Correlated Trial Wave Functions for Quantum Monte Carlo Calculations

By: Cody Petrie

I am a first year graduate student doing research in computational nuclear physics. During my first semester here at ASU I have learned how to use methods like Variational and Diffusion Monte Carlo. I have used these methods to solve problems like the quantum harmonic oscillator. I have been developing as a computational physicist since my Sophomore year in my undergraduate degree at BYU. While there I computationally solved Maxwell's equations for the reflection of extreme ultraviolet light from thin film surfaces. I then compared these calculations to reflection experiments that I did at BYU and at the Advanced Light Source at Berkley National Laboratory. At the end of my time there I also worked on understanding Direct Simulation Monte Carlo to solve for plasma systems. I also have experience in computational Bayesian statistics and using the Finite Difference Time Domain method to computationally solve Maxwell's equations. At ASU I am further developing my passion and skills to do physics. I have completed two of the four core courses thus far with A letter grades in both classes. I have also contributed to the physics department by being a TA for the physics 122 lab two semesters in a row. I have continued to develop a love of research while here at ASU. Working with Kevin Schmidt I have already improved the way I think about solving physics problems, specifically in research. My research with him focuses on solving quantum many body problems for nuclear physics.

Quantum many body problems are often very difficult to solve due to the large number of degrees of freedom. Using Quantum Monte Carlo (QMC) methods to solve these problems, such as nuclei and nuclear matter problems, allows us to solve the large dimensional integrals using sampling methods. The method that we are currently using is the Auxiliary Field Diffusion Monte Carlo (AFDMC) method developed by Schmidt and Fantoni in 1999. The accuracy of many QMC methods depends on how close the trial wave function is to the actual ground state wave function of the system. Typically the simplest trial wave function is the mean field wave function which consists of a sum of Slater determinants, enforcing an antisymmetric wave function, with correlation factors. Currently independent pair terms have not been included in the correlation. I will be working this summer to include these correlation terms in the trial wave function. From this we hope to see an even better correlation between the calculations and the experimental measurements. The main goal of this project is to include these terms which will improve our trial wave function, and also allow me the experience I need to start working on other projects. Once I have an understanding of the current methods for solving these many body problems I expect to contribute to the field by improving the existing methods and developing new ways to solve these problems. Being able to better predict the quantum states and energies of nuclear systems could improve our understanding of nucleon-nucleon interactions. Specifically the interactions that occur between nuclear systems with large degrees of freedom such as heavy nuclei.

Having the funding to do research this summer would allow the chance to spend the necessary time learning the algorithms involved in AFDMC. To be able to develop as a computational physicist here at ASU it is critical that I have the time to develop my research early on in my time here. Being able to start research early on at ASU will allow me to accomplish much in furthering our understanding of physics and upholding the long standing tradition of research and intellectual development at this institution.