Nonequilibrium relaxation study of the anisotropic antiferromagnetic Heisenberg model on the triangular lattice

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Antiferromagnet on the two-dimensional triangular lattice has been intensively studied as one of the most fundamental models for the geometrically frustrated systems.1 For the isotropic Heisenberg model with nearest-neighbor interactions, it is believed that the ground state of the system exhibits a three-sublattice 120° long-range order,2 whereas the magnetic ordering is no longer retained against thermal fluctuations.3 Nevertheless, an interesting possibility was proposed by Kawamura and Miyashita,4,5 that is, an unconventional topological transition at a finite temperature (T) — Z2 vortex transition. From the symmetry point of view, the Z2 vortex transition is different from the conventional Berezinskii-Kosterlitz-Thouless (BKT) transition which occurs in the presence of anisotropy.6,7 The relation between these two topological transitions, however, is not fully understood yet. In particular, it is still unclear how the system behaves in the region of vanishing anisotropy.

Experimentally, several materials with triangular layered structure have been studied, and recently, the Z2 vortex attracts renewed interests for understanding of their peculiar properties. One of the peculiar properties is anomalous enhancement of the spin relaxation time. Critical divergence of the relaxation time is observed in an anomalously wide range of temperatures.8,9,10 As the anisotropy decreases, both the critical temperatures steeply decrease, while the BKT critical region becomes divergently wide. We elucidate a sharp "V" shape of the phase diagram around the isotropic Heisenberg point, which suggests that the isotropic case is exceptionally singular and the associated Z2 vortex transition will be isolated from the BKT and chiral transitions. We discuss the relevance of our results to peculiar behavior of the spin relaxation time observed experimentally in triangular antiferromagnets.

KEYWORDS: geometrical frustration, triangular lattice, Heisenberg model, nonequilibrium relaxation, BKT transition, chiral transition, Z2 vortex transition

Effect of exchange anisotropy on the relaxation time of spin and vector chirality is studied for the antiferromagnetic classical Heisenberg model on the triangular lattice by using the nonequilibrium relaxation Monte Carlo method. We identify the Berezinskii-Kosterlitz-Thouless (BKT) transition and the chiral transition in a wide range of the anisotropy, even for very small anisotropy of ~ 0.01%. As the anisotropy decreases, both the critical temperatures steeply decrease, while the BKT critical region becomes divergently wide. We elucidate a sharp "V" shape of the phase diagram around the isotropic Heisenberg point, which suggests that the isotropic case is exceptionally singular and the associated Z2 vortex transition will be isolated from the BKT and chiral transitions. We discuss the relevance of our results to peculiar behavior of the spin relaxation time observed experimentally in triangular antiferromagnets.

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Experimentally, several materials with triangular layered structure have been studied, and recently, the Z2 vortex attracts renewed interests for understanding of their peculiar properties. One of the peculiar properties is anomalous enhancement of the spin relaxation time. Critical divergence of the relaxation time is observed in an anomalously wide range of temperatures.8,9,10 As the anisotropy decreases, both the critical temperatures steeply decrease, while the BKT critical region becomes divergently wide. We elucidate a sharp "V" shape of the phase diagram around the isotropic Heisenberg point, which suggests that the isotropic case is exceptionally singular and the associated Z2 vortex transition will be isolated from the BKT and chiral transitions. We discuss the relevance of our results to peculiar behavior of the spin relaxation time observed experimentally in triangular antiferromagnets.

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in exchange interactions affects the behavior of relaxation time. We determine the finite-T phase diagram precisely by varying the anisotropy, and uncover the exceptionally singular nature of the isotropic Heisenberg case.

Our model Hamiltonian is defined in the form

$$H = J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z), \quad (1)$$

where $J$ is the antiferromagnetic exchange interaction, and $S_i = (S_i^x, S_i^y, S_i^z)$ is a vector representing the classical spin at site $i$ (we normalize as $|S_i| = 1$); the summation $\langle ij \rangle$ runs over the nearest-neighbor bonds of the triangular lattice. We introduce here the exchange anisotropy $\lambda$. For the XY anisotropy ($\lambda < 1$), it is known that both BKT and chiral transitions occur at different but very close temperatures.15,16 On the other hand, for the Ising anisotropy ($\lambda > 1$), it is known that two different BKT transitions occur separately for the longitudinal $S^z$ and the transverse $(S^x, S^y)$ components.17,18 It is, however, still controversial how these four transitions behave as the system approaches the isotropic Heisenberg point $\lambda = 1$. We will discuss this issue later.

We calculate the relaxation time of the model (1) by using the nonequilibrium relaxation (NER) method.19 In this method, the relaxation time is directly computed by analyzing the relaxation process from an initial ordered state in terms of the Monte Carlo (MC) dynamics. We typically perform the relaxation up to $10^5$ MC steps by using the standard Metropolis local update for the system size $N_s = L \times L$ up to $L = 4002$ under the periodic boundary conditions. We confirm that the finite-size effect is negligibly small. The results are averaged over eight independent MC runs. We choose the initial state to be a three-sublattice $120°$ state; spins are set to be in the $xy$ plane for $\lambda \leq 1$, while they are in the $xz$ plane with aligning one of three spins to the $z$ direction for $\lambda > 1$. The ground state is slightly different from the $120°$ state in the Ising case $\lambda > 1$, but this deviation does not af-

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fect the long-time behavior of relaxation process. We set $J = 1$ and the Boltzmann constant $k_B = 1$.

In Fig. 1, we demonstrate how the NER method works in the XY limit ($\lambda = 0$), as an example. We calculate the dynamical spin correlation function $G(t)$ defined as

$$G(t) = \frac{1}{N_s^2} \sum_i \langle \mathbf{S}_i(t) \cdot \mathbf{S}_i(0) \rangle,$$

(2)

where $\mathbf{S}_i(t)$ denotes the spin configuration at site $i$ and MC step $t$. As shown in Fig. 1(a), $G(t)$ changes from an exponential decay in the high-$T$ paramagnetic phase to a power-law decay in the low-$T$ BKT phase. The BKT transition temperature $T_{BKT}$ is determined by the divergence of the relaxation time $\tau$ estimated from the high-$T$ exponential behavior, $G(t) \sim \exp(-t/\tau)$. We employ the scaling analysis by using $G(t) = \tau^{-\alpha} f(t/\tau)$, which enables us to estimate $\tau$ up to $\sim 10^5$. The results are plotted in Fig. 1(b). The divergent behavior of $\tau$ at low $T$ is well fitted by the BKT scaling $\tau = g(T) = a \exp[b/(T - T_{BKT})^{1/2}]$. Here we choose the $T$ range for the fit by monitoring the weighted residual defined by $R_w = \frac{1}{N_T} \sum_{i=1}^{N_T} \left( \frac{\tau_i - g(T_i)}{g(T_i)} \right)^2$, where $N_T$ is the number of the data ($T_i$): We fit the range of low-$T$ data which gives $R_w$ less than 0.002. The fit gives an estimate of the transition temperature $T_{BKT} = 0.400(1)$, which is consistent with the previous estimate. At the same time, the fitting procedure defines $\bar{\tau} = 0.440(10)$, below which $\tau$ follows the BKT scaling. The region $T_{BKT} < T < \bar{\tau}$ represents the BKT critical region in which $G(t)$ obeys the universal behavior [see the inset of Fig. 1(b)]. We confirm a similar universal scaling for all the following data.

We study the critical behavior of $\tau$ in this way for various values of the anisotropy $\lambda$. The results for $\lambda < 1$ are shown in Fig. 2(a). As approaching the Heisenberg case with $\lambda \to 1$, $T_{BKT}$ decreases monotonically, while $\bar{\tau}$ first decreases but increases for $\lambda > 0.9$: As a result, the width of the BKT critical region becomes wider as $\lambda \to 1$. This is more clearly observed in Fig. 2(b), which plots the normalized relaxation time $\tilde{\tau} = \tau/\alpha$ on the basis of the BKT scaling $\tau = a \exp[b/(T - T_{BKT})^{1/2}]$. In fact, as shown in Fig. 2(c), the relative width of the critical region, $\Delta T_{BKT} = (T - T_{BKT})/T_{BKT}$, appears to diverge logarithmically or more strongly with decreasing the anisotropy.

As anticipated from the diverging $\Delta T_{BKT}$, $\tau$ for the isotropic Heisenberg case can be fitted by the BKT scaling in the entire range of $T$ calculated, as shown in Fig. 2(d). The fitting naively suggests that $\tau$ diverges at $T^* = 0.282(4)$. Similar behavior was seen in the spin correlation length, for which it was argued that a crossover takes place from the BKT behavior to another $T$ dependence and the correlation length does not diverge except for $T = 0.22, 23$. Our data are consistent with such analyses as shown in Fig. 2(d). We return to this point later. Besides the crossover, the crucial observation here is that the isotropic case $\lambda = 1$ looks quite singular since the apparent BKT critical behavior is observed in the divergently wide range of $T$.

Let us further discuss the singular behavior as $\lambda \to 1$ from the viewpoint of the vector spin chirality. We study the dynamical chiral correlation function defined as

$$\kappa(t) = \frac{1}{2N_s} \sum_{\mathbf{R}_i} \langle \kappa_{\mathbf{R}_i}(t) \cdot \kappa_{\mathbf{R}_i}(0) \rangle,$$

(3)
Fig. 3. (Color online) Relaxation of the vector chiral order parameter (a) in the XY limit ($\lambda = 0$) and (b) very close to the Heisenberg point ($\lambda = 0.9999$). (c) Scaling plot of the relaxation time of the chirality, $\tau_{\kappa}$. Solid lines for $\lambda \leq 0.99$ represent the power-law fit $\tau_{\kappa} \propto (T - T_*)^{-z\nu}$. The dashed curve for the Heisenberg case $\lambda = 1$ is the fit to the BKT criticality, i.e., $\tau_{\kappa} \propto \exp[b/(T - T_*)^{1/2}]$. (d) Relaxation in the Heisenberg case.

where the summation $R_i$ runs over all the unit triangles, and $\kappa^2$ is the $z$ component of the vector chirality $\kappa^2 = \frac{1}{2} (S_1 \times S_2 + S_2 \times S_3 + S_3 \times S_1)^z$ for each triangle of three spins $S_1$, $S_2$, and $S_3$. The vector chirality exhibits a true long-range order in the anisotropic cases, and therefore, we expect that $\kappa(t)$ decays exponentially above a chiral transition temperature $T_c$, while it approaches a nonzero constant below $T_c$. At $T = T_c$, $\kappa(t)$ shows a power-law decay. This is indeed the case as demonstrated in Figs. 3(a) and 3(b) for $\lambda = 0.0$ and 0.9999, respectively. The results give the estimates $T_c = 0.413(1)$ for $\lambda = 0.01\%$ and $T_c = 0.290(5)$ for $\lambda = 0.9999$. It is noteworthy that the chiral transition is clearly discernible even for very small anisotropy of 0.01% ($\lambda = 0.9999$).

Similar to the analysis of $\sigma$ in Fig. 2, we examine the behavior of the relaxation time of the chirality, $\tau_{\kappa}$, by varying the anisotropy $\lambda$. The results for $\lambda < 1$ are summarized in Fig. 3(c). For $\lambda < 1$, $\tau_{\kappa}$ shows a power-law divergence $\tau_{\kappa} \propto (T - T_*)^{-z\nu}$, with the same exponent $z\nu \approx 1.9$. At $\lambda = 0.999$ the data show a crossover from a BKT-like behavior at high $T$ to the power-law divergence near $T_c$. In the isotropic case $\lambda = 1$, $\tau_{\kappa}$ shows a stronger divergence than the power law and is well fitted by the BKT scaling $\tau_{\kappa} \propto \exp[b/(T - T_{\kappa}^{*})^{1/2}]$ with $T_{\kappa}^{*} = 0.284(3)$. The relaxation process at $\lambda = 1$ is shown in Fig. 3(d); $\kappa(t)$ exhibits a power-law decay even at much lower $T$ than $T_{\kappa}^{*}$. The results seemingly suggest a BKT-type transition in the vector chiral degree of freedom at $T_{\kappa}^{*}$, as seen at $T^{*}$ in the spin sector [Fig. 2(d)]. These behaviors in the vector chirality also illustrate a singularity of the isotropic Heisenberg case. We will discuss $T^{*}$ and $T_{\kappa}^{*}$ in comparison with the $Z_2$ vortex transition temperature later.

Collecting the data of the relaxation of spin and vector chirality, we map out the finite-$T$ phase diagram as a function of the anisotropy $\lambda$. We also study the Ising anisotropic cases ($\lambda > 1$), where two different BKT transitions take place: one is for the $z$ component of spin $S^z$, and the other is for the $xy$ components $S^x$, $S^y$. The latter transition accompanies a quasi-long-range ordering of the vector chirality, and occurs at a lower $T$ than the former. The two BKT transition temperatures are determined from the dynamical spin correlation function for the corresponding spin component [cf. Eq. (2)].

Figure 4(a) summarizes our phase diagram around the isotropic Heisenberg point $\lambda \sim 1$. In the $XY$ anisotropic region $\lambda < 1$, the chiral transition always occurs at a slightly higher $T$ than the BKT transition. Both two transition temperatures decrease more rapidly as $\lambda \to 1$. Similar decrease is observed in the two BKT transitions when approaching from the Ising anisotropic case $\lambda > 1$. Especially, the BKT transition temperature for the $xy$ components shows a nonmonotonic $\lambda$ dependence. Consequently, the phase diagram exhibits a sharp “V shape”, which illuminates the singularity of the Heisenberg case $\lambda = 1$. To our knowledge, this peculiar form in the very vicinity of $\lambda = 1$ has not been elucidated before.

The question is the fate of the transition temperatures as $\lambda \to 1$, in particular, their relation to the $Z_2$ vortex transition predicted for $\lambda = 1$. Figure 4(b) shows the asymptotic behavior of the chiral and BKT transition temperatures in comparison with a recent estimate of $Z_2$ vortex transition temperature $T_v$. We plot the data as a function of $1/|\ln(1 - \lambda)|$, with considering an analyti-
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