Random collection of notes that will go toward my dissertation

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1 Correlated Mixed Expectation Values

One of the main goals of the AFDMC method is to calculate expectation values of the form

$$\langle \mathcal{O} \rangle = \frac{\langle \Psi(\tau) | \, \mathcal{O} \, | \Psi(\tau) \rangle}{\langle \Psi(\tau) | \Psi(\tau) \rangle}. \tag{1}$$

In practice we calculate mixed expectation values due to the complexity of operating through the propagator on the left.

$$\langle \mathcal{O} \rangle_{\text{mixed}} = \frac{\langle \Psi(\tau) | \, \mathcal{O} \, | \Psi_T \rangle}{\langle \Psi(\tau) | \Psi_T \rangle} \tag{2}$$

If the real expectation value is written as a perturbation of the variational expectation value, $\langle \mathcal{O} \rangle \approx \langle \mathcal{O} \rangle_T + \delta \langle \mathcal{O} \rangle$ where $\langle \mathcal{O} \rangle_T = \frac{\langle \Psi_T | \mathcal{O} | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$. This is a good assumption as long as the trial wave function is close to the true ground state wave function. In general the expectation value can be approximated up to leading order in δ to be

$$\langle \mathcal{O} \rangle \approx \frac{\langle \Psi(\tau) | \, \mathcal{O} \, | \Psi_T \rangle}{\langle \Psi(\tau) | \Psi_T \rangle} + \frac{\langle \Psi_T | \, \mathcal{O} \, | \Psi(\tau) \rangle}{\langle \Psi_T | \Psi(\tau) \rangle} - \langle \mathcal{O} \rangle_T. \tag{3}$$

For diagonal matrix elements this can be simplified to $\langle \mathcal{O} \rangle \approx 2 \langle \mathcal{O} \rangle_{mixed} - \langle \mathcal{O} \rangle_T$. For operators that commute with the propagator, like the Hamiltonian, it turns out that $\langle \mathcal{O} \rangle \approx \langle \mathcal{O} \rangle_{mixed}$. This can be seen if you split up the propagator in the limit that imaginary time is large,

$$\langle H \rangle_{mixed} = \frac{\langle \Psi_T | \, e^{-H\tau/2} H e^{-H\tau/2} \, | \Psi_T \rangle}{\langle \Psi_T | \, e^{-H\tau/2} e^{-H\tau/2} \, | \Psi_T \rangle}, \tag{4}$$

which gives in the limit of large τ,

$$\lim_{\tau \to \infty} \langle H \rangle_{mixed} = E_0. \tag{5}$$

The correlation and potential operators only change the spin-isospin states of the walkers. The walkers are used to build a Slater matrix which is then updated according to the various correlation and potential operators. A simple Slater matrix has the form

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

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where $|\mathbf{r}_i s_i\rangle$ are the walkers containing the positions, spins and isospins of the particles and $|k\rangle$ contain the radial model states and spin-isospin singlet and triplet states. This matrix is updated from S to a new matrix S' for each operator. An arbitrary number of operators can be included by updating the matrix for each additional operator. Since expectation values are given by determinants of matrices that have been operated on, the identity $\det S^{-1} S' = \frac{\det S'}{\det S}$ can be used.

To reduce the number of operators done in the inner loops, the ratio of determinants for a pair of operators is written in the form

$$\frac{\langle \Phi | O_{ij} | R, S \rangle}{\langle \Phi | R, S \rangle} = \sum_{s=1}^{4} \sum_{s'=1}^{4} \mathrm{d2b}(s, s', ij) \langle ss' | O_{ij} | s_i s_j \rangle, \tag{7}$$

where

$$\mathrm{d2b}(s, s', ij) = \frac{\langle \Phi | R, s_1, \ldots, s_{i-1}, s, s_{i+1}, \ldots, s_{j-1}, s', s_{j+1}, \ldots, s_A \rangle}{\langle \Phi | RS \rangle} \tag{8}$$

can be calculated in an outer loop, with $R = \mathbf{r}_1, \ldots, \mathbf{r}_A$ and $S = s_1, \ldots, s_A$. The distributions, d2b can be calculated from a precalculated sxz

$$\mathrm{d2b}(s, s', ij) = \det \begin{pmatrix} \mathrm{sxz}(s, i, i) & \mathrm{sxz}(s, i, j) \\ \mathrm{sxz}(s', j, i) & \mathrm{sxz}(s', j, j) \end{pmatrix} \tag{9}$$

where

$$\mathrm{sxz}(s, i, j) = \sum_k S_{jk}^{-1} \langle k | \mathbf{r}_i, s \rangle. \tag{10}$$

Here we are concerned with two-body operators but it is simple to generalize to one-body and three-body operators. Additional operators can be included by updating the Slater matrix and inverse matrices.

In the case of expectation values with correlated wave functions the number of operators can be much greater than two and the sxz need to be updated for each additional operator,

$$\mathrm{sxzi}(s, m, n) = \sum_k S_{nk}'^{-1} S_{km}'(s), \tag{11}$$

where the updated matrix is given by

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

To calculate sxzi the inverse matrix needs to be calculated and multiplied by this updated matrix. The inverse matrix is calculated by taking the ratio of determinants and again using the identity $\det S^{-1} S'' = \frac{\det S''}{\det S}$, where $\det S^{-1} S''$ is the determinant of the 2x2 sub-matrix, as shown on the right side of equation 13. Here S' is the matrix with the ith column changed and S'' is the matrix with first the ith and then the jth columns changed.

$$\frac{\det S''}{\det S} = \frac{\det S'}{\det S} \sum_m S_{jm}'^{-1} S_{mj}'' = \begin{cases} \sum_{nm} S_{in}^{-1} S_{ni}'' S_{jm}^{-1} S_{mj}'' - \sum_{nm} S_{im}^{-1} S_{mj}'' S_{jn}^{-1} S_{ni}'' & j \neq i \\ \sum_l S_{il}^{-1} S_{li}'' & j = i \end{cases} \tag{13}$$

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To find the updated inverse matrix the terms multiplying S''_{mj} are gathered. Noting that when $j \neq i$, $S''_{mi} = S'_{mi}$ and the updated inverse can be written as

$$S'^{-1}_{jm} = \begin{cases} S^{-1}_{jm} - \dfrac{\sum_n S^{-1}_{jn} S'_{ni}}{\sum_l S^{-1}_{il} S'_{li}} S^{-1}_{im} & j \neq i \\ \dfrac{S^{-1}_{im}}{\sum_n S^{-1}_{in} S'_{ni}} & j = i \end{cases}. \tag{14}$$

Multiplying this by the updated matrix gives

$$\text{sxzi}(s,n,m) = \begin{cases} \text{sxz}(s,n,m) - \dfrac{\sum_k S^{-1}_{mk}\langle k|O_i|\vec{r}_i s_i\rangle}{\sum_k S^{-1}_{ik}\langle k|O_i|\vec{r}_i s_i\rangle}\text{sxz}(s,n,i) & n,m \neq i \\ \dfrac{\text{sxz}(s,n,i)}{\sum_k S^{-1}_{ik}\langle k|O_i|\vec{r}_i s_i\rangle} & m=i; n \neq i \\ \sum_k S^{-1}_{mk}\langle k|O_i|\vec{r}_i s\rangle - \dfrac{\sum_k S^{-1}_{mk}\langle k|O_i|\vec{r}_i s_i\rangle}{\sum_k S^{-1}_{ik}\langle k|O_i|\vec{r}_i s_i\rangle} \sum_k S^{-1}_{ik}\langle k|O_i|\vec{r}_i s\rangle & n=i; m \neq i \\ \dfrac{\sum_k S^{-1}_{ik}\langle k|O_i|\vec{r}_i s\rangle}{\sum_k S^{-1}_{ik}\langle k|O_i|\vec{r}_i s_i\rangle} & n=m=i \end{cases}. \tag{15}$$

This can be written more simply as

$$\text{sxzi}(s,n,m) = \begin{cases} \text{sxz}(s,n,m) - \dfrac{\text{di}(m)}{\text{di}(i)}\text{sxz}(s,n,i) & n,m \neq i \\ \dfrac{\text{sxz}(s,n,i)}{\text{di}(i)} & m=i; n \neq i \\ \text{opi}(s,m) - \dfrac{\text{di}(m)}{\text{di}(i)}\text{opi}(s,i) & n=i; m \neq i \\ \dfrac{\text{opi}(s,i)}{\text{di}(i)} & n=m=i \end{cases}, \tag{16}$$

where the opi terms is a sum of sxz terms multiplied by operators and stands for "operator i,"

$$\text{opi}(s,m) = \sum_k S^{-1}_{mk}\langle k|O_i|\vec{r}_i s\rangle = \sum_{k,s'} S^{-1}_{mk}\langle k|\vec{r}_i s'\rangle\langle s'|O_i|s\rangle = \sum_{s'} \text{sxz}(s',i,m)\langle s'|O_i|s\rangle. \tag{17}$$

The di term is similar to the opi term except that it has $|s_i\rangle$ on the right hand side. This looks like a ratio of determinants and so the name stands for "determinant i."

$$\text{di}(m) = \sum_k S^{-1}_{mk}\langle k|O_i|\vec{r}_i s_i\rangle = \sum_s \text{opi}(s,m)\langle s|s_i\rangle \tag{18}$$

1.1 Calculations with linear correlations

The two most common calculations are of the wave function and the expectation value of the Hamiltonian. To calculate the wave function with linear correlations, first the walkers are operated on by each possible operator and stored in a variable called spx. A variable containing the functions and the operations is stored in the variable f2b.

$$\text{f2b}(iz,jz,ij) = \text{f2b}(iz,jz,ij) + f_{\alpha\beta}(r_{ij}) * \text{spx}(iz,\alpha,i) * \text{spx}(jz,\beta,j) \tag{19}$$

The ratio of determinants, correlated wave function over uncorrelated wave function, is then calculated by sum(d2b*f2b).

The expectation value of the potential includes correlation and potential operators, where one term in the sum may have the form $\left(1 + O_{ij}^c\right) O_{kl}^p$ where the O_{ij}^c and O_{ij}^p are really two operators, the correlation operators being $O_{ij}^c = O_i^c O_j^c$ and similar for the potential operators O_{ij}^p. The sxz needs to be updated twice, once for O_i^c and once for O_j^c, before it can be used for the calculation of the potential. A subroutine called sxzupdate is called twice, which updates the sxz for each operator. This updated sxz is then used to calculate the d2b values that will be multiplied by the potential operators, $\langle ss'| O_{kl}^p |s_k s_l\rangle$. The expectation value is then calculated using the updated d2b similar to the wave function described above.

1.2   Calculations with quadratic correlations

To do calculations with quadratic correlations a subroutine called paircorrelation loops through all of the linear correlation operators updating sxz twice for each pair of operators. This can be seen by looking at one term in the sum of correlations, $1 + O_{ij}^c + O_{ij}^c O_{kl}^c$. The first set of operators, O_{ij}^c is handled as before, and then paircorrelation uses these same operators to update sxz. The updated sxz are then used to calculate and add the additional terms corresponding to quadratic correlations to d2b. The subroutine paircorrelation includes the function values $f_{\alpha\beta}$ in each pair update, allowing the ratio of determinants to be calculated in the same way as before, sum(d2b*f2b).

One term in the sum of the expectation value of the potential may have the form $\left(1 + O_{ij}^c + O_{ij}^c O_{kl}^c\right) O_{mn}^p$, which can be written in a more instructive way combining the i and j operators, $\left(1 + O_{ij}^c \left(1 + O_{kl}^c\right)\right) O_{mn}^p$. When the sxz is updated for the $O_i^c O_j^c$ operators the d2b values corresponding to the linear term are added as before, however paircorrelation is also called which updates sxz for the $O_k^c O_l^c$ operators as well. The resulting sxz is now updated for all 4 of the quadratic correlation operators. This sxz is then used to add the d2b values which are then multiplied by the potential operators, $\langle ss'| O_{mn}^p |s_m s_n\rangle$.

1.3   Operator Breakup

In cartesian coordinates the $v6'$ operators, $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$, $\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, S_{ij} and $S_{ij} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, where $S_{ij} = 3\boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$, can be written by 39 operators, 3 for the $\tau_{i\alpha} \tau_{j\alpha}$, 9 for the $\sigma_{i\alpha} \sigma_{j\beta}$ and 27 for the $\sigma_{i\alpha} \sigma_{j\beta} \tau_{i\gamma} \tau_{j\gamma}$ operators, where the α, β and γ indecies loop over the cartesian coordinates x, y, and z. If instead of using cartesian coordinates the coordinates $\hat{r}_{ij}$ plus two orthogonal coordinates are used the number of required operators can be reduced to just 15. This is because the $\boldsymbol{\sigma}_i \cdot \hat{r}_{ij}$ term in the tensor operator only leaves one nonzero piece, unlike the cartesian breakup which leaves all three. Now the operators are 3 for the $\tau_{i\alpha} \tau_{j\alpha}$, 3 for the $\sigma_{i\alpha} \sigma_{j\alpha}$ and 9 for the $\sigma_{i\alpha} \sigma_{j\alpha} \tau_{i\beta} \tau_{j\beta}$ operators, where α and β now loop over the 3 new coordinates, $\hat{r}_{ij}$ plus two orthogonal coordinates.

2   Motivation

Understanding the interactions between nucleons has been a lengthy and difficult task to persue for science. Despite the difficulty, science has been making continuous steps along the way. In 1935 Hideki Yukawa proposed the idea that this interaction, called the strong

force, was governed by quanta or exchange particles [1]. These particles were later called gluons. From this idea was born the idea of the Yukawa potential, which is still used in modified form in many nuclear models today. The range of the force proposed by Yukawa was based on the mass of the exchange particle, and the strength of the force was based only on the distance separating the particles. Today we often use potentials that depend on the separation distance between the particles, but also their relative spins and isospins. These interactions can be quite complicated making a true understanding of the strong force difficult to achieve.

Currently it is believed that Quantum Chromodynamics (QCD) is the most correct theory to describe the strong force. However, due to asymptitic freedom at low energies, this theory becomes quite difficult to use and so other, approximate methods are often used to study the strong interaction. This is why we use Monte Carlo simulations to investigate different aspects of the strong interaction.

Continuing to better understand the interactions between nuclei will advance our understanding of many important processes in the universe.

3 Hartree Fock Method

Hartree Fock (HF) is a method used to solve quantum many body problems. One can assume, as inspired by the independent particle model, that the wave function is an antisymmetrized product of unknown single particle orbitals,

$$\psi_{\mathrm{HF}} = \mathcal{A}\prod_{i=1}^{A}\phi_i(\mathbf{r}_i, s_i) = \frac{1}{A!}\det\,\phi_i(\mathbf{r}_i, s_i), \tag{20}$$

where the determinant is called a Slater determinant. This simple wave function assumes that the particles have no interaction other than some potential given by the average of all the other particles, as in mean field theory. HF is then used to determine the single-particle orbitals by minimizing the total energy, i.e. the expectation value of the Hamiltonian. We assume a Hamiltonian with kinetic energy for each particle and a two-body interactions potential of the form

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{A}\nabla_i^2 + \sum_{i<j}\hat{V}_{ij}. \tag{21}$$

The variational principle is then used to minimize the expectation value of the energy, $E = \langle\psi_{\mathrm{HF}}|\,H\,|\psi_{\mathrm{HF}}\rangle$. This is done by varying the single particle orbitals until a minimum in the energy is reached. The minimum energy is an upper bound on the true energy of the system, as given by the variational principle, and the set of orbitals that give the minimum energy gives an estimate to the true wave function of the system.

To do this you can first write the Hamiltonian in terms of single and pair particle operators.

$$H = \sum_{i=1}^{A}\hat{h}_i + \sum_{i<j}\hat{V}_{ij} \tag{22}$$

Then we will write the energy in terms of single particle states $\phi_i(x_i)$ and the operators above. You start with $E_{\text{HF}} = \langle \phi_{\text{HF}} | H | \phi_{\text{HF}} \rangle$, and after some algebra you can show that

$$E_{\text{HF}} = \sum_i \langle i | \sum_j \hat{h}_j | i \rangle + \sum_{i<j} \left(\langle ii | \sum_{k<l} V_{kl} | jj \rangle - \langle ij | \sum_{k<l} V_{kl} | ji \rangle \right). \tag{23}$$

We then use the method of Lagrange's undetermined multipliers to minimize the above energy. If we allow the orbitals to vary, $\phi_i \rightarrow \phi_i + \delta\phi_i$, it can be shown that you get the hartree-fock equations, which are Schrödinger-like equations for the single-particle orbitals, ϕ_i. More on this later.

4 Ab-initio No-Core Shell Model

To describe the No-Core Shell Model (NCSM) I am first going to briefly describe the Shell Model. The nuclear Shell Model is largely inspired by the atomic Shell Model. Both Shell Models rely on the Pauli exclusion principle, which requires that electrons stack up one at a time in each of the angular momentum states available. Since nucleons are spin 1/2, each angular momentum state can have two particles, one with spin up and the other with spin down. In the ground state the total spin of a particle is given by any unpaired particles. In the No-Core Shell Model all particles are allowed to contribute to the angular momentum properties of the nucleus, not just the unpaired particles.

5 Quantum Monte Carlo

Quantum Monte Carlo (QMC) calculations use statistical sampling to solve large integrals that would otherwise be intractable. There are many good resources from which to learn about the many different QMC methods, List some here. Here I will describe the methods that I have used in this dissertation, those being Variational, Diffusion, and auxiliary Field Diffusion Monte Carlo methods.

5.1 Variational Monte Carlo

Before I describe Variational Monte Carlo (VMC), I need to introduce the ideas of Monte Carlo Integration, and the Metropolis algorithm, which will both be used later. to understand VMC.

5.1.1 Monte Carlo Integration

I will illustrate Monte Carlo Integration by imagining that we want to integrate the function $g(\mathbf{R})$ where $\mathbf{R} = \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_n$i, so

$$I = \int g(\mathbf{R}) d\mathbf{R}. \tag{24}$$

We can rewrite this integral in terms of a probability density called an importance function $P(\mathbf{R})$, and $f(\mathbf{R}) = g(\mathbf{R})/P(\mathbf{R})$.

$$I = \int f(\mathbf{R})P(\mathbf{R})d\mathbf{R} \tag{25}$$

Now if the $\mathbf{R}$ are distributed according to $P(\mathbf{R})$ then this integral is the expectation value of $f(\mathbf{R})$, which can be computed by drawing an infinite number of samples of $f(\mathbf{R})$ and taking the average.

$$I = \lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} f(\mathbf{R}_n) \tag{26}$$

The integral can then be approximated by taking a large number of samples giving us

$$I \approx \frac{1}{N}\sum_{n=1}^{N} f(\mathbf{R}_n). \tag{27}$$

This method of integration is useful especially when the dimensions of the integration increase. In many-body quantum mechanics the dimension of the integrals can be quite large, including several dimensions for each particle in the calculation. Monte Carlo Integration only needs to sample each of these dimension decreasing the work required by a substantial amount.

5.1.2 Metropolis Algorithm

Let's assume that we are doing Monte Carlo Integration as described above, but the importance function, $P(\mathbf{R})$, from which the random variables $\mathbf{R}$ are drawn is a simple invertible function. We can then simply generate a random variable from the uniform distribution, u, and then figure out what value of x gives us that value given $P(x) = u$. This works quite well assuming the function $P(x)$ is invertible. But let's say that we can't invert it. This is where the Matropolis algorithm comes in, allowing us to get random samples from $P(x)$ even if it's noninvertible. The Metropolis algorithm is a Markov Chain method that uses only the previous point to determine where the next move will be, i.e. the step doesn't depend on history other than the previous step. These are the steps to the algorithm.

1. Start at a random position, $\mathbf{R}$.

2. Propose a move to a new position $\mathbf{R}'$, pulled from a distribution $T(\mathbf{R}'|\mathbf{R})$, where T can be a Gaussian centered on the current position. This makes sure that too large of steps aren't taken.

3. The probability of accepting the move is given by

$$A(\mathbf{R}'|\mathbf{R}) = \frac{P(\mathbf{R}')}{P(\mathbf{R})} \tag{28}$$

4. If $A \geq 1$, then the move is accepted. Otherwise a random number, u,is generated from a uniform distribution between 0 and 1, and the move is accepted if $A > u$.

5.1.3 VMC

Variational Monte Carlo starts with a trial wave function, ψ_T, that should have some non-zero overlap with the actual ground state wave function, and a Hamiltonian, $\hat{H}$. The expectation value of the Hamiltonian in the trial state gives what is called the variational energy. This variational energy is then an upper bound on the true ground state wave function.

$$E_V = \frac{\int \psi_T^*(\mathbf{R}) \hat{H} \psi_T(\mathbf{R}) d\mathbf{R}}{\int \psi_T^*(\mathbf{R}) \psi_T(\mathbf{R}) d\mathbf{R}} \leq E_0 \tag{29}$$

Multiplying the top integrand by $\psi_T(\mathbf{R})\psi_T^{-1}(\mathbf{R})$ we can rewrite the variational energy as

$$E_V = \frac{\int |\psi_T(\mathbf{R})|^2 \, \psi_T^{-1}(\mathbf{R}) \hat{H} \psi_T(\mathbf{R}) d\mathbf{R}}{\int |\psi_T(\mathbf{R})|^2 \, d\mathbf{R}} \leq E_0. \tag{30}$$

Random walkers are generated, $\{\mathbf{R}_n : n = 1, N\}$, from the distribution $P(\mathbf{R}) = |\Psi_T(\mathbf{R})|^2 / \int |\Psi_T(\mathbf{R})|^2 d\mathbf{R}$. The local energy at each point is found using $E_L(\mathbf{R}) = \Psi_T^{-1}(\mathbf{R}) \hat{H} \Psi_T(\mathbf{R})$. Now rewriting E_V in terms of E_L we get

$$E_V = \int P(\mathbf{R}) E_L(\mathbf{R}) d\mathbf{R}. \tag{31}$$

The local energy can then be sampled using the Metropolis method described above to give the energy.

$$E_V \approx \frac{1}{N} \sum_{n=1}^{N} E_L(\mathbf{R}_n). \tag{32}$$

At this point certain parameters in Ψ_T can be varied until a minimum in the energy is found. A minimum in the energy will be produced when $\Psi_T \to \Psi_0$.

5.2 Diffusion Monte Carlo

Diffusion Monte Carlo (DMC) solves for the ground state by letting the walkers diffuse in imaginary time. You start with the Schrödinger equation

$$\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t}. \tag{33}$$

Now we substitute time for imaginary time using $\tau = it/\hbar$ and notice that this looks similar to the diffusion equation.

$$\hat{H}\Psi = -\frac{\partial \Psi}{\partial \tau} \tag{34}$$

At this point we assume that the solution will consist of exponentials, but we shift the energies by the ground state energy, $V \to V - E_0$ and $E_n \to E_n - E_0$.

$$\Psi(\mathbf{R}, \tau) = \sum_{n=0}^{\infty} c_n \phi_n(\mathbf{R}) e^{-\tau(E_n - E_0)} \tag{35}$$

Then one of the key parts of DMC is that as you let $\tau \to \infty$ all of the states higher than the ground state die because the difference $E_n - E_0$ is non-zero and the intinity τ kills the exponential. This leaves only the ground state.

$$\lim_{\tau \to \infty} \Psi(\mathbf{R}, \tau) = \sum_{n=0}^{\infty} c_n \phi_n(\mathbf{R}) e^{-\tau(E_n - E_0)} \tag{36}$$

5.2.1 Model states: $|\Phi\rangle$

The Slater determinants in the trial wave function are overlaps of the walkers with single particle model states. For a system with spin

$$|s_i\rangle = \begin{pmatrix} a_i \\ b_i \\ c_i \\ d_i \end{pmatrix} = a_i \, |p \uparrow\rangle + b_i \, |p \downarrow\rangle + c_i \, |n \uparrow\rangle + d_i \, |n \downarrow\rangle \,, \tag{37}$$

and K single particle states this would be

$$D = \begin{vmatrix} a_1 \phi_1(\mathbf{r}_1) & a_2 \phi_1(\mathbf{r}_2) & \dots & a_A \phi_1(\mathbf{r}_A) \\ a_1 \phi_2(\mathbf{r}_1) & a_2 \phi_2(\mathbf{r}_2) & \dots & a_A \phi_2(\mathbf{r}_A) \\ \dots & \dots & \dots & \dots \\ b_1 \phi_1(\mathbf{r}_1) & b_2 \phi_1(\mathbf{r}_2) & \dots & b_A \phi_1(\mathbf{r}_A) \\ b_1 \phi_2(\mathbf{r}_1) & b_2 \phi_2(\mathbf{r}_2) & \dots & b_A \phi_2(\mathbf{r}_A) \\ \dots & \dots & \dots & \dots \\ d_1 \phi_1(\mathbf{r}_1) & d_2 \phi_1(\mathbf{r}_2) & \dots & d_A \phi_1(\mathbf{r}_A) \\ \dots & \dots & \dots & \dots \\ d_1 \phi_K(\mathbf{r}_1) & d_2 \phi_K(\mathbf{r}_2) & \dots & d_A \phi_K(\mathbf{r}_A) \end{vmatrix} . \tag{38}$$

The single particle model states are made up of a radial and spin, iso-spin dependent parts,

$$\phi_k = \Phi_{nj} \left[C^j_{cl,m_s} Y_{l,m_l}(\hat{r}_i) \chi_s(s_i) \right]_{j,m_j}, \tag{39}$$

where Φ_{nj} is the radial part and the rest contains the spherical harmonics $Y_{l,m_l}(\hat{r}_I)$ and spin and iso-spin states where the Clebsch-Gordan coefficients ensure the correct j and m_j quantum numbers, and the different states are given by the index k. To accurately describe the wave function of an open shell nuclei each state with the correct total angular momentum and parity J^π and isospin T is included as a seperate Slater determinant.

$$\langle RS | \Phi \rangle_{J^\pi, T} = \sum_n c_n D\{\phi_k(\mathbf{r}_i, s_i)\} \tag{40}$$

Here the c_n coefficients are variational parameters used to minimize the energy given a set of possible state configurations. One of the simplest examples of an open shell nuclei would be ^{6}He whose ground state is a $J^\pi = 0^+$ state. The two protons and two of the neutrons could be in the full $(1S_{1/2})^2$ shell while the two remaining neutrons could be in the $(1P_{3/2})^2$ shell with their $m_j = \pm 3/2, \pm 1/2$ values being equal an opposite to ensure

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that $J = 0$. This state given two possible determinants. Other possible configurations for the two remaining neutrons would be $(1P_{1/2})^2$ with one possible determinant, $(1D_{5/2})^2$ with three possible determinants, $(2S_{1/2})^2$ with one possible determinant and $(1D_{3/2})^2$ with two possible determinants giving a total of nine possible determinants. Notice that the two neutrons could be in a combination of S and D shells but never an S and P or D and P to ensure the parity of the state is positive. The number of determinants used for open shell nuclei will control how accurate the trial wave function is but for closed shell nuclei such as ^{4}He or ^{16}O a single slater determinant describing the full shell configuration is sufficient.

The radial part Φ_{nj} of the single particle states are obtained as bound state solutions to the single particle Schrödinger equation with a Woods-Saxon potential wine-bottle potential add reference here maybe.

$$v(r) = V_s \left[\frac{1}{1 + e^{(r-r_s)/a_s}} + \alpha_s e^{(-r/\rho_s)^2} \right] \tag{41}$$

Here the parameters, V_s, r_s, a_s, α_s and ρ_s are variational parameters used to shape the potential to obtain a minimum in energy.

A simple example of this would be the deuteron. The deuteron is in a iso-spin singlet state, $\frac{1}{\sqrt{2\pi}}(|pn\rangle - |np\rangle)$. To show how the model state, $|\Phi\rangle$ would be built for this I will assume all entries are 1, though in practice the could all take on different numbers to account for the different spacial and spin dependencies of the state. Let's assume that both the neutron and the proton are in a spin up state. In this case the $\Phi(k, i)$ terms, where $k, i = 1, 2$, would take on the following values.

$$\phi(1,1) = (1,0,0,0) = p\uparrow_1 \tag{42}$$
$$\phi(2,1) = (0,0,1,0) = n\uparrow_1 \tag{43}$$
$$\phi(1,2) = (1,0,0,0) = p\uparrow_2 \tag{44}$$
$$\phi(2,2) = (0,0,1,0) = n\uparrow_2 \tag{45}$$

The determinant of the Slater matrix can then be written as

$$\Psi_T = \det(S) = \begin{vmatrix} \langle k_1|s_1\rangle & \langle k_1|s_2\rangle \\ \langle k_2|s_1\rangle & \langle k_2|s_2\rangle \end{vmatrix} = \begin{vmatrix} p_1 & p_2 \\ n_1 & n_2 \end{vmatrix} = p_1 n_2 - n_1 p_2, \tag{46}$$

which is the singlet state that we wanted to start with.

6 Wave function with independent pair correlations

One of the simplest many particle wave functions is a antisymmetrized product of single particle orbitals. This is often called a Slater Determinant. This wave function represents that long range part of the interactions leaving our short range correlations. The simplest short range correlation that can be formed is Jastrow-like correlation only dependent on space Add reference here.

$$|\psi_T\rangle = \prod_{i<j} f(r_{ij}) |\phi\rangle \tag{47}$$

This does not include any spin-isospin correlations, and also is not cluster decomposable. The most general form for correlations that can be spin-isospin dependent and are cluster decomposable is an exponential form.

$$|\psi_T\rangle = \prod_{i<j} f_c(r_{ij}) e^{\sum_p f_p(r_{ij})\mathcal{O}_{ij}^p} |\phi\rangle \tag{48}$$

If we then assume that the correlations are small we can then expand the exponential to first order getting

$$|\psi_T\rangle = \prod_{i<j} f_c(r_{ij}) \left(1 + \sum_p f_p(r_{ij})\mathcal{O}_{ij}^p\right) |\phi\rangle . \tag{49}$$

From here I'm going to expand this out showing why we previously have use the wave function that we did, and why we are adding the independent pair terms as we have. I will do this by assuming $A = 3$ for convenience. Expanding this out we get

$$\left[f_c(r_{12})\left(1 + \sum_p f_p(r_{12})\mathcal{O}_{12}^p\right)\right]\left[f_c(r_{13})\left(1 + \sum_p f_p(r_{13})\mathcal{O}_{13}^p\right)\right]\left[f_c(r_{23})\left(1 + \sum_p f_p(r_{23})\mathcal{O}_{23}^p\right)\right] \tag{50}$$

$$= f_c(r_{12})f_c(r_{13})f_c(r_{23})\left(1 + \sum_p f_p(r_{12})\mathcal{O}_{12}^p + \sum_p f_p(r_{13})\mathcal{O}_{13}^p + \sum_p f_p(r_{23})\mathcal{O}_{23}^p \right. \tag{51}$$

$$\left. + \sum_p f_p(r_{12})\mathcal{O}_{12}^p \sum_q f_q(r_{13})\mathcal{O}_{13}^q + \sum_p f_p(r_{12})\mathcal{O}_{12}^p \sum_q f_q(r_{23})\mathcal{O}_{23}^q + \sum_p f_p(r_{13})\mathcal{O}_{13}^p \sum_q f_q(r_{23})\mathcal{O}_{23}^q\right) \tag{52}$$

$$= \left[\prod_{i<j} f_c(r_{ij})\right]\left[1 + \sum_{i<j}\sum_p f_p(r_{ij})\mathcal{O}_{ij}^p + \sum_{i<j}\sum_p f_p(r_{ij})\mathcal{O}_{ij}^p \sum_{k<l}\sum_q f_q(r_{kl})\mathcal{O}_{kl}^q + \ldots\right] . \tag{53}$$

In the example with $A = 3$ we only get up to quadratic terms, but you can imagine many more terms if you have more particles. With previous calculations we have approximated this by only taking up to the linear term.

$$|\psi_T\rangle = \left[\prod_{i<j} f_c(r_{ij})\right]\left[1 + \sum_{i<j}\sum_p f_p(r_{ij})\mathcal{O}_{ij}^p\right] |\phi\rangle . \tag{54}$$

What I have done here is kept some, but not all, of the quadratic terms.

$$|\psi_T\rangle = \left[\prod_{i<j} f_c(r_{ij})\right]\left[1 + \sum_{i<j}\sum_p f_p(r_{ij})\mathcal{O}_{ij}^p\left(1 + \sum_{k<l,\text{ip}}\sum_q f_q(r_{kl})\mathcal{O}_{kl}^q\right)\right] |\phi\rangle \tag{55}$$

The sum $\sum_{k<l,\text{ip}}$ is a sum over all of the kl pairs that don't have a particle that matches either the ith or the jth particle. This is the independent pair sum.

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6.1 Fully Quadratic, and why there is a $\frac{1}{2}$

It turns out that if you take all of the quadratic terms you get something like

$$|\psi_T\rangle = \left[\prod_{i<j} f_c(r_{ij})\right]\left[1 + \sum_{i<j}\sum_p f_p(r_{ij})\mathcal{O}_{ij}^p + \frac{1}{2}\sum_{i<j}\sum_p f_p(r_{ij})\mathcal{O}_{ij}^p \sum_{k<l,ij\neq kl}\sum_q f_q(r_{kl})\mathcal{O}_{kl}^q\right]|\phi\rangle. \tag{56}$$

You can see when when you work out the symmetrization operator (along with the sum over $i < j$ particle pairs. You have something like

$$\mathcal{S}\prod_{i<j}(1 + \mathcal{O}_{ij}) = \frac{1}{A!}\sum_{\{p\}}^{A!}\prod_{i<j}(1 + \mathcal{O}_{ij}), \tag{57}$$

where $A!$ are the number of possible permutations for A particles. The product works out to look like

$$(1 + \mathcal{O}_{12})(1 + \mathcal{O}_{13})\dots(1 + \mathcal{O}_{(A-1)(A)}). \tag{58}$$

Since you never get the operators on the same particles before the permutations you will never get the same particles afterwards (so 1213 will never turn into 2525 or 2552 (which would be 2525)), and since operators on different particles commute you will always get sums like $i < j$. There will be $A!$ permutations and each permutation of the products will produce 1 of each of the sets of pairs. Each permutation will produce a 1246 for example, but they will be produced from different terms. The factor of a $\frac{1}{2}$ is simply because of the way I have written the sums. The way I've written the sums I get 1246 and 4612, but those are the same. If I was to write

$$|\psi_T\rangle = \left[\prod_{i<j} f_c(r_{ij})\right]\left[1 + \sum_{i<j}\sum_p f_p(r_{ij})\mathcal{O}_{ij}^p + \sum_{ij<kl}\sum_p f_p(r_{ij})\mathcal{O}_{ij}^p \sum_q f_q(r_{kl})\mathcal{O}_{kl}^q\right]|\phi\rangle. \tag{59}$$

then the factor of a half goes away. *The only problem is I've **ignored commutation terms** that come from switching 2412 to 1224 (wince the f functions for the 2's don't commute).* Notice that both quadratic wave functions scale as A^4 but with different factors. The number of 2-body terms in the fully quadratic scales as $\frac{1}{8}(A^4 - 2A^3 - A^2 + 2A)$. You can figure this out by saying that there are $A(A-2)/2$ pairs, then there are $N(N-1)/2$ of those pairs, where N is the number of pairs $N = A(A-1)/2$. The number of independent pair terms also scales as A^4, but as $\frac{1}{8}A(A-1)(A-2)(A-3) = \frac{1}{8}(A^4 - 6A^3 + 11A^2 - 6A)$.

6.2 $f^p(r_{ij})$ functions in the correlations

In the 2015 review they mention that the $f_{S,T}(r)$ functions are calculated from a Schrödinger-like equation

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + v_{S,T}(r) + \lambda_{S,T}(r)\right] = 0.$$

This equation comes from the fact that when two particles get close to eachother the potential get's really large, think Lennard-Jones potential that is infinite at 0. This gives large energies

in the local energy unless something cancels it. The above equation is the result of trying to cancel these large potential terms. If particles 1 and 2 get close then $v(r_{ij})$ gets large and the corresponding derivative terms must cancel this. The dominant derivative term I don't see where other terms would even come from is the ∇^2 term and the λ encodes all the rest.

7 Some notes about the Pfaffian wave function

Here are a few useful properties of the pfaffian of a skew-symmetric matrix.

1. If you multiply row i and column i by a constant the resulting pfaffian will be multiplied by that constant. Just a row or column will multiply the pfaffian by the square root of that constant.

2. Simultaneously interchanging two rows (and corresponding columns) will change the sign of the pfaffian.

3. Adding the multiple of a row (and a corresponding addition with a column) to another row (and column) will not change the pfaffian.

In the code there are a few things that I want to make sure I understand before I continue on.

1. How they build the ϕ_{ij}.

2. How they calculate the pfaffian.

3. How they calculate the potential

    (a) How do they do $\mathcal{O}_i \phi ij$, etc?

To address how they build ϕ_{ij} let's start in wavebcs.f90 in the hpsi subroutine. The pf(2,2,A,A) parameter in the code I think would be best as pf(si,sj,i,j), where i and j are the particles and si and sj are the spins (up and down) of each neutron. The pf for 2 specific particles is passed to pairfn in orbital.f90, where it's calculated as

$$pf(1,2) = vk(1) + \sum_{i=2}^{nk} 2vk(i)\cos(\mathbf{k}_i \cdot \mathbf{r}), \tag{60}$$

where the vk are the amplitudes for each k vector, and the factor of 2 accounts for the fact that each i has a positive and a negative value, except for the zero case, $vk(1)$. For each set of particles the pf(2,1)=-pf(1,2) which is assume comes in when forming the singlet state. This is done when the radial part of the pair-state, pf is dotted with the spin states with dotsp in wavebcs.f90. It calculates for each particle i

$$dotsp(j) = |\uparrow\rangle_i |\uparrow\rangle_j \,\phi(1,1) + |\uparrow\rangle_i |\downarrow\rangle_j \,\phi(1,2) + |\downarrow\rangle_i |\uparrow\rangle_j \,\phi(2,1) + |\downarrow\rangle_i |\downarrow\rangle_j \,\phi(2,2) \tag{61}$$

$$= \left(|\uparrow\rangle_i |\downarrow\rangle_j - |\downarrow\rangle_i |\uparrow\rangle_j\right)\phi(1,2) \tag{62}$$

$$= \text{spin-singlet * radial ij function}, \tag{63}$$

where we have used $\phi(1,1)$ and $\phi(2,2)$ are zero and $\phi(1,2) = -\phi(2,1)$. Also, the 1 and 2 in ϕ refer to spin up and down respectively.

The k vectors are stored in the code as ak and are calculated, along with their weights in setupk in kshell.f90. It calculated ak as $ak = 2\pi/L * ik$ where ik is the standard k vectors (0,0,0), (0,0,1), etc, so the ak are ready to dot into the **r** vectors. The vk are read into setupk.

The calculate the pfaffian the skew-symmetric matrix is first formed. In this case it's simply the dotsp calculated above for each particle i. In the code they also include single particle terms which are then used to build a determinant I believe. The pfaffian is then calculated using the subroutine pfaf from pfaffian.f90. See Kevin's notes about how to calculate the pfaffian and decide how much to include in this, since it seems semi-complicated.

7.1 Calculate the Pfaffian

First of all the pfaffian is defined as $\text{Pf}(A) = \mathcal{A}[\phi_{12}\phi_{34}\ldots\phi_{N-1,N}]$, where A is the skew symmetrix matrix

$$A = \begin{pmatrix} 0 & \phi_{12} & \phi_{13} & \cdots & \phi_{1N} \\ -\phi_{12} & 0 & \phi_{23} & \cdots & \phi_{2N} \\ -\phi_{13} & -\phi_{23} & 0 & \cdots & \phi_{3N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\phi_{1N} & -\phi_{2N} & \phi_{3N} & \cdots & 0 \end{pmatrix}. \tag{64}$$

To calculate the pfaffian the code uses the property that for block diagonal (each skew-symmetric) matricies the pfaffian can be written as

$$\text{Pf}(A) = \text{Pf}\begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix} = \text{Pf}(A_1)\text{Pf}(A_2). \tag{65}$$

So if you can use Gaussian elemination to write the matrix A_1 as something like

$$A_1 = \begin{pmatrix} 0 & \phi_{12} \\ -\phi_{12} & 0 \end{pmatrix}, \tag{66}$$

and then $\text{Pf}(A)$ will be $\phi_{12}\text{Pf}(A_2)$. If the matrix is more than 4x4 then you could then use the process again to calculate the pfaffian of A_2.

Kevin showed this for a 4x4 matrix. He showed that you could write the Gaussian eliminated block matrix as

$$A'' = \begin{pmatrix} 0 & a_{12} & 0 & 0 \\ -a_{12} & 0 & 0 & 0 \\ 0 & 0 & 0 & a_{34} + \frac{a_{14}a_{23}}{a_{12}} - \frac{a_{13}a_{24}}{a_{12}} \\ 0 & 0 & -a_{34} - \frac{a_{14}a_{23}}{a_{12}} + \frac{a_{13}a_{24}}{a_{12}} & 0 \end{pmatrix}. \tag{67}$$

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He also points out that this operation can be calculated as

$$A'' = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \frac{a_{23}}{a_{12}} & -\frac{a_{13}}{a_{12}} & 1 & 0 \\ \frac{a_{24}}{a_{12}} & -\frac{a_{14}}{a_{12}} & 0 & 1 \end{pmatrix} \underbrace{\begin{pmatrix} 0 & a_{12} & a_{13} & a_{14} \\ -a_{12} & 0 & a_{23} & a_{24} \\ -a_{13} & -a_{23} & 0 & a_{34} \\ -a_{14} & -a_{24} & -a_{34} & 0 \end{pmatrix}}_{A} \begin{pmatrix} 1 & 0 & \frac{a_{23}}{a_{12}} & \frac{a_{24}}{a_{12}} \\ 0 & 1 & -\frac{a_{13}}{a_{12}} & -\frac{a_{14}}{a_{12}} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (68)$$

8 Derive Exponential Wave Function

The most general form of the fully correlated wave function is the exponentially correlated wave function given by

$$|\Psi_T\rangle = \left[\prod_{i<j} f_c(r_{ij}) \right] e^{\sum_{i<j,p} f_p(r_{ij})\mathcal{O}_{ij}^p} |\Phi\rangle \quad (69)$$

The exponential is to maintain cluster decomposition of the wave function. The Jastrow spin-isospin independent correlations are handeled independent of my piece of the code and so I will ignore them here which effectively leaves me with

$$|\Psi_T\rangle = e^{\sum_{i<j,p} f_p(r_{ij})\mathcal{O}_{ij}^p} |\Phi\rangle, \quad (70)$$

where the operators in the sum are the standard $v6'$ operators, $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$, $\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, S_{ij} and $S_{ij}\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, where $S_{ij} = 3\boldsymbol{\sigma}_i \cdot \hat{r}_{ij}\boldsymbol{\sigma}_j \cdot \hat{r}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$. In an effort to write this an a sum of squared single particle operators (to be used with the Hubbard Stratanovich transformation) these operators can be written in the form

$$\exp\left(\sum_{i<j,p} f_p(r_{ij})\mathcal{O}_{ij}^p \right) = \exp\left(\frac{1}{2}\sum_{i\alpha,j\beta} \sigma_{i\alpha} A_{i\alpha,j\beta}^{\sigma} \sigma_{j\beta} + \frac{1}{2}\sum_{i\alpha,j\beta} \sigma_{i\alpha} A_{i\alpha,j\beta}^{\sigma\tau} \sigma_{j\beta}\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j + \frac{1}{2}\sum_{i,j} A_{i,j}^{\tau} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j \right). \quad (71)$$

These matricies are simply another way to write the $f^p(r_{ij})$ function. Writting the operators in this form is discussed in more detail in appendix 10. In the code (in psicalc.f90) these matricies are actually called "ftau(npart,npart)", "fsig(3,npart,3,npart)" and "fsigtau(3,npart,3,npart)". These matricies are zero when $i = j$, symmetric and can be written in terms of their eigenvalues and vectors.

$$\sum_{j\beta} A_{i\alpha,j\beta}^{\sigma} \psi_{n,j\beta}^{\sigma} = \lambda_n^{\sigma} \psi_{n,i\alpha}^{\sigma} \quad (72)$$

$$\sum_{j\beta} A_{i\alpha,j\beta}^{\sigma\tau} \psi_{n,j\beta}^{\sigma\tau} = \lambda_n^{\sigma\tau} \psi_{n,i\alpha}^{\sigma\tau} \quad (73)$$

$$\sum_{j} A_{i,j}^{\tau} \psi_{n,j}^{\tau} = \lambda_n^{\tau} \psi_{n,i}^{\tau} \quad (74)$$

The operators can then be written as

$$\exp\left(\sum_{i<j,p} f_p(r_{ij})\mathcal{O}_{ij}^p \right) = \exp\left(\frac{1}{2}\sum_{n=1}^{3A} (O_n^{\sigma})^2 \lambda_n^{\sigma} + \frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{3A} (O_{n\alpha}^{\sigma\tau})^2 \lambda_n^{\sigma\tau} + \frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{A} (O_{n\alpha}^{\tau})^2 \lambda_n^{\tau} \right), \quad (75)$$

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where the operators are given by

$$O_n^\sigma = \sum_{j,\beta} \sigma_{j,\beta} \psi_{n,j,\beta}^\sigma$$

$$O_{n\alpha}^{\sigma\tau} = \sum_{j,\beta} \tau_{j,\alpha} \sigma_{j,\beta} \psi_{n,j,\beta}^{\sigma\tau} \qquad (76)$$

$$O_{n\alpha}^\tau = \sum_j \tau_{j,\alpha} \psi_{n,j}^\tau.$$

Now this is ready to use with the Hubbard Stratanovich transformation

$$e^{-\frac{1}{2}\lambda O^2} = \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{x^2}{2} + \sqrt{-\lambda}xO}. \qquad (77)$$

Writting this set of correlation operators in a more compact way,

$$\exp\left(\sum_{i<j,p} f_p(r_{ij})\mathcal{O}_{ij}^p\right) = \exp\left(\frac{1}{2}\sum_{n=1}^{15A} (O_n)^2 \lambda_n^\sigma\right) \qquad (78)$$

allows for the application of the HS transformation, after breaking it into $15A$ exponentials and ignoring the commutation terms.

$$\exp\left(\frac{1}{2}\sum_{n=1}^{15A} (O_n)^2 \lambda_n^\sigma\right) = \prod_{n=1}^{15A} \frac{1}{\sqrt{2\pi}} \int dx_n e^{-x_n^2/2} e^{\sqrt{\lambda_n}x_n O_n}. \qquad (79)$$

The auxiliary fields can then be drawn from the gaussian distribution, $\exp\left(-x_n^2/2\right)$ and the correlations can be written as follows.

$$\Psi_T(R,S) = \langle RS| \prod_{n=1}^{15A} \frac{1}{N} \sum_{\{x_n\}}^N \frac{1}{\sqrt{2\pi}} e^{\sqrt{\lambda_n}x_n O_n} |\Phi\rangle. \qquad (80)$$

8.1 Cluster Decomposability

A physical multi-particle system has the property of cluster decomposability. This is that when two systems A_1 and A_2, are separated by large distances their composite wavefunction will asymptotically approach

$$|A_1 + A_2\rangle \rightarrow |A_1\rangle |A_2\rangle. \qquad (81)$$

The exponentially correlated trial wave function is cluster decomposable. If a system were split into two parts A_1 and A_2, any pair correlation with a particle in each system would have no contribution to the total wave function because any such correlation would be zero inside the exponential. This is not a property held by the linear or quadratically correlated wave functions.

For example, a system of four particles split into two subsystems and separated by a large distance where the two systems are A_{12} containing particles 1 and 2, and A_{34} containing

particles 3 and 4. Any correlations that correlate particles in different subsystems will be zero. For the linear correlated wave function this will leave the correlationsof the form

$$\langle RS| \left[1 + f_p(r_{12})\mathcal{O}^p_{12} + f_p(r_{34})\mathcal{O}^p_{34}\right] |\Phi\rangle \,, \tag{82}$$

where there is an implicit sum over p operators. This is not of the form $|A_{12} + A_{34}\rangle = |A_{12}\rangle |A_{34}\rangle$ and is thus not cluster decomposable. A similar analysis can be done for the quadratically correlated wave function.

One of the advantages to the exponentially correlated wave function is that is maintains cluster decomposibility. The most basic form for the exponentially correlated wave function ignoring spin-isospin independent Jastrow correlations is

$$\Psi_T = \langle RS| e^{\sum\limits_{i<j} f_p(r_{ij})\mathcal{O}^p_{ij}} |\Phi\rangle \,. \tag{83}$$

Again, any correlations that correlate particles from the two different systems will be zero and the wave function becomes

$$\Psi_T = \langle RS| e^{f_p(r_{12})\mathcal{O}^p_{12}+f_p(r_{34})\mathcal{O}^p_{34}} |\Phi\rangle \tag{84}$$

$$= \langle RS| e^{f_p(r_{12})\mathcal{O}^p_{12}}e^{f_p(r_{34})\mathcal{O}^p_{34}} |\Phi\rangle \,. \tag{85}$$

The walkers $|RS\rangle$ and states $|Phi\rangle$ can be broken up into parts that correspond to the different subsystems and so the wave function can be written as

$$\Psi_T = {}_{12}\langle RS| e^{f_p(r_{12})\mathcal{O}^p_{12}} |\Phi\rangle_{12} \, {}_{34}\langle RS| e^{f_p(r_{34})\mathcal{O}^p_{34}} |\Phi\rangle_{34} \,. \tag{86}$$

This is the same form as equation 81 and is thus a sully cluster decomposed wave function.

9   Exponential of an Operator

To start I'll write down the exponential correlations in their full form. They look something like this

$$\prod_{n=1}^{15A} \frac{1}{\sqrt{2\pi}} \int dx_n e^{-x_n^2/2} e^{\sqrt{-\lambda_n}x_n O_n} \,. \tag{87}$$

This is after the Hubbard-Staratanovich transformation has been applied to the correlations so that the correlations can be sampled from single-particle operators. If they are sampled they take a form something like

$$\prod_{n=1}^{15A} \frac{1}{\sqrt{2\pi}} \sum_{x_n}^{N} \frac{1}{N} e^{\sqrt{-\lambda_n}x_n O_n} \,. \tag{88}$$

It might also be important to note that we have added plus-minus sampling to this... but I'll add that and the square root of the matrix stuff in later.

Now I will talk about each individual operator that we have in the correlations. The 15A operators are $\tau_{\alpha i}$ (3A), $\sigma_{\alpha i}$ (3A), and $\sigma_{\alpha i}\tau_{\beta j}$ (9A). Assuming the basis is $|p\uparrow, p\downarrow, n\uparrow, n\downarrow\rangle$ and stored as a column vector we can write the operators in matrix form as follows.

$$\tau_x = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \qquad \tau_y = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix} \qquad \tau_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

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

$$\sigma_x\tau_x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \qquad \sigma_x\tau_y = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \qquad \sigma_x\tau_z = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

$$\sigma_y\tau_x = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \qquad \sigma_y\tau_y = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \qquad \sigma_y\tau_z = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix}$$

$$\sigma_z\tau_x = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \qquad \sigma_z\tau_y = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix} \qquad \sigma_z\tau_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Now those are easy enough to figure out if you just look at the pauli matricies on a simple spin-1/2 system. But what we really want is the exponential of these matricies with an extra factor up top that looks something like

$$e^{\sqrt{-\lambda_n}x_n O_n}. \tag{89}$$

I'm going to rewrite this with an i in it as

$$e^{i\gamma O_n}, \tag{90}$$

where the $\gamma = \sqrt{\lambda_n}x_n$, for each particular operator. In this way the exponentiated matricies can be written in terms of regular matricies. Plugging this into Mathematica I get the following.

$$e^{i\gamma\tau_x} = \begin{pmatrix} \cos\gamma & 0 & i\sin\gamma & 0 \\ 0 & \cos\gamma & 0 & i\sin\gamma \\ i\sin\gamma & 0 & \cos\gamma & 0 \\ 0 & i\sin\gamma & 0 & \cos\gamma \end{pmatrix} \quad e^{i\gamma\tau_y} = \begin{pmatrix} \cos\gamma & 0 & \sin\gamma & 0 \\ 0 & \cos\gamma & 0 & \sin\gamma \\ -\sin\gamma & 0 & \cos\gamma & 0 \\ 0 & -\sin\gamma & 0 & \cos\gamma \end{pmatrix} \quad e^{i\gamma\tau_z} = \begin{pmatrix} e^{i\gamma} & 0 & 0 & 0 \\ 0 & e^{i\gamma} & 0 & 0 \\ 0 & 0 & e^{-i\gamma} & 0 \\ 0 & 0 & 0 & e^{-i\gamma} \end{pmatrix}$$

$$e^{i\gamma\sigma_x} = \begin{pmatrix} \cos\gamma & i\sin\gamma & 0 & 0 \\ i\sin\gamma & \cos\gamma & 0 & 0 \\ 0 & 0 & \cos\gamma & i\sin\gamma \\ 0 & 0 & i\sin\gamma & \cos\gamma \end{pmatrix} \quad e^{i\gamma\sigma_y} = \begin{pmatrix} \cos\gamma & \sin\gamma & 0 & 0 \\ -\sin\gamma & \cos\gamma & 0 & 0 \\ 0 & 0 & \cos\gamma & \sin\gamma \\ 0 & 0 & -\sin\gamma & \cos\gamma \end{pmatrix} \quad e^{i\gamma\sigma_z} = \begin{pmatrix} e^{i\gamma} & 0 & 0 & 0 \\ 0 & e^{-i\gamma} & 0 & 0 \\ 0 & 0 & e^{i\gamma} & 0 \\ 0 & 0 & 0 & e^{-i\gamma} \end{pmatrix}$$

$$
e^{i\gamma\sigma_x\tau_x} = \begin{pmatrix} \cos\gamma & 0 & 0 & i\sin\gamma \\ 0 & \cos\gamma & i\sin\gamma & 0 \\ 0 & i\sin\gamma & \cos\gamma & 0 \\ i\sin\gamma & 0 & 0 & \cos\gamma \end{pmatrix}
\quad
e^{i\gamma\sigma_x\tau_y} = \begin{pmatrix} \cos\gamma & 0 & 0 & \sin\gamma \\ 0 & \cos\gamma & \sin\gamma & 0 \\ 0 & -\sin\gamma & \cos\gamma & 0 \\ -\sin\gamma & 0 & 0 & \cos\gamma \end{pmatrix}
\quad
e^{i\gamma\sigma_x\tau_z} = \begin{pmatrix} \cos\gamma & i\sin\gamma & 0 & 0 \\ i\sin\gamma & \cos\gamma & 0 & 0 \\ 0 & 0 & \cos\gamma & -i\sin\gamma \\ 0 & 0 & -i\sin\gamma & \cos\gamma \end{pmatrix}
$$

$$
e^{i\gamma\sigma_y\tau_x} = \begin{pmatrix} \cos\gamma & 0 & 0 & \sin\gamma \\ 0 & \cos\gamma & -\sin\gamma & 0 \\ 0 & \sin\gamma & \cos\gamma & 0 \\ -\sin\gamma & 0 & 0 & \cos\gamma \end{pmatrix}
\quad
e^{i\gamma\sigma_y\tau_y} = \begin{pmatrix} \cos\gamma & 0 & 0 & -i\sin\gamma \\ 0 & \cos\gamma & i\sin\gamma & 0 \\ 0 & i\sin\gamma & \cos\gamma & 0 \\ -i\sin\gamma & 0 & 0 & \cos\gamma \end{pmatrix}
\quad
e^{i\gamma\sigma_y\tau_z} = \begin{pmatrix} \cos\gamma & \sin\gamma & 0 & 0 \\ -\sin\gamma & \cos\gamma & 0 & 0 \\ 0 & 0 & \cos\gamma & -\sin\gamma \\ 0 & 0 & \sin\gamma & \cos\gamma \end{pmatrix}
$$

$$
e^{i\gamma\sigma_z\tau_x} = \begin{pmatrix} \cos\gamma & 0 & i\sin\gamma & 0 \\ 0 & \cos\gamma & 0 & -i\sin\gamma \\ i\sin\gamma & 0 & \cos\gamma & 0 \\ 0 & -i\sin\gamma & 0 & \cos\gamma \end{pmatrix}
\quad
e^{i\gamma\sigma_z\tau_y} = \begin{pmatrix} \cos\gamma & 0 & \sin\gamma & 0 \\ 0 & \cos\gamma & 0 & -\sin\gamma \\ -\sin\gamma & 0 & \cos\gamma & 0 \\ 0 & \sin\gamma & 0 & \cos\gamma \end{pmatrix}
\quad
e^{i\gamma\sigma_z\tau_z} = \begin{pmatrix} e^{i\gamma} & 0 & 0 & 0 \\ 0 & e^{-i\gamma} & 0 & 0 \\ 0 & 0 & e^{-i\gamma} & 0 \\ 0 & 0 & 0 & e^{i\gamma} \end{pmatrix}
$$

10 Write potential as squared ops for AFDMC

The spin-isospin dependent potential can be written in the form

$$
V = \sum_p \sum_{i<j} u^p(\hat{r}_{ij}) \mathcal{O}_{ij}^p. \tag{91}
$$

I'm going to just write this out in terms of the simplest set of terms, the $\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$ terms.

$$
V = \sum_{i<j} u^\tau(\hat{r}_{ij}) \mathcal{O}_{ij}^p \tag{92}
$$

$$
= \sum_{i<j} u^\tau(\hat{r}_{ij}) \left(\tau_{ix}\tau_{jx} + \tau_{iy}\tau_{jy} + \tau_{iz}\tau_{jz} \right) \tag{93}
$$

$$
= \sum_{i<j} u^\tau(\hat{r}_{ij}) \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j \tag{94}
$$

$$
= \sum_\alpha \sum_{i<j} u^\tau(\hat{r}_{ij}) \tau_{i\alpha}\tau_{j\alpha}. \tag{95}
$$

These can be rewritten in terms in a martix made of of the u values. In the case of the τ operators this is simple because $A_{i,j}^\tau = u^\tau(\hat{r}_{ij})$. If I rewrite the potential using this, and doing a full sum over all i and j and then dividing by 2 I get

$$
V = \frac{1}{2} \sum_{\alpha,i,j} A_{i,j}^\tau \tau_{i\alpha}\tau_{j\alpha} \tag{96}
$$

Now I want to write this matrix in terms of it's eigenvalues and eigenvectors, which are defined as

$$
A^\tau \psi_n^\tau = \lambda_n^\tau \psi_n^\tau, \tag{97}
$$

or if you want to write them in the matrix multiplication form

$$
\sum_j A_{i,j}^\tau \psi_{n,j}^\tau = \lambda_n^\tau \psi_{n,i}^\tau. \tag{98}
$$

Now I want to write out the A matrix in terms of it's eigenvalues and eigenvectors. I do this using eigenvector decompositon. This is defined as

$$
A = Q\Lambda Q^{-1}, \tag{99}
$$

where Q is the matrix of eigenvectors (so $Q_{ab} = \psi_{ab}$, the ath eigenvector for the bth particle, for example), and Λ is the diagonal matrix of eigenvalues (so $\Lambda_{ab} = \delta_{ab}\lambda_a$). I didn't prove this, but it's roughly believable when you consider the eigenvalue equation, and doing it for each component. Also, if Q is a symmetric square matrix, which it is for us, then you can write $Q^{-1} = Q^T$i. What we have in the potential is $A_{i,j}^\tau$, so we need to write the eigenvector decomposition in terms of the ij^{th} entry. This can be done by using the definitions of matrix multiplication.

$$(A\psi)_i = \sum_j A_{ij}\psi_j \tag{100}$$

$$(AB)_{ij} = \sum_\alpha A_{i\alpha}B_{\alpha j} \tag{101}$$

I'll now use these two equations to get A_{ij} from the definition of eigenvalue decomposition.

$$A_{ij} = \left(Q\Lambda Q^T\right)_{ij} \tag{102}$$

$$= \sum_\alpha \sum_\beta Q_{i\beta}\Lambda_{\beta\alpha}Q_{\alpha j}^T \tag{103}$$

$$= \sum_\alpha \sum_\beta Q_{i\beta}\delta_{\beta\alpha}\lambda_\alpha Q_{\alpha j}^T \tag{104}$$

$$= \sum_\alpha \lambda_\alpha Q_{i\alpha}Q_{\alpha j}^T \tag{105}$$

$$= \sum_\alpha \lambda_\alpha \psi_{i\alpha}\psi_{j\alpha} \tag{106}$$

Now plug this into the equation that we had earlier for the potential to get

$$V = \frac{1}{2}\sum_{\alpha,i,j} A_{i,j}^\tau \tau_{i\alpha}\tau_{j\alpha} \tag{107}$$

$$= \frac{1}{2}\sum_{\alpha,i,j}\sum_n \lambda_n^\tau \psi_{i,n}\psi_{j,n}\tau_{i\alpha}\tau_{j\alpha} \tag{108}$$

$$= \frac{1}{2}\sum_\alpha \sum_n \left(\mathcal{O}_{n\alpha}^\tau\right)^2 \lambda_n^\tau, \tag{109}$$

where

$$\mathcal{O}_{n\alpha}^\tau = \sum_i \tau_{i\alpha}\psi_n^\tau. \tag{110}$$

A similar analysis can be done for the $\mathcal{O}_n^\sigma$ and $\mathcal{O}_{n\alpha}^{\sigma\tau}$ operators.

10.1 Importance Sampling

Fill in here!

10.2 Controlling the run away kinetic energy

11 One Pion Exchange potential

When I get a little for QFT under my belt I'll tackle this.

12 Alessandro Roggero's Correlations

A possible form for spin iso-spin dependent correlations (tensor-tau only here) could be written as

$$S_{ki} \rightarrow S'_{ki} = \left[1 + \sum_d^3 \sum_j^A f_{t\tau}(r_{ji}) \hat{r}_{ji} \cdot \sigma_i \tau_i^d \right] S_{ki}, \tag{111}$$

where the S_{ki} is the usual Slater matrix, and the wave function is given by

$$\Psi_T = \sum_{y_d = \pm 1} det[S'], \tag{112}$$

there being a 6 total auxiliary fields (± 1 for each of the three y_d). One of the main motivations for these correlations (I think) is their improvement on the 2-particle only coupling of the linear correlations, which still being relatively resonable to evaluate. Notice that when taking the determinant for an A nucleon system there will be terms that couple from 1 to A nucleons.

One of the issues with this wave function are the off diagonal correlations that are induced in the correlations function. For example with the
Add a little bit about Alessandro's correlations here One of the problems with the Alessandro's correlations is that they break T^2 and T_z symmetry. That is, there are terms like explain here how it breaks T^2 and T_z and explain how linear or other correlations don't. Also explain how J^2 and J_z are only broken if you include the $\sigma_i \cdot \sigma_j$ terms, which aren't included for now.

One solution to this is to multiply the correlations by a term $e^{-\alpha T^2}$ such that alpha is large enough to exponentially reduce the T^2 and T_z breaking. This added piece to the correlations would take the form

$$\exp\left(-\alpha T^2\right) = \exp\left(-\alpha \sum_\beta \sum_{i,j} \tau_{i\beta} \tau_{j\beta}\right). \tag{113}$$

The Hubbard-Stratanovich transformation can be used on these operators by writting them as an exponential of squared one-body operators.

$$\exp\left(-\alpha T^2\right) = \exp\left(-\alpha \sum_\beta \left(\sum_j \tau_{j\beta}\right)^2\right). \tag{114}$$

In a standard AFDMC calculation the sum over β would then be approximated by a product over β where the commutator terms are small as long as the factor α is small. However, α

must be large in order to eliminate T^2 breaking terms from the wave function and thus this approximation can't be used. Instead we have used the identity

$$\exp\left(\sum_\beta A_\beta\right) = \mathcal{S}\prod_\beta \exp(A_\beta), \tag{115}$$

where the symmetrization operator $\mathcal{S} = \frac{1}{N!}\sum_\pi P_\pi$, permutes the cartesian coordinates $\beta = xyz$. With this identity and the Hubbard-Stratanovich transformation we can write the correlations as

$$\exp\left(-\alpha\sum_\beta\left(\sum_j \tau_{j\beta}\right)^2\right) = \mathcal{S}\prod_\beta \exp\left(-\alpha\left(\sum_j \tau_{j\beta}\right)^2\right) \tag{116}$$

$$= \mathcal{S}\prod_\beta \int dx_\beta \exp\left(-x_\beta^2/2\right)\exp\left(i\sqrt{2\alpha}x_\beta\sum_j \tau_{j\beta}\right) \tag{117}$$

$$\approx \mathcal{S}\prod_\beta \frac{1}{N}\sum_{n=1}^N \exp\left(i\sqrt{2\alpha}x_{n\beta}\sum_j \tau_{j\beta}\right), \tag{118}$$

where the sum over n is a sum over the N sampled configurations of the 3 auxiliary fields. The sum over i can be brought out of the exponential as a product because the operators on different particles all commute. Also the symmetrization operator can be written as a sum over the $3! = 6$ permutations of the β coordinates giving us

$$\frac{1}{6N}\prod_j \sum_{P(xyz)} \sum_{n=1}^N \exp\left(i\sqrt{2\alpha}x_{nx}\tau_{jx}\right)\exp\left(i\sqrt{2\alpha}x_{ny}\tau_{jy}\right)\exp\left(i\sqrt{2\alpha}x_{nz}\tau_{jz}\right) \tag{119}$$

The exponential operators on each particle look identical and can be written in a matrix representation as

$$\exp\left(i\sqrt{2\alpha}x_{nx}\tau_{jx}\right) = \begin{pmatrix} \cos(a_{xn}) & 0 & i\sin(a_{xn}) & 0 \\ 0 & \cos(a_{xn}) & 0 & i\sin(a_{xn}) \\ i\sin(a_{xn}) & 0 & \cos(a_{xn}) & 0 \\ 0 & i\sin(a_{xn}) & 0 & \cos(a_{xn}) \end{pmatrix} \tag{120}$$

$$\exp\left(i\sqrt{2\alpha}x_{ny}\tau_{jy}\right) = \begin{pmatrix} \cos(a_{yn}) & 0 & \sin(a_{yn}) & 0 \\ 0 & \cos(a_y) & 0 & \sin(a_{yn}) \\ -\sin(a_{yn}) & 0 & \cos(a_{yn}) & 0 \\ 0 & -\sin(a_{yn}) & 0 & \cos(a_{yn}) \end{pmatrix} \tag{121}$$

$$\exp\left(i\sqrt{2\alpha}x_{nz}\tau_{jz}\right) = \begin{pmatrix} e^{ia_{zn}} & 0 & 0 & 0 \\ 0 & e^{ia_{zn}} & 0 & 0 \\ 0 & 0 & e^{-ia_{zn}} & 0 \\ 0 & 0 & 0 & e^{-ia_{zn}} \end{pmatrix}, \tag{122}$$

where $a_{xn} = \sqrt{2\alpha}x_{xn}$, $a_{yn} = \sqrt{2\alpha}x_{yn}$, $a_{zn} = \sqrt{2\alpha}x_{zn}$ and in our basis the iso-spin matricies are

$$
\tau_x = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \qquad \tau_y = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix} \qquad \tau_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{123}
$$

Owing to the clean matrix representation of these operators the symmetrized product of exponential operators can be written as one matrix,

$$
\mathcal{M}_{jn} = \frac{1}{6} \sum_{P(xyz)} = \begin{pmatrix} A & 0 & B & 0 \\ 0 & A & 0 & B \\ C & 0 & D & 0 \\ 0 & C & 0 & D \end{pmatrix}, \tag{124}
$$

where

$$
A = e^{ia_{zn}} \cos(a_{xn}) \sin(a_{yn}) \tag{125}
$$
$$
B = \cos(a_{zn}) \left(i \cos(a_{yn}) \sin(a_{xn}) + \cos(a_{xn}) \sin(a_{yn}) \right) \tag{126}
$$
$$
C = \cos(a_{zn}) \left(i \cos(a_{yn}) \sin(a_{xn}) - \cos(a_{xn}) \sin(a_{yn}) \right) \tag{127}
$$
$$
D = e^{-a_{zn}} \cos(a_{xn}) \cos(a_{yn}). \tag{128}
$$

This matrix can then be build and operated on each of the particles.

$$
\exp\left(-\alpha T^2\right) \approx \frac{1}{N} \prod_{j=1}^{A} \sum_{n=1}^{N} \mathcal{M}_{jn} \tag{129}
$$

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Equation 6 in Kevin's notes is

$$P(J, M) |\psi_T\rangle = \frac{2J + 1}{16\pi^2} \int_0^{4\pi} d\alpha \int_0^{\pi} d\beta \int_0^{2\pi} d\gamma \sin(\beta) D_{M,M}^{J*}(\alpha, \beta, \gamma) R(\alpha, \beta, \gamma) |\psi_T\rangle. \quad (130)$$

For the isospin case where $T{=}0$ and $M{=}0$ this can be written as

$$P(0, 0) |\psi_T\rangle = \frac{1}{16\pi^2} \int_0^{4\pi} d\alpha \int_0^{\pi} d\beta \int_0^{2\pi} d\gamma \sin(\beta) e^{-i\sum_i \tau_{zi}\alpha} e^{-i\sum_i \tau_{yi}\beta} e^{-i\sum_i \tau_{zi}\gamma} |\psi_T\rangle, \quad (131)$$

where $D_{0,0}^0(\alpha, \beta, \gamma) = 1$ and the general rotation is $R(\alpha, \beta, \gamma) = e^{-\frac{i}{\hbar}T_z\alpha} e^{-\frac{i}{\hbar}T_y\beta} e^{-\frac{i}{\hbar}T_z\gamma}$, where $T_\delta = \hbar \sum_i \tau_{\delta i}$.

Since the exponential of the pauli operators can be written easily as a matrix I have done this in the code.

$$M_y(\beta) = ety = e^{-i\beta\tau_y} = \begin{pmatrix} \cos(\beta) & 0 & -\sin(\beta) & 0 \\ 0 & \cos(\beta) & 0 & -\sin(\beta) \\ \sin(\beta) & 0 & \cos(\beta) & 0 \\ 0 & \sin(\beta) & 0 & \cos(\beta) \end{pmatrix} \quad (132)$$

$$M_z(\alpha) = etz = e^{-i\alpha\tau_z} = \begin{pmatrix} e^{-i\alpha} & 0 & 0 & 0 \\ 0 & e^{-i\alpha} & 0 & 0 \\ 0 & 0 & e^{i\alpha} & 0 \\ 0 & 0 & 0 & e^{i\alpha} \end{pmatrix} \quad (133)$$

where the pauli matricies are

$$ty = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}, \quad ty = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \quad (134)$$

With these matricies defined this way the isospin projection can be written as

$$P(0, 0) |\psi_T\rangle = \frac{1}{16\pi^2} \int_0^{4\pi} d\alpha \int_0^{\pi} d\beta \int_0^{2\pi} d\gamma \sin(\beta) \prod_i M_z(\alpha, i) \prod_i M_y(\beta, i) \prod_i M_z(\gamma, i) |\psi_T\rangle. \quad (135)$$

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13　Results

I have calculated binding energies with and without the independent pair correlations and compared the results. In both cases we have used the v6 potential and the same operators for the correlations. In each case the weights for each operator was determined variationally. Calculations were done for systems, ^{4}He and ^{16}O and the binding energies are reported in table 1 with and without independent pairs correlations and compared to the experimental value.

Table 1: Binding energies in MeV for ^{4}He and ^{16}O as calculated with and without independent pair correlations (IPC) compared to experimental energies.

	Linear	IndPair	Quadratic	Expt.
^{4}He	-27.0(3)	-26.3(3)	-28.5(2)	-28.295
^{16}O	-114(3)	-132(3)	-143.3(3)	-127.619

I have also calculated the binding energy per nucleon of symmetric nuclear matter with density $\rho = 0.16\text{fm}^{-1}$ of 28 particles with periodic boundary conditions. The energy per nucleon was -14.3(2) MeV without the independent pair correlations and -16.6(2) MeV with the independent pair correlations.
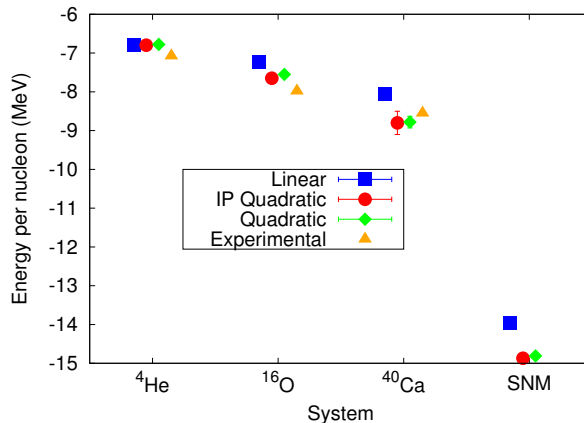

Figure 1: Binding energies for ^{4}He and ^{16}O as calculated with linear, independent pair, and quadratic correlations. Also, the energy per nucleon of symmetric nuclear matter as calculated from 28 particles in a periodic box. All calculations are compared to their expected values.

References

[1] H. Yukawa. On the interaction of elementary particles. i. *Proceedings of the Physico-Mathematical Society of Japan. 3rd Series*, 17:48, 1935.