The Phase Transition of the Spin-1/2 Heisenberg Model with a Spatially Staggered Anisotropy on the Square Lattice.

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Puzzled by the indication of a new critical theory for the spin-1/2 Heisenberg model with a spatially staggered anisotropy on the square lattice as suggested in \cite{1}, we re-investigate the phase transition of this model induced by dimerization. We focus on studying the finite-size scaling of the observables $\rho_1 L$ and $\rho_2 L$, where $L$ stands for the spatial box sizes used in the simulations and $\rho_i$ with $i \in \{1, 2\}$ is the spin-stiffness in $i$-direction. We find by performing finite-size scaling using the observable $\rho_2 L$, which corresponds to the spatial direction with a fixed antiferromagnetic coupling, one would suffer a much less severe correction compared to that of using $\rho_1 L$. Therefore $\rho_2 L$ is a better quantity than $\rho_1 L$ for finite-size scaling analysis concerning the limitation for the availability of large volumes data in our study. Remarkably, by employing the method of fixing the aspect-ratio of spatial winding numbers squared in the simulations, even from $\rho_1 L$ which receives the most serious correction among the observables considered in this study, we arrive at a value for the critical exponent $\nu$ which is consistent with the expected $O(3)$ value by using only up to $L = 64$ data points.

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I. INTRODUCTION

Heisenberg-type models have been studied in great detail during the last twenty years because of their phenomenological importance. For example, it is believed that the spin-1/2 Heisenberg model on the square lattice is the correct model for understanding the undoped precursors of high $T_c$ cuprates (undoped antiferromagnets). Further, due to the availability of efficient Monte Carlo algorithms as well as the increasing power of computing resources, properties of undoped antiferromagnets on geometrically non-frustrated lattices have been determined to unprecedented accuracy \cite{2, 3, 4, 5, 8, 9}. For instance, using a loop algorithm, the low-energy parameters of the spin-1/2 Heisenberg model on the square lattice are calculated very precisely and are in quantitative agreement with the experimental results \cite{4}. Despite being well studied, several recent numerical investigation of anisotropic Heisenberg models have led to unexpected results \cite{6, 10, 11}. In particular, Monte Carlo evidence indicates that the anisotropic Heisenberg model with staggered arrangement of the antiferromagnetic couplings may belong to a new universality class, in contradiction to the theoretical $O(3)$ universality prediction \cite{3}. For example, while the most accurate Monte Carlo value for the critical exponent $\nu$ in the $O(3)$ universality class is given by $\nu = 0.7112(5)$ \cite{12}, the corresponding $\nu$ determined in \cite{3} is shown to be $\nu = 0.689(5)$. Although subtlety of calculating the critical exponent $\nu$ from performing finite-size scaling analysis is demonstrated for a similar anisotropic Heisenberg model on the honeycomb lattice \cite{13}, the discrepancy between $\nu = 0.689(5)$ and $\nu = 0.7112(5)$ observed in \cite{3} remains to be understood.

In order to clarify this issue further, we have simulated the spin-1/2 Heisenberg model with a spatially staggered anisotropy on the square lattice. Further, we choose to analyze the finite-size scaling of the observables $\rho_1 L$ and $\rho_2 L$, where $L$ refers to the box sizes used in the simulations and $\rho_i$ with $i \in \{1, 2\}$ is the spin stiffness in $i$-direction. The reason for choosing $\rho_1 L$ and $\rho_2 L$ is twofold. First of all, these two observables can be calculated to a very high accuracy using loop algorithms. Secondly, one can measure $\rho_1$ and $\rho_2$ separately. In practice, one would naturally either measure $\rho_s$ which is the average of $\rho_1$ and $\rho_2$ in order to increase the statistics, or $\rho_2$, which corresponds to the spatial direction with a fixed antiferromagnetic coupling, would not be used for data analysis since more measurements is required in order to obtain a good statistics for this observable. However for the model considered here, it is useful to measure quantities which are sensitive to anisotropy. Surprisingly, as we will show later, the observable $\rho_2 L$ receives a much less severe correction than $\rho_1 L$ does. Hence $\rho_2 L$ is a better observable than $\rho_1 L$ (or $\rho_s L$) for finite-size scaling analysis concerning the limitation for the availability of large volumes data in this study. In addition, instead of using a fixed aspect-ratio of spatial box sizes as done in most Monte Carlo calculations, in our investigation we employ the method of fixing the aspect-ratio of spatial winding numbers squared in the simulations which we will introduce briefly later. Remarkably, combining the idea of fixing the aspect-ratio of spatial winding numbers squared in the simulations and finite-size scaling analysis, unlike the unconventional value for $\nu$ observed in \cite{3}, even from $\rho_1 L$ which suffers a very serious correction, we arrive at a value for $\nu$ which is
consistent with that of $O(3)$ by using only up to $L = 64$ data points.

This paper is organized as follows. In section II the anisotropic Heisenberg model and the relevant observables studied in this work are briefly described. Section III contains our numerical results. In particular, the corresponding critical point as well as the critical exponent $\nu$ are determined by fitting the numerical data to their predicted critical behavior near the transition. Finally, we conclude our study in section IV.

II. MICROSCOPIC MODEL AND CORRESPONDING OBSERVABLES

The Heisenberg model considered in this study is defined by the Hamilton operator

$$H = \sum_{(xy)} J \vec{S}_x \cdot \vec{S}_y + \sum_{(x'y')} J' \vec{S}_{x'} \cdot \vec{S}_{y'},$$

where $J'$ and $J$ are antiferromagnetic exchange couplings connecting nearest neighbor spins $(xy)$ and $(x'y')$, respectively. Figure 1 illustrates the Heisenberg model described by Eq. (1). To study the critical behavior of this anisotropic Heisenberg model near the transition driven by the anisotropy, in particular to determine the critical point as well as the critical exponent $\nu$, the spin stiffnesses in the 1- and 2-directions which are defined by

$$\rho_{si} = \frac{1}{3L^2}(W_i^2),$$

are measured in our simulations. Here $\beta$ is inverse temperature and $L$ refers to the spatial box sizes. Further $W_i^2$ is the winding number squared in the $i$-direction. By carefully investigating the spatial volumes and the $J'/J$ dependence of $\rho_{si}L$, one can determine the critical point as well as the critical exponent $\nu$ with high precision.

III. DETERMINATION OF THE CRITICAL POINT AND THE CRITICAL EXponent $\nu$

To calculate the relevant critical exponent $\nu$ and to determine the location of the critical point in the parameter space $J'/J$, one useful technique is to study the finite-size scaling of certain observables. For example, if the transition is second order, then near the transition, the observable $\rho_{si}L$ for $i \in \{1, 2\}$ should be described well by the following finite-size scaling ansatz

$$O_L(t) = (1 + bL^{-\omega})g_\omega(tL^{1/\nu}),$$

where $O_L$ stands for $\rho_{si}L$, $t = (J_s - J)/J_c$ with $j = (J'/J)$, $b$ is some constant, $\nu$ is the critical exponent corresponding to the correlation length $\xi$ and $\omega$ is the confluent correction exponent. Finally $g_\omega$ appearing above is a smooth function of the variable $tL^{1/\nu}$. From Eq. (3), one concludes that the curves of different $L$ for $O_L$, as functions of $J'/J$, should have the tendency to intersect at critical point $(J'/J)_c$ for large $L$. In the following, we will employ the finite-size scaling formula, Eq. (3), for $\rho_{si}L$ with $i \in \{1, 2\}$ to calculate the critical exponent $\nu$ and the critical point $(J'/J)_c$. Without losing the generality, in our simulations we have fixed $J$ to be 1.0 and have varied $J'$. Further, the box size used in the simulations ranges from $L = 6$ to $L = 64$. We also use large enough $\beta$ so that the observables studied here take their zero-temperature values. Figure 2 shows the observables $\rho_sL$ and $\rho_{s2}L$ as functions of $J'/J$. The figure clearly indicates the phase transition is second order since different $L$ curves for both $\rho_sL$ and $\rho_{s2}L$ tend to intersect at a particular point in the parameter space $J'/J$. What is the most striking observation from our results is that the observable $\rho_sL$ receives a much severe correction than

FIG. 1: The anisotropic Heisenberg model considered in this study.

FIG. 2: $\rho_sL$ (upper panel) and $\rho_{s2}L$ (lower panel) as functions of $J'/J$. 
ρsL (upper panel) and ρs2L (lower panel) to Eq. 3. While the circles and squares on these two panels are the numerical Monte Carlo data from the simulations, the solid curves are obtained by using the results from the fits.

where ρ2L does. This can be understood from the trend of the crossing among these curves of different L in figure 2. Therefore one expects a better determination of ν can be obtained by applying finite-size scaling analysis to ρ2L. Before presenting our results, we would like to point out that since data from large volumes might be essential in order to determine the critical exponent ν accurately as suggested in 12, we will use the strategy employed in 12 for our data analysis as well. A Taylor expansion of Eq. 5 up to fourth order in tL^{1/ν} is used to fit the data of ρ2L. The critical exponent ν and critical point (J'/J)c calculated from the fit using all available data of ρ2L are given by 0.6934(13) and 2.51962(3), respectively. The upper panel of figure 3 demonstrates the result of the fit. Notice both ν and (J'/J)c obtain are consistent with the corresponding results found in 11. By eliminating some data points of small L, we can reach a value of 0.700(3) for ν by fitting ρ2L with L ≥ 26 to Eq. 3. On the other hand, with the same range of L (L ≥ 26), a fit of ρsL to Eq. 3 leads to ν = 0.688(2) and (J'/J)c = 2.5193(2), both of which are consistent with those obtained in 11 as well (lower panel in figure 3). By eliminating more data points of ρsL with small L, the values for ν and (J'/J)c calculated from the fits are always consistent with those quoted above. What we have shown clearly indicates that one would suffer the least correction by considering the finite-size scaling of the observable ρs2L. As a result, it is likely one can reach a value for ν consistent with its O(3) prediction, namely ν = 0.7112(5) if large volume data points for ρ2L are available. Here we do not attempt to carry out such a task of obtaining data for L > 64. Instead, we employ the technique of fixing the aspect-ratio of spatial winding numbers squared in the simulations. Surprisingly, combining the idea of fixing the aspect-ratio of winding numbers squared and finite-size scaling analysis, even from the observable ρs3L which is found to receive the most severe correction among the observables considered here, we reach a value for the critical exponent ν consistent with ν = 0.7112(5) without additionally obtaining data points for L > 64. The motivation behind the idea of fixing the aspect-ratio of spatial winding numbers squared in the simulations is as follows. Intuitively the winding numbers squared W^2_i and W^2_j play the role of the quantity (L_i/L'_i)^2 for the system, here L_i and L'_i with i ∈ {1, 2} are the spatial box size used in the simulations and the linear physical length of the system in i-direction, respectively. Indeed it is demonstrated in 8 that rectangular lattice is more suitable than square lattice for studying the spatially anisotropic Heisenberg model with different antiferromagnetic couplings J_i, J_f in 1- and 2-directions. The idea of fixing the aspect-ratio of spatial winding numbers squared quantifies the method used in 8. In general for a fixed L_2, one can vary L_1 and J'/J in order to reach the criterion of a fixed aspect-ratio of spatial winding numbers squared in the simulations. For our study here, without obtaining additional data, this method is implemented as follows. First of all, we calculate (W^2_i)/(W^2_j) for the data point at J'/J = 2.5196 with L = 40 which we denote by w_f. Notice since only the aspect-ratio of the linear physical lengths squared is fixed, we choose L'_i = L for our finite-size scaling analysis. After obtaining this number, a linear interpolation for other data points of ρs1 based on (w_i/w_f)^(-1/2) is performed in order to reach the criterion of a fixed aspect-ratio of spatial winding numbers squared in the simulations. The w appearing above is the corresponding (W^2_i)/(W^2_j) for other data points. Further, we keep the number |w_i/w_f - 1| smaller than 0.055 so that the interpolation results are reliable. A fit of the interpolated (ρs1)wL data to Eq. 3 with w being fixed to its O(3) value (ω = 0.78) leads to ν = 0.706(7) and (J'/J)_c = 2.5196(1) for 36 ≤ L ≤ 64 (figure 4). The subscript "w" appearing above stands for interpolation. Letting ω be a fit parameter results in consistent ν = 0.707(8) and (J'/J)_c = 2.5196(7). Further, we always arrive at consistent results with ν = 0.706(7) and (J'/J)_c = 2.5196(1) from the fits using L > 36 data. The
value of $\nu$ we calculate from the fit is in good agreement with the expected $O(3)$ value $\nu = 0.7112(5)$. The critical point $(J'/J)_c = 2.5196(1)$ is consistent with that found in [1] as well. To avoid any bias, we perform another analysis for the same set of Monte Carlo data without interpolation. By fitting this set of original data points to Eq. 3 with a fixed $\omega = 0.78$, we arrive at $\nu = 0.688(7)$ and $(J'/J)_c = 2.5197(1)$ (figure 5), both of which again agree quantitatively with those determined in [1]. Finally we would like to make a comment regarding the choice of $w_f$. In principle one can calculate $w_f$ for any $L$ and for any $J'/J$ close to the critical point. However since it is shown in [13] that data points of larger volumes is essential for a quick convergence of $\nu$, it will be desirable to choose $w_f$ such that the set of interpolated data contains sufficiently many data points from large volumes. For example, using the $w_f$ obtained at $J'/J = 2.5191$ ($J'/J = 2.5196$) with $L = 40$ ($L = 44$), we reach the results of $\nu = 0.704(7)$ and $(J'/J)_c = 2.5196(1)$ ($\nu = 0.705(7)$ and $(J'/J)_c = 2.5196(1)$) from the fit with a fixed $\omega = 0.78$. These values for $\nu$ and $(J'/J)_c$ agree with what we have obtained earlier. Interestingly, it seems that the idea of fixing the aspect-ratio of winding numbers squared determines the critical exponent $\nu$ more accurately than the conventional method of fixing the aspect-ratio of box sizes in the simulations. It would be interesting to explore this new method systematically including applying it to the study of phase transition for other spatially anisotropic Heisenberg models.

IV. DISCUSSION AND CONCLUSION

In this letter, we revisit the phase transition of the spin-1/2 Heisenberg model with a spatially staggered anisotropy. We find that the observable $\rho_{s2}L$ suffers a much less severe correction compared to that of $\rho_{s1}L$, hence is a better quantity for finite-size scaling analysis. Further, by employing the method of fixing the aspect-ratio of spatial winding numbers squared in the simulations, we arrive at $\nu = 0.706(7)$ for the critical exponent $\nu$ which is consistent with the most accurate Monte Carlo $O(3)$ result $\nu = 0.7112(5)$ by using only up to $L = 64$ data points derived from $\rho_{s1}L$.

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![FIG. 4: Fit of interpolated ($\rho_{s1}$) data to Eq. 3 While the circles are the numerical Monte Carlo data from the simulations, the solid curves are obtained by using the results from the fit.](image1)

![FIG. 5: Fit of original $\rho_{s1}L$ data to Eq. 3 While the circles are the numerical Monte Carlo data from the simulations, the solid curves are obtained by using the results from the fit.](image2)

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