RICC Usage Report for Fiscal Year 2009

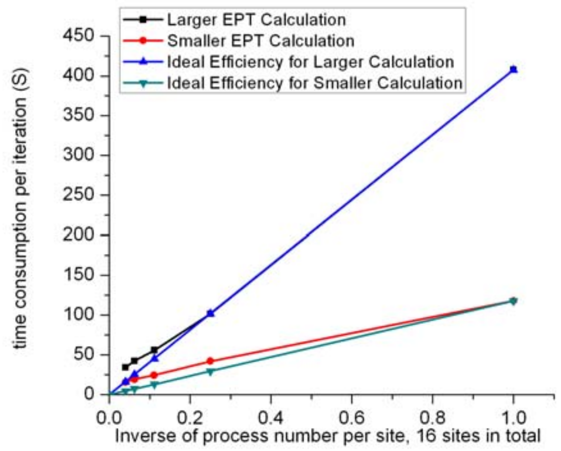
Project Title:

Large scale simulation for many electron system

Name: Lihua Wang

Affiliation: 和光研究所 基幹研究所 柚木計算物性物理研究室

1. It is important to find a new, precise yet efficient and general method to study the strongly correlated quantum system, since the current other algorithms see some limitations while they made great achievements in many applications. The new non-uniform Entanglement Perturbation Theory (EPT) and its generalization to two-dimensional (2D) were developed in this project. The results proved that it reflected the correct physics when applied to both 2D fermion system and 2D spin system. Besides, it adopted several high efficient algorithms both in novel mathematic structure and large-scale parallelization on many CPUs.
2. The usage status of the system is strongly related to the calculation method we used.
   First, the calculation method. For a lattice structure, we need to find the converged local wave functions on every site in EPT. Therefore, it is an iteration procedure. During each iteration, we perform matrix product and solve the generalized eigenvalue problem for all the sites at the same time. So naturally it has the high efficiency in parallelization if we divide our CPU usage into many small groups and let different group working on individual sites. Furthermore, the communication and collaboration are balanced in that the group-wide communication is intensive, the communication between groups is maintained minimum. See the following figure for the efficiency achieved by our moderate calculation on a few hundred CPU.



   Second. We used many CPU hours.
3. We report the EPT's core idea and its application to the antiferromagnetic spin chains in the attached paper. We also successfully test our methods on a 4x4 Heisenberg model on the triangular lattice, a 4x4 J1-J2 model lattice, a 4x4 Hubbard model lattice and a 8x8 Heisenberg model on the square lattice.
4. We got a general and high efficient non-uniform 2D EPT algorithm for both fermion, boson and spin strongly correlated systems
5. We are going to do EPT calculation on a reasonably large 2D fermion, boson and spin system (around 10x10), collecting precise data and investigate more fundamentally insightful many-body physics.
6. Like described above, we'd keep improving our testified method and apply it to those interesting problems. What we achieved now by using 66.2% of the CPU time in this period includes: a) a multiple level parallelizable,

precise EPT algorithm for both spin, boson and fermion. b) We collected data from EPT calculation for spin train with and without the external magnetic field. c) We also performed an extremely large calculation for an infinite system. There we developed an efficient way to solve the regular and the generalized eigenvalue problems for very large matrices which might bear novel mathematical interests. In the next period, we just make use of the achievement from this period to do more interesting physics like we repeated several time above.

7. I have a “General User” account and could not complete my allocated computation time. The reason is not that my calculation doesn't need this much time. Instead, it is because in the late of this period, in Feb and Mar, my submitted jobs were often put in queue and were not able to run for weeks. Before Feb, the situation was much better though. I just miss those days very much and feel very painful now.

Fiscal Year 2009 List of Publications Resulting from the Use of RICC

[Publication]

L. Wang, S. Yunoki and S.G. Chung, Entanglement Perturbation Theory for the spin system I : Antiferromagnetic Spin Chains, preprint

[Proceedings, etc.]

L. Wang, S.G. Chung and S. Yunoki, Entanglement Perturbation Theory for the spin system II : Spin Ladder

[Oral presentation at an international symposium]

Submitted the abstract to SCES 2010, The international conference on strongly correlated electron systems.