Low Temperature Thermodynamic of Spin Model Formed by XX Chains Coupled via Ising spins

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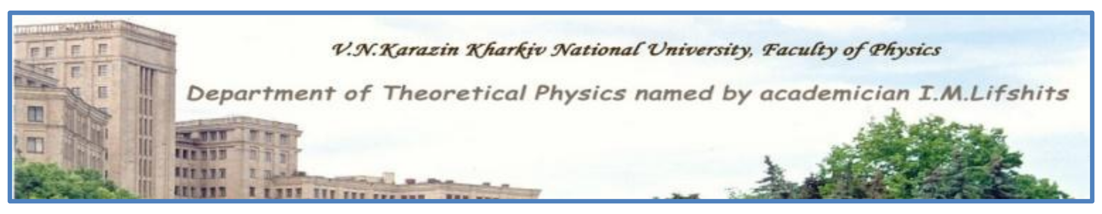
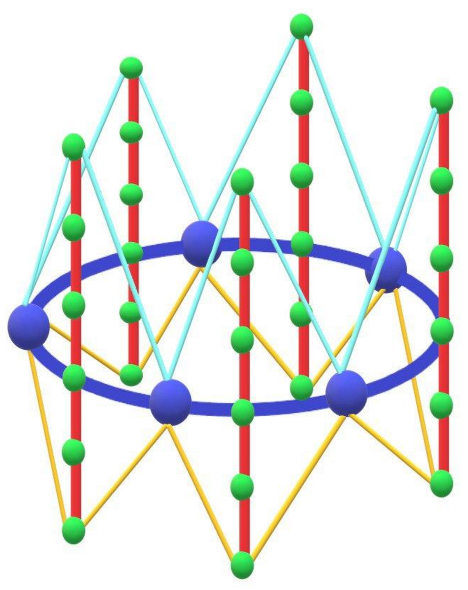


Low temperature thermodynamics of model spin system formed by open finite spin-1/2 XX chains coupled through Ising spins-S into periodical structure via one intermediate lattice site with the same number and two first and last sites of each XX chains was theoretically studied.
The model Hamiltonian has the following form



$$\hat{\mathbf{H}} = -\sum_{l=1}^{L}\Big[g_0\mu_B H\sigma_l^z + \left(\sigma_l^z + \sigma_{l+1}^z\right)\left(J_0 S_{l,n_0}^z + J_1 S_{l,1}^z + J_2 S_{l,N}^z\right) + \sum_{n=1}^{N} g\mu_B H S_{l,n}^z + J\sum_{n=1}^{N-1}\left(S_{l,n}^x S_{l,n+1}^x + S_{l,n}^y S_{l,n+1}^y\right)\Big]. \quad (1)$$

We can consider the eigenvalues of all Ising spins operators, as the parameters of the Hamiltonian (1). Due to the commutation relations of Ising spins σ_l^z and model Hamiltonian all $\sigma_l = -S, \ldots, S$. The Hamiltonian have a simple block form, which permits us to use standard **transfer-matrix technique** for numerical simulation of the model thermodynamics.

$$\hat{\mathbf{H}} = \sum_{l=1}^{L} \mathbf{H}(\sigma_{l,n_0}, \sigma_{l+1,n_0}) \quad (2)$$

Jourdan-Wigner Transformation + diagonalization for XX chains

$$\hat{\mathbf{H}}(\sigma_l,\sigma_{l+1}) = E_0(\sigma_l,\sigma_{l+1}) + \sum_{k_{\sigma_l,\sigma_{l+1}}} \varepsilon(k_{\sigma_l,\sigma_{l+1}}) a^\dagger_{k_{\sigma_l,\sigma_{l+1}}} a_{k_{\sigma_l,\sigma_{l+1}}}$$

Partition function of effective XX chain with "impurity" spin 1/2 at both ends and lattice site l, n_0

$$Z_{\sigma_l,\sigma_{l+1}} = \exp\left(-\frac{E_0(\sigma_l,\sigma_{l+1})}{T}\right)\prod_{k_{\sigma_l\sigma_{l+1}}}\left[1+\exp\left(\frac{\varepsilon(k_{\sigma_l\sigma_{l+1}})}{T}\right)\right]$$

Total partition function for (1)

$$Z_L = \mathrm{Tr}\left(\exp\left(-\frac{\hat{\mathbf{H}}_1}{T}\right)\right) = \mathrm{Tr}\left(\exp\left(-\frac{1}{T}\sum_l \hat{\mathbf{H}}(\sigma_l,\sigma_{l+1})\right)\right) =$$

$$\mathrm{Tr}\left(\exp\left(-\frac{1}{T}\hat{\mathbf{H}}(\sigma_1,\sigma_2)\right)\cdot\exp\left(-\frac{1}{T}\hat{\mathbf{H}}(\sigma_2,\sigma_3)\right)\ldots\exp\left(-\frac{1}{T}\hat{\mathbf{H}}(\sigma_L,\sigma_1)\right)\right) = \mathrm{Tr}\left(Z^L_{\sigma_l,\sigma_{l+1}}\right);$$

For the Hamiltonian (2) the transfer-matrix is the 2x2 matrix, if Ising spins S=1/2

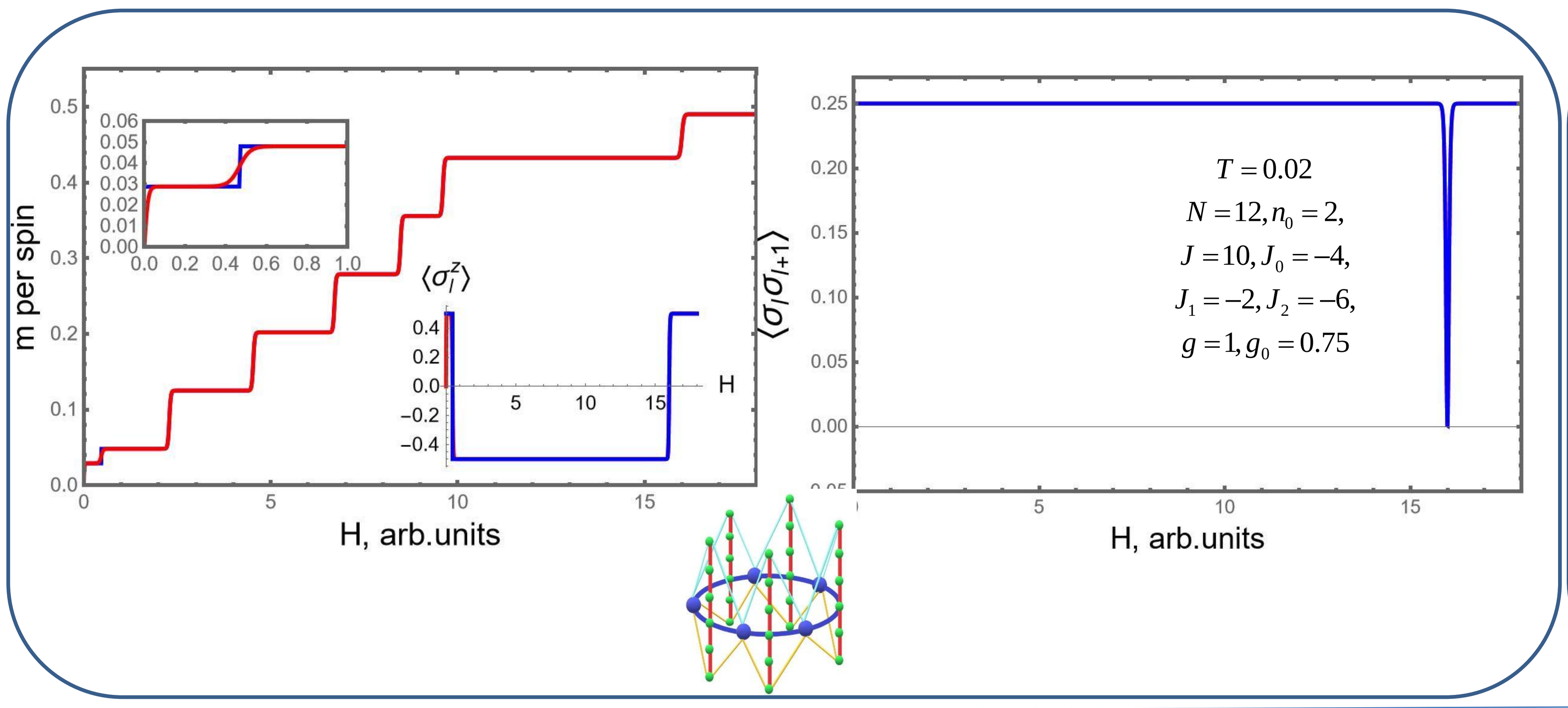
$$Z_L = \lambda_+^L + \lambda_-^L; \quad \lambda_\pm = \frac{1}{2}(Z_{11}+Z_{22}) \pm \sqrt{\frac{1}{4}(Z_{11}-Z_{22})^2 + Z_{12}Z_{21}};$$

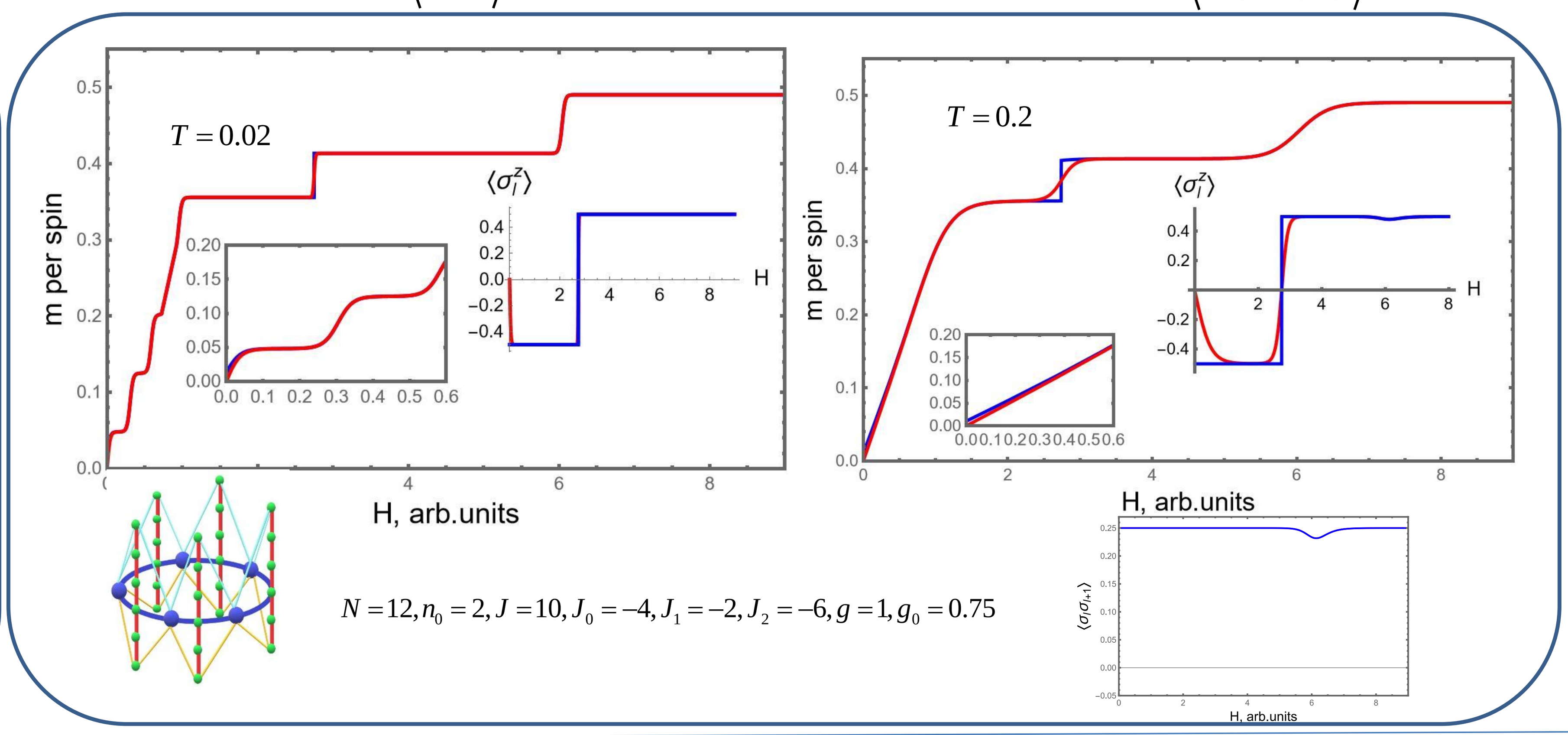
Some analytical formulae

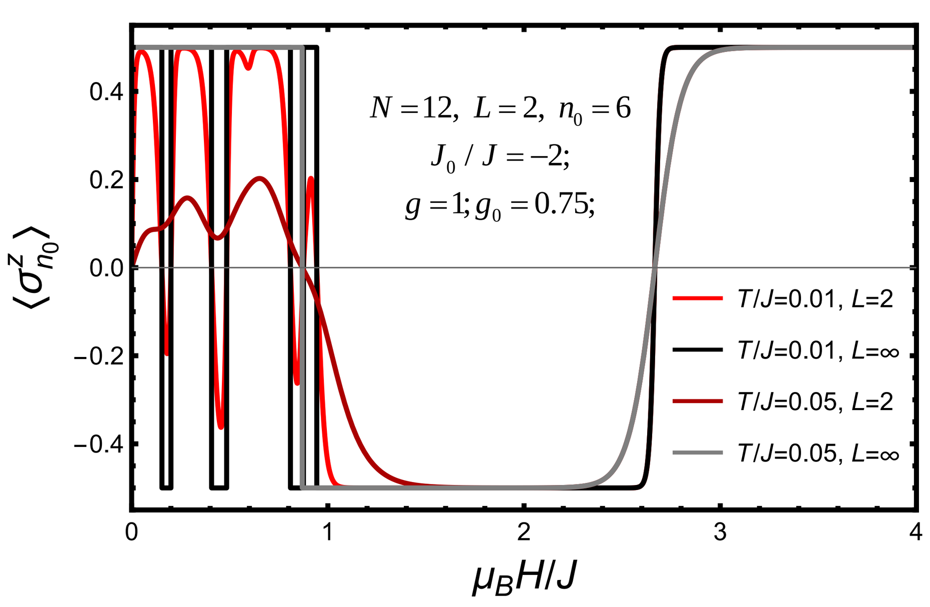
$$\left\langle \sigma_{n_0}^z \right\rangle = \frac{1}{2}\sqrt{1+\frac{4Z_{12}^2}{(Z_{11}-Z_{22})^2}}\left(\frac{\lambda_+^L - \lambda_-^L}{\lambda_+^L + \lambda_-^L}\right).$$

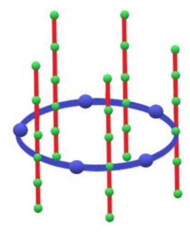
$$\left\langle \sigma_{l,n_0}^z \sigma_{l+1,n_0}^z \right\rangle = \frac{1}{8}\left\{\frac{(Z_{11}+Z_{22})\left(\lambda_+^{L-1}+\lambda_-^{L-1}\right)}{\left(\lambda_+^L+\lambda_-^L\right)} + \frac{(Z_{11}-Z_{22})^2 - 4Z_{12}^2}{\sqrt{(Z_{11}-Z_{22})^2+4Z_{12}^2}}\left[\frac{\left(\lambda_+^{L-1}-\lambda_-^{L-1}\right)}{\left(\lambda_+^L+\lambda_-^L\right)}\right]\right\}.$$

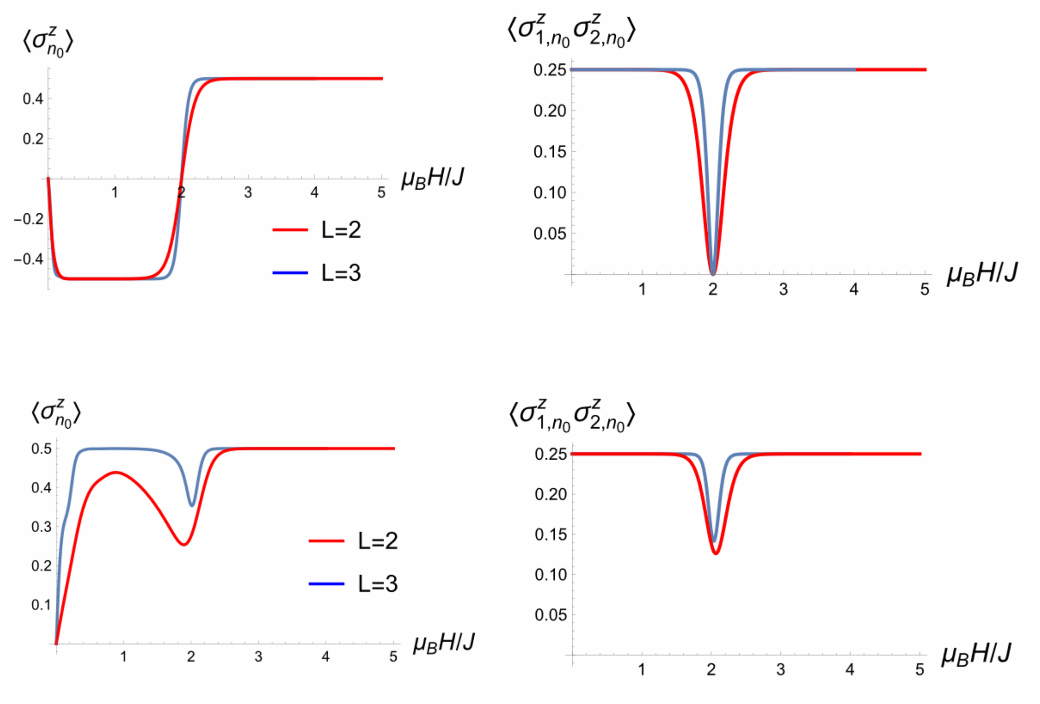
Field Dependence of Magnetization and Average values of decorated spins $\langle \sigma_l^z \rangle$ and pair correlation function $\langle \sigma_l^z \sigma_{l+1}^z \rangle$



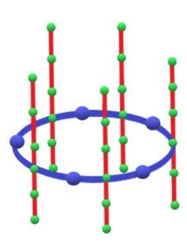




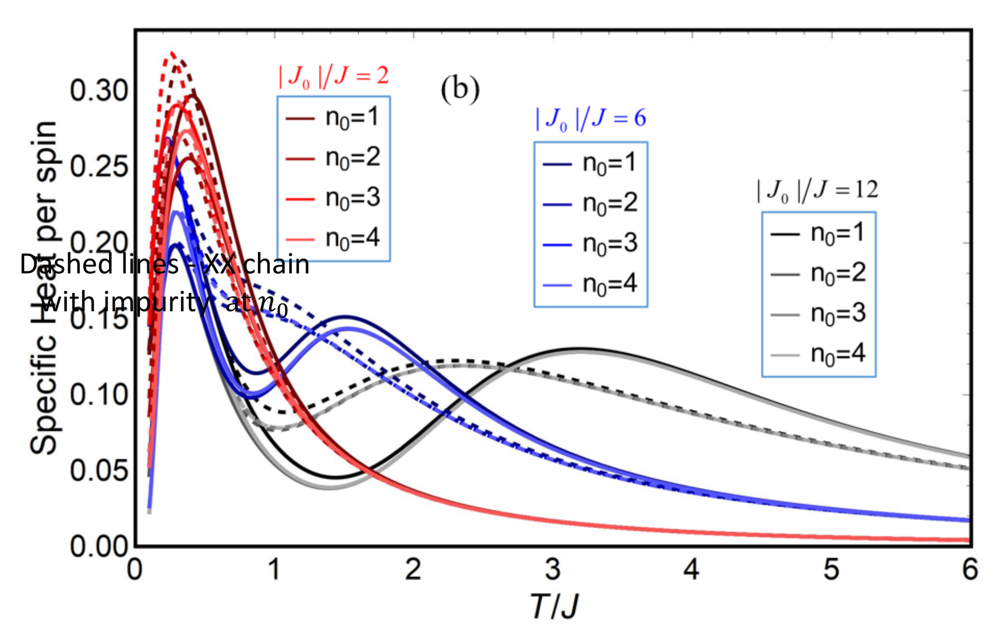




$N = 10;\ S = 1/2;\ T/J = 0.05;\ J_0/J = -2;\ g = 1.1;\ g_0 = 1$



Specific heat at zero magnetic field



Summary:

- The field and temperature dependences of the main magnetic characteristics like magnetization, specific heat, the field dependences of , and the pairwise correlation functions for the nearest neighboring decorating spins were calculated numerically.
- For the case of the large values of the g-factor in XX chains and antiferromagnetic Ising interaction, simple analytical calculations indicate that the pair correlation functions for neighbor Ising spins can take zero value at some critical fields. This behavior is associated with additional degeneracy of the exact energy spectrum.
- Field dependence of magnetization demonstrates two intermediate plateaus for strong AF and FM Ising interactions at very low temperatures.
- We found numerically three maxima behavior of zero field temperature dependence of specific heat at some values of model parameters.

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