Research Project Request

Quantum Monte Carlo Calculations of Nucleon Systems and Cold Atom Gases

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Abstract

This research project request is for 500,000 SUs on Stampede. We will use Quantum Monte Carlo methods to study nucleon systems and cold atom gases. One of our goals is to include explicitly the pionic degrees of freedom in the simulations. We also plan to study vortex excitations in both cold atom gases and low-density neutron matter. Our large-scale highly-parallel code has been successfully used to calculate properties of nuclear matter, neutron matter and medium-mass nuclei in the past.

1 Research Objectives

This allocation request is intended to provide the computational resources to carry out the project *Quantum Monte Carlo (QMC) Calculations of Nucleon Systems* supported by the National Science Foundation grant PHY-1404405, and related projects.

Many nuclear processes in our universe occur under extreme conditions in supernovae and neutron stars. The properties of nuclei and nuclear matter under these conditions, which are difficult or impossible to reproduce in the laboratory, must necessarily be calculated theoretically. These data are needed to understand astrophysically important systems and processes such as neutron rich matter, neutron stars, supernovae, and r-process nucleosynthesis and neutrino scattering. The quantum many-particle methods developed within this project have broad applications across many areas of physics, including nuclear physics, cold atomic gas research, and electronic structure. Methods previously developed within this project have been applied in each of these areas.

The results of this project are relevant for the nuclear physics program at the Department of Energy Office of Science, that has identified the knowledge of the structure of nuclei and nuclear

matter as one of the most important scientific questions in nuclear physics in the most recent Nuclear Science Advisory Committee long-range plan. This proposal consists mainly of two projects, which we describe in the following sections.

1.1 Improved QMC simulations for nuclei and nuclear matter

Most QMC simulations of nuclear matter model particles interacting via instantaneous two- and three-body potentials [1]. Usually these potentials are derived from chiral effective field theories for nuclear structure by approximately integrating out the field degrees of freedom. Our goal is to include explicitly the low energy degrees of freedom of the pion field in the QMC simulations, while the high energy degrees of freedom will be included in the instantaneous potentials. We will develop an expression for the low energy components of the pion field, the potential for the high energy degrees of freedom, the Hamiltonian of the system and suitable wavefunctions for this problem.

In QMC the results are highly dependent on the accuracy of the wave function. Currently the trial wave function is only correlated up to linear order as in [2]. We will be including quadratic correlations to the trial wave functions of nuclei and nuclear matter.

1.2 Strongly paired fermionic systems: cold atoms and neutron matter

Strongly paired fermions are important in many contexts, for example cold Fermi atom experiments and low-density neutron matter [3, 4]. Developing a quantitative understanding of strongly paired Fermi systems is important since they are a unique regime for quantum many-body physics. Cold atom experiments can provide direct tests of the equation of state and the pairing gap in the strongly paired regime, and provide a benchmark of many-body theories in these systems.

Ultracold atomic gases and low-density neutron matter are unique in the sense that both exhibit pairing gaps of the order of the Fermi energy [5]. The neutron scattering length is about -18.5 fm which is significantly larger than the interparticle spacing and the interaction range 2.7 fm, therefore low density neutron matter is near unitarity. In this regime both dilute cold fermion atoms and neutron matter have similar properties [6]. The possibility of tuning particle-particle interactions experimentally in cold atomic gases provides an emulation of low-density neutron matter, which is beyond direct experimental reach. We have studied the vortex structure in cold atomic gases [7] and we intend to extended these calculations to direct simulations of vortices in superfluid neutron matter using nuclear Hamiltonians.

Superfluidity of neutron matter is of great interest across astrophysics, nuclear physics and many-body physics [8]. The occurrence of superfluidity in neutron matter is one of many examples of pairing effects in low-density many-fermion systems. One signature of superfluidity is the formation of quantized vortices and many questions remain to be answered concerning the structure of the vortex core in neutron matter. This project will be to simulate vortex excitations in superfluid

neutron matter using QMC methods. Possible properties to be calculated are the vortex excitation energy, the superfluid pairing gap and the equation of state.

2 Computational Methods

We will use QMC methods, in particular Auxiliary Field Diffusion Monte Carlo (AFDMC) methods, which have proven to be very successful in calculating ground state properties including momentum distributions, as we have shown in our article for Reviews of Modern Physics [1]. The AFDMC code has been successfully used to calculate properties of nuclear matter, neutron matter, and medium-mass nuclei [2]. The results of [9] showed the relation between the symmetry energy and properties of neutron stars.

We have written a large-scale highly-parallel code to achieve high precision calculations for many properties of medium-mass nuclei. The AFDMC code calculates the ground-state of the nucleus through a branching random walk algorithm, and can be used to compute other properties including radii and momentum distributions.

2.1 Algorithm and implementation

The AFDMC code has been developed by the investigators of this project. The AFDMC method is used to extract the ground-state component of the system from the variational ansatz describing the system. This is done with a projection in imaginary-time, i.e. we calculate

$$\lim_{n\to\infty} \left[e^{-H\delta\tau}\right]^n \Psi_T(R,S) \to \Psi_0(R',S'), \tag{1}$$

where $R = (r_1, \cdots, r_N)$ are the coordinates of nucleons, $S = (s_1, \cdots, s_N)$ are complex numbers indicating their spin and isospin projections, and $\Psi_T(R,S)$ is a trial variational wave function. The algorithm is a branching random walk that requires the diagonalization of $3N \times 3N$ matrices (N is the number of particles) at each step of the random walk. AFDMC is written in Fortran90 and MPI, and uses the vendor optimized BLAS and LAPACK libraries to perform matrix diagonalizations at each step.

The AFDMC algorithm is a variant of Diffusion Monte Carlo, where each step involves:

1. Diffuse nucleon's positions, $R \to R'$ according to the kinetic energy T of the Hamiltonian.
2. Rotate nucleon's spins, $S \to S'$, according to the spin and isospin-dependent potential.
3. Calculate the weight W of the new configuration, and generate N replicas of the new configuration according to $N = [W + \eta]$, where η is a random number uniformly distributed from 0 to 1.

This algorithm is implemented by considering a collection of configurations (called *walkers*) that are simultaneously evolved in imaginary-time. The parallelization is accomplished by spreading the configurations among the nodes. However, AFDMC is not embarrassingly parallel because the branching term generates fluctuations in the number of configurations, of the order up to 10%, and the calculation of observables requires an average over walkers at the same imaginary-time. We employ a dynamic load rebalancing after each time step to redistribute walkers across nodes.

3 Application efficiencies

The AFDMC code is written in Fortran90 and MPI. We describe in detail the performance and scaling of our code in the additional document submitted with this proposal. The most relevant feature that we present in that document is the scaling in Stampede.

We used our startup allocation (TG-PHY140003, PI Kevin Schmidt) to test the performance of the code on Stampede. Up to 4096 cores, the largest number tested, the code scales strongly. We intend to perform simulations with a maximum number of 1024 cores.

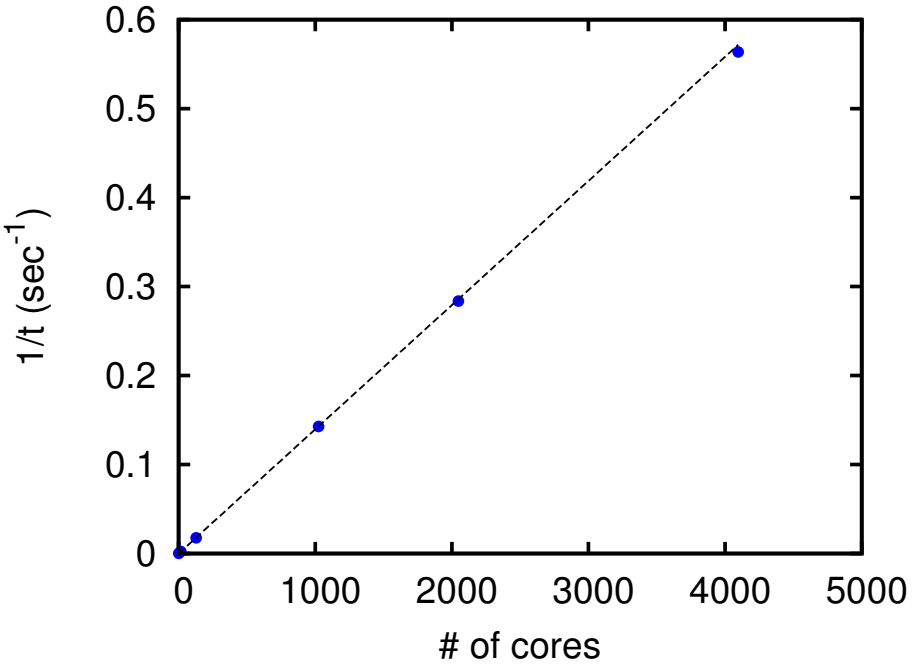

Figure 1: Scaling on Stampede using the time to propagate 10000 configurations of an ^{16}O nucleus for 100 steps.

4 Computational Research Plan and Justification for Requested Resources

As discussed in Sec. 2, the simulations depend on a trial variational wave function. The variational parameters are determined using the stochastic reconfiguration method [10]. Once these parameters are determined, we can proceed with the computation of physical quantities of interest.

4.1 Improved QMC simulations for nuclei and nuclear matter

We base our estimates on the amount of SUs and storage used in [1] and references therein. We want to perform simulations with different system sizes, ranging from one nucleon plus the pion field up to four nucleons plus the pion field, a total of four systems. For each system we require:

- variational optimization of the parameters: for these systems the average amount of SUs necessary for the optimization is approximately 20,000 SUs.
- production runs: longer runs are necessary to compute quantities such as energy of the system, density and other distribution functions, with small variances. We estimate 50,000 SUs for these computations.

4.2 Strongly paired fermionic systems

We base our estimates on the amount of SUs and storage used in [7], the most similar calculation in terms of computational cost. We want to perform simulations with different system sizes, for example 10 different systems with the number of particles varying between 38 and 66 particles. We would also like to vary the interaction strength between particles, for 10 different values of the interaction strength. Hence the total would be of 100 different systems. For each system we require:

- variational optimization of the parameters: for these systems sizes the number of parameters is between 20 and 40 parameters, and the average amount of SUs necessary for the optimization is approximately 400 SUs.
- production runs: longer runs are necessary to compute quantities such as energy of the system, density and other distribution functions, with small variances. We estimate 1,500 SUs for these computations.

4.3 Summary of the requested resources

We present in Table 1 the amount of SUs requested for each task. We are requesting a total of 500,000 SUs on Stampede. The systems of the *Explicit pion field* project require more computation

time (approximately 50 times the variational optimization and 30 times for the production runs) than the systems of the *Strongly paired fermionic systems* because of extra degrees of freedom. In Eq. 1 we have the S coordinates corresponding to spin and isospin projections. These only need to be sampled for the first project, thus the difference in computation times. We also included SUs for the code development, in order to ensure performance and scaling during execution.

Table 1: Justification for the requested amount of SUs

	Explicit pion field	Strongly paired fermionic systems
Development	20,000	10,000
Variational optimization	80,000	40,000
Production	200,000	150,000
Subtotal	300,000	200,000
Total: 500,000 SUs		

As for storage needs, we request the default value. The size of input, output and configuration files is of approximately 50 Mb per system. As the simulations are independent, there is no need to store all of them at the same time at Stampede. We are capable of handling the post-processing of the simulations in our local computing environment.

5 Additional considerations

We believe that we have enough funding, through the NSF grant, and qualified staff to complete the work plan described in this project.

5.1 Qualifications of the PIs and team

PIs

Kevin Schmidt

update Stefano Gandolfi is a nationally and internationally recognized scientist in Many-Body Nuclear Theory. During the past 4 years he has published 25 papers and given 34 invited talks, including many at major national and international conferences. He has about 1,400 citations on Google Scholar. As a result of his excellent work, Gandolfi received the International Union of Pure and Applied Physics prize for young researchers in nuclear physics in 2013. He has led a program in Quantum Monte Carlo at the Institute of Nuclear Theory in 2013.

Graduate students

Lucas Madeira is a PhD student at Arizona State University. He received his Bachelor degree and Masters degree in Physics from the University of Campinas, Brazil. He has experience with High Performance Computing including MPI and OpenMP.

Cody Petrie is a PhD student at Arizona State University. He received a BS in Physics from Brigham Young University in 2014. He has been computational nuclear physics for the past year and a half.

References

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