmetric matter

It's easy to calculate with different numbers of neutrons and protons.

Removing size dependence is important.



These are for Argonne v_6'.

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

Spin-Orbit isospin exchange – 3-body Commutator terms

These both require 3-body breakups for our choice of basis.

Spin-orbit isospin exchange interaction has terms like

$$p_1\sigma_1\tau_1\tau_2 v(r)$$

We can break these up using 2 Hubbard-Stratonovich transformations

$$\begin{aligned} & e^{-\frac{p^2}{2}\Delta t - ipO_1O_2\Delta t} \\ = & \frac{1}{2\pi}\int dx \int dy e^{-\frac{x^2+y^2}{2}} \cdot \\ & \cdot e^{ipx\Delta t^{1/2} - \sqrt{x}y(O_1+O_2)\Delta t^{1/4} - x(O_1^2+O_2^2)\Delta t^{1/2}/2 - O_1^2O_2^2\Delta t/2} \end{aligned}$$

With importance sampling like we use for the Hubbard-Stratonovich transformation we get a modified gaussian distribution and a local energy weight - Low variance.

Work in progress...

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. These three-operator breakups are now possible with low variance.
- Physics of neutron rich nuclei can be studied...