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On the energy spectrum of a spin lattice formed by a finite number of coupled spin-$\frac{1}{2}$ XY chains

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Abstract

We studied the energy spectrum of a spin lattice formed by m XY spin-$\frac{1}{2}$ chains with Ising inter-chain coupling. For strong ferromagnetic coupling we found that the lowest-energy states for non-zero numbers of inverted spins on each XY chain have n-magnon bound character if $n = ml - 1$, where $l = 2, 3, \ldots$. For a spin tube formed by three XY chains with strong ferromagnetic inter-chain coupling, the lowest-energy states are described by the XXZ spin-$\frac{1}{2}$ chain model with antiferromagnetic coupling.

1. Introduction

Quasi-one-dimensional quantum spin systems such as spin ladders formed by a small number of spin chains have been studied extensively in recent years [1–3]. These systems are relevant to a number of quasi-one-dimensional compounds such as $SrCu_2O_3$, $CuGeO_3$ (two-chain ladders) and $Sr_2Cu_3O_5$ (three-chain ladder). There is a family of compounds, $La_{4n+4}Cu_{2n+8}O_{8n+14}$, which, as special cases, contains four- and five-chain ladder structures [1]. According to the theoretical predictions, isotropic Heisenberg even- and odd-chain spin-$\frac{1}{2}$ ladders should have surprisingly different properties [1, 4]; this has been confirmed experimentally. A large variety of theoretical techniques, both analytical and numerical, have been used to study the ladder systems. Nevertheless, there is relatively little information available concerning anisotropic spin ladders. These systems may also exhibit unusual behaviour because of strong quantum fluctuations in low dimensions. One such system is a ladder formed by two coupled XY spin-$\frac{1}{2}$ chains with inter-chain interaction of the Ising type proposed by Shiba [5]. This model can be reduced to a 1D Hubbard model by means of the Jordan–Wigner transformation [6], the exact spectrum of which is available via the Bethe ansatz technique [7]. For a simple generalization of the above ladder model to the case of different intra-chain exchange integrals, which is of interest as a lattice model of spin-dependent hopping phenomena, there are only a few conclusions regarding the exact energy spectrum and some numerical estimates available [8].

In this paper we will study the lowest-energy states of the anisotropic spin ladder system formed by m spin-$\frac{1}{2}$ XY chains (the m-chain ladder) with Ising-type interaction between neighbour chains. First, we will give some general conclusions on the exact spectrum of

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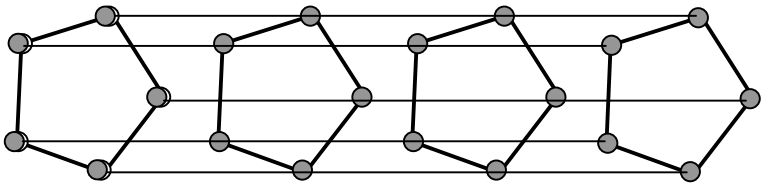

Figure 1. The spin tube formed by five XY spin-$\frac{1}{2}$ chains with inter-chain interaction of the Ising type.

the model using a symmetry of the lattice Hamiltonian. To obtain more detailed information concerning the energy spectrum we will use both perturbation theory (PT) in the limit of strong inter-chain coupling and a numerical study using the density-matrix renormalization-group method (DMRG). The main attention will be paid to the case of periodic boundaries in the direction perpendicular to the XY chains. This permits us to skip some unimportant but cumbersome details of the PT analysis. On the other hand, the corresponding lattice is of interest as one of the simplest strongly correlated electron models of non-carbon nanotubes.

2. General properties of the model energy spectrum

Let us consider a spin lattice formed by m coupled XY spin-$\frac{1}{2}$ chains described by the Hamiltonian

$$\boldsymbol{H} = -\sum_{i=1}^{N}\sum_{j=1}^{m}\{J_0 \boldsymbol{S}^z_{i,j}\boldsymbol{S}^z_{i,j+1} + J_1(\boldsymbol{S}^x_{i,j}\boldsymbol{S}^x_{i+1,j} + \boldsymbol{S}^y_{i,j}\boldsymbol{S}^y_{i+1,j}) + 2\mu h \boldsymbol{S}^z_{i,j}\}, \qquad (1)$$

where $\vec{\boldsymbol{S}}_{i,j} = (\boldsymbol{S}^x_{i,j}, \boldsymbol{S}^y_{i,j}, \boldsymbol{S}^z_{i,j})$ is a spin-$\frac{1}{2}$ operator located on ith site of the jth chain. $\vec{\boldsymbol{S}}_{i,m+1} \equiv \vec{\boldsymbol{S}}_{i,1}$ because of the cylindrical form of the lattice (figure 1); μ is a Bohr magneton and h is a longitudinal magnetic field.

Since the operators $\sum_i \boldsymbol{S}^z_{i,j}$ ($j = 1, 2, \ldots, m$) are integrals of motion, the eigenstates of (1) can be characterized by setting m quantum numbers describing the numbers of inverted spins on each XY chain. In the case of only one non-zero quantum number, the tube Hamiltonian can be easily reduced to the exactly solvable XY chain model [9]. For two non-zero quantum numbers that correspond to a pair of neighbouring XY chains, the model Hamiltonian is equivalent to the linear Hubbard model in an external longitudinal magnetic field with a well known exact solution [7].

To use the unitary transformation [9]

$$\boldsymbol{S}^x_{i,j} \to (-1)^i \boldsymbol{S}^x_{i,j}, \qquad \boldsymbol{S}^y_{i,j} \to (-1)^i \boldsymbol{S}^y_{i,j}, \qquad \boldsymbol{S}^z_{i,j} \to \boldsymbol{S}^z_{i,j}, \qquad (2)$$

we can change the sign of J_1. Hence, the energy spectrum of (1) does not depend on the sign of J_1. We can choose this sign in such a way that in the space of the eigenfunctions of the z-projection of the total spin, all non-diagonal elements of (1) have non-positive values. On the other hand, for given values of the Hamiltonian parameters J_0, $J_1 \neq 0$, and the set of quantum numbers N_j, the Hamiltonian matrix cannot be reduced to a block-diagonal form by permutations of its rows. Therefore, according to Perron–Frobenius theorem, the lowest eigenstate of (1) from the corresponding subspace is non-degenerate. For even N, a similar conclusion is valid also for periodic boundaries along the XY chains (lattice on a torus). This allows us to use translation symmetry of the lattice to investigate the nature of the excitation spectrum—similarly to in the consideration of isotropic spin chains [9, 10]. To do this, let us

consider the state

$$\Psi_{k,j} = \exp\left\{ \mathrm{i}k \sum_{n=1}^{N} n S_{n,j}^{z} \right\} \Psi_0 = \boldsymbol{Q}_{k,j} \Psi_0, \qquad k = \frac{2\pi}{N}\lambda, \qquad \lambda = 1, 2, \ldots, \tag{3}$$

where Ψ_0 is the lowest eigenstate of (1) in the subspace with specified values of the quantum numbers $N_1, N_2, \ldots, N_m$.

With the help of the unitary operator $\boldsymbol{U}$ that displaces all spins by one unit cell cyclically, it can easily be shown that

$$\langle \Psi_0 | \Psi_{k,j} \rangle = \langle \Psi_0 | \boldsymbol{U} \boldsymbol{Q}_{k,j} \boldsymbol{U}^{+} | \Psi_0 \rangle = \langle \Psi_0 | \Psi_{k,j} \rangle \exp(\mathrm{i}kN_j). \tag{4}$$

Therefore, $\langle \Psi_0 | \Psi_{k,j} \rangle = 0$ at $0 < N_j < N$. We omit here simple but cumbersome manipulations with the spin operators; it can be shown that for large values of N and $k = 2\pi/N$,

$$\langle \Psi_{k,j} | \boldsymbol{H} | \Psi_{k,j} \rangle = \langle \Psi_0 | \boldsymbol{Q}_{k,j}^{+} \boldsymbol{H} \boldsymbol{Q}_{k,j} | \Psi_0 \rangle \leqslant \langle \Psi_0 | \boldsymbol{H} | \Psi_0 \rangle + \frac{2\pi}{N} |J_1|. \tag{5}$$

The average $\langle \Psi_{k,j} | \boldsymbol{H} | \Psi_{k,j} \rangle$ is an upper boundary for the exact energy of the first excited state of $\boldsymbol{H}$ in the corresponding subspace. Therefore the relation (5) shows that the difference in energy between the lowest-energy state and the first excited state from the subspace with specified values of the quantum numbers $N_1, N_2, \ldots, N_m$ tends to zero in the thermodynamic limit if at least one of this number satisfies the condition $0 < N_j < N$.

With the help of the identity $\boldsymbol{Q}_{k,j}^{+} \boldsymbol{Q}_{l,j} = \boldsymbol{Q}_{l-k,j}$ it can also be shown that $\langle \Psi_{l,j} | \Psi_{k,j} \rangle = 0$ at $|l-k|N_j \neq 2\pi n (n = 0, 1, 2, \ldots)$. In other words, the functions Ψ_k are to be orthogonal among themselves, for example, at small non-zero values of $k \neq l$ and N_j. Therefore, according to the variational description of the eigenvalues, there are quasi-continuous excitation spectra in all the subspaces with $0 < N_j \ll N$.

The lattice Hamiltonian (1) is mapped to the 1D Hubbard-like model by means of Jordan–Wigner transformation [6, 9]:

$$\begin{aligned} \boldsymbol{H} &= \boldsymbol{H}_1 - \frac{(J_0 + 4\mu h) N m}{4} + (J_0 + 2\mu h) \sum_{j=1}^{m} N_j, \\ \boldsymbol{H}_1 &= -\tfrac{1}{2} \left(\sum_{i=1}^{N-1} \sum_{j=1}^{m} J_1 \boldsymbol{a}_{i,j}^{+} \boldsymbol{a}_{i+1,j} + \text{H.c.} \right) - J_0 \sum_{i=1}^{N} \sum_{j=1}^{m} \boldsymbol{a}_{i,j}^{+} \boldsymbol{a}_{i,j} \boldsymbol{a}_{i,j+1}^{+} \boldsymbol{a}_{i,j+1}. \end{aligned} \tag{6}$$

Here $\boldsymbol{a}_{ij}^{+}$ is a spinless Fermi operator describing the creation of a j-type particle on the ith 1D lattice site. The number of j particles coincides with the number N_j, and the total number of particles in $\boldsymbol{H}_1$ coincides with the number of inverted spins $\sum_{j=1}^{m} N_j$ in Hamiltonian (1). To apply the unitary hole–particle transformation for even j: $\boldsymbol{a}_{ij} \to (-1)^i \boldsymbol{a}_{ij}^{+}$, we can easily show that, similar to the case for the ordinary 1D Hubbard model [7, 11], the energy spectrum of $\boldsymbol{H}_1$ satisfies the following relation between positive and negative values of J_0:

$$\tilde{E}(N_1, N_2, N_3, \ldots, N_m; |J_0|) = 2|J_0| \sum_{i=1}^{m/2} N_{2i-1} + \tilde{E}(N_1, N - N_2, N_3, \ldots, N - N_m; -|J_0|). \tag{7}$$

Therefore, the energy spectrum of (1) in zero magnetic field for even m satisfies the following simple relation:

$$E(N_1, N_2, N_3, \ldots, N_m; |J_0|) = E(N_1, N - N_2, N_3, \ldots, N - N_m; -|J_0|). \tag{8}$$

It is easily seen that a similar relation is valid for a strip-type lattice formed by an arbitrary number of XY chains.

For more than two non-zero quantum numbers which correspond to the neighbouring XY chains, we can find only some of the eigenstates of the Hamiltonian (1) by means of Bethe ansatz. Let us consider for simplicity an infinite tube-type lattice formed by three XY chains. The stationary states with three inverted spins ($N_1 = N_2 = N_3 = 1$) obey the following set of finite-difference equations:

$$\begin{aligned}\left[E - E_f - 6\mu h - J_0\left(3 - \delta_{m_1,m_2} - \delta_{m_2,m_3} - \delta_{m_1,m_3}\right)\right]A_{m_1m_2m_3} + \frac{J_1}{2}(A_{m_1+1m_2m_3} \\ + A_{m_1-1m_2m_3} + A_{m_1m_2+1m_3}A_{m_1m_2-1m_3} + A_{m_1m_2m_3+1} + A_{m_1m_2m_3-1}) = 0. \end{aligned} \tag{9}$$

Here $E_f = -3N(\mu h + J_0/4)$ is the energy of the 'ferromagnetic' state (parallel orientation of all spins), δ_{m_1,m_2} is a Kronecker symbol, $A_{m_1m_2m_3}$ is the wavefunction in the lattice site representation. The inequalities $2\mu h > |J_1|$, $J_0 > 0$ are sufficient conditions for this 'ferromagnetic' state to be the ground state.

In each region $m_{Q1} \leqslant m_{Q2} \leqslant m_{Q3}$, the Bethe-type wavefunction has the following form:

$$A_{m_1,m_2,m_3} = \sum_P a_{PQ} \exp[\mathrm{i}(k_{P1}m_{Q1} + k_{P2}m_{Q2} + k_{P3}m_{Q3})], \tag{10}$$

where P and Q are permutations of the quasi-momenta k_1, k_2, k_3 and the coordinates m_1, m_2, m_3 respectively. With the help of this function one can obtain only some of the possible solutions due to the additional restriction $A_{mmm} = 0$ which follows from (9), (10) at $m_1 = m_2 = m_3$. This is consistent with the statement of [12] concerning the failure of Bethe ansatz solutions of generalizations of the Hubbard chain to arbitrary permutation symmetry. The Bethe ansatz wavefunction describes only the states with scattering of three magnons and 'partly bound' states with scattering of a one-magnon state by a two-magnon bound state. The corresponding energies of states with scattering are the sums of the one-magnon energies:

$$\varepsilon_{k_1k_2k_3} = \varepsilon_{k_1} + \varepsilon_{k_2} + \varepsilon_{k_3}, \qquad \varepsilon_k = 2\mu h + J_0 - J_1\cos k, \qquad -\pi \leqslant k < \pi. \tag{11}$$

These states obey the Pauli exclusion principle. For 'partly bound states', energies are the sums of energies of one-magnon states (ε_k) and energies of two-magnon bound states $\varepsilon_q^{(b)}$:

$$\begin{aligned}\varepsilon_{kq} &= \varepsilon_k + \varepsilon_q^{(b)} \\ \varepsilon_q^{(b)} &= 4\mu h + 2J_0 - \frac{|J_0|}{J_0}\left(J_0^2 + 4J_1^2\cos^2\left(\frac{q}{2}\right)\right)^{1/2}, \qquad -\pi \leqslant q < \pi. \end{aligned} \tag{12}$$

3. The case of strong ferromagnetic coupling

Let us first consider the lowest-energy states of the spin tube formed by three XY chains and described by the Hamiltonian (1) at $h = 0$. The exact energy spectrum of the tube can be characterized by three quantum numbers N_1, N_2 and N_3 in accordance with the numbers of inverted spins on each XY chain. In the case of $J_1 = 0$ we have a system of non-interacting unit cells (triangles) with a highly degenerate energy spectrum. For big negative values of J_0 and finite numbers of inverted spins, simple analysis shows that the lowest energy of the infinite lattice at $h = 0$ has the form

$$E(N_1, N_2, N_3) = E_f + (J_0 - |J_1|)(N_1 + N_2 + N_3). \tag{13}$$

For positive values of J_0 the structure of the energy spectrum is more complicated. If $N_1 = N_2 = N_3 = 1$ the lowest energy corresponds to the state with three inverted spins on the same unit cell (the three-spin complex). For $J_1 = 0$ such a state has the same energy as a ferromagnetic state. For $\alpha = |J_1/J_0| \ll 1$ the energy of a three-spin complex can be estimated by means of PT for degenerate energy states. We omit here simple but cumbersome

PT calculations; we found that the lowest energies of three-spin complex at $h = 0$ are described by the formula

$$E_3(k) = -|J_1|\{\tfrac{1}{4}(3\alpha + \tfrac{5}{16}\alpha^3) + \tfrac{3}{8}(\alpha^2 - \tfrac{1}{4}\alpha^4)\cos k\} + \mathrm{O}(\alpha^5), \qquad -\pi < k \leqslant \pi. \tag{14}$$

For simplicity, E_f is chosen as a reference energy.

Note that the same formula for the energy can be easily obtained from (9) by making successive approximations.

Let us now consider the energy states of a tube with an arbitrary number of three-spin complexes. Up to third PT order in J_1, these states are described by the following Hamiltonian:

$$\boldsymbol{H} = -|J_1| \sum_i \{\tfrac{3}{4}\alpha \boldsymbol{n}_i(1 - \boldsymbol{n}_{i+1}) + \tfrac{3}{16}\alpha^2(\boldsymbol{a}_i^+ \boldsymbol{a}_{i+1} + \boldsymbol{a}_{i+1}^+ \boldsymbol{a}_i)\} \tag{15}$$

where $\boldsymbol{a}_i^+$ is spinless Fermi operator describing the creation of a three-spin complex on the ith unit cell; $\boldsymbol{n}_i = \boldsymbol{a}_i^+ \boldsymbol{a}_i$.

With the help of Jordan–Wigner transformation it can be shown that $\boldsymbol{H}$ is equivalent to the Hamiltonian of the linear antiferromagnetic XXZ spin-$\frac{1}{2}$ chain:

$$\boldsymbol{H} = \frac{3}{8}\sum_i \left\{ 2\frac{J_1^2}{J_0}\left(\boldsymbol{S}_i^z \cdot \boldsymbol{S}_{i+1}^z - \frac{1}{4}\right) - \frac{J_1^3}{J_0^2}(\boldsymbol{S}_i^x \cdot \boldsymbol{S}_{i+1}^x + \boldsymbol{S}_i^y \cdot \boldsymbol{S}_{i+1}^y) \right\}. \tag{16}$$

Therefore the ground state of a tube at strong ferromagnetic coupling corresponds to the subspace with the z-projection of total spin $M = 0$. In the presence of a longitudinal magnetic field h there is a zero-temperature phase transition to the state with a maximum value of M at $h = \frac{1}{8\mu}\alpha|J_1|$.

The three-spin complex begins to interact with the one-magnon state only in second PT order in J_1. Therefore, if we add one inverted spin to the infinite system with one three-spin complex, the lowest energy will correspond to the sum of the lowest energies of this complex and that of the free one-magnon state (figure 2). The lowest one-magnon energy is equal to $J_0 - |J_1|$. Therefore, the lowest energy of the infinite tube for the state with four inverted spins has the form

$$E_4^0 = E_3^0 + J_0 - |J_1|. \tag{17}$$

For five inverted spins in zero PT order in J_1 the lowest energy corresponds to the configuration with two-spin and three-spin complexes (figure 3). But these complexes interact in first PT order in J_1. The corresponding PT estimate for the lowest energy has the following form:

$$E_5^0 = J_0 - 0.5|J_1| - \frac{7J_1^2}{8J_0} + \mathrm{O}(J_1^3). \tag{18}$$

Therefore the energy of five-magnon complex should be lower than the lowest energy of the combination of isolated two-spin and three-spin complexes. For the case of six inverted spins we have a configuration with two three-spin complexes (3 + 3) that interact in fourth PT order in J_1 only. Therefore for an infinite lattice the lowest energy of the state with six inverted spins is equal to double the lowest energy of the three-spin complex. The case of seven inverted spins is similar to the case of four inverted spins because the lowest zero-PT-order configuration has the form (3 + 3 + 1). Only for eight inverted spins with zero-PT-order configuration (3 + 2 + 3) do we have interaction in the first PT order in J_1. Therefore the lowest energy of the state with eight inverted spins corresponds to the eight-spin complex.

To generalize this consideration let us consider the lowest energy of the spin complex formed by $3n + 2$ inverted spins up to second PT order in J_1:

$$E_{3n+2}^0 = J_0 - |J_1|\cos\left(\frac{\pi}{n+2}\right) - \frac{J_1^2}{2J_0}\left[\frac{1}{n+2}\sin^2\left(\frac{\pi}{n+2}\right) + \frac{3}{2}\right]. \tag{19}$$

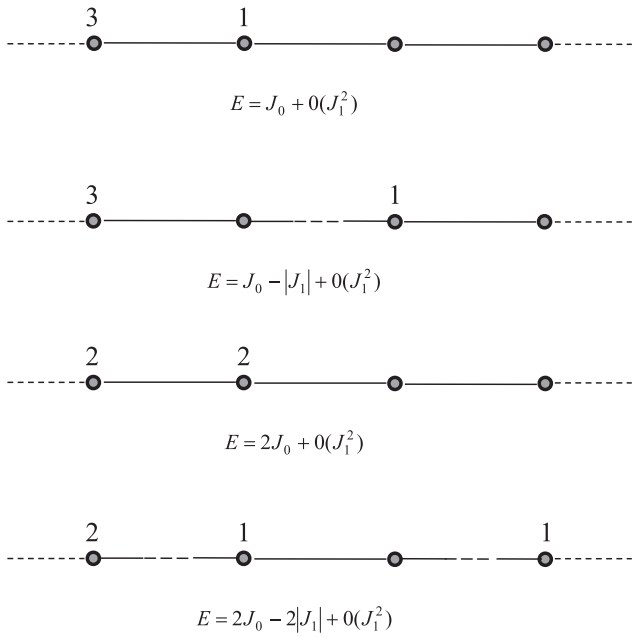

Figure 2. The inverted spin distributions and the corresponding lowest energies for the three-chain spin tube with $N_1 = 2$, $N_2 = 1$, $N_3 = 1$ in the limit of strong ferromagnetic inter-chain coupling. The dark circles correspond to the unit cells of the tube.

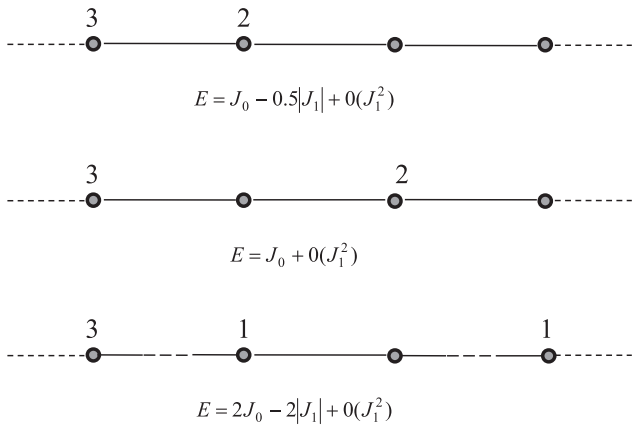

Figure 3. The inverted spin distributions and the corresponding lowest energies for the three-chain spin tube with $N_1 = 2$, $N_2 = 2$, $N_3 = 1$ in the limit of strong ferromagnetic inter-chain coupling.

To compare this energy with the sum of the lowest energies of the $(3n - 1)$-spin complex and the single three-spin complex for large n, we obtain for the bound energy ΔE the following expression:

$$\Delta E = E^0_{3n+2} - E^0_3 - E^0_{3n+1} = -|J_1|\frac{\pi^2}{n^3} + \frac{3}{4}\frac{J_1^2}{J_0}. \tag{20}$$

Obviously the $(3n+2)$-spin complex has the lowest energy in the corresponding subspace only if $\Delta E < 0$. Therefore the number n does not exceed the critical value

$$n^* = \left(\frac{4\pi^2}{3\alpha}\right)^{1/3}. \tag{21}$$

Perturbative analysis of the bound character of the lowest-energy states can be easily performed for the case of a spin tube or strip formed by $m > 3$ coupled XY chains. This leads to the simple rule that the lowest-energy state with N inverted spins has a bound character if $N = ml - 1$, with $l = 2, 3, \ldots$.

4. DMRG study of the case of ferromagnetic coupling

In order to study the lowest-energy states of the three-chain spin tube in the case of an arbitrary inter-chain coupling, we applied the standard infinite-system DMRG algorithm proposed by White [13, 14]. The number of dominant density-matrix eigenstates r that were retained at each DMRG iteration was varied from 16 to 64. The accuracy of the calculations decreased along with the increase of the total number of inverted spins N. Thus, for appropriate accuracy of the estimate of the lowest state energy for $N = 3$ and $\alpha = 0.2$ it is sufficient to retain only 16 states at each iteration. The increasing of the number of dominant states r to 64 does not change the corresponding energy estimate to five digits. Note also that the PT expansion (14) gives for this energy the estimate $-E_3^0/|J_1| = 0.165\,48$ which is close to the DMRG estimate 0.165 43. For $N > 3$ the value of r should be increased. We found that for $N \leqslant 8$, $r = 40$ provides sufficient accuracy for lowest-state-energy estimates. We also found that the accuracy of the calculations increases along with the decrease of α in the region $(0.1 < \alpha < 1)$. At $\alpha = 0.2$ the DMRG gives for the lowest energy of the state with $n = 4$ the estimate $-E_4^0/|J_1| = 3.8347$. According to (17) this energy should be equal to 3.8346. The corresponding DMRG estimate for the lowest energy of the state with six inverted spins shows that this energy is equal to double the lowest energy for $n = 3$. So, our DMRG calculations agree well with the results of PT analysis in the limit of strong ferromagnetic coupling.

We also study the dependence of the bound energy of the complexes of five and eight inverted spins on the value of α (figure 4). The results of this study show that the corresponding bound states appear only if the ferromagnetic coupling is sufficiently strong, in agreement with PT analysis. Unfortunately, we could not check the accuracy of formula (21) because of a convergence problem for big values of n.

5. Summary and conclusions

We performed analytical and numerical studies of the spectrum of the anisotropic spin lattice formed by a finite number of XY spin-$\frac{1}{2}$ chains with inter-chain interaction of Ising type. We found the conditions for the absence of the energy gap in the exact spectrum for strip-type and tube-type lattices formed by arbitrary numbers of infinite XY chains. For strong ferromagnetic inter-chain coupling we found that the lowest-energy states with non-zero numbers of inverted spins on each XY chain have n-magnon bound character if $n = ml - 1$, with $l = 2, 3, \ldots$. For the spin tube formed by three XY chains this conclusion is in a good agreement with the results of numerical simulation of lowest-energy states by means of the DMRG method. The perturbative analysis for this spin tube gives the condition at which the n-magnon bound state corresponds to the lowest energy. The DMRG study for $n = 5, 8$ also demonstrates that the lowest-energy states have bound character if the ferromagnetic inter-chain coupling exceeds some critical value.

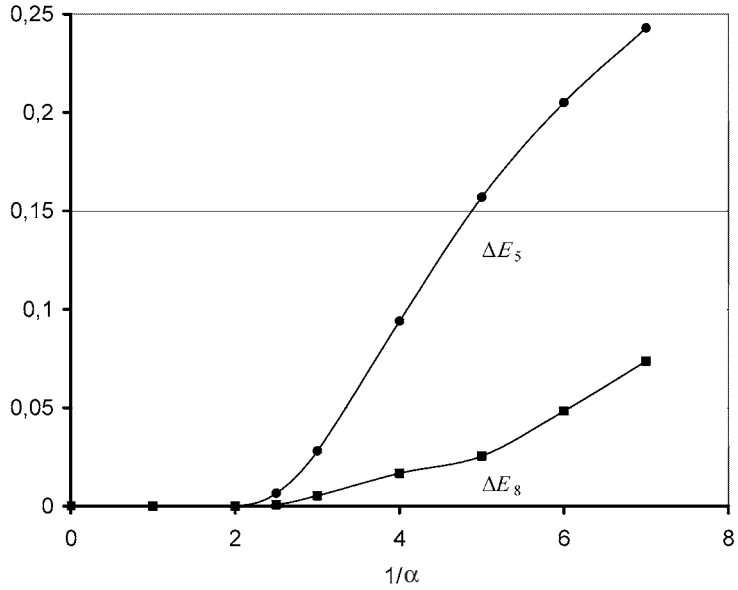

Figure 4. The bound energies for the states with five and eight inverted spins as a function of α^{-1}.

It is shown that the lowest-energy states of the spin tube formed by three chains with strong inter-chain ferromagnetic coupling are described by the XXZ spin-$\frac{1}{2}$ chain model with antiferromagnetic coupling. Therefore there is a critical value of the longitudinal magnetic field $h \sim J_1^2/J_0$ at which the transition between the states with minimal and maximal values of the z-projection of the total spin M appears.

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