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Constrained path calculations of the ^{4}He and ^{16}O nuclei

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Abstract. We give results for the energy of the ^{4}He and ^{16}O nuclei using the auxiliary field diffusion Monte Carlo and a path constraint. We compare the results with previous FHNC and cluster Monte Carlo calculations.

PACS. 21.10.Dr Binding energies and masses – 21.60.Ka Monte Carlo models

1 Introduction

While Monte Carlo methods have been very successful in calculating the properties of systems with central potentials, accurate Monte Carlo results for nuclei with spin-isospin potentials have been obtained only by summing rather than sampling the spin-isospin degrees of freedom [1,2]. The problem with summing over the spin states is that for a nucleus with A nucleons and N neutrons, the number of spin-isospin states is

$$\frac{A!}{N!(A-N)!}2^A\,, \tag{1}$$

which grows exponentially with A. For systems that conserve isospin, the number of states can be reduced but not by a large factor. The exponential behavior of the spin sums has limited these calculations to light nuclei. The number of nucleons that can be included has increased according to Moore's law with an addition of about 1 nucleon every 2 years.

The auxiliary field diffusion Monte Carlo (AFDMC) method, which samples the spin-isospin states, with the addition of a path constraint to control the fermion sign problem, has given good results for pure neutron matter [3,4]. For nuclei, the strong tensor force in the isosinglet channel makes sampling the spin-isospin states more difficult. We will review the application of the method to the v_6 interaction and apply it to the alpha-particle and ^{16}O. Our results indicate that the path constraint built on the simple single determinant trial wave function, while sufficient to bind both the alpha and ^{16}O, gives an energy several MeV per particle too high. More accurate calculations will require a better trial function or an otherwise improved constraint.

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2 The v_6 Hamiltonian

We take the Hamiltonian to be

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

where i and j label the two nucleons, r_{ij} is the distance separating the two nucleons, and the $O^{(p)}$ include spin and isospin operators, and M is the maximum number of operators (*i.e.* 18 in v_{18} models). The mass m is the average nucleon mass.

We use v_6 models where the two-body potiental is truncated at the $M = 6$ level. The six $O^n(i,j)$ terms are the central operator, and the spin-isospin operators $\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j$, $\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j$, $\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j$, t_{ij}, and $t_{ij}\boldsymbol{\tau}\cdot\boldsymbol{\tau}_j$, where t_{ij} is the tensor operator $3\boldsymbol{\sigma}_i\cdot\hat{\boldsymbol{r}}_{ij}\boldsymbol{\sigma}_j\cdot\hat{\boldsymbol{r}}_{ij} - \boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j$. The $\boldsymbol{\tau}_i$ and $\boldsymbol{\sigma}_i$ are the Pauli matrices for the isospin and spin of particle i. We have simply truncated the Urbana v_{14} [5] and Argonne v_8' [1,6] potentials at the v_6 levels.

While the neutron-proton mass difference, Coulomb interactions, spin-orbit interactions, and three-body potentials can be done with an increase in complexity, we want first to see how well the method performs on this simplified Hamiltonian.

3 Spin sampling

Before describing the auxiliary field diffusion Monte Carlo method, we look at the simpler case of a variational calculation.

We can define a wave function

$$\Psi_T(R,S) = \langle R,S|\Psi_T\rangle\,, \tag{2}$$

as the amplitude for finding the nucleus with nucleons at positions $R \equiv \boldsymbol{r}_1, \boldsymbol{r}_2, ...\boldsymbol{r}_A$ and an A particle spin-isospin state S. There are many choices for the representation of the spin state. We specify the basis states by giving a spinor for each of the particles. That is four complex numbers for each particle which give the amplitude of finding the particle as a proton-up, proton-down, neutron-up, neutron-down.

A variational Monte Carlo calculation of the energy requires the evaluation of

$$\langle H\rangle = \frac{\int \mathrm{d}R \sum_{S,S'} \Psi_T^*(R,S) H_{S,S'} \Psi_T(R,S')}{\int \mathrm{d}R \sum_S \Psi_T^*(R,S)\Psi_T(R,S)}\,. \tag{3}$$

We can write this in two ways depending on whether we plan to sum or sample the spins. Spin summing corresponds to writing

$$P_1(R) = \frac{\sum_S \Psi_T^*(R,S)\Psi_T(R,S)}{\int \mathrm{d}R \sum_S \Psi_T^*(R,S)\Psi_T(R,S)}\,, \tag{4}$$

$$E_1(R) = \frac{\sum_{S,S'} \Psi_T^*(R,S) H_{S,S'} \Psi_T(R,S')}{\sum_S \Psi_T^*(R,S)\Psi_T(R,S)}\,, \tag{5}$$

$$\langle H\rangle = \int \mathrm{d}R\; E_1(R) P_1(R)\,, \tag{6}$$

and sampling the spatial coordinates of the particles from $P_1(R)$ using, for example, the Metropolis method. Notice if Ψ_T is Ψ_0 the ground state, $E_1(R) = E_0$ so good trial functions will give low variance. The number of terms in the spin sum in the numerator of P_1 and E_1, grows exponentially in A.

Alternatively, we can sample both the positions R and the spin-isospin S from

$$P_2(R,S) = \frac{\Psi_T^*(R,S)\Psi_T(R,S)}{\int \mathrm{d}R \sum_S \Psi_T^*(R,S)\Psi_T(R,S)}\,, \tag{7}$$

and evaluate using

$$E_2(R) = \frac{\Psi_T^*(R,S)\sum_{S'} H_{S,S'}\Psi_T(R,S')}{\Psi_T^*(R,S)\Psi_T(R,S)}\,, \tag{8}$$

$$\langle H\rangle = \sum_S \int \mathrm{d}R\; E_2(R,S) P_2(R,S)\,. \tag{9}$$

Notice if Ψ_T is Ψ_0 the ground state, $E_2(R) = E_0$ so again good trial functions will give low variance.

Metropolis sampling of this form does not require any spin sum. The number of terms in the spin sum of $E_2(R,S)$ above is of order A^2 with pairwise potentials, since each term can at most change the spin or isospin of the particles in the pair. Full spin-isospin sums are normally done because the physics leads to forms of the trial function where the computational complexity to calculate $\Psi_T(R,S)$ for a single value of S is the same as calculating all values of S. For example, in the pair-product form

$$\Psi_T(R,S) = \langle R,S|\prod_{i<j} f_{ij}^c[1 + \sum_{p\neq 1} u_{ij}^{(p)} O^{(p)}(i,j)]|\Phi_0\rangle\,. \tag{10}$$

For each of the $A(A-1)/2$ different i,j values, $O^{(p)}(i,j)$ couples to 4 or 8 other terms. Roughly, A such factors alone couple to all spin-isospin states; the computational complexity is the same whether all the spin-isospin amplitudes are calculated or just a single value. If trial wave functions can be devised that both contain the physically appropriate correlations and can be evaluated efficiently for a single spin-isospin configuration, sampling with Monte Carlo methods is straightforward.

4 The auxiliary field method

Since we cannot use good trial functions to sample spins for large A, we require an alternative method of selecting spin samples. We apply the auxiliary field and constrained path ideas of S. Zhang, J. Carlson, and J. Gubernatis [7,8] to the spin-isospin part of the nuclear Hamiltonian, while sampling the spatial part as in Green's function or diffusion Monte Carlo.

The basic diffusion Monte Carlo method writes the Schrödinger equation in imaginary time (measured in units of energy^{-1}).

$$(H - E_T)|\Psi(t)\rangle = -\frac{\partial}{\partial t}|\Psi(t)\rangle\,, \tag{11}$$

which is a diffusion equation in R space. The formal solution is

$$|\Psi(t)\rangle = e^{-(H-E_T)t}|\Psi(0)\rangle\,. \tag{12}$$

Expanding the initial state in eigenstates of H,

$$\begin{aligned} H|n\rangle &= E_n|n\rangle\,,\\ |\Psi(0)\rangle &= \sum_n a_n|n\rangle\,, \end{aligned} \tag{13}$$

shows that the long-time solution converges to the lowest-energy state not orthogonal to $|\Psi(0)\rangle$.

$$|\Psi(t)\rangle = e^{-(E_0-E_T)t}\left[a_0|0\rangle + \sum_{n\neq 0} e^{-(E_n-E_0)t} a_n|n\rangle\right]\,. \tag{14}$$

For short-time propagation, the Trotter expansion can be used to calculate an approximate propagator

$$e^{-H\Delta t} = e^{-V\frac{\Delta t}{2}} e^{-\frac{P^2}{2m}\Delta t} e^{-V\frac{\Delta t}{2}} + O(\Delta t^3)\,. \tag{15}$$

In R representation the $P^2/2m$ term is the free propagator, and the V terms do not couple different R values. The $P^2/2m$ terms are diagonal in spin-isospin (this is modified if the physical unequal masses of the protons and neutrons

are used) so that the spin-isospin dependence is entirely in the potential. The free propagator is

$$G(R,R',\Delta t) = \langle R|e^{-(H-E_T)\Delta t}|R'\rangle\,,$$
$$= \left[\frac{1}{2\pi\sigma^2}\right]^{\frac{3A}{2}} e^{-\frac{(R-R')^2}{2\sigma^2}} e^{-[\frac{V(R)+V(R')}{2}-E_T]\Delta t}\,,$$
$$\sigma^2 = 2\frac{\hbar^2}{2m}\Delta t\,. \tag{16}$$

Given positions for all the nucleons, we can obtain new positions in the next step by sampling the Gaussian.

The potential propagator matrix elements are

$$\langle RS'|\exp(-V\Delta t)|RS\rangle\,, \tag{17}$$

which for the v_6 potential has essentially the same form as the pair-product wave function. We have already seen that computational complexity makes the evaluation of this matrix element unfeasible beyond small A. We therefore need to find a sensible way to sample the spin-isospin S' given the original spin-isospin state.

Furthermore, we would like the spin propagation to be local in some sense. That is, as $\Delta t \to 0$ we want our propagator to go smoothly to the identity and the walker remains the same as $\Delta t \to 0$. One way to do this is to use a general spinor basis. For example, starting with a spin-up particle rather than flipping the spin with a small probability in the next time step, we sample spinors that have a small down amplitude.

We therefore look for a method which will propagate a state represented by an outer product of spinors, one for each particle, to another state of the same form. One way is to write the spin-isospin part of the propagator as

$$\sum_{\text{samples}} \prod_{i=1}^{A} [a_i + \boldsymbol{b}_i\cdot\boldsymbol{\sigma}_i + \boldsymbol{c}_i\cdot\boldsymbol{\tau}_i + \boldsymbol{\sigma}_i\cdot\overleftrightarrow{\boldsymbol{d}}_i\cdot\boldsymbol{\tau}_i]\,. \tag{18}$$

The Hubbard-Stratonovich or auxiliary field method accomplishes this breakup. For example,

$$\exp(-\sigma_{x1}\sigma_{x2}v_{12}^{\sigma}\Delta t)$$
$$= \cosh(v_{12}^{\sigma}\Delta t)[1-\sigma_{x1}\sigma_{x2}\tanh(v_{12}^{\sigma}\Delta t)]$$
$$= \cosh(v_{12}^{\sigma}\Delta t)\frac{1}{2}\sum_{\epsilon=\pm1}\left[1+\epsilon\sigma_{x1}\sqrt{\tanh(-v_{12}^{\sigma}\Delta t)}\right]\,,$$
$$\left[1+\epsilon\sigma_{x2}\sqrt{\tanh(-v_{12}^{\sigma}\Delta t)}\right]\,.$$

As $\Delta t \to 0$ this goes smoothly to 1, and for nonzero Δt, the spinors each get multiplied by a near-unit 2×2 matrix. The ϵ variables are sampled using the Monte Carlo method.

The breakup above requires 3 Hubbard-Stratonovich variables for each pair of particles for a spin-exchange and tensor interaction, or $3A(A-1)/2$ variables.

To reduce this number, we diagonalize the interaction in spin-isospin space. This requires order (A^3) operations, but the trial wave function determinant has the same complexity. This breakup is similar to those used in auxiliary field breakups in Shell Model Monte Carlo.

For A particles, the v_6 interaction can be written as

$$V = \sum_{i<j}\left[\sum_{p=1}^{6} v_p(r_{ij})O^{(p)}(i,j)\right] = V_{si}+V_{sd}$$
$$= V_{si} + \frac{1}{2}\sum_{i,\alpha,j,\beta}\sigma_{i,\alpha}A^{(\sigma)}_{i,\alpha,j,\beta}\sigma_{j,\beta}$$
$$+\frac{1}{2}\sum_{i,\alpha,j,\beta}\sigma_{i,\alpha}A^{(\sigma\tau)}_{i,\alpha,j,\beta}\sigma_{j,\beta}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j$$
$$+\frac{1}{2}\sum_{i,j}A^{(\tau)}_{i,j}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j\,.$$

Here, V_{si} is the spin-independent part of the potential and V_{sd} is the spin-dependent part.

The A-matrices are zero when $i=j$ and they are symmetric. Note however, that we can include an arbitrary nonzero $i=j$ term if we include a corresponding central counterterm. This can shift the spectrum of the operators to make, for example, all the eigeinvalues negative if desired. Since the A-matrices are real and symmetric they have real eigenvalues and eigenvectors. The eigenvectors and eigenvalues are defined by

$$\sum_{j,\beta}A^{(\sigma)}_{i,\alpha,j,\beta}\boldsymbol{\psi}^{\sigma}_n(j)\cdot\hat{x}_\beta = \lambda^{(\sigma)}_n\boldsymbol{\psi}^{\sigma}_n(i)\cdot\hat{x}_\alpha\,. \tag{19}$$

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

$$V_{sd} = \frac{1}{2}\sum_{i,j,n}\boldsymbol{\sigma}_i\cdot\boldsymbol{\psi}^{(\sigma)}_n(i)\lambda^{(\sigma)}_n\boldsymbol{\psi}^{(\sigma)}_n(j)\cdot\boldsymbol{\sigma}_j$$
$$+\frac{1}{2}\sum_{i,j,n}\boldsymbol{\sigma}_i\cdot\boldsymbol{\psi}^{(\sigma\tau)}_n(i)\lambda^{(\sigma\tau)}_n\boldsymbol{\psi}^{(\sigma\tau)}_n(j)\cdot\boldsymbol{\sigma}_j\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j$$
$$+\frac{1}{2}\sum_{i,j,n}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j\psi^{(\tau)}_n(i)\lambda^{(\tau)}_n\psi^{(\tau)}_n(j)\,. \tag{20}$$

We want the squares of operators so we write

$$V_{sd} = \frac{1}{2}\sum_{n=1}^{3A}(O^{(\sigma)}_n)^2\lambda^{(\sigma)}_n \tag{21}$$
$$+\frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{3A}(O^{(\sigma\tau)}_{n\alpha})^2\lambda^{(\sigma\tau)}_n \tag{22}$$
$$+\frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{A}(O^{(\tau)}_{n\alpha})^2\lambda^{(\tau)}_n\,, \tag{23}$$

with

$$O^{(\sigma)}_n = \sum_i\boldsymbol{\sigma}_i\cdot\boldsymbol{\psi}^{(\tau)}_n(i)$$
$$O^{(\sigma\tau)}_{n\alpha} = \sum_i\tau_{i\alpha}\boldsymbol{\sigma}_i\cdot\boldsymbol{\psi}^{(\sigma\tau)}_n(i)$$
$$O^{(\tau)}_{n\alpha} = \sum_i\tau_{i\alpha}\psi^{(\tau)}_n(i)\,. \tag{24}$$

The Hubbard-Stratonovich transformation is

$$e^{-\frac{1}{2}\lambda_n O_n^2 \Delta t} = \left(\frac{\Delta t|\lambda_n|}{2\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \mathrm{d}x e^{-\frac{1}{2}\Delta t|\lambda_n|x^2 - \Delta t s \lambda_n O_n x}, \tag{25}$$

where s is 1 for $\lambda < 0$, and s is i for $\lambda > 0$.

Our O_n do not 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 $3A \times 3A$ matrices and one $A \times A$ matrix.

Once the Hubbard-Stratonovich variables have been sampled, the resulting propagator acting on a walker consisting of the positions and spinors for each particle gives a single new walker.

5 The path constraint

We still have the usual fermion sign problem. In this case the overlap of our walkers with the trial function will be complex. We constrain the path to regions where the real part of the overlap with our trial function is positive. For spin-independent potentials this reduces to the fixed-node approximation.

6 The trial wave function

We use the simplest trial function

$$|\Psi_T\rangle = \left[\prod_{i<j} f_{ij}^c\right] \mathcal{A}\left[\prod_i \phi_i(\boldsymbol{r}_i - R_{\mathrm{cm}}, s_i)\right], \tag{26}$$

where $\mathcal{A}$ is an antisymmetrization operator, ϕ are single-particle orbitals, and R_{cm} is the center-of-mass position of the nucleus. Given a set of positions and spinors, the antisymmetrization produces a determinant of single-particle orbitals. For the nuclei here we have chosen s-orbitals for the alpha-particle and s- and p-orbitals for ^{16}O, constructed as the orbitals of the Wood-Saxon well. The parameters of the well were adjusted to give roughly the correct nuclear radius. The trial wave function is translationally invariant and requires no center-of-mass correction.

The overlap of our walker with the trial function is the determinant of the space-spin orbitals evaluated at the walker position and spinor for each particle multiplied by a central Jastrow product.

7 The algorithm

Our algorithm becomes:

1. Sample $|R, S\rangle$ initial walkers from $|\langle\Psi_T|R, S\rangle|^2$ using Metropolis Monte Carlo.
2. Propagate in the usual diffusion Monte Carlo way with a drifted Gaussian for half a time step.
3. Diagonalize, for each walker, the potential matrix.
4. Loop over the eigenvectors, sampling the corresponding Hubbard-Stratonovich variable and update the spinors. We use the matrix elements $\langle\Psi_T|\boldsymbol{\sigma}_i|R, S\rangle$, $\langle\Psi_T|\boldsymbol{\tau}_i|R, S\rangle$, and $\langle\Psi_T|\boldsymbol{\sigma}_i\boldsymbol{\tau}_i|R, S\rangle$ as replacements to the operators in the exponential to approximately predict the relative weights of the positive and negative samples from the Hubbard-Stratonovich variables. Then propagate with the correct operators and divide by these important sampling probabilities. This preferentially samples the values that we predict will give a larger weight. Since the sampled probabilities are divided out we change only the variance not the averages.
5. Propagate with a drifted Gaussian for the remaining half of a time step.
6. Combine all weight factors and evaluate new value of $\langle\Psi_T|R, S\rangle$. If the real part is less than 0, enforce the constrained path by dropping the walker.
7. Evaluate the averages of $\langle\Psi_T|R, S\rangle$ and $\langle\Psi_T|H|R, S\rangle$ to calculate the energy.
8. Repeat steps 2 through 7 as necessary until convergence.

8 Results and discussion

We show the results with the v_6 truncated potentials in table 1. Since our trial function contains no tensor correlations, the variational estimate is not bound. However the auxiliary field diffusion Monte Carlo gives a bound result. Unfortunately, the path constraint imposed by our simple wave function is not sufficient to obtain a good answer. For the alpha-particle, Joe Carlson [9] has calculated the energy with the Argonne v_8' truncated to v_6 as -22.8 ± 0.2 MeV. We see that our constraint gives an energy that is about 5 MeV too high. The exact energy for the ^{16}O nucleus is not known. However, correlated basis function calculations [10] with the Urbana v_{14} potential truncated at the v_6 level give an energy of -82.40 MeV which is within our error bars. This indicates that our method is giving energies that are roughly on par with these variational calculations, but presumably are above the correct energy by something of the order of 1-2 MeV per nucleon as in the alpha-particle. With the same CM correction, the cluster MC result [11] using just their expectation of the v_6 part of the Argonne v_{14} potential [12] and the kinetic

Table 1. The calculated ground-state energy in MeV for the v_6 truncated Argonne v_8' and Urbana v_{14} potentials.

Nucleus	Potential	$E_{\mathrm{Constrained}}$
^{4}He	Urbana	$-20.7(3)$
^{4}He	Argonne	$-17.9(1)$
^{16}O	Urbana	$-84(2)$
^{16}O	Argonne	$-57(3)$

energy is −86.6 MeV. Previous constrained path AFDMC calculations [13] using v_4-type potentials (without tensor force) gave an energy lower than FHNC in nuclear matter and in a very good agreement with accurate few-body variational calculations for the alpha-particle.

From these results it is clear that while qualitative inclusion of the effect of the tensor forces is being included even with our crude trial function for the constraint, accurate calculations will require better constraints or a method without constraints in order to give trustworthy results for nuclear binding energies. We are working in this direction.

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