

## Trial Wave Functions in Nuclear Physics

By: Cody Petrie

I am in my fourth year as a physics graduate student and have completed the core courses with a GPA of 4.0. I have completed the oral qualifying exam as well as the written and oral comprehensive exams. I am working with Kevin Schmidt at ASU and Joe Carlson and Stefano Gandolfi at Los Alamos National Laboratory to improve the trial wave function used in Quantum Monte Carlo (QMC) calculations. We have one publication submitted and in review currently. While at ASU I have improved and honed my skills in computational nuclear physics. I have had the opportunity to work with a couple of different high performance computers across the country doing QMC simulations to calculate the binding energies of light to medium nuclei as well as nuclear matter. I have learned about Variational, Diffusion, and Auxiliary Field Diffusion Monte Carlo methods and how to implement them in nuclear physics applications. I have also had the opportunity to TA for a variety of courses at ASU including, most recently, the online based 113 and 122 physics labs which has been an interesting and instructive experience. I have also been an adjunct professor of physics at Mesa Community College and have participated as an instructor in a summer course teaching and ASU sponsored course and inspiring young scholars in Mexico as part of the Clubes de Ciencia program. As a result my passion, love to do and teach physics has continued to grow while being here at ASU.

Solving many-body problems, particularly in nuclear physics where the exact interactions aren't fully known, gets increasingly difficult as the number of particles increases. This is why we use QMC methods which sample the large dimensional integrals to give us an approximate answer with less computation. The success of a QMC simulation depends on the accuracy of a trial wave function. If the trial wave function is not close to the actual wave function, the simulation may take a long time to converge to the correct answer, if it ever converges at all. I have been working to improve the trial wave function. The simplest wave function is an antisymmetrized product of single particle orbitals. This is often in the form of a single, or sum, of Slater determinants. However this simple form only includes the mean field, and does not include any interactions between the particles. To improve this simple wave function we have added spin-isospin dependent correlations which ideally would be in the form of an exponential of spin-isospin operators, which obeys cluster decomposition. However, to decrease the computational cost we have, up until now, only included linear terms where you have operators like  $O_{ij}$ , which correlates the  $i$  and  $j$  particles. I have added quadratic correlations which includes two pairs of particles and has the form  $O_{ij}O_{kl}$ . Adding these correlations improved the energy calculations for  ${}^4\text{He}$ ,  ${}^{16}\text{O}$  and nuclear matter at saturation density, with respect to the linear correlations only.

These calculations have taught us that including extra terms in the expansion of the correlations does improve the wave function, but the computational cost is too great to use these correlations for calculations of large nuclear systems. As a result I will be using the Hubbard-Stratonovich transformation to write the exponential correlations in terms exponentials of single particle operators, which we can calculate. The Hubbard-Stratonovich transformation is currently used in another part of the code to sample spin-isospin states of the system. With an improved trial wave function I would be able to perform calculations on larger nuclear systems as well as study other interesting topics such as alpha particle clustering in nuclear matter, which could lend us great insight into the field of neutron star structure and formation.

This fellowship would give me the chance to make progress on new projects like including the exponential correlations into the trial wave function, or studying the formation of alpha particle clusters in nuclear matter. I would be able to devote more time to completing my dissertation and focusing on further publishing my research, while decreasing the financial burden of raising a family at the same time. I have learned a great deal about computational nuclear physics while studying here at ASU and this fellowship would aid my learning and progress.