Mechanism for lifting the degeneracy
in the double-exchange spin ice model on a kagomé lattice:
Dodecamer formation

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Abstract

We investigated the double-exchange spin ice model on a kagomé lattice by Monte Carlo simulation in order to study a mechanism for lifting the degeneracy in frustrated electron systems. We show specific heat and vector spin chirality data on a finite lattice. Specific heat has a double-peak structure: A broad peak and a sharp peak are at $k_B T/t \sim 0.15$ and $0.015$, respectively, where $t$ is the transfer integral of electrons. The broad peak corresponds to a crossover to the spin ice-like state, on the other hand, the sharp one a transition to a dodecagonal spin cluster (dodecamer) state. We discuss the interplay between the formation of the dodecamer state and the lifting of the macroscopic degeneracy.

Key words: Dodecamer; Cluster order; Frustration; Double-exchange; Monte-Carlo calculation

Macroscopic degeneracy is one of the well-known properties in frustrated systems. However, such a degeneracy should be lifted at $T = 0$ in realistic systems because of the third law of thermodynamics. Considering these circumstances, it is significant to investigate mechanisms to lift the degeneracy. In particular, a peculiar mechanism is expected in electron systems with the frustration: The motion of electrons plays an important role for lifting macroscopic degeneracy, which may lead to some kinds of exotic phases.

In order to see such a mechanism, we investigate a double-exchange spin ice (DESI) model on a kagomé lattice by a Monte-Carlo (MC) simulation [1], where the kagomé lattice consists of corner-shared up- and down-triangles. The DESI model is the Anderson-Hasegawa model [2] with a following condition: Localized spins have uniaxial anisotropies that they are forced to point either inward (in-spin) or outward (out-spin) for an up-triangle. In this case, localized spins are coplanar. The uniaxial anisotropies and ferromagnetic interaction between the nearest-neighbor (n.n.) spins due to the Anderson-Hasegawa mechanism cause the frustration in the model for the same reason seen in the spin ice systems [3].

From our previous MC calculations, following results have been obtained [1]: At sufficiently low temperatures, a dodecagonal localized spin cluster, “dodecamer” [see Fig. 1], is realized in a wide doping region $n \simeq 1/3 \sim 1/2$, where $n$ is the number of particles per site. The dodecamer order is driven by both the kinetic energy gain and the frustration.

In this paper, specific heat and vector spin chirality data of the system are shown, in wide temperature range in order to investigate a relation between the
The chemical potential $\mu = 0$. We can see a double-peak structure: A broad peak is seen at $k_B T / t \sim 0.15$ and a sharp peak is at $k_B T / t \sim 0.015$, where $t$ is the transfer integral of electrons.

To clarify the origin of the broad peak, we check a spin configuration of the system. A vector spin chirality is defined for triangles in the kagomé lattice which has the form, $\vec{v} = -\frac{1}{3} \left( \vec{S}_i \times \vec{S}_j + \vec{S}_j \times \vec{S}_k + \vec{S}_k \times \vec{S}_i \right)$, where $i$, $j$, and $k$ represents three sites of a triangle. Here, we set $|\vec{S}_i| = 1$. We only consider the $z$-component of $\vec{v}$, because localized spins are coplanar in the system. Each triangle is allowed to take “three-out” ($v^z = -3$), “three-in” ($v^z = -3$), “two-in one-out” ($v^z = 1$) or “one-in two-out” ($v^z = 1$) spin structures. At sufficiently high temperatures, all of these patterns are realized equally; i.e., $\langle v^z \rangle = 0$, since both one-in two-out and two-in one-out have a three-fold degeneracy. On the other hand, as the temperature is lowered, three-out and three-in states are excluded, because they have higher energy than the others due to the n.n. ferromagnetic interaction. Then, the system has $\langle v^z \rangle \rightarrow 1$. This situation is similar to the spin ice systems [3]. Thus, we call such states an “ice state”, hereafter.

Temperature dependence of $\langle v^z \rangle$ are shown in Fig. 2. $\langle v^z \rangle$ grows as the temperature is lowered, and almost saturates below the broad peak. This means that the system becomes the ice state at the broad peak temperature. Thus, we conclude that the broad peak of the specific heat data corresponds to a crossover to the ice state. Note that the ice state still has the macroscopic degeneracy due to the frustration.

Next, let us consider the sharp peak in the specific heat data. We investigated a dodecamer structure factor $D_q$ in Ref [1]. The largest peak of $D_q$ is defined as $\tilde{D}_q$, which shows a rapid change at $k_B T / t \sim 0.015$. Temperature dependence of $D_q$ indicates that there is an inflection point in this temperature range. The sharp peak temperature is almost consistent with that of the inflection point. Thus, it is considered that the sharp peak corresponds to a phase transition from the ice state to the dodecamer state, which is smeared out by the finite-size effect.

In conclusion, the process for lifting the degeneracy in the system is as follows: At intermediate temperatures, the n.n. ferromagnetic interaction leads the system to the ice state, which still has the macroscopic degeneracy. According to this result, the short-range correlation is considered to be insufficient to lift the degeneracy, often seen in the classical spin systems. Furthermore, at sufficiently low temperature region, the effective long-range interaction is relevant in order to gain the kinetic energy, and the degeneracy is lifted by the dodecamer formation accompanied with the translational symmetry breaking.
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