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

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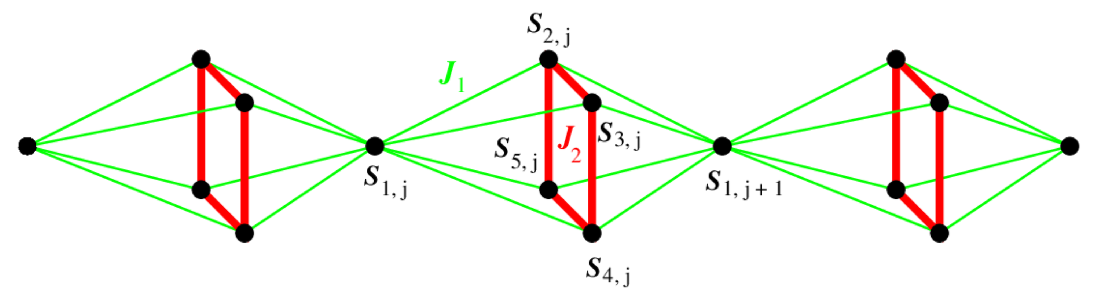
Introduction

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

$$H = \sum_{(ij)} J_{ij}\mathbf{s}_i \cdot \mathbf{s}_j - hS^z, \quad S^z = \sum_{i=1}^{N} s_i^z. \qquad (1)$$



J. Strečka et al., Phys. Rev. B **95**, 224415 (2017); Physica B **536**, 364 (2018).

The main goal of the present research is to investigate a strength of the bipartite entanglement between the nearest- and next-nearest-neighbor spin from square plaquettes of the spin-1/2 Heisenberg octahedral chain.

- $|\uparrow\uparrow\uparrow \ldots \uparrow\rangle$ – ground state of H (only for big h),
- $\sum_i \alpha_i s_i^- |\uparrow\uparrow\uparrow \ldots \uparrow\rangle$ – one-magnon state with energy ε_k,
- Ideal geometry, $J_1 = J_3 = J_4 = J_5 = J$, $J_2 > 2J$

$$\frac{1}{2}\left(s_{m,1}^- - s_{m,2}^- + s_{m,3}^- - s_{m,4}^-\right)|\uparrow\uparrow\uparrow \ldots \uparrow\rangle \qquad (2)$$

J. Schulenburg et al., Phys. Rev. Lett. **88**, 167207 (2002); H.-J. Schmidt, J. Phys. A **35**, 6545 (2002).

Regime of strong frustration: $J_2/J_1 \geq 2$

- Ground state of H, only for big h:

$$|0\rangle_j = |\uparrow_{2,j}\uparrow_{3,j}\uparrow_{4,j}\uparrow_{5,j}\rangle$$

- One-magnon state on square plaquette (moderate magnetic fields):

$$|1\rangle_j = \frac{1}{2}\big(|\downarrow_{2,j}\uparrow_{3,j}\uparrow_{4,j}\uparrow_{5,j}\rangle - |\uparrow_{2,j}\downarrow_{3,j}\uparrow_{4,j}\uparrow_{5,j}\rangle + |\uparrow_{2,j}\uparrow_{3,j}\downarrow_{4,j}\uparrow_{5,j}\rangle - |\uparrow_{2,j}\uparrow_{3,j}\uparrow_{4,j}\downarrow_{5,j}\rangle\big);$$

- Two-magnon state on square plaquette (small magnetic fields):

$$|2\rangle_j = \frac{1}{\sqrt{3}}\big(|\uparrow_{2,j}\downarrow_{3,j}\uparrow_{4,j}\downarrow_{5,j}\rangle + |\downarrow_{2,j}\uparrow_{3,j}\downarrow_{4,j}\uparrow_{5,j}\rangle\big) - \frac{1}{\sqrt{12}}\big(|\uparrow_{2,j}\uparrow_{3,j}\downarrow_{4,j}\downarrow_{5,j}\rangle + |\uparrow_{2,j}\downarrow_{3,j}\downarrow_{4,j}\uparrow_{5,j}\rangle + |\downarrow_{2,j}\uparrow_{3,j}\uparrow_{4,j}\downarrow_{5,j}\rangle + |\downarrow_{2,j}\downarrow_{3,j}\uparrow_{4,j}\uparrow_{5,j}\rangle\big).$$

Localized magnons and thermodynamics

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

$$\mathcal{H}_{\rm eff} = E_{\rm FM}^0 - 2hN - h\sum_{j=1}^{N} S_{1,j}^z - \mu_1\sum_{j=1}^{N} n_{1,j} - \mu_2\sum_{j=1}^{N} n_{2,j}, \qquad (3)$$

- $E_{\rm FM}^0 = N(2J_1 + J_2)$ – zero-field energy of the fully polarized ferromagnetic state;
- $\mu_1 = J_1 + 2J_2 - h$ – chemical potential of the first kind of monomeric particles;
- $\mu_2 = 2J_1 + 3J_2 - 2h$ – chemical potential of the second kind of monomeric particles;
- $n_{1,j} = 0, 1$ and $n_{2,j} = 0, 1$ – occupation numbers of both kinds of the monomeric particles.

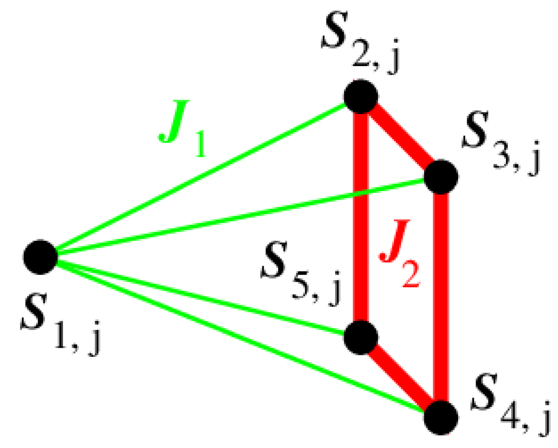
J. Strečka et al., Phys. Rev. B **95**, 224415 (2017); Physica B **536**, 364 (2018).

- $\mathcal{Z}_{\rm eff} = e^{-\beta N(2J_1+J_2-2h)}\prod_{j=1}^{N}\sum_{S_{1,j}^z} e^{\beta h S_{1,j}^z} \times \sum_{n_{1,j}}\sum_{n_{2,j}}(1-n_{1,j}n_{2,j})e^{\beta(\mu_1 n_{1,j}+\mu_2 n_{2,j})} = e^{-\beta N(2J_1+J_2-2h)}\left[2\cosh\left(\frac{\beta h}{2}\right)\right]^N\left(1+e^{\beta\mu_1}+e^{\beta\mu_2}\right)^N$, $\beta = 1/(k_B T)$.
- $F_{\rm eff} = -k_B T \lim_{N\to\infty}\frac{1}{N}\ln\mathcal{Z}_{\rm eff} = 2J_1 + J_2 - 2h - k_B T\ln\left[2\cosh\left(\frac{\beta h}{2}\right)\right] - k_B T\ln\left(1+e^{\beta\mu_1}+e^{\beta\mu_2}\right)$;
- $M = -\frac{\partial F_{\rm eff}}{\partial h} = 2 + \frac{1}{2}\tanh\left(\frac{\beta h}{2}\right) - \frac{e^{\beta\mu_1}+2e^{\beta\mu_2}}{1+e^{\beta\mu_1}+e^{\beta\mu_2}}$.

Concurrence and correlation functions

$$C_{nn} = \max\left\{0, 4|\langle\hat{S}_{2,j}^x\hat{S}_{3,j}^x\rangle| - 2\sqrt{\left(\frac{1}{4}+\langle\hat{S}_{2,j}^z\hat{S}_{3,j}^z\rangle\right)^2 - \left(\frac{1}{2}\langle\hat{S}_{2,j}^z+\hat{S}_{3,j}^z\rangle\right)^2}\right\},$$

$$C_{nnn} = \max\left\{0, 4|\langle\hat{S}_{2,j}^x\hat{S}_{4,j}^x\rangle| - 2\sqrt{\left(\frac{1}{4}+\langle\hat{S}_{2,j}^z\hat{S}_{4,j}^z\rangle\right)^2 - \left(\frac{1}{2}\langle\hat{S}_{2,j}^z+\hat{S}_{4,j}^z\rangle\right)^2}\right\},$$

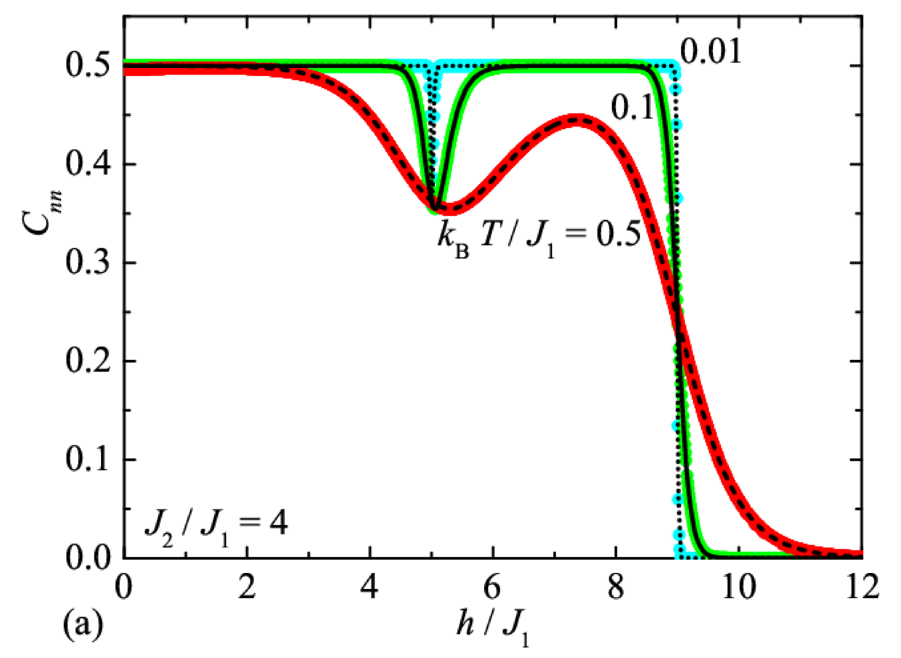


$$\langle\hat{S}_{2,j}^\alpha\hat{S}_{3,j}^\alpha\rangle = \frac{1}{\mathcal{Z}_{\rm eff}}\sum_{\{S_{1,j}^z\}}\sum_{\{n_{1,j}\}}\sum_{\{n_{2,j}\}}\sum_{k=0}^{2}\langle k|\hat{S}_{2,j}^\alpha\hat{S}_{3,j}^\alpha|k\rangle_j\, e^{-\beta\mathcal{H}_{\rm eff}} = \frac{C_{kk}^{\alpha\alpha} + C_{kk}^{\alpha\alpha}e^{\beta\mu_1} + C_{kk}^{\alpha\alpha}e^{\beta\mu_2}}{1+e^{\beta\mu_1}+e^{\beta\mu_2}},$$

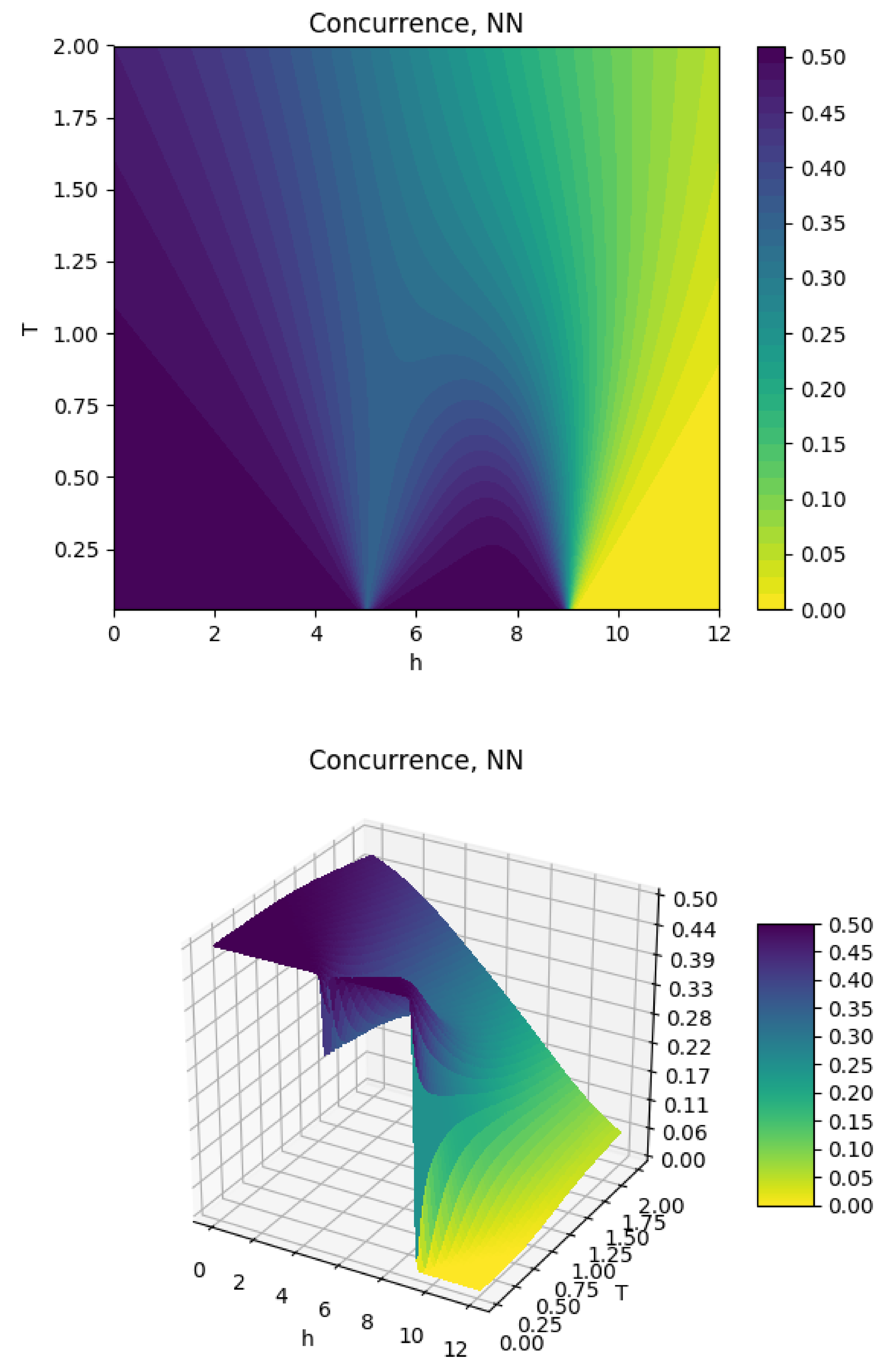
$$C_{kk}^{\alpha\alpha} = \langle k|\hat{S}_{2,j}^\alpha\hat{S}_{3,j}^\alpha|k\rangle_j, \quad (k = 0, 1, 2; \alpha = x, z).$$

L. Amico, A. Osterloh, F. Plastina, R. Fazio, and G. M. Palma, Phys. Rev. A, **69**, 022304 (2004).

Concurrence, nearest-neighbor spins

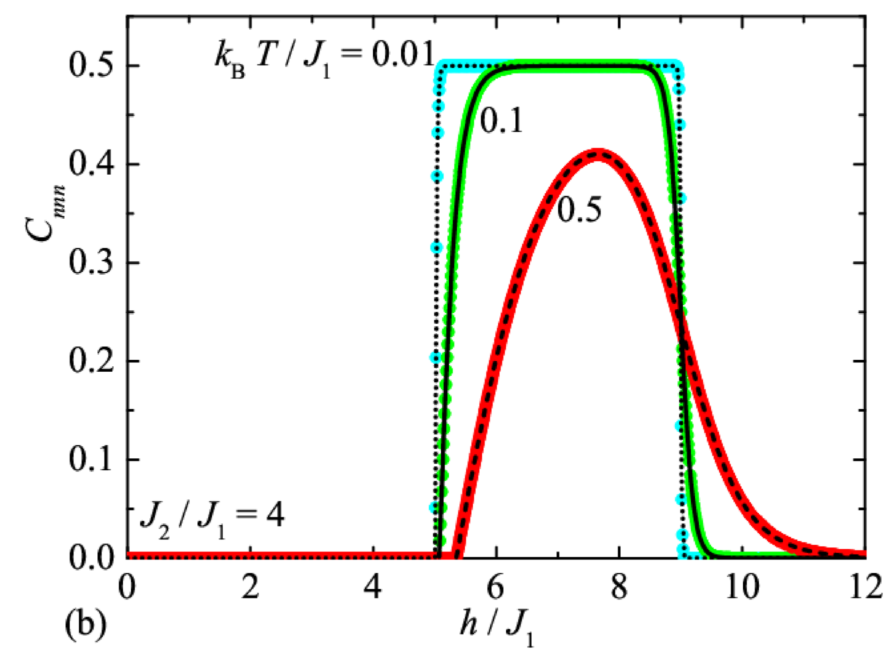


Isothermal dependencies of the quantum concurrence on a magnetic field, which quantifies the bipartite entanglement between the nearest-neighbor (a) spin pairs within square plaquettes.

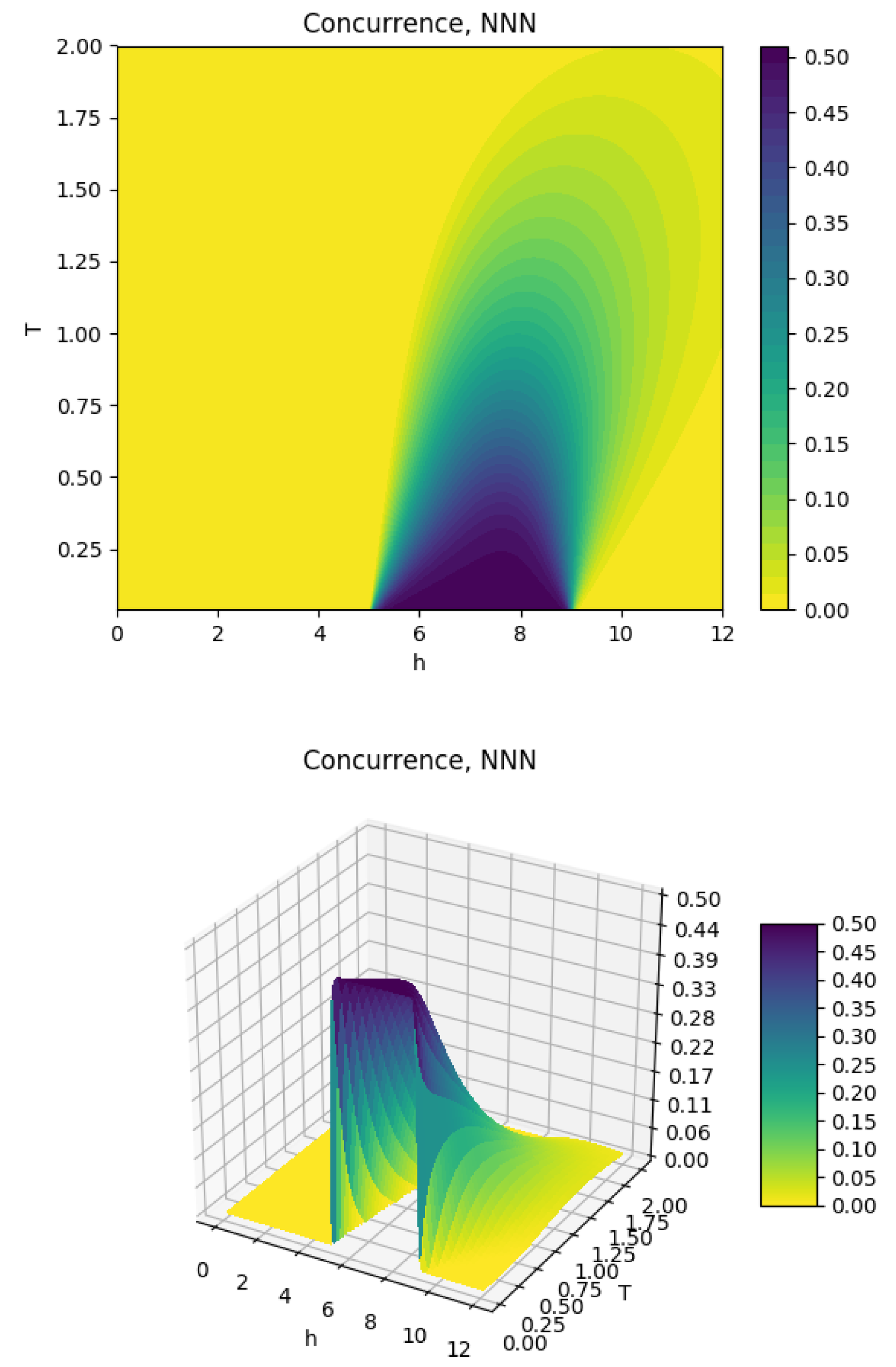


Density plots of the concurrence C_{nn} as a function of magnetic field and temperature.

Concurrence, next-nearest-neighbor spins

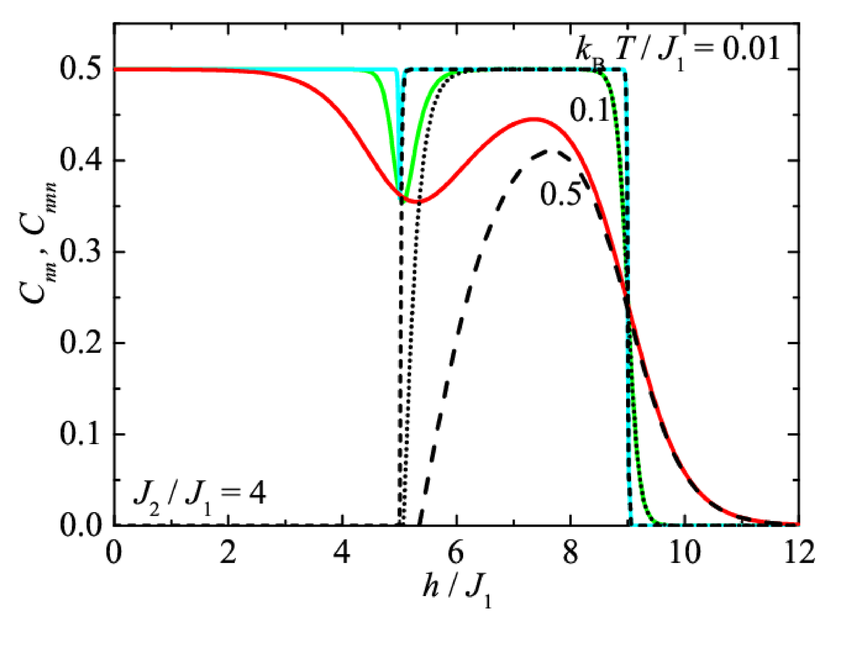


Isothermal dependencies of the quantum concurrence on a magnetic field, which quantifies the bipartite entanglement between next-nearest-neighbor (b) spin pairs within square plaquettes.



Density plots of the concurrence C_{nnn} as a function of magnetic field and temperature.

Concurrences C_{nn} and C_{nnn}



A comparison between the concurrences C_{nn} and C_{nnn}.

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.
- J. Strečka, O. Krupnitska and J. Richter, EPL, **132** 30004 (2020).