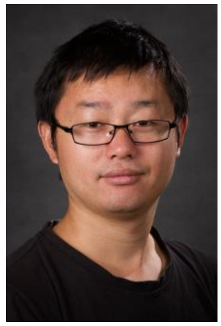
WILLIAM & MARY

CHARTERED 1693

Final Oral Examination for the Ph. D. Degree

Department of Physics



# Hao Shi

## "Computational Studies of Strongly Correlated Quantum Matter"

Monday, 27 March 2017, 1:30 p.m.

Earl Gregg Swem Library, Ford Room

Williamsburg, Virginia 23187-8795

Open to the Public

Abstract: The study of strongly correlated quantum many-body systems is an outstanding challenge. Highly accurate results are needed for the understanding of practical and fundamental problems in condensed-matter physics, high energy physics, material science, quantum chemistry and so on. Our familiar mean-field or perturbative methods tend to be ineffective. Numerical simulations provide a promising approach for studying such systems. The fundamental difficulty of numerical simulation is that the dimension of the Hilbert space needed to describe interacting systems increases exponentially with the system size. Quantum Monte Carlo (QMC) methods are one of the best approaches to tackle the problem of enormous Hilbert space. They have been highly successful for boson systems and unfrustrated spin models. For systems with fermions, the exchange symmetry in general causes the infamous sign problem, making the statistical noise in the computed results grow exponentially with the system size. This hinders our understanding of interesting physics such as high-temperature superconductivity, metal-insulator phase transition. In this thesis, we present a variety of new developments in the auxiliary-field quantum Monte Carlo (AFQMC) methods, including the incorporation of symmetry in both the trial wave function and the projector, developing the constraint release method, using the force-bias to drastically improve the efficiency in Metropolis framework, identifying and solving the infinite variance problem, and sampling Hartree-Fock-Bogoliubov wave function. With these developments, some of the most challenging many-electron problems are now under control. We obtain an exact numerical solution of two-dimensional strongly interacting Fermi atomic gas, determine the ground state properties of the 2D Fermi gas with Rashba spin-orbit coupling, provide benchmark results for the ground state of the two-dimensional Hubbard model, and establish that the Hubbard model has a stripe order in the underdoped region.

Bio: Hao Shi was born in Gugao, China, on July 13, 1986. He is fascinated with science and math since he was a kid. In 2008, he graduated with a Bachelor of Science degree in Physics from Nanjing University in Nanjing, China. In the same year, he joined Renming University in Beijing, China to study computational physics. He entered the College of William and Mary and joined Dr. Shiwei Zhang's computational condensed matter physics group in Fall 2011. His research focuses on studying strongly correlated systems by Auxiliary Field Quantum Monte Carlo and other numerical methods. After graduation, he will work as a postdoctoral fellow at Center for Computational Quantum Physics in Flatiron Institute.