Exact results for Ising models on the triangular Kagomé lattice

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A two-dimensional Ising model on a particular topological structure, a "triangles-in-triangles" Kagomé structure, which is called a triangular-Kagomé lattice, is investigated. In this model, we consider two interaction parameters J_{aa} and J_{ab}, corresponding to the interactions among spins on the inner sites and between spins on the inner and vertex sites of the triangular in the Kagomé lattice, respectively. By summing over all spins at inner sites in the partition function, we arrive at the partition function of the Kagomé lattice. The effective interaction of the corresponding Kagomé lattice is always ferromagnetic, even for antiferromagnetic J_{aa}. The critical properties of the system depend only on $J_{aa}/|J_{ab}|$. When $J_{aa}/|J_{ab}|>-1$, the system has long range order at low temperature. However, when $J_{aa}/|J_{ab}|<-1$, the partition function of the triangular-Kagomé lattice can be related to that of the Kagomé lattice with effective interaction at a temperature higher than its critical temperature. Therefore, the system will be in paramagnetic phase at all temperatures for $J_{aa}/|J_{ab}|<-1$. The phase diagram for $J_{aa}/|J_{ab}|$ is given exactly.

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Since Onsager solved exactly the problems of the Ising model for the case of a square lattice,[1] the same problems for many other two-dimensional lattices, such as triangular,[2,3] honeycomb,[4,5] Kagomé lattice[6] and so on, have been treated by several authors. When the interaction is antiferromagnetic, some of them are very frustrated, such as triangular and Kagomé lattices, and in these cases there is no long range order at finite temperature.

Recently $Cu_9X_2(cpa)_6$ (cpa=carboxypentonic acid; X=F, Cl, Br) was discovered to form a particular topological structure, a "triangles-in-triangles" Kagomé structure,[7,8] which was called a triangular-Kagomé lattice. The structure of this compound is shown in Fig. 1. As shown in Fig. 1, a triangular-Kagomé lattice is made by dividing each triangle in the Kagomé lattice into four small triangles. The triangular-Kagomé lattice has two geometrically inequivalent sites *a* and *b*, as shown in Fig. 1, although both sites have four neighbors.

The magnetic properties of these systems have also been studied recently. The magnetic susceptibility observed under 10 kG obeyed the Curie-Weiss law down to 150 K with Weiss temperatures of −237, −226, and −243 K for X=F, Cl, Br, respectively.[9–12] These large negative values suggest very strong antiferromagnetic exchange interactions, which may be on the order of hundreds k_B. The magnetization in magnetic field up to 38 T does not reach full saturation, which shows that the antiferromagnetic exchange interactions are much stronger than this field. In an electron-spin resonance experiment,[13] the transmission spectra observed in a triangular-Kagomé lattice show that the resonance field remains constant as the temperature is decreased. In inelastic neutron scattering measurements,[14] dispersionless scattering around 6.5 meV is observed, which indicates a single-site excitation with about $70k_B$. It is noticeable that this single-site excitation is smaller than that caused by the antiferromagnetic exchange interactions. Thus, it may relate to spin flipping under other weaker interactions instead of the strong antiferromagnetic ones.

Based on these experiments and the consideration of exchange paths, it is expected that the interaction J_{aa} among sites *a* is antiferromagnetic and that its strength is much stronger than the interaction J_{ab} between sites *a* and *b*, which is always ferromagnetic. Further, Mekata has interpreted the magnetic properties in terms of the plaquette ordering model, which assumes a 120° arrangement of three moments on each triangular plaquette and a random freezing of the remaining paramagnetic moments. This interpretation is apparently based on a classical Heisenberg spins model, which corresponds to spin→∞.

For this compound, the magnetic moments come from Cu^{2+} with spin 1/2. Therefore, the spin-1/2 Heisenberg model may be more appropriate than the classical Heisenberg spin for this compound. Theoretical study for the spin-1/2 Heisenberg model on the triangular-Kagomé lattice also exists, based on the linear Holstein-Primakoff spin wave theorem.[15] The spin-1/2 Heisenberg model is a quantum magnetic model and is very difficult to treat. Until now, no

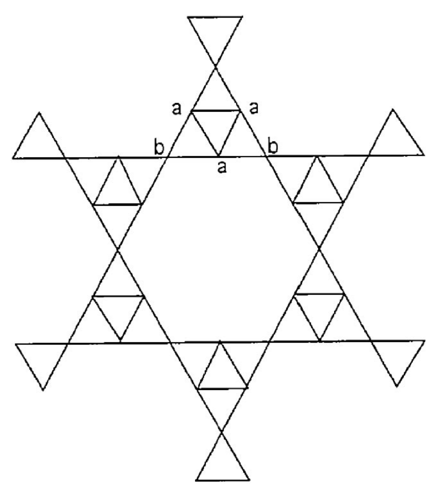

FIG. 1. Schematic drawing of triangular-Kagomé lattice. The two geometrically inequivalent sites *a* and *b* are shown.

exact solutions exist for any two-dimensional Heisenberg model, regardless of the spin value.

In this report, we adapt an Ising-type interaction instead of the Heisenberg type, i.e., we ignore the quantum fluctuation in the spin-$1/2$ Heisenberg model. The Ising model can also be seen as a limiting case of the classical Heisenberg model with infinite easy-axis anisotropy, which may result in some discrepancy with experiments. However, it is fascinating that the model of Ising-type interaction can be solved exactly. Furthermore, the antiferromagnetic interaction J_{aa} in the Ising model will cause both types of triangles, $\triangle aaa$ and $\triangle aab$, to be frustrated. The existence of all these frustrated triangles will result in some properties similar to those observed in other frustrated Ising models, among which are that, no long range order exists in finite temperature, the ground states are very degenerate, and the entropy is nonzero at absolute zero temperature. We shall investigate the effect of the frustrated triangular plaquette in this model in detail.

We shall exactly solve the transition temperature of the Ising model on triangular-Kagomé lattice with only the nearest-neighbor interaction by the decimation of spins on site a.[16] The Hamiltonian of this system is

$$H_0 = -J_{aa}\sum_{\langle i,j\rangle}\sigma_i\sigma_j - J_{ab}\sum_{\langle i,l\rangle}\sigma_i S_l, \tag{1}$$

where σ_i, $S_l = \pm 1$ are spin variables for sites a and b, respectively, i and j are site labels for site a, and l is the site label for site b. $\Sigma_{\langle ..\rangle}$ indicates the summation is over corresponding nearest-neighbor pairs. From Hamiltonian (1), we find that simultaneously changing the sign of J_{ab} and reversing the definition of directions of all the b spins, the Hamiltonian is invariant. Thus, the critical properties should not depend on the sign of the interaction J_{ab}, although their magnetization is different.

The partition function of the model is given by

$$Z(K_{aa},K_{ab}) = \sum_{\{\sigma_i\}\{S_l\}}\exp[-\beta H_0], \tag{2}$$

where $\beta = 1/k_B T$, $K_{aa} = \beta J_{aa}$, and $K_{ab} = \beta J_{ab}$. The triangular-Kagomé lattice is different from the Kagomé lattice by considering more detailed structures in the triangles in the Kagomé lattice, as shown in Fig. 1, i.e., one $\triangle aaa$ and three $\triangle aab$ are defined clearly for the triangular-Kagomé lattice, instead of only a large $\triangle bbb$ as in the Kagomé lattice. It is noticeable that in the triangular-Kagomé model, each of the three sites a in the large triangle $\triangle bbb$ can only couple with its vertex on a b site, except the interactions among themselves. Therefore, we can first sum over the spins on sites a for a fixed spin configuration of site b. It can be found that after the decimation of the spins on sites a, the triangle $\triangle bbb$ is transformed to an Ising model coupled between sites b directly with an effective interaction strength K; i.e.,

$$\begin{aligned}\sum_{\sigma_4,\sigma_5,\sigma_6}&\exp\{(K_{ab}\,[(S_1+S_2)\sigma_4+(S_1+S_3)\sigma_5+(S_2+S_3)\sigma_6]\\&+K_{aa}(\sigma_4\sigma_5+\sigma_5\sigma_6+\sigma_6\sigma_4)\}\\&=A\exp[K(S_1S_2+S_2S_3+S_3S_1)],\end{aligned} \tag{3}$$

where

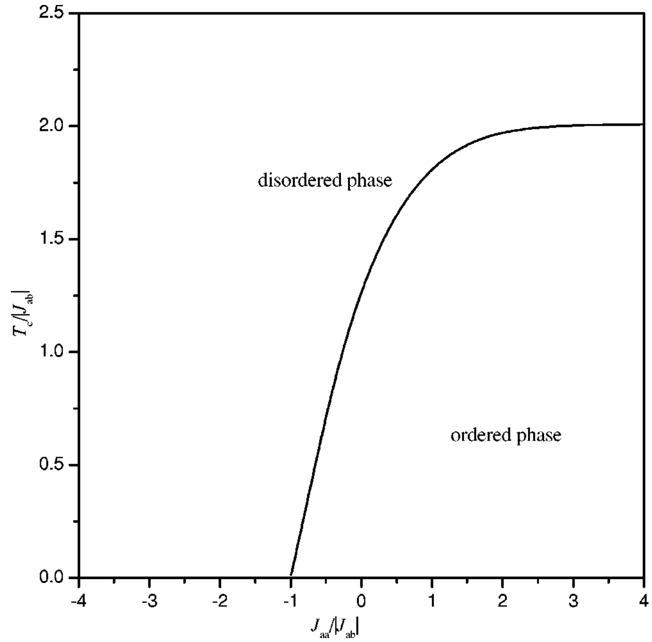

FIG. 2. Phase diagram of the Ising model on the triangular-Kagomé lattice.

$$e^{4K} = \frac{e^{3K_{aa}}\cosh(6K_{ab}) + 3e^{-K_{aa}}\cosh(2K_{ab})}{(e^{3K_{aa}} + 3e^{-K_{aa}})\cosh(2K_{ab})}, \tag{4}$$

and

$$A = 2e^{K}(e^{3K_{aa}} + 3e^{-K_{aa}})\cosh(2K_{ab}). \tag{5}$$

If the decimation is carried out on the whole lattice, the triangular-Kagomé lattice will be transformed into the Kagomé lattice. The relation between the partition function of the Ising model on triangular-Kagomé lattice $Z(K_{aa},K_{ab})$ and that on the Kagomé lattice $Z_k(K)$ is

$$Z(K_{aa},K_{ab}) = A^N \times Z_k(K), \tag{6}$$

where N is the number of the triangles on the Kagomé lattice. Now, we have established a mapping relation between the partition function of the Ising model on the triangular-Kagomé lattice and that on the Kagomé lattice, and the latter has exact results already.[6]

From Eq. (4), we can easily find that the effective interaction strength K is an even function of J_{ab}, which shows that the critical properties of the model do not depend on the sign of the interaction J_{ab} as described previously. Furthermore, in Eq. (4) the numerator is always larger than its denominator. Thus, the effective interaction strength K is always larger than zero, corresponding to a ferromagnetic Ising model on the Kagomé lattice. The singular part in Eq. (6) can only result from the partition function of the Ising model on the Kagomé lattice, which has a logarithmically divergent specific heat at the critical temperature $e^{4K^c} = 3 + 2\sqrt{3}$.[6] By use of the relationship between the Kagomé model and the triangular-Kagomé model as described in Eq. (4), the critical temperature of the Ising model for the triangular-Kagomé lattice is

$$\frac{\exp\left(3\frac{J_{aa}}{|J_{ab}|}K_{ab}^c\right)\cosh(6K_{ab}^c) + 3\exp\left(-\frac{J_{aa}}{|J_{ab}|}K_{ab}^c\right)\cosh(2K_{ab}^c)}{\left[\exp\left(3\frac{J_{aa}}{|J_{ab}|}K_{ab}^c\right) + 3\exp\left(-\frac{J_{aa}}{|J_{ab}|}K_{ab}^c\right)\right]\cosh(2K_{ab}^c)} = 3 + 2\sqrt{3}, \tag{7}$$

where $K_{ab}^c = |J_{ab}|/k_B T_c$, which is only a function of $J_{aa}/|J_{ab}|$. Figure 2 shows the critical temperature $k_B T_c/|J_{ab}|$ as a function of $J_{aa}/|J_{ab}|$.

From Fig. 2, we can see that there exists a long range order phase at low temperature in the region $J_{aa}/|J_{ab}| > -1$. For the region $J_{aa}/|J_{ab}| < -1$, no long range order exists. To illustrate what happens at $J_{aa}/|J_{ab}| = -1$, we emphasize the following fact. If J_{aa} is antiferromagnetic, all triangles of the system have an odd number of antiferromagnetic bonds, which means that all triangles are frustrated. However, if $J_{aa}/|J_{ab}| > -1$, the wrong bond can be located only at J_{aa} for the ground state of the triangle $\triangle aab$. Therefore, in the ground state of the large triangles $\triangle bbb$, all spins at site a are parallel aligned. The alignment of the spins on sites a and b are parallel or antiparallel according to the sign of J_{ab}, so that the spins on sites b are also parallel aligned. In this case, the ground state of the whole system is twofold degenerate and can be effectively related to a ferromagnetic Ising model on the Kagomé lattice at any temperature. Therefore, it has long range order at low temperature and a finite critical temperature. It is not surprising now that a fully frustrated Ising model has long range order at low temperature. For example, the exact solution of the Ising model on a Kagomé lattice with anisotropic ferromagnetic and antiferromagnetic interaction and a magnetic field[17] also shows finite critical temperature for a frustrated case similar to our case. In fact, in these cases the systems are not "really frustrated," because the ground state in the large triangle is twofold degenerate in spite of all small triangles being frustrated.

For the case of $J_{aa}/|J_{ab}| < -1$, the situation is different. In this case, the frustrated triangle $\triangle aaa$ becomes dominant and should be in the lowest energy state, which is two spins in one direction and the other in opposite direction. Then, the spin on site b neighboring the two parallel-aligned spins of sites a is decisively determined. However, the spins on the other two sites b can be in either direction without energy changes. The ground state of the whole system in this case is infinitely degenerate. This implies that the frustrated triangle $\triangle aaa$ will block off the effective interaction between sites b for the large triangle $\triangle bbb$. Our calculation shows that the effective interaction is always ferromagnetic, but with an effective temperature higher than the critical point for all temperature regions. Therefore, the system is always in paramagnetic phase for $J_{aa}/|J_{ab}| < -1$ and no phase transition will occur.

In summary, exact solutions of the Ising model with two kinds of interactions on triangular-Kagomé lattice have been obtained by the decimation of some spins, which transforms the triangular-Kagomé lattice into the Kagomé lattice. The phase diagram is given as a function of $J_{aa}/|J_{ab}|$. We also investigated the effects of frustration in the Ising model on triangular-Kagomé lattice in detail. Our results show that the existence of the long range order is determined only by the degeneracy of the ground state.

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