Magnetic properties of a spin-1/2 Ising-Heisenberg Cairo pentagonal model

Hamid Arian Zad
Alikhanyan National Science Laboratory, Alikhanyan Br. 2, 0036 Yerevan, Armenia
E-mail: arianzad.hamid@mshdiau.ac.ir

Nerses Ananikian
Alikhanyan National Science Laboratory, Alikhanyan Br. 2, 0036 Yerevan, Armenia
CANDLE Synchrotron Research Institute, Acharyan 31, 0040 Yerevan, Armenia
E-mail: ananik@mail.yerphi.am

Abstract. In the present paper, the specific heat and magnetic property studies of a spin-1/2 Ising-Heisenberg Cairo pentagonal structure are reported. The model has been comprehensively investigated by F. C. Rodrigues et al. in Ref. [28] without external magnetic field. Here, we consider the mentioned Cairo pentagonal model in the presence of an external tunable magnetic field and examine the low-temperature magnetization process, as well as, the specific heat of the model by using the transfer matrix approach. We find that the model shows magnetization intermediate plateaus at zero and $\frac{1}{2}$ of the saturation magnetization accompanied with the growing single Schottky peak in the specific heat curve versus temperature. Each magnetization jump is in accordance with the merging of each two peaks of the specific heat curve when the magnetic field increases. This is reminiscent of the ground state phase transition from one plateau to one another. We also deduce that the magnetic field and the isotropic coupling constant considered for the dimers have substantial effects on the temperature dependence of the specific heat.

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1. Introduction

Obtaining a profound perception about interacting quantum many-body systems like low-dimensional magnetic materials with competing interactions or geometrical frustration have become an intriguing research object in a number of subjects such as condensed matter physics, material science and inorganic chemistry. In these particular areas many investigations concerned about quantum ferrimagnetic chains have been carried out, due to that they present a relevant combination of ferromagnetic and antiferromagnetic phases. As a result of zero and finite temperature phase transitions, these materials present various ground states and thermal properties [1–9].
Spin ladders can be count as attractive models among these systems. The latter consist of square-shaped topological units along the ladder [9–19].

During the past two decades it has become possible to synthesize a large variety of compounds such as $A_2Cu_3(PO_4)_3$ with $A = Ca, Sr$ [20], $Cu_3Cl_6(H_2O)_2 \cdot 2H_2SO_4$ [21, 22], the ferromagnetic diamond chains in polymeric coordination compound $Cu_3(TeO_3)_2Br_2$ [23] and the natural mineral azurite ($Cu_3(CO_3)_2(OH)_2$) [24, 25], which can be properly introduced in terms of Heisenberg spin models. Recently, A. Baniodeh et al. verified experimentally the ground state as well as low-temperature thermodynamic properties of material $[Fe_{10}Gd_{10}(Me-tea)_{10}(Me-teaH)_{10}(NO_3)_{10} \cdot 20MeCN]$ as a saw-tooth spin chain in detail [26]. Motivated by the compound $Bi_2Fe_3O_9$, in Ref. [27] M. Rojas et al. offered a general solution for the frustrated Ising model on the Cairo pentagonal lattice. Afterwards, F. C. Rodrigues et al. designed an interesting spin model for one stripe of the Cairo pentagonal Ising-Heisenberg lattice, then they investigated in detail zero-temperature phase transition and some thermodynamic parameters for such model in Ref. [28].

Quantum phase transitions have been one of the most interesting topics of strongly correlated systems during the last decade. It is basically a phase transition at zero temperature where the quantum fluctuations play the dominant role [18, 19, 29–34]. Further studies to investigate these quantum spin models have provided precise outcomes for the ground-state phase transition in the presence of an external magnetic field, which can be induced through the exchange couplings [35–38]. It is quite noteworthy that the ground state and thermodynamics of the spin ladders constituted by higher spins have been particularly examined as well [4, 37].

Magnetization curves of low-dimensional quantum ferromagnets/antiferromagnets are topical issue of current research interest, in order to they often exhibit intriguing features such as magnetization plateaus. The spin-1/2 quantum chain in a transverse magnetic field [39, 40], the spin-1/2 quantum spin ladder [18, 41], spin-1/2 Ising-Heisenberg diamond chain in a transverse magnetic field [2, 7, 8, 31–33] are a few exactly solved quantum spin models for which magnetization varies smoothly with rising absolute magnetic field until reaches its saturation magnetization. The specific heat of magnetic materials, as an applicable topic in statistical physics, has attracted much attention over the past two decades, since it usually exhibits an anomalous thermal behavior by altering other parameters of the Hamiltonian such as coupling constants, spin exchange anisotropy and magnetic field etc. Such a function can be typically approximated under a certain thermodynamic condition by the Schottky theory [9, 42]. The associated round maximum of the specific heat, the so-called Schottky peak, has been experimentally detected in various magnetic compounds [43–45].

In solid state physics and material science, most of the theoretical treatments are based on numerical techniques. Hence, an analytical approach to describe the ground state, magnetic and thermodynamic properties of the quantum spin systems such as the magnetization and specific heat, is definitely required. A promising method is the transfer-matrix formalism which has widely been applied to a number of strongly correlated systems at zero-temperature, as well as, low-temperature for studying the ground- and low-lying state properties of spin models. In the following of the analytical discussion in Ref. [28], we here investigate the magnetic and thermodynamic properties of the spin-1/2 Ising-Heisenberg Cairo pentagonal model in the presence of an external magnetic field using the transfer matrix method.

The paper is organized as follows. In Sec. 2 we describe the exactly solvable model and present the thermodynamic solution of the model with in the transfer-matrix
formalism. In Sec. 3, we numerically discuss the magnetization process and specific heat behavior of the model in the presence of an external homogeneous magnetic field. Finally, the most significant results will be summarized together in Sec. 4.

2. Model and exact solution within the transfer matrix formalism

The Hamiltonian of the spin model shown in Fig. 1 can be expressed as

\[ H = \sum_{i=1}^{N} \left( \mathcal{H}_{i,i}^{ab} + \mathcal{H}_{i,i+1}^{cd} \right) + H_z, \]

where

\[ \mathcal{H}_{i,i}^{ab} = -J(S_{a,i} \cdot S_{b,i})_\Delta - J_0(\sigma_{1,i} + \sigma_{4,i}) S_{z,i}^a - J_0(\sigma_{3,i} + \sigma_{4,i}) S_{z,i}^b, \]
\[ \mathcal{H}_{i,i+1}^{cd} = -J'(S_{c,i} \cdot S_{d,i})_\Delta' - J_0(\sigma_{3,i} + \sigma_{4,i}) S_{z,i}^c - J_0(\sigma_{1,i+1} + \sigma_{2,i+1}) S_{z,i}^d, \]
\[ H_z = -g\mu_B B_z \sum_{i=1}^{N'} \left[ S_{z,i}^a + S_{z,i}^b + S_{c,i}^z + S_{d,i}^z \right] + \sum_{\{\sigma_1,i, \sigma_2,i, \sigma_3,i, \sigma_4,i\}}. \]

where \( N' \) is the number of unit blocks. The XXZ interaction between pair spins of ab-dimer can be given by

\[ J(S_{a,i} \cdot S_{b,i})_\Delta = J(S_{a,i}^x S_{b,i}^x + S_{a,i}^y S_{b,i}^y) + \Delta S_{z,i}^a S_{z,i}^b. \]

Analogously, for the cd-dimer we have following definition

\[ J'(S_{c,i} \cdot S_{d,i})_\Delta' = J'(S_{c,i}^x S_{d,i}^x + S_{c,i}^y S_{d,i}^y) + \Delta' S_{z,i}^c S_{z,i}^d. \]

The nodal spins localized on the \( i \)-th rung are representing by the pure Ising-type exchange coupling \( J_0 \). \( 2S = \sigma \) for which \( \sigma = \{\sigma^x, \sigma^y, \sigma^z\} \) are Pauli operators (with \( \hbar = 1 \)). Final part of the Hamiltonian (1) accounts for the Zeeman's energy of magnetic moments in the external magnetic field \( B = g\mu_B B_z \).

The cornerstone of our further calculations is based on the commutation relation between different block Hamiltonians \([\mathcal{H}_i, \mathcal{H}_j] = 0\), which will allow us to characterize the partition function of the ladder under consideration and represent it as a product over block partition functions

\[ Z = \text{Tr} \left[ \prod_{i=1}^{N'} \exp \left( -\beta \left[ \mathcal{H}_{i,i}^{ab} + \mathcal{H}_{i,i+1}^{cd} + H_z \right] \right) \right], \]
where \( \mathcal{H}_z = (\mathcal{H}^{ab})^z + (\mathcal{H}^{cd})^z \) represents the Zeeman’s energy of each twodimers in the block Hamiltonian. \( \beta = \frac{1}{k_B T} \) for which \( k_B \) is the Boltzmann’s constant and \( T \) signifies the temperature. Hence, we can figure out the \( 4 \times 4 \) transfer matrix \( \mathcal{W} \) as follows

\[
\mathcal{W} = T_{ab} T_{cd} = \sum_{k=1}^{4} \exp \left[ -\beta \mathcal{E}_k (\sigma_{1,i} \sigma_{2,i} \sigma_{3,i} \sigma_{4,i}) \right] \times \sum_{k=1}^{4} \exp \left[ -\beta \mathcal{E}_k (\sigma_{3,i} \sigma_{4,i} \sigma_{1,i+1} \sigma_{2,i+1}) \right].
\]

(6)

\( \mathcal{E}_k \) denotes eigenvalues of the Hamiltonian \( \mathcal{H}^{ab} + (\mathcal{H}^{cd})^z \) and can be given by

\[
\mathcal{E}_{1,2} = -\Delta \pm \frac{1}{2} \sqrt{(2B + J(\sigma_{1,i} + \sigma_{2,i} + \sigma_{3,i} + \sigma_{4,i}))}.
\]

\[
\mathcal{E}_{3,4} = \frac{\Delta}{2} \pm \frac{1}{2} \sqrt{J_0^2 (\sigma_{1,i} + \sigma_{2,i} - \sigma_{3,i} - \sigma_{4,i})^2 + J^2}.
\]

(7)

Analogously, the corresponding eigenenergies for cd-dimer are given by

\[
\tilde{\mathcal{E}}_{1,2} = -\Delta' \pm \frac{1}{2} \sqrt{(2B + J'(\sigma_{1,i+1} + \sigma_{2,i+1} + \sigma_{3,i+1} + \sigma_{4,i}))}.
\]

\[
\tilde{\mathcal{E}}_{3,4} = \frac{\Delta'}{2} \pm \frac{1}{2} \sqrt{J_0^2 (\sigma_{1,i+1} + \sigma_{2,i+1} - \sigma_{3,i} - \sigma_{4,i})^2 + J'^2}.
\]

(8)

Since we seek eigenvalues of the transfer matrix \( \mathcal{W} \) in the thermodynamic limit \( N \to \infty \), the largest eigenvalue \( \Lambda_{\text{max}} \) has the most effect on the thermodynamic properties of the system, whereas other three smaller eigenvalues are almost effectless and their contribution can be completely neglected. Hence, the free energy per block can be obtained from the largest eigenvalue of the transfer matrix \( \mathcal{W} \) as

\[
f = -\frac{1}{\beta} \lim_{N \to \infty} \ln \frac{1}{N} Z = -\frac{1}{\beta} \ln \Lambda_{\text{max}}.
\]

(9)

Now one can utilize the thermodynamic relations to evaluate various quantities that would be investigated. The specific heat, entropy, and magnetization per block can be consequently defined as

\[
M = -\left( \frac{\partial f}{\partial T} \right)_B, \quad S = -\left( \frac{\partial f}{\partial B} \right)_T, \quad C = -T \left( \frac{\partial^2 f}{\partial B^2} \right)_B.
\]

(10)

### 3. Results and discussion

The following section introduces the most interesting results obtained from the study of the magnetization processes and the specific heat behavior of the spin-1/2 Ising-Heisenberg Cairo pentagonal model under different circumstances. Figure 2 illustrates the magnetic field dependences of magnetization in the unit of its saturation for various fixed values of the exchange anisotropy parameter \( \Delta \). Panel 2 (a) demonstrates the magnetization per block against the magnetic field at low temperature \( T = 0.1 J_0 \) and fixed value of the isotropic coupling constant \( J = 0.45 J_0 \) where several amounts of the anisotropy \( \Delta \) are considered. On the other hand, panel 2 (b) displays this quantity versus the magnetic field at stronger coupling constant \( J = 1.5 J_0 \) for the same set of other parameters to the case (a). It is quite obvious that the magnetization curve shows intermediate plateaus at zero and \( \frac{1}{4} \) of saturation magnetization for anisotropy range \( \Delta < -1.5 J_0 \). The 0–plateau gradually disappears upon increasing the anisotropy property close to the value \( \Delta = -1.5 J_0 \), also the magnetic-position of the intermediate 1/2–plateau shifts toward lower magnetic fields. That means, for higher values of \( \Delta/J_0 \), magnetization jumps accompanying the quantum phase transition between different magnetization plateaus; from 0–plateau to \( \frac{1}{4} \)-plateau and
Figure 2. Magnetization per saturation value $M/M_s$ of the spin-1/2 Ising-Heisenberg Cairo pentagonal model as a function of external magnetic field $B/J_0$ at low temperature $T = 0.1J_0$ for fixed value of $J = 0.45J_0$ and several exchange anisotropies $\Delta = \{-3J_0, -2.5J_0, -2J_0, -1.5J_0, -J_0, -0.5J_0, 0, 0.5J_0, 2J_0\}$. (b) The magnetization per saturation value $M/M_s$ of the model for the fixed value $J = 1.5J_0$, where other parameters are taken as panel (a).

It is evident from this figure that increasing the exchange coupling $J/J_0$ has substantial effect on the magnetization behavior versus the magnetic field. As a matter of fact, with increase of the exchange coupling $J/J_0$ the width of the intermediate $\frac{1}{2}$—plateau gradually decreases, while the width of the zero-plateau simultaneously increases. Consequently, upon increasing $J/J_0$ the magnetization jump between plateaus occurs in the stronger magnetic field. From the ground phase transition perspective, when the coupling constant $J/J_0$ increases the transition from antiferromagnetic state in turn from $\frac{1}{2}$—plateau to the saturation magnetization occur at lower magnetic fields. Further increase of the anisotropy results in disappearing the $\frac{1}{2}$—plateau such that at high anisotropies the magnetization behaves as a horizontal line at its saturation value (gold line marked with hexagons). We plot in panel 2 (b) the low-temperature magnetization per saturation as a function of the magnetic field ($B > 0$) where fixed value of $J = 1.5J_0$ is considered. Other parameters have been taken as the case 2 (a).
Figure 3. (a) The specific heat of the spin-1/2 Ising-Heisenberg Cairo pentagonal model as a function of the temperature for several fixed values of the magnetic field $B/J_0$, where other parameters are taken as $J = 0.45J_0$ and $\Delta = -1.5J_0$. The temperature dependence of the specific heat for different magnetic fields and fixed values of $J = 1.5J_0$ and $\Delta = -1.5J_0$.

Now let us examine the effects of the exchange coupling $J/J_0$ and the magnetic field $B/J_0$ on the temperature dependence of the specific heat. To this end, we display in Fig. 3(a) the temperature dependence of the specific heat for the model under consideration for the several fixed values of the magnetic field by supposing $J = 0.45J_0$ and $\Delta = -1.5J_0$. Blue solid line marked with hexagons represents the specific heat curve for $J = 0.45J_0$ and $\Delta = -1.5J_0$ when the magnetic field is absence ($B = 0$). This line is the same specific heat curve plotted in Ref. [28]. Actually, we plotted this line for better understanding the effects of external magnetic

$(M/M_s = 0)$ to the state with the corresponding magnetization $M/M_s = 1/2$, as well as, from state $M/M_s = 1/2$ to the fully polarized state (ferromagnetic state) occur for the stronger magnetic fields. Moreover, it can be understood that for the stronger coupling constant $J/J_0$ the intermediate magnetization plateaus disappear for the stronger exchange anisotropy $\Delta/J_0$ (for example compare marked lines plotted in the both panels 2 (a) and 2 (b) together).
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field and isotropic coupling constant $J/J_0$ on the specific heat behavior and make some stimulating comparisons between our results and their counterpart discussed in Ref. [28]. By inspecting this figure one can see that the specific heat exhibits a triple-peak when $B = 0$. With increase of the magnetic field, first two smaller peaks merge together and make a bigger peak at higher temperature (see green dotted-dash line corresponds to $B = 0.2J_0$). With further increase of the magnetic field, all peaks merge together and make a single Schottky-peak (black solid line marked with diamonds). Interestingly, when the magnetic field increases further that $B = J_0$, a small second peak arises at low temperature. So, in this condition the specific heat has a double-peak temperature dependence. Comparisons between two figures 3(a) and 2(a) manifests that procedure of merging peaks together and making a bigger peak is accompanying with the magnetization jumps from 0−plateau to 1/2−plateau (merging first small peak with the second one, see again the evolution from blue solid line marked with hexagons to green dotted-dash line depicted in Fig. 3(a)). The intermediate magnetization 1/2−plateau coincides the single Schottky peak existence. Ultimately, the magnetization jump from 1/2−plateau to the saturation magnetization is in coincidence with the arising of a small peak when the magnetic field increases further than $B = J_0$ (trace the evolution from black solid line marked with diamonds to the pink dotted-dash line marked with cycles illustrated in Fig. 3(a)).

To gain an overall insight into the coupling constant $J/J_0$ effects on the specific heat, let us also examine the specific heat behavior of the spin-1/2 Ising-Heisenberg Cairo pentagonal model for the different values of $J/J_0$, which can be particularly interesting especially for the case when the model is putted in the presence of a tunable magnetic field. We have depicted in Fig. 3(b) typical dependences of the specific heat on the temperature for several fixed magnetic fields by assuming $J = 1.5J_0$ and $\Delta = -1.5J_0$. The interesting point to observe from this figure is that the specific heat does not show the triple-peak even for the case $B = 0$. Nevertheless, a particular double-peak temperature dependence is observed whose peaks merge together upon increasing the magnetic field and ultimately make a Schottky-type maximum at higher temperature and strong magnetic fields accompanied with the magnetization jump from one plateau to another. Another interesting thing is that the Schottky-type maximum appears for the remarkably stronger magnetic fields rather than the case when we considered fixed value $J = 0.45J_0$ for the model. This phenomenon demonstrates that for the case $J = 1.5J_0$ the magnetization jump from 0−plateau to 1/2−plateau occurs for the stronger magnetic fields compared with the case $J = 0.45J_0$.

4. Conclusions

In this paper, we have theoretically investigated the thermodynamic properties and magnetic behavior of the spin-1/2 Ising-Heisenberg Cairo pentagonal model in the presence of an external tunable magnetic field. To do so, we have examined the magnetization process and specific heat of this model by means of solution within the transfer-matrix formalism.

In terms of numerical investigations, we understood that the magnetization has intermediate plateaus at zero and 1/2 of the saturation magnetization. These plateaus rigorously depend on the both isotropic and anisotropic Heisenberg exchange couplings considered for the dimers. In fact, increase of the exchange anisotropy parameter leads to weaken the critical magnetic field in which the magnetization jump occurs from
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0−plateau to 1/2−plateau. But on the other hand, increasing the isotropic coupling constant $J/J_0$ results in increasing the width of the 0−plateau and decreasing the width of the 1/2−plateau.

Furthermore, it has been already demonstrated that in the absence of magnetic field, the specific heat curve of the model manifests three separated peaks. Here, we declared that the magnetic field and the isotropic coupling constant variations can remarkably alter the shape and the temperature-position of these peaks. Namely, the magnetic field increment leads to merging two smaller peaks together, hence, the specific heat has just a double-peak. With further increase of the magnetic field all peaks merge together and create a single Schottky peak. The created single Schottky peak denotes existence of the intermediate 1/2−plateau. Moreover, we concluded that merging and separating each pairs of peaks are accompanied with a magnetization jump from one plateau to one another. Varying the exchange coupling $J/J_0$ has substantial effect on the specific heat behavior versus temperature that is in an excellent coincidence with the magnetization response to this variation. As a result, the specific heat variations with respect to the magnetic field are in a good accordance with the low-temperature magnetization process of the spin-1/2 Ising-Heisenberg Cairo pentagonal model.

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