# Magnetic properties of the Heisenberg–Ising model of nanomagnets on the base of transition metal polymeric complexes

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## Abstract

This work is devoted to the theoretical study of thermodynamics of mixed spin model built from Ising spin-1/2 rings, which are decorated by three-spin fragments with XXZ Heisenberg interaction. This system has translational symmetry.

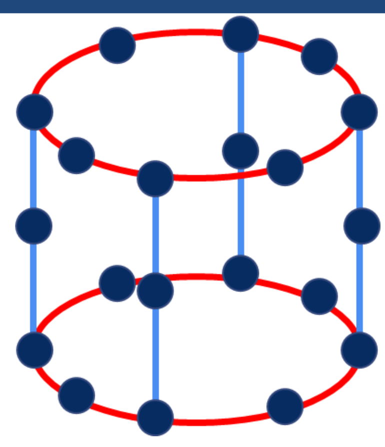
## System structure

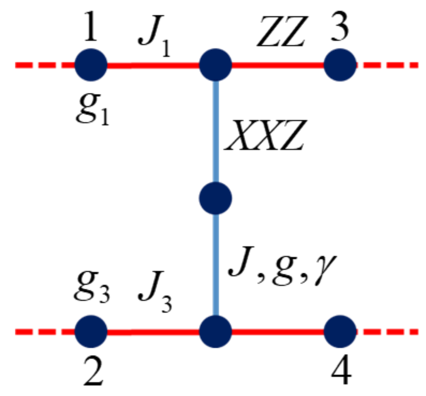
This spin system contains finite XXZ chains connected by Ising spin rings. The system Hamiltonian has the following form:

$$\hat{\mathbf{H}} = -\sum_{l=1}^{L}\Big[g_1\mu_B H\sigma_{l,1}^z + g_3\mu_B H\sigma_{l,3}^z + J_1\left(\sigma_{l,1}^z+\sigma_{l+1,1}^z\right)S_{l,1}^z + J_3\left(\sigma_{l,3}^z+\sigma_{l+1,3}^z\right)S_{l,3}^z + $$
$$+\sum_{n=1}^{3} g\mu_B H S_{l,n}^z + J\sum_{n=1}^{2}\left(S_{l,n}^x S_{l,n+1}^x + S_{l,n}^y S_{l,n+1}^y + \gamma S_{l,n}^z S_{l,n+1}^z\right)\Big]$$

Periodic boundary conditions:

$$\sigma_{L+1,1} = \sigma_{1,1}$$
$$\sigma_{L+1,3} = \sigma_{1,3}$$






## Thermodynamics of the system

We used transfer matrix method to perform simulation of system's low temperature properties. Transfer-matrix element:

$$T_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} = e^{-\frac{E_0}{T}}\left(1+e^{-\frac{\varepsilon_{1,1}}{T}}+e^{-\frac{\varepsilon_{1,2}}{T}}+e^{-\frac{\varepsilon_{1,3}}{T}}+e^{-\frac{\varepsilon_{2,1}}{T}}+e^{-\frac{\varepsilon_{2,2}}{T}}+e^{-\frac{\varepsilon_{2,3}}{T}}+e^{-\frac{\varepsilon_{3}}{T}}\right)$$

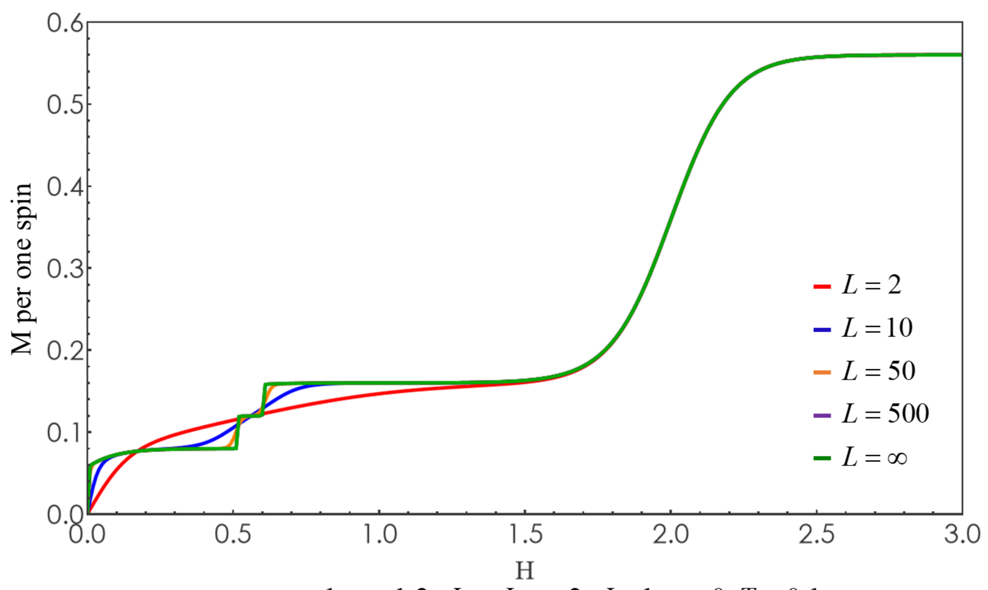
Partition function and free energy:

$$Z=\sum_{i=1}^{4}\lambda_i^L \qquad F=-T\ln Z \qquad F_{\text{inf}} = -T\ln\lambda_{\max}$$

Partition function for system without translational symmetry:

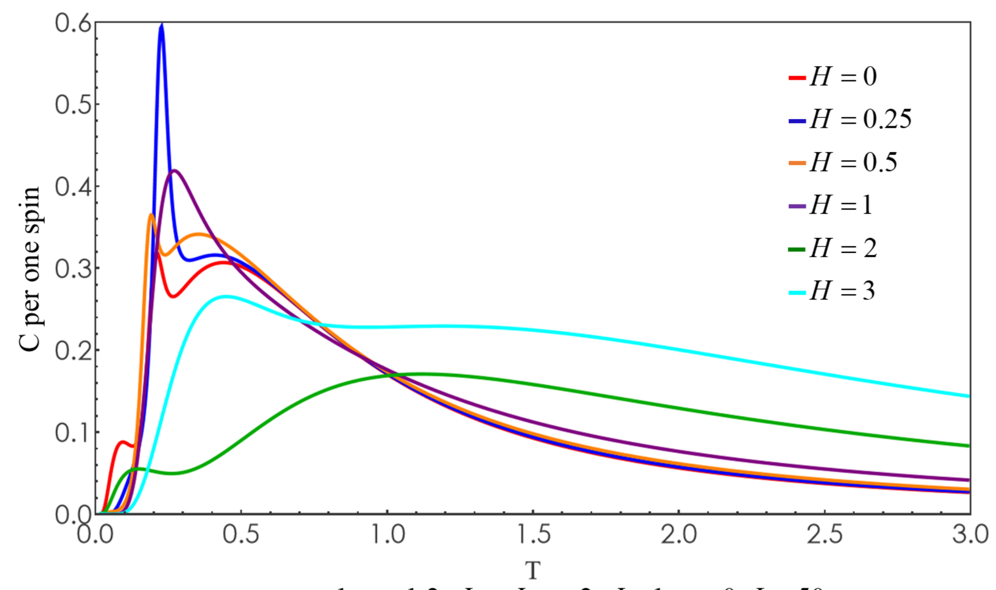
$$Z=\sum_{1}^{4^L}\prod_{1}^{L} e^{-\frac{E_0}{T}}\left(1+e^{-\frac{\varepsilon_{1,1}}{T}}+e^{-\frac{\varepsilon_{1,2}}{T}}+e^{-\frac{\varepsilon_{1,3}}{T}}+e^{-\frac{\varepsilon_{2,1}}{T}}+e^{-\frac{\varepsilon_{2,2}}{T}}+e^{-\frac{\varepsilon_{2,3}}{T}}+e^{-\frac{\varepsilon_{3}}{T}}\right)$$

Magnetization



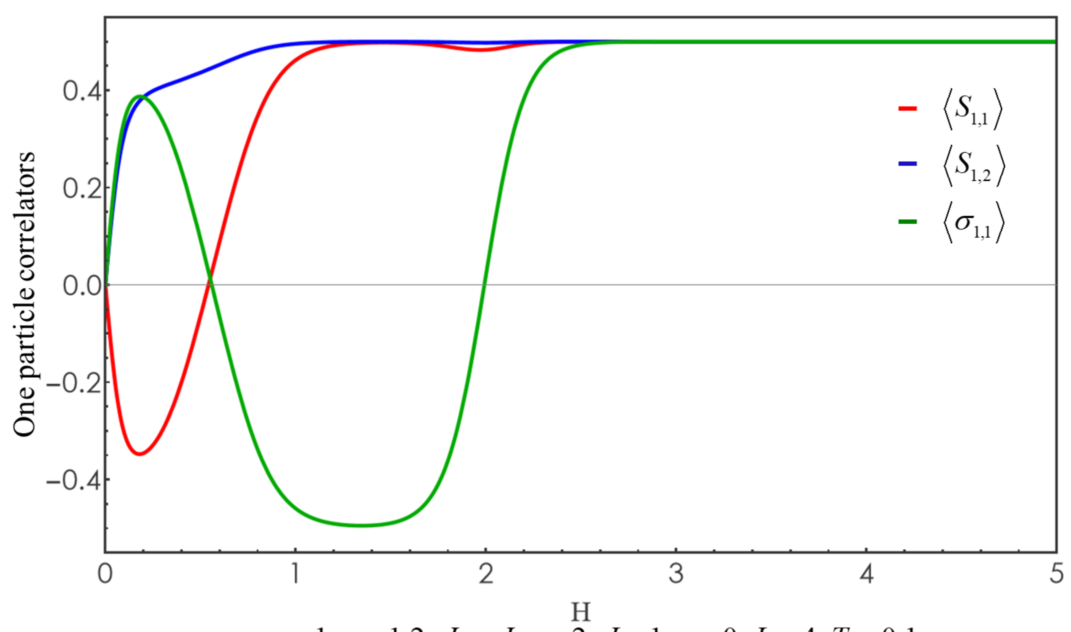

$g_1=g_3=1,\ g=1.2,\ J_1=J_3=-2,\ J=1,\ \gamma=0,\ T=0.1$

Heat capacity

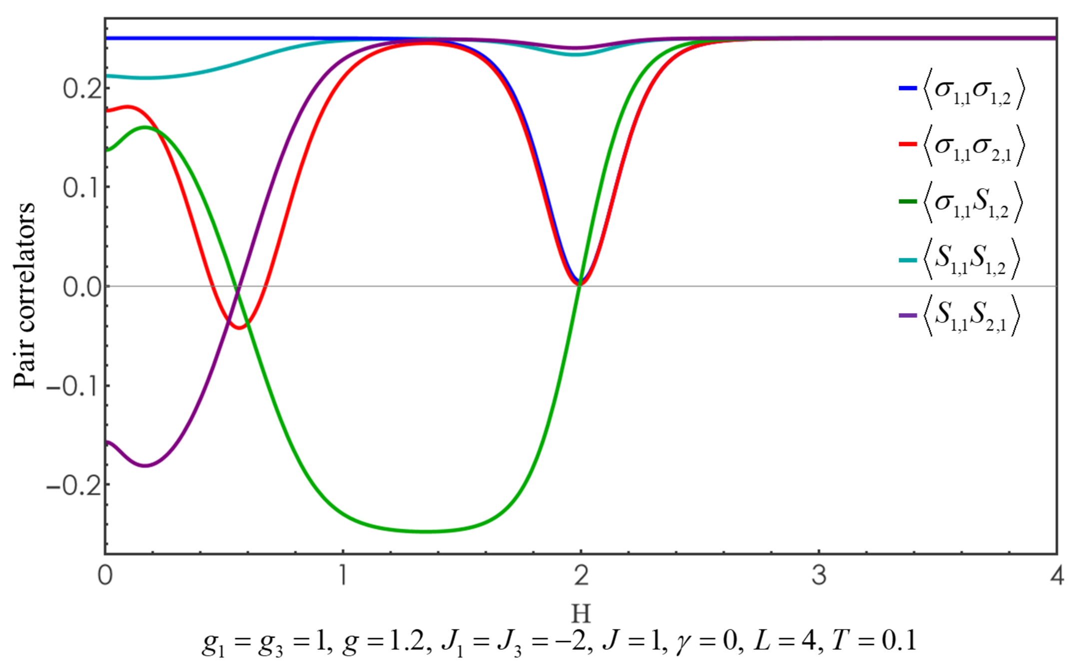



$g_1=g_3=1,\ g=1.2,\ J_1=J_3=-2,\ J=1,\ \gamma=0,\ L=50$

## One and two particle correlators



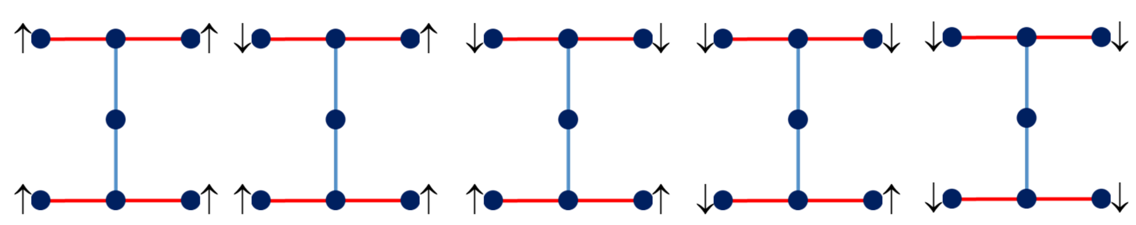

$g_1=g_3=1,\ g=1.2,\ J_1=J_3=-2,\ J=1,\ \gamma=0,\ L=4,\ T=0.1$




$g_1=g_3=1,\ g=1.2,\ J_1=J_3=-2,\ J=1,\ \gamma=0,\ L=4,\ T=0.1$

For the case of big g-factors on XXZ chains and antiferromagnetic Ising interactions, nearest neighbor Ising spin correlators are equal to zero at some fixed values of magnetic field.

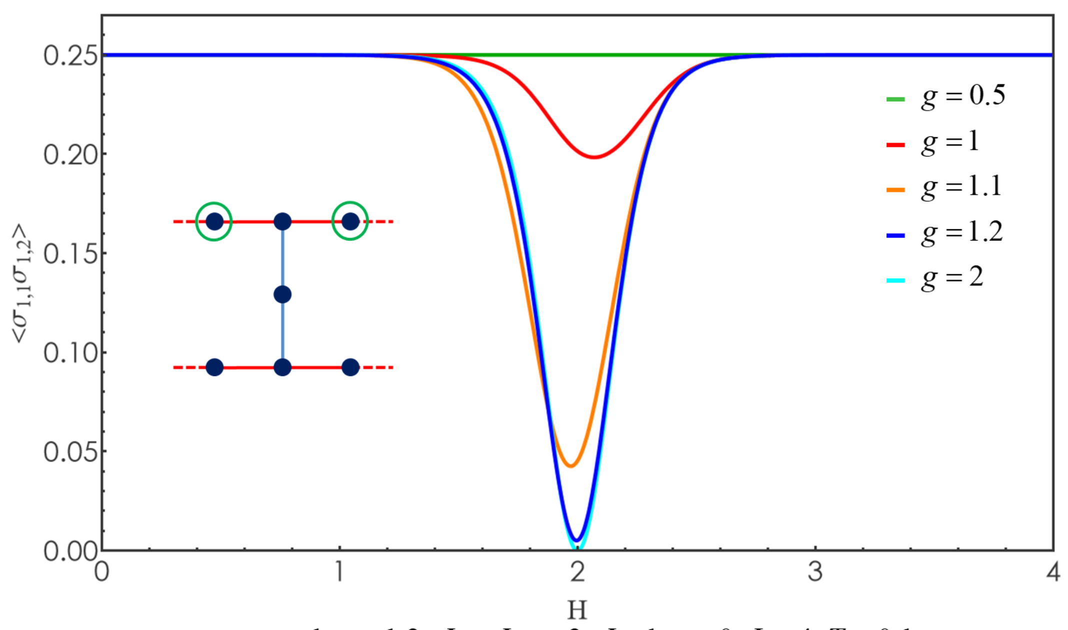
The reason of this effect is that the orientation of XXZ spins along magnetic field becomes preferable earlier than for Ising spins. In this case the energy changes starts to depend only on Ising spin configuration as it is shown below



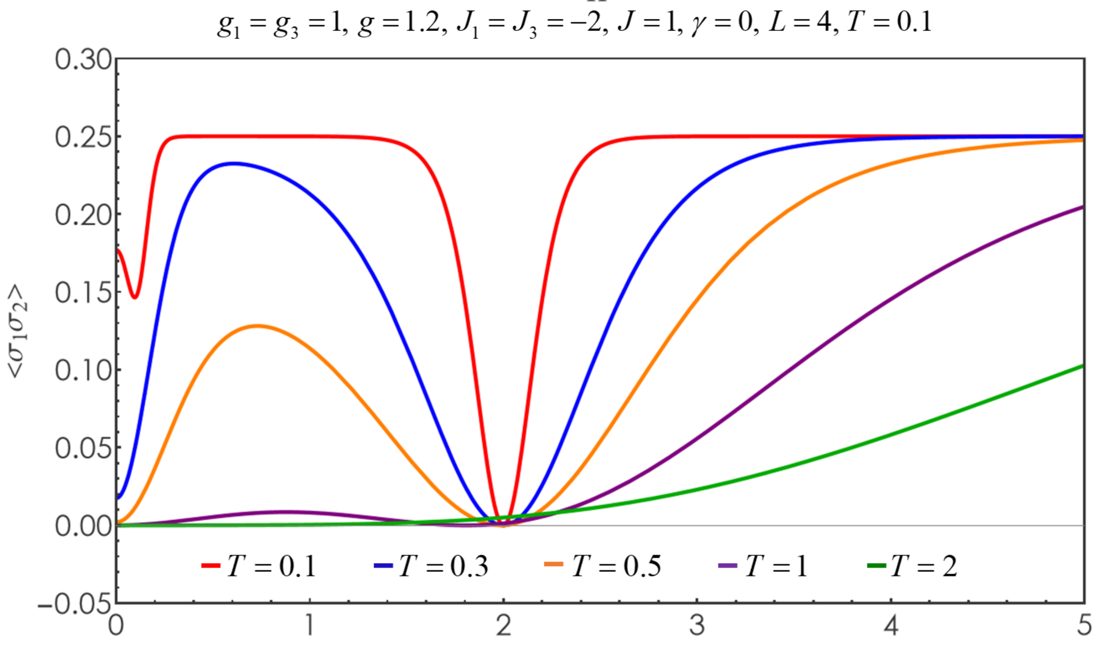
$E=-(g_1H+J_1)$ $\quad E=-(g_1H+J_1)/2$ $\quad E=0$ $\quad E=(g_1H+J_1)/2$ $\quad E=g_1H+J_1$

The spin configurations have the same energies at the field

$$H=\frac{-J_1}{g_1}$$



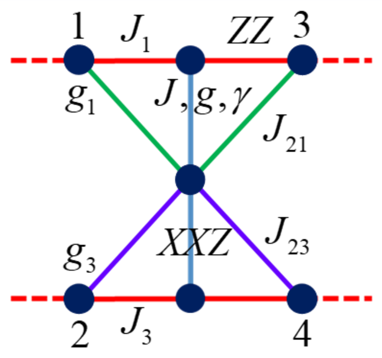

$g_1=g_3=1,\ g=1.2,\ J_1=J_3=-2,\ J=1,\ \gamma=0,\ L=4,\ T=0.1$



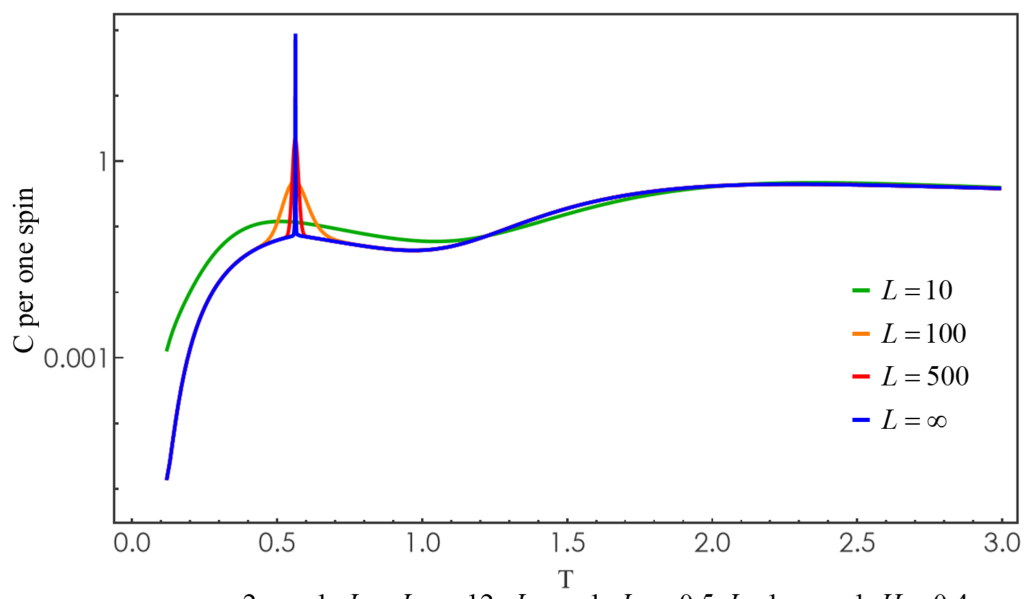

$g_1=g_3=1,\ g=2,\ J_1=J_3=-2,\ J=1,\ \gamma=0,\ L=4,\ T=0.1$

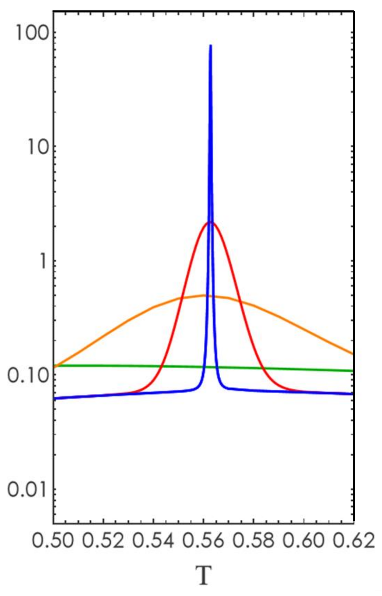
## Pseudo-phase transition

Hamiltonian of new system:

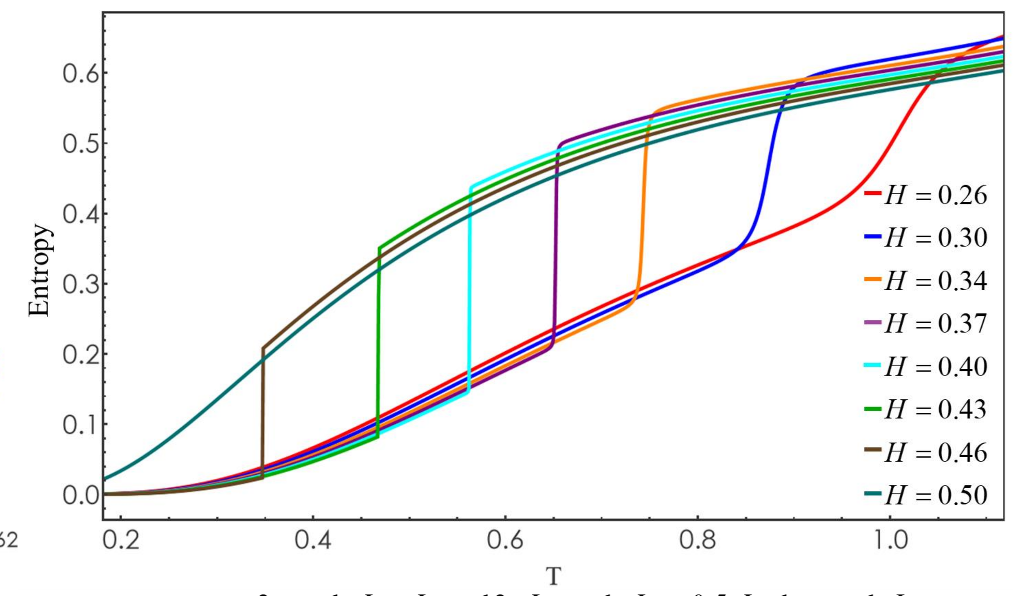



$$\hat{\mathbf{H}} = -\sum_{l=1}^{L}\Big[g_1\mu_B H\sigma_{l,1}^z + g_3\mu_B H\sigma_{l,3}^z + J_1\left(\sigma_{l,1}^z+\sigma_{l+1,1}^z\right)S_{l,1}^z +$$
$$+J_3\left(\sigma_{l,3}^z+\sigma_{l+1,3}^z\right)S_{l,3}^z + \left(J_{21}\left(\sigma_{l,1}^z+\sigma_{l+1,1}^z\right)+J_{23}\left(\sigma_{l,3}^z+\sigma_{l+1,3}^z\right)\right)S_{l,2}^z +$$
$$+\sum_{n=1}^{3} g\mu_B H S_{l,n}^z + J\sum_{n=1}^{2}\left(S_{l,n}^x S_{l,n+1}^x + S_{l,n}^y S_{l,n+1}^y + \gamma S_{l,n}^z S_{l,n+1}^z\right)\Big].$$




$g_1=g_3=2,\ g=1,\ J_1=J_3=-12,\ J_{21}=-1,\ J_{23}=0.5\ J=1,\ \gamma=-1,\ H=0.4$




$g_1=g_3=2,\ g=1,\ J_1=J_3=-12,\ J_{21}=-1,\ J_{23}=0.5\ J=1,\ \gamma=-1,\ L=\infty$

## Summary

Partition function and thermodynamic characteristics were calculated using classic transfer-matrix method. The phenomenon of zero correlation between Ising spins in some special magnetic field was found and explained. Existence of pseudo-phase transition for spin cylinder with additional Ising bonds was shown.

## References

[1] Rojas O., Strečka J., de Souza S. M. Thermal entanglement and sharp specific-heat peak in an exactly solved spin-1/2 Ising-Heisenberg ladder with alternating Ising and Heisenberg inter–leg couplings. Solid State Communications. 2016. Vol. 246. P. 68–75