Phys730 Final-Project Proposal

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Numerical Solution of Frustrated Quantum Heisenberg Spin Chain

Introduction

The spin-half quantum Heisenberg spin chain is a model of mutually interacting quantum spins arranged at a regular intervals along a line. The nature of interaction is antiferromagnetic $(J > 0)$, meaning that they favor the opposite alignment of spins.The simple and natural way to incorporate frustration is to consider the next-nearest-neighbor interation in the Hamiltoian. The nearest- and next-nearest-neighbor interactions favor incompatible spin orderings, and the competition between them gives rise to *frustration*. The Hamiltonian is

$$\hat{\mathbf{H}} = \sum_{i=0}^{N-1} \left[J_1 \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1} + J_2 \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+2} \right],$$

where N is the length of the chain, and S_i is the spin at site i.
There is a special, exactly solvable point $(J_2/J_1 = 0.5)$, called Majumdar Ghosh point (MGP). At MGP ,the doubly degenerate ground state energy per spin is $E_0/N = -3/8$.

Computational Method

The Python programming language will be used for the simulation. Hamiltonian matrix is sparse, a matrix in which most of the elements are zero. So, *scipy.sparse* from *SciPy* will be used which require less memory space to represent a sparse matrix, and allows for speeding up calculations involving these matrices. The simulation will be carried out over a range of tuning parameter J_2/J_1, the ratio between the strength of next-nearest- and nearest-neighbor interactions, on finite-size systems of increasing size with result extrapolated to infinite-size limit. Numerical results will be compared to the known result at MGP.

Tool

NumPy
SciPy
matplotlib