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Magnetic Susceptibility and Magnetization Plateau in Triangular Spin Cluster

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The magnetic susceptibility and the magnetization as a function of magnetic field are calculated exactly for the antiferromagnetic Ising and Heisenberg models of a triangle cluster. Both characters of the bending of the inverse susceptibility as a function of temperature and the 1/3 plateau of magnetization found in the Monte Carlo simulation study for the triangle based lattice systems survive even in a single triangle cluster. The quantum effect and the spin magnitude are discussed concerning the characters.

KEYWORDS: triangle cluster, antiferromagnetic, Ising, Heisenberg, susceptibility, plateau

§ 1. Introduction

Our recent Monte Carlo (MC) simulation study of the $s = 1/2$ antiferromagnetic Ising spin systems on triangular and kagomé lattices has shown the peculiar characters in the magnetic susceptibility and the magnetization under the magnetic field. Those are the downward bending in the inverse of magnetic susceptibility from the Curie-Weiss like form at the characteristic temperature T^* with decreasing temperature and the appearance of the 1/3 magnetization plateau for $T < T^*$ in the magnetization process. Such anomaly of magnetic susceptibility has been indicated by Sano,[1] in his MC simulation study both for the Ising and Heisenberg models on the triangular lattice. After then, for the Heisenberg model, totally different low temperature behavior was proposed by the high temperature series expansion,[2] but for Ising model any attention has not been paid.[3] On the other side, the 1/3 magnetization plateau in the triangular lattice is well recognized

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to appear for both models.[4-7] However the correlation between these two characters has not been discussed carefully, up to now.

In a general argument, the spin correlation of the geometrically frustrated spin systems is known to be restricted in short distance.[8] A motivation is therefore directed toward the investigation of the equilateral triangle spin cluster, which is the unit structure of triangular and kagomé lattices.

In this investigation, we give the exact calculations of the magnetic susceptibility as a function of temperature and the magnetization under the magnetic field in a triangular cluster of $s=1/2$ antiferromagnetic Ising and Heisenberg models, and in addition the $s=1$ Ising model, to discuss the effects of quantum fluctuation and the spin magnitude on those quantities. The obtained results are briefly discussed as the character of frustrated triangle spin structure, suppressing the long range order down to very low or zero temperature.

The paper is constructed as follows: In the next section, eigen states are calculated for $s = 1/2$ Ising and Heisenberg models. In § 3 and § 4, the magnetic susceptibility and the magnetization under the magnetic field are calculated, respectively. The final section is devoted for conclusions and discussions. The result of the MC simulation study will be published in the future issue.

§ 2. Eigen states of triangle cluster

We first calculate the eigen states of three spin triangle cluster. The state functions of three spins {I II III} are denoted as

$$|\phi_1\rangle=|\uparrow\uparrow\uparrow\rangle, |\phi_2\rangle=|\downarrow\downarrow\downarrow\rangle, |\phi_3\rangle=|\uparrow\uparrow\downarrow\rangle, |\phi_4\rangle=|\uparrow\downarrow\uparrow\rangle,$$

$$|\phi_5\rangle=|\downarrow\uparrow\uparrow\rangle, |\phi_6\rangle=|\uparrow\downarrow\downarrow\rangle, |\phi_7\rangle=|\downarrow\uparrow\downarrow\rangle, |\phi_8\rangle=|\downarrow\downarrow\uparrow\rangle, \tag{1}$$

where up- and down-arrows denote respective spins of magnitude 1/2, respectively.

For s = 1/2 Ising model, the spin Hamiltonian for the triangular cluster is given as

$$\tilde{H}=4H=\sigma_{\mathrm{I}}\sigma_{\mathrm{II}}+\sigma_{\mathrm{II}}\sigma_{\mathrm{III}}+\sigma_{\mathrm{III}}\sigma_{\mathrm{I}}-h(\sigma_{\mathrm{I}}+\sigma_{\mathrm{II}}+\sigma_{\mathrm{III}}), \tag{2}$$

where $\sigma_i = 2s_i^z$. The s_i^z is z component of ith spin $\boldsymbol{s}_i$ and h the magnetic field. H is the Hamiltonian for the original spin variable $\boldsymbol{s}$ in usual expression. The exchange coupling constant is chosen as an energy unit. The corresponding energies for $\tilde{H}$ are calculated as

$$E_1=3(1-h),\ E_2=3(1+h),\ E_{3,4,5}=-(1+h),\ E_{6,7,8}=-(1-h). \tag{3}$$

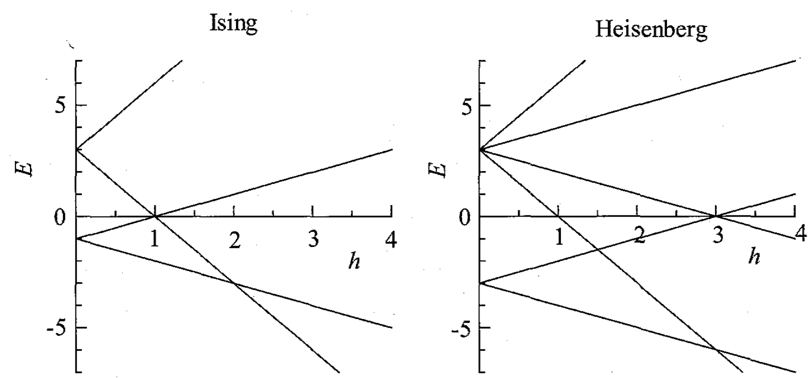

Fig.1. Energy spectra of Ising and Heisenberg model triangle clusters as a function of magnetic field h.

Table 1. Eigenvalues and eigen functions of the Heisenberg model triangle cluster. The former is given in units of exchange coupling constant.

eigenvalues	eigen functions
$\varepsilon_1 = 3(1-h)$	$\|\phi_1>$
$\varepsilon_2 = 3(1+h)$	$\|\phi_2>$
$\varepsilon_3 = -(3+h)$	$\frac{1}{\sqrt{2}}(\|\phi_4> - \|\phi_5>)$ $\frac{1}{\sqrt{6}}(-2\|\phi_3> + \|\phi_4> + \|\phi_5>)$
$\varepsilon_4 = 3-h$	$\frac{1}{\sqrt{3}}(\|\phi_3> + \|\phi_4> + \|\phi_5>$
$\varepsilon_5 = -(3-h)$	$\frac{1}{\sqrt{2}}(\|\phi_7> - \|\phi_8>)$ $\frac{1}{\sqrt{6}}(-2\|\phi_6> + \|\phi_7> + \|\phi_8>)$
$\varepsilon_6 = 3+h$	$\frac{1}{\sqrt{3}}(\|\phi_6> + \|\phi_7> + \|\phi_8>)$

For the case of vanishing magnetic field $h = 0$, the ground state is the 6-fold degenerate doublet and the excited state 2-fold degenerate quartet. By the magnetic field, the degeneracy of ground states is lifted into two 3-fold states and also that of the 2-fold degenerate excited state is also dissolved.

The Hamiltonian of the spin-1/2 Heisenberg model triangle cluster is expressed as

$$\tilde{H} = 4H = 4(s_{\mathrm{I}} \cdot s_{\mathrm{II}} + s_{\mathrm{II}} \cdot s_{\mathrm{III}} + s_{\mathrm{III}} \cdot s_{\mathrm{I}}) - h(\sigma_{\mathrm{I}} + \sigma_{\mathrm{II}} + \sigma_{\mathrm{III}}). \tag{4}$$

The eigenvalues and the corresponding eigen functions in a complete form are solved as in Table1.

The energy spectrum for both models is figured in Fig. 1 as a function of magnetic field. For the case of $h = 0$, the ground doublet state degenerates in 4-fold with energy $E = -3$ and the excited state is 4-fold degenerate quartet with energy $E = 3$. As also in Ising model, the ground state degeneracy is not lifted completely, against the excited state. In both models, the ground state changes from doublet state to quartet one for greater value than 2 or 3 of h by level crossing for Ising or Heisenberg model, respectively.

§ 3. Magnetic susceptibility

The longitudinal (z component) uniform magnetic susceptibility per spin is expressed in general form as

$$\chi = \frac{1}{3T}[<(\sum_i \sigma_i)^2> - <\sum_i \sigma_i>^2], \tag{5}$$

where $< >$ denotes the thermal average,

$$<A> = \frac{1}{Z}\,\mathrm{Tr}\, \mathrm{e}^{-\beta\tilde{H}} A,$$

Z is the partition function of the system at $h = 0$, the symbol Tr denotes the trace operation and β the inverse temperature $1/T$ in units of Boltzmann constant.

The longitudinal uniform susceptibility of Ising model χ_{I} is expressed as

$$\chi_{\mathrm{I}} = \frac{1}{T} \cdot \frac{1+3\mathrm{e}^{-4\beta}}{3+\mathrm{e}^{-4\beta}}, \tag{6}$$

explicitly. The inverse of this magnetic susceptibility is drawn in Fig. 2 as a function of temperature. As can be seen in the figure, the inverse magnetic susceptibility shows the distinct downward deviation at $T_{\mathrm{I}}^* \sim 1.2$ from high temperature Curie-Weiss like linear form. Below the temperature T_{I}^* it decreases with temperature linearly like a Curie law, that is, toward the vanishing at zero temperature. This might be accounted by mixing of the quartet excited state with the doublet ground state for $T \geq T_{\mathrm{I}}^*$. The temperature dependence of susceptibility is globally resembled to those found in the MC simulation study for Ising model on the triangular and the kagomé lattices.

The magnetic susceptibility for the Heisenberg model is also calculated to see whether the bending of the inverse magnetic susceptibility found in the Ising model is

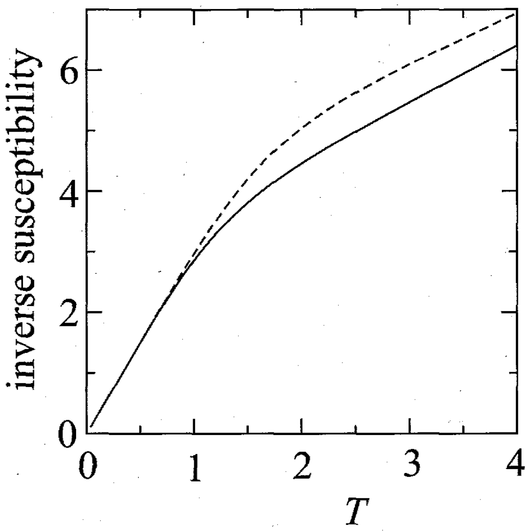

Fig. 2. The inverse longitudinal uniform susceptibility as a function of T. The solid line denotes for the Ising model, χ_{I}^{-1}, and the broken line for the Heisenberg one, χ_{H}^{-1}, analytically given in eqs. (6) and (7) , respectively.

affected by the quantum effect or not. The exact expression of magnetic susceptibility for the Heisenberg model χ_{H} is given as

$$\chi_{\mathrm{H}}=\frac{1}{3T}\cdot\frac{1+5e^{-6\beta}}{1+e^{-6\beta}}. \tag{7}$$

This expression is drawn in Fig. 2 together with the result of the Ising model. The similar bending as in Ising model is also seen in the Heisenberg model at the characteristic temperature $T_{\mathrm{H}}^{*}\sim 1.5$, somewhat higher than that of Ising model $T_{\mathrm{I}}^{*}\sim 1.2$.

The magnetic susceptibilities for two models show the similar temperature dependence qualitatively, except the difference in the value of T^{*}. This difference comes from that of the magnitude of excitation gap, 1.5 times greater in the Heisenberg model than the Ising one. The coincidence of the Curie and Curie-Weiss constants at low and high temperatures, respectively, in two models is easily found as same limiting values at $T\rightarrow 0$ and $T\rightarrow\infty$ in eqs. (6) and (7) . Then it may be claimed that the magnetic susceptibility, and furthermore the bending in it, do not seem to be affected by the quantum effect as far as the triangle cluster is considered. Such bending of magnetic susceptibility was firstly shown by Sano[1)] on the MC simulation study of the Ising and Heisenberg models on the triangular lattice by showing the absence of temperature dependence of average squared magnetization $< m^2 >$, which is proportional to the magnetic susceptibility, at low temperature region. The present result for cluster are in good correspondence with the behavior of $< m^2 >$ in Ref. 1 for both models.

§ 4. Magnetization plateau

The magnetization per spin is calculated by the following formulation,

$$m=\frac{1}{3}< \sum_i s_i^z >. \tag{8}$$

In the case of Ising model, the magnetization m_{I} is expressed as

$$m_{\mathrm{I}} = \frac{e^{3\beta(h-1)} - e^{-3\beta(h+1)} + e^{\beta(1+h)} - e^{\beta(1-h)}}{e^{3\beta(h-1)} + e^{-3\beta(h+1)} + 3(e^{\beta(1+h)} + e^{\beta(1-h)})}. \tag{9}$$

This function is drawn as a function of magnetic field h for two values of T in Fig. 3. As shown in the figure, the 1/3 plateau appears in the magnetization in cases of the lower temperature than T_{I}^*. Where the magnetic field at the plateau region is about the energy scale of the exchange coupling constant.

For Heisenberg model, the magnetization m_{H} is expressed as

$$m_{\mathrm{H}} = \frac{1}{3} \cdot \frac{3(e^{-3\beta(1-h)} - e^{-3\beta(h+1)}) + 2(e^{\beta(3+h)} - e^{\beta(3-h)}) + e^{\beta(h-3)} - e^{-\beta(h+3)}}{e^{-3\beta(1-h)} + e^{-3\beta(h+1)} + 2(e^{\beta(3+h)} + e^{\beta(3-h)}) + e^{\beta(h-3)} - e^{-\beta(h+3)}}, \tag{10}$$

and this function shows similar behavior as Ising model, depicting the 1/3 plateau in the case of $T < T_{\mathrm{H}}^*$, as shown in Fig. 3.

At low temperature and low field limit $(T, h \ll 1)$, eqs. (9) and (10) have same limiting expression $m_{\mathrm{I}}(T\to 0, h\to 0) = m_{\mathrm{H}}(T\to 0, h\to 0) = \frac{1}{3}\tanh(\beta h)$ and it is seen in the same gradient of the initial rising at low temperature case $(T=0.5)$ in Fig. 3. At absolute zero temperature, this limiting value for weak field has finite value of 1/3, in contrast to the result of Ising-like anisotropic Heisenberg model by the explicit numerical diagonalization method.[6] The magnitude of h at steep rising from 1/3 plateau up to full polarization $(m = 1)$ for sufficiently low temperature case $(T \ll T^*)$ is well accounted from the values of h for the level crossing.

§ 5. Conclusions and discussions

The longitudinal uniform magnetic susceptibility and the magnetization as functions of temperature and external magnetic field, respectively, have been calculated in this study for the $s = 1/2$ Ising and Heisenberg spin triangle clusters.

We can recognize the distinct bending in the inverse magnetic susceptibility drawn as a function of temperature in spin clusters of both of the Ising and Heisenberg models. Even for a single triangle cluster survives the bending found in our MC simulation study for the triangular and kagomé lattices of $s = 1/2$ Ising spin.

The 1/3 magnetization plateau has been revealed in the magnetization processes for both spin models on triangle cluster, as the temperature was decreased below the temperature T^*, at which the inverse magnetic susceptibility shows the bending in each spin model. Such plateau was also found in MC study of Ising spin triangular and kagomé lattice systems.

It should be noticed that any quantitative difference is not found between two spin models for the calculated quantities. Furthermore, such characters of magnetic susceptibility and magnetization have also been found for the case of spin magnitude $s = 1$ Ising model, though the explicit expressions and figures are not shown here. The ground state of Heisenberg model on the triangular lattice is the symmetry breaking ordered state, [9-12] contrasting with the disorder state of the Ising model on the same lattice and of both models on the kagomé lattice. Even in the case of different ground state in the lattice systems, the finite temperature magnetic excitation seems to be governed by local doublet-quartet one. This fact is a peculiar character of the two-dimensional frustrated system, retaining the disorder down to low temperature.

From the present cluster calculation and the MC simulation study, we can speculate that the magnetic susceptibility and the magnetization plateau originate in the local low energy states. We may fairly well expect that the low energy states of triangle based lattices, such as triangular and kagomé lattices, are well approximated as the direct product of the low energy states of the local triangle. These similarities between the cluster and the lattice should be studied in the near future, in the relation to the concept of the geometrically frustrated structure.[13,14] Therein the low energy excitation is not affected so much by the quantum effect and by the spin magnitude. For further confirmation concerning the quantum effect, the exact calculation of magnetic susceptibility for the Heisenberg spin cluster of finite size is now in progress, toward the resolution of previous confliction.[1,2]

Finally in the relation with the experimental observations,[13,14] some discussions have ever been given for the deviation in the inverse magnetic susceptibility at low temperature from the Curie-Weiss behavior.[15] However, those discussions are restricted to the phenomenological one. The present exact calculation based on two spin models gives the theoretical basis of their phenomenological two-population model.[15] The experiments of the magnetic susceptibility and the magnetization process should be paid the attention in the relationship between them.

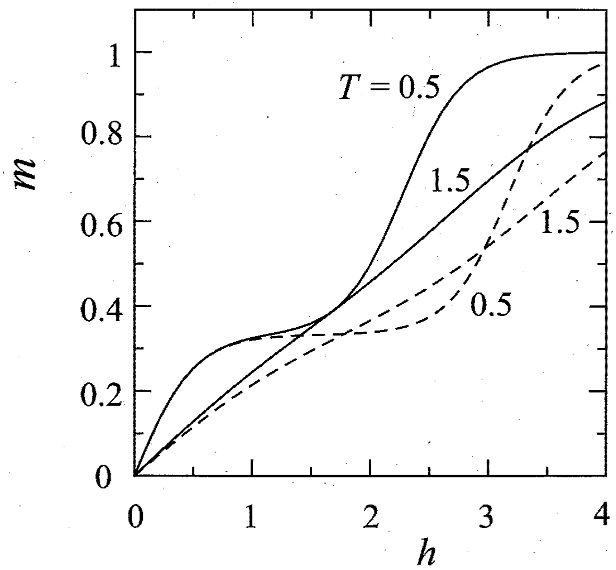

Fig. 3. The magnetization as a function of h for T = 0.5 sufficiently lower than T^* and T= 1.5 nearly equal value to T^* for both models. The solid line depicts for the Ising model and the broken line for the Heisenberg one, analytically given in eqs. (9) and (10), respectively.

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