Correlated Trial Wave Functions for Quantum Monte Carlo Calculations

By: Cody Petrie

I am in my second year as a physics graduate student and have completed the core courses and now have a GPA of 4.0. I have also completed the oral qualifying exam. Currently I am working with Kevin Schmidt doing computational nuclear physics. Though I had experience before coming to ASU my understanding of how to do computational physics has grown immensely since being here at ASU. I have had the chance to work with a couple of different high performance computers across the country doing Quantum Monte Carlo (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 been trained in the basics of nuclear and particle physics in class and within my research group. I have also had the opportunity to TA for four semesters at ASU, teaching students about basic Newtonian physics as well as electricity and magnetism and other interesting topics in physics. As a result my passion, love, and understanding of physics has continued to grow since 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 the 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 for our calculations by adding quadratic correlations. 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. A simple improvement to this is to add a Jastrow-like correlation, which correlates particles according to their relative distance. We have also added spin-isospin correlations. Up until now these correlations have only included linear terms where you have operators, like $O_{ij,}$ which correlates the i and j particles. I have added terms that have included the k and l particles, which are distinct from i and j, and have the form $O_{ij}O'_{kl}$. Adding these correlations has shown to decrease the binding energies and statistical errors or ^{16}O and symmetric nuclear matter of density $\rho=0.16\ fm^{-3}$ with respect to the linear correlations only. I have also done calculations for ^{4}He, which caused the energy to increase, but the statistical error to decrease. This summer I will potentially be doing some other comparison calculations and then publishing this work in an appropriate physics journal. In addition, I will be working to develop ways to improve the algorithm and trial wave function which will give new insights into the true nucleon-nucleon interactions.

If I receive this fellowship I would be able to devote the time needed to publish the work that I am currently finishing up and it would give me the chance to explore new avenues of exciting research. It would give me the chance to develop and hone my skills nuclear physics and with QMC methods. Being able to develop these skill early on in my program here at ASU would ensure my success in the future as a computational nuclear physicist.