A REGULARLY ALTERNATING ISING–HEISENBERG CHAIN. METHOD OF DECORATION-ITERATION TRANSFORMATION

B.M. LISNII

Institute for Condensed Matter Physics, Nat. Acad. Sci. of Ukraine
(1, Sventsits'kyi Str., L'viv 79011, Ukraine; e-mail: lisnyj@icmp.lviv.ua)

UDC 536.75, 538.913-405

A regularly alternating spin-1/2 Ising–Heisenberg chain with the XYZ anisotropic Heisenberg interaction is considered. By using the method of decoration-iteration transformation, the exact results concerning the free energy, the magnetizations of the Ising and Heisenberg sublattices, and a number of spin correlations are obtained. The role of XY anisotropy in the Heisenberg interaction is demonstrated for the process of magnetization.

1. Introduction

A significant interest in the study of regularly alternating Ising–Heisenberg chains is caused by the possibility to obtain the exact results for their physical characteristics. The first example of such a chain with the isotropic Heisenberg interaction is given in [1]. The case of the anisotropic Heisenberg interaction in this chain was considered recently in [2]. If a regularly alternating spin chain contains sites involved in the Ising interaction, the exact results for its physical characteristics can be obtained with the use of the decoration-iteration transformation [3–5]. By this transformation, such a chain is reduced to the classical Ising chain with the temperature-dependent interaction of the nearest neighbors and the temperature-dependent field [5], and the exact results for its physical characteristics are well known (see, e.g., [6]). Moreover, regularly alternating Ising–Heisenberg chains can be a model for certain magnetic materials [7], which is another important argument in favor of their study.

The exact results for the thermodynamic characteristics of a regularly alternating Ising–Heisenberg chain, the primitive cell of which contains one Ising atom and two Heisenberg atoms positioned in series (Fig. 1), were obtained by the decoration-iteration transformation in [5]. In this case, the XXZ anisotropic Heisenberg interaction was taken into account. For two Heisenberg atoms of the k-th primitive cell, such an interaction has the form

$$J[\Delta(\hat{S}^x_{k,1}\hat{S}^x_{k,2}+\hat{S}^y_{k,1}\hat{S}^y_{k,2})+\hat{S}^z_{k,1}\hat{S}^z_{k,2}].$$

If the parameter of anisotropy Δ is zero, the chain is an ordinary Ising chain. But if this parameter is essentially great, we have the system of noninteracting pairs of sites with the isotropic XY interaction between the sites of a pair. But within the model given in [5], we cannot, under any conditions, obtain a regularly alternating anisotropic XY chain, in which the anisotropic XY interaction would be regularly changed along the chain. Therefore, it is of interest to consider the most general case of the Heisenberg interaction with the XYZ anisotropy for a chain with such a structure as that in [5]. The exact solution within such a general model can be of independent interest. In addition, such a model allows one to get a regularly alternating anisotropic XY chain for certain sets of the interaction constants, so that its exact solution can be obtain within the appproach based on the Jordan–Wigner fermionization and the use of continued fractions [8]. Thus, by analyzing the results for a regularly alternating Ising–Heisenberg chain with the XYZ anisotropic Heisenberg interaction, we can compare two methods: the first uses the decoration-iteration procedure [5] and the second involves continued fractions [8]. Finally, one may also expect that the exact results for such a model will be useful in the analysis of the properties of real systems: experimental data for the magnetization process can depend on the direction of an applied external magnetic field, which testifies to the anisotropy of the exchange interaction.

In the present work, by using the decoration-iteration transformation, we will get the exact results for the thermodynamic characteristics of a regularly alternating spin-1/2 Ising–Heisenberg chain which possesses the same structure as the chain in [5], but has, as distinct from it, the XYZ anisotropic Heisenberg interaction.

2. Model. Free Energy

Consider a regularly alternating spin-1/2 Ising–Heisenberg chain in the external magnetic field. The chain is composed of N primitive cells. A primitive cell contains one Ising atom and two Heisenberg atoms positioned in series (Fig. 1). The total Hamiltonian of the system has the form

$$\hat{\mathcal{H}} = \sum_{k=1}^{N} \hat{\mathcal{H}}_k,$$

$$\hat{\mathcal{H}}_k = J_1 \hat{S}^x_{k,1}\hat{S}^x_{k,2} + J_2 \hat{S}^y_{k,1}\hat{S}^y_{k,2} + J_3 \hat{S}^z_{k,1}\hat{S}^z_{k,2} + J_{\rm I}(\hat{\mu}^z_k \hat{S}^z_{k,1} + \hat{S}^z_{k,2}\hat{\mu}^z_{k+1}) - \frac{h_{\rm a}}{2}(\hat{\mu}^z_k + \hat{\mu}^z_{k+1}) - h_{\rm b}(\hat{S}^z_{k,1} + \hat{S}^z_{k,2}), \quad (1)$$

where $\hat{\mu}^z_k$ and $\hat{S}^\alpha_{k,i}$ ($\alpha = x, y, z; i = 1, 2$) stand for components of the standard spin-1/2 operators which describe Ising and Heisenberg atoms, respectively, which belong to the k-th primitive cell (Fig. 1). The parameters J_1, J_2, J_3 describe the XYZ anisotropic interaction between two neighboring Heisenberg atoms; the parameter $J_{\rm I}$ describes the interaction of Ising atoms with the nearest Heisenberg atoms; and $h_{\rm a}$ and $h_{\rm b}$ are the magnetic fields acting on the Ising and Heisenberg atoms, respectively. The total Hamiltonian of the chain is the sum of the Hamiltonians $\hat{\mathcal{H}}_k$ which correspond to primitive cells. In this case, each $\hat{\mathcal{H}}_k$ corresponds also to a pair of Ising atoms ($\hat{\mu}^z_k$ and $\hat{\mu}^z_{k+1}$) located in neighboring primitive cells. As for the structure of the Hamiltonian $\hat{\mathcal{H}}_k$, it describes all the interactions of Heisenberg atoms of the k-th primitive cell with the nearest neighbors.

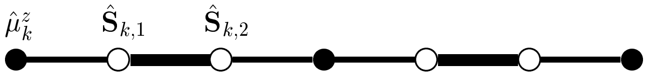

Fig. 1. Fragment of a regularly alternating spin-1/2 Ising–Heisenberg chain. Black circles denote Ising atoms with spin $\hat{\mu}^z_k$, and light circles stand for Heisenberg atoms with spin $\hat{\mathbf{S}}_{k,i}$. Spins of the k-th primitive cell ($\hat{\mu}^z_k$, $\hat{\mathbf{S}}_{k,1}$, and $\hat{\mathbf{S}}_{k,2}$) are shown

With regard for the commutativity of the Hamiltonians $\hat{\mathcal{H}}_k$ ($[\hat{\mathcal{H}}_k, \hat{\mathcal{H}}_j] = 0$ at $k \neq j$), the partition function of the system $\mathcal{Z} = \mathrm{Sp}\exp(-\beta\hat{\mathcal{H}})$ can be partially factorized, i.e.

$$\mathcal{Z} = \mathrm{Sp}_{\{\hat{\mu}^z\}} \prod_{k=1}^{N} \mathrm{Sp}_{\hat{\mathbf{S}}_{k,1},\hat{\mathbf{S}}_{k,2}} \exp(-\beta\hat{\mathcal{H}}_k). \quad (2)$$

In this formula, $\beta = (k_{\rm B}T)^{-1}$, $k_{\rm B}$ is the Boltzmann constant, T is the absolute temperature, $\mathrm{Sp}_{\{\hat{\mu}^z\}}$ means the trace over the states of Ising spins, and $\mathrm{Sp}_{\hat{\mathbf{S}}_{k,1},\hat{\mathbf{S}}_{k,2}}$ is the trace over the states of Heisenberg spins of the k-th cell. We now pass to a matrix representation of $\hat{\mathcal{H}}_k$ in the basis constructed on the eigenfunctions of the operators $\hat{S}^z_{k,i}$, determine the eigenvalues of the matrix $\hat{\mathcal{H}}_k$, and get

$$\mathrm{Sp}_{\hat{\mathbf{S}}_{k,1},\hat{\mathbf{S}}_{k,2}} \exp(-\beta\hat{\mathcal{H}}_k) = 2\exp\left(\frac{\beta h_{\rm a}(\hat{\mu}^z_k + \hat{\mu}^z_{k+1})}{2}\right) \times \left\{ \mathrm{ch}\left(\beta\sqrt{\frac{(J_1 - J_2)^2}{16} + \frac{(J_{\rm I}(\hat{\mu}^z_k + \hat{\mu}^z_{k+1}) - 2h_{\rm b})^2}{4}}\right) \times \exp\left(-\frac{\beta J_3}{4}\right) + \exp\left(\frac{\beta J_3}{4}\right) \times \mathrm{ch}\left(\beta\sqrt{\frac{(J_1 + J_2)^2}{16} + \frac{J_{\rm I}^2(\hat{\mu}^z_k - \hat{\mu}^z_{k+1})^2}{4}}\right) \right\}. \quad (3)$$

The partially factorized partition function (2) has a structure which allows one to use the decoration-iteration transformation [3–5]:

$$\mathrm{Sp}_{\hat{\mathbf{S}}_{k,1},\hat{\mathbf{S}}_{k,2}} \exp(-\beta\hat{\mathcal{H}}_k) = A\exp[\beta R\hat{\mu}^z_k\hat{\mu}^z_{k+1} + \beta h_0(\hat{\mu}^z_k + \hat{\mu}^z_{k+1})/2]. \quad (4)$$

In order to determine the unknown parameters A, R, and h_0 of the transformation, we use the available degree of freedom of the Ising spins $\hat{\mu}^z_k$ and $\hat{\mu}^z_{k+1}$, each of the spins can take values $\pm\frac{1}{2}$. Thus, we get the following formulas for these parameters:

$$A = (A_1 A_2 A_3^2)^{1/4}, \quad \beta R = \ln\left(\frac{A_1 A_2}{A_3^2}\right),$$

$$\beta h_0 = \beta h_{\rm a} - \ln\left(\frac{A_1}{A_2}\right), \tag{5}$$

where

$$A_{1,2} = 2\,{\rm ch}\left(\beta\sqrt{\frac{(J_1-J_2)^2}{16}+\frac{(J_{\rm I}\pm 2h_{\rm b})^2}{4}}\right)\times$$

$$\times\exp\left(-\frac{\beta J_3}{4}\right) + 2\exp\left(\frac{\beta J_3}{4}\right){\rm ch}\left(\beta\frac{J_1+J_2}{4}\right),$$

$$A_3 = 2\,{\rm ch}\left(\beta\sqrt{\frac{(J_1-J_2)^2}{16}+h_{\rm b}^2}\right)\exp\left(-\frac{\beta J_3}{4}\right)+$$

$$+2\exp\left(\frac{\beta J_3}{4}\right){\rm ch}\left(\beta\sqrt{\frac{(J_1+J_2)^2}{16}+\frac{J_{\rm I}^2}{4}}\right).$$

It is worth noting that the structure of formulas (5) is the same as in [5], and the coefficients A_1, A_2, A_3 coincide in the partial case where $J_1 = J_2 \neq J_3$ with the corresponding coefficients in [5].

The decoration-iteration transformation realizes the mapping of the initial Ising–Heisenberg chain (1) on a spin-1/2 Ising chain with effective interaction R under the action of the external effective magnetic field h_0 [see (4)]. After this transformation, the determination of the partition function of an Ising–Heisenberg chain $\mathcal{Z}$ (2) is reduced to that of the partition function of an Ising chain $\mathcal{Z}_{\rm I}$:

$$\mathcal{Z}(\beta, J_1, J_2, J_3, J_{\rm I}, h_{\rm a}, h_{\rm b}) =$$

$$= A(\beta, J_1, J_2, J_3, J_{\rm I}, h_{\rm b})^N \mathcal{Z}_{\rm I}(\beta R, \beta h_0), \tag{6}$$

where

$$\mathcal{Z}_{\rm I} = {\rm Sp}_{\{\hat\mu^z\}}\prod_{k=1}^{N}\exp[\beta R\hat\mu_k^z\hat\mu_{k+1}^z + \beta h_0(\hat\mu_k^z+\hat\mu_{k+1}^z)/2].$$

For the partition function of an Ising chain, we have [6]

$$\mathcal{Z}_{\rm I} = \lambda_1^N + \lambda_2^N,$$

where the eigenvalues of the transfer matrix are

$$\lambda_{1,2} = \exp\left(\frac{\beta R}{4}\right){\rm ch}\left(\frac{\beta h_0}{2}\right)\pm$$

$$\pm\sqrt{\exp\left(\frac{\beta R}{2}\right){\rm sh}^2\left(\frac{\beta h_0}{2}\right)+\exp\left(-\frac{\beta R}{2}\right)}.$$

By using this result for $\mathcal{Z}_{\rm I}$, we obtain the free energy per primitive cell (3 atoms) in the thermodynamic limit as

$$f \equiv \lim_{N\to\infty}\frac{-k_{\rm B}T\ln\mathcal{Z}}{N} = -\frac{1}{\beta}\ln A - \frac{1}{\beta}\ln\lambda_1. \tag{7}$$

The entropy s and the heat capacity c per primitive cell can be calculated with the use of the well-known thermodynamic relations. It is convenient to take them in the form

$$s = k_{\rm B}\beta^2\left(\frac{\partial f}{\partial\beta}\right)_{h_{\rm a},h_{\rm b}}, \qquad c = -\beta\left(\frac{\partial s}{\partial\beta}\right)_{h_{\rm a},h_{\rm b}}.$$

3. Magnetization. Spin Correlations

As was noted in [5], by differentiating the free energy f with respect to the magnetic fields $h_{\rm a}$ and $h_{\rm b}$, respectively, one can obtain the magnetizations of the Ising and Heisenberg sublattices. To calculate the average values of operator structures of the type $f_1(\hat\mu_i^z,\ldots,\hat\mu_j^z)$ i $f_2(\hat S_{k,1}^\alpha, \hat S_{k,2}^\gamma, \hat\mu_k^z, \hat\mu_{k+1}^z)$, where the indices $\alpha,\gamma = x,y,z$ stand for components of the spin operators, we will use the relations [5]

$$\langle f_1(\hat\mu_i^z,\ldots,\hat\mu_j^z)\rangle = \langle f_1(\hat\mu_i^z,\ldots,\hat\mu_j^z)\rangle_{\rm I},$$

$$\langle f_2(\hat S_{k,1}^\alpha, \hat S_{k,2}^\gamma, \hat\mu_k^z, \hat\mu_{k+1}^z)\rangle =$$

$$= \left\langle\frac{{\rm Sp}_{\hat{\mathbf S}_{k,1},\hat{\mathbf S}_{k,2}} f_2(\hat S_{k,1}^\alpha, \hat S_{k,2}^\gamma, \hat\mu_k^z, \hat\mu_{k+1}^z)\exp(-\beta\hat{\mathcal H}_k)}{{\rm Sp}_{\hat{\mathbf S}_{k,1},\hat{\mathbf S}_{k,2}}\exp(-\beta\hat{\mathcal H}_k)}\right\rangle \tag{8}$$

which can be easily obtained from formulas (2) and (4). In these relations, the notations $\langle\ldots\rangle$ and $\langle\ldots\rangle_{\rm I}$ mean the standard averaging in the Ising–Heisenberg model and the averaging in the Ising model equivalent to it, respectively. The calculation of the magnetizations and the correlations of the nearest neighbors can be also performed by differentiating the partition function (6).

The magnetization of the Ising sublattice $m_{\rm a}^z \equiv \frac{1}{2}\langle\hat\mu_k^z + \hat\mu_{k+1}^z\rangle$ and the correlation function $q_{\rm ii}^{zz}(n) \equiv \langle\hat\mu_k^z\hat\mu_{k+n}^z\rangle$ can be obtained with the use of the first relation in (8) and the well-known exact results for an Ising chain [6]:

$$m_{\rm a}^z = \frac{1}{2}\langle\hat\mu_k^z + \hat\mu_{k+1}^z\rangle_{\rm I} = \frac{{\rm sh}\left(\frac{\beta h_0}{2}\right)}{2\sqrt{{\rm sh}^2\left(\frac{\beta h_0}{2}\right)+e^{-\beta R}}},$$

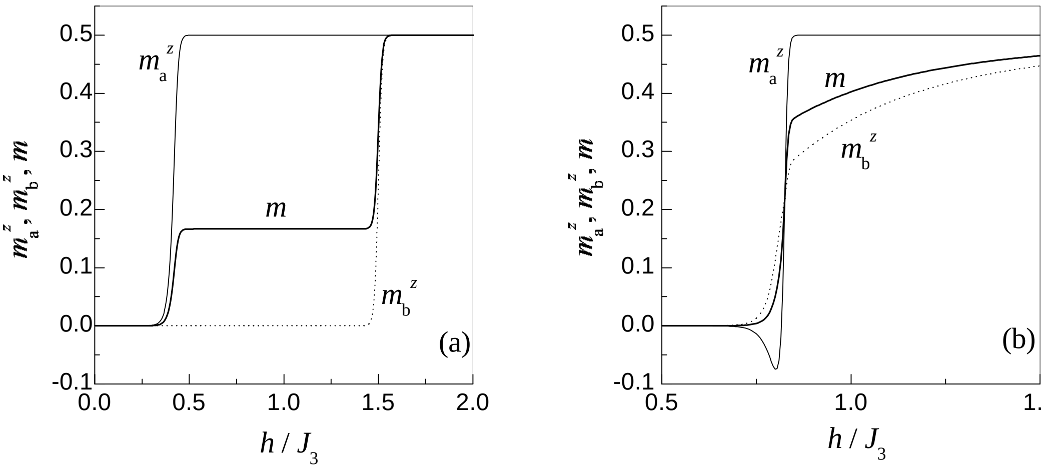

Fig. 2. Dependence of the magnetizations $m_{\rm a}^z$, $m_{\rm b}^z$ and $m = (m_{\rm a}^z + 2m_{\rm b}^z)/3$ on the external magnetic field $h \equiv h_{\rm a} = h_{\rm b}$ at a low temperature $k_{\rm B}T/J_3 = 0.01$. The curves are constructed for such values of the parameters: $J_1/J_3 = J_2/J_3 = J_{\rm I}/J_3 = 1$ [5] (a); $J_1/J_3 = -J_2/J_3 = J_{\rm I}/J_3 = 1$ (b)

$$q_{\rm ii}^{zz}(n) = \langle \hat\mu_k^z \hat\mu_{k+n}^z \rangle_{\rm I} = \frac{{\rm sh}^2\left(\frac{\beta h_0}{2}\right) + \left(\frac{\lambda_2}{\lambda_1}\right)^n e^{-\beta R}}{4\left({\rm sh}^2\left(\frac{\beta h_0}{2}\right) + e^{-\beta R}\right)}.$$

The magnetization of the Heisenberg sublattice $m_{\rm b}^z \equiv \frac{1}{2}\langle \hat S_{k,1}^z + \hat S_{k,2}^z \rangle$ is determined by differentiating the partition function (6):

$$m_{\rm b}^z = \lim_{N\to\infty} \frac{1}{2N\beta\mathcal{Z}}\frac{\partial \mathcal{Z}}{\partial h_{\rm b}} =$$

$$= \frac{1}{2}\left(\frac{A_{1\rm b}}{A_1} - \frac{A_{2\rm b}}{A_2} + 2\frac{A_{3\rm b}}{A_3}\right) - 2m_{\rm a}^z\left(\frac{A_{1\rm b}}{A_1} + \frac{A_{2\rm b}}{A_2}\right) +$$

$$+ 2q_{\rm ii}^{zz}(1)\left(\frac{A_{1\rm b}}{A_1} - \frac{A_{2\rm b}}{A_2} - 2\frac{A_{3\rm b}}{A_3}\right),$$

where

$$A_{1\rm b,2b} = \frac{(J_{\rm I} \pm 2h_{\rm b})e^{-\frac{\beta J_3}{4}}}{\sqrt{(J_1 - J_2)^2 + 4(J_{\rm I} \pm 2h_{\rm b})^2}} \times$$

$$\times\, {\rm sh}\left(\frac{\beta}{4}\sqrt{(J_1 - J_2)^2 + 4(J_{\rm I} \pm 2h_{\rm b})^2}\right),$$

$$A_{3\rm b} = \frac{2h_{\rm b}e^{-\frac{\beta J_3}{4}}}{\sqrt{(J_1 - J_2)^2 + 16h_{\rm b}^2}}\,{\rm sh}\left(\frac{\beta}{4}\sqrt{(J_1 - J_2)^2 + 16h_{\rm b}^2}\right).$$

It should be noted that, in the case where $J_1 = J_2 \neq J_3$, the result for $m_{\rm b}^z$ coincides with the relevant result in [5]. In the same way, we calculated the correlation functions of the nearest neighbors as

$$q_{\rm hh}^{\alpha\alpha} \equiv \langle \hat S_{k,1}^\alpha \hat S_{k,2}^\alpha \rangle,\ \alpha = x, y, z,$$

$$q_{\rm ih}^{zz} \equiv \frac{1}{2}\langle \hat\mu_k^z \hat S_{k,1}^z + \hat S_{k,2}^z \hat\mu_{k+1}^z \rangle.$$

These correlation functions look as

$$q_{\rm hh}^{\alpha\alpha} = \lim_{N\to\infty} -\frac{1}{N\beta\mathcal{Z}}\frac{\partial \mathcal{Z}}{\partial J_{i(\alpha)}} =$$

$$= -\frac{1}{\beta}\left(\frac{1}{A}\frac{\partial A}{\partial J_{i(\alpha)}} + q_{\rm ii}^{zz}(1)\frac{\partial(\beta R)}{\partial J_{i(\alpha)}} + m_{\rm a}^z\frac{\partial(\beta h_0)}{\partial J_{i(\alpha)}}\right),$$

$$q_{\rm ih}^{zz} = \lim_{N\to\infty} -\frac{1}{2N\beta\mathcal{Z}}\frac{\partial \mathcal{Z}}{\partial J_{\rm I}} = -\frac{1}{2\beta}\left(\frac{1}{A}\frac{\partial A}{\partial J_{\rm I}} + \frac{1}{\lambda_1}\frac{\partial \lambda_1}{\partial J_{\rm I}}\right),$$

where the subscripts include the function $i(\alpha)$: $i(x) = 1$, $i(y) = 2$, $i(z) = 3$. The calculation of derivatives present in these formulas is simple, but cumbersome.

We now illustrate the effect caused by the XY anisotropy of the Heisenberg interaction (Fig. 2). The presence of XY anisotropy in the Heisenberg interaction changes significantly the character of the dependence of the magnetizations $m_{\rm a}^z$ and $m_{\rm b}^z$ on the external magnetic field $h \equiv h_{\rm a} = h_{\rm b}$ at low temperatures: the plateau-like behavior disappears (see Fig. 2,a,b). We also indicate the appearance of an interval of values of the field h, in which the magnetization $m_{\rm a}^z$ is contrariwise oriented to the field h (Fig. 2,b). This is due to the fact that the effective field $h_0 = h - \beta^{-1}\ln(A_1/A_2)$ (5) which acts on the Ising spins can be contrariwise oriented to the field h.

4. Final Remarks

We now sum up the results of the present work. Within the method of decoration-iteration transformation, we have obtained the exact results for the thermodynamic characteristics of a regularly alternating spin-1/2 Ising–Heisenberg chain with XYZ anisotropic Heisenberg interaction, namely for the free energy, the magnetizations of the Ising and Heisenberg sublattices, and a number of spin correlations. If one passes from the XYZ anisotropic to the XXZ anisotropic Heisenberg interaction, these results coincide with the relevant results in work [5].

The influence of a change of the anisotropy of the Heisenberg interaction – from XXZ to XYZ – on the process of magnetization at low temperatures is illustrated in Fig. 2.

For certain values of the interaction constants, the free energy (7) can correspond, in contrast to the free energy for a model in [5], to a regularly alternating anisotropic XY chain which was exactly solved within another method – with the use of the Jordan–Wigner transformation and continued fractions [8]. The discussion of the application of the Jordan–Wigner fermionization to decorated spin chains will be given in the future work.

The author thanks Prof. O. Derzhko who attracted the author's attention to the given problem and gave fruitful advices and remarks.

1. E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961).
2. H. Yao, J. Li, and Ch. Gong, Solid State Commun. **121**, 687 (2002).
3. I. Syozi, Prog. Theor. Phys. **6**, 341 (1951).
4. M. Fisher, Phys. Rev. **113**, 969 (1959).
5. J. Strečka and M. Jaščur, J. Phys.: Cond. Matter **15**, 4519 (2003).
6. R.J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Acad. Press, London, 1982).
7. J. Strečka, M. Jaščur, M. Hagiwara, K. Minami, Y. Narumi, and K. Kindo, Phys. Rev. B **72**, 024459 (2005).
8. O. Derzhko, J. Richter, T. Krokhmalskii, and O. Zaburannyi, Phys. Rev. E **69**, 066112 (2004).

Received 01.10.07.
Translated from Ukrainian by V.V. Kukhtin

РЕГУЛЯРНОЗМІННИЙ ЛАНЦЮЖОК ІЗІНГА–ГАЙЗЕНБЕРГА. МЕТОД ДЕКОРАЦІЙНО-ІТЕРАЦІЙНОГО ПЕРЕТВОРЕННЯ

Б.М. Лісний

Р е з ю м е

Розглядається регулярнозмінний спін-1/2 ланцюжок Ізінга–Гайзенберга з XYZ анізотропною взаємодією Гайзенберга. Методом декораційно-ітераційного перетворення отримано точні результати для вільної енергії, намагніченостей ізінгівської і гайзенбергівської підґраток, а також для ряду спінових кореляцій. Продемонстровано роль XY-анізотропії у взаємодії Гайзенберга для процесу намагнічення.