6. Computational Materials Science Research Team

6.1. Team members

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6.2. Research Activities

Solid state materials exhibit different properties ranging from metals, semi-conductors, insulators, magnets, and superconductors. A wide variety of these properties of materials are determined by quantum mechanical behaviors of a large number ($\sim 10^{23}$) of electrons. Thus, in order to understand materials properties, predict new behaviors, and design new materials, we must understand correctly the quantum mechanical motion of electrons that are described by Schrodinger equation. However, simulating many electron systems is computationally highly demanding and requires a massively parallel computer system such as the K computer in AICS.

The computational materials science research team conducts researches on developing new simulation methods/codes to search for a new quantum state of matter and to design new materials, specially in strongly correlated materials. Strongly correlated materials are a class of systems where Coulomb interactions between electrons are larger than the electron kinetic energy. These materials include various transition metal oxides such as high-Tc cuprate superconductors, colossal magneto resistive manganites, and organic conductive materials. The electronic states of weakly correlated materials such as semiconductors, where Coulomb interactions between electrons are only perturbative, can be well described by a single Slater determinant (one-particle approximation), and thus the standard density functional theory with an appropriate approximation works the best for weakly correlated materials. Instead, it is well known that the one-particle description is a poor approximation (and very often breaks down) for strongly correlated materials, and thus the standard method based on the density functional theory cannot be simply applied. Therefore, lots of efforts have been focused currently on developing new numerical methods to simulate strongly correlated materials.

The computational materials science research team focuses mainly on the following projects:

1) We develop a quantum Monte Carlo (QMC) method for a Hubbard-type model with more than 10,000 electrons where there is no sign problem.

2) We develop a density matrix renormalization group (DMRG) method to simulate two-dimensional Hubbard-type and quantum spin models for clusters as large as 16x16 and both at zero and at finite temperatures.

3) We develop a dynamical DMRG method and a time-dependent DMRG method to calculate

dynamical quantities as well as to simulate non-equilibrium quantum dynamics.

4) We offer highly efficient routines to perform in the K computer matrix-vector and matrix-matrix operations which are necessary in quantum many-body simulations such as the ones listed above.

With these newly developing methods, we conduct fundamental researches in strongly correlated quantum systems including various 3d transition metal oxides, low-dimensional organic materials, quantum spin systems, and cold atoms in optical lattices. We also plan to develop a first-principles simulation for strongly correlated materials.

6.3. Research Results and Achievements

6.3.1. QMC using the auxiliary field Monte Carlo technique

Among many QMC techniques to simulate interacting many electron systems like Hubbard model, we have developed the auxiliary field Monte Carlo method at zero temperature, which was originally proposed by J. E. Hirsch in 1985, by highly optimizing the code for the K computer. Describing one Slater determinant of many electrons in a single node (i.e., a Slater determinant not distributed to multiple nodes), we were able to use up to 24576 nodes with quite high efficiency of about 50% of the peak performance.

We have applied this method to the two-dimensional single-band Hubbard model, one of the simplest models to describe high-T_c cuprate superconductors and carbon sheets (graphene). Previously, the auxiliary field Monte Carlo method has been applied extensively to Hubbard-type models, and the largest lattice size reached was about N=600 sites by a German group in 2010. Using the K computer, we have reached up to N=2596 sites, about 4 times larger than the previous study. Note that the computational complexity scales like N^3. Thus it could have not been possible without the K computer.

Using this state-of-the-art QMC method, we have stared re-examined the ground state phase diagram of the half-filled Hubbard model on the honeycomb lattice, a model of graphene, as a function of the on-site Coulomb repulsion. This study is motivated by very recent finding of a possible spin liquid phase in the phase diagram of this model. This finding has surprised many researchers in this field because it is widely believed that a stable spin liquid appears most likely in geometrically frustrated systems and the Hubbard model on the honeycomb lattice is not frustrated. We are hoping to establish the grand state phase diagram of this model and resolve this issue of spin liquid.

6.3.2. DMRG

We have developed dynamical DMRG to calculate the one-particle excitation spectra for strongly correlated quantum systems. DMRG is known to be the best numerical method for one-dimensional quantum systems with extremely high precision. Extending DMRG to higher spatial dimensions is not trivial since the computational cost increases exponentially. To achieve high performance in the K computer, we have optimized the code using both MPI (and MPI2) and OpenMP. This improvement was necessary to simulate strongly correlated quantum systems in higher spatial dimensions even for quasi one-dimensional systems like several-leg ladders.

We have applied the dynamical DMRG to simulate cold fermionic atoms in quasi one-dimensional optical lattices with site dependent interactions. Depending the sign of local interactions, we have found a variety of phases at half-filling, including a possible superfluid phase. We have also studied the one-particle excitation spectra to characterize the nature of different phases.

6.4. Schedule and Future Plan

In the next academic year, we will conduct the following research.

6.4.1. QMC for a large number of interacting electrons

What prevents us from reaching even large lattice sites up to 10,000 sites in the K computer is the memory capacity available in each node. To simulate larger sites, we must distribute a Slater determinant into several nodes. So far we have used only a single node to describe a Slater determinant. In the next academic year, we are planning to develop a simulation code (using the auxiliary field Monte Carlo technique) in which a Slater determinant is distributed into several (4-6) nodes. A large size simulation is essential particularly when we want to study the phase boundary of a continuous quantum phase transition where the order parameter becomes inevitably small, thus requiring a careful finite-size scaling analysis.

6.4.2. DMRG for two-dimensional quantum systems

To simulate two-dimensional quantum systems, we will develop highly parallelized DMRG method at zero temperatures as well as finite temperatures. We have already developed highly parallelized DMRG code for one-dimensional systems, and in this academic year we will extend this to higher spatial-dimensions. Using this method, we are planning to study the ground state phase diagrams as well as various excitation spectra, including one-particle excitation spectra, linear and non-linear optical conductivities, and magnetic excitation spectra, for geometrically frustrated quantum spin systems and Hubbard-type interacting electrons.

6.4.3. Time-dependent DMRG to simulate quantum dynamics in strongly correlated systems

Time-dependent DMRG (t-DMRG) is the only reliable method thus far to simulate non-equilibrium quantum dynamics in strongly correlated systems. Thus, it is crucial to develop a highly efficient code of t-DMRG in the K computer. We have been developing a t-DMRG for the K computer, and we will continue doing it in this academic year. The main goal in this academic year is to improve the performance much better both for a single node and for a moderate number of nodes, before trying massively parallel simulations. For this purpose, we will take a simple model such as Hubbard-like models for cold atoms in optical lattices.

6.5. Publication, Presentation and Deliverables

(1) Papers

1. S. Zhang, S. Yamagiwa, M. Okumura, and S. Yunoki, "Performance Acceleration of Kernel Polynomial Method Applying Graphics Processing Units", IPDPS/APDCM 11, p. 564-571 (2011).

2. Q. Zhang, S. Hikino, and S. Yunoki, "First-principles study of the spin-mixing conductance in Pt/Ni$_{81}$Fe$_{19}$ junctions", Appl. Phys. Lett. 99, 172105 (2011).

3. H. Watanabe, T. Shirakawa, and S. Yunoki, "Spin-orbit-induced Mott insulator in 5d electron systems", J. Phys. Soc. Jpn. 80, SB006 (2011).

4. T. Shirakawa, H. Watanabe, and S. Yunoki, "Microscopic study of electronic and magnetic properties for Ir oxide", J. Phys. Soc. Jpn. 80, SB010 (2011).

5. T. Saitou, A. Koga, and A. Yamamoto, "Metal-insulator transition in optical lattice system with site-dependent interactions", arXiv:1204.4188 (2012).

(2) Invited Talks

1. S. Yunoki, "Microscopic study of spin-orbit-induced Mott insulator in Ir oxides ", Nanjing University (China) (Octobor, 2011).

2. S. Yunoki, "Microscopic study of spin-orbit-induced Mott insulator in Ir oxides ", SISSA (Italy) (February, 2012).

(3) Posters and presentations

1. S. Zhang, S. Yamagiwa, M. Okumura, and S. Yunoki, "Performance Acceleration of Kernel Polynomial Method Applying Graphics Processing Units", 13th Workshop on Advances in Parallel and Distributed Computational Models (APDCM2011), Anchorage (USA) (May, 2011).

2. H. Watanabe, T. Shirakawa, and S. Yunoki, "Variational Monte Carlo study for superconductivity in multi-orbital systems", The 26th International Conference on Low Temperature Physics, Beijing (China) (August, 2011).

3. Q. Zhang and S. Yunoki, "Magnetic Properties and Improper Ferroelectricity in LaFeO$_3$/LaCrO$_3$ Superlattices", The 26th International Conference on Low Temperature Physics, Beijing (China) (August, 2011).

4. Q. Zhang, G. Chen, X.-G. Gong, and S. Yunoki, "d^0 Ferromagnetic Surface in HfO$_2$", The 26th International Conference on Low Temperature Physics, Beijing (China) (August, 2011).

5. V. Badaut, T. Shirakawa, and S. Yunoki, "A Haldane-Anderson model study for the iron spin and charge state in Myoglobin", The 26th International Conference on Low Temperature Physics, Beijing (China) (August, 2011).

6. A. Yamamoto, S. Yamada, and M. Machida, "A novel quantum phase of one-dimensional fermionic optical lattices with spatially alternating interactions" (24aBA-6), The 67th Annual Meeting of the Physical Society of Japan, Osaka (Japan) (March, 2012).

7. T. Saitou, A, Koga, and A. Yamamoto, "Metal-insulator transition of fermionic optical lattices with spatially modulated on-site interactions" (24pAD-2), The 67th Annual Meeting of the Physical Society of Japan, Osaka (Japan) (March, 2012).

8. S. Yamada, J, Igarashi, M. Okumura, H. Onishi, A. Yamamoto, and M. Machida, "A DMRG study of superfluid correlations in a repulsive Hubbard model in a confined potential" (27aBG-13), The 67th Annual Meeting of the Physical Society of Japan, Osaka (Japan) (March, 2012).

(4) Patents and Deliverables
 - None