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Mixed Heisenberg chains: I. The ground-state problem

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Abstract. We consider a mechanism for competing interactions in alternating Heisenberg spin chains due to the formation of local spin-singlet pairs. The competition of spin-1 and spin-0 states reveals hidden Ising symmetry of such alternating chains.

1. Introduction

During the last few years mixed quantum spin chains have attracted some interest from theorists. Exactly solvable versions with sophisticated Hamiltonians have been studied via Bethe *ansatz* [1–3]. Very recently, numerical methods [4, 5] and matrix-product techniques [6] have been applied to these spin systems. Different kinds of alternating chain with XXZ-like interactions have been investigated by using finite-size calculations and conformal invariance [7]. The subjects of interest in this paper are alternating spin chains, in which each second site of the chain is considered as a compound, a kind of dumb-bell configuration. Two dumb-bell spins 1/2 interact with each other via the Heisenberg interaction with a coupling constant J_0, either ferromagnetically, or antiferromagnetically. Each first site of the chain is occupied (A) by a usual quantum spin (we shall consider the cases of spin $1/2, 1, 3/2, 2$), or (B) by a compound spin too (see figure 1). This spin is supposed to be antiferromagnetically coupled (coupling constant $J_1 < 0$) to the spins of the nearest dumb-bells. In spite of the short-range Heisenberg interactions, variations of J_0 may result in first-order transitions at zero temperature.

Realizations of such one-dimensional chains are shown in figure 1(a) and 1(b). The Hamiltonian in case A can be written as

$$H^{(a)} = -\mathcal{J}_1 \sum_{\langle \rho, r \rangle} \boldsymbol{s}(\rho) \cdot (\boldsymbol{\sigma}(r_1) + \boldsymbol{\sigma}(r_2)) - \mathcal{J}_0 \sum_{\langle r_1, r_2 \rangle} \boldsymbol{\sigma}(r_1) \cdot \boldsymbol{\sigma}(r_2) \tag{1}$$

whereas in case B it becomes

$$H^{(b)} = -\mathcal{J}_1 \sum_{\langle \rho, r \rangle} (\boldsymbol{s}(\rho_1) + \boldsymbol{s}(\rho_2)) \cdot (\boldsymbol{\sigma}(r_1) + \boldsymbol{\sigma}(r_2)) - \mathcal{J}_0' \sum_{\langle \rho_1, \rho_2 \rangle} \boldsymbol{s}(\rho_1) \cdot \boldsymbol{s}(\rho_2) - \mathcal{J}_0 \sum_{\langle r_1, r_2 \rangle} \boldsymbol{\sigma}(r_1) \cdot \boldsymbol{\sigma}(r_2). \tag{2}$$

Except for one special case which is described by model B, we concentrate our efforts on model A. The Hamiltonians in (1) and (2) can also be represented as follows:

$$H^{(a,b)} = H_1 + H_0^{(a,b)} \qquad H_1 = -\mathcal{J}_1 \sum_{\langle \rho, r \rangle} \boldsymbol{S}(\rho) \cdot \boldsymbol{S}(r) \tag{3}$$

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and

$$H_0^{(a)} = -\frac{1}{2}\mathcal{J}_0 \sum_r \boldsymbol{S}^2(r) \tag{4}$$

$$H_0^{(b)} = -\frac{1}{2}\mathcal{J}_0' \sum_\rho \boldsymbol{S}^2(\rho) - \frac{1}{2}\mathcal{J}_0 \sum_r \boldsymbol{S}^2(r). \tag{5}$$

When making transformations from Hamiltonians (1) and (2) to (4) and (5), we have discarded irrelevant constant terms. The coordinates of the spins in the dumb-bells, r_1 and r_2, are replaced by a single coordinate r (in model B ρ_1 and ρ_2 are also replaced by their common value ρ). Note that model B transforms into model A when $\mathcal{J}_0' \to \infty$.

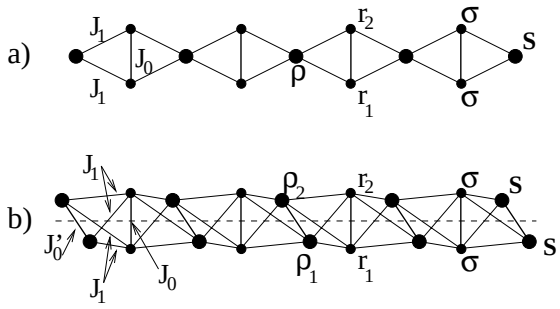

Figure 1. Shown are chain fragments of length $k = 4$. Model A: spins s $(= 1/2, 1, 3/2, 2)$ occupy sites ρ, and spins σ are arranged in dumb-bells. Model B: spins s are in dumb-bells, too, which are shown orthogonal to the σ-dumb-bells.

The two spins, $\boldsymbol{\sigma}(r_1)$ and $\boldsymbol{\sigma}(r_2)$, are incorporated into the *compound* spin: $\boldsymbol{S}(r) = \boldsymbol{\sigma}(r_1) + \boldsymbol{\sigma}(r_2)$, which is either 0, or 1. This reveals a hidden Ising symmetry of the original Heisenberg models (1) and (2). In fact, Hamiltonian H_1 does not generate any transitions between the total spin states 0 and 1 of any compound spin. Thus we can introduce spin-0 states on (some) r-sites which are a type of intrinsic 'defect'. Governed by the $\mathcal{J}_0$-terms, these 'defects' regulate a separation of the original chain into an ensemble of finite chain fragments decoupled from each other. Their structure can be defined as follows: a chain fragment of length k ($k \geqslant 1$) consists of $k+1$ spins s and k spins 1. The spins of these two groups alternate with each other. A chain fragment can be formally described as $(s, 1)^k s$. Chain fragments are isolated from each other by spins 0.

For convenience, we enumerate the lattice sites r with integer numbers, and half-integers are reserved for sites ρ.

All of the energies are suitably measured in units of $\mathcal{J}_1$ which is supposed to be negative. Thus, we set $\mathcal{J}_1 = -1$. Below we shall determine the phase diagram of the chains with $s = 1/2, 1, 3/2, 2$ depending on the parameter $\mathcal{J}_0$ in model A, and both $\mathcal{J}_0$ and $\mathcal{J}_0'$ in model B.

Our analysis includes elements of a rigorous analytical approach, a linear programming method, and numerical methods. Here we use the density matrix renormalization group (DMRG) method [8, 9] which is most appropriate to our problem.

A detailed description of the DMRG algorithm which we have used to compute ground-state energies of finite open chains can be found in appendix A. It was implemented in C++ and ran on a SUN UltraSparc 2 workstation with two 167 MHz processors and 256 Mbyte memory. In order to achieve the desired accuracy, we kept up to $N = 100$ block states

during each DMRG step. The whole project consumed about 400 hours of CPU time. No parallelization was used.

2. The ground-state problem. Model A

For convenience, we include into the definition of a chain fragment of length k a spin-0 state, say, from its right. Then a chain fragment of length k is represented by $(s,1)^k(s,0)$. This classification needs the 'empty' chain fragments to be included: any of these 'empty' fragments is spin s with spin 0, attached from its right, i.e. $(s,0)$. Conventionally, a nearest spin from the left of any chain fragment *is also* 0, but it is incorporated into the nearest-from-the-left chain fragment.

Let us suppose that we have succeeded in determining the ground-state energies of Hamiltonian H_1 for all finite chain fragments, i.e. $\{\epsilon_0, \epsilon_1, \epsilon_2, \ldots, \epsilon_k, \ldots\}$. Then, the contribution of $H_0^{(a)}$ will be $-k\mathcal{J}_0$ for the chain fragment of length k. The ground-state energy (per compound spin) of the chain, consisting of N_0 'empty' chain fragments, N_1 chain fragments of length 1, ..., and N_k chain fragments of length k, etc, is

$$\mathcal{E}_{\mathrm{g.s}} = \sum_{k\geqslant 0}(\epsilon_k - k\mathcal{J}_0)w_k. \tag{6}$$

In (6) we introduced the 'probabilities' $w_k = N_k/\mathcal{N}$, $k \geqslant 0$, with $\mathcal{N}$ being the total number of compound spins. Expressing $\mathcal{N}$ in terms of the numbers N_k of the various chain fragments is equivalent to the constraint

$$1 = \sum_{k\geqslant 0}(k+1)w_k \tag{7}$$

imposed on the set of 'probabilities'. Of course, all of the w_k are non-negative. Equations (6) and (7) constitute a linear programming problem which demands that extrema of the energy (6) should be searched for at the vertices of the polygon defined by (7). This method has been efficiently applied to the problem of competitive interactions, leading to complex modulated structures [10–13]. For this particular problem, it can be easily proven that each vertex is characterized by only one non-zero 'probability' value. For example, the vertex with $w_0 = 1$ corresponds to the perfect structure with the periodicity element $(s,0)$, its energy being $\mathcal{E} = 0$ (we denote this regular spin configuration by $\langle 0\rangle$); and $w_1 = 1/2$ (a configuration conventionally denoted by $\langle 1\rangle$) corresponds to the periodicity element $(s,1,s,0)$ with energy $\mathcal{E} = (\epsilon_1 - \mathcal{J}_0)/2$. For the $\langle k\rangle$ state, $N_k = \mathcal{N}/(k+1)$ and the periodicity element can be represented as $((s,1)^k, s, 0)$. The energy of this spin configuration is given by

$$\mathcal{E}_k = (\epsilon_k - k\mathcal{J}_0)/(k+1). \tag{8}$$

Numerical methods which are outlined in appendix A allow us to analyse characteristic first-order transitions. They happen at zero temperature and are controlled by $\mathcal{J}_0$. For $s = 1/2$ the set of energies $\{\epsilon_i\}$ is given in table 1 (left-hand column). According to the Lieb–Mattis theorem, a ferrimagnetic ground state would be realized with a total spin $k/2$, if we dealt with a periodic alternating chain, consisting of k spins 1/2 and k spins 1, coupled antiferromagnetically. In our case, a chain fragment with k spins 1 and $k+1$ spins 1/2 will exhibit the total spin $S_k = (k-1)/2$ ($k \geqslant 1$) in the ground state. Low-lying excitations are asymmetric. Their hierarchy is as follows: the lowest excitations are triplets which correspond to $\Delta S = -1$, or the total spin $(k-3)/2$ ($k \geqslant 3$). The next-lowest excitations are triplets too, but with $\Delta S = +1$ (the total spin is $(k+1)/2$). The singlet excitations are

Table 1. The ground-state energies of H_1 and the function $e_{\rm int}(k)$ for the chain fragments, consisting of k spins 1 and $k+1$ spins s, 1/2, 3/2 and 2 in three successive columns.

	$s = 1/2$		$s = 3/2$		$s = 2$	
k	ϵ_k	$e_{\rm int}(k)$	ϵ_k	$e_{\rm int}(k)$	ϵ_k	$e_{\rm int}(k)$
0	0	0.453 733	0	0.150 038	0	0.111 298
1	−2	−0.092 173	−4	0.011 951	−5	0.005 167
2	−3.381 5016	−0.019 581	−7.872 7492	0.001 114	−9.898 7531	0.000 282
3	−4.819 1715	−0.003 157	−11.735 772	0.000 003	−14.792 914	−0.000 009
4	−6.270 5355	−0.000 426	−15.597 742	−0.000 054	−19.686 790	−0.000 017
5	−7.724 2539	−0.000 051	−19.459 627	−0.000 026	−24.580 654	−0.000 012
6	−9.178 3024	−0.000 005	−23.321 522	−0.000 009	−29.474 518	−0.000 007
7	−10.632 391	0.000 000	−27.183 429	−0.000 003	−34.368 384	−0.000 004
8	−12.086 485	0.000 000	−31.045 338	0.000 000	−39.262 251	−0.000 003
9	−13.540 579	0.000 000	−34.907 251	0.000 000	−44.156 119	−0.000 002
10	−14.994 673	0.000 000	−38.769 163	0.000 000	−49.049 987	−0.000 001

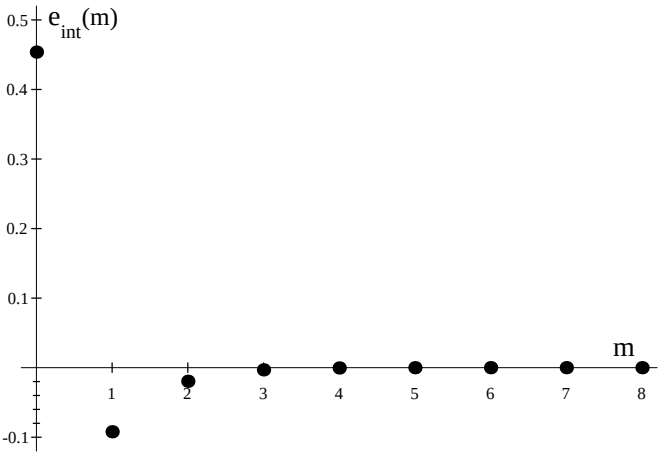

Figure 2. Shown are a few first points of $e_{\rm int}(m)$ (model A, $s = 1/2$).

lying above both triplet excitations. Only the triplet excitations with $\Delta S = -1$ will give rise to a gapless mode in the limit $k \to \infty$.

Comparison of the ground-state energy expressions (8) at various vertices clearly shows that three configurations are competitive in the global ground state: this is $\langle 0 \rangle$ for $\mathcal{J}_0 < -2$, which changes to $\langle 1 \rangle$ for $-2 < \mathcal{J}_0 < 2e_\infty + 2 \approx -0.910$. Beyond this region, i.e. for $-0.910 < \mathcal{J}_0$, the $\langle \infty \rangle$ state becomes energetically favourable. The numerical data for the set $\{\epsilon_k\}$ can be represented as

$$\epsilon_k = ke_\infty + e_0 + e_{\rm int}(k) \tag{9}$$

where $e_\infty \approx -1.454\,12$ is the energy per element $(s, 1, s)$ of the perfect periodic spin structure $\langle \infty \rangle \equiv (s, 1)^\infty$, $s = 1/2$. The energy due to the open ends is $e_0 \approx -0.453\,52$, and the remaining part, $e_{\rm int}(k)$, can be interpreted as the interaction between the chain fragment ends which apparently tends to zero for $k \to \infty$. This function $e_{\rm int}(k)$ plays an important role in establishing the succession of phase transitions. In appendix B we perform a rigorous analysis, according to which *a succession is given by a broken line*,

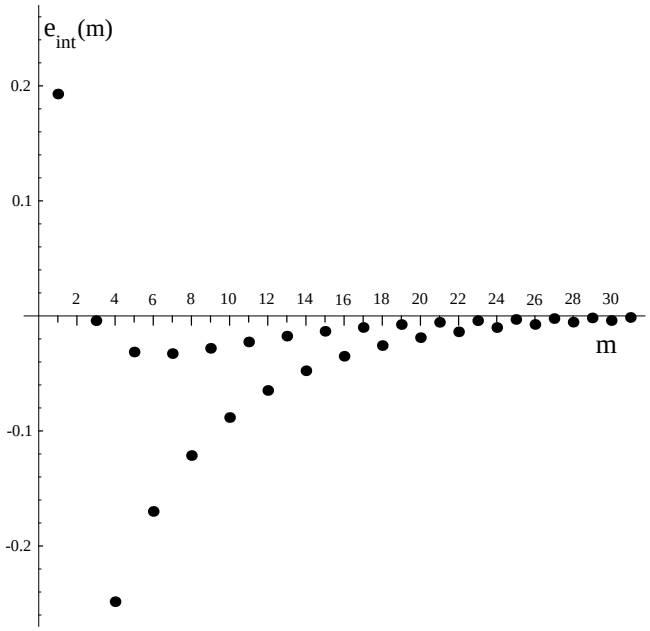

Figure 3. Shown are two subsets of $e_{\rm int}(m)$ for *m odd* and *even*. The points for $m = 2$ and $m = 0$ are situated far below at -0.4056 and -1.2086, respectively. $e_{\rm int}(2k + 1)$ of model B coincides with $e_{\rm int}(k)$ of model A.

which is concave upwards and envelops $e_{\rm int}(k)$ from below. This broken line includes the points corresponding to periodic structures with the shortest chain fragment ($k = 0$ in model A) and infinitely long chain fragments, $k \to \infty$.

For $s = 1/2$, $e_{\rm int}(k)$ is shown in figure 2. Thus, the energetically favourable configurations can be $\langle 0\rangle$, $\langle 1\rangle$ and $\langle\infty\rangle$.

For $s = 1$, the function $e_{\rm int}(k)$ is the upper curve in figure 3, related to the odd integers $m = 2k + 1$. According to appendix B we have successive phase transitions

$$\langle 0\rangle \to \langle 1\rangle \to \langle 2\rangle \to \langle 3\rangle \to \langle\infty\rangle$$

at $\mathcal{J}_0^{(0,1)} = -3$, $\mathcal{J}_0^{(1,2)} = -2.660\,425$, $\mathcal{J}_0^{(2,3)} = -2.582\,746$, and $\mathcal{J}_0^{(3,\infty)} = -2.577\,340$, which are determined from equation (8) and the data of table 2 (right-hand column). In accordance with the Lieb–Mattis theorem, the value of the spin of the ground state of a chain fragment is $S_k = 1$, independently of the length.

For $s = 3/2$, the total spin in the ground state is $S_k = (3 + k)/2$, whereas for $s = 2$, $S_k = k + 2$. A succession of phase transitions can be easily identified by making use of table 1 (middle and right-hand columns). It is the same in these two cases:

$$\langle 0\rangle \to \langle 1\rangle \to \langle 2\rangle \to \langle 3\rangle \to \langle 4\rangle \to \langle\infty\rangle.$$

The last two transitions occur at $\mathcal{J}_0^{(3,4)}$ and $\mathcal{J}_0^{(4,\infty)}$ whose values slightly differ from $\mathcal{J}_0^{(2,3)}$.

Note that a transformation $\langle 0\rangle \to \langle\infty\rangle$ via a few intermediate first-order transitions proceeds due to quantum effects. In fact, if H_1 is confined to a pure Ising form, then $e_{\rm int}(k) \equiv 0$. The system undergoes a direct transition $\langle 0\rangle \to \langle\infty\rangle$ at $\mathcal{J}_0 = -2s$. A transition point is highly degenerate: chain fragments of any length are allowed as well as any sequence of them.

Table 2. The ground-state energies of H_1 and the function $e_{\rm int}(k)$ for the chain fragments, consisting of spins 1. For model B, the data of the computations are given in the left-hand (right-hand) column for chain fragments of even (odd) total lengths, $2k$ $(2k+1)$. For model A, only the numerical data in the right-hand column should be used.

k	ϵ_{2k}	$e_{\rm int}(2k)$	ϵ_{2k+1} or ϵ_k	$e_{\rm int}(2k+1)$ or $e_{\rm int}(k)$
0	0	−1.208	0	0.193 484
1	−2	−0.405 032	−3	−0.003 548
2	−4.645 7513	−0.247 815	−5.830 2125	−0.030 792
3	−7.370 2750	−0.169 371	−8.634 5320	−0.032 144
4	−10.124 637	−0.120 765	−11.432 932	−0.027 575
5	−12.894 560	−0.087 720	−14.230 359	−0.022 035
6	−15.674 010	−0.064 202	−17.028 266	−0.016 973
7	−18.459 853	−0.047 076	−19.827 036	−0.012 775
8	−21.250 218	−0.034 473	−22.626 683	−0.009 455
9	−24.043 879	−0.025 167	−25.427 099	−0.006 902
10	−26.839 978	−0.018 298	−28.228 140	−0.004 975
11	−29.637 889	−0.013 240	−31.029 675	−0.003 542
12	−32.437 147	−0.009 530	−33.831 576	−0.002 474
13	−35.237 402	−0.006 818	−36.633 771	−0.001 701
14	−38.038 394	−0.004 842	−39.436 175	−0.001 138
15	−40.839 927	−0.003 407	−42.238 735	−0.000 730

In contrast to this, a spin-wave approach 'overestimates' quantum effects for $s \geqslant 3/2$: $e_{\rm int}(k)$ of the spin-wave approach may not differ much from the numerical data, but for $s \geqslant 3/2$ it always decays monotonically with k and thus would lead always to an infinite set of first-order transitions

$$\langle 0\rangle \to \langle 1\rangle \to \cdots \to \langle k\rangle \to \cdots \to \langle \infty\rangle.$$

Exceptional is the case of $s = 1/2$ for which the spin-wave approach exhibits a global minimum of $e_{\rm int}(k)$ at $k = 1$. This results in the same succession of transitions, $\langle 0\rangle \to \langle 1\rangle \to \langle \infty\rangle$, as obtained within the exact numerical scheme.

3. The ground-state problem. Model B

The subject of this section is model B, where σ and s are both spins 1/2; thus the equivalent model described by Hamiltonian (3) deals with chain fragments consisting of compound spins 1 only. The ground-state energies and excitations of finite spin-1 chains described by Hamiltonian H_1 have been studied by Kennedy [14] in the framework of the Lanczos method.

It is more suitable to enumerate the chain by integers, say *odd* and *even* for ρ- and r-sites, respectively. Our consideration can be restricted to $\mathcal{J}_0' \geqslant \mathcal{J}_0$. Relation (9), which can be used for spin-1 chain fragments as well, is apparently not identical for chain fragments consisting of even or odd numbers of sites. This does not concern e_∞, whose value is common to both types of chain fragment, but concerns e_0 [15] and $e_{\rm int}(k)$. The total spin in the ground state is zero or one; it depends on the length of the chain fragments, even or odd.

The linear programming method will be used again to select those chain fragments which may be candidates to form the ground state. The following four types of fragment should be taken into consideration: $(1^{2k+1}, 0)_r$, $(1^{2k+1}, 0)_\rho$, $(1^{2k}, 0)_r$, and $(1^{2k}, 0)_\rho$. We denote

their total numbers as $N^{(r)}_{2k+1}$, $N^{(\rho)}_{2k+1}$, $N^{(r)}_{2k}$, and $N^{(\rho)}_{2k}$, respectively, and the corresponding 'probabilities' as $w^{(r)}_{2k+1}$, $w^{(\rho)}_{2k+1}$, $w^{(r)}_{2k}$, and $w^{(\rho)}_{2k}$, e.g. $w^{(r)}_{2k+1} = N^{(r)}_{2k+1}/\mathcal{N}$. Here $\mathcal{N}$ is the total number of sites of both types, r and ρ. As in the prior consideration, a spin-0 state is attached from the right to any finite spin-1 chain fragment. Indices r and ρ specify the type of the rightmost site, which is occupied by spin 0. Certainly, this definition incorporates 'empty' chain fragments 0_r and 0_ρ into the scheme. Not all of the numbers N mentioned above are independent, e.g. the leftmost sites of $(1^{2k}, 0)_r$ and $(1^{2k+1}, 0)_\rho$ are both of the r-type. They evidently follow all of those chain fragments which have a rightmost site of type ρ. Thus, the following 'conservation law' holds:

$$\sum_k (N^{(r)}_{2k} + N^{(\rho)}_{2k+1}) = \sum_m N^{(\rho)}_m$$

which yields

$$\sum_k w^{(r)}_{2k} = \sum_k w^{(\rho)}_{2k}. \tag{10}$$

The total number of lattice sites $\mathcal{N}$ expressed in terms of $N^{(r)}$ and $N^{(\rho)}$ gives rise to the equation

$$1 = \sum_{k\geqslant 0} (2(2k+1)w^{(r)}_{2k} + (2k+2)(w^{(\rho)}_{2k+1} + w^{(r)}_{2k+1}) \tag{11}$$

and the energy per site is

$$\mathcal{E} = \sum_k (2(\varepsilon_{2k} - k\mathcal{J}_0' - k\mathcal{J}_0)w^{(r)}_{2k} + (\varepsilon_{2k+1} - (k+1)\mathcal{J}_0' - k\mathcal{J}_0)w^{(r)}_{2k+1} + (\varepsilon_{2k+1} - k\mathcal{J}_0' - (k+1)\mathcal{J}_0)w^{(\rho)}_{2k+1}. \tag{12}$$

In this equation we should use the energies ε_m given in table 2. Note that the set $\{\varepsilon_{2k+1}\}$ coincides with $\{\epsilon_k\}$ used in model A.

As we have assumed $\mathcal{J}_0' \geqslant \mathcal{J}_0$, the contribution of chain fragments $(1^{2k+1}, 0)_\rho$ to the energy is not competitive with the one for the $(1^{2k+1}, 0)_r$ fragments; see equation (12). Thus, in the problem of finding the ground-state energy, we must check the contribution of two sorts of vertex. The first kind is defined as $w^{(r)}_{2k} = w^{(\rho)}_{2k} = 1/(4k+2)$ with energy

$$\mathcal{E}_{2k} = \frac{1}{2k+1}(\varepsilon_{2k} - k\mathcal{J}_0' - k\mathcal{J}_0). \tag{13}$$

For the second kind we get $w^{(r)}_{2k+1} = 1/(2k+2)$ and the energy reads

$$\mathcal{E}_{2k+1} = \frac{1}{2k+2}(\varepsilon_{2k+1} - (k+1)\mathcal{J}_0' - k\mathcal{J}_0). \tag{14}$$

We shall denote the corresponding regular structures as $\langle\langle 2k\rangle\rangle$ and $\langle\langle 2k+1\rangle\rangle$ in accordance with the numbers of spin-1 sites in the chain fragments. Note that in the second case the periodicity is $2k+2$, whereas in the first case it is $4k+2$. Expressions (13) and (14) can be rewritten as

$$\mathcal{E}_m = \frac{1}{m+1}\left(\varepsilon_m - m\frac{\mathcal{J}_0' + \mathcal{J}_0}{2} - \theta_m\frac{\mathcal{J}_0' - \mathcal{J}_0}{2}\right) \tag{15}$$

where $\theta_m = 0$ or 1 for m even or odd. Except for the last term in the r.h.s., equation (15) has a form similar to equation (8).

Shown in figure 3 is $e_{\rm int}$ at $\mathcal{J}_0' = \mathcal{J}_0$. If, however, $\mathcal{J}_0' > \mathcal{J}_0$, then the subset $\{e_{\rm int}(m, \text{even})\}$ increases as compared with $\{e_{\rm int}(m, \text{odd})\}$. Having figure 3 as a prerequisite, we can describe all possible transformations as a function of $\mathcal{J}_0' - \mathcal{J}_0$.

(i) As long as $e_{\rm int}(0)$ remains below $e_{\rm int}(7)$, which is the absolute minimum of the $\{e_{\rm int}(m, \text{odd})\}$ subset, our system only undergoes the $\langle\langle 0\rangle\rangle \rightarrow \langle\langle\infty\rangle\rangle$ transition.

(ii) If $e_{\rm int}(0)$ rises above $e_{\rm int}(7)$, but remains below the continuation of the straight line connecting the points at $m = 5$ and at $m = 7$, then two transitions $\langle\langle 0\rangle\rangle \rightarrow \langle\langle 7\rangle\rangle \rightarrow \langle\langle\infty\rangle\rangle$ take place.

(iii) Next, if $e_{\rm int}(0)$ rises above the continuation of the line connecting the points at $m = 5$ and $m = 7$, but remains below the continuation of the line connecting the points at $m = 3$ and $m = 5$, then the three transitions $\langle\langle 0\rangle\rangle \rightarrow \langle\langle 5\rangle\rangle \rightarrow \langle\langle 7\rangle\rangle \rightarrow \langle\langle\infty\rangle\rangle$ take place.

(iv) The scheme can be continued.

(v) Finally, at sufficiently large $\mathcal{J}_0' - \mathcal{J}_0$, we get a maximal possible number of first-order transitions: $\langle\langle 0\rangle\rangle \rightarrow \langle\langle 1\rangle\rangle \rightarrow \langle\langle 3\rangle\rangle \rightarrow \langle\langle 5\rangle\rangle \rightarrow \langle\langle 7\rangle\rangle \rightarrow \langle\langle\infty\rangle\rangle$.

The phase diagram is shown in figure 4.

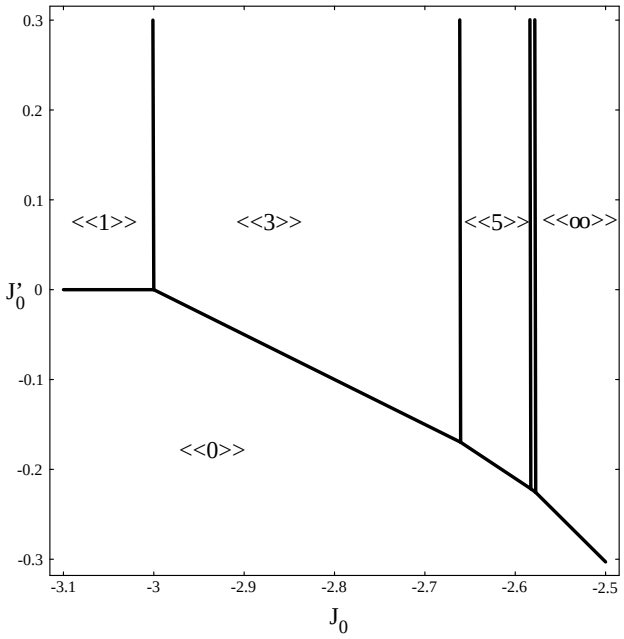

Figure 4. The phase diagram for model B is shown in the $(\mathcal{J}_0, \mathcal{J}_0')$ plane. A narrow area between $\langle\langle 5\rangle\rangle$ and $\langle\langle\infty\rangle\rangle$ belongs to the $\langle\langle 7\rangle\rangle$ phase. The line, which separates the $\langle\langle 0\rangle\rangle$ phase from the others, changes its slope from -1 through $-3/4$, $-2/3$, $-1/2$ to 0.

4. Discussion and conclusions

The model considered in this paper is probably the simplest representative of the family of Heisenberg models which possess the intrinsic property of a hidden Ising symmetry. The compound spins of our model form a regular sublattice within a one-dimensional chain: We have considered only the case of alternating chains; however, any periodicity within a system of compound spins is allowed.

We have restricted ourselves to the compound spin values 0 and 1. In principle, a more complex construction for compound spins can be used, i.e. instead of dumb-bells, three spins 1/2 may form a triangle. Then a compound spin is allowed to be 3/2 and 1/2. A treatment of

this case is more difficult, because all possible modulations in a distribution of spins 3/2 and 1/2 should be considered within the ensemble of infinite chains; there are no spin-0 breakers like in the models of this work. Another possibility would be associated with σ constituents of compound spins of a higher value than 1/2, say 1. Then, increasing $\mathcal{J}_0$ from large negative values to moderate negative ones, we could pass through a few regimes, starting from a periodic structure of elements $(s, 0)$ through a few structures whose periodicity elements are $((s, 1)^k, s, 0)$ to $(s, 1)^\infty$, then, most likely, a few intermediate structures $(s, 2)^k, s, 1$ will finally lead to a perfect $(s, 2)^\infty$ chain. However, the analysis of the phase diagram between perfect $(s, 1)^\infty$ and $(s, 2)^\infty$ structures is somewhat difficult because of the absence of spin-0 breakers.

For dealing with these more complicated systems, one could use a spin-wave approach, although it is tedious for finite systems, but well defined. We have employed this approach in order to compare our 'exact' numerical results with this approximate analytical scheme. For $s = 1/2$ these two schemes qualitatively lead to the same global minimum of $e_{\rm int}(k)$ at $k = 1$, thus exhibiting the identical succession of transitions. We have observed that for $s \geqslant 3/2$, $e_{\rm int}(k)$ is *always* a monotonically decreasing function. This means that the occurrence of a negative minimum in $e_{\rm int}(k)$ should be due to non-linear terms of a spin-wave expansion. It is clearly seen from table 1 that this minimum is extremely small ($\sim 10^{-4} e_{\rm int}(0)$) even at $s = 3/2$ or 2, but it exists and has an important influence on the succession of phase transitions versus $\mathcal{J}_0$. As this minimum occurs at $k = 4$, which is a rather short length, and thus is well controlled numerically, we are absolutely sure of the existence of the minima. The data obtained from the spin-wave approach are given in table 3. Evidently they do not differ much from our 'exact' numerical results, decreasing very rapidly with k. Exceptional is the $s = 1$ case, where $e_{\rm int}(k)$ decreases slowly, as within the 'exact' numerical scheme, although monotonically.

Table 3. The spin-wave approximation. The ground-state energies of Hamiltonian H_1 and the function $e_{\rm int}(k)$ for the chain fragments, consisting of k spins 1 and $k + 1$ spins s, 1/2, 3/2, and 2, are shown in three successive columns.

	$s = 1/2$		$s = 3/2$		$s = 2$	
k	ϵ_k	$e_{\rm int}(k)$	ϵ_k	$e_{\rm int}(k)$	ϵ_k	$e_{\rm int}(k)$
0	0	0.370 671	0	0.184 008	0	0.131 569
1	−2	−0.192 873	−4	0.012 081	−5	0.004 480
2	−3.292 8932	−0.049 311	−7.837 7223	0.002 433	−9.876 8944	0.000 497
3	−4.693 7567	−0.013 719	−11.667 585	0.000 644	−14.750 229	0.000 073
4	−6.120 3597	−0.003 866	−15.496 108	0.000 194	−19.623 201	0.000 012
5	−7.554 0280	−0.001 079	−19.324 313	0.000 063	−24.496 123	0.000 002
6	−8.989 7014	−0.000 297	−23.152 429	0.000 022	−29.369 036	0.000 001
7	−10.425 941	−0.000 081	−26.980 516	0.000 008	−34.241 947	0.000 000
8	−11.862 337	−0.000 022	−30.808 595	0.000 003	−39.114 859	0.000 000
9	−13.298 777	−0.000 006	−34.636 671	0.000 001	−43.987 770	0.000 000
10	−14.735 228	−0.000 002	−38.464 745	0.000 000	−48.860 681	0.000 000

We suppose that this important property of $e_{\rm int}(k)$ exhibiting a minimum, more and more shallow, will be valid for larger s-values, too, but we cannot say definitely whether the minimum persists at finite k-values or shifts to $k \to \infty$.

The next article in this series, which will be published elsewhere, is devoted to the thermodynamics of mixed Heisenberg chains. Certainly, all of the transitions will be smeared out due to thermal fluctuations. However, the system must show big changes

in the physical properties, such as the specific heat and the magnetic susceptibility, if $\mathcal{J}_0$ is in a transitional area. In fact, as the chain fragments of finite lengths possess total non-zero spins, which do not interact with spins of the nearest chain fragments, they form a system of paramagnetic spins. Thus, the susceptibility will exhibit a Curie-like behaviour at low temperatures. The prefactor will be temperature dependent, too, because the values of paramagnetic spins and their concentrations strongly correlate with the length distribution of the chain fragments.

We illustrate this by taking an example from the forthcoming article. Let us consider model A with $s = 1/2$ and $\mathcal{J}_0 \approx -2$, i.e. where only the chain fragments $(s, 1, s, 0)$ and $(s, 0)$ are competitive. The former is practically in a singlet state, while the latter represents a purely paramagnetic spin 1/2; their concentration in a lattice varies with T as

$$\frac{1}{2}\frac{1+\sqrt{1+4w}}{1+4w+\sqrt{1+4w}} \qquad w = \exp(\mathcal{J}_0 + 2)/T.$$

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Appendix A

To calculate the ground-state energies of the finite chain fragments $(S_1, S_2)^k S_1$ we used a slightly modified version of the well-known density matrix renormalization group (DMRG) method introduced by White [8, 9]. Here we give a brief sketch of this method.

Let us consider the following finite fragment, which consists of three spin-S_1 sites and two spin-S_2 sites:

$$\underset{i_1}{\boxed{S_1}}\ \underset{i_2}{\boxed{S_2}}\ \underset{i_3}{\boxed{S_1}}\ \underset{i_4}{\boxed{S_2}}\ \underset{i_5}{\boxed{S_1}}\ . \tag{A1}$$

Each box denotes a single-spin Hilbert space with basis states numbered with the corresponding index i_ν in the lower row. For the moment, i_1, i_3, and i_5 are identical, as are i_2 and i_4. The Hamiltonian for the chain (A1) can be divided into the following contributions:

$$\begin{aligned} H = {} & H^B_{i_1,j_1} + H^B_{i_5,j_5} + H^{S_2}_{i_2,j_2} + H^{S_2}_{i_4,j_4} + H^{S_1}_{i_3,j_3} \\ & + H^{BS_2}_{i_1 i_2,j_1 j_2} + H^{BS_2}_{i_5 i_4,j_5 j_4} + H^{S_1 S_2}_{i_3 i_2,j_3 j_2} + H^{S_1 S_2}_{i_3 i_4,j_3 j_4}. \end{aligned} \tag{A2}$$

The first five terms are on-site contributions; the others couple neighbouring sites. At this stage, H^B, H^{BS_2} are identical to H^{S_1}, $H^{S_1 S_2}$, respectively.

The first step of the algorithm now is to compute the lowest eigenvalue of the Hamiltonian (A2) and the corresponding eigenstate by using the Lanczos method. The eigenvalue is directly the ground-state energy ϵ_2 of the fragment $(S_1, S_2)^2 S_1$, and the corresponding eigenstate $\phi_{i_1 i_2 i_3 i_4 i_5}$ serves as the 'target state' of the subsequent DMRG step. From this target state we calculate the density matrix for the combined $i_1 i_2$ Hilbert space:

$$\rho_{i_1 i_2, j_1 j_2} = \sum_{i_3, i_4, i_5} \phi_{i_1 i_2 i_3 i_4 i_5} \phi_{j_1 j_2 i_3 i_4 i_5}. \tag{A3}$$

Clearly, the eigenvectors of ρ corresponding to the largest eigenvalues give the most important contributions to the target state $\phi_{i_1 i_2 i_3 i_4 i_5}$. The idea of the DMRG method is to reduce the dimension of the $i_1 i_2$ Hilbert space by projecting all of the operators onto the eigenstates of ρ belonging to the N largest eigenvalues. Let U be the rectangular matrix that contains these N normalized eigenvectors as columns [16]. This matrix U allows us to combine the Hilbert spaces i_1 and i_2 into a new single Hilbert space i_1' while limiting its dimension to at most N. All operators A acting on $i_1 i_2$ are transformed into operators A' acting on i_1' via

$$A' = UAU^{\dagger}. \tag{A4}$$

We then arrive at the situation

$$\underset{i_1'}{\boxed{S_1 S_2}} \quad \underset{i_3}{\boxed{S_1}} \quad \underset{i_5'}{\boxed{S_2 S_1}} \; . \tag{A5}$$

Note that i_5' is the reflected version of i_1'. The length of the chain can now be increased by inserting an (S_1, S_2) pair, yielding

$$\underset{i_1'}{\boxed{S_1 S_2}} \quad \underset{i_2'}{\boxed{S_1}} \quad \underset{i_3'}{\boxed{S_2}} \quad \underset{i_4'}{\boxed{S_1}} \quad \underset{i_5'}{\boxed{S_2 S_1}} \tag{A6}$$

where we have renamed i_3 as i_2'. The Hamiltonian for the chain (A6) again has the structure (A2), but with interchanged roles of S_1 and S_2, and new operators

$$\begin{aligned} H^{B}_{\text{new}} &= U\left[H^{B} \otimes 1 + 1 \otimes H^{S_2} + H^{BS_2}\right] U^{\dagger} \\ H^{BS_1}_{\text{new}} &= \sum_{\nu} (U\left[1 \otimes B^{\nu}\right] U^{\dagger}) \otimes A^{\nu} \end{aligned} \tag{A7}$$

provided that the original interaction is given by

$$H^{S_1 S_2} = \sum_{\nu} A^{\nu} \otimes B^{\nu}. \tag{A8}$$

This completes the DMRG step. The Lanczos method is now applied to the new full Hamiltonian for chain (A6); the lowest eigenvalue gives the energy ϵ_3 of the chain fragment $(S_1, S_2)^3 S_1$, and the corresponding eigenvector serves as the target state for the subsequent DMRG step.

The algorithm described above is a straightforward generalization of the standard 'infinite-system method' of White [8] to alternating symmetric spin chains. It differs from the original algorithm in two points: (1) it contains an additional spin i_3 in the centre of the chain; and (2) the role of S_1 and S_2 has to be interchanged at every DMRG step. We did not use the extended 'finite-system method', as agreement with competing pure Lanczos calculations was already satisfactory and could be systematically increased by using larger N.

Appendix B

In this appendix we show how a succession of first-order transitions takes place. We start by noting that the $\langle 0 \rangle$ structure is optimal when $\mathcal{J}_0$ has a large negative value and the $\langle \infty \rangle$ phase is realized at large positive $\mathcal{J}_0$.

Let us define the $\mathcal{J}_0$-parameter as $\mathcal{J}_0^{(m,n)}$, when two phases, $\langle m \rangle$ and $\langle n \rangle$, are at equilibrium, i.e., $\mathcal{E}_m = \mathcal{E}_n$. Then we can employ representation (9) to determine the following

equations:

$$e_\infty - \mathcal{J}_0^{(k-1,k)} - e_0 = (k+1)e_{\rm int}(k-1) - ke_{\rm int}(k) \tag{B1}$$

$$e_\infty - \mathcal{J}_0^{(k,k+1)} - e_0 = (k+2)e_{\rm int}(k) - (k+1)e_{\rm int}(k+1). \tag{B2}$$

From equations (B1) and (B2) we obtain

$$\mathcal{J}_0^{(k,k+1)} - \mathcal{J}_0^{(k-1,k)} = (k+1)(e_{\rm int}(k+1) - 2e_{\rm int}(k) + e_{\rm int}(k-1)). \tag{B3}$$

Thus, we come to the *first* conclusion: if $e_{\rm int}(k)$ is concave upwards at any k, we have a full succession of transitions: $\langle 0\rangle \to \langle 1\rangle \to \langle 2\rangle \to \cdots \to \langle\infty\rangle$.

Suppose now that the condition for $e_{\rm int}(k)$ does not hold. For instance, if for $0 < j < m$ $e_{\rm int}(k+j)$ satisfies the inequalities

$$e_{\rm int}(k+j) > e_{\rm int}(k) + \frac{j}{m}(e_{\rm int}(k+m) - e_{\rm int}(k)) \tag{B4}$$

then a generalization of equations (B1) and (B2) is

$$\mathcal{J}_0^{(k,k+j)} = e_\infty - e_0 - e_{\rm int}(k) + \frac{k+1}{j}(e_{\rm int}(k+j) - e_{\rm int}(k)). \tag{B5}$$

Taking into account inequalities (B4), one simply obtains $\mathcal{J}_0^{(k,k+j)} > \mathcal{J}_0^{(k,k+m)}$. These last inequalities show that all intermediate phases whose 'energies' $e_{\rm int}(\ell)$ are above the enveloping line cannot be realized as ground states at any value of $\mathcal{J}_0$. An important consequence is that if $e_{\rm int}$ achieves an absolute minimum at some k, this results in a direct transition $\langle k\rangle \to \langle\infty\rangle$. A convenient expression for the critical value $\mathcal{J}_0^{(k,\infty)}$ can be derived from (B5):

$$\mathcal{J}_0^{(k,\infty)} = \mathcal{J}_0^{(k-1,k)} + (k+1)(e_{\rm int}(k-1) - e_{\rm int}(k)). \tag{B6}$$

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