Loop Cluster Monte Carlo Simulation of Quantum Magnets Based on Global Union-find Graph Algorithm

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The study of strongly-correlated quantum systems is the foremost area of research in contemporary statistical and condensed-matter physics [1], where the computational approaches are of increasing importance during recent years. From the view point of the computational condensed-matter physics, challenges are: supersolid in frustrated spin/bosonic lattice models, where diagonal and offdiagonal long-range orders coexist [2]; cold atoms on optical lattice, in which one can compare experiments with computations directly [3]; deconfined criticality, a direct continuous quantum phase transition between long-range ordered phase with incompatible symmetries [4], [5]; long-range and strongly anisotropic interactions, in which one observes effective reduction of spatial dimensions, exotic boundary effects, etc [6].

In order to tackle such important problems in strongly-correlated quantum systems, numerical simulations on large lattices are generally required, as the correlation length sometimes reaches millions of lattice constants and in many cases it indeed diverges due to strong fluctuations. Demands on unbiased and efficient simulation algorithms thus become stronger and stronger in recent years.

The quantum Monte Carlo method is one of the most promising tools as in principle it can simulate rather large lattices in any dimensions in *statistically exact* ways [7]. However, it is widely known that the conventional quantum Monte Carlo method based on local updates of world lines suffers from several drawbacks; ergodicity problem, fine-mesh slowing down, etc. Especially, in the vicinity of the quantum criticality the autocorrelation time in the Markov chain diverges as L^z, where L is the linear size of the lattice and $z \simeq 2$ the dynamical exponent. This is called the *critical slowing down*. The loop algorithm invented in 1993 [8], [9] and its extensions solve (or at least reduce) most of the drawbacks in the conventional method [10]–[12].

The loop algorithm, which is a kind of cluster algorithm, realizes updates of world-line configuration by flipping non-local objects, called *loops*. It has been shown that it is fully ergodic and drastically reduces the autocorrelation time, often by orders of magnitude, especially at low temperatures. Furthermore, by using the continuous-time version of the algorithm, one can completely eliminate the discretization error originating from the Suzuki-Trotter decomposition; simulations can be performed directly in the so-called Trotter limit.

Recently, the importance of the non-floating-point operations (e.g., graph algorithms) in high-performance computing has been widely realized, especially in the field of data-intensive applications [13]. Here, we present the world's first peta-scale cluster algorithm quantum Monte Carlo simulation on the K computer based on global union-find algorithm on a graph of about 1.1 trillion vertices and edges, solving the fundamental problems in statistical and condensed-matter physics.

In this poster presentation, after introducing the loop cluster algorithm, we discuss in detail how effectively the parallel graph algorithm is implemented using the OpenMP-MPI hybrid parallelization. By using the nonlocal update scheme based on the union-find graph algorithm, one can simulate such a huge system without any convergence problem. We show that the global graph algorithm is performed very efficiently up to 24,576 nodes (196,608 cores) of the K computer by means of the OpenMP-MPI hybrid scheme combined with several new techniques; asynchronous wait-free union-find algorithm, butterfly-type global union-find algorithm, majority-vote trick, process mapping optimization, etc. Compared with the conventional local flip quantum Monte Carlo updates performed on a single core, we have achieved $8\,(\text{threads}) \times 81\% \times 24,576\,(\text{nodes}) \times 46\% \simeq 10^5$-fold speed-up by parallelization. Together with $2,621,440 \times 310,690 \simeq 10^{12}$-fold acceleration of the Monte Carlo dynamics by eliminating the critical slowing down by the nonlocal cluster updates, we have virtually achieved 10^{17}-fold speed-up in total. We also represent the result of the quantum Monte Carlo simulation

of the spin-4 antiferromagnetic Heisenberg chain. We have successfully estimated the magnitude of the first excitation gap and the antiferromagnetic correlation length for the first time as 0.000799 ± 0.000005 and $10,400 \pm 70$, respectively.

The benchmark results presented in this paper have been obtained by early access to the K computer at the RIKEN Advanced Institute for Computational Science. The simulation program was developed based on the ALPS library [14], [15]. This work was supported by Grand Challenges in Next-Generation Integrated Nanoscience, Next-Generation Supercomputer Project and the Strategic Programs for Innovative Research (SPIRE) from the MEXT, and the Computational Materials Science Initiative (CMSI), Japan [16].

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