Influence of a spatial anisotropy on presence of the intermediate one-half magnetization plateau of a spin-1/2 Ising-Heisenberg branched chain*

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Abstract

A spin-1/2 Ising-Heisenberg branched chain constituted by regularly alternating Ising spins and Heisenberg dimers involving an additional side branching is exactly solved in a magnetic field by the transfer-matrix method. The spin-1/2 Ising-Heisenberg branched chain involves two different Ising and one Heisenberg coupling constants. The overall ground-state phase diagram is formed by three different ground states emergent depending on a mutual interplay between the magnetic field and three considered coupling constants: the modulated quantum antiferromagnetic phase, the quantum ferrimagnetic phase, and the classical ferromagnetic phase. It is shown that the interaction anisotropy connected to two different Ising coupling constants substantially influences a breakdown of the intermediate one-half magnetization plateau, which represents a macroscopic manifestation of the quantum ferrimagnetic phase.

Keywords: Ising-Heisenberg branched chain, magnetization plateau, interaction anisotropy

1. Introduction

Quantum Heisenberg spin chains provide an intriguing platform for an investigation of quantum magnetism using fully rigorous calculation methods being completely free of any uncontrolled approximation [1]. A few exactly solved Ising-Heisenberg and Heisenberg branched spin chains have recently attracted considerable attention, because they may exhibit striking quantum critical points of Kosterlitz-Thouless and Gaussian type [2–4]. Moreover, the Ising-Heisenberg and Heisenberg branched spin chains are not only purely theoretical models, but they are closely related to a few real-world experimental realizations from the family of polymeric coordination compounds [5, 6]. In the present work we will investigate a spin-1/2 Ising-Heisenberg branched chain whose magnetic structure is inspired by the heterobimetallic coordination polymer [(Tp)2Fe2(CN)6(OCH3)(bap)Cu2(CH2OH)-2CH3OH] (Tp=tris(pyrazolyl)hydroborate, bapH = 1,3-bis(amino)-2-propanol) to be further abbreviated as [Fe2Cu2]∞.

2. Model and method

The spin-1/2 Ising-Heisenberg branched chain, which is inspired by magnetic structure of the heterometallic coordination polymer [Fe2Cu2]∞ originally reported in
Ref. [6], can be defined through the Hamiltonian:

\[
\hat{\mathcal{H}} = \sum_{i=1}^{N} \left[ J \hat{S}_{1,i} \cdot \hat{S}_{2,i} + J_{1} \left( \hat{S}_{1,i}^{z} \sigma_{1,i}^{z} + \hat{S}_{2,i}^{z} \sigma_{1,i+1}^{z} \right) \right]
+ J_{2} \hat{S}_{1,i}^{z} \sigma_{1,i}^{z} - h \left( \hat{S}_{1,i}^{z} + \hat{S}_{2,i}^{z} + \sigma_{1,i}^{z} + \sigma_{1,i+1}^{z} \right). \tag{1}
\]

Here, $\sigma_{j}^{\alpha}$ ($\alpha = x, y, z$) are the spin-1/2 operators ascribed to the Ising and Heisenberg spins, which are schematically shown in Fig. 1 as orange and blue circles, respectively. This schematic illustration additionally involves also notation for three considered coupling constants: the coupling constant $J > 0$ stands for the antiferromagnetic Heisenberg exchange interaction within the dimeric units from a backbone of the polymeric chain, while the coupling constants $J_{1}$ and $J_{2}$ correspond to two different Ising-type exchange interactions between the nearest-neighbor Ising and Heisenberg spins. Finally, the Zeeman’s term $h$ accounts for a magnetostatic energy of the Ising and Heisenberg spins in a magnetic field, $N$ is the total number of unit cells and the periodic boundary condition $\sigma_{1,N+1} = \sigma_{1,1}$ is imposed for simplicity. For further convenience, the total Hamiltonian (1) can be rewritten as a sum of the cell Hamiltonians $\hat{\mathcal{H}} = \sum_{i=1}^{N} \hat{\mathcal{H}}_{i}$, where each cell Hamiltonian $\hat{\mathcal{H}}_{i}$ is defined by:

\[
\hat{\mathcal{H}}_{i} = J \hat{S}_{1,i} \cdot \hat{S}_{2,i} + J_{1} \left( \hat{S}_{1,i}^{z} \sigma_{1,i}^{z} + \hat{S}_{2,i}^{z} \sigma_{1,i+1}^{z} \right) + J_{2} \hat{S}_{1,i}^{z} \sigma_{1,i}^{z} - h \left( \hat{S}_{1,i}^{z} + \hat{S}_{2,i}^{z} + \sigma_{1,i}^{z} + \sigma_{1,i+1}^{z} \right). \tag{2}
\]

The cell Hamiltonians $\hat{\mathcal{H}}_{i}$ obviously commute, i.e. $[\hat{\mathcal{H}}_{i}, \hat{\mathcal{H}}_{j}] = 0$, which means that the partition function of the spin-1/2 Ising-Heisenberg branched chain can be partially factorized into the following product:

\[
Z = \sum_{\{\sigma_{1,j}\}} \prod_{j=1}^{N} \text{Tr}_{[S_{1,j},S_{2,j}]} e^{-\beta H_{i}} = \sum_{\{\sigma_{1,j}\}} \prod_{i=1}^{N} \text{Tr}(\sigma_{1,i}^{z}, \sigma_{1,i+1}^{z}),
\]

where $\beta = 1/(k_{B}T)$, $k_{B}$ is the Boltzmann’s factor, $T$ is the absolute temperature, $\text{Tr}_{[S_{1,j},S_{2,j}]}$ denotes a trace over degrees of freedom of the Heisenberg dimer from the $i$-th unit cell and $\sum_{\{\sigma_{1,j}\}}$ denotes a summation over all possible configurations of the Ising spins from a backbone of the branched chain. The expression $\text{Tr}(\sigma_{1,i}^{z}, \sigma_{1,i+1}^{z}) = \text{Tr}_{[S_{1,j},S_{2,j}]} e^{-\beta H_{i}}$ is the usual transfer matrix obtained after tracing out spin degrees of freedom of two Heisenberg spins and the Ising spin $\sigma_{2,i}$ from the $i$-th unit cell. To proceed further with the calculations, we have to calculate eigenvalues of the cell Hamiltonian (2) by performing a straightforward diagonalization in the local basis of the Heisenberg spins from the $i$-th unit cell:

\[
E_{ii,1,2} = J \pm \frac{J_{1}}{2} \left( \sigma_{1,i}^{z} + \sigma_{1,i+1}^{z} \right) + J_{2} \sigma_{1,i}^{z} \pm h_{1},
\]

\[
E_{ii,3,4} = -\frac{J}{2} \pm \frac{1}{2} \sqrt{J_{1}^{2} \left( \sigma_{1,i}^{z} + \sigma_{1,i+1}^{z} \right)^{2} + J_{2}^{2}},
\]

which should be shifted by the field term $\frac{h_{1}}{2} \left( \sigma_{1,i}^{z} + \sigma_{1,i+1}^{z} \right) - h \sigma_{2,i}^{z}$ accounting for Zeeman’s energy of the Ising spins. The corresponding eigenvectors read:

\[
\left| \phi_{1} \right\rangle = |\uparrow\rangle_{1,i} |\downarrow\rangle_{1,i+1}, \quad \left| \phi_{2} \right\rangle = |\downarrow\rangle_{1,i} |\uparrow\rangle_{1,i+1},
\]

\[
\left| \phi_{3} \right\rangle = c_{+} |\uparrow\rangle_{1,i} |\downarrow\rangle_{1,i+1} + c_{-} |\downarrow\rangle_{1,i} |\uparrow\rangle_{1,i+1}, \quad \left| \phi_{4} \right\rangle = c_{+} |\downarrow\rangle_{1,i} |\uparrow\rangle_{1,i+1} - c_{-} |\uparrow\rangle_{1,i} |\downarrow\rangle_{1,i+1},
\]

where

\[
c_{\pm} = \frac{1}{\sqrt{2}} \left[ 1 \pm \frac{J_{1}}{2} \sqrt{J_{1}^{2} \left( \sigma_{1,i}^{z} + \sigma_{1,i+1}^{z} \right)^{2} + J_{2}^{2}} \right]. \tag{4}
\]

In this way one gets an explicit expression for the transfer matrix $T(\sigma_{1,i}^{z}, \sigma_{1,i+1}^{z})$:

\[
T(\sigma_{1,i}^{z}, \sigma_{1,i+1}^{z}) = \sum_{\{\sigma_{1,j}\}} \sum_{j=1}^{4} e^{-\beta E_{j,i}} = 2 e^{-\frac{\beta}{2} \left( J_{1} (\sigma_{1,i}^{z} + \sigma_{1,i+1}^{z}) + J_{2} \sigma_{1,i}^{z} \right)}
\times \left( e^{-\frac{\beta}{2} \left( J_{1} \sigma_{1,i}^{z} + J_{1} \sigma_{1,i+1}^{z} + J_{2} \sigma_{1,i}^{z} + 2h_{1} \right)} \right)
+ e^{-\frac{\beta}{2} \left( J_{1} \sigma_{1,i}^{z} + J_{1} \sigma_{1,i+1}^{z} - J_{2} \sigma_{1,i}^{z} + 2h_{1} \right)}
+ e^{-\frac{\beta}{2} \left( J_{1} \sigma_{1,i}^{z} - J_{1} \sigma_{1,i+1}^{z} + J_{2} \sigma_{1,i}^{z} + 2h_{1} \right)}
+ e^{-\frac{\beta}{2} \left( J_{1} \sigma_{1,i}^{z} - J_{1} \sigma_{1,i+1}^{z} - J_{2} \sigma_{1,i}^{z} + 2h_{1} \right)}
\times \left( e^{-\frac{\beta}{2} \left( J_{1} \sigma_{1,i}^{z} + J_{1} \sigma_{1,i+1}^{z} + J_{2} \sigma_{1,i}^{z} + 2h_{1} \right)} \right).
\]

The partition function of the spin-1/2 Ising-Heisenberg
branched chain can be expressed in terms of two eigenvalues $\lambda_+$ and $\lambda_-$ of the transfer matrix (5):

$$Z = \sum_{(\sigma_1)} \prod_{i=1}^N T(\sigma_{1,i}^r, \sigma_{i+1}^r) = \text{Tr} T^N = \lambda_+^N + \lambda_-^N,$$

which can be written in this compact form:

$$\lambda_\pm = \frac{1}{2} \left(T_1 + T_2 \pm \sqrt{(T_1 - T_2)^2 + 4T_1T_2}\right).$$

The parameters $T_i (i = 1 - 4)$ mark four elements of two-by-two transfer matrix (5):

$$T_1 = T(+, +), \quad T_2 = T(-, -), \quad T_3 = T(+, -), \quad T_4 = T(-, +),$$

which correspond to four possible states of the Ising spins $\sigma_{1,i}^r$ and $\sigma_{i+1}^r$ (± applies for $\sigma = \pm 1/2$). In thermodynamic limit $N \to \infty$ the Gibbs free energy can be expressed through larger eigenvalue of the transfer matrix:

$$G = -k_bT \lim_{N \to \infty} \frac{1}{N} \ln Z = -k_bT \ln \lambda_+.$$

Other quantities can be subsequently derived from the Gibbs free energy (8) using standard relations.

### 3. Results and discussion

Let us begin discussion of the most interesting results by a comprehensive analysis of the ground state. It turns out that the spin-1/2 Ising-Heisenberg branched chain may exhibit just three different ground states referred to as the quantum antiferromagnetic phase (QAF):

$$|\text{QAF}\rangle = \prod_{i=1}^{N/2} \left|\left\{ \uparrow \right\} \left| \uparrow \downarrow \right\rangle \sigma_{1,i}^r \left( a_+ \uparrow \downarrow - a_- \downarrow \uparrow \right) s_{1,2\cdots 1,2\cdots 1} \sigma_{2,3}^r \left( a_+ \downarrow \uparrow - a_- \uparrow \downarrow \right) s_{1,2\cdots 2,3\cdots 1} \right\}.$$

the quantum ferrimagnetic phase (QFI):

$$|\text{QFI}\rangle = \prod_{i=1}^N \left| \left\{ \uparrow \right\} \left| \uparrow \downarrow \right\rangle \sigma_{1,i} \left( b_+ \downarrow \uparrow - b_- \uparrow \downarrow \right) s_{1,i} s_{2,i} \right\},$$

and the saturated paramagnetic phase (SPP):

$$|\text{SPP}\rangle = \prod_{i=1}^N \left| \left\{ \uparrow \right\} \left| \uparrow \downarrow \right\rangle \sigma_{1,i} \left( \uparrow \downarrow \right) s_{1,i} s_{2,i} \right\}.$$

For a shorthand notation the QAF and QFI ground states are defined through the probability amplitudes:

$$a_\pm = \frac{1}{\sqrt{2}} \left( 1 \pm \frac{J_1 + J_2}{\sqrt{(J_1 + J_2)^2 + J^2}} \right),$$

and

$$b_\pm = \frac{1}{\sqrt{2}} \left( 1 \pm \frac{J_2}{\sqrt{(J_2)^2 + J^2}} \right).$$

It is worth mentioning that the QAF ground state with translationally broken symmetry is consistent with existence of zero magnetization plateau in a zero-temperature magnetization curve due to a null total magnetization, while the QFI ground state is responsible for presence of the intermediate one-half plateau if the total magnetization is scaled with respect to its saturation value.

The ground-state phase diagrams of the spin-1/2 Ising-Heisenberg branched chain are plotted in Fig. 2 in the $J_1 / J - h / J$ plane for four selected values of the interaction anisotropy $J_2 / J_1$. It can be concluded that the ground-state phase diagrams are formed regardless of the interaction anisotropy $J_2 / J_1$ by the same three ground states.
QAF, QFI and SPP as previously reported in Ref. [4] for the isotropic case with \( J_2/J_1 = 1 \), see Fig. 2(a). The interaction anisotropy, i.e. the decline of the interaction ratio from the value \( J_2/J_1 = 1 \), merely causes an extension of the QFI ground state down to lower values of the interaction ratio \( J_1/J \). On the other hand, the QAF ground state is gradually suppressed by the interaction anisotropy (i.e. when the interaction ratio \( J_2/J_1 \) decreases) until the QAF ground state completely disappears from the phase diagram in the limit \( J_2/J_1 \to 0 \).

To verify the aforementioned behavior, a few typical isothermal magnetization curves of the spin-1/2 Ising-Heisenberg branched chain are displayed in Fig. 3 for the fixed value of the interaction anisotropy \( J_2/J_1 = 0.1 \) and three selected values of the interaction ratio \( J_1/J = 3.0, -3.0 \) and \(-6.0\), respectively. It can be seen that a relatively wide one-half plateau and narrow zero plateau can be observed by considering the antiferromagnetic Ising coupling \( J_1/J = 3.0 \) [see Fig. 3(a)], while the width of zero plateau extends and of one-half plateau shrinks by considering the ferromagnetic Ising coupling \( J_1/J = -3.0 \) [see Fig. 3(b)]. If the ferromagnetic Ising interaction is sufficiently strong one detects a mere existence of zero plateau and a full breakdown of the one-half plateau (see Fig. 3(c) for \( J_1/J = -6.0 \)). It is noteworthy that the depicted magnetization curves are in a perfect accordance with the established ground-state phase diagrams (c.f. Figs. 2 and 3), whereby the intermediate one-half plateau is absent if a relative strength of the ferromagnetic Ising coupling constant exceeds the particular value ascribed to a triple coexistence point of the QAF, QFI and SPP ground states.

4. Conclusion

In the present paper we have exactly solved using the transfer-matrix method the spin-1/2 Ising-Heisenberg branched chain with two different Ising and one Heisenberg coupling constants in a magnetic field. It has been verified that the investigated quantum spin chain may exhibit just three different ground states QAF, QFI and SPP depending on a mutual interplay between the magnetic field and three considered coupling constants. The QAF and QFI ground states with a quantum entanglement between the Heisenberg dimers are responsible for presence of intermediate zero and one-half plateaus in zero- and low-temperature magnetization curves, whereby a relative size of the intermediate magnetization plateaus depends basically on the interaction anisotropy. A full breakdown of the intermediate one-half magnetization plateau has been additionally detected for the particular case with sufficiently strong ferromagnetic Ising coupling constants.

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