Classical Heisenberg antiferromagnet on a triangular lattice in the presence of single-ion anisotropy

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Abstract. The Heisenberg antiferromagnet on a triangular lattice is one of the prototype examples of frustrated systems and has been studied for several decades. In the presence of magnetic fields, the system exhibits a phase diagram consisting of exotic phases. At low temperatures successive magnetic phase transitions occur as the magnetic field is increased. We analyze the ground states of the system to obtain the critical fields at zero temperature. It is also shown through Monte Carlo simulations that the easy-axis single-ion anisotropy in classical Heisenberg antiferromagnet results in the expansion of the uud-phase region.

1. Introduction
Frustrated systems are a very attractive topic in magnetism studies [1, 2] and the triangular lattice antiferromagnet (TLAF) is one of the well-known frustrated systems. Although the TLAF composed of Heisenberg spins is a simple model, it has a variety of interesting physical properties.

In the square lattice the antiferromagnetic spins can align antiparallel to one another without any difficulty. On an equilateral triangle, in contrast, the third spin cannot satisfy both two nearest-neighbor spins simultaneously when two adjacent spins align antiparallel; it is called a geometrical frustration. In that case, the resulting ground state of TLAF has a $120^\circ$ spin structure which is twofold degenerate [3].

According to Mermin-Wagner theorem [4], it is impossible for any continuous symmetry to be broken spontaneously in two-dimensional (2D) lattice of Heisenberg spin system at finite temperatures, implying that no long-range order can emerge in two dimensions. An interesting possibility of a quasi-long range order still exists with a topological phase transition in 2D lattice [5, 6], which is called Berezinskii-Kosterlitz-Thouless (BKT) transition. Below the BKT transition temperature, vortex-antivortex pairs are bound tightly while free vortices are available above the critical temperature.

The 2D TLAF with magnetic fields is known to exhibit exotic phases due to the competition between magnetic fields and exchange interactions [7]. Earlier studies [8, 9] have revealed that there emerge interesting coplanar phases such as the Y state and the 2:1 canted state as well as a colinear phase called the uud state. The three distinct phases were confirmed in the experiments of quasi-2D TLAF materials such as $\text{Ba}_3\text{NiNb}_2\text{O}_9$ [10], $\text{Rb}_4\text{Mn(MoO}_4)_3$ [11], and $\text{Ba}_3\text{CoNb}_2\text{O}_9$ [12]. A lot of interesting properties of TLAF have also been examined in extensive theoretical studies [7–9, 13, 14].

In this work, we consider the TLAF in the presence of external magnetic fields and easy-axis single-ion anisotropy. At zero temperature we apply the analytic method to the ground-state...
energy for competing phases, obtaining the critical magnetic fields between the equilibrium phases. At finite temperatures we investigate the thermodynamic properties of the system for various magnetic fields with emphasis on the effects of the easy-axis anisotropy. The phase diagram reveals that the uud-phase region widens with the territory of Y phase shrinking as the strength of anisotropy increases.

This paper is organized as follows: In Sec. 2, we give a brief description of the Hamiltonian of the model, numerical methods, and order parameters to be investigated. The results are presented in Sec. 3, which includes the analytic results at zero temperature and the Monte Carlo (MC) simulation results on the phase diagram at finite temperatures. We summarize our results in Sec. 4.

2. Model and Methods

We consider the classical Heisenberg model, which is described by the Hamiltonian

\[ \mathcal{H} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i S_i^z - D \sum_i (S_i^z)^2, \]

where \( \mathbf{S}_i \) is a Heisenberg spin at \( i \)th site, the sum \( \langle i,j \rangle \) runs over nearest-neighbor sites, \( D \) is the strength of the single-ion anisotropy, and \( h \) is the magnetic field in the \( z \)-direction. We study the model with antiferromagnet exchange interactions \( J > 0 \) and easy-axis single-ion anisotropy \( D > 0 \) on a triangular lattice in periodic boundary conditions.

We have performed parallel-tempering MC simulations [15] based on Metropolis algorithm. Typically \( 1.1 \times 10^6 \) MC steps have been performed and the first \( 1 \times 10^5 \) steps were discarded for equilibration. We have prepared 10 - 50 replicas of \( N = L \times L \) spins and replicas at adjacent temperatures are exchanged every 10 MC steps. In this work we have used linear sizes \( L = 30, 60, \) and 120.

We use two order parameters to characterize various phases. The spin stiffness \( \rho_s \) plays the role of a convenient order parameter for BKT phase transition associated with quasi-long-range order. In the \( S^x - S^y \) plane, \( \rho_s \) is defined by [16]

\[ \rho_s = -\frac{2}{3\sqrt{3}N} \sum_{a=1}^{3} \left[ \left\langle J \sum_{\langle i,j \rangle} (\mathbf{e}_a \cdot \mathbf{r}_{ij})^2 S_i^x S_j^y \right\rangle + \frac{1}{T} \left( \left\langle J \sum_{\langle i,j \rangle} (\mathbf{e}_a \cdot \mathbf{r}_{ij}) S_i^+ S_j^- \right\rangle \right)^2 \right], \]

where \( S_i^\pm = (S_i^x, S_i^y) \), \( \mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j \), and \( \{ \mathbf{e}_a \} = \{(1, 0), (1, 2/\sqrt{3}), (-1, 2/\sqrt{3})\} \). It represents the rigidity of spin structure when spins are twisted about \( \mathbf{z} \)-axis, and it is known to exhibit a universal jump from zero to \( \rho_s = \frac{2}{3} T_{BKT} \) at the BKT transition temperature \( T_{BKT} \) [17].

We also consider a complex order parameter, \( \psi^z \equiv \psi_1^z + i\psi_2^z \), which is associated with the breaking of the \( C_3 \) lattice symmetry for \( S^z \) [8]

\[ \psi_1^z = \frac{\sqrt{6}}{N} \sum_{\alpha} [S_{\alpha A}^z + S_{\alpha B}^z - 2S_{\alpha C}^z], \]

\[ \psi_2^z = -\frac{3\sqrt{2}}{N} \sum_{\alpha} [S_{\alpha B}^z - S_{\alpha A}^z], \]

where the sum of \( \alpha \) runs over all primitive unit cells and \( S_{\alpha a} \) is the spin on the sublattice \( a = A, B, C \) in the unit cell \( \alpha \). The magnitude of complex order parameter \( O^{zz} \) is given by

\[ O^{zz} \equiv |\psi^z|, \]

which is \( 4\sqrt{6}/3 \) in the state with a perfect uud structure.
3. Results

3.1. Phase transitions at zero temperature

We first consider phase transitions at zero temperature as the magnetic field is varied. We consider three trial spin configurations for ordered states [7] as well as a saturated state along the magnetic field. For each phase given in Fig. 1 we find the optimal configuration which minimizes the energy for a given magnetic field \( h \) and single-ion anisotropy \( D \). By the comparison of the energies of the phases, we can determine the ground state for \( h \).

For small \( h \) the ground state turns out to be Y phase, whose energy is

\[
E_Y = -\frac{1}{2} \left( \frac{3J + h}{3J + D} \right)^2 - 3J + D + h. \tag{6}
\]

As the magnetic field is increased, the angle \( \theta \) shown in Fig. 1(a) decreases gradually, and the Y state is connected continuously to the uud state at \( h_c1 = 3J + 2D \). The energy of the uud state is

\[
E_U = -3J - h + 3D, \tag{7}
\]

which is obviously higher than \( E_Y \) for \( h < h_c1 \).

The 2:1 canted phase near the uud phase exhibits a spin configuration in Fig. 1(c). To the quartic order in \( \theta_1 \) and \( \theta_2 \), the energy of the 2:1 canted phase is calculated to be

\[
E_{C1} \approx -3J - h + 3D - \frac{6(h-6D)(h+2D)[3J(h-6D) - (h-2D)(h+2D)]^2}{6J[4(h+8D)(h-2D)^3 - (h-8D)(h+2D)^3] - 3J(h-6D)(h+2D)^3 + (h-8D)(h+2D)^4} \tag{8}
\]

The condition for \( E_U \leq E_{C1} \) gives \( h \leq h_{c2} \), where

\[
h_{c2} \equiv \frac{3J + \sqrt{9J^2 - 8D(9J - 2D)}}{2}. \tag{9}
\]

Above \( h_{c2} \) the 2:1 canted phase is stable and with the increase of the magnetic field \( h \) its configuration turns gradually to that in Fig. 1(d) near the boundary with the saturated state. The energy of the spin configuration is

\[
E_{C2} \approx 9J - 3h + 3D + \frac{18(h - 2D)(-9J + h - 2D)^2}{18J(h - 8D) + (h - 2D)(h - 8D - 51J)} \tag{9}
\]
Figure 2. (color online) The magnetic-field dependence of ground-state magnetizations $M_z$ in the $z$-direction for $D/J = 0.05$. The (green) squares and (red) circles indicate $M_z$ for linear sizes $L = 30$ and $60$, respectively, which are obtained from MC simulations at $T/J = 0.0001$. The solid line represents the magnetization derived analytically in the text. The Y, uud, 2:1 canted, and saturated phases are denoted by $Y$, $U$, $C$, and $S$, respectively. The dashed lines represent analytical results for the critical magnetic fields $h_{c1}, h_{c2}$, and $h_{c3}$. In the inset we magnify the region around the uud phase, where the system exhibits a 1/3 magnetization plateau.

and the state is transformed continuously to the saturated state at the magnetic field $h_{c3} = 9J + 2D$. The energy of the saturated state is

$$E_S = 9J - 3h + 3D,$$

which yields $E_{C2} < E_S$ for $h < h_{c3}$.

In Fig. 2 we present the MC simulation results with the analytic results at zero temperature for $D/J = 0.05$. (The MC simulation has been performed at $T/J = 0.0001$ which is very close to zero temperature.) Figure 2 demonstrates that the analytic results for magnetization are in good agreement with the simulation results. At zero temperature we find four distinct magnetic phases as in the case of zero anisotropy. In the presence of the easy-axis anisotropy, a 1/3 magnetization plateau appears in a finite region while no such magnetization plateau exists for zero anisotropy since the uud phase exists only at one value of magnetic field $h/J = 3.0$.

3.2. Phase transition at finite temperatures

We now investigate the phase transitions at finite temperatures by performing MC simulations under the magnetic field $h$. We calculate two order parameters, the spin stiffness $\rho_s$ and the $C_3$ order parameter $O^{zz}$ which we introduced in Sec. 2. Figure 3 displays $\rho_s$ and $O^{zz}$ as a function of temperature for $h = 1.2J$. In Fig. 3(a) we observe that $\rho_s$ becomes finite below a certain critical temperature $T_{BKT}$, which indicates the emergence of quasi-long-range order for $xy$ components of spins for $T < T_{BKT}$. The increase of the $C_3$ order parameter $O^{zz}$ at low temperatures, shown in Fig. 3, determines the critical temperature $T_c$ where the $C_3$ symmetry is broken for $S^z$. It turns out that $T_c$ is higher than $T_{BKT}$, and the phase for $T_{BKT} < T < T_c$ is identified as the uud phase.
Figure 3. (color online) (a) Spin stiffness $\rho_s$ and (b) $C_3$ order parameter $O^{zz}$ as a function of temperature $T$ for $h/J=1.2$. The (red) triangles, (yellow) circles, and (green) squares indicate the data for linear size $L = 30, 60$ and $120$, respectively. The solid line denotes a universal-jump line. The numerical errors are smaller than the size of symbols.

Figure 4. (color online) (a) Spin stiffness as a function of magnetic field $h$ for $L = 120$ and $D/J = 0.20$. The region with $\rho_s = 0$ indicates the uud phase regime. (b) Critical magnetic fields $h_{c1}$ and $h_{c2}$ in units of $J$ as a function $D/J$. The (yellow) filled circles and (green) open squares represent the data for $T/J = 0.05$ and $0.10$, respectively. The solid lines indicate the critical fields at zero temperature, and the dotted lines are the best fits of the critical fields at finite temperatures.

In Fig. 4(a) we plot $\rho_s$ as a function of $h$ at temperature $T = 0.05J$. The plot shows a region with $\rho_s = 0$, indicating that the uud phase is stable for $h_{c1}(T) < h < h_{c2}(T)$. As shown in Fig.4(b), $h_{c2}$ which separates the uud phase from the 2:1 canted phase increases linearly with $D$ while the increase of $D$ results in the reduction of the critical magnetic field $h_{c1}$ between the Y and the uud phases. Accordingly, the region of the uud phase is expanded by the increase of the easy-axis anisotropy. It is also observed that $h_{c1}$ reduces significantly as the temperature is increased. On the other hand, $h_{c2}$ is rather insensitive to the temperature $T$.

3.3. Phase diagram
The computation of two order parameters $\rho_s$ and $O^{zz}$ in the plane spanned by the temperature $T$ and the magnetic field $h$ yields the phase diagram at finite temperatures. In Fig. 5 we plot
Figure 5. (color online) $T$--$h$ phase diagram for various values of $D$. The (green) filled triangles and (red) open squares represent the phase boundaries for $D/J = 0$ and 0.05, respectively. The BKT transitions are denoted by the solid lines while the dotted lines indicate the continuous transition associated with the $C_3$ sublattice symmetry. Two (yellow) circles indicate the analytic results for critical fields at zero temperature for $D/J = 0.5$.

the phase diagrams for $D/J = 0.00$ and 0.05 up to the magnetic field $h = 4J$. The overall shape of the phase diagram in the presence of the easy-axis anisotropy is similar to that for $D = 0$; $h_{c1}$ is reduced linearly by the increase of temperature while thermal fluctuations do not have much effect on $h_{c2}$. The critical temperature $T_c$ has its maximum around $h = 2J$, which is also very similar to the case of $D = 0$. One prominent difference for $D > 0$ compared with $D = 0$ is that the uud phase region is enlarged with increasing $D$. Although $h_{c1}$ is rather insensitive to $D$, $h_{c2}$ as well as $T_c$ is increased by the introduction of $D$.

4. Summary
In summary, we have investigated the effects of the easy-axis anisotropy on the TLAF. Through the analysis of the ground state we have obtained the critical magnetic fields, which has been shown to be consistent with MC results. We have also performed MC simulations at finite temperatures. The easy-axis anisotropy turns out to enlarge the region of the uud phase in the phase diagram. It can be understood from the tendency for the easy-axis anisotropy to align the spins along the $z$-axis, which makes the uud phase be energetically more favorable.

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