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27 - Exact Diagonalization on Pyrochlore System

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In quantum physics, if we can find the eigenstates $|\phi_i\rangle$ of a Hamiltonian H, and the respective eigenergies E_i, we can calculate many aspects such as time evolution, or its thermal properties. Exact diagonalization is a method which can solve the Hamiltonian numerically. For a small Hamiltonian system, we can find the eigenvalues by solve the characteristic polynomial equation of the matrix. However, as the system goes larger, the calculation will go exponentially. Instead of calculating the eigenstates directly, We will use the unitary transformation matrix to block diagonalise the Hamiltonian first. As a consequence, instead of solving the Hamiltonian directly, we will solve each block. In order to find the unitary transformation matrix U, we will use the symmetry of the Hamiltonian, and with the help of group theory, we can construct U matrix and do the block diagonalization.
The space group for Pyrochlore is No.227, it contains the point group O_h with space translations. Here we consider the conventional cell contains 16 sites, and use three translations T1:$(0, 1/2, 1/2)$, T2:$(1/2, 0, 1/2)$ and T3:$(1/2, 1/2, 0)$. Additionally, we also use the subgroup D_2 and the time reversal symmetry. As a result, we will block diagonalise the Hamiltonian into 32 blocks, which can be analyze easily.

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