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POS-F42 – Exact Diagonalization on Pyrochlore System with Lattice Distortion

Wednesday 9 June 2021 13:47 (2 minutes)

Exact diagonalization is a powerful method to analyze a crystal system. In our research, we apply the exact diagonlization method on 16 site spin 1/2 Pyrochlore system. The Hamiltonian of this system can be expressed as a 65536 times 65536 matrix, then we use point group D_3 and FCC translational group to block diagonalise this matrix. Finally, we apply Lapack subroutine to get the eigenvalues and eigenstates of this 16 sites system. Moreover, we also consider a lattice distortion which reduce the full spce group Fd3m to F43m. With small varying of the exchange constants J_{ij}, we can analyze the ground state energy and the total system energy changing through the lattice distortion. Moreover, using the result from exact diagonalization, we are also able to find the quantum entanglement between different sites in the system with lattice distortion.

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