Quadratically Correlated Trial Wave Functions for Nuclear Quantum Monte Carlo Calculations

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We have done binding energy calculations for ^{4}He, ^{16}O, ^{40}Ca and symmetric nuclear matter. The calculations have been done using Auxiliary Field Diffusion Monte Carlo with two improved trial wave functions, both including up to quadratic correlations. We show that these wave functions decrease the binding energy of each system as compared to the previously used wave function with up to linear correlations. We show that though these wave function cost more in terms of computation time, they do improve the binding energy estimates for nuclear systems.

INTRODUCTION

The study of the nuclear force has proven to be one of the more difficult problems to solve in physics. This is due to the complex nature of the nuclear interaction. There have been a number of phenomenological models that have had good success describing the strong force. Some of these are the CD-Bonn [1], Nijmegen [2, 3] and Argonne [4] two-body potentials and the Urbana [5] and Illinois [6] three-body potentials. There are a variety of methods that use these models to solve for properties of nuclear systems. Two main classes of methods are basis set methods like the no core shell model [7, 8], the coupled-cluster method [9], the self-consistent Green's function methods [10, 11] and Quantum Monte Carlo methods such as Green's Function Monte Carlo and Auxiliary Fields Diffusion Monte Carlo [12]. Basis set methods have had good success in calculating the properties of nuclei but are limited only to soft potentials like the CD-Bonn and Nijmegen models. We use the Auxiliary Field Diffusion Monte Carlo (AFDMC) method which is well suited for a variety of local potentials with hard and soft cutoffs. It is currently limited to mostly local (velocity independent) potentials, but some recent progress has been made with non-local potentials [13–15]. This makes the Argonne potentials good candidates for AFDMC. All calculations for this work were done with the AFDMC method using the Argonne AV6′ which is a refitting of the first six operators of the two-body Argonne AV18 potential, the first six operators being $[1, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, S_{ij}] \otimes [1, \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j]$.

The AFDMC methods evolves a trial wave function in imaginary time to extract out the ground state properties of the system using the imaginary time propagator.

$$\Psi(\tau) = e^{-(H-E_T)\tau}\Psi_T(0) \tag{1}$$

Currently the AFDMC method has been able to do statistically significant calculations for nuclei as large ^{40}Ca and neutron matter with 66 particles and periodic boundary conditions [12]. The accuracy of the AFDMC method depends heavily on the accuracy of the trial wave function. This is the case due to the constraint used to solve the fermion sign problem [16], without which the exact solution could be obtained with a bad wave function. In either case a good wave function will decrease the variance of the calculation. An accurate but low cost wave function could be used to do accurate calculation for much larger systems which could advance our understanding of nuclear structure, neutron star formation and structure as well as the r-process for nucleosynthesis that occurs in supernovae [17–21].

TRIAL WAVE FUNCTION

An accurate trial wave function would account for the complex nuclear correlations, but this can be difficult to do in practice. One of the simplest trial wave functions is a single or linear combination of a few Slater determinants. This is an antisymmetrized product of single particle states. The single particle states ensure the right quantum numbers and the spatial components are obtained by a Hartree-Fock calculation with Skyrme forces [22]. Short range correlations are taken into account with Jastrow-like spin-isospin independent and dependent correlation terms,

$$|\psi_T\rangle_{exp} = \left[\prod_{i<j} f_c(r_{ij})\right]\left[e^{\sum_{i<j}\sum_p f_p(r_{ij})\mathcal{O}^p_{ij}}\right]|\phi\rangle\,, \tag{2}$$

where the operators, $\mathcal{O}^p_{ij}$, are the same six operators used for the potential. The $f_c(r_{ij})$ and $f_p(r_{ij})$ function come from solving Schrödinger-like equations as discussed in [23].

The calculation of the exponential correlations scales exponentially with the number of particles and so to directly calculate this wave function can be very difficult. Previous work [22] has done calculations of light and medium mass nuclei, symmetric and asymmetric nuclear matter with different two-body interactions using an expansion of these exponential correlations, truncated at the linear term. We have expanded a nearly equivalent

symmetrized product trial wave function to include up to quadratic terms,

$$|\psi_T\rangle_{sp} = \left[\prod_{i<j} f_c(r_{ij})\right]\left[\mathcal{S}\prod_{i<j}\left(1+\sum_p f_p(r_{ij})\mathcal{O}^p_{ij}\right)\right]|\phi\rangle\,, \tag{3}$$

where $\mathcal{S}$ is the symmetrization operator. The symmetrized product wave function and exponential correlations are exactly the same up to linear order.

Expanding the symmetrized product wave function to quadratic order gives

$$|\psi_T\rangle_{fq} = \left[\prod_{i<j} f_c(r_{ij})\right]\left[1+\sum_{i<j}\sum_p f_p(r_{ij})\mathcal{O}^p_{ij} + \frac{1}{2}\sum_{i<j}\sum_p f_p(r_{ij})\mathcal{O}^p_{ij}\sum_{\substack{k<l\\ ij\neq kl}}\sum_q f_q(r_{kl})\mathcal{O}^q_{kl}\right]|\phi\rangle\,. \tag{4}$$

This is called the full quadratic wave function. We have used this wave function in addition to a variation called the independent pair wave function given by

$$|\psi_T\rangle_{ip} = \left[\prod_{i<j} f_c(r_{ij})\right]\left[1+\sum_{i<j}\sum_p f_p(r_{ij})\mathcal{O}^p_{ij} + \frac{1}{2}\sum_{i<j}\sum_p f_p(r_{ij})\mathcal{O}^p_{ij}\sum_{k<l,\mathrm{ip}}\sum_q f_q(r_{kl})\mathcal{O}^q_{kl}\right]|\phi\rangle\,, \tag{5}$$

where the sum over kl pairs only includes particles that are not included in the ij pair. For example, if the ij pair includes particles 12 then the kl pairs 13 and 24 would not be permitted, while pairs 34 and 56 would be included. Since none of the operators act on the same particle all of the operators commute, removing the need for a symmetrization. Thus the terms $\frac{1}{2}(f_p(r_{12})\mathcal{O}^p_{12}f_q(r_{34})\mathcal{O}^q_{34} + f_q(r_{34})\mathcal{O}^q_{34}f_p(r_{12})\mathcal{O}^p_{12})$ is calculated as $f_p(r_{12})\mathcal{O}^p_{12}f_q(r_{34})\mathcal{O}^q_{34}$. This wave function reduces the numbers of operators needed while still capturing most of the relevant physics.

CALCULATIONS

To do these calculations the walkers, which contains the positions, spins and isospins of each particle, are used to build a Slater matrix

$$S_{ki} = \langle k|\mathbf{r}_i s_i\rangle = \sum_{s=1}^{4}\langle k|\mathbf{r}_i s\rangle\langle s|s_i\rangle\,, \tag{6}$$

where $|\mathbf{r}_i s_i\rangle$ are the walkers and $|k\rangle$ contain the radial model states and ls or j angular momentum states. The Slater matrix is updated by each of the operators. These updates are done with the aid of the identity $\det S^{-1}S' = \frac{\det S'}{\det S}$, where S' is the matrix that has been updated by one operator. To reduce the number of operations done in the inner loops the ratio of determinants for a pair of operators, $\mathcal{O}_{ij} = \mathcal{O}_i\mathcal{O}_j$, is written in the form

$$\frac{\langle\Phi|\,O_{ij}\,|R,S\rangle}{\langle\Phi|R,S\rangle} = \sum_{s=1}^{4}\sum_{s'=1}^{4} d_{2b}(s,s',ij)\,\langle ss'|\,O_{ij}\,|s_i s_j\rangle\,, \tag{7}$$

where

$$d_{2b}(s,s',ij) = \frac{\langle\Phi|R,s_1,\ldots,s,s_{i+1},\ldots,s',s_{j+1},\ldots,s_A\rangle}{\langle\Phi|RS\rangle}, \tag{8}$$

with $R = \mathbf{r}_1,\ldots,\mathbf{r}_A$, $S = s_1,\ldots,s_A$, and s and s' are one of the four spin-isospin states neutron-up, neutron-down, proton-up, proton-down. The d_{2b} are calculated in an outer loop from the precalculated matrix elements $P_{s,ij}$,

$$d_{2b}(s,s',ij) = \det\begin{pmatrix} P_{s,ii} & P_{s,ij}\\ P_{s',ji} & P_{s',jj}\end{pmatrix} \tag{9}$$

where

$$P_{s,ij} = \sum_k S^{-1}_{jk}S_{ki}(s_i\to s). \tag{10}$$

Though this only addressed two-body operators this method can be generalized to other N-body operators as well. To include additional operators the matrix elements $P_{s,ij}$ need to be updated

$$P'_{s,mn} = \sum_k S'^{-1}_{nk}S'_{km}(s_m\to s) \tag{11}$$

where

$$S'_{km}(s) = \begin{cases} S_{km} & m\neq i\\ \langle k|\,O_i\,|\mathbf{r}_i,s_i\rangle & m=i\end{cases}. \tag{12}$$

To calculate the updated inverse matrix the identity $\det(S^{-1}S'') = \det S''/\det S$ is used. Both sides of the identity are expanded and like terms are grouped noting that when $j\neq i$, $S''_{mi} = S'_{mi}$.

Calculations with Linear and Quadratic Wave Functions

The wave function with linear correlations is calculated by first operating on the walkers with each possible operator and calculating the sum of each term $\sum_{ss'} d_{2b}(s,s',ij)\,\langle ss'|\,f(\mathbf{r}_{ij})\mathcal{O}_{ij}\,|s_i s_j\rangle$. The expectation value of the potential with the linear wave function includes correlation and potential operators, where one term in the sum may have the form $\left(1+\mathcal{O}^c_{ij}\right)\mathcal{O}^p_{kl}$ where

the correlation, $\mathcal{O}^c_{ij}$, and potential operators, $\mathcal{O}^p_{ij}$, are four potentially distinct operators. For this calculation the P matrix is updated twice, once for $\mathcal{O}^c_i$ and once for O^c_j, where $O^c_{ij} = O^c_i O^c_j$. The ratio of determinants is calculated in a similar way as the wave function above, except that the updated distribution, d''_{2b}, is used.

The quadratic wave function includes all of the pieces from the linear wave function and a piece with two additional operators. One possible term in the sum of correlations is $1 + \mathcal{O}^c_{ij} + \mathcal{O}^c_{ij}\mathcal{O}^c_{kl}$. The operators up to linear terms are handled identically to the method described above. The quadratic product of operators is handled in practically the same was as the potential with the linear wave function, as described above. That is, the P matrix is updated twice, once for $\mathcal{O}^c_i$ and once for $\mathcal{O}^c_j$ and the ratio of determinants is calculated with the updated distributions. The calculation of the correlation operators for the quadratic wave function requires $\mathcal{O}(A^4)$ operations whereas the linear correlations requires $\mathcal{O}(A^2)$.

The only part with the expectation value of the potential with the quadratic wave function that is different than above is the product of six operators $\mathcal{O}^c_{ij}\mathcal{O}^c_{kl}\mathcal{O}^p_{mn}$. A total of four updates are used to calculate this term.

A total of four updates are used to calculate the quadratically correlated term for the potential, $\mathcal{O}^c_{ij}\mathcal{O}^c_{kl}\mathcal{O}^p_{mn}$. The linear terms are handled as before. After including the updated distributions for the $\mathcal{O}^c_{ij}$ term, the same distributions were updated two more times for the $\mathcal{O}^c_{kl}$ term. These quadratically updated distributions are then used to calculate the expectation value of the potential in the usual way. To calculate the potential with the quadratic wave function required $\mathcal{O}(A^6)$ operations compared to the $\mathcal{O}(A^4)$ operations required for the linear wave function.

Mixed Expectation Values

We have calculated the ground state energy for ^{4}He, ^{16}O, ^{40}Ca and symmetric nuclear matter (SNM) with 28 particles with periodic boundary conditions at the nuclear saturation density, $\rho = 0.16\text{fm}^{-3}$. Ideally the expectation value would be calculated with fully propagated states, however operating though the propagator can be difficult and so in practice mixed expectation values are used.

$$\langle \mathcal{O} \rangle_m = \frac{\langle \Psi(\tau) | \mathcal{O} | \Psi_T \rangle}{\langle \Psi(\tau) | \Psi_T \rangle} \tag{13}$$

If the operator commutes with the Hamiltonian, and thus the unconstrained propagator, the mixed expectation value gives the ground state energy in the large imaginary time limit and so the energy can be calculated as $\langle H \rangle = \lim_{\tau\to\infty} \langle H \rangle_m$. If the operator does not commute with the propagator the real expectation value is written as a perturbation of the variational expectation value, $\langle \mathcal{O} \rangle_T = \langle \Psi_T | \mathcal{O} | \Psi_T \rangle / \langle \Psi_T | \Psi_T \rangle$ and the expectation value can be approximated as

$$\langle \mathcal{O} \rangle \approx \frac{\langle \Psi(\tau) | \mathcal{O} | \Psi_T \rangle}{\langle \Psi(\tau) | \Psi_T \rangle} + \frac{\langle \Psi_T | \mathcal{O} | \Psi_{(}\tau) \rangle}{\langle \Psi_T | \Psi(\tau) \rangle} - \langle \mathcal{O} \rangle_T , \tag{14}$$

which for diagonal matrix elements is simply $\langle \mathcal{O} \rangle \approx 2 \langle \mathcal{O} \rangle_m - \langle \mathcal{O} \rangle_T$.

Due to the fermion sign problem the propagation is constrained using the constrained-path method [16]. This approximation limits the propagation of the wave function to regions where the propagated and trial wave function have non-zero overlap. As a result the propagator and the Hamiltonian do not commute anymore and the resulting energy estimates are not strict upper bounds to the ground state energy. This can accounted for by using a method such as the forward walking method to release the constraint and check the accuracy of the constrained calculation.

RESULTS

The results for the energy calculations are reported in Table I. The energies for each system decreased as the new correlations were added, which was expected with an improved wave function. The optimization parameters for ^{4}He had to be re-optimized using the new correlations to produce a decrease in energy, though the parameters used for ^{16}O, ^{40}Ca and SNM were only optimized for linear correlations due to the computational cost of optimization. To compare the efficiency of each wave function the scaling factor was calculated, which was the ratio of the average time to complete one block of calculation for each of the new wave functions compared to the linear wave function. The results are shown in Table II. Scaling for the fully quadratic wave function was greater than that of the independent pair wave function, and for ^{16}O, ^{40}Ca and SNM it was approximately twice as large. This is due in part to the explicit symmetrization that is required for the quadratic wave function. The scaling for the fully quadratic wave function could be improved if the symmetrization was only done on non-independent pair terms. However, given that the energies of each

TABLE I. Energy (per particle*) in MeV for ^{4}He, ^{16}O, ^{40}Ca and symmetric nuclear matter as calculated with all three types of correlations compared to experimental energies where available [24].

	Linear	IndPair	Quadratic	Expt.
^{4}He	-27.17(4)	-27.46(4)	-27.22(6)	-28.296
^{16}O	-115.7(9)	-121.5(1.5)	-120.0(1.4)	-127.619
^{40}Ca	-320(5)	-358(4)	-354(6)	-348.464
SNM*	-13.92(6)	-14.80(7)	-14.70(11)	

TABLE II. Scaling for both quadratic wave functions as compared to the linear wave function. The scaling was calculated as the ratio of the average time it took to complete one block of calculation.

	IndPair	Quadratic
^{4}He	1.73	2.00
^{16}O	30.74	58.83
^{40}Ca	720.91	1473.94
SNM	64.77	133.59

system were similar for both the independent pair and the fully quadratic wave functions this indicates that the independent pair wave function captures most of the relevant physics.

CONCLUSION

In conclusion, we were able to improve on the simple linearly expanded wave function by expanding to quadratic terms. Two wave function were formed from these quadratic terms, one which included all the terms and one that only included independent pair terms. Binding energy calculations were done for ^{4}He, ^{16}O, ^{40}Ca and SNM and it was found that both wave functions decreased the binding energies of each system. The independent pair wave function required less computation while still capturing most of the relevant physics. Though both wave function improved the accuracy of the trial wave function, both require large computational cost. Including these additional correlations, or the full exponential correlations, while maintaining a low computational cost will be the goal of future work.

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