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Susceptibility of the Kagomé Lattice Ising Model

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We explicitly calculate the zero-field magnetic susceptibility of the anisotropic Kagomé lattice Ising model on two different varieties of the parameter space. One of them is the limit $H = 0$ of the solubility condition, obtained in a previous paper by Giacomini, for the model with magnetic field. The other one is the disorder variety of the model, for which a dimensional reduction occurs. These varieties do not contain any nontrivial critical behavior of the model. A functional relation is also established, which relates the zero-field susceptibility for ferromagnetic and competing interactions.

KEY WORDS: Ising model; magnetic susceptibility; exact results.

The exact expression for the initial magnetic susceptibility is not known for any of the two-dimensional Ising models, except in very special cases: the superexchange model of Fisher[(1)] and the triangular[(2)] and checkerboard[(3)] lattices restricted to the disorder variety, where the model decouples and becomes unidimensional.

In the critical region of the square lattice model, a large amount of information on the susceptibility has been obtained in recent years.[(4–14)] These results have been found, in general, by combining the fluctuation-dissipation theorem with the many exact results that have been accumulated for the two-spin correlation functions.

However, an explicit expression for the susceptibility at all temperatures obtained through the fluctuation-dissipation theorem has not been found so far.

In this work, the explicit expression for the initial (zero-field) susceptibility of the anisotropic Kagomé lattice Ising model (see Fig. 1) is obtained when a special relation between the three interaction parameters of the model is satisfied. This result is derived from the relation established

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in a previous paper[15] between the partition functions of the anisotropic Kagomé and honeycomb lattice Ising models with a magnetic field. In particular, for the free energy per site, this relation is as follows:

$$f_{\mathrm{Kag}}(K_1, K_2, K_3, H) = \tfrac{1}{3}\log(A_1 A_2 A_3) + \tfrac{1}{3}\log R^2 + \tfrac{2}{3} f_{\mathrm{honey}}(L_1, L_2, L_3, \bar{H})$$

where $f_{\mathrm{Kag}} = (1/3N)\log Z_{\mathrm{Kag}}$ and $f_{\mathrm{honey}} = (1/2N)\log Z_{\mathrm{honey}}$. Here $3N$ and $2N$ are the numbers of sites of the Kagomé and honeycomb lattices, respectively. The parameters L_i, $\bar{H}$, A_i, and R are given in terms of K_i and H as follows:

$$\exp(4L_i) = \cosh(2M_i + H)\cosh(2M_i - H)[\cosh(H)]^{-2}, \quad i = 1, 2, 3 \tag{2a}$$

$$\exp(4\bar{H}) = \prod_{i=1}^{3} \cosh(2M_i + H)\,[\cosh(2M_i - H)]^{-1} \tag{2b}$$

$$\sinh(2K_i)\sinh(2M_i) = 1/\alpha, \quad i = 1, 2, 3 \tag{2c}$$

$$R^2 = (\alpha^2/2)\sinh(2K_1)\sinh(2K_2)\sinh(2K_3) \tag{2d}$$

$$A_i = 2[\cosh(2M_i + H)\cosh(2M_i - H)\cosh^2(H)]^{1/4}, \quad i = 1, 2, 3 \tag{2e}$$

with

$$\alpha = (1 - t_1^2)(1 - t_2^2)(1 - t_3^2) \times [16(1 + t_1 t_2 t_3)(t_1 + t_2 t_3)(t_2 + t_3 t_1)(t_3 + t_1 t_2)]^{-1/2} \tag{2f}$$

and $t_i = \tanh(K_i)$. Here, M_1, M_2, and M_3 are auxiliary parameters, defined in terms of K_1, K_2, and K_3 by means of Eqs. (2c) and (2f). Moreover,

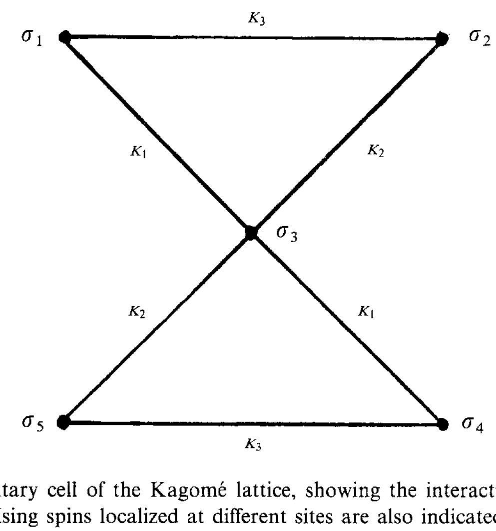

Fig. 1. An elementary cell of the Kagomé lattice, showing the interaction parameters. The Ising spins localized at different sites are also indicated.

the parameters L_1, L_2, and L_3 are the interaction coefficients of the honeycomb lattice model.

From (1) and (2) one can easily deduce a relation between the initial magnetic susceptibility of both models. Taking into account that

$$\left.\frac{\partial L_i}{\partial H}\right|_{H=0} = \left.\frac{\partial A_i}{\partial H}\right|_{H=0} = 0, \qquad i = 1, 2, 3 \tag{3a}$$

$$\left.\frac{\partial^2 \bar{H}}{\partial H^2}\right|_{H=0} = 0 \tag{3b}$$

$$\left.\frac{\partial \bar{H}}{\partial H}\right|_{H=0} = \frac{1}{2}\sum_{i=1}^{3} \tanh(2M_i) \tag{3c}$$

$$\left.\frac{\partial^2 L_i}{\partial H^2}\right|_{H=0} = -\frac{1}{2}\tanh^2(2M_i) \tag{3d}$$

$$\left.\frac{1}{A_i}\frac{\partial^2 A_i}{\partial H^2}\right|_{H=0} = 1 - \frac{1}{2}\tanh^2(2M_i) \tag{3e}$$

we obtain

$$\begin{aligned}\chi_{0,\mathrm{Kag}}(K_1, K_2, K_3) = 1 &- \frac{1}{6}\sum_{i=1}^{3} \tanh^2(2M_i) \\ &- \frac{1}{3}\sum_{i=1}^{3}\left[\tanh^2(2M_i)\,\frac{\partial f_h(L_1, L_2, L_3, \bar{H}=0)}{\partial L_i}\right] \\ &+ \frac{1}{6}\left[\sum_{i=1}^{3}\tanh(2M_i)\right]^2 \chi_{0,\mathrm{honey}}(L_1, L_2, L_3)\end{aligned} \tag{4}$$

where

$$\chi_{0,\mathrm{Kag}} = \left.\frac{\partial^2 f_{\mathrm{Kag}}(K_1, K_2, K_3, H)}{\partial H^2}\right|_{H=0} \tag{5a}$$

$$\chi_{0,\mathrm{honey}} = \left.\frac{\partial^2 f_{\mathrm{honey}}(L_1, L_2, L_3, \bar{H})}{\partial \bar{H}^2}\right|_{\bar{H}=0} \tag{5b}$$

When $H = 0$ the parameters L_i are given by

$$\exp(2L_i) = \cosh(2M_i) \tag{6}$$

As can be seen from (4), if the condition

$$\sum_{i=1}^{3} \tanh(2M_i) = 0 \tag{7}$$

is imposed, the coefficient of $\chi_{0,\text{honey}}$ becomes null and $\chi_{0,\text{Kag}}$ can be exactly evaluated, the nearest neighbor correlation functions

$$\partial f_{\text{honey}}(L_1, L_2, L_3, \bar{H}=0)/\partial L_i$$

being known exactly for arbitrary values of L_1, L_2, L_3.

Taking into account (2c), Eq. (7) imposes the following condition on the interaction parameters K_i:

$$\frac{1}{\alpha}\left(\frac{1}{\tanh(2K_1)+\tanh(2K_2)\tanh(2K_3)} + \frac{1}{\tanh(2K_2)+\tanh(2K_3)\tanh(2K_1)} + \frac{1}{\tanh(2K_3)+\tanh(2K_1)\tanh(2K_2)}\right)=0 \tag{8}$$

which factorizes into two independent equations.

The first of these is $1/\alpha=0$, which, explicitly written by using (2f), reads as follows:

$$(1+t_1t_2t_3)(t_1+t_2t_3)(t_2+t_1t_3)(t_3+t_1t_2)=0 \tag{9}$$

for finite values of parameters K_i.

The surface defined by (9) is the disorder variety of the model with zero field.[16] On this variety there is a dimensional reduction. The partition function behaves as a zero-dimensional model and the correlation functions have a one-dimensional behavior. Moreover, when Eq. (9) is satisfied, we have

$$\tanh(2M_i)=0, \qquad \cosh^2(2M_i)=1 \tag{10}$$

The corresponding model on the honeycomb lattice is trivial: two interaction parameters become zero and the third is equal to $i\pi/2$. For this case the free energy of the honeycomb lattice model is singular, and we have an indeterminate limit in expression (4). In consequence, it is not possible to calculate $\chi_{0,\text{Kag}}$ on the disorder variety by this method. The explicit expression of $\chi_{0,\text{Kag}}$ on this variety can be obtained by the decimation method. We explain this method in the Appendix, and we quote here only the final expression for χ_0 on the disorder variety:

$$\chi_{0,\text{Kag}}=\frac{1}{3}+\frac{2}{3}\,\frac{(1+t_1)(1+t_2)(1-t_1t_2)^2(1+t_1t_2+t_1^2t_2^2)}{(1-t_1)(1-t_2)(1+t_1^2t_2^2)^2} \tag{11}$$

with

$$t_3 = -t_1 t_2 \tag{12}$$

Other independent solutions can be obtained by using the invariance of the free energy and condition (9) with respect to permutations of t_1, t_2, and t_3. This expression is only valid for real values of the interaction parameters K_1, K_2, K_3, as explained in the Appendix. The simple, purely algebric, character of (11) and the absence of singularities (with the exception of the trivial one for K_1 or K_2 equal to ∞) are consequences of the dimensional reduction that occurs on the variety (9).

The second possibility for satisfying Eq. (8) is to impose the following condition on the parameters K_i:

$$\frac{1}{\tanh(2K_1)+\tanh(2K_2)\tanh(2K_3)} + \frac{1}{\tanh(2K_2)+\tanh(2K_3)\tanh(2K_1)} + \frac{1}{\tanh(2K_3)+\tanh(2K_1)\tanh(2K_2)} = 0 \tag{13}$$

It can be shown that this is just the limit $H=0$ of the solubility condition found in ref. 15 for the Kagomé lattice Ising model with magnetic field. In contrast to (9), this equation does not factorize into a set of nonsymmetric conditions, and it does not impose a dimensional reduction on the system.

It is evident that there are no solutions of Eq. (13) in the ferromagnetic region, where K_1, K_2, and K_3 are positive. For the "physical" solutions of (13), the following cases are possible: (i) the three interactions are negative; (ii) one is positive and the other two are negative; (iii) one interaction is negative and the other two are positive. Hence, the system can be in the antiferromagnetic "frustrated" region [case (i)], or in a region of competing interactions with or within "frustration" [cases (iii) and (ii), respectively]. By contrast, when the disorder condition (9) is satisfied, the system is always "frustrated."

Unfortunaly, the surface (13) has no intersection, for the physical (real) region of the parameter space, with the critical variety of the model. Taking into account (4), (6), and the explicit expression of $f_{\text{honey}}(L_1, L_2, L_3, \bar{H}=0)$ (see, for example, ref. 17), we finally obtain the following expression for $\chi_{0,\text{Kag}}$ on the surface (13):

$$\chi_{0,\mathrm{Kag}} = \frac{1}{12\pi^2} \int_0^{2\pi} \int_0^{2\pi} \times \frac{A - B\cos\omega_1 - C\cos\omega_2 - D\cos(\omega_1+\omega_2)}{1 + C_1C_2C_3 - S_2S_3\cos\omega_1 - S_3S_1\cos\omega_2 - S_1S_2\cos(\omega_1+\omega_2)}\, d\omega_1\, d\omega_2 \tag{14}$$

where

$$A = (C_1 + C_2C_3)(C_1 - S_1) + (C_2 + C_1C_3)(C_2 - S_2) + (C_3 + C_1C_2)(C_3 - S_3)$$
$$B = (C_1 - S_1)C_1S_2S_3, \quad C = (C_2 - S_2)C_2S_3S_1, \quad D = (C_3 - S_3)C_3S_1S_2 \tag{15}$$

with

$$C_i = \cosh 2L_i = \frac{1}{2}\frac{2\alpha^2\sinh^2 2K_i + 1}{\alpha\sinh 2K_i\,(1+\alpha^2\sinh^2 2K_i)^{1/2}}$$
$$S_i = \sin 2L_i = \frac{1}{2}\frac{1}{\alpha\sinh 2K_i\,(1+\alpha^2\sinh^2 2K_i)^{1/2}} \tag{16}$$

The integral expression (14) can be calculated in terms of elliptic functions of the first and third kinds, but the resulting expressions are very complicated, and do not give additional insight when compared to the integral representation.

In general, if the initial susceptibility is known for the Kagomé lattice, it can also be calculated for the honeycomb lattice and, in turn, for the triangular lattice. (For a review see ref. 17.) Unfortunately, the same mechanism that enables us to obtain expression (14) [condition (13)] rules out the possibility of extending our result to other two-dimensional lattices.

Let us now return to the general case of the relation between $\chi_{0,\mathrm{Kag}}$ and $\chi_{0,\mathrm{honey}}$, given by (4). From this equation, a relation can be obtained between $\chi_{0,\mathrm{Kag}}(K_1, K_2, K_3)$ and $\chi_{0,\mathrm{Kag}}(K_1, -K_2, -K_3)$. If we change M_1 by $-M_1$, Eq. (4) becomes

$$\chi_0(K_1, -K_2, -K_3) = 1 - \frac{1}{6}\sum_{i=1}^{3}\tanh^2(2M_i) - \frac{1}{3}\sum_{i=1}^{3}\left[\tanh^2(2M_i)\frac{\partial f_h(L_1, L_2, L_3, \bar{H}=0)}{\partial L_i}\right] + \frac{1}{6}\left[-\tanh(2M_1) + \tanh(2M_2) + \tanh(2M_3)\right]^2 \chi_{0,\mathrm{honey}}(L_1, L_2, L_3) \tag{17}$$

where we have taken into account that L_1, L_2, and L_3 are invariant by the change of sign of M_1.

From Eqs. (4) and (17) it can be deduced that

$$\chi_{0,\mathrm{Kag}}(K_1, -K_2, -K_3)$$
$$= \frac{1-p}{12\pi^2} \int_0^{2\pi} \int_0^{2\pi}$$
$$\times \frac{A - B\cos\omega_1 - C\cos\omega_2 - D\cos(\omega_1+\omega_2)}{1 + C_1C_2C_3 - S_2S_3\cos\omega_1 - S_3S_1\cos\omega_2 - S_1S_2\cos(\omega_1+\omega_2)}$$
$$\times d\omega_1\, d\omega_2 + p\chi_{0,\mathrm{Kag}}(K_1, K_2, K_3) \tag{18}$$

where p is given by

$$p = \frac{[-\tanh(2M_1) + \tanh(2M_2) + \tanh(2M_3)]^2}{[\tanh(2M_1) + \tanh(2M_2) + \tanh(2M_3)]^2} \tag{19}$$

This functional relation for $\chi_{0,\mathrm{Kag}}$ is valid for arbitrary values of K_1, K_2, K_3, with the exception of the values that satisfy condition (7). If K_1, K_2, K_3 are all positive and on the critical variety of the model, (18) enables us to obtain information on the critical behavior of the susceptibility on a region of competing interactions (the critical variety is invariant with respect to the change of sign of two of the three interaction parameters). It is deduced from Eq. (18) that the dominant singularity of $\chi_{0,\mathrm{Kag}}(K_1, -K_2, -K_3)$ is the same as that of $\chi_{0,\mathrm{Kag}}(K_1, K_2, K_3)$, but the correction terms are different, owing to the contribution of the integral term in the right-hand side of (18). These contributions are of the form $t^n \log(t)$, where $t = (T_c - T)/T_c$ is the reduced temperature and n is an integer.

To summarize, in this paper we have found exact expressions for the zero-field susceptibility of the anisotropic Kagomé lattice Ising model. The first expression, given by (11), is valid on the disorder variety (12), and the second one, given by (14), holds on the variety defined by condition (13). Also, we have found a functional relation for $\chi_{0,\mathrm{Kag}}$, given by Eq. (18). This relation enables us to obtain information about the critical behavior of the susceptibility in a region of competing interactions of the parameter space of the model.

APPENDIX. SUSCEPTIBILITY OF THE KAGOMÉ LATTICE ISING MODEL ON THE DISORDER VARIETY

In order to obtain the expression of the susceptibility on the disorder variety, we apply a local criterion, found be means of a decimation method, in refs. 16 and 18. This local criterion can be stated as follows: when the following condition is satisfied

$$\sum_{\sigma_1, \sigma_2, \sigma_3} W(\sigma_1, \sigma_2, \sigma_3, \sigma_4, \sigma_5) = \lambda \tag{A1}$$

where λ is a constant independent of σ_4 and σ_5, then the partition function per site in the thermodynamic limit is given by

$$Z^{1/3N} = \lambda^{1/3} \tag{A2}$$

Here, $W(\sigma_1, \sigma_2, \sigma_3, \sigma_4, \sigma_5)$ is the Boltzmann weight associated to the elementary cell of the Kagomé lattice shown in Fig. 1, and is given by

$$\begin{aligned} &W(\sigma_1, \sigma_2, \sigma_3, \sigma_4, \sigma_5) \\ &\quad = \exp\{K_1(\sigma_1\sigma_3 + \sigma_3\sigma_4) \\ &\qquad + K_2(\sigma_2\sigma_3 + \sigma_3\sigma_5) + K_3(\sigma_1\sigma_2 + \sigma_4\sigma_5) \\ &\qquad + H\sigma_3 + H/2(\sigma_1 + \sigma_2 + \sigma_4 + \sigma_5) \\ &\qquad + H_1(\sigma_1 - \sigma_4) + H_2(\sigma_2 - \sigma_5)\} \end{aligned} \tag{A3}$$

where H_1 and H_2 are auxiliary fields that are canceled when the Boltzmann weights associated to all cells of the lattice are multiplied away. These auxiliary fields are introduced in order to verify condition (A1) with the minimal constraints on the parameters of the model.

From (A1) and (A3), by giving all possibles values to σ_4 and σ_5, we obtain the following equations:

$$\begin{aligned} &\cosh(2K_1 + 2K_2 + H)e^{2K_3 + 2H} + \cosh(H)e^{2K_3 + 2H_1 + 2H_2} \\ &\quad + \sum_{i \neq j; i; j = 1}^{2} \cosh(2K_i + H)e^{H + 2H_j} = \lambda \\ &\cosh(H)e^{2K_3 - 2H_1 - 2H_2} + \cosh(2K_1 + 2K_2 - H)e^{2K_3 - 2H} \\ &\quad + \sum_{i \neq j; i, j = 1}^{2} \cosh(2K_i - H)e^{-H - 2H_j} = \lambda \\ &\cosh(2K_1 - 2K_2 + H)e^{-2K_3} + \cosh(H)e^{-2K_3 + 2H_1 - 2H_2} \\ &\quad + \cosh(2K_1 + H)e^{H - 2H_2} + \cosh(2K_2 - H)e^{-H + 2H_1} = \lambda \\ &\cosh(H)e^{-2K_3 - 2H_1 + 2H_2} + \cosh(-2K_1 + 2K_2 + H)e^{-2K_3} \\ &\quad + \cosh(2K_2 + H)e^{H - 2H_1} + \cosh(2K_1 - H)e^{-H + 2H_2} = \lambda \end{aligned} \tag{A4}$$

The zero-field susceptibility is given by

$$\chi_{0,\mathrm{Kag}} = \left. \frac{\lambda\, \partial^2\lambda/\partial H^2 - (\partial\lambda/\partial H)^2}{3\lambda^2} \right|_{H=0} \tag{A5}$$

Explicit expression for λ, $\partial\lambda/\partial H$, and $\partial^2 \lambda/\partial H^2$ can be found, for the case $H=0$, from Eqs. (A4). After a very lengthly algebra we found the final expression given by Eq. (12) in the text and valid on the variety (13). Other independent solutions can be obtained by using the permutation symmetry of the model with respect to K_1, K_2, K_3. This type of disorder solution is valid only for real values of the parameters of the model, as is discussed in ref. 18.

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