Towards Monte Carlo Simulations on Large Nuclei

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Abstract

This paper describes a previously published method to compute properties on neutron matter using variational Monte Carlo simulations, and presents initial work done to use similar methods on large nuclei. Necessary changes to account for protons in these calculations are outlined. In addition, steps taken to optimize the run-time of these calculations are described.

I. Introduction

Properties of large nuclei, such as the ground state wave function, energy, and density distribution, are poorly characterized due to the expanse of the required computational calculations. While light nuclei have been studied extensively, calculations on heavier species are rare. Characterizing large nuclei is important to our understanding of nuclear, atomic, and even molecular processes. Thus, a better method must be found to make such calculations.

Wlazłowki et al. [1] recently published a method of performing variational Monte Carlo calculations on neutron matter comprised of up to 340 neutrons on a 10^3 discretized lattice. This work represents a significant step in the treatment of large systems, and acts as a starting point to study more complex systems such as nuclei. This paper will describe the computational process used by Wlazłowki et al. to perform calculations on neutron matter, as well as characterize changes that are being made in order to use a similar method to study large nuclei.

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II. Quantum Monte Carlo

This section provides a brief overview of Quantum Monte Carlo in general and the specific calculations used by Wlazłowki et al. This method was taken as a starting point to perform calculations on nuclei.

The basic principle of Quantum Monte Carlo is to use imaginary time evolution to project out the ground state wavefunction of a many-body system,

$$\lim_{\tau\to\infty} e^{-\tau\hat{H}}\psi_0 \to \psi \tag{1}$$

where ψ_0 is an arbitrary initial trial state that overlaps the ground state of the system.

In order to actually perform computational calculations, the Trotter Decomposition method is used to rewrite this expression in terms of small iterative imaginary time steps, $\Delta\tau$.

$$\lim_{\Delta\tau\to 0, N\to\infty} e^{-N\Delta\tau\hat{H}}\psi_0 \to \psi \tag{2}$$

The following approximation can then be made to break the Hamiltonian into its kinetic and

potential components.

$$e^{-\Delta\tau\hat{H}} \approx e^{\frac{-\Delta\tau\hat{T}}{2}} e^{-\Delta\tau\hat{V}} e^{\frac{-\Delta\tau\hat{T}}{2}} \quad (3)$$

Thus, the imaginary time evolution of the ket can be written as

$$e^{-\tau\hat{H}} |\psi_0\rangle = \left(e^{\frac{-\Delta\tau\hat{T}}{2}} e^{-\Delta\tau\hat{V}} e^{\frac{-\Delta\tau\hat{T}}{2}}\right)^N |\psi_0\rangle \quad (4)$$

Note that the bra is evolved in a identical manner independently.

Since $\hat{T}$ is a one-body operator and ψ_0 can be expressed as a Slater Determinant, calculation of $e^{-\Delta\tau\hat{T}}\psi_0$ simply returns another Slater Determinant. However, calculation of $e^{-\Delta\tau\hat{V}}\psi_0$ returns a sum of Slater Determinants, causing the evolution problem at hand to increase exponentially.

The Hubbard-Stratonovich Transformation, expressed here in its continuous form,

$$e^{-\left(\frac{\Delta\tau}{2}\right)\lambda\hat{A}^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx e^{\frac{-x^2}{2}} e^{x\sqrt{-\Delta\tau\lambda}\hat{A}} \quad (5)$$

can be used to express $e^{-\Delta\tau\hat{V}}$ in terms of solely one-body operators, preventing this exponential scaling.

Applying this transformation to the iterative evolution process results in a multi-dimensional integral that can be expressed in the form

$$\prod_n^N \int dx_{n,i}\, \rho(x) \hat{O}(x) \quad (6)$$

where $\rho(x)$ is defined as some probability density and $\hat{O}(x)$ is a one-body evolution operator.

In order to accurately converge upon the ground state wave function, the number of imaginary time steps, N, must be sufficiently large. Thus, calculation must be done over a nearly infinite dimensional space. Accounting for every contribution to this integral is a time-consuming and impractical effort. Thus, Monte Carlo methods are used, where contributions are randomly sampled across the parameter space. This method allows for considerably faster and more accurate convergence.

III. Fermion Sign Problem

Few calculations of this size have been attempted previously because Quantum Monte Carlo simulations have limited applicability in fermionic systems. In order to successfully use Monte Carlo techniques, the integrand of the multi-dimensional integral in question must be positive definite. While this is the case for bosonic systems, due to antisymmetry, fermionic integrals oscillate, taking on both positive and negative values. This leads to cancellations and a loss of significance in calculations. This occurrence is known as the fermion sign problem.

In order to avoid this sign problem, Wlazłowki et al. define an effective Hamiltonian

$$\hat{H}_{ev} = \hat{T} + \hat{V}_{ev} \quad (7)$$

in which V_{ev} is spin-independent and attractive in momentum space. Defining the potential in such a manner keeps the integrand positive definite, thus eliminating the sign problem.

The approximate ground state wave function can be found by evolving the bra and ket wavefunctions with the evolution Hamiltonian as described in the above section. The remaining components of the full potential,

$$\delta\hat{V} = \hat{V} - \hat{V}_{ev} \quad (8)$$

can then be treated pertubatively, such that to leading order,

$$E \lesssim \langle\psi| \hat{H}_{ev} |\psi\rangle + \langle\psi| \delta\hat{V} |\psi\rangle . \quad (9)$$

IV. Addition of Protons

This section describes work in progress to use the methods described above to move from calculations on neutron matter to calculations on nuclei. Adding protons to the systems requires that several changes must be made, namely, the trial wave function used, definition of the evolution potential, and treatment of the perturbative corrections to the potential.

I. Trial Wave Function

In the previous calculations done by Wlazłowki et al. on neutron matter, plane waves were used as trial wave functions. Neutron matter is in a gaseous state, meaning that the neutrons can be treated as approximately free particles, and plane waves are adequate as a first approximation to the wave function.

This is no longer the case for nuclei, where interactions between particles are mush stronger. Trial wave functions for calculations on nuclei are instead based on the eigenfunctions of the three-dimensional harmonic oscillator,

$$\Psi_n = NH_{n_x}(x)H_{n_y}(y)H_{n_z}(z)\mathrm{e}^{-r^2/2r_0^2} \qquad (10)$$

where

$$r_0^2 = \frac{\hbar}{m\omega} \qquad (11)$$

In order to define an appropriate trial wave function, r_0^2 must be calculated based on the total quantum number n of the system, and the product of the three Hermite polynomials of order n_x, n_y, and n_z, must also be found.

II. Evolution Potential

In addition to the trial wave function, the evolution potential must also be updated from calculations on neutron matter to calculations on nuclei. This follows because while neutron matter has uniform density, nuclei do not. Potential interactions between nucleons are not only dependent on the distance between nucleons, expressed as k in momentum space, but also where in the nuclei those nucleons are located, defined by r. Viewing the nuclei as spherically symmetric, there is a direct correlation between r, and the density, n. Thus, we require a definition of the evolution potential that is dependent on both k and n.

For both neutron matter and nuclei, the evolution potential can be described as the sum of three Yukawa interactions and a constant,

$$V_{ev} = \sum_{i=\pi,\sigma,\omega} \frac{V_i M_i^2}{k^2 + M_i^2} + V_0 \qquad (12)$$

where each term represents interactions by pion exchange, sigma boson exchange, and omega boson exchange, respectively. In each case, V describes the strength of the interaction, while M refers to the mass of the particle in the exchange. V_π and M_π are known from previous experiments, while the four remaining parameters are fit at each density to minimize phase shifts.

To perform calculations on neutron matter, evolution potentials were constructed at various constant densities (See Figure 1).

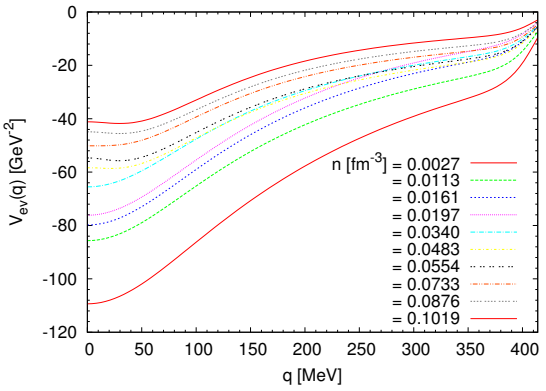

Figure 1: *Evolution potential vs. momentum at various constant densities. Figure from Wlazłowki et al. [1]*

For calculations on nuclei, these potentials are needed as a function of density as well as momentum. Interpolation between the constant density curves was considered, but ultimately proved to compromise the speed of calculations. Instead, the σ and ω parameters were recalculated using the results at the previous density as a starting point in an effort to create smooth curves. These points were then fitted to third and fourth-degree polynomials.

Redefining these parameters as continuous functions allows for the rapid calculation of the evolution potential at any value of n and k, as depicted in Figure 4. The validity of these new evolution potentials was assessed by recalculating approximate ground state energies for neutron matter at four densities. These values are compared to the previous results reported by Wlazłowki et al. in Table 1. At low densi-

ties, the approximate energies calculated from the new potentials match those of calculated from the old potential curves to within error. At higher densities, the new potentials report slightly higher energies, a discrepancy which can be further studied and possibly corrected.

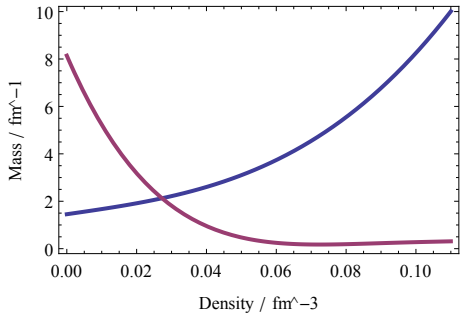

Figure 2: *Polynomial fits for mass parameters as a function of density. Blue = M_σ, purple = M_ω*

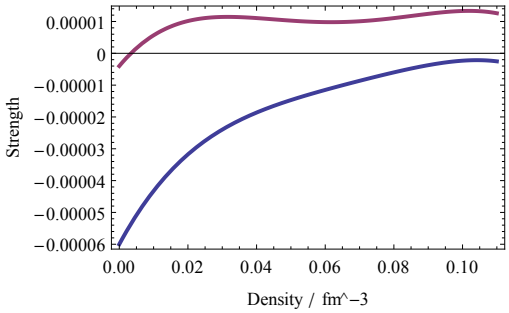

Figure 3: *Polynomial fits for strength parameters as a function of density. Blue = V_σ, purple = V_ω*

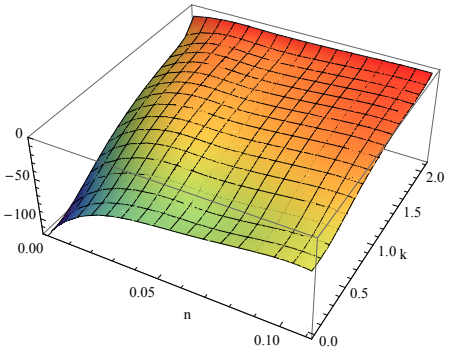

Figure 4: *Evolution potential surface for varying n (in fm^{-3}) and k (in fm^{-1}). Potentials are given in GeV^2.*

Density	Previous V	New V
0.00655	2.154 ± 0.025	2.151 ± 0.332
0.0113	3.048 ± 0.016	2.939 ± 0.279
0.0554	8.250 ± 0.012	8.560 ± 0.130
0.1019	12.862 ± 0.007	13.518 ± 0.019

Table 1: *Comparison of $\langle\psi|\,\hat{H}_{ev}\,|\psi\rangle$ calculated from old and new evolution potentials. Densities are given in fm^{-3}, potentials are given in MeV/N.*

III. Isospin Dependence

After computing the expectation value of the evolution Hamiltonian, corrections are made to the ground state energy via perturbation theory. Many of these components of the full potential have isospin dependence. Some of the potential terms, such as the one describing one-pion exchange [2],

$$V_{1\pi} = \frac{g_A^2}{4f_\pi^2}\vec{\tau}_1\cdot\vec{\tau}_2\frac{\vec{\sigma}_1\cdot\vec{q}\,\vec{\sigma}_2\cdot\vec{q}}{q^2+m_\pi^2} \tag{13}$$

have explicit dependence on $\vec{\tau}$, the isospin matrix.

Other components of the potential are not applicable in neutron matter due to the Pauli Principle. For example, the three-body contact force shown in Figure 5 does not contribute in neutron matter as it is impossible to have three distinguishable particles interacting. However, there is a contribution to the potential from this term when protons are introduced into the system. Cases like these must be accounted for in order to accurately describe the potential of the system.

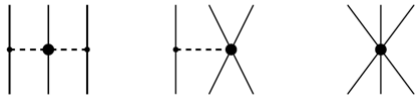

Figure 5: *Feynman diagrams depicting three-body force contributions to the interaction potential at next-to-next-to-leading-order (NNLO). From left to right: two-pion exchange, one-pion exchange, and contact interactions. Figure from Machleidt and Entem. [2]*

V. CUDA and Parallel Programming

Nuclei, with the addition of protons, are more complex systems than neutron matter. In order to deal with the growing complexity of the problem, computational efforts are in the process of being moved from a CPU platform to a GPU platform, where more transistors are devoted to data processing.

The parallel programming and computing platform CUDA was used to help parallelize the code and make use of both host and device memory. In CUDA, kernels are set up as parallel portions of code to be executed on the device by an array of parallel threads which constitute a block. This basic set-up is shown in Figure 5.

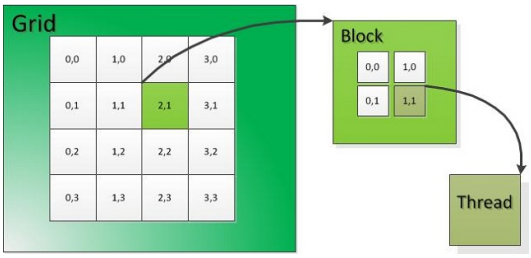

Figure 6: *Schematic of the CUDA grid system depicting blocks and threads. Figure from cs.cmu.edu.*

In order to optimize the nuclei calculations, a separate stream is created for each wavefunction to be evolved. This allows the kernel evolution operators to be run in parallel, evolving each wavefunction at the same time, and reducing computational run-time.

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References

[1] G. Wlazłowski, J. W. Holt, S. Mororz, A. Bulgac, K. J. Roche. arXiv:1403.3753 (2014)

[2] R. Machleidt, D. R. Entem. Phys. Rept. **503**, 1 (2011)