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The ground-state properties of the one-dimensional heterospin chain (5/2, 1/2, 1/2) with alternating exchange

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Abstract

The ground-state properties of the ferrimagnetic spin chain consisting of $(5/2, 1/2, 1/2)$ trimers with antiferromagnetic exchange between the $5/2$ and $1/2$ spins and ferromagnetic exchange between the $1/2$ and $1/2$ spins are analysed in the framework of the quantum renormalization group in real space and the matrix product method. The results are compared with a spin-wave calculation for a spin chain with two types of spin, $(5/2, 1)$. The ground-state energy, the average magnetizations and the correlation length are found as functions of the ratio between the antiferromagnetic and ferromagnetic exchange. The analysis shows that the trimer spin chain is characterized by strong quantum fluctuations reducing the average magnetizations and possesses an extremely short correlation length.

1. Introduction

In recent years the magnetic properties of a new series of molecule-based heterospin magnets with a general formula $[Mn(hfac)_2BNO_R]$ have been a subject of theoretical and experimental investigation. The magnetic properties of the compounds strongly depend on the chemical formula and spin configurations in space [1]. In these compounds the manganese ions and diradical 5-R-1, 3-bis(*N-tert*-butil-*N*-oxy-amino) benzene (BNO_R) molecules (R = H, F, Cl, Br) form one-dimensional (1D) zigzag polymeric chains. The spins of the NO groups of the diradical are ordered ferromagnetically with a large value of the energy of the exchange coupling. The exchange interaction between the 3d electrons of the divalent Mn ion and the 2p electrons of the NO group is antiferromagnetic. The 1D complex with R = H is ordered antiferromagnetically below 5.5 K due to a negative inter-chain interaction while the compounds with R = Cl, Br show ferrimagnetic order below 4.8 and 5.3 K, respectively. The compounds have three-spin periodicity along the 1D chains.

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In reference [2] it was suggested that some of these compounds can be interpreted as 1D ferrimagnetic spin-chain systems where $(1/2, 5/2, 1/2)$ trimers with intra-block antiferromagnetic $5/2$–$1/2$ exchange (J_a) interact ferromagnetically (J_f) through the $1/2$ spins of the middle nitroxide groups. However, the relationship of the ferromagnetic (J_f) and antiferromagnetic (J_a) exchange interactions in the Mn–R–Mn spin chains (R = NO) is still far from being understood [3]. In view of this, it is of interest to see how the ground-state properties of the chain depend on the ratio J_f/J_a.

Recently, mixed-spin chains with two kinds of spin coupled antiferromagnetically have attracted much interest—especially the simplest case of such chains with spins 1 and $1/2$. It has been found that the ground state which is a multiplet of spin $N/2$ (the Lieb–Mattis theorem [4]) shows elementary excitations of two distinct types. The lower branch has ferromagnetic features reducing the ground-state magnetization and has a gapless dispersion relation. The other excitations have antiferromagnetic character and are separated by a gap from the ground state which manifests itself in the thermodynamic properties. Intensive analytical and numerical studies of the simplest quantum ferrimagnetic chains have provided the possibility of carrying out a useful analysis of the ground-state properties of more complicated one-dimensional magnetic structures. In the current paper some of the analytical methods developed are applied to the 1D system Mn–R–Mn consisting of three types of spin (one spin $S_{\mathrm{Mn}} = 5/2$, and two spins $S_{\mathrm{R=NO}} = 1/2$).

2. Results and discussion

2.1. The model

We consider the model of the 1D $(5/2, 1/2, 1/2)$ spin chain presented in figure 1 and described by the Hamiltonian

$$\hat{H} = J_a \sum_n \vec{S}_{1n} \cdot \vec{S}_{2n} + J_f \sum_n \vec{S}_{2n} \cdot \vec{S}_{3n} + \frac{J_a}{2}\left(\sum_n \vec{S}_{3n} \cdot \vec{S}_{1n+1} + \sum_n \vec{S}_{3n-1} \cdot \vec{S}_{1n}\right) \tag{1}$$

where $\vec{S}_{1n}$, $\vec{S}_{2n}$ and $\vec{S}_{3n}$ are respectively spin-$\frac{5}{2}$, spin-$\frac{1}{2}$ and spin-$\frac{1}{2}$ operators on the nth elementary magnetic cell. Due to the translational invariance, the last two terms in equation (1) coincide. The exchange interaction exists only between nearest neighbours and all bonds are antiferromagnetic between $\frac{5}{2}$ and $\frac{1}{2}$ spins ($J_a > 0$) and ferromagnetic between $\frac{1}{2}$ and $\frac{1}{2}$ spins ($J_f < 0$). The present Hamiltonian can be divided up into a part corresponding to the intra-block interactions:

$$\hat{H}_B = \sum_n J_a \vec{S}_{1n} \cdot \vec{S}_{2n} + J_f \vec{S}_{2n} \cdot \vec{S}_{3n} \tag{2}$$

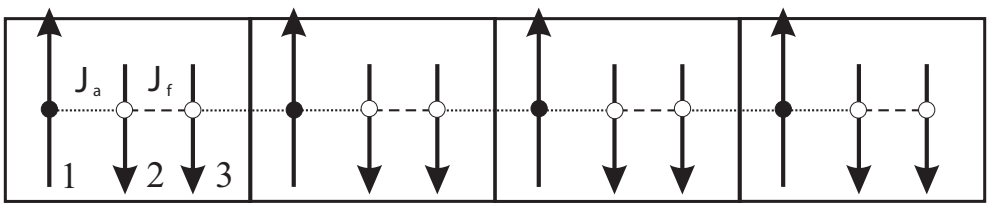


Figure 1. The Heisenberg spin chain $(5/2, 1/2, 1/2)$ with mixed exchange.

and a part corresponding to the inter-block interactions:

$$\hat{H}_{BB} = J_a \sum_n \vec{S}_{3n} \cdot \vec{S}_{1n+1}. \tag{3}$$

It is convenient to consider the states of an isolated block in the summary spin representation SM_S. The complete set of wave functions contains a quartet ($S = 3/2$), twelve states for $S = 5/2$ and eight states for $S = 7/2$. We assume that each block state $|\frac{5}{2}\frac{1}{2}\frac{1}{2}SM_S\rangle$ with spin S and its projection M_S presents a linear combination:

$$\left|\frac{5}{2}\frac{1}{2}\frac{1}{2}SM_S\right\rangle = \alpha_2^S \left|\frac{5}{2}\frac{1}{2}\frac{1}{2}(S_{13}=2)SM_S\right\rangle + \alpha_3^S \left|\frac{5}{2}\frac{1}{2}\frac{1}{2}(S_{13}=3)SM_S\right\rangle \tag{4}$$

where the coefficients α_2^S, α_3^S are estimated by diagonalization of the block energy:

$$\hat{H}_B(n) \left|\frac{5}{2}\frac{1}{2}\frac{1}{2}SM_S\right\rangle = E_S^0 \left|\frac{5}{2}\frac{1}{2}\frac{1}{2}SM_S\right\rangle. \tag{5}$$

The unitary transformation from one scheme with the addition of three angular momenta to another one is determined by the ratio which connects the states with the different intermediate couplings S_{ij} of the ith and jth spins and the same quantum numbers SM_S; for example,

$$\left|\frac{5}{2}\frac{1}{2}\frac{1}{2}(S_{13})SM_S\right\rangle = \sum_{S_{23}=0,1} (-1)^{S+5/2+S_{23}} [S_{13}, S_{23}]^{1/2} \begin{Bmatrix} 5/2 & 1/2 & S_{13} \\ 1/2 & S & S_{23} \end{Bmatrix} \left|\frac{5}{2}\frac{1}{2}\frac{1}{2}(S_{23})SM_S\right\rangle \tag{6}$$

where $\{\cdots\}$ is the $6j$-symbol and $[S] = 2S + 1$. The weight of the singlet state ($S_{23} = 0$) in the functions $|\frac{5}{2}\frac{1}{2}\frac{1}{2}SM_S\rangle$ can be easily obtained from equation (6). It equals zero for the state $S = 3/2$, with the energy $E_{3/2}^0 = -\frac{7}{4}J_a + \frac{1}{4}J_f$, $\alpha_2^{3/2} = 1$, $\alpha_3^{3/2} = 0$. For the state with $S = 5/2$, the energy is

$$E_{5/2}^0 = -\frac{1}{4}J_a - \frac{1}{4}J_f \pm \frac{1}{2}\sqrt{9J_a^2 - J_aJ_f + J_f^2}. \tag{7}$$

We take the states with the lower energy. Their coefficients

$$\alpha_2^{5/2} = \frac{\frac{\sqrt{35}}{2}(J_a - J_f)}{\sqrt{\frac{35}{4}(J_a - J_f)^2 + (7J_a - J_f - 6E_{5/2}^0)^2}} \qquad \alpha_3^{5/2} = \sqrt{1 - \left(\alpha_2^{5/2}\right)^2} \tag{8}$$

allow one to determine the weight of the singlet state:

$$\left|\alpha_0^{5/2}\right|^2 = \left(\frac{\alpha_2^{5/2}\sqrt{15} - \alpha_3^{5/2}\sqrt{21}}{6}\right)^2 \tag{9}$$

and that of the triplet one:

$$\left|\alpha_1^{5/2}\right|^2 = \left(\frac{\alpha_2^{5/2}\sqrt{21} + \alpha_3^{5/2}\sqrt{15}}{6}\right)^2. \tag{10}$$

The state $S = 7/2$ has the highest energy $E_{7/2}^0 = \frac{5}{4}J_a + \frac{1}{4}J_f$ and will be dropped in further calculations. In two opposite limits $J_a \gg |J_f|$ and $J_a \ll |J_f|$, the description of the block states is simplified. If the condition $\delta \gg 1$ ($\delta = |J_f|/J_a$) is fulfilled, the energy of the state with $S = 5/2$ is $E_{5/2}^0 \approx -\frac{1}{2}J_a + \frac{1}{4}J_f$ and the corresponding coefficients are

$$\alpha_2^{5/2} \approx \sqrt{7/12}(1 - 5/(4\delta)) \qquad \alpha_3^{5/2} \approx \sqrt{5/12}(1 + 7/(4\delta)).$$

Thus, the weight of the singlet state ($S_{23} = 0$) is negligible, $35/(16\delta^2) \ll 1$, and one can consider a spin chain $(5/2, 1)$ instead of the spin chain $(5/2, 1/2, 1/2)$ with the following Hamiltonian:

$$H = J\sum_n \vec{S}_{1n}\cdot\vec{S}_{2n} + J\sum_n \vec{S}_{2n}\cdot\vec{S}_{1n+1} \qquad (S_1 = 5/2, S_2 = 1) \tag{11}$$

where the J corresponds to the previous antiferromagnetic exchange coupling $J = J_a/2$. This fact allows us to compare the matrix product method (MPM) and real-space quantum renormalization group (QRG) results in the limit of strong ferromagnetic exchange with the SW theory of the ferrimagnetic spin chain $(5/2, 1)$. In the opposite limit, $\delta = 0$, the weight of the singlet state is $|\alpha_0^{5/2}|^2 = \frac{15}{36}$ and that of the triplet one is $|\alpha_1^{5/2}|^2 = \frac{21}{36}$.

2.2. The real-space quantum renormalization group

In reference [5] it has been shown that some important features of the physics of ferromagnetic quantum spin chains can be captured by a QRG in real space. The real-space QRG method is less complicated than the MPM, though it is based on a similar block renormalization [6]. To apply the real-space QRG technique, one divides the spin lattice into small blocks and obtains the lowest-energy states $\{|\alpha\rangle\}$ of each isolated block. The effect of inter-block interactions is then taken into account by constructing an effective Hamiltonian H^{eff} which now acts on a smaller Hilbert space embedded in the original one. In this new Hilbert space each of the former blocks is treated as a single site. We choose the $S = 3/2$ multiplet basis kets as the states to be retained in the real-space QRG procedure to find the effective low-energy Hamiltonian. The higher-energy states of the $S = 5/2$ and $S = 7/2$ multiplets are neglected. The effective Hamiltonian $H^{eff} = Q^\dagger H Q$ is constructed via the embedding operator

$$Q = \prod_{i=1}^{N} Q_i \qquad \text{with } Q_i = \sum_{\alpha=1}^{m} |\alpha\rangle\langle\alpha|$$

for each ith block where m is the number of low-energy states that are retained and N is the number of lattice cells. By using the ratios ($S_1 = \frac{5}{2}$ and $S_{2,3} = \frac{1}{2}$)

$$\left\langle \left(\frac{5}{2}\frac{1}{2}\frac{1}{2}\right)\frac{3}{2}M_S \middle| \vec{S}_1 \middle| \left(\frac{5}{2}\frac{1}{2}\frac{1}{2}\right)\frac{3}{2}M'_S \right\rangle = \frac{7}{5}\left\langle \frac{3}{2}M_S \middle| \vec{S} \middle| \frac{3}{2}M'_S \right\rangle \tag{12}$$

$$\left\langle \left(\frac{5}{2}\frac{1}{2}\frac{1}{2}\right)\frac{3}{2}M_S \middle| \vec{S}_{2,3} \middle| \left(\frac{5}{2}\frac{1}{2}\frac{1}{2}\right)\frac{3}{2}M'_S \right\rangle = -\frac{1}{5}\left\langle \frac{3}{2}M_S \middle| \vec{S} \middle| \frac{3}{2}M'_S \right\rangle \qquad (S = 3/2) \tag{13}$$

one can obtain the effective spin operators of the renormalized chain:

$$Q_i^\dagger \vec{S}_{1i} Q_i = \frac{7}{5}\vec{S}_i \qquad Q_i^\dagger \vec{S}_{2i} Q_i = -\frac{1}{5}\vec{S}_i \qquad Q_i^\dagger \vec{S}_{3i} Q_i = -\frac{1}{5}\vec{S}_i. \tag{14}$$

Equation (14) allows one to find the renormalized form of the initial Hamiltonian $H = H_B + H_{BB}$:

$$H_B^{eff} = -\frac{7}{4}J_a N + \frac{1}{4}J_f N \qquad H_{BB}^{eff} = -\frac{7}{25}J_a \sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+1} \tag{15}$$

where the spin chain is assumed to obey the periodic boundary condition. As is seen from equations (15), the effective low-energy Hamiltonian describing a trimer ferrimagnetic Heisenberg chain coincides with that of a spin-3/2 Heisenberg ferromagnet with a renormalized constant $\frac{7}{25}J_a > 0$. This is a consequence of the more general fact that a low-energy behaviour of a ferrimagnetic chain corresponds to a gapless ferromagnet. The energy per block is

$$E/N = -\frac{7}{4}J_a + \frac{1}{4}J_f - \frac{7}{25}J_a\left(\frac{3}{2}\right)^2. \tag{16}$$

In the real-space QRG theory the ground state $|0\rangle$ is replaced by $Q|0'\rangle$ where $|0'\rangle$ is the ground state of the effective Hamiltonian Hilbert space; then the average magnetization per cell for each block spin is

$$\langle S_1^z \rangle = \langle 0| \frac{1}{N} \sum_{i=1}^{N} S_{1i}^z |0\rangle = 2.1 \tag{17}$$

and

$$\langle S_2^z \rangle = \langle S_3^z \rangle = \langle 0| \frac{1}{N} \sum_{i=1}^{N} S_{2,3i}^z |0\rangle = -0.3. \tag{18}$$

The accuracy of the real-space QRG method is determined by the number of states retained. But as will be seen in the further consideration, the qualitative real-space QRG results correlate well with more precise values found in the MPM in the situation where $|J_f|/J_a \to 0$.

2.3. The matrix product method

There has recently been considerable progress in the study of the one-dimensional quantum ferrimagnetic spin chain achieved by using the matrix product (MP) states technique. In reference [7] a new version of the MP states approach to the description of quantum spin chains has been suggested. It is useful for the variational description of quantum ferrimagnetic chains whose ground state has non-zero momentum S. The rotational symmetry is spontaneously broken in the ground state, which results in a ferrimagnetic long-range order.

We use the method of constructing the matrix product states with fixed quantum numbers of the total spin and its z-projection. From the physical point of view, the construction is justified if the system has a tendency to weak ferromagnetism when the equivalence between the states $|SM_S\rangle$ and $|S - M_S\rangle$ is lost. We will suppose that the ground state of the trimer spin chain has the total spin $S = \frac{3}{2}N$. This assumption may be justified in the nearest-neighbour approximation. It is also in good agreement with magnetization measurements on the compounds in the ordered state at low temperatures [8]. Further, for consistency, the results obtained will be compared with the model of a ferrimagnetic spin chain (5/2, 1) in the limit of strong ferromagnetic exchange $\delta \gg 1$.

The matrix product ground state $|\Omega\rangle$ of the spin chain with N unit cells is defined as

$$|\Omega\rangle = \mathrm{Tr}(\hat{g}_1 \hat{g}_2 \cdots \hat{g}_N). \tag{19}$$

The elementary matrices $\hat{g}_i$ are the matrices composed from the spin states of the ith magnetic elementary cell. They can be constructed via

$$\hat{g}^{\frac{3}{2}\frac{3}{2}} = \sum_{k\lambda} C_{\frac{3}{2}}^{k\lambda} \sum_{q\mu} \begin{bmatrix} k & \lambda & \frac{3}{2} \\ q & \mu & \frac{3}{2} \end{bmatrix} \hat{X}^{kq} \left| \left(\frac{5}{2}\frac{1}{2}\frac{1}{2} \right) \lambda\mu \right\rangle \tag{20}$$

where $[\cdots]$ are the Clebsch–Gordan coefficients, $C_{3/2}^{k\lambda}$ are the variable constants. We choose the simplest case of a 2×2 matrix space which corresponds to the neglect of the states with $S = 7/2$. The basis of the matrix space consists of the matrices

$$\begin{aligned} \hat{X}^{00} &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad & \hat{X}^{10} &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ \hat{X}^{11} &= \begin{pmatrix} 0 & 0 \\ -\sqrt{2} & 0 \end{pmatrix} \qquad & \hat{X}^{1-1} &= \begin{pmatrix} 0 & \sqrt{2} \\ 0 & 0 \end{pmatrix}. \end{aligned} \tag{21}$$

Hereinafter, the notation

$$C_{\frac{3}{2}}^{0\frac{3}{2}} \equiv u \qquad C_{\frac{3}{2}}^{1\frac{3}{2}} \equiv v \qquad C_{\frac{3}{2}}^{1\frac{5}{2}} \equiv w \qquad \left| \left(\frac{5}{2}\frac{1}{2}\frac{1}{2} \right) SM_S \right\rangle \equiv |SM_S\rangle$$

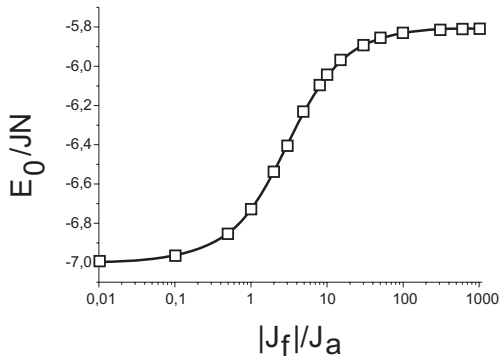
is used. Then the most general form of the elementary matrix with $S = M_S = 3/2$ is

$$\hat{g}^{\frac{3}{2}\frac{3}{2}} = \begin{pmatrix} (u - \sqrt{\frac{3}{5}}v)\left|\frac{3}{2}\frac{3}{2}\right\rangle - \frac{2}{\sqrt{15}}\omega\left|\frac{5}{2}\frac{3}{2}\right\rangle & \frac{2}{\sqrt{3}}\omega\left|\frac{5}{2}\frac{5}{2}\right\rangle \\ -\frac{2}{\sqrt{5}}v\left|\frac{3}{2}\frac{1}{2}\right\rangle - \sqrt{\frac{2}{15}}\omega\left|\frac{5}{2}\frac{1}{2}\right\rangle & (u + \sqrt{\frac{3}{5}}v)\left|\frac{3}{2}\frac{3}{2}\right\rangle + \frac{2}{\sqrt{15}}\omega\left|\frac{5}{2}\frac{3}{2}\right\rangle \end{pmatrix}. \tag{22}$$

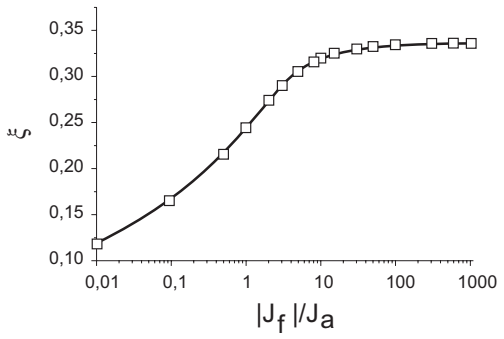
On introducing the transfer matrix $\hat{G} = (\hat{g}^{\frac{3}{2}\frac{3}{2}})^{\dagger} \otimes \hat{g}^{\frac{3}{2}\frac{3}{2}}$, the ground-state energy per block is given as

$$\frac{E_{MP}}{N} = \frac{\mathrm{Tr}(((\hat{g}_1^{\frac{3}{2}\frac{3}{2}})^{\dagger} \otimes ((J_a(\vec{S}_1 \cdot \vec{S}_2) + J_f(\vec{S}_2 \cdot \vec{S}_3))\hat{g}_1^{\frac{3}{2}\frac{3}{2}}))\hat{G}^{N-1})}{\mathrm{Tr}(\hat{G}^N)} + J_a \frac{\mathrm{Tr}(((\hat{g}_1^{\frac{3}{2}\frac{3}{2}})^{\dagger} \otimes (\vec{S}_3\hat{g}_1^{\frac{3}{2}\frac{3}{2}}))((\hat{g}_2^{\frac{3}{2}\frac{3}{2}})^{\dagger} \otimes (\vec{S}_1\hat{g}_2^{\frac{3}{2}\frac{3}{2}}))\hat{G}^{N-2})}{\mathrm{Tr}(\hat{G}^N)} \tag{23}$$

where the sign $\otimes$ means the outer matrix product. This expression includes two independent variational parameters $\tilde{v} = v/u$ and $\tilde{w} = w/u$ which are assumed to be the same throughout the chain. Its numerical minimization in the thermodynamic limit $N \to \infty$ gives $E_{MP}^{\min}$. The dependence of the ground-state energy per site on the ratio of the ferromagnetic and antiferromagnetic exchange constants is presented in figure 2(a). As is seen from the plot, the ground-state energy per block varies from the value $-5.805J$ ($|J_f|/J_a \gg 1$), which coincides with the ground-state energy per block of the $(5/2, 1)$ mixed-spin chain, up to the value $-7.0J$



(a)



(b)

Figure 2. The ground-state energy per trimer (a) and the correlation length ξ in lattice units (b) as functions of $|J_f|/J_a$.

($|J_f|/J_a \to 0$). The last value is the doubled energy of an isolated $(5/2, 1)$ block. For convenience the energy is given in units of the exchange parameter J of the Hamiltonian (11).

The values $\tilde{v}$ and $\tilde{w}$ found allow one to calculate average spin values and spin correlation functions. The quantum averages can be calculated using the transfer-matrix technique:

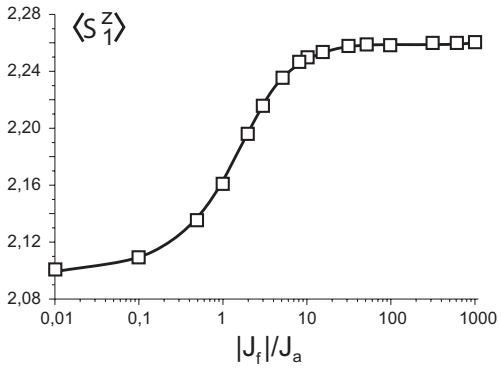
$$\left\langle S_i^z \right\rangle = \frac{\mathrm{Tr}((\hat{g}_1^{\frac{3}{2}\frac{3}{2}})^\dagger \otimes (\hat{S}_i^z \hat{g}_1^{\frac{3}{2}\frac{3}{2}})\hat{G}^{N-1})}{\mathrm{Tr}(\hat{G}^N)} \qquad i = 1, 2, 3. \tag{24}$$

The dependencies $\langle S_i^z \rangle$ on the δ-parameter are presented at figures 3(a) and 3(b). These dependencies are rather weak. It should be noted that the quantum fluctuations suppressing the average value of the sublattice magnetizations decrease with increase of δ, while the total magnetization remains constant. In the same manner one obtains

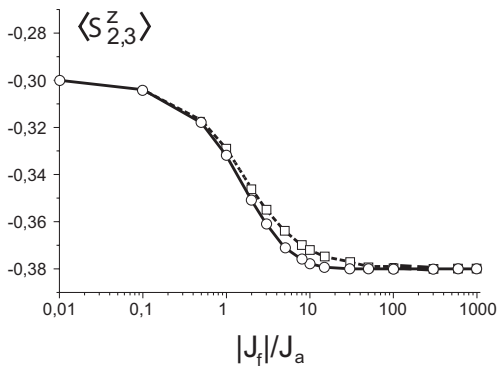
$$\left\langle S_{1i}^z S_{nj}^z \right\rangle = \frac{\mathrm{Tr}((\hat{g}_1^{\frac{3}{2}\frac{3}{2}})^\dagger \otimes (\hat{S}_i^z \hat{g}_1^{\frac{3}{2}\frac{3}{2}})\hat{G}^{n-2}(\hat{g}_n^{\frac{3}{2}\frac{3}{2}})^\dagger \otimes (\hat{S}_j^z \hat{g}_n^{\frac{3}{2}\frac{3}{2}})\hat{G}^{N-n})}{\mathrm{Tr}(\hat{G}^N)}. \tag{25}$$

For example, the correlation function for $i = j = 1$ behaves as

$$\left\langle S_{1i}^z S_{nj}^z \right\rangle = a + b \exp\left(-\frac{n}{\xi}\right) \tag{26}$$



(a)



(b)

Figure 3. The average magnetization of the Mn spin ($S = 5/2$) (a) and the nitroxide group ($s_1 = s_2 = 1/2$) $\langle S_2^z \rangle$ (circles) and $\langle S_3^z \rangle$ (squares) (b) as functions of $|J_f|/J_a$.

with the extremely short correlation length

$$\xi^{-1} = \log\left(\frac{1+\frac{3}{5}\tilde{v}^2+\frac{4}{15}\tilde{w}^2+\sqrt{\frac{12}{5}\tilde{v}^2+\frac{4}{3}\tilde{w}^2(\frac{4}{5}\tilde{v}^2+\frac{2}{15}\tilde{v}^2)}}{1+\frac{3}{5}\tilde{v}^2+\frac{4}{15}\tilde{w}^2-\sqrt{\frac{12}{5}\tilde{v}^2+\frac{4}{3}\tilde{w}^2(\frac{4}{5}\tilde{v}^2+\frac{2}{15}\tilde{v}^2)}}\right). \tag{27}$$

The dependence of the correlation length on the parameter $\delta = |J_f|/J_a$ is presented in figure 2(b). As can be seen, at $\delta \gg 1$ the correlation length is a constant: $\xi \approx 0.336$ (in lattice units); the coefficients in equation (27) are $a = \langle S_1^z \rangle^2 \approx 5.108$ and $b \approx 7.556$. The length ξ decreases as $\delta \to 0$, which corresponds to a decreasing of the triplet-state weight in the block states.

2.4. Comparison with spin-wave theory

One can compare the MP results with the results of the spin-wave theory suggested for a mixed-spin (S_1, S_2) chain when the elementary cell consists of two spins [9, 10]. The analysis of the Hamiltonian for the (5/2, 1) model equation (11) gives the ground-state energy per block:

$$\frac{E_0}{N} = -2JS_1S_2 + \frac{1}{N}\sum_k\left(-J(S_1+S_2)+J\sqrt{(S_1-S_2)^2+4S_1S_2\sin^2\left(\frac{k}{2}\right)}\right) \approx -5.899J. \tag{28}$$

The average magnetization values for the sublattices are

$$\langle S_{1n}^z \rangle = S_1 - \frac{1}{\pi}\int_0^\pi \mathrm{d}k\ \sinh^2 u_k \approx S_1 - 0.2308 \approx 2.269 \tag{29}$$

$$\langle S_{2n}^z \rangle = -S_2 + \frac{1}{\pi}\int_0^\pi \mathrm{d}k\ \sinh^2 u_k \approx -S_2 + 0.2308 \approx -0.769 \tag{30}$$

where the value of u_k is defined through the ratio

$$\tanh(2u_k) = \frac{2\sqrt{S_1S_2}}{S_1+S_2}\cos\left(\frac{k}{2}\right).$$

We also note that in the reference [11] an analogous problem has been considered using the Schwinger boson mean-field theory (SBMFT). It yields the following magnetization values: $\langle S_{1n}^z \rangle \approx 2.303$ and $\langle S_{2n}^z \rangle \approx -0.803$.

In contrast to the case for the alternating-spin chain (1, 1/2), the SW results agree very well with the MP variational results at $\delta \gg 1$ ($\tilde{v} \approx -0.754$, $\tilde{w} \approx -0.913$), both as regards the average spin values $\langle S_{1n}^z \rangle \approx 2.260$, $\langle S_{2n}^z \rangle + \langle S_{3n}^z \rangle \approx -0.760$ and as regards the ground-state energy per block $E_{MP}^{min}/N \approx -5.805J$. However, as in the previous investigations, the spin-wave correlation length

$$\xi \sim \frac{\sqrt{S_1S_2}}{S_1-S_2} \approx 1.054$$

considerably exceeds the MP result (in the SBMFT, $\xi \approx 0.641$).

3. Conclusions

The analytical consideration presented is an attempt to classify the typical properties of the ground state of the collinear trimer 1D spin chain (5/2, 1/2, 1/2) with two types of exchange interaction J_f, J_a as a function of $|J_f|/J_a$. The ground-state energy, the average magnetizations

and the correlation length are found using the real-space quantum renormalization group and matrix product methods. The results are compared with the spin-wave theory analysis for the dimer spin chain (5/2, 1) in the limit of $|J_f|/J_a \gg 1$ and they are presented in table 1. One may conclude that, in contrast to the model of the alternating-spin chain (1, 1/2), the spin-wave theory and the matrix product method give close values; however, to draw any definite conclusions as regards the consistency, further numerical investigations would be required. On the whole, it should be noted that the ground state of the trimer spin chain is characterized by strong quantum fluctuations reducing the average magnetization of spins and possesses an extremely short correlation length when there are gapless excitations. Calculations of the excitation spectrum and the thermodynamic properties within our model are in progress and the results will be reported elsewhere.

Table 1. The features of the ground state of the ferrimagnetic spin chain ($\frac{5}{2}$, 1) treated by different approaches.

	Real-space QRG	SW	MPM
$m(S = 5/2)$	2.1	2.269	2.260
$m(S = 1)$	−0.6	−0.769	−0.760
E_0/N	$-4.769J$	$-5.899J$	$-5.805J$

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