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The energy spectrum of a spin-1/2 ladder with mixed interactions

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Abstract

We studied the energy spectrum of two coupled XY spin-1/2 chains with different exchange integrals and inter-chain interaction of Ising type. The thorough analytical treatment of two-magnon states was given for finite and infinite lattice strips. To study the case of macroscopic number of inverted spins we used the corresponding density matrix renormalization group (DMRG) simulation. We also derived the self-consistent Bardeen–Cooper–Schrieffer (BCS) estimates for the lowest energies of the system. The comparison of the BCS and the DMRG estimates has shown incorrect behaviour of the BCS approximation for energy as a function of the intra-chain exchange integrals. To use the analytical results for two-magnon bound states we proposed a simple approximate formula for the lowest n-magnon energies of an infinite ladder with a more correct dependence on model parameters.

1. Introduction

The investigation of the spin-1/2 ladder systems has received much interest from the theoretical and experimental points of view [1]. These systems are relevant to a number of quasi-one-dimensional compounds such as $SrCu_2O_3$ and $CuGeO_3$. A variety of theoretical techniques, both analytical and numerical, are used to study the related two-chain spin-1/2 ladder with isotropic antiferromagnetic interactions. One of the simplest anisotropic spin-1/2 one-dimensional systems is the 1D XY model. It adequately describes a number of real compounds [2–4], and simultaneously has a simple structure of the energy spectrum [5, 6]. Therefore it is of interest to consider a system of two coupled XY chains because there is relatively little information about anisotropic spin ladder systems. One such system is a ladder formed by two coupled XY spin-1/2 chains with inter-chain interaction of Ising type proposed by Shiba [7]. This model can be reduced to the 1D Hubbard model by means of Jordan–Wigner transformation, the exact spectrum of which is available via the Bethe ansatz technique [7, 8]. We will study a simple generalization of the anisotropic spin ladder system to consider the case of different intra-chain exchange integrals. Such a model may be of interest for the

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theoretical predictions of the magnetic structure of quasi-one-dimensional bimetallic molecular magnets with each unit cell containing two spins of the same spin value. We will give an analytical consideration of the two-magnon spectrum of the ladder, paying special attention to the conditions of the existence of the bound states. The Jordan–Wigner transformation in the case of different intra-chain integrals leads to the 1D Hubbard-like model with spin dependent hopping integrals and a richer structure of the excitation spectrum. Unfortunately, we were unable to obtain the exact n-magnon spectrum ($n > 2$). Therefore, we will apply a slightly modified BCS self-consistent approximation [9, 10], and the numerical DMRG infinite system method proposed by White [11]. To compare the results of these considerations we will propose a simple approximation for the lowest eigenvalues of the ladder Hamiltonian, which gives more accurate estimates in comparison with the BCS approach. We believe also that the results of our consideration of energy spectrum are of interest for the investigation of the phenomena of spin-dependent transport.

2. Some analytical results for the exact spectrum of the spin ladder with mixed interactions and related Hubbard-like model

Let us consider the double spin-1/2 chain (the ladder structure with two legs) with different constants of XY exchange interaction in the legs and Ising interaction in the rungs (figure 1). The constant magnetic field is applied along the z-axis. Bohr magnetons in XY chains are supposed to be different. The Hamiltonian of our system has the form

$$\boldsymbol{H} = -\sum_{\alpha,n} 2\mu_\alpha h S^z_{\alpha,n} - \sum_{\alpha,n} J_\alpha (S^x_{\alpha,n} S^x_{\alpha,n+1} + S^y_{\alpha,n} S^y_{\alpha,n+1}) - J_0 \sum_{n} S^z_{1,n} S^z_{2,n} \qquad \alpha = 1, 2 \quad (1)$$

where $\vec{S}_{1,n}$, $\vec{S}_{2,n}$ are spin-1/2 operators for the first and the second chains, J_1, J_2 are coupling constants along the XY chains, J_0 describes the Ising exchange interaction between the chains, h is the constant magnetic field directed along the z-axis and μ_1, μ_2 are corresponding magnetons. Let us first consider the general properties of the exact spectrum of the ladder Hamiltonian.

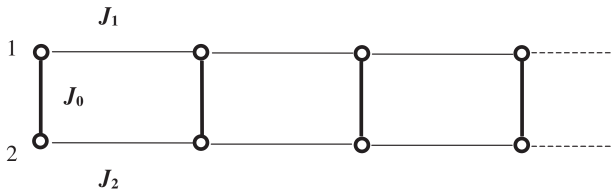

Figure 1. Two coupled XY spin-1/2 chains with different exchange integrals and inter-chain interaction of Ising type.

Since the operators, $\sum_n S^z_{\alpha,n}$, $\alpha = 1, 2$ are integrals of motion the eigenvalues of (1) can be classified according to the numbers of inverted spins N_1 and N_2 for the first and second legs of the ladder, respectively. To use the unitary transformation [5]

$$S^x_{\alpha,n} \to (-1)^n S^x_{\alpha,n} \qquad S^y_{\alpha,n} \to (-1)^n S^y_{\alpha,n} \qquad S^z_{\alpha,n} \to S^z_{\alpha,n} \quad (2)$$

we can change signs of J_α for one spin chain or for both simultaneously for a ladder with an even number of unit cells (rungs) N. Hence, the energy spectrum of (1) does not depend on signs of J_α for even N. We can choose these signs by such a way that in the space of the eigenfunctions of z-projection of total spin of the ladder all non-diagonal elements of (1) have non-positive values. On the other hand, for given values of Hamiltonian parameters h,

$J_\alpha \neq 0$, J_0, N_1 and N_2 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 and specified values of the above parameters. For the strip-type ladder (open boundary conditions) this conclusion is valid also for odd N.

In the case of $J_1 = J_2$ and open boundary conditions the lattice Hamiltonian (1) is mapped to the 1D Hubbard model by means of Jordan–Wigner transformation [7]. For $J_1 \neq J_2$ this transformation leads to the 1D Hubbard-like model with spin dependent hopping integrals:

$$\boldsymbol{H} = \boldsymbol{H}_1 - \mu_1 h(N - 2N_1) - \mu_2 h(N - 2N_2) - \frac{J_0(N - 2N_1 - 2N_2)}{4}$$
$$\boldsymbol{H}_1 = -\frac{1}{2}\left(\sum_{i=1}^{N-1} J_1 a_{i\alpha}^{+} a_{i+1\alpha} + J_2 a_{i\beta}^{+} a_{i+1\beta} + \text{h.c.}\right) - J_0 \sum_{i=1}^{N} a_{i\alpha}^{+} a_{i\alpha} a_{i\beta}^{+} a_{i\beta}. \tag{3}$$

Here the total number of particles in H_1 coincides with the number of inverted spins $(N_1 + N_2)$ in Hamiltonian (1), and the numbers of α and β particles coincide with the numbers N_1 and N_2 respectively. To apply unitary hole–particle transformation for α particles $a_{i\alpha} \rightarrow (-1)^i a_{i\alpha}^{+}$ we can easily show that, similar to ordinary 1D Hubbard model [8, 12], the energy spectrum of H_1 satisfies the following relation between positive and negative values of J_0

$$E(N_1, N_2; |J_0|) = N_1|J_0| + E(N_1, N - N_2; |J_0|). \tag{4}$$

In the strong magnetic field the ground state of (1) is 'ferromagnetic' with all spins 'upwards' $(N_1 = N_2 = 0)$. Obviously, the condition $h \geqslant \max(J_\alpha/2\mu_\alpha)$, $\alpha = 1, 2$, and $J_0 > 0$ is a sufficient condition for ferromagnetic character of the ground state. The stationary states of (1) with n inverted spins are described by the Schrödinger equation

$$(\boldsymbol{H} - E_0)|n\rangle = \varepsilon|n\rangle$$
$$|n\rangle = \sum_{m_1 \ldots m_n} A_{m_1 \ldots m_n}^{\alpha_1 \ldots \alpha_n} S_{\alpha_1 m_1 \ldots}^{-} S_{\alpha_n m_n}^{-} |0\rangle \qquad \alpha_i = 1, 2 \qquad i = 1, 2, \ldots, n \tag{5}$$

where $E_0 = -(\mu_1 + \mu_2)Nh - J_0 N/4$ is the energy of the 'ferromagnetic' state, ε is the energy of the state with n inverted spins measured from E_0, $|0\rangle$ is the vector of the ferromagnetic state and $A_{m_1 \ldots m_n}^{\alpha_1 \ldots \alpha_n}$ is the wavefunction in the lattice site representation.

If the inverted spins are located on only one of the XY chains, the corresponding eigenvalue problem (5) can be solved exactly. The Ising interaction leads only to an additive term $J_0/2$ to the energy of one-particle states of the one-dimensional XY chain

$$E = \sum_{i=1}^{n} \varepsilon_{k_i}^{\alpha} \qquad \varepsilon_k^{\alpha} = 2\mu_\alpha h + J_0/2 - J_\alpha \cos k \qquad \alpha = 1, 2 \tag{6}$$

where $k_i = \pi l_i/(N + 1)$ for the linear chains [5, 6], and $k_i = \pi(2l_i + 1)/N$, or $k_i = 2l_i\pi/N$, $l_i = 0, 1, \ldots, N - 1$ for periodic boundary conditions [13, 14] with even and odd number of excitations n, respectively (the case of periodic boundary conditions cannot be exactly reduced to the ideal Fermi gas model). It should be noted that these excitations obey the Pauli exclusion principle.

If the inverted spins are located on both chains the excitations are scattered, and the bound states can be formed due to the Ising inter-chain interaction. For the positive values of J_0 these bound states give the main contribution in low-temperature properties of the model.

Let us consider the two-magnon energy spectrum of (1) with one inverted spin on each XY chain and with the periodic boundary conditions. In this case we can introduce the total quasi-momentum of the pair of inverted spins due to the translation symmetry of the lattice and seek for a solution of (5) in the form

$$A^{12}_{m_1m_2} = \exp\left(\frac{\mathrm{i}k(m_1+m_2)}{2}\right) f_l \qquad l = m_1 - m_2 = 0, 1, \ldots, N-1$$
$$k = \frac{2\pi r}{N} \qquad r = 0, 1, \ldots, N-1. \tag{7}$$

From (5) and (7) we derive the following equation for f_l:

$$f_l[\varepsilon - 2(\mu_1+\mu_2)h - J_0] + \frac{J}{2}(\mathrm{e}^{\mathrm{i}\varphi} f_{l+1} + \mathrm{e}^{-\mathrm{i}\varphi} f_{l-1}) = 0 \qquad l \neq 0$$
$$J = (J_1^2 + J_2^2 + 2J_1J_2\cos k)^{1/2} \qquad \tan(\varphi) = \frac{J_1 - J_2}{J_1 + J_2}\tan\left(\frac{k}{2}\right) \tag{8}$$

with the boundary conditions

$$f_0[\varepsilon - 2(\mu_1+\mu_2)h] + \frac{J}{2}(\mathrm{e}^{\mathrm{i}\varphi} f_1 + \mathrm{e}^{-\mathrm{i}\varphi} f_{-1}) = 0 \tag{9}$$
$$f_l = \mathrm{e}^{\mathrm{i}kN/2} f_{l+N} \qquad l \leqslant 0 \text{ and } f_l = \mathrm{e}^{\mathrm{i}kN/2} f_{l-N} \qquad l \geqslant 0. \tag{10}$$

We will seek for the general solution of the problem (8)–(10) in the form

$$f_l = \mathrm{e}^{-\mathrm{i}\varphi l}(A_j x^l + B_j x^{-1}) \qquad j = \begin{cases} 1 & l \leqslant 0 \\ 2 & l \geqslant 0. \end{cases} \tag{11}$$

Here the parameter x satisfies the characteristic equation

$$x^{2N} - 2x^N \cos\varphi' N + 1 = 2\beta \sum_{n=1}^{N} x^{2n-1} \tag{12}$$

and $\varphi' = k/2 + \varphi$, $\beta = J_0/J$ and

$$\varepsilon = 2(\mu_1+\mu_2)h + J_0 - \frac{J}{2}\left(x + \frac{1}{x}\right). \tag{13}$$

The parameter x is to be either complex of the form $x = \mathrm{e}^{\mathrm{i}q}$, or real due to the real values of ε. In the limit $N \to \infty$ the complex values of x correspond to the continuous spectrum, and real x (it can be selected with $|x| \leqslant 1$) corresponds to bound states. For the infinite ladder we have only one boundary equation (9), and the energy of the continuous spectrum is

$$\varepsilon = 2(\mu_1+\mu_2)h + J_0 - (J_1^2 + J_2^2 + 2J_1J_2\cos k)^{1/2}\cos q$$
$$0 \leqslant k < 2\pi \qquad 0 \leqslant q < \pi \tag{14}$$

with two orthogonal wavefunctions

$$f_l^{(1)} = \begin{cases} A_1' \,\mathrm{e}^{-\mathrm{i}\varphi l}(2\beta\sin ql + \mathrm{e}^{\mathrm{i}ql}\sin q) & l \leqslant 0 \\ A_1' \,\mathrm{e}^{-\mathrm{i}\varphi l}\,\mathrm{e}^{\mathrm{i}ql}\sin q & l \geqslant 0 \end{cases}$$
$$f_l^{(2)} = \begin{cases} B_2' \,\mathrm{e}^{-\mathrm{i}\varphi l}\,\mathrm{e}^{-\mathrm{i}ql}\sin q & l \leqslant 0 \\ B_2' \,\mathrm{e}^{-\mathrm{i}\varphi l}(-2\beta\sin ql + \mathrm{e}^{-\mathrm{i}ql}\sin q) & l \geqslant 0 \end{cases} \tag{15}$$

for any given value of q.

The wavefunctions (7) can be written as

$$A^{12(1)}_{m_1m_2} = \begin{cases} A_1''[\mathrm{e}^{\mathrm{i}k_1m_1+\mathrm{i}k_2m_2}(1+\mathrm{i}a_{12}) - \mathrm{e}^{\mathrm{i}(k_2-2\varphi)m_1+\mathrm{i}(k_1+2\varphi)m_2}] & m_1 \leqslant m_2 \\ A_1''\mathrm{i}a_{12}\,\mathrm{e}^{\mathrm{i}k_1m_1+\mathrm{i}k_2m_2} & m_1 > m_2 \end{cases}$$
$$A^{12(2)}_{m_1m_2} = \begin{cases} B_2''\mathrm{i}a_{12}\,\mathrm{e}^{\mathrm{i}(k_2-2\varphi)m_1+\mathrm{i}(k_1+2\varphi)m_2} & m_1 \leqslant m_2 \\ B_2''[(1+\mathrm{i}a_{12})\,\mathrm{e}^{\mathrm{i}(k_2-2\varphi)m_1+\mathrm{i}(k_1+2\varphi)m_2} - \mathrm{e}^{\mathrm{i}k_1m_1+\mathrm{i}k_2m_2}] & m_1 > m_2 \end{cases} \tag{16}$$

where

$$k_1 = \frac{k}{2} - \varphi + q \qquad k_2 = \frac{k}{2} + \varphi - q \qquad a_{12} = \frac{\sin q}{\beta} = \frac{J_1 \sin k_1 - J_2 \sin k_2}{J_0}.$$

In terms of k_1 and k_2, the energy (14) has the form $\varepsilon = \varepsilon^1_{k_1} + \varepsilon^2_{k_2}$ with ε^α_k defined in (6), but k_1 and k_2 are not good quantum numbers. For $q = 0$ (this is equivalent to $J_1 \sin k_1 = J_2 \sin k_2$) the wavefunctions (16) are equal to zero. Thus, we have a Pauli-like exclusion principle for the continuous spectrum of two-magnon excitations.

For real x with $|x| \leqslant 1$ the wavefunction must be bounded as $l \to \pm\infty$. Therefore $A_1 = B_2 = 0$, in (11), and instead of (12) we have

$$2\beta + x - \frac{1}{x} = 0. \tag{17}$$

Thus, for the infinite ladder two-magnon bound states with energy

$$\varepsilon = 2(\mu_1 + \mu_2)h + J_0 - \left(\frac{|J_0|}{J_0}\right)(J_0^2 + J_1^2 + J_2^2 + 2J_1J_2\cos k)^{1/2} \qquad 0 \leqslant k < 2\pi \tag{18}$$

exist for any value of the Ising inter-chain interaction and for any value of total quasi-momentum k of a pair of inverted spins. For positive J_0 the local energy level (18) lies under the low boundary of the continuous spectrum (14) with the same value of k. For negative J_0 this local level has the maximal energy.

Full study of the spectrum of (1) requires some numerical estimates. Therefore, we performed the exact diagonalization of the finite systems (up to 20 unit cells). For small system sizes these estimates are subject to finite-size effects. It is therefore of interest to examine how these effects influence the results of the above analytical consideration. For finite chains of length N one can easily obtain from (12) the following inequalities for model parameters at which the bound states exist:

$$J_0 > \frac{1}{N}(J_1^2 + J_2^2 + 2J_1J_2\cos k)^{1/2}(1 - \cos\varphi' N) \tag{19}$$

and

$$|J_0| > \frac{1}{N}(J_1^2 + J_2^2 + 2J_1J_2\cos k)^{1/2}(1 - (-1)^N\cos\varphi' N) \tag{20}$$

for positive and negative J_0 respectively. In the case of $k = 0$ it is easily seen that for either positive J_0 (all N) or negative J_0 and even N the bound state exists at any value of $|J_0|$. The same result can be obtained for even N and $k = \pi$. For negative J_0 and odd N the bound state with $k = 0$ exists only if the ladder length N exceeds the critical values defined by the inequality

$$N > \frac{2(J_1 + J_2)}{|J_0|} \qquad N \text{ is odd.} \tag{21}$$

Note also that for odd N condition (19) is transformed to (20) by the substitution $k \to 2\pi - k$.

To study the case $k \neq 0, \pi$, let us consider the minimal value of $|J_0|$ at which the local energy level exists as a function of J_2/J_1. The zeros of this function correspond to the absence of restrictions for the value of J_0, and they can be found from (19) and (20) by means of simple transformations. For even N we obtain the following relation between model parameters:

$$J_2/J_1 = \frac{\sin[2\pi(r - r')/N]}{\sin[2\pi r'/N]}. \tag{22}$$

Here the integer r corresponds to the total quasi-momentum $k \neq 0, \pi$;

$$r' = \begin{cases} 1, 2, \ldots, r & 0 < r < \dfrac{N}{2} \\[2ex] r - \dfrac{N}{2}, r - \dfrac{N}{2} + 1, \ldots, \dfrac{N}{2} - 1 & \dfrac{N}{2} < r < N. \end{cases}$$

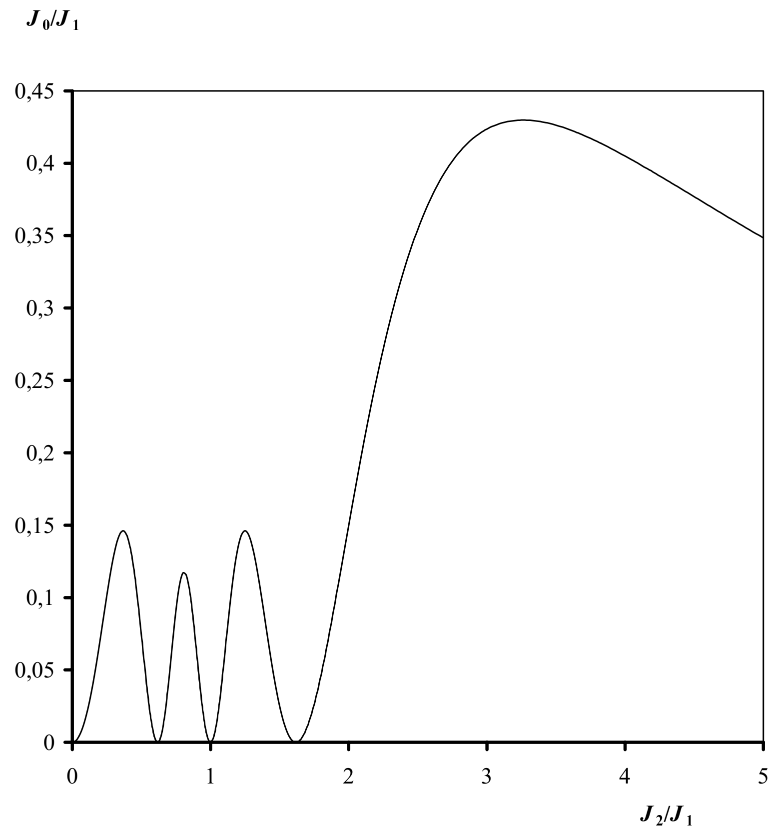

Figure 2. Dependence of critical value of J_0 on the values of J_2 for $N = 10$ and $r = 4$.

For odd N and positive J_0 we have the same formula (22) but with

$$r' = \begin{cases} 1, 2, \ldots, r & 0 < r \leqslant \dfrac{N-1}{2} \\ r - \dfrac{(N-1)}{2}, \ldots, \dfrac{(N-1)}{2} & \dfrac{N-1}{2} < r \leqslant N-1. \end{cases}$$

For odd N and negative J_0 we have

$$J_2/J_1 = \frac{\sin[\pi(2r - 2r' - 1)/N]}{\sin[\pi(2r' + 1)/N]} \tag{23}$$

where

$$r' = \begin{cases} 0, 1, 2, \ldots, r - 1 & 0 < r \leqslant \dfrac{(N-1)}{2} \\ r - \dfrac{(N+1)}{2}, \ldots, \dfrac{(N-3)}{2} & \dfrac{(N-1)}{2} < r \leqslant N-1. \end{cases}$$

In all cases for finite values J_2/J_1 the number of zeros equals r for $r < N/2$ and $N - r$ for $r > N/2$. Some numerical results of this consideration for even and odd N are depicted in figure 2 and figure 3, respectively.

In the limiting cases of a 'comb' structure ($J_1 = 0$ or $J_2 = 0$) for finite even N, the local level appears at arbitrarily small values of $|J_0|$. For odd N there are nonzero critical values of

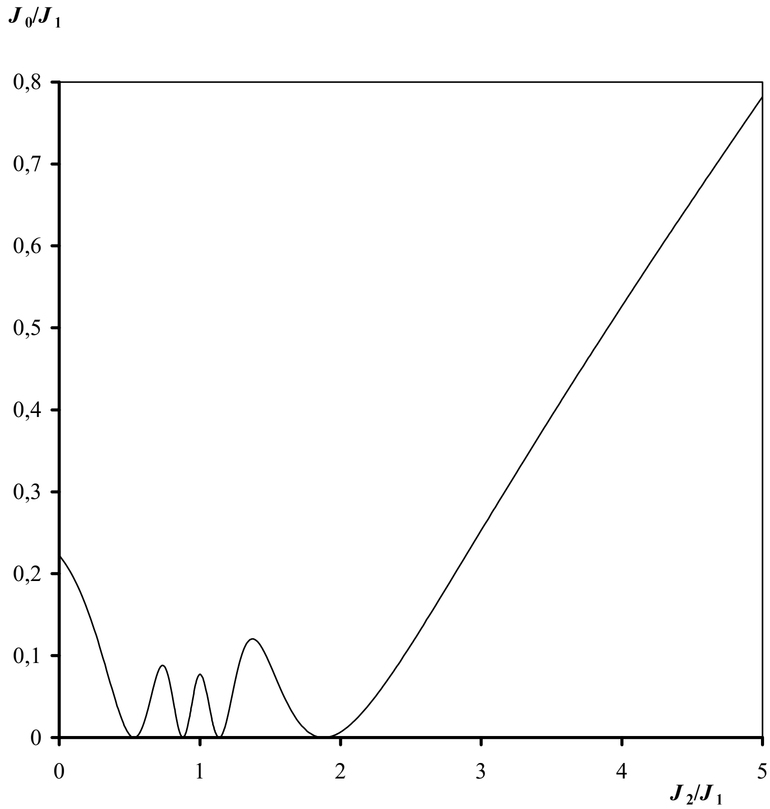

Figure 3. Dependence of critical value of J_0 on the values of J_2 for $N = 9$ and $r = 5$.

Ising interaction J_0 if k is specified by $(N+1)/2 \leqslant r \leqslant N$ for $J_0 > 0$, and $0 \leqslant r \leqslant (N-1)/2$ for $J_0 < 0$. These critical values are given by (21) with $J_1 = 0$ or $J_2 = 0$.

It should be noted that all of the above analysis for the character of the two-magnon spectrum can be easily applied to the case of N inverted spins with the distributions $N_1 = 1$, $N_2 = N - 1$ or $N_2 = 1$, $N_1 = N - 1$ if symmetry relation (4) is taken into account.

3. BCS approximation

In the general case for $N_1 + N_2 > 2$, the study of the exact spectrum of (1) cannot be performed analytically. Therefore an approximate consideration is of interest. Because of the symmetry relation (4) for the lowest energy at specified values of quantum numbers N_1 and N_2, we may restrict our consideration to the case of positive values of J_0. This corresponds to the attractive 1D Hubbard-like model. In the symmetric case ($J_1 = J_2$) the energy states of this model can be found with a good accuracy by means of the variational BCS-like approximation [9, 10]. Therefore, we will apply the same approach to the study of the spectrum of (1) with macroscopic values of N_1 and N_2. Without loss of generality let us consider only the spectrum of Hamiltonian H_1. The derivation of BCS equations for H_1 is similar to the well known symmetric case and will not be presented here. For $N \gg 1$ they are

$$1 = \frac{J_0}{2N}\sum_k \frac{1}{\sqrt{(\omega_k^2 + \Delta^2)}} \tag{24}$$

$$\frac{1}{N}\sum_k \frac{\omega_k}{\sqrt{(\omega_k^2 + \Delta^2)}} = 1 - n \tag{25}$$

$$\frac{E}{N} = -\frac{1}{N}\sum_k \sqrt{(\omega_k^2 + \Delta^2)} - \frac{n^2 J_0}{4} + \frac{\Delta^2}{J_0} + \left(\mu + \frac{nJ_0}{2}\right)(n-1) \tag{26}$$

where $\omega_k = \frac{1}{2}(J_1 + J_2)\cos(k) - \mu - nJ_0/2$, $n = (N_1 + N_2)/N$ is the density of particles in H_1 and the sums are carried out over the first Brillouin zone $(-\pi < k \leqslant \pi)$.

For given values of J_1, J_2, n and J_0 equations (25) and (26) determine the chemical potential μ and the BCS parameter Δ. It is easily seen that the BCS estimates of energy E as a function of J_1 and J_2 satisfy the relation

$$E(J_1, J_2) = E(J_1', J_2') \qquad \text{if } J_1 + J_2 = J_1' + J_2'. \tag{27}$$

In the absence of a magnetic field and sufficiently large values of J_0 the ground state of the ladder corresponds to quantum numbers $N_1 = N_2 = N/2$. In this case it can be shown that $\mu + nJ_0/2 = 0$ and for $N \to \infty$ the ground state energy per unit cell ε_0 has the form

$$\varepsilon_0 = -\frac{2}{\pi}\sqrt{I^2 + \Delta^2}\, E\left(\frac{I}{\sqrt{I^2 + \Delta^2}}\right) - \frac{J_0}{4} + \frac{\Delta^2}{J_0} \tag{28}$$

where $I = \frac{1}{2}(J_1 + J_2)$, and the BCS parameter is defined from the equation

$$K\left(\frac{I}{\sqrt{I^2 + \Delta^2}}\right) = \frac{\pi\sqrt{I^2 + \Delta^2}}{J_0}.$$

In these expressions, $K(x)$ and $E(x)$ are full elliptic integrals of the first and second kind respectively.

4. The DMRG study

In order to obtain more information about the energy spectrum of (1), we applied the standard infinite system DMRG algorithm proposed by White. For two-magnon states the results of DMRG simulations coincides with the analytical estimations with an accuracy of five digits if 16 states are kept for each of DMRG iterations. We also studied three- and four-magnon lowest energy states. For three and four inverted spins the lowest energy of the infinite system coincides with the sum of corresponding two-magnon and one-magnon solutions. For an infinite lattice strip such a coincidence is to be expected from the above analytical treatment. We also considered the case of macroscopic number of inverted spins, which corresponds to the value $S^z = 0$. In this case we kept 32–80 states, and performed up to 2000 iterations to reach convergence. The truncation error as given by the sum of density matrix eigenvalues of the discarded states was equal to 10^{-6} for the calculations with 80 states. The results of DMRG simulation showed a violation of the BCS relation (27) for the energy. Thus, after 2000 DMRG iterations with 80 states kept we obtained the value $\varepsilon_0 = -2.7911$ for $J_1 = 2.0$, $J_2 = 1.0$, $J_0 = 5.0$, and $\varepsilon_0 = -2.7882$ for $J_1 = 1.5$, $J_2 = 1.5$, $J_0 = 5.0$ (symmetric case). The exact value of ε_0 coincided with the second DMRG estimate with an accuracy of five digits (we have found this via the well known analytical formula for the ground state energy of the 1D Hubbard model [8]). According to (27) estimates of ε_0 for both sets of parameters should

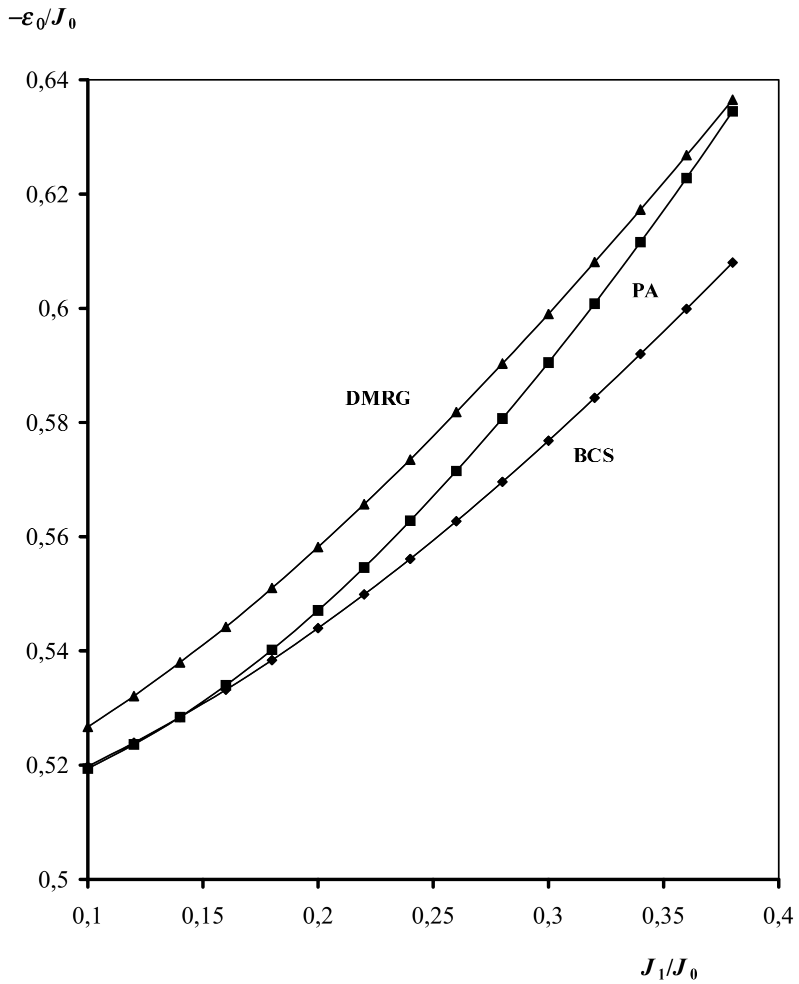

Figure 4. Lowest energies per rung of infinite ladder with $N_1 = N_2 = \frac{1}{2}N$ and $J_2 = 1$ as a function of J_1. PA is a 'pair' approximation for the energy by formula (29).

be coincident. Hence the BCS approach does not reproduce correctly the dependence of ε_0 on the values of intra-chain integrals. Since two different pair of inverted spins cannot occupy the same rung of the ladder for sufficiently large values of $|J_0|$ one half of the lowest bound two-magnon energy gives the lower bound for the exact energy per unit cell with specified values of $N_1 = N_2 = N/2$. This estimate is free from the BCS mistake. Let us suppose that we have a regular distribution of the quasi-impulses k of the pairs of inverted spins similar to the distribution of quasi-impulses for the ground state of an ordinary XY chain in the absence of a magnetic field. The corresponding estimate for the lowest energy of H_1 has the following form:

$$\varepsilon_0 = -\frac{1}{\pi}\sqrt{J_0^2 + (J_1 + J_2)^2}\, E\left(\frac{2\sqrt{J_1 J_2}}{\sqrt{J_0^2 + (J_1 + J_2)^2}}\right). \tag{29}$$

Despite the simple structure, this formula gives a more accurate estimate for the lowest energy of the state with $S^z = 0$ in comparison with the BCS approach. The corresponding energy estimates by formulae (28) and (29) and DMRG results are given in figure 4.

5. Summary and conclusion

We performed analytical and numerical studies of the excitation spectrum of the double XY spin chain with inter-chain interaction of Ising type. This model is equivalent to the generalization of the 1D Hubbard model to the case of spin dependent hopping. We found that two-magnon bound states for the infinite system exist at any value of Ising inter-chain interaction J_0 and total quasi-momentum k of the pair of inverted spins. For positive J_0 and a given k, the local level lies below the continuous spectrum. For negative J_0 it is above the continuous spectrum.

In the case of periodic boundary conditions and finite systems, which are of interest as a model of the corresponding mesoscopic rings, the conditions for the existence of two-magnon bound states have unexpectedly more complicated structure. For odd N and $k = 0$, we found that for negative J_0 there is a critical value of the chain length N at which the bound state exists. For positive J_0 (all N) and negative J_0 (even N) the bound state with $k = 0$ exists for any value of J_0. The same result was obtained for even N and $k = \pi$. In contrast, for the symmetric case $J_1 = J_2$ the bound state exists for all nonzero values of J_0.

To study n-magnon energy states we performed self-consistent BCS and DMRG calculations for an infinite ladder in the subspace $S^z = 0$. Even though the BCS approach gives a very accurate estimate of the ground state energy for the 1D Hubbard model, it does not reproduce correctly the dependence of the energy on the values of spin dependent hopping integrals. Using ideas of the above exact consideration for two-magnon bound states we derived a simple formula for an approximate estimation of the ground state energy, which is more accurate in comparison with the corresponding BCS estimate.

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