RICC Usage Report for Fiscal Year 2010

Project Title:

Large scale parallel numerical simulation for strongly correlated quantum systems

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1. **Background and purpose of the project, relationship of the project with other projects**

There are high demands on novel numerically exact algorithms to investigate the rich physics of low-dimensionality, frustrations, etc, including order-disorder and so on.

2. **Specific usage status of the system and calculation method**

We develop the entanglement perturbation theory (EPT) as the numerical method. We also develop a novel non-linear spin wave theory (NLSWT) as an analytical tool. Both works utilized RICC's nice computational recourses via large-scale parallelization (NLSWT does need corporation of numerical simulation, though it is analytical.)

3. **Result**

We obtained 3 major results in this fiscal year

a) We benchmarked the EPT for finite 2D with the spin 1/2 Heisenberg model on square lattices where the correct ground state energy is obtained. We then apply this algorithm to the model on triangular lattices which are featured by the geometric frustration. Our robust and efficient algorithm not only enables simulation on a moderately large system but also predicts a forth new 4-sublattice phase in the ground state phase diagram.

b) We developed a novel NLSWT. It goes beyond the border of other SWT regarding the treatment of the negative energy excitation by LSWT. It is found that the stable collinear spin configuration of spin 1/2 antiferromagnetic Heisenberg model on a triangular lattice is extended to that verified by various numerical simulations including ours. Plus, the incommensurate spiral spin configuration is found by our work to be unstable, which is consistent with our numerical study (But the 4-sublattice spin configuration is the exception).

c) We developed EPT for the infinite quasi-1D quantum system where the problem is converted to a statistical treatment through density matrix while the quantum feature is correspondingly embedded in the entangled localized density matrices. This entanglement can be reduced in a systematical way. Hence infinite quasi-1D spin lattice can be simulated with a concrete convergence. As the first application, we apply this method to the spin 1/2 Heisenberg model on infinite zigzag chains with ferromagnetic nearest neighboring interaction and antiferromagnetic next nearest neighboring interaction. The results disapprove the infinite Dimer-Neel phase switches in the region of the xxz anisotropy, 0.95~1.00, on the Lifshitz line.

4. **Conclusion**

Our method, EPT, is one of the promising many-body numerical methods, which utilizes large-scale computational resources with a good efficiency.

5. **Schedule and prospect for the future**

6. **If you wish to extend your account, provide usage situation (how far you have achieved, what calculation you have completed and what is yet to be done) and what you will do specifically in the next usage term.**

   Although I will leave Riken soon, I hope I can use RICC in an appropriate way in the future.

7. **If you have a "General User" account and could not complete your allocated computation time, specify the reason.**

   63%

8. **If no research achievement was made, specify the reason.**

   The schedule is often busy.

Fiscal Year 2010 List of Publications Resulting from the Use of RICC

[Publication]

1. L.Wang, S.G.Chung and S. Yunoki, *Entanglement perturbation theory for infinite quasi-1D quantum systems*

2. L.Wang and S.G. Chung, *A novel nonlinear spin wave theory for the spin 1/2 antiferromagnetic Heisenberg model on a triangular lattice*

3. L.Wang, T. Shirakawa, H. Watanabe and S. Yunoki, *A numerical study for two-dimensional spin 1/2 antiferromagnets: a generalization of Entanglement Perturbation Theory to two-dimensional systems*

[Proceedings, etc.]

4. L.Wang, T. Shirakawa, H. Watanabe and S. Yunoki, *A numerical study for two-dimensional spin 1/2 antiferromagnets: a generalization of Entanglement Perturbation Theory to two-dimensional systems, Proceeding of SCES2010,* Journal of Physics: Conference Series