Multiple frustration-induced plateaus in a magnetization process of the mixed spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ Ising-Heisenberg diamond chain

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Abstract. Magnetization process of the mixed spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ Ising-Heisenberg diamond chain is examined by combining three exact analytical techniques: Kambe projection method, decoration-iteration transformation and transfer-matrix method. Multiple frustration-induced plateaus in a magnetization process of this geometrically frustrated system are found provided that a relative ratio between the antiferromagnetic Heisenberg- and Ising-type interactions exceeds some particular value. By contrast, there is just a single magnetization plateau if the frustrating Heisenberg interaction is sufficiently small compared to the Ising one.

1. Introduction
The spin-$\frac{1}{2}$ quantum Heisenberg model on the diamond chain has enjoyed a considerable research interest since two unusual tetramer-dimer and dimer-monomer phases were theoretically predicted by Takano et al. [1] as a consequence of the mutual interplay between quantum fluctuations and geometric frustration. Another stimulus for investigating diamond chain models was triggered by a recent discovery of molecular solids Bi$_4$Cu$_3$V$_2$O$_{14}$ [2], Cu$_3$(CO$_3$)$_2$(OH)$_2$ [3], Cu$_3$(TeO$_3$)$_2$Br$_2$ [4], which represent possible experimental realizations of the diamond chain compounds. Motivated by these experiments, several phenomenological models have been suggested and solved with the aim to bring insight into a frustrated magnetism of the diamond chain compounds (see [5] and references therein). In the present work, we will develop an exact analytical treatment for the mixed spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ Ising-Heisenberg diamond chain that should clarify how the geometric frustration influences a possible magnetization scenario.

2. Model and its exact solution
Let us write the total Hamiltonian of the mixed spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ Ising-Heisenberg diamond chain as a sum over plaquette Hamiltonians $\hat{H} = \sum_k \hat{H}_k$, where each plaquette Hamiltonian $\hat{H}_k$ involves all the interaction terms included within kth diamond-shaped plaquette

$$\hat{H}_k = J_H \hat{S}_{3k-1} \cdot \hat{S}_{3k} + J_I (\hat{S}_{3k-1}^z + \hat{S}_{3k}^z)(\hat{\mu}_{3k-2}^z + \hat{\mu}_{3k+1}^z) - H_H (\hat{S}_{3k-1}^z + \hat{S}_{3k}^z) - H_I (\hat{\mu}_{3k-2}^z + \hat{\mu}_{3k+1}^z)/2. \quad (1)$$

Here, $\hat{\mu}_k^z$ and $\hat{S}_k = (\hat{S}_k^x, \hat{S}_k^y, \hat{S}_k^z)$ denote spatial components of the spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ operators, the parameter $J_H > 0$ labels the isotropic antiferromagnetic interaction between the nearest-neighbouring Heisenberg spins and the parameter $J_I > 0$ accounts for the antiferromagnetic interactions.
Ising-type interaction between the Heisenberg spins and their nearest Ising neighbours. The last two terms determine the magnetostatic Zeeman’s energy of the Ising and Heisenberg spins in an external magnetic field $H_I$ and $H_H$ oriented along the $z$-axis.

Exact solution for the aforedescribed Ising-Heisenberg diamond chain can be obtained by combining three exact analytical techniques: the Kambe projection method [6], the generalized decoration-iteration transformation [7] and the transfer-matrix method [8]. First, let us take advantage of a commutation relation between different plaquette Hamiltonians $[\hat{H}_i, \hat{H}_j] = 0$ valid for each $i \neq j$ to partially factorize the partition function

$$Z = \sum_{\{\mu_k\}} \text{Tr}(s_k) \exp(-\beta\hat{H}) = \sum_{\{\mu_k\}} \sum_{k=1}^{N} \text{Tr}_k \exp(-\beta\hat{H}_k).$$

Here, $\beta = 1/(k_BT)$ ($k_B$ is Boltzmann’s constant, $T$ is the absolute temperature), the symbols $\sum_{\{\mu_k\}}$ and $\text{Tr}(s_k)$ denote a summation over spin degrees of freedom of all Ising and Heisenberg spins, respectively. To proceed further with calculation, it is necessary to perform a trace over spin degrees of freedom of two Heisenberg spins from $k$th diamond plaquette as indicated by the symbol $\text{Tr}_k$ shown on the rhs of Eq. (2). This calculation can easily be accomplished by making use of the Kambe projection method [6], since the Hamiltonian $\hat{H}_k$ can also be viewed as the Hamiltonian of the spin-3/2 Heisenberg dimer in the effective field $H_{eff} = H_H - J_I(\mu_{3k-2} + \mu_{3k+1})$. Consequently, the complete set of eigenvalues $E_k$ corresponding to the plaquette Hamiltonian $\hat{H}_k$ can be expressed solely as a function of two quantum spin numbers $S_{tot}$ and $S_{tot}^z$.

$$E_k(S_{tot}, S_{tot}^z) = -15J_I/4 + J_HS_{tot}(S_{tot} + 1)/2 - S_{tot}^zH_{eff} - H_I(\mu_{3k-2} + \mu_{3k+1})/2,$$

which determine the total quantum spin number of the spin-3/2 Heisenberg dimer and its projection towards the $z$-axis. According to the basic laws of quantum mechanics, the total quantum spin number of the spin-3/2 dimer gains four different values $S_{tot} = 0, 1, 2, 3$, while the quantum spin number $S_{tot}^z$ gains $2S_{tot} + 1$ different values $S_{tot}^z = -S_{tot}, -S_{tot} + 1, \ldots, S_{tot}$ for each allowed value of $S_{tot}$. The energy eigenvalues (3) can be then used to obtain the relevant trace of the last expression on rhs of Eq. (2), whose explicit form immediately implies a possibility of performing the generalized decoration-iteration transformation [7]

$$\text{Tr}_k \exp(-\beta\hat{H}_k) = \exp[\beta H_I(\mu_{3k-2} + \mu_{3k+1})/2] \sum_{n=0}^{3} \sum_{m=-n}^{n} \exp[-\beta J_In(n + 1)/2] \cosh(\beta H_{eff}m)$$

$$= A \exp[\beta R \mu_{3k-2} + \mu_{3k+1}] + \beta H(\mu_{3k-2} + \mu_{3k+1})/2].$$

Note that unimportant constant term exp(15/2) has been for simplicity omitted from lhs of Eq. (4) as it does not basically change physics of the studied system. It should be mentioned, however, that the decoration-iteration transformation (4) must hold for arbitrary combination of spins states of two Ising spins $\mu_{3k-2}$ and $\mu_{3k+1}$ involved therein. This self-consistency condition unambiguously determines so far not specified mapping parameters $A$, $R$ and $H$

$$A = (W_+W_-W^2)^{1/4}, \quad R = \ln(W_+W_-) - 2\ln W, \quad H = \beta H_I - \ln W_+ + \ln W_-,$$

which can be uniquely expressed through the functions $W_\pm = F(\pm 1)$ and $W = F(0), where

$$F(x) = \sum_{n=0}^{3} \sum_{m=-n}^{n} \exp[-\beta J_In(n + 1)/2] \cosh(\beta m(J_1x + H_I)).$$

It is easy to verify that the transformation (4) establishes a precise mapping relationship between the mixed spin-1/2 and spin-3/2 Ising-Heisenberg diamond chain and its corresponding spin-1/2 Ising linear chain with the nearest-neighbour coupling $R$ and the effective magnetic field $H$.
given by Eqs. (5) and (6). A direct substitution of the mapping transformation (4) into Eq. (2) actually connects partition functions of both these models through the relation

\[ Z(\beta, J_I, J_H, H) = A^N Z_{\text{Ising}}(\beta, R, H). \] (7)

It is noteworthy that the partition function \( Z_{\text{Ising}} \) of the spin-1/2 Ising linear chain can simply be attained with the help of the transfer-matrix method (see for instance Ref. [8]) and thus, our exact calculation is formally completed. In this respect, the mapping relation (7) can also be used to obtain exact results for the Helmholtz free energy \( F = -\beta^{-1} \ln Z \) and subsequently, both the sublattice magnetization \( m_I = -\frac{1}{2N} \left( \frac{\partial F}{\partial H} \right) \) and \( m_H = -\frac{1}{N} \left( \frac{\partial F}{\partial H} \right) \).

3. Results and discussion

Now, let us step forward to a discussion of the most interesting numerical results obtained for magnetization process. Before doing so, it is useful to mention that magnetic properties of the frustrated Ising-Heisenberg diamond chain with other two particular values of the Heisenberg spins \( S = 1/2 \) and 1 have been detailed discussed in our previous work [5]. The main objective of the present work is therefore to investigate magnetization curves of the mixed spin-1/2 and spin-3/2 Ising-Heisenberg diamond chain, which should serve for the sake of comparison with the recently published results [5] and would shed light on how the scenario of magnetization process depends on a magnitude of the Heisenberg spins.

To simplify further discussion, let us first rescale all interaction parameters with respect to the Ising-type interaction \( J_I \) by introducing the following set of dimensionless parameters: \( \alpha = J_I/H, \ h = H_I/J_I = H_H/J_I \) and \( t = k_B T/J_I \) as describing a strength of the geometric frustration, external field and temperature, respectively. The total magnetization \( m = (m_I + 2m_H)/3 \) together with both sublattice magnetization \( m_I \) and \( m_H \) is plotted in Fig. 1 against the reduced magnetic field for several values of the frustration parameter \( \alpha \). As one can see, we have altogether found six different types of magnetization curves. If the frustration parameter is \( \alpha < 1/3 \) [see Fig. 1(a)], there exists just a single intermediate magnetization plateau before the magnetization tends towards its saturation value. On the other hand, two or three intermediate magnetization plateaus can be observed provided that the frustration parameter is from the interval \( 1/3 < \alpha < 1/2 \) [Fig. 1(b)] or \( \alpha > 1/2 \) [see Figs. 1(c)–(f)], respectively. It is quite obvious from this analysis that the geometric frustration can be regarded as the driving force behind appearance of the greater number of intermediate magnetization plateaus.

It is worthwhile to remark that the identified magnetization plateaus appear at 1/7, 3/7 and 5/7 of the saturation magnetization when normalizing the total magnetization with respect to its saturation value. All these fractional values are in accordance with the Oshikawa-Yamanaka-Affleck rule [9], which has been proposed as a necessary condition for the formation of quantized plateaus. As it could be readily understood from the relevant results for the sublattice magnetization, the spin arrangements emerging at intermediate plateau regions with the same value of the total magnetization might significantly differ. However, the precise nature of spin arrangements to emerge at different plateau regions requires a more comprehensive analysis of the ground-state phase diagram, which is left as a challenging task for our future work.

It should be also mentioned that the stepwise magnetization curves with an abrupt change(s) of the magnetization observable at critical fields occur merely at zero temperature, while there are no real magnetization jumps at any finite temperatures. It turns out, however, that the magnetization curve exhibits a rather rapid continuous increase in the vicinity of critical fields whenever the temperature is set sufficiently small. Contrary to this, the magnetization curves are gradually smeared out when the temperature is raised from zero and consequently, the plateau structure gradually diminishes from the magnetization curves above \( t \sim 0.4 \).

In conclusion, we have developed an exact analytical treatment that enables to study the magnetization process of the mixed spin-1/2 and spin-3/2 Ising-Heisenberg diamond chain.
Figure 1. The total magnetization $m$ (solid lines) and the sublattice magnetization $m_\parallel$ (dotted lines), $m_H$ (dashed lines) as functions of the external magnetic field at very low temperature $t = 0.01$ for several values of the frustration parameter (a) $\alpha = 0.2$, (b) $\alpha = 0.4$, (c) $\alpha = 0.8$, (d) $\alpha = 1.3$, (a) $\alpha = 1.8$, (b) $\alpha = 2.0$.

Within the framework of this exact method, we have found a rigorous evidence for multiple frustration-induced plateaus, whereas the number of intermediate plateaus basically depends on a strength of the frustration parameter $\alpha$. It is noteworthy, moreover, that the developed exact analytical treatment can be rather easily generalized to account for the magnetization scenario of the mixed spin-1/2 and spin-S Ising-Heisenberg diamond chain, which will be dealt with in our subsequent more comprehensive study.

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