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The energy spectrum and thermodynamics of the finite spin-1/2 XX chain with Ising-type Impurities

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The energy spectrum and thermodynamics of two one-dimensional spin systems: the finite XX-chain with periodic boundaries and one zz (Ising) bond, and open ends XX-chain with two zz-impurities at the both ends have been investigated. The conditions for the appearance of the energy states, localized in the vicinity of impurity spins, have been derived. The peculiarities of field and temperature dependences of the basic thermodynamic characteristics of these models have been studied.
Keywords: spin Hamiltonian, XY-chain, XX-chain, spin, energy spectrum, thermodynamic characteristics.

Исследованы энергетический спектр и термодинамика двух одномерных спиновых систем – конечной XX-цепочки с дополнительной zz (изинговской) связью, замыкающей цепочку в кольцо, и XX-цепочки с открытыми концами с двумя zz-примесями на концах. Показано, что в спектре могут существовать локализованные вблизи примесных спинов состояния, найдены условия их появления. Исследованы полевые и температурные зависимости основных термодинамических характеристик моделей.
Ключевые слова: спиновый гамильтониан, XY-цепочка, XX-цепочка, спин, энергетический спектр, термодинамические характеристики.

Досліджено енергетичний спектр і термодинаміку двох одновимірних спінових систем – кінцевого XX-ланцюжка з додатковим zz (ізінговским) зв'язком, який замикає ланцюжок в кільце, і XX-ланцюжка з відкритими кінцями з двома zz-домішками на кінцях. Показано, що в спектрі можуть існувати локалізовані поблизу домішкових спінів стани, знайдено умови їх появи. Досліджено польові і температурні залежності основних термодинамічних характеристик моделей.
Ключові слова: спіновий гамільтоніан, XY-ланцюжок, XX ланцюжок, спін, енергетичний спектр, термодинамічні характеристики.

Low-dimensional spin models occupy special place in quantum theory of magnetism due to the fact that such systems in some cases may have exact analytical solutions [1, 2]. Usually, the real magnets are characterized by different types of heterogeneity, so the theoretical study of the influence of impurities on the energy spectrum and the thermodynamics of such structures is of great interest.

This work is devoted to the study of the energy spectrum and the thermodynamics of two exactly solvable spin models: finite isotropic XY-chain, or so called XX-chain, with periodic boundaries ("ring") and impurity Ising spin S_1 which is described by the Hamiltonian

$$\mathbf{H}_{ring} = -g_0\mu_B H S_0^z - J_0\left(S_1^z + S_N^z\right)S_0^z - g\mu_B H\sum_{n=1}^{N} S_n^z - J\sum_{n=1}^{N-1}\left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y\right) \tag{1}$$

and open ends finite XX chain ("line") with two different edge impurity Izing spins S_1, S_2 described by the Hamiltonian

$$\begin{aligned}\mathbf{H}_{line} = &-\mu_B H\left(g_0 S_0^z + g_{N+1}S_{N+1}^z\right) - J_0 S_0^z S_1^z - J_{N+1}S_N^z S_{N+1}^z \\ &-g\mu_B H\sum_{n=1}^{N} S_n^z - J\sum_{n=1}^{N-1}\left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y\right).\end{aligned} \tag{2}$$

Here $J>0$ is the exchange integral for spin-1/2 XX chain, J_0, J_{N+1} are the exchange integrals of Ising (or *zz*)-type interactions with impurity spins, μ_B is the Bohr magneton, g, g_0 and g_{N+1} are g-factors for chain and impurities respectively, H is the longitudinal uniform magnetic field. Positive and negative values of Ising interactions correspond to ferromagnetic (FM) and antiferromagnetic (AF) type of exchange. These Hamiltonians describe some kind of well-known broken-chain effect in real quasi-one dimensional magnets [3, 4].

Z-projections of the impurity spins are the good quantum numbers due to the commutation of the Hamiltonians (1) and (2) with the z-projection of the impurity spin operators ($\sigma_i = -S_i, \ldots, +S_i$, $i = 1, 2$), and z-component of the XX-chain total spin. The models stationary states can be classified by all the possible values of these projections:

The model Hamiltonians split into the sum of the finite XX-chain Hamiltonians with the effective "impurity" spins ($s = 1/2$) at the ends. After Jordan-Wigner transformation [1] the Hamiltonians and and take the form

$$\mathbf{H}_{ring} = \sum_{\sigma_0=-S_1}^{S_1} \mathbf{H}(\sigma_0), \quad \mathbf{H}(\sigma_0) = E_0(\sigma_0) + \left(g\mu_B H + J_0\sigma_0\right)\left(a_1^+ a_1 + a_N^+ a_N\right)$$
$$+ g\mu_B H \sum_{n=2}^{N-1} a_n^+ a_n - \frac{J}{2}\sum_{n=1}^{N-1}\left(a_n^+ a_{n+1} + a_{n+1}^+ a_n\right), \tag{3}$$
$$E_{ferro}(\sigma_0) = -\left(g_0\mu_B H + J_0\right)\sigma_0 - \frac{g\mu_B HN}{2}, \quad \sigma_0 = -S_1, \ldots, S_1,$$

and

$$\mathbf{H}_{line} = \sum_{\sigma_{N+1}=-S_2}^{S_2} \sum_{\sigma_0=-S_1}^{S_1} \mathbf{H}(\sigma_0, \sigma_{N+1}),$$
$$\mathbf{H}(\sigma_0, \sigma_{N+1}) = E_{ferro}(\sigma_0, \sigma_{N+1}) + \left(g\mu_B H + J_0\sigma_0\right) a_1^+ a_1$$
$$+ \left(g\mu_B H + J_{N+1}\sigma_{N+1}\right) a_N^+ a_N + g\mu_B H \sum_{n=2}^{N-1} a_n^+ a_n - \frac{J}{2}\sum_{n=1}^{N-1}\left(a_n^+ a_{n+1} + a_{n+1}^+ a_n\right);$$
$$E_{ferro}(\sigma_0, \sigma_{N+1}) = -\left(g_0\mu_B H + \frac{J_0}{2}\right)\sigma_0 \tag{4}$$
$$-\left(g_{N+1}\mu_B H + \frac{J_{N+1}}{2}\right)\sigma_{N+1} - \frac{g\mu_B HN}{2},$$
$$\sigma_0 = -S_1, \ldots, S_1, \quad \sigma_{N+1} = -S_2, \ldots, S_2,$$

respectively. Here a_n^+, a_n are the creation and annihilation operators for spinless fermions. The Ising interactions of impurity spins in , are described by additional Zeeman type terms. Spin-1/2 XX chain is a well-known example of an exactly solvable spin system [1, 2].

We used one particle Schrödinger equation in the lattice site representation to diagonalize the Hamiltonians and . As a result, we derived the following dispersion relations for the exact energy spectrum for the "ring":

$$\frac{1 \pm x_\sigma^{N+1}}{x_\sigma(1 \pm x_\sigma^{N-1})} = \alpha_0, \tag{5}$$

and for the "line"

$$\left(\alpha_0 + \frac{1}{x_\sigma}\right)\left(\alpha_{N+1} + \frac{1}{x_\sigma}\right) - (\alpha_0 + x_\sigma)(\alpha_{N+1} + x_\sigma)x_\sigma^{2(N-1)} = 0. \tag{6}$$

respectively, and calculated the normalized wave functions. In both cases excitation energy defines by

$$\varepsilon\left(x_\sigma\right) = h - \frac{J}{2}\left(x_\sigma + \frac{1}{x_\sigma}\right), \tag{7}$$

where $h = g\mu_B H$, $\sigma = \sigma_0$, $\sigma = \sigma_{0,}\,\sigma_{N+1}$ for the "ring" and for the "line" respectively, and

$$\alpha_0 = \frac{2J_0\sigma_0}{J};\quad \alpha_{N+1} = \frac{2J_{N+1}\sigma_{N+1}}{J}, \sigma_0 = -S_1,..,+S_1;\quad \sigma_{N+1} = -S_2,..,+S_2.$$

For quasi-continuous band the parameter $x_\sigma = \exp(ik_\sigma)$, and

$$\varepsilon_{k_\sigma} = h - J\cos k_\sigma, \tag{8}$$

with $\sigma = \sigma_0$ for the "ring" and $\sigma = \sigma_{0,}\,\sigma_{N+1}$ for the "line".

It was shown that the sufficiently strong Ising interactions of impurities with the main chain lead to the appearance of localized levels with real parameter x ($|x| < 1$). For cyclic chain two critical values of the parameter α are defined from the conditions for the emergence of levels :

$$\left|\alpha_{1c}\right| > 1;\quad \left|\alpha_{2c}\right| > \frac{N+1}{N-1}. \tag{9}$$

The critical length of the open chain (the condition of the appearance of the next level at given values of α_0, α_{N+1}) has the form:

$$N_c = \frac{\alpha_0\alpha_{N+1} - 1}{(\alpha_0 \pm 1)(\alpha_{N+1} \pm 1)}, \tag{10}$$

and for infinite chain ($N \to \infty$)

$$|\,\alpha_0\,| > 1; |\,\alpha_{N+1}\,| > 1. \tag{11}$$

The partition functions for above "ring" and "line" models are the sum of partition functions of finite XX chains with impurities described by the Hamiltonians $\mathbf{H}(\sigma_0)$ and $\mathbf{H}(\sigma_0, \sigma_{N+1})$ respectively

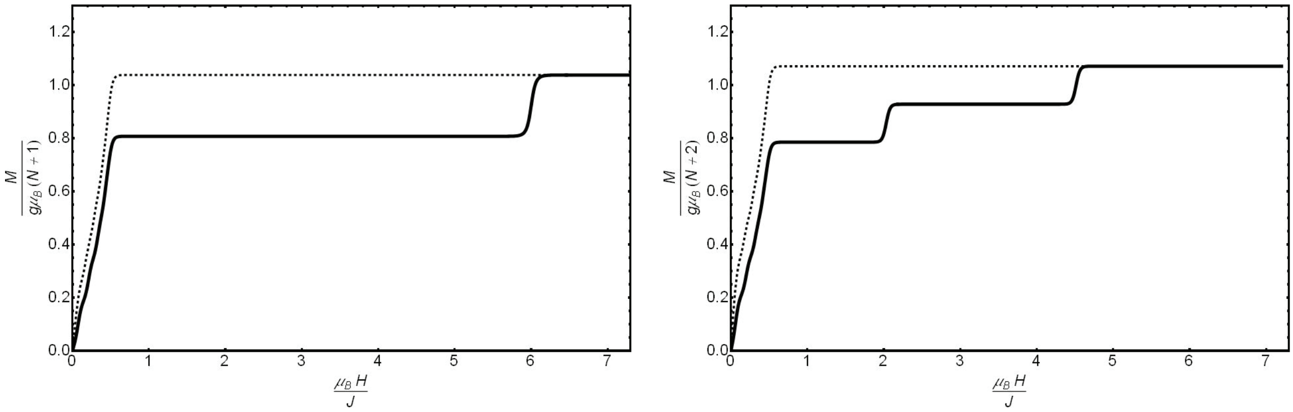
$$Z_{ring} = \sum_{\sigma_0=-S_1}^{S_1} Z(\sigma_0) = \sum_{\sigma_0=-S_1}^{S_1} e^{\frac{1}{T}\left((h_0+J_0)\sigma_0 + \frac{hN}{2}\right)} \prod_\lambda \left\{1 + e^{-\frac{1}{T}\left[h - \frac{J}{2}\left(x_{\lambda\sigma_0} + \frac{1}{x_{\lambda\sigma_0}}\right)\right]}\right\}, \tag{12}$$

$$Z_{line} = \sum_{\sigma_{N+1}=-S_2}^{S_2} \sum_{\sigma_0=-S_1}^{S_1} Z(\sigma_0, \sigma_{N+1}) =$$

$$\sum_{\sigma_{N+1}=-S_2}^{S_2} \sum_{\sigma_0=-S_1}^{S_1} e^{\frac{1}{T}\left((h_0+J_0)\sigma_0 + (h_{N+1}+J_{N+1})\sigma_{N+1} + \frac{hN}{2}\right)} \prod_\lambda \left\{1 + e^{-\frac{1}{T}\left[h - \frac{J}{2}\left(x_{\lambda\sigma_0\sigma_{n+1}} + \frac{1}{x_{\lambda\sigma_0\sigma_{n+1}}}\right)\right]}\right\}; \tag{13}$$

$$h_0 = g_0\mu_B H;\quad h_{N+1} = g_{N+1}\mu_B H.$$

One can calculated easily all the thermodynamic quantities of "ring" and "line" models from and . For example, the magnetization for "line" has the form



a *b*

Fig. 1. Field dependence of the magnetization per spin at $T = 0.05K$ for $N = 12$, $g = 2$, $J = 1K$ for (a) "ring" with $S_0 = 1.5$, $g_0 = 1$, $J_0 = -6K$ (b) "line" with $S_1 = 1.5$, $S_2 = 1$, $g_0 = 1$, $g_{N+1} = 1.5$, $J_0 = -6K$, $J_{N+1} = -4K$.

$$\frac{M_{line}}{\mu_B} = \left\{ \sum_{\sigma_0=-S_0}^{S_0} \sum_{\sigma_{N+1}=-S_{N+1}}^{S_{N+1}} e^{\left[(J_0+h_0)\sigma_0+(J_{N+1}+h_{N+1})\sigma_{N+1}\right]/T} \left[\left(g_0\sigma_0 + g_{N+1}\sigma_{N+1}\right) \prod_{\lambda} 2\text{ch}\frac{\varepsilon_\lambda(\sigma_0,\sigma_{N+1})}{2T} \right.\right.$$

$$\left.\left. + g\sum_{\lambda} \text{sh}\frac{\varepsilon_\lambda(\sigma_0,\sigma_{N+1})}{2T} \prod_{\lambda'\neq\lambda} 2\text{ch}\frac{\varepsilon_{\lambda'}(\sigma_0,\sigma_{N+1})}{2T} \right]\right\} \tag{14}$$

$$\times \left\{ \sum_{\sigma_0=-S_0}^{S_0} \sum_{\sigma_{N+1}=-S_{N+1}}^{S_{N+1}} e^{\left[(J_0+h_0)\sigma_0+(J_{N+1}+h_{N+1})\sigma_{N+1}\right]/T} \prod_{\lambda} 2\text{ch}\frac{\varepsilon_\lambda(\sigma_0,\sigma_{N+1})}{2T} \right\}^{-1}$$

We performed the simulation of the field and the temperature dependencies of the magnetization and heat capacity. One may expect the big effect of impurities, if there are localized levels. The sign of Ising interaction is also important. For AF Ising interaction the field dependence of the "ring" magnetization at very low temperatures, one can see jump associated with the spin-flip of impurity spin in sufficiently strong magnetic field for "ring" (fig. 1a) and two jumps for "line" (fig. 1b). At very low temperatures, the field dependence of the specific heat for both chains has complex form with the multiple maxima. Additional peaks of specific heat for AF Ising interaction of impurities with XX chain we associate with the local impurity levels and the spin-flip of an impurity spin in strong fields (fig. 2).

Average values of z-projections of impurity spins $\left\langle S_0^z \right\rangle, \left\langle S_{N+1}^z \right\rangle$ are

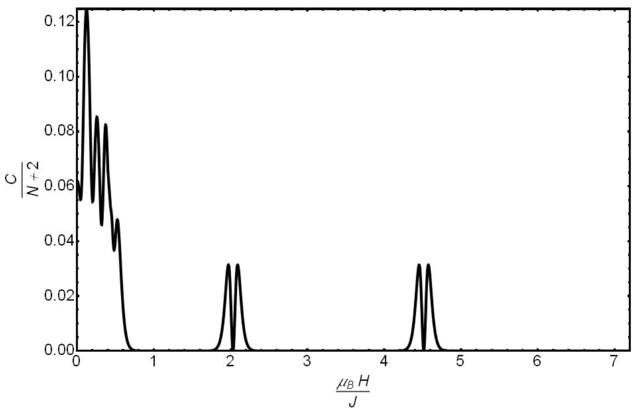


Fig.2. Field dependence of the specific heat per spin at $T = 0.05K$ for "line" with $S_1 = 1.5$, $S_2 = 1$, $g_0 = 1$, $g_{N+1} = 1.5$, $J_0 = -6K$, $J_{N+1} = -4K$.

$$\left\langle S_0^z \right\rangle = \frac{\sum\limits_{\sigma_0=-S_0}^{S_0} \sigma_0 Z(\sigma_0)}{\sum\limits_{\sigma_0=-S_0}^{S_0} Z(\sigma_0)}, \tag{15}$$

for "ring" and

$$\left\langle S_0^z \right\rangle = \frac{\sum\limits_{\sigma_0=-S_1}^{S_1} \sum\limits_{\sigma_{N+1}=-S_2}^{S_2} \sigma_0 Z(\sigma_0, \sigma_{N+1})}{\sum\limits_{\sigma_0=-S_2}^{S_2} \sum\limits_{\sigma_{N+1}=-S_2}^{S_2} Z(\sigma_0, \sigma_{N+1})}; \quad \left\langle S_{N+1}^z \right\rangle = \frac{\sum\limits_{\sigma_0=-S_1}^{S_1} \sum\limits_{\sigma_{N+1}=-S_2}^{S_2} \sigma_{N+1} Z(\sigma_0, \sigma_{N+1})}{\sum\limits_{\sigma_0=-S_1}^{S_1} \sum\limits_{\sigma_{N+1}=-S_2}^{S_2} Z(\sigma_0, \sigma_{N+1})} \qquad (16)$$

for "line". The longitudinal pair spin-spin correlation function $\left\langle S_0^z S_{N+1}^z \right\rangle$ for impurities in "line" has the form

$$\left\langle S_0^z S_{N+1}^z \right\rangle = \frac{\sum\limits_{\sigma_0=-S_1}^{S_1} \sum\limits_{\sigma_{N+1}=-S_2}^{S_2} \sigma_0 \sigma_{N+1} Z(\sigma_0, \sigma_{N+1})}{\sum\limits_{\sigma_0=-S_1}^{S_1} \sum\limits_{\sigma_{N+1}=-S_2}^{S_2} Z(\sigma_0, \sigma_{N+1})}. \qquad (17)$$

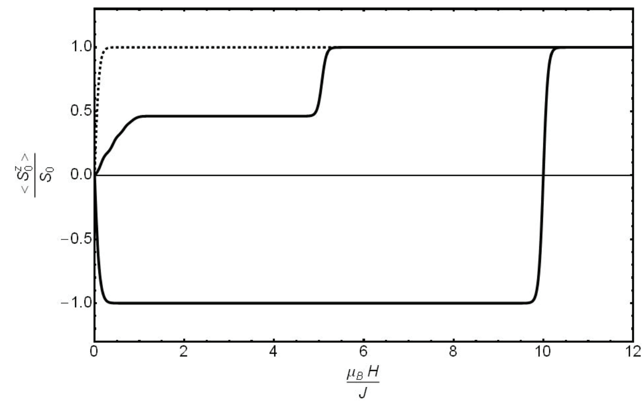


Fig 3. Comparative behavior of $\left\langle S_0^z \right\rangle / S_0$ for "ring" and for "line' of N = 12 spins in the XX chain for the same values of all g-factors for T=0.1K, $S_1 = S_2$ =1/2, $g = g_0 = g_{N+1}$ = 1, J=1K, $J_0 = J_{N+1}$ = –10K.

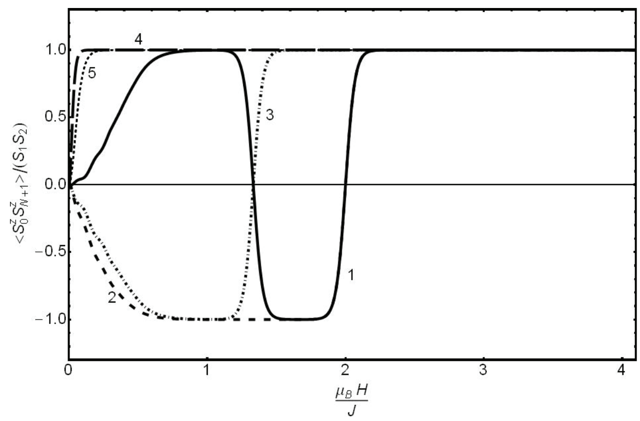


Fig. 4. The ratio of longitudinal pair spin-spin correlation functions to impurity spins values $\left\langle S_0^z S_{N+1}^z \right\rangle / S_1 S_2$ for the two impurity sites in "line" at $S_1 = S_2$ =1/2, g = 2, $g_0 = g_{N+1}$ = 1.5, J = 1K at =0.05K (1) J_0 = –6K, J_{N+1} = –4K; (2) J_0 = –6K, J_{N+1} = 4K; (3) (1) J_0 = 6K, J_{N+1} = –4K; (4) J_0 = 6K, J_{N+1} = 4K; (5) product Brillouin functions for free spinsю

The behavior of the average z-projection of impurity spins and longitudinal impurities spin-spin correlation functions at zero and non-zero temperature were studied numerically. It was shown that under certain conditions, the average z-spin projection for impurity sites at T = 0 may have the finite jumps and non-monotonic dependence on the magnetic field at low temperatures. The behavior of an impurity spin in a closed chain and open chain can differ substantially (fig. 3). This is due to the fact that in the closed chain the impurity spin interacts directly with the two neighboring spins. Peculiarities of this behavior are clearly visible at AF impurity interactions with the XX chain. Even for the same g-factors in the case of closed chain in weak field, the impurity spin is oriented oppositely to the field. In open chain in all fields average z- projection of impurity spin is positive. The longitudinal pair spin-spin correlation functions $\left\langle S_0^z S_{N+1}^z \right\rangle$ for the two impurity spins in "line" is shown on fig. 4. For sufficiently strong AF Ising interactions with opposite signs the corresponding correlation functions demonstrate non-monotonic field dependencies.

1. E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. 16, 407 (1961).
2. Zvyagin A.A., Quantum Theory of One-Dimensional Spin Systems, Cambridge Scientific Publishers, Cambridge, 2010. – 330 p.
3. A. Klumper, D.C. Johnston, Phys. Rev. Lett., 84, 4701 (2000).
4. 4. Y. Liu, J.E. Drumheller, R.D. Willett, Phys. Rev., B52, 15327 (1995).