Magnetic properties of decorated spin ladder systems

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Abstract

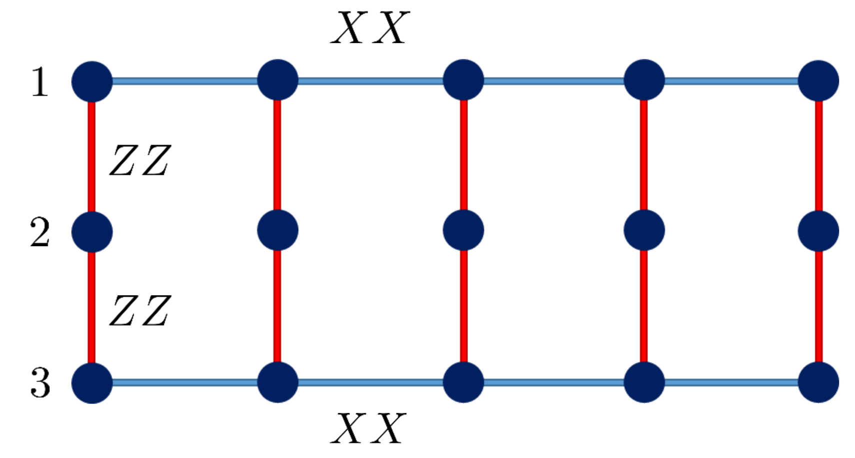
This work is devoted to the theoretical study of the decorated spin ladder built from two finite open spin-½ chains with XX interaction, connected vertically through additional Ising spins-S. This ladder structure has three spin unit cells.

System structure

Decorated spin ladder contains two finite XX chains connected by Ising spin decorations. Hamiltonian [1]:

$$\mathbf{H} = -g_1\mu_B H\sum_{n=1}^{N} S_{1,n}^z - g_2\mu_B H\sum_{n=1}^{N} S_{2,n}^z - g_3\mu_B H\sum_{n=1}^{N} S_{3,n}^z -$$

$$-J_1\sum_{n=1}^{N-1}\left(S_{1,n}^x S_{1,n+1}^x + S_{1,n}^y S_{1,n+1}^y\right) - J_3\sum_{n=1}^{N-1}\left(S_{3,n}^x S_{3,n+1}^x + S_{3,n}^y S_{3,n+1}^y\right) - J_2\sum_{n=1}^{N} S_{2,n}^z\left(S_{1,n}^z + S_{3,n}^z\right)$$



Methods

Application of Jordan-Wigner transformation gives us:

$$\mathbf{H} = -g_1\mu_B H\sum_{n=1}^{N}\left(\frac{1}{2} - a_{1,n}^\dagger a_{1,n}\right) - g_3\mu_B H\sum_{n=1}^{N}\left(\frac{1}{2} - a_{3,n}^\dagger a_{3,n}\right) - g_2\mu_B H\sum_{n=1}^{N} S_{2,n}^z$$

$$-\frac{J_1}{2}\sum_{n=1}^{N-1}\left(a_{1,n}^\dagger a_{1,n+1} + a_{1,n+1}^\dagger a_{1,n}\right) - \frac{J_3}{2}\sum_{n=1}^{N-1}\left(a_{3,n}^\dagger a_{3,n+1} + a_{3,n+1}^\dagger a_{3,n}\right)$$

$$-J_2\sum_{n=1}^{N} S_{2,n}^z\left(1 - a_{1,n}^\dagger a_{1,n} - a_{3,n}^\dagger a_{3,n}\right)$$

Due to commutation between Hamiltonian and operators of z-projection of Ising spin operators we can replace operators S_{2n}^z by their eigen values σ_n.

This is simplified version of the Hamiltonian.

$$\mathbf{H} = E_0 + \sum_{n=1}^{N}\left(g_1\mu_B H + J_2\sigma_n\right)a_{1,n}^\dagger a_{1,n} + \sum_{n=1}^{N}\left(g_3\mu_B H + J_2\sigma_n\right)a_{3,n}^\dagger a_{3,n}$$

$$-\frac{J_1}{2}\sum_{n=1}^{N-1}\left(a_{1,n}^\dagger a_{1,n+1} + a_{1,n+1}^\dagger a_{1,n}\right) - \frac{J_3}{2}\sum_{n=1}^{N-1}\left(a_{3,n}^\dagger a_{3,n+1} + a_{3,n+1}^\dagger a_{3,n}\right)$$

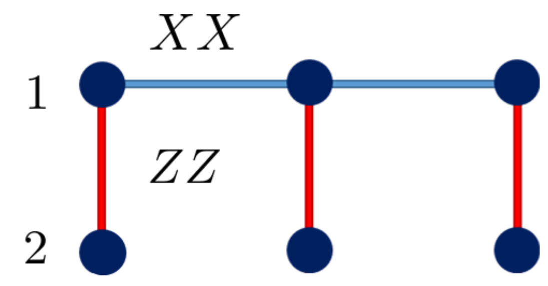
$$E_0 = -\frac{1}{2}\mu_B H\left(g_1 + g_3\right)N - \left(g_2\mu_B H + J_2\right)\sum_{n=1}^{N}\sigma_n$$

For one inverted spin we have the following equation:

$$\mathbf{H}|1\rangle = \left(E_0 + \varepsilon\right)|1\rangle$$

$$|1\rangle = \sum_{n=1}^{3}\left(U_n a_{1,n}^\dagger + V_n a_{3,n}^\dagger\right)|0\rangle;$$

Our spin ladder system can be separated into two chains with the same set of pendant Ising spins.



$$\begin{cases}\left(\varepsilon - g_1\mu_B H - J_2\sigma_1\right)U_1 + \frac{J_1}{2}U_2 = 0;\\ \left(\varepsilon - g_1\mu_B H - J_2\sigma_2\right)U_2 + \frac{J_1}{2}\left(U_1 + U_3\right) = 0;\\ \left(\varepsilon - g_1\mu_B H - J_2\sigma_3\right)U_3 + \frac{J_1}{2}U_2 = 0;\end{cases}$$

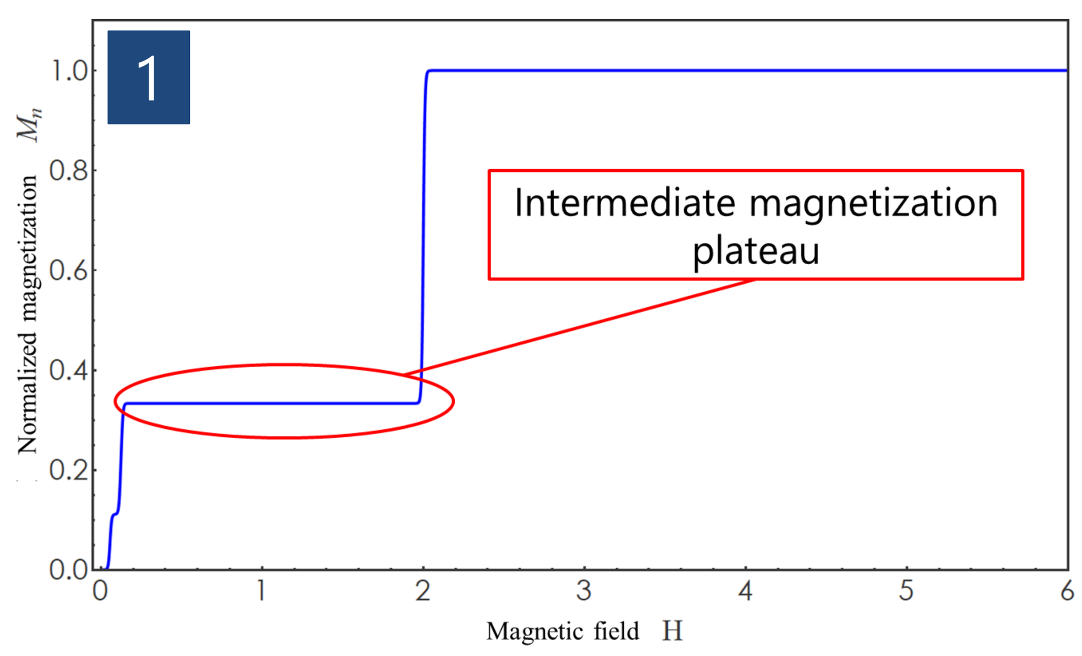
$$\mathrm{Det}\begin{vmatrix} h_1 + J_1\sigma_1 - \varepsilon & -\frac{J_1}{2} & 0 \\ -\frac{J_1}{2} & h_1 + J_1\sigma_2 - \varepsilon & -\frac{J_1}{2} \\ 0 & -\frac{J_1}{2} & h_1 + J_1\sigma_3 - \varepsilon \end{vmatrix} = 0$$

Solution of this equation gives us energy values which can be used for calculation of partition function.

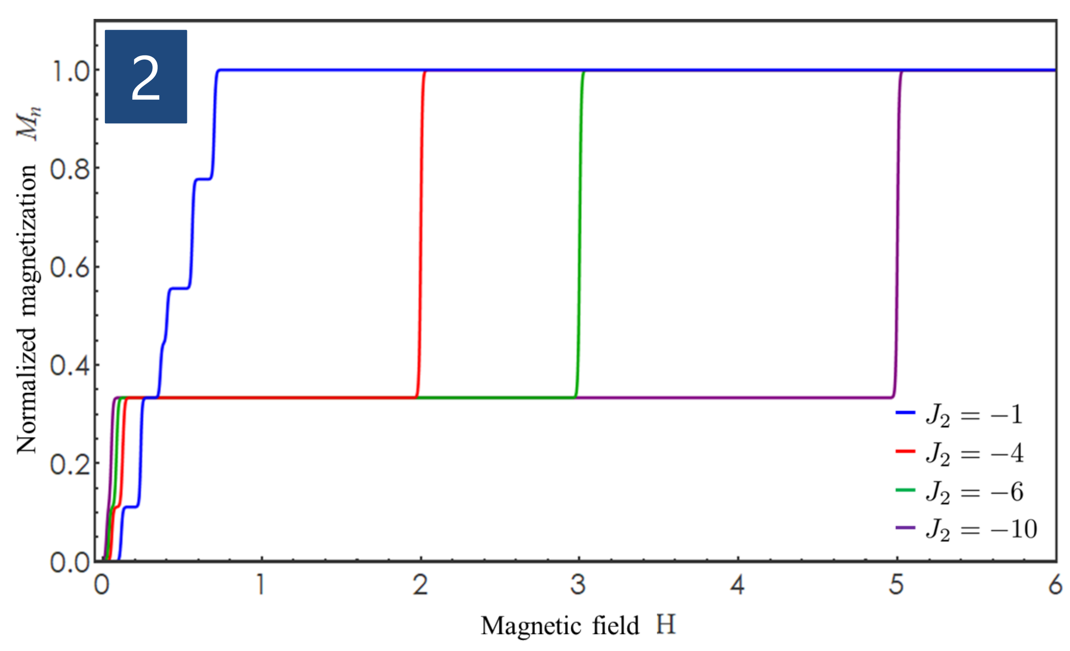
$$Z = \sum_{i=1}^{2^N} e^{-\frac{E_{0,i}}{T}}\prod_{j=1}^{N}\left(1 + e^{-\frac{\varepsilon_{1,i,j}}{T}}\right)\left(1 + e^{-\frac{\varepsilon_{3,i,j}}{T}}\right)$$

Calculation for three and more rungs system were performed in program Wolfram Mathematica 14.0.

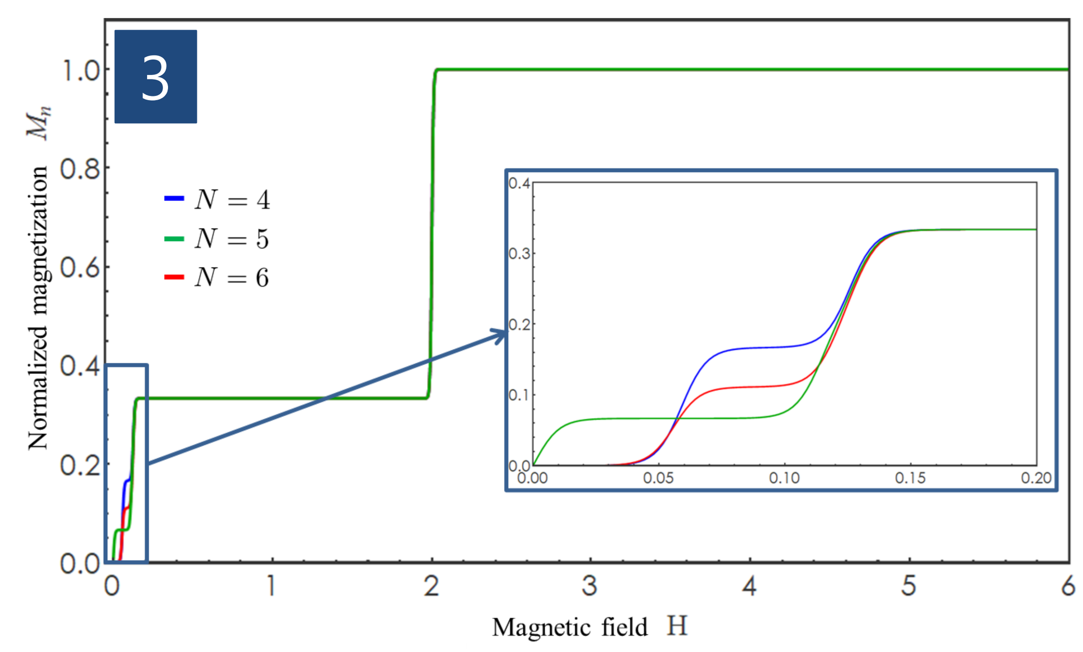
Results



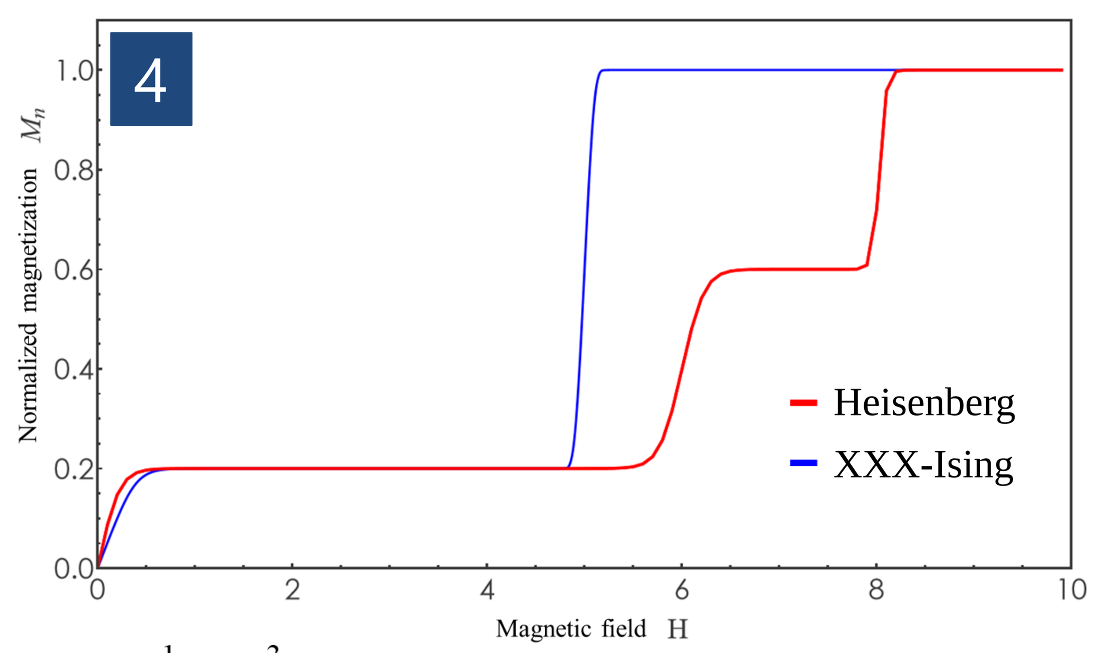
$J_1 = 1, J_2 = -4, J_3 = 1, g_1 = 2, g_2 = 2, g_3 = 2, \mu = 1, N = 6, T = 0.01$



$J_1 = 1, J_3 = 1, g_1 = 2, g_2 = 2, g_3 = 2, \mu = 1, N = 6, T = 0.01$

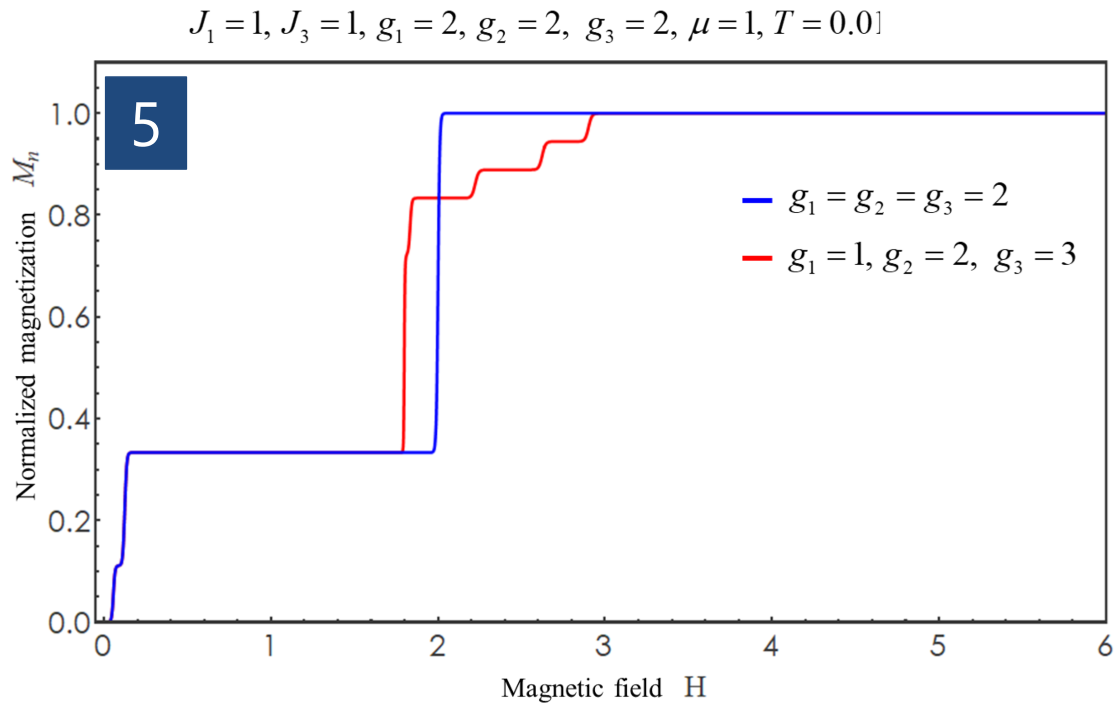


$J_1 = 1, J_2 = -4, J_3 = 1, g_1 = 2, g_2 = 2, g_3 = 2, \mu = 1, T = 0.01$

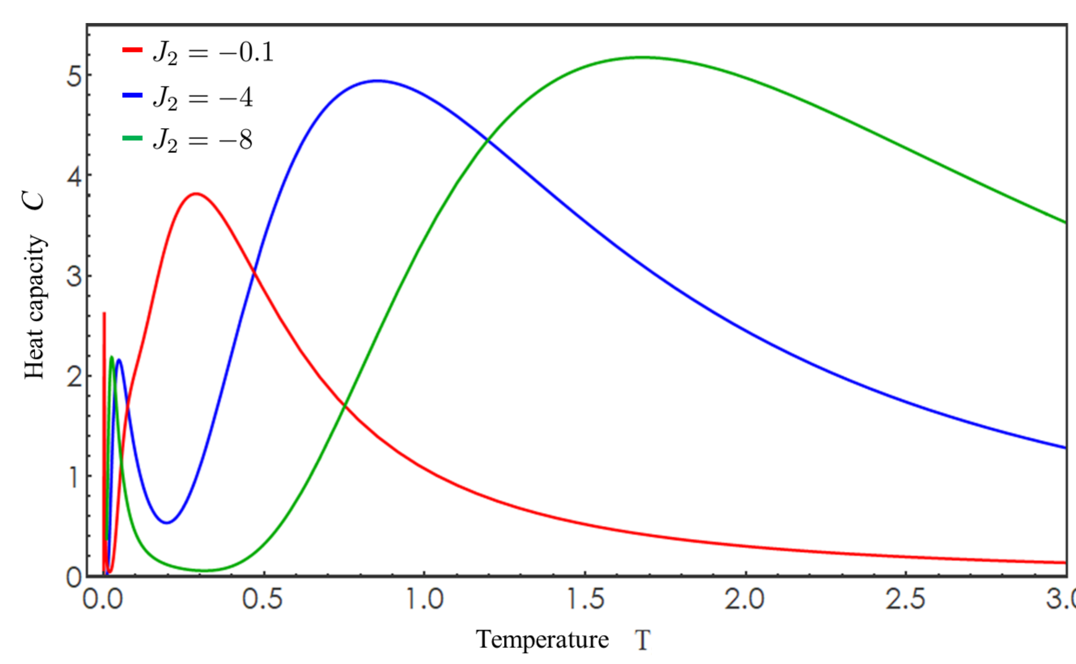


$S_1 = S_3 = \frac{1}{2}, S_2 = \frac{3}{2}, J_1 = J_3 = -0.1, J_2 = -4, g_1 = g_2 = g_3 = 1, \mu = 1, N = 3, T = 0.1$

$$\mathbf{H} = -\sum_{i=1}^{L}\left[J_1\left(\mathbf{S}_{1,i}\mathbf{S}_{1,i+1} + \mathbf{S}_{3,i}\mathbf{S}_{3,i+1}\right) + J_2\left(\mathbf{S}_{1,i} + \mathbf{S}_{3,i}\right)\bar{\mathbf{S}}_{2,i}\right] - h\mathbf{S}_{total}^z$$



$J_1 = 1, J_2 = -4, J_3 = 1, \mu = 1, N = 6, T = 0.01$



$J_1 = 1, J_2 = -4, J_3 = 1, g_1 = 2, g_2 = 2, g_3 = 2, \mu = 1, N = 6, H = 0$

Fig. 4 was obtained for two systems: isotropic Heisenberg spin coupling and for XXX chains and Ising coupling in rungs.

Summary

We found that the antiferromagnetic mixed spin ladder model with dominant coupling in rungs may have the intermediate plateaus in magnetization profile. We also found that in contrast to isotropic spin ladder model, similar anisotropic model with dominant Ising-type interactions in rungs has only one intermediate magnetization plateau.

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References

[1] V. O. Cheranovskii, E.V. Ezerskaya, S. Ye. Kononenko, Low Temp. Phys. 50, 152 (2024). https://doi.org/10.1063/10.0024327