DSQSS - A PIMC-based quantum lattice model solver [1]

Naoki KAWASHIMA
Institute for Solid State Physics, University of Tokyo
Kashiwa-no-ha, Kashiwa, Chiba 277-8581

Among many numerical solutions to the quantum many-body problems on lattices, the path-integral Monte Carlo method (PIMC) has probably the most broad range of applicability [1]. By using PIMC, we can calculate the thermal expectation values of observables of interest with no systematic error for larger systems than can be handled by exact methods. The method works in arbitrary dimension at finite temperature as long as the system is free from the sign problem. The Monte Carlo method generally suffers from the slow convergence near the critical point ('critical slowing down'). For discrete space problems, several update methods, e.g., the loop algorithm and the directed-loop algorithm (DLA), have been developed to overcome the critical slowing down. These methods have been extended for massive parallelization for modern supercomputers.

While the loop-type update algorithms are quite powerful in selected problems, the worm-type update algorithm, the DLA included, are more frexible in various applications. Representative examples are boson systems and, equivalently, antiferromagnets with uniform magnetic field. In spite of these broad range of applicability, very few DLA-based open-source software has been available for parallel computation. Therefore, we proposed to develop one in the ISSP software-development/improvement project, to make it easier for non-experts to run DLA simulation on pararell machines without much effort.

Specifically, We are developing a PIMC program package for quantum lattice problems, which we call DSQSS (Discrete Space Quantum Systems Solver). Since DSQSS adopts the DLA for update scheme, it can update configurations effectively even under a symmetry-breaking field, DSQSS supports arbitrary Hamiltonians and lattices while it comes with additional tools to make it easier to define standard Hamiltonians and lattices. For example, models such as XXZ model defined on hypercubic lattice are pre-defined in DSQSS. As a result, in many cases of interest, users can perform QMC calculation by providing only a small amount of information (typically a few ten lines of text file) to define the condition of the simulation precisely. DSQSS also offers the parallelized multi worm algorithm for massively parallel calculation.

[1] This report is based on collaboration of Y. Motoyama (ISSP), K. Yoshimi (ISSP), A. Masaki-Kato (Hitachi Ltd.), N. K., and T. Kato (ISSP).

[2] The software website is
https://github.com/issp-center-dev/dsqss