Research Project Renewal

Quantum Monte Carlo Calculations of Nucleon Systems and Cold Atom Gases

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Abstract

This research project renewal request is for 50,000 SUs on Stampede2. We describe our progress on cold atom gases simulations and nucleon systems calculations. We propose a project related to strongly-interacting Fermi gas systems. We present our progress on explicitly including the pionic degrees of freedom in the nuclear Monte Carlo simulations, and we introduce the next steps, related to larger nuclei. We also have been developing improved trial wave functions for nuclei and nuclear matter, and we intend to continue our research by extending these wave functions to other nucleon systems. In summary, we will continue to employ Quantum Monte Carlo methods to study nucleon systems and cold atom gases, by using our large-scale highly-parallel code, which has been successfully used to calculate properties of cold gases, nuclear matter, neutron matter, and medium-mass nuclei.

1 Research Objectives

This allocation renewal request is intended to provide the computational resources to continue 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.

In this document we summarize the advances we have achieved, in addition to the proposed plan for the current cycle. In Sec. 1.1 we describe an interesting project involving cold atomic Fermi gases. The inclusion of explicit pion field contributions in simulations of nucleon systems is discussed in Sec. 1.2. In Sec. 1.3 we present our study of improved wave functions for nuclei and nuclear matter.

1.1 Three-component Fermi gas

There are three relevant length scales in an attractive two-component Fermi gas: the effective range of the potential r_e, the s-wave scattering length a, and $n^{-1/3}$ the interparticle distance (n being the number density). The diluteness condition corresponds to $n^{-1/3} \gg r_e$, while the BEC scheme coincides with $1/(na^3) \gg 1$, and the BCS scheme $1/(na^3) \ll -1$. At the heart of the BEC-BCS crossover there is the unitary regime, $1/(na^3) = 0$, which is a strongly interacting system with short-range interactions of remarkable properties.

In a three-component Fermi gas there are two more main ingredients: the competition between pairing and binding among different atom pairs, and the role of three-body correlations. The Thomas effect (the collapse of the three-body system as $r_e \to 0$ at fixed a) and the Efimov effect (the accumulation of three-body bound states at threshold as a$\to \infty$ at fixed r_e) are consequences of the strong attraction among three resonating particles. These can occur only if the three particles in the system can overlap in space, which is forbidden by the Pauli exclusion principle in the case of only two species.

At zero temperature, the properties of the system depend on 4 parameters: the three scattering lengths (a_{12}, a_{13}, a_{23}) and the three-body parameter. The authors in Ref. [1] used qualitative arguments and found a rich phase diagram for this system. There were several reports of experimental realizations of a three-component ^{6}Li gas. One of them attributed enhanced three-body recombination in the gas to an excited Efimov trimer state [2]. Another work studied the atom loss in a mixture of atoms and dimers, and found two peaks corresponding to the degeneracy points of the energy levels of the dimers and the ground- and first-excited Efimov trimers [3].

Our objective with this project is to determine properties (such as phase diagrams, equations of state, and pairing gaps) of a dilute gas with three fermionic species at zero temperature. We will employ variational and diffusion Monte Carlo methods to determine properties of these systems. These are many-body methods that have been successfully used by us to calculate properties of strongly-interacting fermionic systems [4–7] using XSEDE resources.

1.2 QMC simulations with explicit contributions from the pion field

In most simulations of nonrelativistic nuclear systems, the wave functions found solving the many-body Schrödinger equations describe the quantum-mechanical amplitudes of the nucleonic degrees of freedom. In those simulations the pionic contributions are encoded in nuclear potentials and electroweak currents, and they determine the low-momentum behavior. In Ref. [6] we presented a novel quantum Monte Carlo formalism in which both relativistic pions and nonrelativistic nucleons are explicitly included in the quantum-mechanical states of the system. We started from the heavy baryon leading order chiral Lagrangian density in which only nucleon and pion degrees of freedom are included,

$$\begin{aligned}\mathcal{L}_0 &= \tfrac{1}{2}\partial_\mu\pi_i\partial^\mu\pi_i - \tfrac{1}{2}m_\pi^2\pi_i\pi_i + N^\dagger\Big[i\partial_0 + \tfrac{\nabla^2}{2M_0} - \tfrac{1}{4f_\pi^2}\epsilon_{ijk}\tau_i\pi_j\partial_0\pi_k - \tfrac{g_A}{2f_\pi}\tau_i\sigma^j\partial_j\pi_i - M_0\Big]N \\ &\quad -\tfrac{1}{2}C_S(N^\dagger N)(N^\dagger N) - \tfrac{1}{2}C_T(N^\dagger\sigma_i N)(N^\dagger\sigma_i N)\,, \end{aligned} \tag{1}$$

where m_π is the pion mass, M_0 is the bare nucleon mass, $f_\pi = 92$ MeV is the pion decay constant, $g_A = 1.26$ is the nucleon axial-vector coupling constant, C_S and C_T are low-energy constants, and $i = x, y, z$. We derived the Hamiltonians for a system composed of A nucleons and pions,

$$\begin{aligned} H &= H_N + H_{\pi\pi} + H_{AV} + H_{WT}, \\ H_N &= \sum_{i=1}^{A}\left[\frac{P_i^2}{2M_P} + M_P + \beta_K P_i^2 + \delta M\right] + \sum_{i<j}^{A}\delta_{R_0}(\boldsymbol{r}_i - \boldsymbol{r}_j)[C_s + C_T\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j], \\ H_{\pi\pi} &= \frac{1}{2}{\sum_{\boldsymbol{k}}}'\left[|\boldsymbol{\Pi}_{\boldsymbol{k}}^c|^2 + \omega_{\boldsymbol{k}}^2|\boldsymbol{\pi}_{\boldsymbol{k}}^c|^2 + |\boldsymbol{\Pi}_{\boldsymbol{k}}^s|^2 + \omega_{\boldsymbol{k}}^2|\boldsymbol{\pi}_{\boldsymbol{k}}^s|^2\right], \\ H_{AV} &= \sum_{i=1}^{A}\frac{g_A}{2f_\pi}\sqrt{\frac{2}{L^3}}{\sum_{\boldsymbol{k}}}'\left\{\boldsymbol{\sigma}_i\cdot\boldsymbol{k}\left[\boldsymbol{\tau}_i\cdot\boldsymbol{\pi}_{\boldsymbol{k}}^s\cos(\boldsymbol{k}\cdot\boldsymbol{r}_i) - \boldsymbol{\tau}_i\cdot\boldsymbol{\pi}_{\boldsymbol{k}}^c\sin(\boldsymbol{k}\cdot\boldsymbol{r}_i)\right]\right\}, \\ H_{WT} &= \sum_{i=1}^{A}\frac{1}{2f_\pi^2L^3}\boldsymbol{\tau}_i\cdot\Bigg[{\sum_{\boldsymbol{k}}}'\cos(\boldsymbol{k}\cdot\boldsymbol{r}_i)\boldsymbol{\pi}_{\boldsymbol{k}}^c\times{\sum_{\boldsymbol{q}}}'\cos(\boldsymbol{q}\cdot\boldsymbol{r}_i)\boldsymbol{\Pi}_{\boldsymbol{q}}^c \\ &\quad + {\sum_{\boldsymbol{k}}}'\cos(\boldsymbol{k}\cdot\boldsymbol{r}_i)\boldsymbol{\pi}_{\boldsymbol{k}}^c\times{\sum_{\boldsymbol{q}}}'\sin(\boldsymbol{q}\cdot\boldsymbol{r}_i)\boldsymbol{\Pi}_{\boldsymbol{q}}^s + {\sum_{\boldsymbol{k}}}'\sin(\boldsymbol{k}\cdot\boldsymbol{r}_i)\boldsymbol{\pi}_{\boldsymbol{k}}^s\times{\sum_{\boldsymbol{q}}}'\cos(\boldsymbol{q}\cdot\boldsymbol{r}_i)\boldsymbol{\Pi}_{\boldsymbol{q}}^c \\ &\quad + {\sum_{\boldsymbol{k}}}'\sin(\boldsymbol{k}\cdot\boldsymbol{r}_i)\boldsymbol{\pi}_{\boldsymbol{k}}^s\times{\sum_{\boldsymbol{q}}}'\sin(\boldsymbol{q}\cdot\boldsymbol{r}_i)\boldsymbol{\Pi}_{\boldsymbol{q}}^s\Bigg]. \end{aligned} \tag{2}$$

Instead of complex amplitudes for the pion fields, we worked with real amplitudes for the sine/cosine modes, hence $\boldsymbol{\pi}_{\boldsymbol{k}}^{c,s}$ denotes the component with momentum $\boldsymbol{k}$ of the field, and the $\boldsymbol{\Pi}_{\boldsymbol{k}}^{c,s}$ are the conjugate momenta. β_K and δM are counter terms, introduced due to our cutoff. The δ_{R_0} function is a smeared off contact used for two-body interactions. The subscript "AV" refers to the pion-nucleon axial-vector coupling, whereas "WT" stands for the Weinberg-Tomozawa tadpole term.

We built the wave functions for A nucleons,

$$\langle RS\Pi|\Psi_T\rangle = \langle RS\Pi| \exp\left\{ -\sum_{\boldsymbol{k}}{}' \left[\frac{\omega_k}{2}(|\boldsymbol{\pi}^c_{\boldsymbol{k}}|^2 + |\boldsymbol{\pi}^s_{\boldsymbol{k}}|^2) + \frac{\alpha_k}{2\omega_k}\left(\boldsymbol{\pi}^c_{\boldsymbol{k}}\cdot\boldsymbol{B}^c_{\boldsymbol{k}} + \boldsymbol{\pi}^s_{\boldsymbol{k}}\cdot\boldsymbol{B}^s_{\boldsymbol{k}}\right) \right.\right.$$
$$\left.\left. -\frac{1}{4}\omega_k\alpha_k^2 G_k^2 \sum_{i<j}^{A} \boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j\boldsymbol{\sigma}_i\cdot\boldsymbol{k}\boldsymbol{\sigma}_j\cdot\boldsymbol{k}\cos(\boldsymbol{k}\cdot\boldsymbol{r}_{ij}) \right] \right\} |\Phi\rangle\,, \tag{3}$$

where R stands for all nucleon positions and S for the spin-isospin degrees of freedom, and Π for all pion amplitudes. The other quantities and the rationale behind this choice of wave function are given in Ref. [6]. We used Eqs.(2) and (3), together with QMC methods, to calculate the renormalization of the nucleon mass as a function of the momentum cutoff, a Euclidean time density correlation function that deals with the short-time nucleon diffusion, and the pion cloud density and momentum distributions. In the two nucleon sector we showed that the interaction of two static nucleons at large distances reduces to the one-pion exchange potential, and we fit the low-energy constants of the contact interactions to reproduce the binding energy of the deuteron and two neutrons in finite volumes.

Currently we are applying this method to light-nuclei, the triton and the alpha particle, $A = 3$ and 4. We found evidences that these systems are overbound, even for relatively small cutoffs. Currently, we are investigating the source of this overbinding, and possible ways of circumventing it.

1.3 Improved trial wave functions for nuclei and nuclear matter

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In QMC calculations, the results are dependent on the accuracy of the trial wave function employed to constrain the path to control the fermion sign problem. The statistical errors also can be reduced with accurate trial functions. We have recently introduced a linearly pair-correlated wave function which has greatly improved the convergence of our results [8]. We are now working on including multiple pair correlations to study their effect. We have written codes to efficiently handle the large number of matrix operations required to include these additional correlations.

We have been able to add quadratic correlations to the trial wave function that we use in nuclear Monte Carlo calculations. These additional correlations have caused the energies to decrease for the nuclei ^{4}He and ^{16}O, as well as for symmetric nuclear matter. The quadratic correlations resulted in an improved trial wave function, but were too expensive to use on larger nuclear systems. Our results for this wave function have been submitted for review to the Physical Review C journal [9]. Linear and quadratic correlations come from an expansion of the exponential correlation. We have begun to include the full set of exponential correlations in the nuclear trial wave function by sampling the terms, and significant progress has been made. We expect to be doing full production

runs with this trial wave function shortly.

We then plan to use these improved wave functions to investigate the clustering of nucleons into alpha particles in mostly neutron matter. We intend to study the convergence of variational and auxiliary field diffusion Monte Carlo with these new wave functions for nuclei and nuclear matter with up to $A = 40$.

2 Computational Methods

We 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 [10]. The AFDMC code has been successfully used to calculate properties of nuclear matter, neutron matter, and medium-mass nuclei [8]. The results of Ref. [11] 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 it 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

$$\lim_{n\to\infty} \left[e^{-H\delta\tau}\right]^n \Psi_T(R,S) \to \Psi_0(R',S'), \tag{4}$$

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 Fortran2008 and MPI, and it 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.

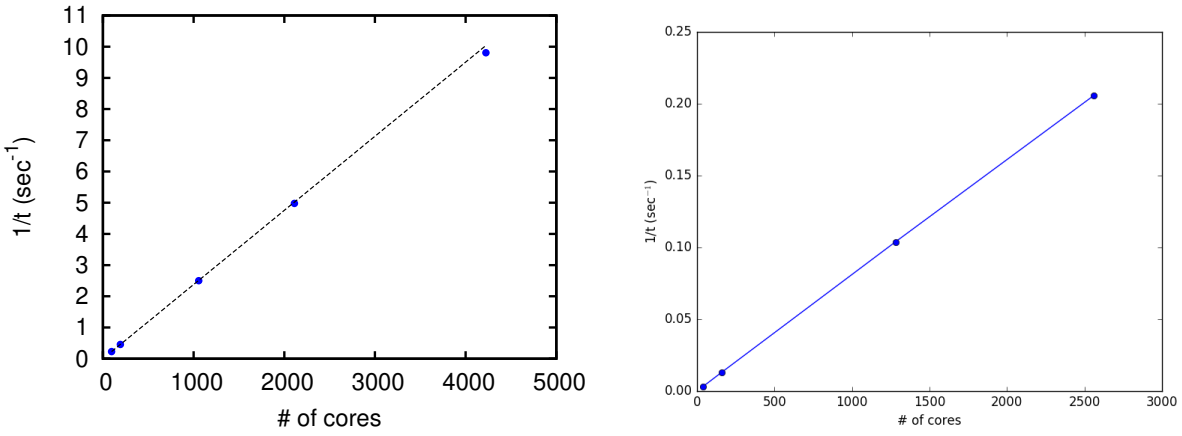
2. Rotate nucleon's spins, $S \to S'$, according to the spin and isospin-dependent potential.

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 quite 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

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 XSEDE resources, namely Stampede2 and SuperMIC. We tested the performance of the code on Stampede2. Up to 4096 ??? cores, the largest number tested, the code scales strongly, Fig. 1a. We also verified that our code scales strongly on SuperMIC, Fig. 1b, up to 2560 cores (the largest number tested).



(a) (b)

Figure 1: Scaling on Stampede2 (a) and SuperMIC (b) 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 [12] and the linear method [13]. Once these parameters are determined, we can proceed with the computation of physical quantities of interest. We base our estimates on the amount of SUs and storage used in [10] and references therein.

4.1 Three-component Fermi gases

We wish to perform simulations for a wide range of systems. Let us denote each component by A, B and C, and N_A, N_B, and N_C the respective number of particles of each component. We wish to investigate the cases: $N_A = N_B = N_C$, equal populations; and $N_A = N_B$ and $N_C = 1$, the polaron problem. The interactions between components can be varied, and the atomic mass of each component can be different as well. This gives rise to several cases that need to be simulated.

We estimate 1,000 SUs for code development, 5,000 SUs for the variational optimization of the parameters, and 11,000 SUs for production runs.

4.2 QMC simulations with explicit contributions from the pion field

We want to perform simulations with different system sizes, ranging from three nucleons plus the pion field up to four nucleons plus the pion field. Several runs are needed for each system, because we have to investigate the behavior of properties as a function of the box size and number of pion modes, for example.

We require approximately 1,000 SUs for code development and 5,000 SUs for the variational optimization of the parameters. Longer runs are necessary to compute quantities such as energy of the system, density and other distribution functions, with small variances. We estimate 11,000 SUs for these computations.

4.3 Improved QMC simulations for nuclei and nuclear matter

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We want to do energy calculations on three systems, ^{4}He, ^{16}O, and symmetric nuclear matter using the new exponential correlations to compare the trial wave function with the linear and quadratic correlations. To do this we will need to optimize a new set of parameters. We estimate that this will require 2,000 SUs for development, 4,000 SUs to optimize the variational parameters for the new correlations, and 18,000 SUs to calculate the energies for the three nuclear systems mentioned above.

With this improved wave function we will be investigating the clustering of alpha particles in mostly neutron matter. We will be doing calculations for a variety of densities to investigate the clustering dependence on density. We estimate that this will require 2,000 SUs for development, 4,000 SUs to optimize the code for mostly neutron matter, and 18,000 SUs to calculate the clustering at a variety of densities.

4.4 Summary of the requested resources

We present in Table 1 the amount of SUs requested for each task. We are requesting a total of 50,000 SUs on Stampede2. We also included SUs for the code development, in order to ensure performance and scaling during execution. As for storage needs, we request the default value of 5 GB per user. 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 Stampede2. We are capable of handling the post-processing of the simulations in our local computing environments.

Table 1: Justification for the requested amount of SUs

	Fermi gases	**Explicit pions**	**Improved QMC simulations**
Development	1,000	1,000	1,000
Variational optimization	5,000	4,000	5,000
Production	11,000	11,000	11,000
Subtotal	17,000	16,000	17,000
Total: 50,000 SUs			

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 Kevin Schmidt in collaboration with Stefano Fantoni developed the auxiliary field diffusion Monte Carlo method. With collaborators he performed the first diffusion and auxiliary field quantum Monte Carlo calculations for paired fermions. He is a fellow of the American Physical society and has published more than 150 papers.

Stefano Gandolfi update is a nationally and internationally recognized scientist in Many-Body Nuclear Theory. He has published more than 50 papers and he has about 3,100 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, among other conferences in 2017 and 2018.

Post-doctoral researcher

Lucas Madeira is a post-doctoral researcher at University of São Paulo. He has several works in collaboration with Kevin Schmidt and Stefano Gandolfi. His research interests include strongly interacting fermionic systems, such as cold atom gases and nucleon systems. He has experience with High Performance Computing including MPI and OpenMP.

Graduate student

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 doing computational nuclear physics for the past four and a half years.

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