Hao Shi

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Education

Ph.D. Physics, College of William and Mary, Williamsburg, VA, USA, 2011-2017.

M.S. study, Computational physic, Renmin University, Beijing, China, 2008-2011.

B.S. Physics, Nanjing University, Nanjing, China, 2004-2008.

Employment History

Flatiron Research Fellow, Flatiron Institute, Simons Foundation, New York, NY, USA, 2017-now.

Research Experience

Center for Computational Quantum Physics *Flatiron Institute* *2017-now*

Research focuses on studying strongly correlated systems by Auxiliary Field Quantum Monte Carlo (AFQMC) and other numerical methods.

- Made AFQMC simulations for Ca2RuO4 materials and determined magnetic and metal-insulator transition.
- Simulated transition metal atom and oxide molecules and got accurate results compared with experiments.
- Studied the multi-band Kanamori model to capture Hund's physics.
- Studied the three-band Hubbard model and determined the accurate phase transition point at Half-filling.
- Worked on repulsive interacting fermion problems with spin-orbit coupling.
- Developed the self-consistent algorithm in AFQMC for realistic materials.
- Applied trial wave functions with enormous number of determinants in AFQMC.
- Developed AFQMCLAB software for general applications of lattice model, quantum chemistry and solids problems.
- Developed finite temperature constraint path Monte Carlo method and reduced the cubic scaling to linear scaling.

College of William and Mary W&M Computational Materials Physics Group 2011-2017

- Developed a variety of new AFQMC methods.
- Used these developments to study the two dimensional Hubbard model; work has served as benchmark in the Simons Foundation Many Electron Collaboration.
- Studied the two-dimensional strongly interacting Fermi atomic gas, provided valuable benchmarks for future studies, and allowed precise comparisons with experiments.
- Made first exact numerical study to determine the ground state properties of the 2D Fermi gas with Rashba spin-orbit coupling.
- More researches include:
  - studied three band Hubbard model.
  - calculated dynamic information in AFQMC.
  - combined Hartree-Fock-Bogoliubov theory with AFQMC.

Renmin University Strongly Correlated Physics Computational Group 2008-2011

- Worked on Exact Diagonalization for the topological phase transition in interacting Haldane model.
- Research experience in Dynamic Mean Field Theory, Continuous Time Quantum Monte Carlo and Density Matrix Renormalization Group.

Service

- Organize the workshop on "Algorithm & Software Development in Auxiliary-field Quantum Monte Carlo Method" New York, February 2018.
- Referee at Physical Review Letter, Physical Review B, and Journal of Chemical Theory and Computation.

Honors

- Arts & Science Distinguished Dissertation Award in Natural and Computational Sciences at the College of William & Mary, May 2017.
- Roy L. Champion Research award, awarded to graduate student in physics who has demonstrated outstanding research achievement, May 2016.
- The Materials Computation Center travel award of $1900 for "4th Les Houches school in computational physics," Les Houches, France, June 2014.
- The Materials Computation Center travel award of $950 for "Quantum Monte Carlo

methods at work for novel phases of matter," Trieste, Italy, Jan 2012.

Presentations

- Invited talk: "Auxiliary Field Quantum Monte Carlo for Transition Metal Systems: from Molecules to Solids"

  Lawrence Livermore National Laboratory, , Livermore, CA, Aug 26 2019.

- Invited talk: "Auxiliary-field quantum Monte Carlo calculationsof the two-dimensional Fermi gas"

  Tsinghua University, Beijing, China, July 2019.

- Invited talk: "Auxiliary Field Quantum Monte Carlo in Simons Many-electron Collaboration: Hubbard Model, Hydrogen Chain, and Transition Metal Systems"

  The 5th Conference on Condensed Matter Physics, Liyang, China, June 2019.

- Invited talk: "Auxiliary Field Quantum Monte Carlo: basics and applications."

  Simons Many Electron Collaboration Summer School, New York, June 2019.

- Invited talk: "Quantum Monte Carlo Study of Strongly Interacting Fermi Gases in Two Dimensions: BCS-BEC Crossover, Spin-orbit Coupling, and Dynamical Response Functions"

  APS March meeting, *Boston*, March 2018.

- Invited talk: "Developments in auxiliary-field quantum Monte Carlo: infinite variance problem and improved trial wave functions"

  Advances in Monte Carlo Techniques for Many-Body Quantum Systems, Seattle, WA, August 2018.

- Invited talk: "Auxiliary field quantum Monte Carlo library for strongly-correlated systems"

  Python quantum chemistry and material simulation software, Pasadena, CA, June 2018.

- Invited talk: "Ground-state properties of the two-dimensional strongly interacting Fermi atomic gas and the interplay between superfluidity and spin-orbit coupling"

  XVIII International Conference on Recent Progress in Many-Body Theories, Niagara Falls, NY, August 2015.

- Invited talk: "Recent developments in auxiliary-field quantum Monte Carlo: magnetic orders and spin-orbit coupling"

  ES2015 Workshop: Developments in electronic structure theory and excited states beyond ground state DFT, Seattle, WA, June 2015.

- Contributed talk: “Auxiliary Field Quantum Monte Carlo Software”

  Flatiron Institute Software Revenue, New York, NY, October 2018.

- Contributed talk: APS March Meeting 2012-2016, Simons Collaboration on the Many Electron Problem Annual Meeting, 2015.

  More invited and contributed talk can be found at: www.boruoshihao.com/research

Publications

1. Metal-insulator and magnetic phase diagram of Ca2RuO4 from auxiliary field quantum Monte Carlo and dynamical mean field theory

   Hongxia Hao, Antoine Georges, Andrew Millis, Brenda M. Rubenstein, Qiang Han, and *Hao Shi*, submit to PRL.

2. Auxiliary field quantum Monte Carlo for multiband Hubbard models: controlling the sign and phase problems to capture Hund's physics

   Hongxia Hao, Brenda M. Rubenstein, *Hao Shi*, Phys. Rev. B 99, 235142 (2019).

3. Ground-state properties of the hydrogen chain: insulator-to-metal transition, dimerization, and magnetic phases

   Mario Motta, Claudio Genovese, Fengjie Ma, Zhi-Hao Cui, Randy Sawaya, Garnet Kin-Lic Chan, Natalia Chepiga, Phillip Helms, Carlos Jimenez-Hoyos, Andrew J. Millis, Ushnish Ray, Enrico Ronca, *Hao Shi*, Sandro Sorella, Edwin M. Stoudenmire, Steven R. White, Shiwei Zhang, arXiv:1911.01618 (2019).

4. Absence of superconductivity in the pure two-dimensional Hubbard model

   Mingpu Qin, Chia-Min Chung, *Hao Shi*, Ettore Vitali, Claudius Hubig, Ulrich Schollwöck, Steven R. White, Shiwei Zhang, arXiv:1910.08931(2019).

5. Direct comparison of many-body methods for realistic electronic Hamiltonians

   Kiel T. Williams, Yuan Yao, Jia Li, Li Chen, *Hao Shi*, Mario Motta, Chunyao Niu, Ushnish Ray, Sheng Guo, Robert J. Anderson, Junhao Li, Lan Nguyen Tran, Chia-Nan Yeh, Bastien Mussard, Sandeep Sharma, Fabien Bruneval, Mark van Schilfgaarde, George H. Booth, Garnet Kin-Lic Chan, Shiwei Zhang, Emanuel Gull, Dominika Zgid, Andrew Millis, Cyrus J. Umrigar, Lucas K. Wagner, arXiv:1910.00045 (2019).

6. Reaching the continuum limit in finite-temperature ab initio field-theory computations in many-fermion systems

   Yuan-Yao He, *Hao Shi*, Shiwei Zhang, Phys. Rev. Lett. 123, 136402 (2019).

7. Metal-insulator transition in the ground-state of the three-band Hubbard model at half-filling

   Ettore Vitali, *Hao Shi*, Adam Chiciak, Shiwei Zhang, Phys. Rev. B 99, 165116 (2019).

8. Finite-temperature Auxiliary-Field Quantum Monte Carlo: Self-Consistent Constraint and Systematic Approach to Low Temperatures

   Yuan-Yao He, Mingpu Qin, *Hao Shi*, Zhong-Yi Lu, Shiwei Zhang, Phys. Rev. B 99, 045108 (2019).

9. Accurate computations of Rashba spin-orbit coupling in interacting systems: from the Fermi gas to real materials

   Peter Rosenberg, *Hao Shi*, Shiwei Zhang, Journal of Physics and Chemistry of Solids, Volume 128, Pages 161-168 (2019).

10. Magnetic orders in the hole doped three-band Hubbard model: spin spirals, nematicity, and ferromagnetic domain walls

    Adam Chiciak, Ettore Vitali, *Hao Shi*, Shiwei Zhang, Phys. Rev. B 97, 235127 (2018).

11. Ultracold atoms in a square lattice with spin-orbit coupling: Charge order, superfluidity, and topological signatures

    Peter Rosenberg, *Hao Shi*, Shiwei Zhang, Phys. Rev. Lett. 119, 265301 (2017).

12. Response functions for the two-dimensional ultracold Fermi gas: dynamical BCS theory and beyond

    Ettore Vitali, *Hao Shi*, Mingpu Qin, Shiwei Zhang, Journal of Low Temperature Physics 189 (5-6), 312-327 (2017).

13. Numerical results on the short-range spin correlation functions in the ground state of the two-dimensional Hubbard model

    Mingpu Qin, *Hao Shi*, Shiwei Zhang, Phys. Rev. B 96, 075156 (2017).

14. Visualizing the BEC-BCS crossover in the two-dimensional Fermi gas: pairing gaps and dynamical response functions from ab initio computations

    Ettore Vitali, *Hao Shi*, Mingpu Qin, Shiwei Zhang, Phys. Rev. A 96, 061601 (2017).

15. Stripe order in the underdoped region of the two-dimensional Hubbard model

Bo-Xiao Zheng*, Chia-Min Chung*, Philippe Corboz*, Georg Ehlers*, Ming-Pu Qin*, Reinhard M. Noack, *Hao Shi**, Steven R. White, Shiwei Zhang, Garnet Kin-Lic Chan, **equal contribution**, Science 358 (6367), 1155-1160 (2017).

16. Quantum Monte Carlo simulation with Hartree-Fock-Bogoliubov wave function

    Hao Shi and Shiwei Zhang, Phys. Rev. B 94, 235119 (2016).

17. Coupling quantum Monte Carlo and independent-particle calculations: self-consistent constraint for the sign problem based on density or density matrix

    Mingpu Qin, *Hao Shi*, and Shiwei Zhang, Phys. Rev. B. 94, 235119 (2016).

18. Cluster size convergence of density matrix embedding theory with an auxiliary field quantum Monte Carlo solver: cellular and dynamical cluster formulations

    Bo-Xiao Zheng, Joshua S. Kretchmer, *Hao Shi*, Shiwei Zhang, and Garnet Kin-Lic Chan, Phys. Rev. B 95, 045103 (2017).

19. Computation of dynamical correlation functions for many fermions systems with auxiliary-field quantum Monte Carlo

    Ettore Vitali, *Hao Shi*, Mingpu Qin, and Shiwei Zhang, **editors' suggestion**, Phys. Rev. B 94, 085140 (2016).

20. A benchmark study of the two-dimensional Hubbard model with auxiliary-field quantum Monte Carlo method

    Mingpu Qin, *Hao Shi*, and Shiwei Zhang, Phys. Rev. B. 94, 085103 (2016).

21. Rashba spin-orbit coupling, strong interactions, and the BCS-BEC crossover in the ground state of the two-dimensional Fermi Gas

    Hao Shi, Peter Rosenberg, Simone Chiesa, and Shiwei Zhang, Phys. Rev. Lett. 117, 040401 (2016).

22. Infinite Variance in Fermion Quantum Monte Carlo Calculations

    Hao Shi and Shiwei Zhang, Phys. Rev. E 93, 033303 (2016).

23. Ground-state properties of strongly interacting Fermi gases in two dimensions

    Hao Shi, Simone Chiesa, and Shiwei Zhang, Phys. Rev. A 92, 033603 (2015).

24. Solutions of the Two Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms

    J. P. F. LeBlanc, Andrey E. Antipov, Federico Becca, Ireneusz W. Bulik, Garnet Kin-Lic Chan, Chia-Min Chung, Youjin Deng, Michel Ferrero, Thomas M. Henderson, Carlos A. Jiménez-Hoyos, E. Kozik, Xuan-Wen Liu, Andrew J. Millis, N. V. Prokof'ev, Mingpu Qin, Gustavo E. Scuseria, *Hao Shi*, B.

V. Svistunov, Luca F. Tocchio, I. S. Tupitsyn, Steven R. White, Shiwei Zhang, Bo-Xiao Zheng, Zhenyue Zhu, and Emanuel Gull, Phys. Rev. X 5, 041041 (2015).

25. CPMC-Lab: A Matlab package for Constrained Path Monte Carlo calculations

Huy Nguyen, *Hao Shi*, Jie Xu and Shiwei Zhang, Computer Physics Communications 185, 12 (2014).

Details about the CPMC-Lab package at http://cpmc-lab.wm.edu/

26. Symmetry-projected wave functions in quantum Monte Carlo calculations

Hao Shi, Carlos A. Jiménez-Hoyos, R. Rodríguez-Guzmán, Gustavo E. Scuseria, and Shiwei Zhang, Phys. Rev. B 89, 125129 (2014).

27. Symmetry in Auxiliary-Field Quantum Monte Carlo Calculations

Hao Shi and Shiwei Zhang, Phys. Rev. B 88, 125132 (2013).

28. Charge-density-wave and topological transitions in interacting Haldane model

Lei Wang, *Hao Shi*, Shiwei Zhang, Xiaoqun Wang, Xi Dai, and X. C. Xie, arXiv:1012.5163 (2010).