Improved Trial Wave Functions for Quantum Monte Carlo Calculations of Nuclear Systems and Their Applications

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Outline and Due Dates

Also add a list of figures???
Oliver will probably want to see pictures of scalings and timings. Scaling/processor etc. Include some nice pictures of these things.

1. Background/Motivation Tuesday Feb 19 Hardest section but really important. Make sure to explain why the stuff we're working on is interesting, this will lead into talking about other methods.
   (a) Other methods like HF and no-core shell model
   (b) General outline of the dissertation
2. Quantum Monte Carlo Friday Feb 22
   (a) VMC
   (b) DMC
   (c) AFDMC
      i. Mixed expectation values, operator breakup
   (d) Hamiltonian - Phenomenogolical + χEFT + some results with AFDMC/GFMC
3. Trial Wave Function Friday Feb 15
   (a) Slater Determinants
   (b) Pfaffian Explain what it's used for (superfluidity etc.) and why it's more efficient than the SD stuff (need many thousands of SD's to do the same thing).
   (c) Spin-Isospin Dependent Correlations
      i. Quadratic Correlations - include results
         A. Results
      ii. Exponential correlations . . . why they aren't working or how to do it, cluster decomposition If not working then don't say much about it. Explain that there are large variances that need to be taken care of etc.

(d) Alessandro's wave function with T^2 fix attempts. Maybe . . . maybe don't include

4. Alpha-clustering Friday Mar 1

   (a) Theory

   (b) Results

5. Conclusion Friday Mar 8

   (a) Future Work

Make sure to include stuff for each member of the committee.

1 Background and Motivation

Mention the recent paper Ground-state properties of doubly magic nuclei from the unitary-model-operator approach with the chiral two- and three-nucleon forces, they do calculations using the Unitary-Model-Operation Aproach (UMOA) on the same light doubly-magic systems that we do but using the χEFT NN and 3N potentials with the similarity renormalization group applied (to soften them?). Nuclear physics sheds light on the extremes. From the structure and processes of atomic nuclei and hypernuclei to the formation and structure of some of the largest objects in the universe, neutron stars. One of the largest obstacles to these regimes stems from our incomplete knowledge of the nuclear interation. Once we settle on a possible interaction, the next obstacle is to solve for properties of many-body nuclear systems using the selected, and often complicated, interaction. Currently the popular choices for 2- and 3-body nuclear interactions come in two flavors, phenomenological and those based in Chiral Effective Field Theory (χEFT). There are a large number of methods that have been developed to solve the many-body nuclear problem, though I will be using the Auxiliary Field Diffusion Monte Carlo (AFDMC) method. Other notable methods are the basis set methods such as no core shell model [1, 2], the coupled-cluster method [3], and the self-consistent Green's function method [4, 5]. For these methods the wave function of the nuclear system is written in terms of a truncated basis, often a harmonic oscillator basis. The momentum cutoff of the basis needs to be higher than the important momenta of the interaction that is being used, in order to do calculations in momentum space. This means however that calculations with sharp potentials (like local hard wall potentials) are difficult to do with basis set methods. They do employ techniques such as Similarity Renormalization Group [6] to soften these types of interaction. This allows them to decrease the number of basis functions used. One of the advantages of basis set methods is that they can use local and non-local, i.e. velocity dependent, potentials. The Quantum Monte Carlo (QMC) methods, which we are using in this work, complement these basis set methods. QMC methods are currently limited to mostly local potentials[1] [7], but can converge for a wide variety of local Hamiltonians. Also, Quantum Monte Carlo methods do not have the momentum cutoff limits or the poor scaling with basis set size of the basis set methods. This is from my comp so maybe work it over a bit

[1] Currently, interactions that are linear in the momentum can be used. Higher order terms are treated perturbatively.

One of the most accurate QMC methods is the Green's Function Monte Carlo (GFMC) method, which has had good success calculating properties of light nuclei and nuclear matter using 2- and 3-body potentials as well as electroweak currents [8]. GFMC has been used to calculate binding energies as well as excited states for nuclei up to ^{12}C as well as the nuclear equation of state (EOS) which has been used to study the structure of neutron stars. Nuclear calculations using the GFMC method are limited due to the explicit sum over spin states when calculating expectation values. In 1999 Schmidt and Fantoni [9] proposed the AFDMC method which is practically identical to GFMC in its Monte Carlo sampling of spatial integrals, however AFDMC uses Monte Carlo to sample the spin-isospin sums as well.

Add a bit about HF and how HF, GFMC, and AFDMC all use a similar form for the wave function

In this study, for simplicity, I have only used the AV6' phenom. potential...

Despite the difficulty, science has been making continuous steps toward that understanding. In 1935 Hideki Yukawa proposed the idea that the nuclear interaction, called the strong force, was governed by quanta or exchange particles called pions [10]. From this idea came 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 was based only on the distance separating the particles. Today we often use potentials that depend on the separation distance between 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 asymptotic freedom, at low energies this theory becomes quite difficult to use and so other, approximate methods are often used to study the strong interaction. We use Quantum Monte Carlo methods to investigate different aspects of the strong interaction.

Many approximate methods exist to solve the nuclear many body problem. Some of these include ??????????

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

2 Quantum Monte Carlo

2.1 Variational Monte Carlo

2.2 Diffusion Monte Carlo

2.3 Auxiliary Field Difusion Monte Carlo

Include a bit about GFMC here and show their good results, but also mention the limitations, which lead to needing AFDMC

2.3.1 Mixed Expectation Values and Operator Breakup

3 Hamiltonian

Phenomenological plus χEFT potentials, and compare the two. What makes them different at NN (same operator structure)?

4 Trial Wave Function

An accurate trial wave function can drastically improve the accuracy of a variational QMC method such as VMC. Most highly accurate trial wave functions are entirely computationally intractable and are never implemented in QMC methods. In addition to being accurate and computationally tractable we seek for wave functions that satisfy known physical properties such as cluster decomposition as well as having an overall antisymmetry with respect to particle exchange due to nucleons obeying fermi statistics.

Cluster decomposition arises from the physical intuition that the wave function of two separate, non-interacting systems, A and B as in Figure 1, can be written as the product of their respective wave functions. Mathematically this can be represented as a product of

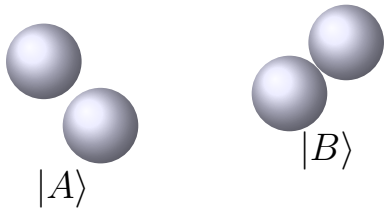

Figure 1: Two non interacting systems A and B, whose composite wave function is the product $|A+B\rangle = |A\rangle\,|B\rangle$.

n-body functions, where n is often 1 or 2 in our situation, though it could be higher. If a system is not cluster decomposable then unphysical correlations between non-interacting systems can occur.

The second property is that the wave function be antisymmetric overall. Since nucleons are fermions and the only degrees of freedom used in these calculations the product of different pieces of the wave function must be antisymmetric. Recent work in QMC has successfully included bosonic degrees of freedom such as pions [11], however that is not the case in this work.

4.1 Slater Determinant

One of the simplest wave functions that satisfies the two properties specified above is the Slater determinant. The Slater determinant has been the starting place for a variety of many-body calculations in nuclear and condensed matter physics alike. In condensed matter the many-body wave functions will often be written in terms of a sum of weighted Slater determinants, where some methods have been able to use a sum of up to 2 billion determinants

[12, 13]. In nuclear physics a single determinant is often used for closed shell calculations and a sum of a small number, $\mathcal{O}(10)$, of weighted determinants is used for open shell systems. A Slater determinant is an antisymmetrized product of single particle (non-interacting) wave functions

$$\Psi_{SD} = \mathcal{A}\left[\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2)\dots\phi_A(\mathbf{r}_A)\right] = \begin{vmatrix} \phi_1(\mathbf{r}_1) & \phi_1(\mathbf{r}_2) & \dots & \phi_1(\mathbf{r}_A) \\ \phi_2(\mathbf{r}_1) & \phi_2(\mathbf{r}_2) & \dots & \phi_2(\mathbf{r}_A) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_K(\mathbf{r}_1) & \phi_K(\mathbf{r}_2) & \dots & \phi_K(\mathbf{r}_A) \end{vmatrix}, \tag{1}$$

where the $\mathcal{A}$ is the antisymitrization operator and the $\phi_i(\mathbf{r}_j)$ are the overlap of the walker positions with the model single particle states. The single particle model states are made up of a radial and spin, iso-spin dependent parts,

$$\phi_k = \Phi_{nj}\left[C^j_{c_l,m_s} Y_{l,m_l}(\hat{r}_i)\chi_s(s_i)\right]_{j,m_j}, \tag{2}$$

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.

$$\langle RS|\Phi\rangle_{J^\pi,T} = \sum_n c_n D\{\phi_k(\mathbf{r}_i, s_i)\} \tag{3}$$

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 and opposite to ensure that $J = 0$. This state has 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.

$$v(r) = V_s\left[\frac{1}{1+e^{(r-r_s)/a_s}} + \alpha_s e^{(-r/\rho_s)^2}\right] \tag{4}$$

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.

The Slater determinant is a mean-field wave function and is often used with Jastrow type short range correlations.

$$addjastrowequationhere \tag{5}$$

These correlations are spin-isospin independent and depend only on the particle separation. These correlations improve upon the uncorrelated Slater determinant wave function significantly Add bit about the functions needing to go to unity to be cluster decomposable ADD PLOT AND CITATION BACKING THIS CLAIM HERE. Make sure to include Jastrow Correlations

4.2 Pfaffian Wave Function

4.3 Spin-Isospin Dependent Correlations

Explain what properties you need, etc.

4.3.1 Quadratic Correlations

Be sure to include results

4.3.2 Exponential Correlations

Why aren't they working

4.3.3 Alessandro's correlations and T^2 fix to them - Maybe just do T^2 fix and apply it to exponential correlations

5 Alpha Particle Formation in Neutron Rich Matter

Include theory here and then talk about the results

6 Conclusion

6.1 Future Work

References

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