Entanglement measure of frustrated Heisenberg octahedral chain within the localized-magnon approach

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Introduction

We consider the spin-1/2 Heisenberg octahedral chain defined through the Hamiltonian

\[ H = \sum_j J_1 S_j \cdot S_j + J_2 S_j \cdot S_{j+1} - h S_j \cdot \hat{S}_z, \quad S^2 = \sum_{j=1}^N S_j^2. \] (1)


Regime of strong frustration: \( J_2/J_1 \geq 2 \)

- Ground state of \( H \), only for big \( h \):
  \[ |0\rangle = |\uparrow\uparrow\uparrow\rangle. \]
- One-magnon state on square plaquette (moderate magnetic fields):
  \[ |1\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\uparrow\rangle \pm |\downarrow\uparrow\uparrow\rangle). \]
- Two-magnon state on square plaquette (small magnetic fields):
  \[ |2\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle). \]

Localized magnons and thermodynamics

Two-component lattice-gas model of hard-core monomers:

\[ H_{\text{eff}} = E_{\text{eff}} - 2hN - h \sum_{j=1}^N S_j^z - \mu_1 \sum_{j=1}^N n_j - \mu_2 \sum_{j=1}^N m_j. \] (3)

For finite-size spin-1/2 Heisenberg octahedral chain with up to 4 unit cells (20 spins).

Concurrences \( C_{\text{00}} \) and \( C_{\text{02}} \)

Density plots of the concurrence \( C_{\text{00}} \) as a function of magnetic field and temperature.

Conclusions

- We have investigated in detail the bipartite entanglement between the nearest-neighbor and next-nearest-neighbor spin pairs of a highly frustrated spin-1/2 Heisenberg octahedral chain in a presence of the external magnetic field.
- To provide an independent check of the localized-magnon method we have performed a full ED of the finite-size spin-1/2 Heisenberg octahedral chain with up to 4 unit cells (20 spins).
- It was shown that the concept of localized magnons can be straightforwardly adapted in order to calculate the quantity concurrence, which may serve as a measure of the pairwise entanglement between nearest-neighbor and next-nearest-neighbor spins.