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Low Temperature Properties of Antiferromagnets on the Kagome Lattice

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Thermodynamic properties of antiferromagnets on the kagome lattice at low temperatures are studied for classical Heisenberg spin systems. In pure Heisenberg model, a coplanar structure is chosen by the entropy effect but it has been turned out to be disorder. Namely, it is not the $\sqrt{3}$-structure in spite of the previous conjectures. The properties are also compared with those of quantum spin systems.
KEYWORDS: kagome antiferromagnet, Monte Carlo method, frustration

1. Introduction

Thermodynamic properties of antiferromagnets on the kagome lattice have been paid much attention because of the macroscopic degeneracy of the ground state due to the frustration.[1] In this lattice, the effect of the frustration is much strong than in the fully frustrated lattice such as the triangular lattice. The ground state of the $S = 1/2$ Ising antiferromagnetic model is the paramagnetic state, namely the spin correlation function decays exponentially[2, 3], which is more disorder than the case of the triangular lattice where the correlation function decays by a power law [4]. In the case of the XY spin system the ground state of the kagome lattice is still macroscopically degenerate although the ground state in the triangular lattice has only microscopic degeneracy due to the symmetry of the order parameter (120° structure: Fig.1(a) which has $Z_2 \times S_1$, a twofold degeneracy and a rotational degeneracy). In the kagome lattice, spins keeps the 120° structure at each triangle, but there exists macroscopic combinations to locate the 120° structures on the kagome lattice because of low connectivity of the lattice. The situation of the degeneracy is equivalent to that in the antiferromagnet 3-state Potts model[5]. In the case of the Heisenberg spin systems, the 120° structures of neighboring triangles can be twisted (Fig. 1(b)), which causes local degeneracy.

In this paper we study ordering properties of the model at low temperatures.

2. Classical system

It has been pointed out that a coplanar structure is chosen by an entropical effect in the Heisenberg system where non-coplanar structures are also degenerate as the grand state. We have investigated how the coplanar structure is formed as the temperature goes down through the quantity

$$X = \sum_i |\vec{\kappa} \cdot \mathbf{n}| \qquad (1)$$

where $\vec{\kappa}$ is the chirality at each triangle[6]

$$\vec{\kappa} = \frac{1}{2\sqrt{3}} \left(\vec{S}_1 \times \vec{S}_2 + \vec{S}_2 \times \vec{S}_3 + \vec{S}_3 \times \vec{S}_1 \right)$$

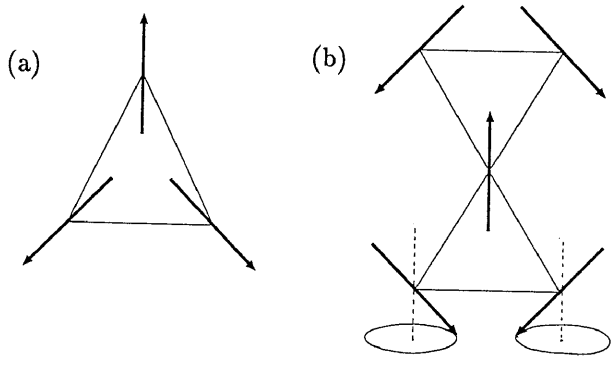


Figure 1: (a) the 120° structures. (b) Twist of the 120° structures

and $\mathbf{n}$ is a normal vector perpendicular to the plane. The plane is chosen to make X maximum. In Fig. 2, the temperature dependence of X is shown Here we find the coplanar structure is suddenly formed at $T < 0.02J$, where J is the coupling constant of the Heisenberg model. We also investigated other parameters to check the coplanar nature and obtained consistent results.

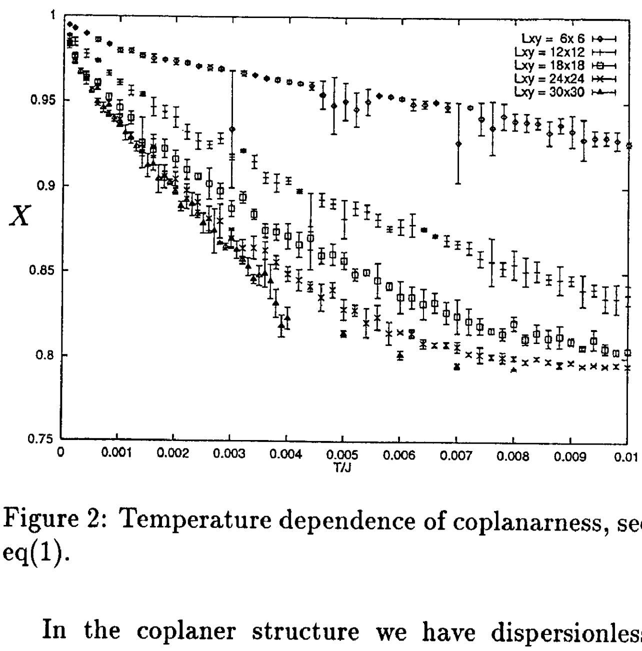


Figure 2: Temperature dependence of coplanarness, see eq(1).

In the coplaner structure we have dispersionless mode which causes a reduction of the specific heat at

$T = 0$ [7, 8, 9]. In Fig. 3, the temperature dependence of the specific heat, C, is given. There the low temperature behavior in $0.02 < T < 0.05$, $C/N \sim k_B$, is consistent with the Dulong-Petit law. Below the temperature region, however, the specific heat decreases as the temperature goes down. The unit cell of the kagome lattice consists of three spins and thus there are 6 modes. One of them has been found to be dispersionless in the harmonic analysis[7]. Due to the higher order correction the mode give a contribution of $k_B/4$ instead of $k_B/2$. Thus at $T = 0$ we expect that

$$C = \frac{Nk_B}{3}\left(5 \times \frac{1}{2} + \frac{1}{4}\right) = \frac{11}{12}Nk_B \qquad (2)$$

In the Fig. 3, the data for $N = 108$ we find a good agreement of C at $T = 0$ with the prediction (2). More precisely C at $T = 0$ have a deviation, which is due to a contribution of global rotations. Namely the total degree of freedom is reduced by 2 for global rotations and the right hand side of (2) should be reduced by 2. For large N, this reduction is negligible but is seen for small lattices such as with $N = 27$.

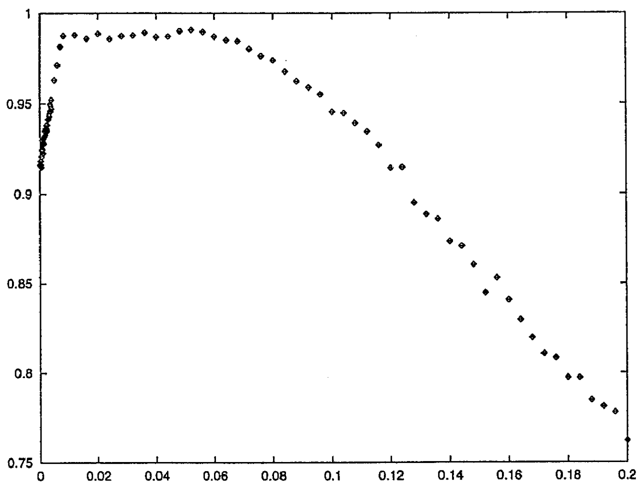


Figure 3: Temperature dependence of the specific heat. N=576.

In Fig. 4, the magnetic susceptibility is also shown, where we find very flat temperature dependence which reminds us the case of the triangular lattice [6].

By entropy effect, the spins lay on a plane but there are still macroscopic degeneracy as the XY case. One may expect that system with Heisenberg model can be ordered due to the entropy effect of a fluctuation perpendicular to the plane. Thus, it has been an interesting problem to determine the spin structure chosen at $T = 0$ for the Heisenberg model. There are two possible spin configurations with long range order. Namely the $\sqrt{3}$- and the q=0-structure (Fig. 5).

So far, there has been some conjectures to support the $\sqrt{3}$-structure [8]. In this paper we study the spin structure at very low temperatures in detail. In order to see which structure is more stable, we have performed Monte Carlo simulation with initial conditions with the the $\sqrt{3}$-structure and the q=0-structure. It turns out that the the $\sqrt{3}$-structure collapses very soon

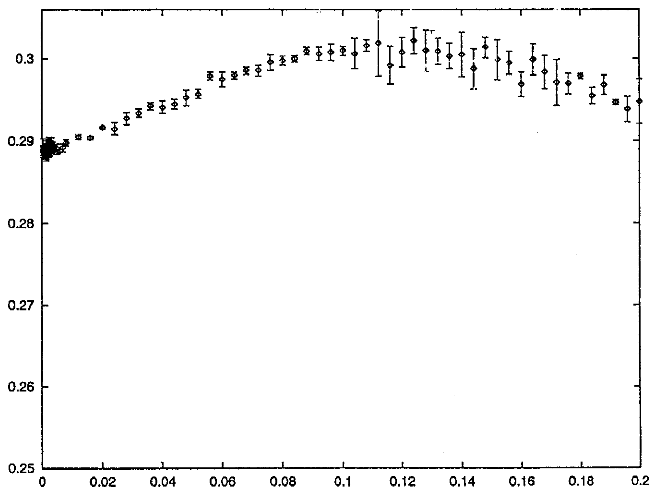
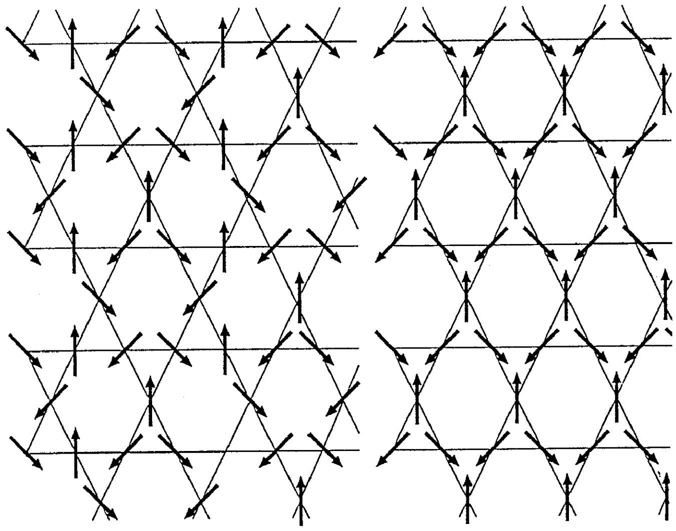


Figure 4: Temperature dependence of the magnetic susceptibility. N=576.



(a) (b)

Figure 5: The ground state spin structures with (a) 3 - and (b) the q=0-structure.

while the q=0-structure stays rather long time. But both structures collapse in long time. Thus we conclude that the the $\sqrt{3}$-structure is not stable at very low temperatures and a mixture of the $\sqrt{3}$-structure and the q=0-structure seems more stable and that the ground state of the Heisenberg model is disorder.

In Fig. 6, data of the specific heat observed along processes with raising the temperature from both initial states, where + and ◇ denote data with the $\sqrt{3}$- and q=0-structures, respectively.

Effect of anisotropy on the thermodynamic properties are also studied and we found that even very small anisotropy cause big changes in the temperature dependences of quantities. In Fig. 7, the dependences on the anisotropy of the specific heat are shown for both Ising-like case and XY-like case, where A is a parameter for

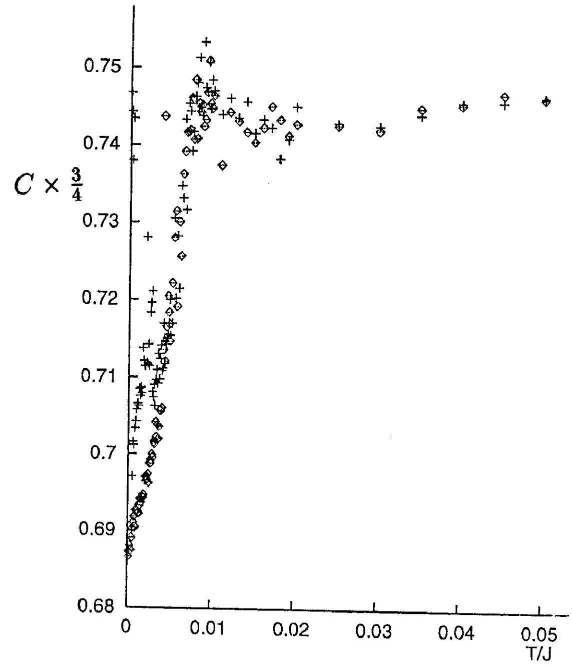


Figure 6: The specific heat observed along processes with raising the temperature from both initial states, where + and ◇ denote data with the root-3 and q=0 structures, respectively. N=576.

the anisotropy:

$$\mathcal{H} = J \sum_{<ij>} (S_i^x S_j^x + S_i^y S_j^y + A S_i^z S_j^z)$$

Here we find that even very small anisotropy causes a sharp peak in the specific heat. It is also find that the reduction of the specific heat at $T = 0$ does not occur in the anisotropic cases.

For all properties reported in this section will be reported elsewhere with more detailed analyses such as size-dependence and error analyses, etc.[10].

3. Quantum system and Discussion

Furthermore, we have studied the ordering nature of the quantum spin systems with $S = 1/2$. So far this model has been studied by the diagonalization method and the high temperature expansion method[11] and has been pointed out to have double peaks in the specific heat. And it has been pointed out that there are various structures in larger lattices[12]. It is, thus, an interesting problem to obtain the specific heat in the thermodynamic limit. For this purpose a study of Quantum Monte Carlo simulation is expected. But because of the negative sign problem quantum Monte Carlo method has not been applied to this model. However, recently one of the authors (S.M.) has proposed a new technique to overcome the negative sign problem named transfer-matrix-Monte Carlo method[13]. This method is applied to the present model[14] and succeeded to investigate larger lattice ($N = 36$ and 72). A preliminary analysis of data shows little changes of the double peak structure. Detail data will be reported elsewhere[14]. The chirality susceptibility $\langle(\sum_i \vec{\kappa})^2\rangle$ shows smooth temperature dependence. On the oth-

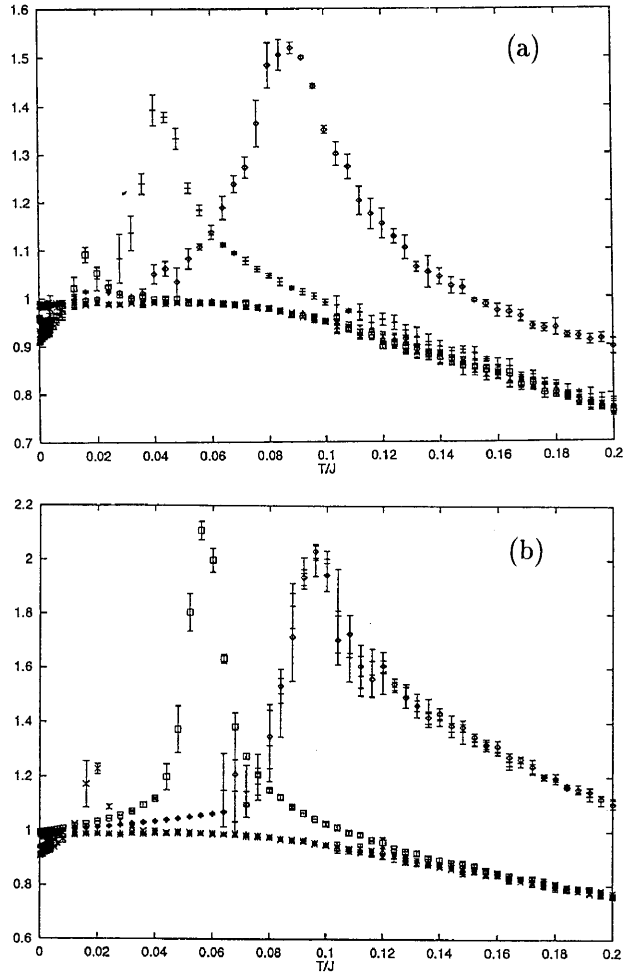


Figure 7: Dependences of the specific heat on the anisotry (a)Ising like case (b) XY like case

erhand, the magnetic susceptibility shows a sharp decrease, which is special for the quantum systems. In Fig. 8, these quantities are shown. At this temperature no sharp change is found in the shart range spin correlation. It is an interesting problem why the susceptibility drops sharply, which usually suggests a existence of a gap in the energy spectrum.

So far, the entropy effect is not clear in quantum system where arrangement of sinlet pairs seems to be more relevant like the RVB state in the triagular lattice[15]. Including the source of the sharp drop of the susceptibility and the peaks of the specific heat, the effect of entropy in other words, degeneracy, in the quantum system is a very interesting problem in the future.

Acknowledgements

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1) V. Elser: Phys. Rev. Lett. 62 (1989) 2405.

2) C. Chappert and P.Bruno: J. Appl. Phys. 64 (1988), 5736.

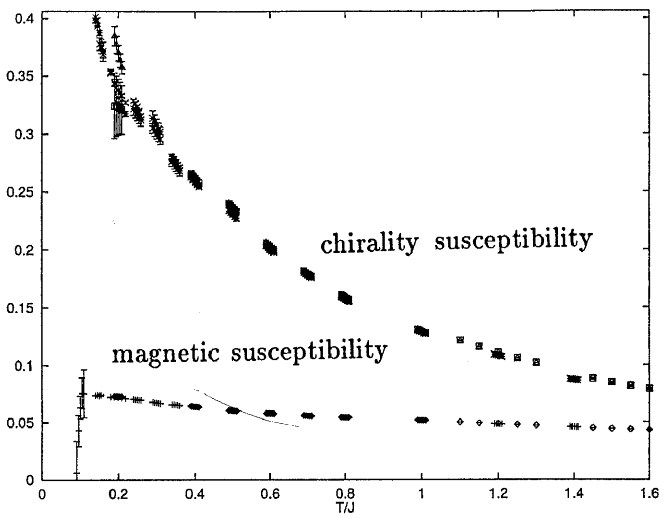

Figure 8: Temperature dependences of the chirality susceptibility and the magnetic susceptibility in the quantum system

3) J. H. Barry, M. Khatun and T. Tanaka, Phys. Rev. B37 (1988) 5193.

4) J. Stephenson:J. Math. Phys. 11 (1970) 413.

5) D. A. Huse and A. D. Rutenberg, Phys. Rev. B45 (1992) 7536.

6) S. Miyashita and H. Shiba: J. Phys. Soc. Jpn. 53 (1984) 1145. H. Kawamura and S. Miyashita: J. Phys. Soc. Jpn. 53 (1984) 9 and 4138.

7) J. T. Chalker, P. C. W. Holdsworth and E. F. Shenker, Phys. Rev. Lett. 68 (1992) 855.

8) Harris et al, Phys. Rev. B45 (1992) 2899.

9) J. N. Reimers and A. J. Berlinsky: Phys. Rev. B48 (1993) 9539.

10) A. Kuroda, T. Yoshino and S. Miyashita, in preparation.

11) N. Elstner and A. P. Young: Phys. Rev. B50 (1994) 6871.

12) H. U. Everts, private communication.

13) S. Miyashita, J. Phys. Soc. Jpn. 63 (1994) 2449.

14) T. Nakanura and S. Miyashita, in preparation.

15) P. Fazakas and P. W. Anderson: Phil. Mag. 30 (1974) 423.