Low temperature thermodynamics of finite spin-1/2 XX Chain with some distorted links

O.S. Dzhenzherov, E.V. Ezerskaya

V. N. Karazin Kharkiv National University, 4 Svoboda sq., Kharkiv, 61022, Ukraine
yezerska@karazin.ua

ORCID: 0000-0002-6896-9550
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We present the results of our analytical and numerical study of quantum stationary states and the thermodynamics of exactly solvable finite linear spin-1/2 XX chain with one or two distorted links. The exact dispersion equations for the stationary states with one inverted spin for both cases have been derived. The corresponding spectrum consists of one quasi-continuous band and some localized impurity levels. The analytical inequalities for the values of the critical model parameters describing the appearance of local energy impurity levels above and below quasi-continuous band are obtained and analyzed. The field and the temperature dependences of the main thermodynamic characteristics of these models are studied. It is shown, that the appearance of the localized levels near the distorted links may effect significantly on the thermodynamic properties at low temperatures, leading to the additional singularities in the field and the temperature dependences of the principal thermodynamic characteristics. For example, the field dependence of $z$-projection of average total spin and the field dependence of the magnetization at zero temperature have the finite jumps associated with the quasi-continuous spectrum, and the impurity levels. The remnants of these jumps at rather low temperature are clearly visible. The average $z$-projections of the spins of distorted link(s) may decrease with the increasing of the magnetic field for some values of model parameters. The temperature dependence of the specific heat may demonstrate additional maxima at very low temperatures. The complex oscillatory pattern of the time dependence of the dynamical longitudinal pair correlation function and the autocorrelation function is associated with the finiteness of the models and the appearance of associated localized energy levels.

Keywords: spin, Heisenberg Hamiltonian, spin-1/2 XX-chain, energy spectrum, thermodynamic characteristics, quantum phase transition.

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Низькотемпературна термодинаміка скінченного ХХ ланцюжка зі спіном $\frac{1}{2}$ з кількома деформованими взаємодіями

О.С. Джержеров, О.В. Єзерська

Харківський національний університет імені В.Н. Каразіна, м. Свободи 4, 61022, Харків, Україна

Проведено теоретичне дослідження квантових стаціонарних станів і термодинаміки точно розв’язуваної моделі скінченного лінійного ХХ ланцюжка зі спіном 1/2 з однією або двома двоцентровими ланками з деформованими зв’язками. Отримано точні дисперсійні співвідношення для стаціонарних станів з одним переверненим спіном для обох випадків. Цей спектр складається з однієї квазінеперервної зони і декількох локалізованих домішкових рівнів. Отримано і проаналізовано аналітичні нерівності для значень критичних параметрів моделей, що описують появу локальних енергетичних домішкових рівнів вище і нижче квазінеперервної зони. Досліджено польові і температурні залежності основних термодинамічних характеристик моделей. Показано, що поява локалізованих рівнів поблизу спотворених ланок може мати суттєвий вплив на термодинамічні властивості при низьких температурах, приводячи до додаткових особливостей на польових і температурних залежностях основних термодинамічних характеристик. Наприклад, польова залежність $z$-проекції середнього повного спина і польова залежність намагніченості при нульовій температурі мають кінцеві скачки, пов’язані як з квазінеперервним спектром, так і домішковими рівнями. Залишки цих стрибків добре видно при дуже низьких температурах. Середні значення $z$-проекції спінів спотворених зв’язків (зв’язків) можуть зменшуватися зі збільшенням магнітного поля для деяких значень параметрів моделі. Температурна залежність питомої теплоємності може демонструвати додаткові максимуми при дуже низьких температурах. Складний коливальний характер залежності від часу динамічної поздовжньої парної кореляційної функції і автокореляційної функції пов’язані зі зв’язаністю моделей і з вищими зв’язаних локалізованих рівнів енергії.

Ключові слова: спин, Гейзенберг, ХХ ланцюжок зі спіном 1/2, енергетичний спектр, термодинамічні характеристики, квантовий фазовий перехід.

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1. Introduction

Last decades the discovery of a big number of new compounds with quasi-one-dimensional and quasi-two-dimensional magnetic structures has given further impetus to the theoretical studies of low-dimensional systems [1-3]. In this context the exactly solvable models like spin-1/2 XX chain attract much attention of theoreticians [1-11]. For many years, above chain model was one of the theoretical instruments for checking the numerical results for more general spin systems, and also applied for adequate simulation of the magnetic properties of real compounds [12, 13]. Any real magnetic material has different types of structure defects. The theoretical study of the influence of these defects on the energy spectrum and the thermodynamics of spin chain structures is of interest.

2. The Hamiltonians

This work is devoted to the theoretical treatment of the low temperature thermodynamics of some exactly solvable quantum models based on spin-1/2 XX-chain. We study analytically and numerically the finite spin-1/2 XX chains with defects of different nature: finite linear XX-chain with one and two distorted XX bond.

The corresponding Hamiltonians for these models have the following form

$$\hat{H} = -g \mu_B H \sum_{n=1}^{N} S_n^z - J \sum_{n=1}^{N} (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) - \sum_{i} \left[ g_i (S_n^z + S_{n+1}^z) - J_i (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) \right]$$

(1)

where $J, J_i > 0$ are the exchange integrals for spin-1/2 XX chain and distorted link(s) respectively, $\mu_B$ is the Bohr magneton, $g, g_i$ are $g$-factors for the chain link(s) respectively, $H$ is the longitudinal uniform magnetic field, and $i = 1 \text{ or } i = 1, 2$ for one or two distorted links respectively.

3. Stationary states with one inverted spin

We diagonalized the Hamiltonian (1) by solving the one particle Schrödinger equation in the lattice site representation and derived the following dispersion relations for the stationary states with one inverted spin

$$\varepsilon = g \mu_B H - \frac{J}{2} \left( x + \frac{1}{x} \right)$$

(2)

for both models and

$$\beta_i = 1 - \frac{2^{(n+1)}}{1 - x^n}$$

$$\beta_i = 1 - \frac{2^{(n+1)}}{1 - x^n} - \alpha_i^2 x^2 = 0$$

(3)

for $i = 1$, and

А.С. Джикензер, Е.В. Єзерська

Харківський національний університет імені В.Н. Каразіна, м. Свободи 4, 61022, Харків, Україна
\[
\left( \beta_i x - \frac{1 - x^{2(n_i+1)}}{1-x^{2n_i}} \right) \left( \beta_i x - \frac{1 - x^{2(n_i+1)}}{1-x^{2n_i}} \right) \times
\]
\[
\left( \beta_i x - \frac{1 - x^{2n_i}}{1-x^{2n_i-1}} \right) \left( \beta_i x - \frac{1 - x^{2n_i}}{1-x^{2n_i-1}} \right) -
\]
\[
- \left( \frac{x}{1-x} \right)^2 \left( \frac{x}{1-x} \right)^2 - \alpha_i^2 x^2 \times
\]
\[
\left( \beta_i x - \frac{1 - x^{2(n_i+1)}}{1-x^{2n_i}} \right) \left( \beta_i x - \frac{1 - x^{2(n_i+1)}}{1-x^{2n_i}} \right) -
\]
\[
- \alpha_i^2 x^2 \left( \beta_i x - \frac{1 - x^{2n_i}}{1-x^{2n_i-1}} \right) \times
\]
\[
\left( \beta_i x - \frac{1 - x^{2n_i}}{1-x^{2n_i-1}} \right) - \alpha_i^2 x^2 = 0
\]

for \( i = 1, 2 \). Here \( \alpha_i = J_i/J \), \( \beta_i = [2(g - g_i)\mu_B H]/J \).

The above spectra consist of one quasi-continuous band
\[
\epsilon = g \mu_B H - J \cos k,
\]
where \( x = \exp(ik) \) is the solutions of (2), (3) with \( |x|=1 \), and may have some localized impurity levels, if \( x \) is the real number with \( |x|<1 \). The total number of localized impurity levels is up to two levels and up to four levels for the models with one and two impurity links, respectively. The analytical inequalities for the values of the critical model parameters describing the appearance of the localized energy impurity levels were found for both models. The corresponding formulas for critical values of model parameters are presented below
\[
\left[ 1+ \frac{1}{2} \left( \frac{1}{n_1} + \frac{1}{n_2} \right) \right] x - \alpha_i^2 = \frac{1}{4} \left( \frac{1}{n_1} - \frac{1}{n_2} \right)^2
\]

for the chain with one distorted link, and
\[
\left( \alpha_i^2 + \delta_1^2 - \gamma_1^2 \right) \left( \alpha_i^2 + \delta_2^2 - \gamma_2^2 \right) =
\]
\[
= \frac{(\alpha_i^2 - \gamma_1^2)(\alpha_i^2 - \gamma_2^2)}{(n_2-1)^2};
\]
\[
\gamma_{1,2} = \pm \beta_{1,2} - 1 \frac{1}{2} \left( \frac{1}{n_{i3}} + \frac{1}{n_{i2} - 1} \right);
\]
\[
\delta_{1,2} = \frac{1}{2} \left( \frac{1}{n_{i3}} - \frac{1}{n_{i2} - 1} \right)
\]

for the chain with two distorted links.

4. Thermodynamics

Using the dispersion relations (2-4), one can investigate the thermodynamic properties of the models.

\( n_1 = 14, n_2 = 5, \quad n_1 = 6, g = 2, \quad g_1 = 2.5, g_2 = 3, \quad J = 1 K, \quad J_1 = 8 K, \quad J_2 = 6 K \).
The remnants of these jumps at rather low temperature are clearly visible (see fig. 2). We associate the maxima and minima in weak fields with quasi-continuous spectra, and additional extrema in strong magnetic field correspond to the localized levels.

In the case of weak interaction with the main XX chain the field dependence of average value of the spins of distorted link may be decreased and even becomes negative with the increasing of magnetic field, and jumps in the critical field along the direction of the magnetic field (see fig. 3a). Pair correlation function (fig. 3b) is negative for nearest neighbors at zero and weak fields. We associate this behavior with antiferromagnetic character of XX exchange interaction.

The temperature dependence of specific heat per spin for both models with the same number of lattice spins and the same parameters for the first “distortion” at \( n_1, n_1 + 1 \) positions in very weak magnetic field is presented at Fig. 4.

The temperature dependence of the specific heat per spin for the model with one distorted bond (dashed line at fig. 4) has no additional low temperature peaks of XX chains with two distorted links (solid line at fig. 4). The low temperature peaks for the model with two distorted links can be associated with the second “distortion” at \( n_2, n_2 + 1 \) for the model with two links.

The absolute values of longitudinal pair dynamical correlation function and autocorrelation function for the spins of distorted link are pictured at fig. 5. These characteristics also affected noticeably by the local levels, which leads to the complex oscillations pattern, including some kind of beats.
5. Summary and conclusions

Two exactly solvable spin-1/2 models with XX exchange interactions with one and two distorted links and finite total number of spins are investigated analytically and numerically.

In particular, we obtained the dispersion equations for the stationary states with one inverted spin are derived, and the analytical relations for the critical values of model parameters which correspond to the appearance of the localized impurity levels. The low temperature thermodynamics of above models are studied numerically.

We found a complex character of the dependence of the heat capacity on applied longitudinal magnetic field with numerous minima and maxima.

The field dependence of z-projection of the average total spin and the field dependence of magnetization at zero temperatures have the finite jumps associated with the quasi-continuous spectrum, and the impurity levels. At rather low temperatures the remnants of these jumps are clearly visible. The average z-projection of the spins of distorted link(s) may decrease with the increasing of the magnetic field for some values of model parameters.

The temperature dependence of specific heat may demonstrate additional maxima at very low temperatures.

The pair dynamical correlation function and autocorrelation function also affected noticeably by the local levels, which results to the complex oscillations patterns. So, the finite nature of the models, and the appearance of the localized levels may effect noticeably on the local thermodynamic characteristics.

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