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On the energy spectrum and thermodynamics of decorated quasi-one-dimensional magnetic systems with uniaxial anisotropy

E. V. Ezerskaya

V. N. Karazin Kharkiv National University, Kharkiv 61022, Ukraine
E-mail: yezerska@karazin.ua

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This paper is devoted to the study of thermodynamics of the quasi-1D spin models with Ising interaction between complex unit cells by transfer-matrix method. The field and the temperature dependences of the main thermodynamic characteristics have been investigated. It is shown that the field dependence of the magnetization at low temperatures for the models of "comb" and "decorated comb", and decorated triangles structures have an intermediate magnetization plateau in case of antiferromagnetic Ising interactions. The temperature dependence of the heat capacity may have several maxima in zero magnetic field. For the chain model of triangles decorated by Ising spins through the one vertex and for the "double decorated comb" some kind of the pseudo-phase transitions in the critical magnetic field is found.

Keywords: spin Hamiltonian, XXZ-model, Ising model, spin chain, thermodynamics, transfer-matrix.

1. Introduction

In recent decades, a large number of materials with quasi-one-dimensional and quasi-two-dimensional magnetic structures were discovered. In particular, high-temperature superconductivity in antiferromagnets gave a strong impetus to the theoretical studies of low-dimensional systems. One of the simplest approaches to the study of above multi-particle systems is the application of the statistical theory of the 1D and 2D Ising model (see, for example [1–3]). For more realistic quantum systems like Heisenberg spin chain or Hubbard chain models until now, the exact solutions were obtained by different variations of the Bethe's method proposed 90 years ago [1–3, 4]. In [5] several generalizations of one-dimensional and two-dimensional exactly solvable quantum spin-1/2 models are proposed. More simple family of exactly solvable quantum models is based on so-called spin-1/2 XY model. By means of the Jordan–Wigner transformation it is possible to find an exact energy spectrum and study the behavior of different thermodynamic quantities for this model (see, for example, [2–4, 6]. The advantage of the above models is their simplicity and possible realizations in a number of applications.

Recently a new type of pseudo-phase transitions was found theoretically for several one-dimensional (1D) spin models. It was shown, the models with complex unit cell may exhibit a peculiar pseudo-transition accompanied with the anomalous response of thermodynamic quantities in close vicinity of pseudo-critical temperature [7, 8].

In this paper, we consider several exactly solvable model spin-1/2 systems for which the transfer-matrix approach can be used to derive a partition function. This permits us to investigate in details the behavior of basic thermodynamic quantities at different temperatures and model parameters. At least for two of the proposed models, the numerical simulation of temperature dependences of specific heat and magnetization demonstrate the existence of pseudo-phase transitions for some values of model parameters. Note also that in [9] the similar numerical approach on the base of standard transfer-matrix technique was used for the exactly solvable quantum model based on spin-1/2 XX chain with the periodically embedded Ising spins but the above pseudo-phase transitions were not found.

2. Models

We consider four quasi-one dimensional spin models with rather simple periodic structure.

The exact energy spectra of the anisotropic spin chains with the four-site unit cell formed by triangles or stripes decorated by one-site spins are studied.

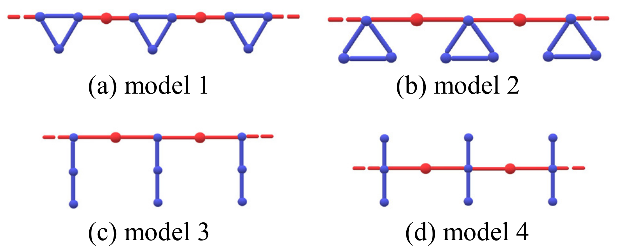

Fig. 1. Structure of models with Hamiltonians (1)–(4).

The Hamiltonian of the (see Fig. 1(a)) formed by the XXZ triangles, which are connected by one side through one-site Ising spins has the form

$$\mathcal{H} = -\sum_{n=1}^{N}\left\{\sum_{i=1}^{3}\left[g\mu_B H S_{in}^z + \right.\right.$$
$$\left.\left. + J(S_{in}^x S_{i+1n}^x + S_{in}^y S_{i+1n}^y + \gamma S_{in}^z S_{i+1n}^z)\right]\right\} - g_0\mu_B H\sum_{n=1}^{N} S_{4n}^z - \quad (1)$$
$$-J_0\sum_{n=1}^{N}\left(S_{4n}^z S_{1n}^z + S_{4n+1}^z S_{2n}^z\right), \quad S_{4n}^\alpha = S_{1n}^\alpha, \ \alpha = x, y, z.$$

Here S_{in}^x ($\alpha = x, y, z$) are the projections of spin-1/2 operator, localized at ith position at nth unit cell, J, γJ are the exchange integrals, which correspond XXZ exchange interactions inside the unit cells and J_0 is the Ising exchange interaction between unit cell, H is the longitudinal magnetic field, μ_B is the Bohr magneton, g, g_0 are the g-factors for unit cells spins and for decoration spins respectively. Periodic boundaries are supposed: $S_{4N+1}^z \to S_{41}^z$.

The Hamiltonian of the model 2 [see Fig. 1(b)] constructed by the XXZ triangles connected through the one vertex has the form

$$\mathcal{H} = -\sum_{n=1}^{N}\left\{\sum_{i=1}^{3}\left[g\mu_B H S_{in}^z + \right.\right.$$
$$\left.\left. + J(S_{in}^x S_{i+1n}^x + S_{in}^y S_{i+1n}^y + \gamma S_{in}^z S_{i+1n}^z)\right]\right\} - \quad (2)$$
$$-g_0\mu_B H\sum_{n=1}^{N} S_{4n}^z - J_0\sum_{n=1}^{N} S_{1n}^z\left(S_{4n}^z + S_{4n+1}^z\right),$$
$$S_{4n}^\alpha = S_{1n}^\alpha, \quad \alpha = x, y, z.$$

The Hamiltonians of model 3 [see Fig. 1(c) and model 4 see Fig. 1(d)] we obtain by broking one connection in triangles in (2)

$$\mathcal{H} = -\sum_{n=1}^{N}\left[g\mu_B H\sum_{i=1}^{3} S_{in}^z + \right.$$
$$\left. + J\sum_{i=1}^{2}\left(S_{in}^x S_{i+1n}^x + S_{in}^y S_{i+1n}^y + \gamma S_{in}^z S_{i+1n}^z\right)\right] - \quad (3)$$
$$-g_0\mu_B H\sum_{n=1}^{N} S_{4n}^z - J_0\sum_{n=1}^{N} S_{1n}^z\left(S_{4n}^z + S_{4n+1}^z\right),$$

$$\mathcal{H} = -\sum_{n=1}^{N}\left[g\mu_B H\sum_{i=1}^{3} S_{in}^z + \right.$$
$$\left. + J\sum_{i=1}^{2}\left(S_{in}^x S_{i+1n}^x + S_{in}^y S_{i+1n}^y + \gamma S_{in}^z S_{i+1n}^z\right)\right] - \quad (4)$$
$$-g_0\mu_B H\sum_{n=1}^{N} S_{4n}^z - J_0\sum_{n=1}^{N} S_{2n}^z\left(S_{4n}^z + S_{4n+1}^z\right).$$

3. Transfer-matrix and thermodynamics

All above Hamiltonians (1)–(4) have the same fragments, for which the z-projection of total spin is the good quantum number. The Hamiltonian can be presented in the form

$$\mathcal{H}(\sigma_1, ..., \sigma_N) = \sum_{n=1}^{N}\mathcal{H}_n(\sigma_n, \sigma_{n+1}), \quad \sigma_{N+1} = \sigma_1, \quad (5)$$

Here σ_n, $n = 1, 2, ..., N$ are the eigenvalues of Ising spins S_{4n}^z at (4, n) positions. So, we omitted "spin decorations" and the Hamiltonian (5) depends now on the additional parameters σ_n. For (5) one can apply the classical transfer matrix method. The partition function is the trace of total transfer-matrix, which has the following form for all above models:

$$T(\sigma_1, \sigma_2) = \exp\left[-\frac{E_{\text{ferro}}(\sigma_1, \sigma_2)}{T}\right]\times$$
$$\times\left(1 + \sum_{i=1}^{3}\exp\left[-\frac{\varepsilon_1^{(i)}(\sigma_1, \sigma_2)}{T}\right] + \sum_{i=1}^{3}\exp\left[-\frac{\varepsilon_2^{(i)}(\sigma_1, \sigma_2)}{T}\right] + \right. \quad (6)$$
$$\left. + \exp\left[-\frac{\varepsilon_3(\sigma_1, \sigma_2)}{T}\right]\right).$$

In principle, Eq. (6) is suitable for calculating the partition function for an arbitrary value of Ising spins. The partition function is the trace of total transfer-matrix $\mathbf{T}^N$

$$Z_N = \mathrm{Tr}(\mathbf{T}^N) = \sum_{i=1}^{2S+1}\lambda_i^N, \quad (7)$$

where λ_i is the Ith eigenvalue of the transfer-matrix (6). We will limit ourselves to the value of spin-1/2, so $\sigma_i = \pm 1/2$, $i = 1, 2$. In this case, the eigenvalues of the transfer matrix are determined by the quadratic equation, and the partition function (7) for the finite system of N unit cells is

$$Z_N = (\lambda_+)^N + (\lambda_-)^N \quad (8)$$

with

$$\lambda_\pm = \frac{T_{11} + T_{22}}{2} \pm \sqrt{\left(\frac{T_{11} - T_{22}}{2}\right)^2 + T_{12}T_{21}}.$$

We would like to remind, that the free energy per spin

$$F = -\frac{T}{4N}\ln\left[(\lambda_+)^N + (\lambda_-)^N\right] \quad (9)$$

for finite system depends on both eigenvalues, and in thermodynamic limit it is defined by only maximal eigenvalue

$$F = -T\ln\left(\lambda_{+}\right). \tag{10}$$

The Hamiltonian of each fragment is the Hamiltonian of spin-1/2 XXZ triangle for models 1 and 2, or XXZ stripe formed by three spin-1/2 for models 3 and 4 in the effective magnetic field, which depends on node number of triangle (stripe).

For example, for model with Hamiltonian (1) $\mathcal{H}_n(\sigma_n,\sigma_{n+1})$ has the form

$$\begin{gathered}\mathcal{H}_n(\sigma_n,\sigma_{n+1}) = -\frac{g_0\mu_B H}{2}(\sigma_n+\sigma_{n+1}) - \\ -\left(g\mu_B H + J_0\sigma_n\right)S_{1n}^z - (g\mu_B H + J_0\sigma_{n+1})S_{2n}^z - \\ -g\mu_B H S_{3n}^z - J\sum_{i=1}^{3}\left(S_{in}^x S_{i+1n}^x + S_{in}^y S_{i+1n}^y + \gamma S_{in}^z S_{i+1n}^z\right), \\ S_{4n}^\alpha = S_{1n}^\alpha, \quad \alpha = x,y,z.\end{gathered} \tag{11}$$

For model with Hamiltonian (2)

$$\begin{gathered}\mathcal{H}_n(\sigma_n,\sigma_{n+1}) = -\frac{g_0\mu_B H}{2}(\sigma_n+\sigma_{n+1}) - \\ -\left[g\mu_B H + J_0(\sigma_n+\sigma_{n+1})\right]S_{1n}^z - g\mu_B H(S_{2n}^z + S_{3n}^z) - \\ -J\sum_{i=1}^{3}\left(S_{in}^x S_{i+1n}^x + S_{in}^y S_{i+1n}^y + \gamma S_{in}^z S_{i+1n}^z\right), \\ S_{4n}^\alpha = S_{1n}^\alpha, \quad \alpha = x,y,z.\end{gathered} \tag{12}$$

For models (3) and (4)

$$\begin{gathered}\mathcal{H}_n(\sigma_n,\sigma_{n+1}) = -\frac{g_0\mu_B H}{2}(\sigma_n+\sigma_{n+1}) - \\ -\left[g\mu_B H + J_0(\sigma_n+\sigma_{n+1})\right]S_{1n}^z - g\mu_B H(S_{2n}^z + S_{3n}^z) - \\ -J\sum_{i=1}^{2}\left(S_{in}^x S_{i+1n}^x + S_{in}^y S_{i+1n}^y + \gamma S_{in}^z S_{i+1n}^z\right),\end{gathered} \tag{13}$$

and

$$\begin{gathered}\mathcal{H}_n(\sigma_n,\sigma_{n+1}) = -\frac{g_0\mu_B H}{2}(\sigma_n+\sigma_{n+1}) - \\ -g\mu_B H(S_{1n}^z + S_{3n}^z) - \left[g\mu_B H + J_0(\sigma_n+\sigma_{n+1})\right]S_{2n}^z - \\ -J\sum_{i=1}^{2}\left(S_{in}^x S_{i+1n}^x + S_{in}^y S_{i+1n}^y + \gamma S_{in}^z S_{i+1n}^z\right).\end{gathered} \tag{14}$$

respectively.

The exact energy spectrum for each XXZ Heisenberg triangles (11), (12) and stripes (13), (14) is obtained easily. One can classify the stationary states of (9)–(12) by the number of inverted spins, starting from the "ferromagnetic state" E_{ferro} the "vacuum" $|0\rangle$ with all three spins "up". For more symmetric models 2 and 4 described by the Hamiltonians (12) and (14), the cubic equation for the stationary states with one or two inverted spins splits on linear and quadratic equations. As an example, we present here the simple result for (12)

$$\begin{gathered}|0\rangle, \quad E_{\text{ferro}} = -\frac{1}{2}\left[3g\mu_B H + \left(g_0\mu_B H + J_0\right)\left(\sigma_1+\sigma_2\right) + \frac{3\gamma J}{2}\right]; \\ |1\rangle, \quad \begin{cases}\varepsilon_1^{(1,2)} = g\mu_B H + \gamma J + \dfrac{1}{2}\left\{J_0\left(\sigma_1+\sigma_2\right) - \dfrac{J}{2} \pm \sqrt{\left[J_0\left(\sigma_1+\sigma_2\right)+\dfrac{J}{2}\right]^2 + 2J^2}\right\}; \\ \varepsilon_1^{(3)} = g\mu_B H + \gamma J + \dfrac{J}{2};\end{cases} \\ |2\rangle, \quad \begin{cases}\varepsilon_2^{(1,2)} = 2g\mu_B H + \gamma J + \dfrac{1}{2}\left\{J_0\left(\sigma_1+\sigma_2\right) - \dfrac{J}{2} \pm \sqrt{\left[J_0\left(\sigma_1+\sigma_2\right)-\dfrac{J}{2}\right]^2 + 2J^2}\right\}; \\ \varepsilon_2^{(3)} = 2g\mu_B H + \gamma J + J_0\left(\sigma_1+\sigma_2\right);\end{cases} \\ |3\rangle, \quad \varepsilon_3 = 3g\mu_B H + J_0\left(\sigma_1+\sigma_2\right).\end{gathered} \tag{15}$$

4. Numerical simulations

Using the above results, we performed numerical simulation of the field and the temperature dependencies of the magnetization and the heat capacity for our systems.

The field dependence of magnetization for antiferromagnetic Ising interactions has several intermediate magnetization plateaus associated with the reversal of the spin directions. As can be seen from Fig. 2 the geometry of the models significantly affects the behavior of the magnetization for the same model parameters, and the dimensional effects are almost invisible at fairly low temperatures.

We modeled the temperature dependence of the heat capacity in the zero magnetic field for all models for different

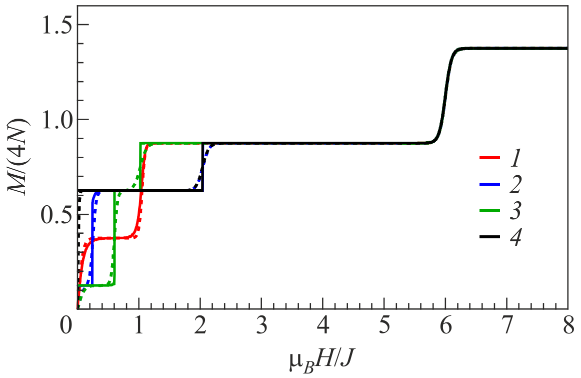

Fig. 2. (Color online) The field dependence of magnetization for models 1–4 at T = 0.1 K for the the same values of parameters $J = 1$ K, $J_0 = -12$ K, $g = 3$, $g_0 = 2$, $\gamma = -2$. Solid lines correspond to infinite number of unit cells, dashed lines correspond to $N = 2$.

numbers of unit cells with strong antiferromagnetic interaction of decorative Ising spins with triangles (stripes) and a sufficiently strong ferromagnetic easy axis anisotropy γ . As can be seen from Figs. 3(a)–3(d) the dimensional effects strongly depend on the geometry of the corresponding model.

For example, the finite size effects for the model 1 are disappeared at $N = 50$. For models 2 and 3, the finite size effects are noticeable for a fairly large number of unit cell. Moreover, there are the additional local minima and maxima [see Fig. 3 (b)]. The heat capacity behavior for the models 3 and 4 in zero magnetic field is very similar. We can expect this effect due to the similar geometrical structure of these two models. Nevertheless, the temperature dependences of $C(T)$ and $\chi(T)$ in the presence of longitudinal magnetic field may differ drastically.

It is known that in one-dimensional models with a finite radius of interaction phase transitions in temperature does not exist. But recently, so-called pseudo-transitions in a critical magnetic field have been discovered theoretically. In [7] such a kind of pseudo-transition was discovered for three-leg Heisenberg–Ising tube. In [8] for the mixed-spin model (1/2 – 1), a pseudo-transition in temperature similar to a lambda point for the second-order phase transitions was observed in the Ising–Heisenberg double tetrahedral chain. We believe that presented here models 2 and 4 have a similar effect. In Figs. 4 and 5 the temperature dependencies of specific heat and magnetic susceptibility with pseudo-phase transition behavior are presented for models 2 and 4, respectively.

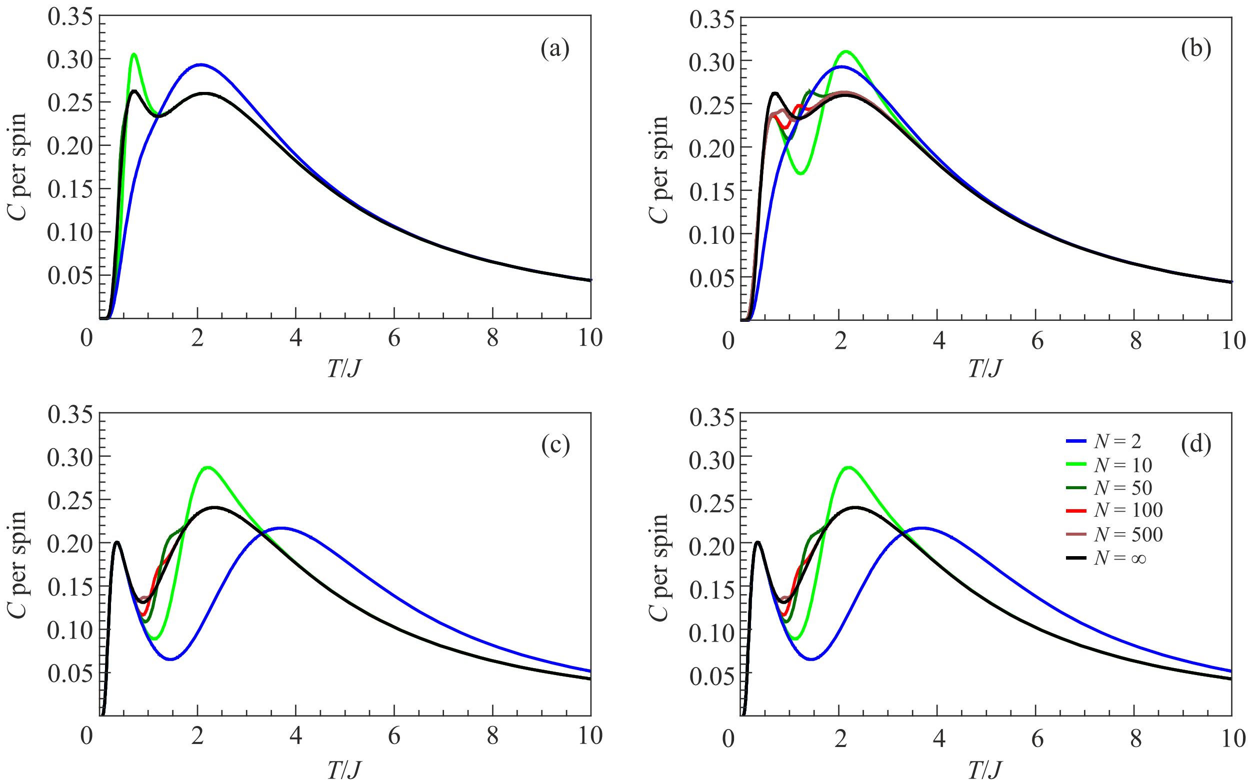

Fig. 3. (Color online) The temperature dependence of heat capacity for models 1–4 in zero magnetic field for different number of unit cells and $J = 1$, $J_0 = -12$, $g = 1$, $g_0 = 2$, $\gamma = 2$; (a) model 1, (b) model 2, (c) model 3, (d) model 4. Plot legends are the same for all figures and are shown at Fig. 3(d).

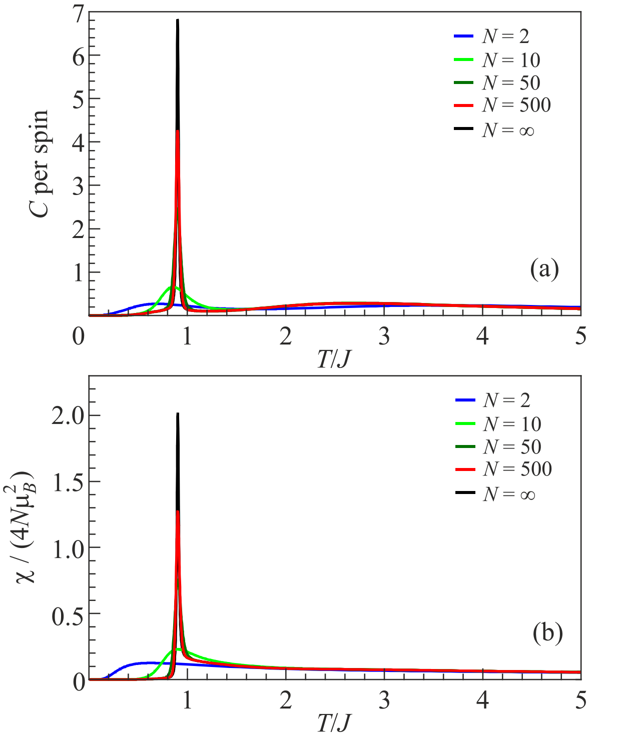

Fig. 4. (Color online) (a) C as T and (b) χ as T at $\mu_B H/J = 1.5$ for pseudo-phase transition for model 2 at $J = 1$, $J_0 = -12$, $g = 1$, $g_0 = 2$, $\gamma = 2$ with increasing of the number of unit cells.

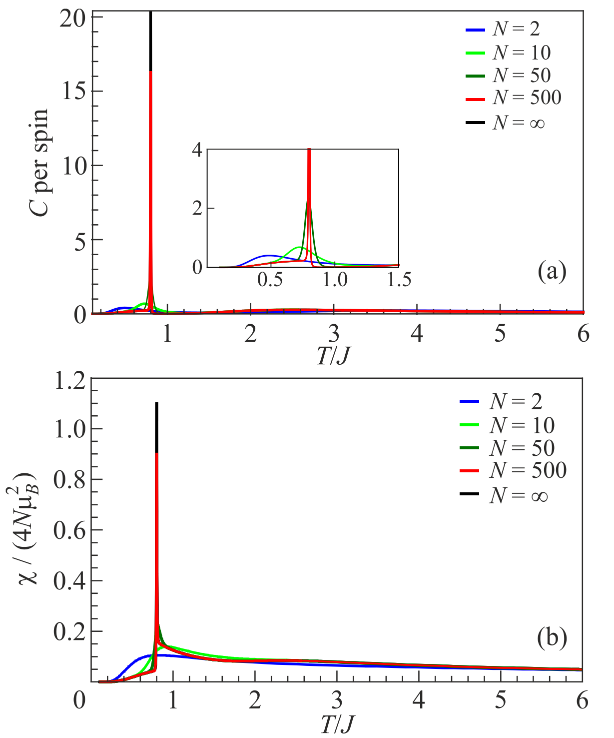

Fig. 5. (Color online) Pseudo-phase transition behavior at $\mu_B H/J = 1$ for model 4. All other parameters as at Fig. 4.

We may suppose, that the pseudo-phase transition is due to special symmetry, which leads to the degeneration of the energy spectrum and the appearance of the flat bands.

5. Conclusions

The low-temperature properties of quasi-one-dimensional spin-1/2 exactly solvable models with “decorated comb”, and decorated triangles structures are investigated. It is shown that the low-temperature dependence magnetization may have one of two intermediate magnetization plateau in case of antiferromagnetic Ising interactions.

The temperature dependence of the heat capacity may have several maxima in zero magnetic field. The temperature dependences of $C(T)$ and $\chi(T)$ in the presence of longitudinal magnetic field may differ drastically for the same values of coupling parameters for the above models with different geometry. For the “double decorated comb” and for the chain model decorated by triangles through the one vertex some kind of the pseudo-phase transitions in the critical magnetic field is determined.

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Про енергетичний спектр та термодинаміку декорованих квазіодновимірних магнітних систем з одновісною анізотропією

E. V. Ezerskaya

Вивчено термодинаміку квазіодновимірних спінових моделей із взаємодією Ізінга між складними елементарними комірками методом трансфер-матриці. Досліджено польові та температурні залежності основних термодинамічних характеристик. Показано, що польова залежність намагніченості при низьких температурах для моделей «гребінця» та «декорованого гребінця», а також оздоблених трикутних структур має проміжне плато намагніченості у разі антиферомагнітних взаємодій Ізінга. Температурна залежність теплоємності може мати кілька максимумів в нульовому магнітному полі. Для моделі трикутників, які поєднані ізінгівськими спінами через одну з вершин трикутників, та «подвійного декорованого гребінця», знайдено псевдофазові переходи у критичному магнітному полі.

Ключові слова: спіновий гамільтоніан, XXZ модель, модель Ізінга, спіновий ланцюжок, термодинаміка, трансфер-матриця.