On the Energy Spectrum and Magnetic Properties of Quasi-One-Dimensional Branched Spin Chain

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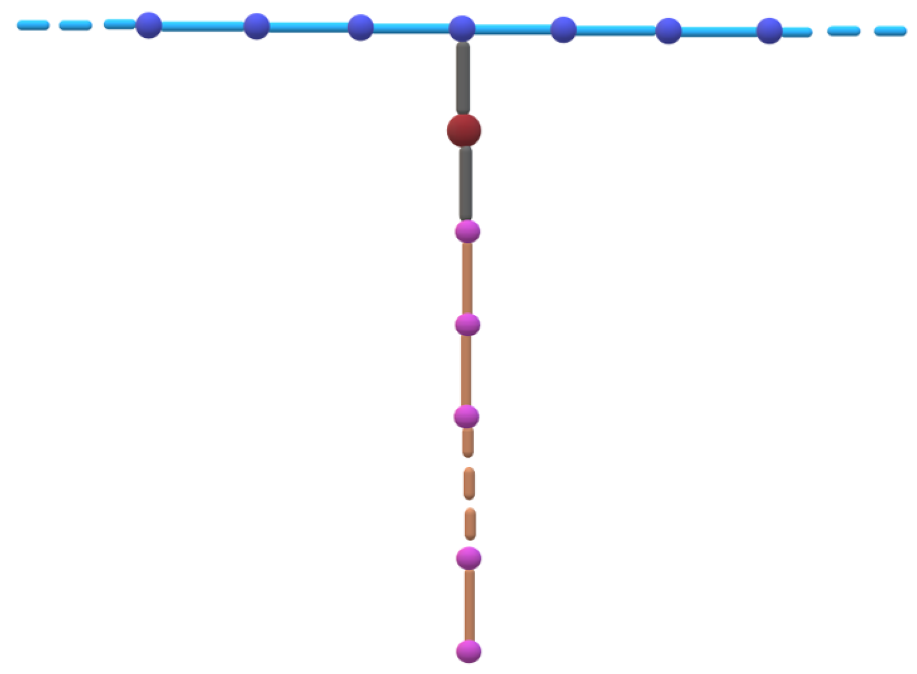
Theoretical study of the exact energy spectrum and low-temperature thermodynamics of two finite spin XX chains connected through the additional Ising spin at one point (T-chain) have been carried out.



$$\hat{\mathbf{H}} = -g_1\mu_B H\sum_{n=1}^{N_1} S^z_{1,n} - J_1 \sum_{n=1,n\neq n_1-1,n_1}^{N_1-1}\left(S^x_{1,n}S^x_{1,n+1}+S^y_{1,n}S^y_{1,n+1}\right)$$
$$-g_2\mu_B H\sum_{n=1}^{N} S^z_{2,n} - J_2\sum_{n=1}^{N_2-1}\left(S^x_{2,n}S^x_{2,n+1}+S^y_{2,n}S^y_{2,n+1}\right)$$
$$-J_1'\left(S^x_{1,n_1-1}S^x_{1,n_1}+S^y_{1,n_1-1}S^y_{1,n_1}+S^x_{1,n_1}S^x_{1,n_1+1}+S^y_{1,n_1}S^y_{1,n_1+1}\right) \qquad (1)$$
$$-g_0\mu_B H S^z_0 - J_0 S^z_0\left(S^z_{1,0}+S^x_{2,1}\right).$$

The Hamiltonian (1) can be reduced to the Hamiltonian of an ideal gas of spinless fermions by Jourdan-Wigner transformation [1, 2].

Good quantum number σ_0 (additional parameter) in (1)

$$\left[\hat{\mathbf{H}}, S^z_0\right]=0, \quad S^z_0 \to \sigma_0 = -S_0,\dots,S_0$$

$$\hat{\mathbf{H}}(\sigma_0) = E_0(\sigma_0) + \sum_{i=1}^{2}\sum_{x_{i,\sigma_0}} \varepsilon_i(x_{i,\sigma_0}) a^{\dagger}_{x_{i,\sigma_0}} a_{x_{i,\sigma_0}};$$

$$E_0(\sigma) = -\frac{1}{2}\mu_B H(g_1N_1+g_2N_2) - (g_0\mu_B H + J_0)\sigma.$$

Dispersion relations for XX chains

We performed analytical study of the corresponding spectrum of stationary states. For the states with one inverted spin this spectrum consists of two independent zones. The additional energy levels of the impurity spin can be split off from zones. We found the conditions for the appearance of localized impurity states.

$$\alpha_1 x_1(1-x_1^{2n_1})(1-x_1^{2(N_1+1-n_1)}) + (1-x_1^2)(1-x_1^{2(N_1+1)}) = 0.$$

$$\alpha_2 x_2\left(1-x_2^{2N_2}\right) + \left(1-x_2^{2(N_2+1)}\right) = 0$$

$$\varepsilon_{i,\sigma_0} = g_i\mu_B H - \frac{J_i}{2}\left(x_{i\sigma_0} + \frac{1}{x_{i\sigma_0}}\right); \quad x_i = x_{i\sigma_0} = \begin{cases}\exp(ik_{i\sigma_0}), \text{"band"}\\ real, |x_i|<1, \text{"bound"}\end{cases}$$

$$\alpha_{1,2} = \frac{2J_0\sigma_0}{J_{1,2}}; \quad i=0,1.$$

Low Temperature Thermodynamics

Partition function

$$Z = \sum_{\sigma_0=-S}^{S} Z(\sigma_0);$$

$$Z(\sigma_0) = \exp\left(-\frac{E_0(\sigma_0)}{T}\right)\prod_{k_{1,\sigma_0}}\left[1+\exp\left(\frac{\varepsilon(x_{1,\sigma_0})}{T}\right)\right]\prod_{k_{2,\sigma_0}}\left[1+\exp\left(\frac{\varepsilon(x_{2,\sigma_0})}{T}\right)\right].$$

Average value of Ising impurity spin

$$\left\langle S^z_0\right\rangle = \frac{\sum_{\sigma_0}\sigma_0 Z(\sigma_0)}{Z}$$

Numerical simulation of the field and the temperature dependences of normalized magnetization, heat capacity and $\left\langle S^z_0\right\rangle$ at different values of system parameters was carried out.

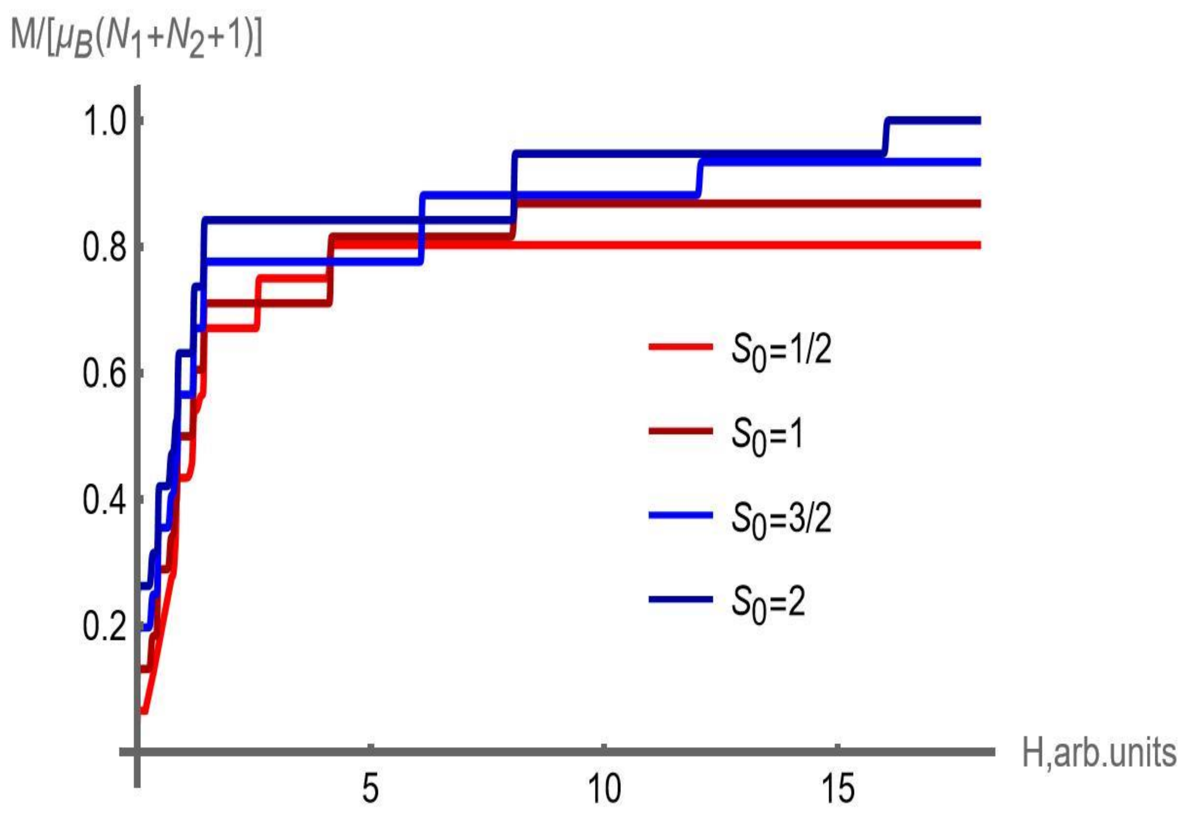


Fig. 1. Field dependence of magnetization per spin at $T=0.01K$

$g_0=2.5,\ g_1=1, g_2=2,\ J_0=-8K, J_1=1K, J_2=3K$

$N_1=N_2=8,\ n_1=4$

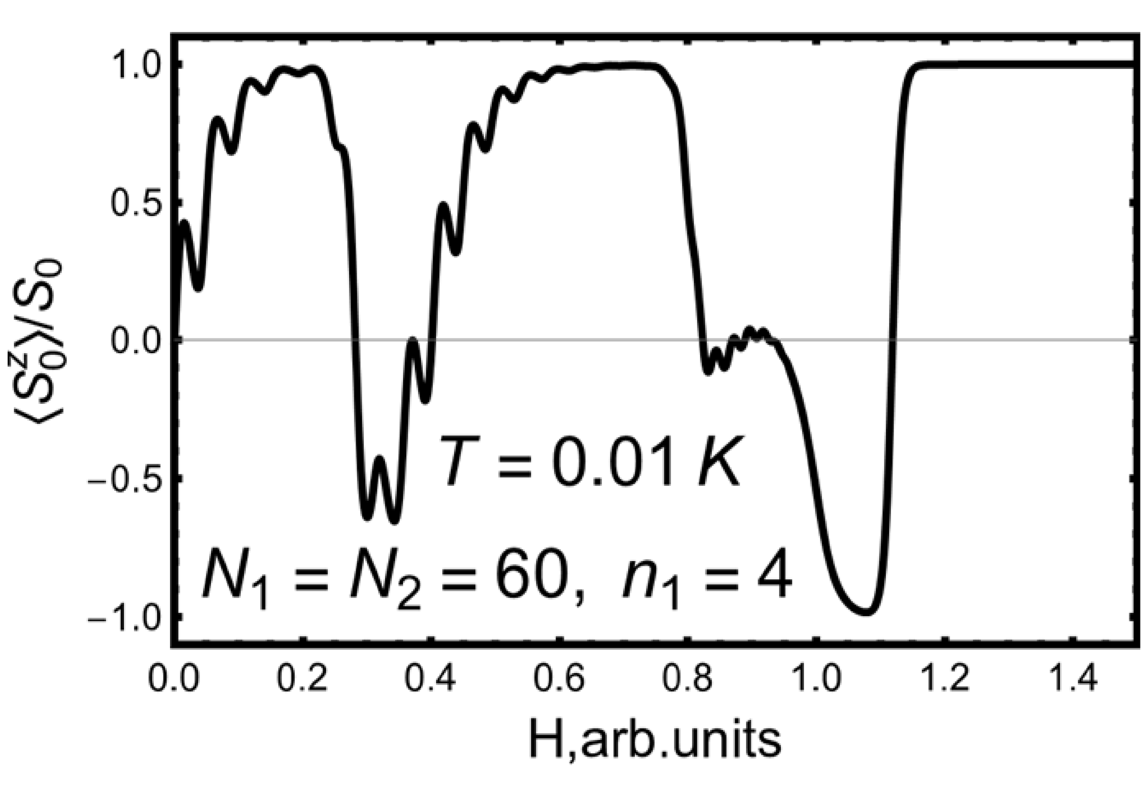


Fig. 2. Field dependence of $\left\langle S^z_0\right\rangle / S_0$ $g_0=0.5,$ $g_1=1, g_2=2, J_0=-1K, J_1=2, J_2=10$

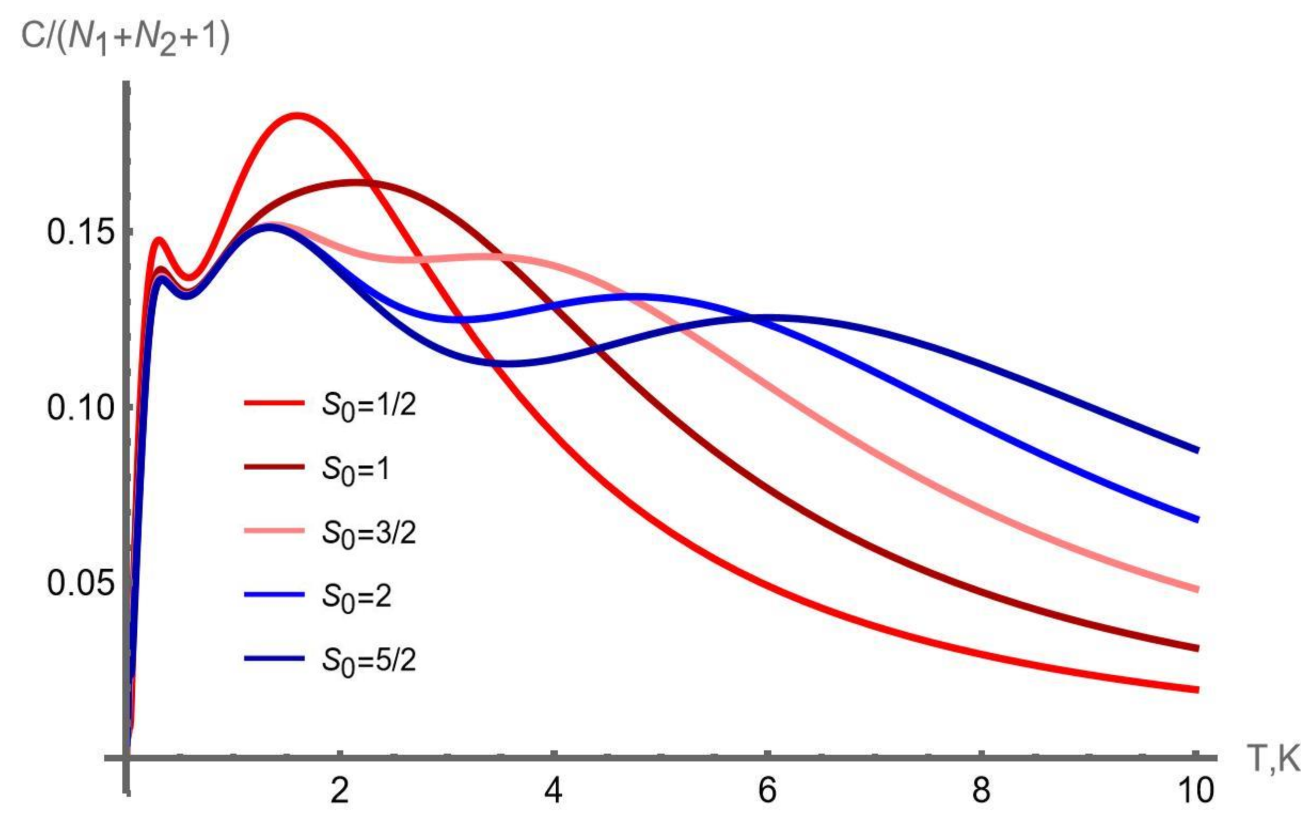


Fig. 3. Temperature dependence of specific heat in zero magnetic field $N_1=N_2=8, n_1=4,$ $J_0=-10K, J_1=1K, J_2=5K$

Summary:

- For strong antiferromagnetic Ising interaction, the field dependence of the magnetization at very low temperatures demonstrates a jump associated with the spin-flip of impurity spins at sufficiently strong magnetic field
- The additional oscillations of an average value of Ising impurity spin with the increase of magnetic field for some values of model parameters were found.
- The possibility of three-peak behavior in zero-field temperature dependence of specific heat was found numerically.

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References

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[2] Zvyagin A.A., Quantum Theory of One-Dimensional Spin Systems, DOI : , Cambridge Scientific Publishers, Cambridge, 2010.