High-performance Parallel Diagonalization for Huge Matrices in Quantum Lattice-fermion Problems

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In order to study novel features of quantum lattice-fermion problems, we develop a new parallel matrix-diagonalization code for solving the ground state including a few excitation states of the model Hamiltonian matrix on the Earth Simulator. In terms of the Hamiltonian matrix-diagonalization, the Lanczos method, which has been so far utilized traditionally, is employed and parallelized. The most time consuming operation in the Lanczos method is the multiplication of the Hamiltonian and a vector, which is a main target for parallelization. However, it is known that the multiplication can not be parallelized effectively through simple distribution of the Hamiltonian matrix due to irregularities of the non-zero elements of the matrix. Especially, the more the number of processors increases, the worse the parallel efficiency becomes. This fact has been a major disadvantage in achieving high parallel efficiency on parallel supercomputers, which have thousands of processors like the Earth Simulator. In this paper, we therefore suggest an alternative parallel algorithm using a physical symmetry in the problem. The algorithm calculates the ground state for the 159-biliom-dimensional Hamiltonian matrix within 6 minutes on the 512 nodes (4096 processors) of the Earth Simulator. The parallelization ratio is beyond 99.99%, and the sustained peak performance is 13.694 TFLOPS (41.8% to the theoretical peak). On the other hand, we examine a new numerical scheme i.e., the preconditioned conjugate gradient (PCG) method instead of the Lanczos method for the diagonalization. The PCG method solves the ground state by minimizing the Rayleigh quotient. We make a preconditioner utilizing an approximation of an eigenvalue, which appear throughout the PCG iteration, and confirm that the preconditioner is quite suitable for the present problem. Using the PCG with the original preconditioner, we succeed in calculating the ground state for the 120-biliom-dimensional Hubbard-Hamiltonian matrix within 1 minute with 16.447 TFLOPS (50.2% of the peak) on the 512 nodes of the Earth Simulator. Note that it takes about 4 minutes for the same size matrix when using the Lanczos method. We find that the PCG method with the suitable preconditioner is much more excellent than the Lanczos method except for the memory usage.

Reference

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