Research Project Renewal

Quantum Monte Carlo Calculations of Nucleon Systems and Cold Atom Gases

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March 14, 2017

Abstract

This research project renewal request is for 1,000,000 SUs on SuperMIC. We describe our progress on cold atom gases simulations, and nucleon systems calculations. One of the proposed goals is to include explicitly the pionic degrees of freedom in the nuclear Monte Carlo simulations. 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 in the past.

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.

The detailed development of the initial proposal is discussed in the document "*Progress Report*", which was submitted alongside this one. 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 our progress on cold fermionic gases, including the study of a vortex line excitation in the unitary Fermi gas, and core structure vortex properties of two-dimensional 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 Strongly paired fermionic systems of cold atoms

Strongly paired fermions are important in many contexts, for example: nuclei, atoms, condensed matter systems, and even neutron stars. Cold atom gases provide a unprecedented clean way to the deal with the fermionic many-body problem. The ingenious usage of magnetic fields can be used to tune the interatomic interactions of the systems, thus reaching a wide spectrum of interaction strengths. 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.

Until very recently, superfluids were classified as either bosonic or fermionic. The Bose-Einstein condensate (BEC) theory was developed to describe bosonic fluids. On the other hand, the Bardeen-Cooper-Schrieffer (BCS) theory was first conceived to describe pairing instability, arising from weak interactions, in a highly degenerate Fermi gas. Later it was realized that the BEC and BCS schemes are limit cases of a continuum of interactions. The possibility of tuning parameters in order to observe the change from one paradigm to the other was conceptually interesting, but real enthusiasm came from the experimental realization of the three-dimensional (3D) BEC-BCS crossover [1]. Right in the middle of this crossover lies a strongly interacting state, the unitary Fermi gas, with remarkable properties.

In our Startup allocation we studied vortices in the unitary Fermi gas [2]. We reported diffusion Monte Carlo results for the ground-state of unpolarized spin-1/2 fermions in a cylindrical container and properties of the system with a vortex-line excitation. We calculated quantities such as: density profiles, the ground- state energy per particle, the superfluid pairing gap, and the excitation energy per particle.

We used the current allocation to study the core structure of two-dimensional Fermi gas vortices in the BEC-BCS crossover region. The study of cold Fermi gases has proven to be a very

rich research field, and the investigation of low-dimensional systems has become an active area in this context [3, 4]. Particularly, the two-dimensional (2D) Fermi gas has attracted much interest recently. It was the object of several theoretical investigations [5–10], but its experimental realization, using a highly anisotropic potential, was a milestone in the study of these systems [11]. Many other studies have been carried out since [12, 13]. QMC methods were successfully employed to compute several properties of the BEC-BCS crossover. The fact that a fully attractive potential in 2D always support a bound-state, and the ability to vary the interaction strength over the entire BEC-BCS crossover regime offers rich possibilities for the study of these systems.

The presence of quantized vortices is an indication of a superfluid state in both Bose and Fermi systems. In 3D, much progress has been made [2,14,15], including the observation of vortex lattices in a strongly interacting rotating Fermi gas of ^{6}Li [16]. With the recent progress on the 2D Fermi gases, it seemed natural to also extend the theoretical study of vortices to these systems. Interest is further augmented in 2D, where a Berezinksii-Kosterlitz-Thouless transition [17, 18] could take place at finite temperatures, and pairs of vortices and antivortices would eventually condense to form a square lattice [19].

We studied properties of a single vortex in a 2D Fermi gas. We considered the ground-state to be a disk with hard walls and total angular momentum zero, and the vortex excitation corresponds to each fermion pair having angular momentum $\hbar$.

Our findings were summarized in the article "Core structure of two-dimensional Fermi gas vortices in the BEC-BCS crossover region" [20], which has been submitted to the Physical Review A journal. We reported $T = 0$ diffusion Monte Carlo results for the ground-state and vortex excitation of unpolarized spin-1/2 fermions in a two-dimensional disk. We investigated how vortex core structure properties behave over the BEC-BCS crossover. We calculated the vortex excitation energy, density profiles, and vortex core properties related to the current. We found a density suppression at the vortex core on the BCS side of the crossover, and a depleted core on the BEC limit. Size-effect dependencies in the disk geometry were carefully studied.

1.2 QMC simulations with explicit contributions from the pion field

Most QMC simulations of nuclear matter model particles interacting via instantaneous two- and three-body potentials [21]. Usually these potentials are either phenomenological or 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 wave functions for this problem.

We have been developing wave functions for systems with $A \leqslant 4$ nucleons, and we are in

the process of implementing them in the code. Once that has been achieved, simulations with one nucleon can help us to determine its bare mass. Simulations with two nucleons will serve as benchmarks to our choice of two-body potentials. The comparison of our results for light-nuclei properties with other numerical calculations and experiments will shed light on the explicit contributions of the pion field.

1.3 Improved trial wave functions for nuclei and nuclear matter

In QMC calculations, the results are dependent on the accuracy of the trial wave function employed to guide the random walk. We have recently introduced a linearly pair-correlated wave function which has greatly improved the convergence of our results [22]. 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.

In the past year 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. We plan to publish these results shortly. These linear and quadratic correlations come from an expansion of the exponential correlation. We plan to include the full set of exponential correlations in the nuclear trial wave function. We then plan to use these improved wave function 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 $A < 40$.

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 [21]. The AFDMC code has been successfully used to calculate properties of nuclear matter, neutron matter, and medium-mass nuclei [22]. The results of Ref. [23] 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

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

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 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.

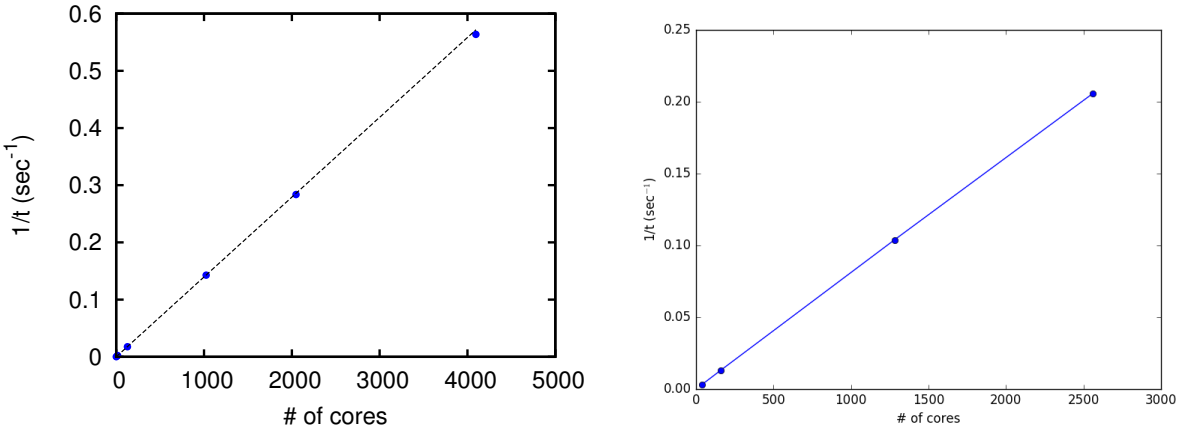
This algorithm is implemented by considering a collection of configurations (called *walkers*) that are simultaneously evolved in imaginary-time. The parallelization is accomplished by spreading the configurations among the nodes. However, AFDMC is not embarrassingly parallel because the branching term 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 XSEDE resources, namely Stampede and SuperMIC.

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, Fig. 1a. During the current allocation (TG-PHY160027), we verified that our code also scales

strongly on SuperMIC, Fig. 1b, up to 2560 cores (the largest number tested), although we intend to perform simulations with a maximum number of 1000 cores.



(a) (b)

Figure 1: Scaling on Stampede (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 [24]. 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 [21] and references therein.

4.1 QMC simulations with explicit contributions from the pion field

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. 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.

For each system we require:

- variational optimization of the parameters: for these systems the average amount of SUs necessary for the optimization is approximately 40,000 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 80,000 SUs for these computations.

4.2 Improved QMC simulations for nuclei and nuclear matter

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 20,000 SUs for development, 40,000 SUs to optimize the variational parameters for the new correlations, and 180,000 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 20,000 SUs for development, 40,000 SUs to optimize the code for mostly neutron matter, and 180,000 SUs to calculate the clustering at a variety of densities.

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 1,000,000 SUs on SuperMIC. 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	**Improved QMC simulations**	
		Exp. correlations	Alpha particle clustering
Development	40,000	20,000	20,000
Variational optimization	160,000	40,000	40,000
Production	320,000	180,000	180,000
Subtotal	520,000	240,000	240,000
Total: 1,000,000 SUs			

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 SuperMIC. We are capable of handling the post-processing of the simulations in our local computing environment at Arizona State University.

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 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 140 papers.

Stefano Gandolfi is a nationally and internationally recognized scientist in Many-Body Nuclear Theory. During the past 4 years he has published 29 papers and given 31 invited talks, including many at major national and international conferences. He has about 2,500 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.

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. 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.

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 two and a half years.

References

[1] C. A. Regal, M. Greiner, and D. S. Jin. Observation of Resonance Condensation of Fermionic Atom Pairs. *Phys. Rev. Lett.*, 92:040403, Jan 2004.

[2] Lucas Madeira, Silvio A. Vitiello, Stefano Gandolfi, and Kevin E. Schmidt. Vortex line in the unitary Fermi gas. *Phys. Rev. A*, 93:043604, Apr 2016.

[3] Stefano Giorgini, Lev P. Pitaevskii, and Sandro Stringari. Theory of ultracold atomic Fermi gases. *Rev. Mod. Phys.*, 80:1215–1274, Oct 2008.

[4] Immanuel Bloch, Jean Dalibard, and Wilhelm Zwerger. Many-body physics with ultracold gases. *Rev. Mod. Phys.*, 80:885–964, Jul 2008.

[5] Mohit Randeria, Ji-Min Duan, and Lih-Yir Shieh. Bound states, Cooper pairing, and Bose condensation in two dimensions. *Phys. Rev. Lett.*, 62:981–984, Feb 1989.

[6] Mohit Randeria, Ji-Min Duan, and Lih-Yir Shieh. Superconductivity in a two-dimensional Fermi gas: Evolution from Cooper pairing to Bose condensation. *Phys. Rev. B*, 41:327–343, Jan 1990.

[7] D. S. Petrov, M. A. Baranov, and G. V. Shlyapnikov. Superfluid transition in quasi-two-dimensional Fermi gases. *Phys. Rev. A*, 67:031601, Mar 2003.

[8] J.-P. Martikainen and P. Törmä. Quasi-Two-Dimensional Superfluid Fermionic Gases. *Phys. Rev. Lett.*, 95:170407, Oct 2005.

[9] J. Tempere, M. Wouters, and J. T. Devreese. Imbalanced Fermi superfluid in a one-dimensional optical potential. *Phys. Rev. B*, 75:184526, May 2007.

[10] Wei Zhang, G.-D. Lin, and L.-M. Duan. Berezinskii-Kosterlitz-Thouless transition in a trapped quasi-two-dimensional Fermi gas near a Feshbach resonance. *Phys. Rev. A*, 78:043617, Oct 2008.

[11] Kirill Martiyanov, Vasiliy Makhalov, and Andrey Turlapov. Observation of a Two-Dimensional Fermi Gas of Atoms. *Phys. Rev. Lett.*, 105:030404, Jul 2010.

[12] Alexey A Orel, Paul Dyke, Marion Delehaye, Chris J Vale, and Hui Hu. Density distribution of a trapped two-dimensional strongly interacting Fermi gas. *New Journal of Physics*, 13(11):113032, 2011.

[13] Vasiliy Makhalov, Kirill Martiyanov, and Andrey Turlapov. Ground-State Pressure of Quasi-2D Fermi and Bose Gases. *Phys. Rev. Lett.*, 112:045301, Jan 2014.

[14] Aurel Bulgac and Yongle Yu. Vortex State in a Strongly Coupled Dilute Atomic Fermionic Superfluid. *Phys. Rev. Lett.*, 91:190404, Nov 2003.

[15] Rajdeep Sensarma, Mohit Randeria, and Tin-Lun Ho. Vortices in Superfluid Fermi Gases through the BEC to BCS Crossover. *Phys. Rev. Lett.*, 96:090403, Mar 2006.

[16] M. W. Zwierlein, J. R. Abo-Shaeer, A. Schirotzek, C. H. Schunck, and W. Ketterle. Vortices and superfluidity in a strongly interacting Fermi gas. *Nature*, 435(7045):1047–1051, Jun 2005.

[17] V. L. Berezinsky. Destruction of long range order in one-dimensional and two-dimensional systems having a continuous symmetry group. 1. Classical systems. *Sov. Phys. JETP*, 32:493–500, 1971.

[18] J M Kosterlitz and D J Thouless. Long range order and metastability in two dimensional solids and superfluids. (Application of dislocation theory). *J. Phys. C*, 5(11):L124, 1972.

[19] S. S. Botelho and C. A. R. Sá de Melo. Vortex-Antivortex Lattice in Ultracold Fermionic Gases. *Phys. Rev. Lett.*, 96:040404, Feb 2006.

[20] Lucas Madeira, Stefano Gandolfi, and Kevin E. Schmidt. Core structure of two-dimensional Fermi gas vortices in the BEC-BCS crossover region. *arXiv pre-print*, 2017. arXiv:1703.01998 [cond-mat.quant-gas].

[21] J. Carlson, S. Gandolfi, F. Pederiva, Steven C. Pieper, R. Schiavilla, K. E. Schmidt, and R. B. Wiringa. Quantum Monte Carlo methods for nuclear physics. *Rev. Mod. Phys.*, 87:1067–1118, Sep 2015.

[22] S. Gandolfi, A. Lovato, J. Carlson, and Kevin E. Schmidt. From the lightest nuclei to the equation of state of asymmetric nuclear matter with realistic nuclear interactions. *Phys. Rev. C*, 90:061306, Dec 2014.

[23] S. Gandolfi, J. Carlson, and Sanjay Reddy. Maximum mass and radius of neutron stars, and the nuclear symmetry energy. *Phys. Rev. C*, 85:032801, Mar 2012.

[24] Michele Casula, Claudio Attaccalite, and Sandro Sorella. Correlated geminal wave function for molecules: An efficient resonating valence bond approach. *The Journal of Chemical Physics*, 121(15):7110–7126, 2004.