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Communication avoiding Neumann expansion preconditioner for LOBPCG method: Convergence property of exact diagonalization method for Hubbard model

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Abstract. The exact diagonalization is the most accurate approach for solving the Hubbard model. The approach calculates the ground state of the Hamiltonian derived exactly from the model. Since the Hamiltonian is a large sparse symmetric matrix, we usually utilize an iteration method. It has been reported that LOBPCG method with a shift-and-invert preconditioner using an approximate eigenvalue can solve the problem efficiently. However, the preconditioner does not take effect for the Hamiltonian whose off-diagonal elements are predominant. In this research, we apply the preconditioner using the Neumann expansion and propose the communication avoiding strategy in consideration of the physical property of the Hubbard model. We show that the preconditioner improves the convergence property and decreases the elapsed time for the Hamiltonian with the predominant off-diagonal elements.

Keywords. LOBPCG method, Neumann expansion, communication avoiding, Hubbard model, quantum lattice systems

1. Introduction

The Hubbard model[1][2], which is one of the strongly-correlated electron systems, has attracted a tremendous number of physicists, since the model exhibits a lot of interesting phenomenon such as High-T_c superconductivity. When we solve the ground state (the smallest eigenvalue and the corresponding eigenvector) of the Hamiltonian derived from the model, we can understand its properties. Therefore, a lot of computational methods have been proposed. The most accurate one is the exact diagonalization which solves the ground state of the Hamiltonian derived exactly from the model. Since the Hamiltonian is a huge sparse symmetric matrix, we usually solve the eigenvalue problem with an iteration method, such as the Lanczos method[3], the LOBPCG method[4][5], and so

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