Phase transition of the $S = \frac{1}{2}$ quantum anisotropic Heisenberg antiferromagnet on the triangular lattice

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We study the $S = \frac{1}{2}$ anisotropic Heisenberg antiferromagnet on finite triangular lattices with $N \leq 24$ sites: $H = 2J \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_j^y S_j^y + \Delta S_i^z S_j^z)$ with $0 \leq \Delta \leq 1$. The specific heat C and the chiral-order parameter $\langle \chi^2 \rangle$ are calculated using a quantum transfer Monte Carlo method. Remarkable differences in the size dependences of C and $\langle \chi^2 \rangle$ are found between the cases of $\Delta \leq 0.4$ and of $\Delta \geq 0.6$. For $\Delta \leq 0.4$, the peak height of C increases with increasing N and an extrapolation of $\langle \chi^2 \rangle$ to the thermodynamic limit gives a finite, nonzero value at low temperatures. In contrast with these, for $\Delta \geq 0.6$, the peak height does not increase and the extrapolation of $\langle \chi^2 \rangle$ gives a smaller value even at very low temperatures indicating the absence of a long-range chiral order. From the results, we suggest that the chiral-ordered phase transition occurs at a finite, nonzero temperature when $\Delta \leq \Delta_c$ with $\Delta_c \gtrsim 0.4$. The phase diagram of the model is predicted.

I. INTRODUCTION

An anisotropic Heisenberg antiferromagnet on the triangular lattice has attracted much interest in recent years. The Hamiltonian of the model is described by

$$H = 2J \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z), \qquad (1)$$

where J (> 0) is the exchange integral and $\langle i, j \rangle$ runs over the nearest neighbor pairs, and S_i^x , S_i^y , and S_i^z are components of the spin \mathbf{S}_i on the *i*th lattice site. $\Delta = 0$ corresponds to the XY model, and $\Delta = 1$ is the Heisenberg model.

In the classical XY model, Miyashita and Shiba¹ showed using the Monte Carlo method, that a long-range chiral order exists at low temperatures, although the long-range order of the spins disappears at finite temperatures. They pointed out that the specific heat diverges logarithmically at the transition temperature T_c and the transition belongs to the universality class of the Ising model. In the classical anisotropic Heisenberg model, Miyashita² pointed out that the chiral-ordered phase persists for $-0.5 < \Delta < 1$.

In the quantum model, however, whether the chiralordered phase exists or not is still in controversy. The ground state properties of the model on finite triangular lattices with N sites have been investigated by several authors using the diagonalization technique. Fujiki and Betts³ studied the S = 1/2 XY and Heisenberg models for $N \leq 21$ and conjectured that the chiral-ordered phase exists in the XY model. Nishimori and Nakanishi⁴ investigated the same models for $N \leq 27$, showed that the extrapolated value of the chiral-order parameter of the XY model was a little smaller than that obtained by Fujiki and Betts, and gave the opposite conjecture. Recently, Leung and Runge⁵ studied the anisotropic Heisenberg model for $N \leq 36$ and suggested that the model has the chiral-ordered phase for $\Delta \sim 0$ and does not for $\Delta = 1$.

Properties of the model at finite temperatures have also been studied. Matsubara and Inawashiro⁶ calculated the specific heat of the S = 1/2 XY model on finite triangular lattices with $N \leq 21$ using a quantum transfer Monte Carlo (QTMC) method⁷ and showed that the peak height of the specific heat increases with increase of N. From the result, they conjectured that a phase transition occurs in the model and estimated the transition temperature of $T_c/J \simeq 0.39$. Fujiki and Betts⁸ studied the same model using the high-temperature series expansion method but they did not find the transition temperature. Recently, Momoi and Suzuki⁹ studied the anisotropic Heisenberg model by applying a supereffective field theory,¹⁰ and found the transition temperature for $-0.5 < \Delta < 0.5$. In particular, they obtained $T_c/J \sim 0.4$ for $\Delta = 0$, which is very close to that of Matsubara and Inawashiro. Having combined the results of spin wave theory,¹¹ they conjectured that the chiralordered phase exists for $-0.5 < \Delta < 1$ as in the classical model.

We ask the following questions in the quantum model. Does the chiral-ordered phase really exist for $\Delta \sim 0$? If so, does the phase persist up to $\Delta \sim 1$? In this paper, we investigate the S = 1/2 anisotropic Heisenberg model with $0 \leq \Delta \leq 1$ at finite temperatures. We treat the model on finite lattices with $N \leq 24$ using the QTMC method. Although the lattices are not so large as those treated in the ground state study, we may obtain fruitful knowledge about the nature of the model. In particular, we may examine whether the phase transition occurs or not from the size dependence of the specific heat as well as the stability of the ground state against thermal disturbance. If it does, we may estimate the transition temperature T_c from the peak temperature of the specific heat and/or the temperature dependence of the chiralorder parameter. In fact, we find evidence of the phase transition for a finite, nonzero range of Δ around $\Delta = 0$

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and estimate T_c . From the results, we predict a phase diagram of the model.

In Sec. II, the QTMC method is presented. In Sec. III, the results of the specific heat and the chiral-order parameter are shown for different Δ , separately. In Sec. IV, the size dependences of these quantities are examined to see whether the phase transition occurs or not. The phase diagram of the model is discussed. Section V contains our summary.

II. FORMALISM

In order to obtain physical quantities of the model at finite temperatures, we use the QTMC method proposed by Imada and Takahashi.⁷ The method is effective for finite systems, because the memory size needed in calculating physical quantities is much smaller than that in the conventional diagonalization method. Moreover, the method does not suffer the negative sign problem which appears in the Suzuki-Trotter formulation.¹²

The thermal average of a physical quantity A of a system with N spins is given by

$$\langle A \rangle = \sum_{i}^{2^{N}} \langle i | A \exp(-\beta H) | i \rangle / \sum_{i}^{2^{N}} \langle i | \exp(-\beta H) | i \rangle , \quad (2)$$

where the sum runs over all the 2^N states of an arbitrary complete orthogonal set and $\beta \equiv 1/T$ with T being the temperature. Here we choose $|i\rangle$ as Ising states. Instead of Eq. (2), we consider the following quantity:

$$\widetilde{\langle A \rangle} = \sum_{k}^{M} \langle \psi_{k} | A \exp(-\beta H) | \psi_{k} \rangle / \sum_{k}^{M} \langle \psi_{k} | \exp(-\beta H) | \psi_{k} \rangle,$$
(3)

where the sum runs over M states each of which is given by

$$|\psi_{k}\rangle = \sqrt{\frac{6}{M}} \sum_{i}^{2^{N}} C_{ik}|i\rangle; \qquad (4)$$

here C_{ik} is a random number in the range $-1 \leq C_{ik} \leq 1$. We can readily show that $\langle A \rangle \rightarrow \langle A \rangle$ for $M \rightarrow \infty$, because $(6/M) \sum_{k}^{M} C_{ik}C_{jk} = \delta_{ij} + O(1/\sqrt{M})$. Hence we use Eq. (3) instead of Eq. (2). A great advantage of using the formula (3) is that we can obtain an approximate value of the average $\langle A \rangle$ by summing up only M terms instead of all the 2^N terms of the Ising states. Using this formula, we can treat systems much larger than those treatable by the rigorous formula (2). Of course, statistical errors of $O(1/\sqrt{M})$ arise, but we may reduce them as M is increased.

In calculating Eq. (3), the following technique can be used. We rewrite Eq. (3) in a symmetric form as

$$\widetilde{\langle A \rangle} = \sum_{k}^{M} \langle \tilde{\psi}_{k} | A | \tilde{\psi}_{k} \rangle \bigg/ \sum_{k}^{M} \langle \tilde{\psi}_{k} | \tilde{\psi}_{k} \rangle, \tag{5}$$

where $|\tilde{\psi}_k\rangle = \exp(-\beta H/2)|\psi_k\rangle$. The calculation of $\exp(-\beta H/2)|\psi_k\rangle$ is made by expanding $\exp(-\beta H/2)$ in term of a power series of $\beta H/2$ and by operating every term to $|\psi_k\rangle$. The convergence of the series is, of course, more rapid for a higher temperature T_0 (or smaller β_0). We start at some higher temperature $T = T_0$ (or some smaller β_0). Once the $|\tilde{\psi}_k\rangle$ for $T = T_0$ is obtained by operating $\exp(-\beta_0 H/2)$ to $|\psi_k\rangle$, we can obtain $|\tilde{\psi}_k\rangle$ for $T = T_0$. In that way, we can readily obtain step by step $|\tilde{\psi}_k\rangle$'s for $T = T_0, T_0/2, T_0/3, \ldots$, using the rapidly converging operator $\exp(-\beta_0 H/2)$.

We calculate the energy, the specific heat, and the chiral-order parameter. The energy and the specific heat are given by

$$E = \langle H \rangle ,$$
 (6)

$$C = \frac{1}{T^2} (\langle H^2 \rangle - \langle H \rangle^2) .$$
 (7)

The z component of the chirality for each upright triangle at \mathbf{R} is defined as

$$\chi^{z}(\mathbf{R}) = \frac{2}{\sqrt{3}} (S_{i}^{x} S_{j}^{y} - S_{i}^{y} S_{j}^{x} + S_{j}^{x} S_{k}^{y} - S_{j}^{y} S_{k}^{x} + S_{k}^{x} S_{i}^{y} - S_{k}^{y} S_{i}^{x}) , \qquad (8)$$

where $i \rightarrow j \rightarrow k$ are taken counterclockwise. The eigenvalues of (8) are ± 1 and 0. The long-range chiral-order parameter is defined as

$$\chi = \frac{1}{N} \sum_{\mathbf{R} \in \Delta} \chi^{z}(\mathbf{R}) , \qquad (9)$$

where **R** runs over all the upright triangles on the lattice. Since the average of χ vanishes because of the symmetry, we calculate the average of its square $\langle \chi^2 \rangle$.



FIG. 1. Finite cluster with lattice sites N = 18. The symbols \circ, \bullet, \Box denote different sublattices.



FIG. 2. The temperature dependence of the specific heat Cfor different Δ : (a) $\Delta = 0.0$, (b) $\Delta = 0.2$, (c) $\Delta = 0.4$, (d) $\Delta = 0.6$, and (e) $\Delta = 1.0$.



FIG. 2 (Continued).

III. RESULTS

We have studied the model with $\Delta = 0.0, 0.2, 0.4, 0.6, 0.8,$ and 1.0 on finite lattices with $N \leq 24$. The lattices are constructed so that the 120° spin structure is possible in the classical system as shown in Fig. 1. The numbers of the states M used in the calculation are as follows: M = 200 for N = 9, 12, 15; M = 80 for N = 18; M = 40-80 for N = 21; M = 15-27 for N = 24. For every lattice, the set of M states is divided into five subsets except for three subsets for N = 24, and quantities of interest are calculated in every subset. Error bars presented in figures given below only mean deviations of the values obtained in different subsets. Since the results depend markedly on whether N is even or odd, we show them separately.

A. Specific heat

In Figs. 2(a)-2(e), we show the specific heat C for different Δ , separately. For odd N, as N is increased, the temperature T_m at which the maximum of C occurs changes together with the peak height C_m . For even N, T_m changes a little but C_m does considerably. It is noted that this difference in N being even or odd is reduced as N is increased.

A considerable difference in the size dependence is seen between the results for $\Delta \leq 0.2$ and $\Delta \geq 0.6$. For $\Delta \leq$ 0.2, as N is increased, C_m becomes larger, suggesting the occurrence of a phase transition in the thermodynamic limit. For $\Delta \geq 0.6$, in contrast with this, C_m does not increase with N. In particular, for even N, it decreases as N is increased. The case of $\Delta = 0.4$ is marginal. A slight increase of C_m is seen only for odd N.

For every Δ , T_m is lowered as N is increased. This is pronounced for odd N and becomes more so as Δ is increased. These size dependences of C_m and T_m will be examined quantitatively in the next section.

B. Chiral-order parameter

In Figs. 3(a)-3(e), we show the chiral-order parameter $\langle \chi^2 \rangle$ for different Δ , separately, together with an extrap-

olated value which will be mentioned in Sec. IV. For odd N, as the temperature is lowered, $\langle \chi^2 \rangle$ monotonically increases and saturates. The usual size dependence is seen at all temperatures, i.e., $\langle \chi^2 \rangle$ decreases with increasing N. For even N, unusual behaviors are seen. $\langle \chi^2 \rangle$ for N = 12 and 18 has its maximum value at a finite temperature. In addition, its size dependence is reversed, i.e., at low temperatures $\langle \chi^2 \rangle$ for N = 24 is larger than that for N = 18. Of course, these unusual properties come from a quantum effect which is reduced as N is increased. In fact, $\langle \chi^2 \rangle$ for N = 24 monotonically increases with decreasing temperature down to a very low temperature, and the difference between the $\langle \chi^2 \rangle$'s for odd and even N becomes smaller as N is increased.

For $\Delta = 0$, as the temperature is lowered, $\langle \chi^2 \rangle$ rapidly increases around T/J = 0.5 and reaches a larger value. It seems that $\langle \chi^2 \rangle$ converges to a finite, nonzero value as $N \to \infty$. As Δ is increased, $\langle \chi^2 \rangle$ is reduced. In addition, the larger the system size N becomes, the more $\langle \chi^2 \rangle$ is reduced, and the size dependence of $\langle \chi^2 \rangle$ becomes larger. For $\Delta \sim 1$, $\langle \chi^2 \rangle$ increases gradually and reaches a value which exhibits a larger size dependence, suggesting $\langle \chi^2 \rangle \to 0$ as $N \to \infty$. Thus we expect that the change in the chiral nature of the model occurs at some value of Δ between $\Delta = 0$ and $\Delta = 1$. This problem will also be discussed in the next section.

IV. DISCUSSION

In the previous section, we show the specific heat C and the chiral-order parameter $\langle \chi^2 \rangle$ for different N. In this section, we examine the N dependence of those values quantitatively and discuss whether the phase transition occurs or not.

A. Size dependence of C_m and T_m

In Figs. 4(a)-4(d), we plot the peak height C_m as a function of $\log_{10} N$. For $\Delta = 0.0$, C_m lies almost on a straight line with a positive slope, like C_m of the classical XY model.¹ A similar N dependence is seen for $\Delta = 0.2$ and 0.4 except for the points of smaller N. In contrast



FIG. 3. The chiral-order parameter $\langle \chi^2 \rangle$ for different Δ : (a) $\Delta = 0.0$, (b) $\Delta = 0.2$, (c) $\Delta = 0.4$, (d) $\Delta = 0.6$, and (e) $\Delta = 1.0$. The symbol \bullet denotes an extrapolated value described in the text.



FIG. 3 (Continued).

with this, C_m for $\Delta = 0.6$ exhibits no systematic increase. These results suggest that C_m for $\Delta \leq 0.4$ increases logarithmically with increasing N, while it remains finite for $\Delta \geq 0.6$; namely, the results predict the occurrence of the phase transition at least for $\Delta \leq 0.4$. We consider the threshold Δ_c below which the phase transition occurs. Assuming that



FIG. 4. The peak height C_m of the specific heat as a function of $\log_{10} N$.

$$C_m = A \log_{10} N + B, \tag{10}$$

we estimate the slope of the line A by using the method of least squares and plot it in Fig. 5. In fact, A > 0for $\Delta \leq 0.4$, but it rapidly decreases around $\Delta = 0.4$ suggesting $\Delta_c \gtrsim 0.4$.

Next, we estimate the peak temperature T_m for $N \rightarrow$ ∞ , which is the critical temperature T_c for $\Delta \leq \Delta_c$. In Figs. 6(a)-6(c), we tentatively plot T_m as a function of $1/N^2$. The values for odd and even N exhibit difference N dependences. For odd $N,\,T_m$ exhibits a larger N dependence and seems to lie on a straight line. On the other hand, for even N, the N dependence is small, and T_m seems to remain almost constant, especially for larger Δ . We estimate T_m for $N \to \infty$ from these results for odd N and even N separately, and show them in Fig. 7. As seen in the figure, the difference between the two values is not large. Note that we also plot T_m as a function of 1/N and make the same estimation of T_m . However, the differences between the two values are much larger than those shown in Fig. 7. Hence we think that our estimation of T_m is plausible. Of course, we cannot rule out other estimations, as well as the latter one described above, because the system size of $N \leq 24$ is not large enough to get a definite value.

A point should be noted. As seen in Fig. 7, T_m is



FIG. 5. The slope of C_m vs $\log_{10} N$ as a function of Δ . These are estimated using the values for $N \ge 15$. The line is a guide to the eye.



FIG. 6. The peak temperature T_m of the specific heat as a function of $1/N^2$. The symbols \circ and \bullet are those for odd and even N, respectively.

almost constant even for $\Delta \geq 0.4$. This means that, as Δ reaches Δ_c from below, T_c reaches some finite, nonzero value T_c^* .

B. Size dependence of the chiral-order parameter

We first consider $\langle \chi^2 \rangle$ at $T \sim 0$. As seen in the previous section, $\langle \chi^2 \rangle$ for even N exhibits unusual temperature and size dependences. We believe these come from a property of the ground state which, of course, does not contribute to physical quantities in the thermodynamic limit at $T \neq 0$. To confirm this, we calculate $\langle \chi^2 \rangle$ for N = 12 and 18 in a space where the ground state is removed. That is,

$$\langle \chi^2 \rangle' = \sum_{k}^{M} \langle \tilde{\psi}'_{k} | \chi^2 | \tilde{\psi}'_{k} \rangle \left/ \sum_{k}^{M} \langle \tilde{\psi}'_{k} | \tilde{\psi}'_{k} \rangle \right.$$
(11)

where

$$|\tilde{\psi_k}\rangle = |\tilde{\psi}_k\rangle - |g\rangle\langle g|\tilde{\psi}_k
angle$$
 (12)



FIG. 7. Extrapolated values of the peak temperatures as functions of Δ . These are obtained using the values for $N \geq 15$.

with $|g\rangle$ being the ground state. In Fig. 8, the result for $\Delta = 0.0$ is shown. In fact, as the temperature is lowered, $\langle \chi^2 \rangle'$ increases monotonically and exhibits the usual size dependence. Then, for even N, we consider $\langle \chi^2 \rangle'$ instead of $\langle \chi^2 \rangle$. Note that we have also calculated $\langle \chi^2 \rangle'$ for odd N and found that the difference between $\langle \chi^2 \rangle$ and $\langle \chi^2 \rangle'$ is negligible at low temperatures.

Now, we estimate $\langle \chi^2 \rangle$ for $N \to \infty$ at $T \sim 0$. In Fig. 9, we plot $\langle \chi^2 \rangle$ as a function of 1/N at the lowest temperature together with those in the ground state for N = 27 and 36 obtained by Leung and Runge.⁵ For $\Delta =$ 0.0 and 0.2, the points lie well on a straight line up to N = 36. For $\Delta \geq 0.4$, they seem to lie on a curve which turns downwards as N increases. Then we estimate $\langle \chi^2 \rangle$ for $N \to \infty$ using the method of least squares with the following function:

$$\langle \chi^2 \rangle = \langle \chi^2 \rangle_{\infty} + a/N + b/N^2.$$
 (13)

The result is plotted in Fig. 10 as a function of Δ . In fact, $\langle \chi^2 \rangle_{\infty}$ has a finite value for $\Delta \leq 0.2$ and drops rapidly at $\Delta \sim 0.4$. For $\Delta \geq 0.6$, $\langle \chi^2 \rangle_{\infty}$ has a small, nonzero value



FIG. 8. The chiral-order parameter $\langle \chi^2 \rangle'$ calculated in a space without the ground state. The lines are those presented in Fig. 3(a).



FIG. 9. The chiral-order parameter as a function of 1/N. $\langle \chi^2 \rangle$ at T/J = 0.133 for N = 9, 15, 21 and at T/J = 0.200 for N = 24. For N = 12 and 18, $\langle \chi^2 \rangle'$ at T/J = 0.133 is plotted. The symbol \bullet is the exact value in the ground state for N = 27 and 36 obtained by Leung and Runge (Ref. 5).

which is almost constant for $0.6 \leq \Delta \leq 1.0$. Of course, from this result alone, we cannot conclude whether it vanishes or not, because the system size of $N \leq 24$ is too small to do it. However, it is natural to think $\langle \chi^2 \rangle_{\infty} = 0$ for $\Delta \geq 0.6$, because it is widely accepted that $\langle \chi^2 \rangle_{\infty} = 0$ for $\Delta = 1$ in the thermodynamic limit. In any case, we find a change in the chiral nature of the model close above $\Delta = 0.4$, i.e., $\Delta_c \gtrsim 0.4$. It is marvelous that both quantities C and $\langle \chi^2 \rangle$ predict a similar value of the threshold of $\Delta_c \gtrsim 0.4$.

Next, we estimate the transition temperature T_c for $\Delta \leq \Delta_c$. From the data of odd N, we estimate $\langle \chi^2 \rangle_{\infty}$ at finite temperatures using Eq. (13). The results are shown in Figs. 3(a)-3(e). As the temperature is increased, $\langle \chi^2 \rangle_{\infty}$ decreases rapidly at $T/J \sim 0.35$, but does not disappear near this temperature. Then we regard the temperature of the inflection point of $\langle \chi^2 \rangle_{\infty}$ as T_c and plot it in Fig. 7. Again we see that T_c estimated



FIG. 10. An estimated value of $\langle \chi^2 \rangle$ at $T \sim 0$ as a function of Δ . The line is a guide to the eye.



FIG. 11. Phase diagram predicted in this study.

here is in good agreement with that estimated from the peak position of the specific heat. Note that we cannot estimate T_c for $\Delta \geq 0.6$, because the inflection point is absent. However, the following point is remarked. Even for $\Delta = 0.6$ and 0.8, the rapid decrease of $\langle \chi^2 \rangle_{\infty}$ occurs around $T/J \sim 0.35$ like that in the case of $\Delta \leq 0.4$. This also suggests that T_c reaches T_c^* as $\Delta \to \Delta_c$.

C. Phase diagram

The phase diagram predicted in the present study is shown in Fig. 11. Properties of the phase diagram are as follows: (i) the chiral-ordered phase appears only for $\Delta \leq \Delta_c$ with $\Delta_c \gtrsim 0.4$, and (ii) the transition temperature T_c is almost constant for $0 \leq \Delta \leq \Delta_c$. Thus the phase boundary separating the paramagnetic phase and the chiral-ordered phase is broken off at some finite, nonzero temperature T_c^* . This suggests the occurrence of some new phase for $\Delta > \Delta_c$ which will become unstable for $\Delta \rightarrow 1$. At present, we cannot identify which phase appears for $\Delta_c < \Delta < 1$. We think, however, that a candidate is a Kosterlitz-Thouless-like phase where the correlation of chiralities $\langle \chi^z(\mathbf{R})\chi^z(\mathbf{R}')\rangle$ decays according to a power law,¹³ because we have also plotted $\langle \chi^2 \rangle$ as a function of N in a log-log form and found that the points for $\Delta > 0.6$ lie almost on a straight line. This problem will be discussed in a separate paper.

It should be noted that the phase diagram predicted here is different from that predicted by Momoi and Suzuki,¹¹ in which the chiral-ordered phase persists up to $\Delta = 1$, although the phase boundaries for $\Delta \leq 0.4$ are in good agreement with each other.

V. SUMMARY

In this paper, we have studied the S = 1/2 quantum anisotropic Heisenberg antiferromagnet on finite triangular lattices with $N \leq 24$ using the QTMC method. We have calculated the specific heat and the chiral-order parameter and examined their size dependences to see whether the phase transition occurs or not. Our results are summarized as follows.

In the specific heat, when $\Delta \leq 0.4$, the peak height

 C_m increases almost linearly with $\log_{10} N$ suggesting the occurrence of the phase transition. The transition temperature is estimated as $T_c/J \lesssim 0.4$ for $\Delta \leq 0.4$ from the peak temperature T_m .

In the chiral-order parameter, the extrapolation to the thermodynamic limit at the lowest temperature suggests that the chiral-ordered phase exists when $\Delta \leq 0.4$. The transition temperature is estimated as $T_c/J \lesssim 0.4$ for $\Delta \leq 0.4$ from the temperature dependence of the extrapolated value.

Both the results are excellently in agreement with each other. We believe, hence, that the chiral-ordered phase

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transition occurs in the model when $\Delta < \Delta_c$ with Δ_c being a little larger than 0.4. The phase diagram of the model has been predicted.

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