Finite-size scaling of the frustrated Heisenberg model on a hexagonal lattice

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We investigate through Monte Carlo simulations the critical behavior of the antiferromagnetic Heisenberg model on a hexagonal lattice. Critical exponents associated with both magnetic and chiral orderings were estimated. The transition temperatures of these two kinds of order were found to be the same within error margins, in agreement with previous results. The calculation of the Binder parameter also demonstrates that the transition is most likely continuous. The exponents obtained agree, for the most part, with those of Kawamura and thus provide further support for the existence of a new universality class.

I. INTRODUCTION

Discussion concerning the existence or not of a new chiral universality class for frustrated spin systems on the stacked triangular lattice still exists.[1] It was Kawamura[2,3] who proposed, based on symmetry arguments and Monte Carlo results, that the critical behavior of the geometrically frustrated antiferromagnetic XY and Heisenberg models on a hexagonal lattice should be described by new universality classes characterized by the following sets of exponents for the $n=3$ case (Heisenberg):[3] $\alpha=0.24(8)$, $\beta=0.30(2)$, $\gamma=1.17(7)$, $\nu=0.59(2)$, $\beta_\kappa=0.55(4)$, $\gamma_\kappa=0.72(8)$, $\nu_\kappa=0.60(3)$ (where the subscript κ refers to the chirality). Kawamura[4] also made some renormalization-group $\epsilon=4-d$ studies which revealed that chirality was a relevant operator and that a new chiral fixed point was associated with it. On the other hand Azaria, Delamotte, and Jolicoeur[5] performed a $2+\epsilon$ renormalization-group calculation and found that the critical behavior of the frustrated Heisenberg antiferromagnet could be described by one of the three following possibilities: either the transition is first order or, if it is continuous, it belongs to the O(4) or mean-field tricritical universality classes. Recently, a few groups have done more sophisticated Monte Carlo simulations in order to test the variety of predictions. Bhattacharya *et al.*[6] reported values for the magnetic exponents which are in close agreement with those of Kawamura. They obtained $\beta/\nu=0.495(10)$, $\gamma/\nu=2.011(14)$, $\nu=0.585(9)$. Loison and Diep[7] also obtained results in agreement with Kawamura. However, none of these groups considered the chiral order parameter. One of the big issues associated with this problem concerns the simultaneous ordering of the chiral and magnetic order parameters. The results of Kawamura seem to support this possibility but there is no *a priori* reason for these two transitions to occur at the same temperature in zero field. The same question arises also in the case of the fully frustrated lattices (generalized Villain model), where simulation results seem to indicate identical transition temperatures.[8] It is only recently, however, that new Monte Carlo techniques (as used here) have provided a means by which to very accurately, and independently, determine transition temperatures.

Both the magnetic and chiral order parameters were considered in our histogram Monte Carlo simulations. This enables us to estimate the magnetic and chiral transition temperatures and the sets of exponents associated with these orderings by finite-size scaling. In Sec. II we present briefly the model and the method we used. The results are presented in Sec. III and our conclusion in Sec. IV.

II. MODEL AND METHOD

We considered the Heisenberg model on a stacked triangular lattice. The Hamiltonian is given by

$$H=J_\parallel \sum_{\langle ij\rangle} \mathbf{S}_i\cdot\mathbf{S}_j + J_\perp \sum_{\langle kl\rangle} \mathbf{S}_k\cdot\mathbf{S}_l \ , \tag{1}$$

where we take nearest-neighbor (NN) ferromagnetic interplane interactions $J_\parallel<0$ and NN antiferromagnetic intraplane interactions $J_\perp>0$, with $|J_\parallel|=|J_\perp|=1$ (all the energies henceforth are expressed in units of $|J_\parallel|$). The spins are thus frustrated on each plaquette of the triangular lattice and we have the well-known 120° structure in the ground state.

The Metropolis algorithm was used, combined with the histogram analysis technique.[9] Lattice sizes $L\times L\times L$, with $L=12$, 15, 18, 21, 24, 27, 30, and 36, and periodic boundary conditions were considered. In order to localize the transition temperature we performed simulations at different nearby temperatures including ones close to the estimated infinite-lattice transition temperature T_c.[2,3] From 10^6 Monte Carlo steps (MCS) for the smaller lattices to 2.6×10^6 MCS for the larger lattices were used for each of these simulations. Histograms were generated for the different magnetic and chiral variables described below. The magnetic order parameter was defined as in Ref. 10. The chiral order parameter for a single triangular plaquette is given by the expression

$$\kappa_p=\frac{2}{3\sqrt{3}} \sum_{\langle ij\rangle} [\mathbf{S}_i\times\mathbf{S}_j]_p \ . \tag{2}$$

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The sum is over the three bonds belonging to the plaquette p. For the XY model κ_p is a scalar but for the Heisenberg model it is a vector. The value of the chiral order parameter for a given configuration is then given by

$$\kappa=\frac{1}{N}\sum_p \kappa_p \ . \tag{3}$$

The chiral order in the ground state is characterized by alternating chirality on adjacent plaquettes. Accordingly, the sum in (3) is on the plaquettes with up- (or down-) pointing chirality. The thermal average is given by

$$\bar{\kappa}=\sqrt{\langle \kappa^2 \rangle} \ . \tag{4}$$

This corresponds to the definition used in Ref. 2.

III. RESULTS

A. Estimation of the transition temperatures

The fourth-order magnetic and chiral cumulants U_L and $U_L^{(\kappa)}$ were used to estimate the transition temperature of the magnetic and chiral order parameters, respectively. This quantity is defined by the following expression:[11]

$$U_L=1-\frac{\langle m^4 \rangle_L}{3\langle m^2 \rangle_L^2} \ . \tag{5}$$

$\langle m^k \rangle_L$ is the thermodynamic average value of the kth power of the magnetic order parameter for the lattice of size L. The same type of expression holds for the chiral order parameter $U_L^{(\kappa)}$. The "cumulant crossing" method[11,12] was used to extract the transition temperatures. It is based on the observation that the temperature T_c^* at which intersect the various curves of $U_L(T)$ for different lattice sizes scale as $\ln^{-1}(L'/L)$, where L' and L are two different lattice sizes. The extrapolated values of the temperature for $\ln^{-1}(L'/L)\rightarrow 0$ correspond to $T_c(L\rightarrow\infty)$. Figure 1 presents the curves of T_c^* as a function of $\ln^{-1}(L'/L)$ for the magnetic and chiral transitions. Table I presents the extrapolated values for the

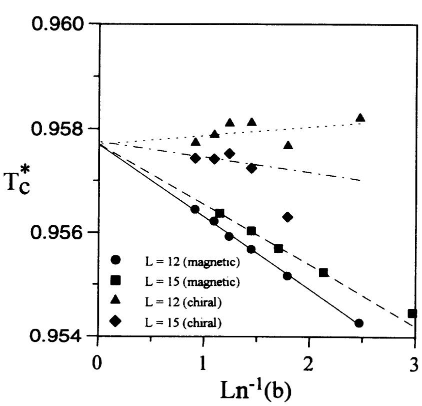

FIG. 1. Critical magnetic and chiral transition temperatures T_c^* obtained by the interception of the fourth-order cumulant values U_L and $U_L^{(\kappa)}$ for lattice sizes L and L' as a function of the inverse logarithm of the scale factor $b=L'/L$.

TABLE I. Estimates for the magnetic and chiral transition temperatures obtained by the extrapolated temperatures at which the magnetic and chiral fourth-order cumulants for lattice size L, U_L, and $U_L^{(\kappa)}$ intercept the cumulants for lattice size L' (see Fig. 1).

Intersection with lattice size L	Transition temperature T_c^* Magnetic	Chiral
12	0.957 69(10)	0.957 7(6)
15	0.957 70(10)	0.957 75(60)

transition temperatures for the different values of L. The chiral transition $T_c^{(\kappa)}$ and the magnetic transition $T_c^{(m)}$ for the infinite lattice are thus estimated as

$$T_c^{(\kappa)}=0.9577(6) \ ,$$

$$T_c^{(m)}=0.9577(2) \ .$$

These results are in agreement with those of the work of Kawamura,[2,3] which reports $T_c^{(m)}=0.958(4)$ and $T_c^{(\kappa)}=0.957(3)$, as well as that of Bhattacharya *et al.*,[6] $T_c^{(m)}=0.9576(2)$. From our results we thus conclude that, within error, the chiral and magnetic transition temperatures are the same.

B. Order of the transition

Azaria, Delamotte, and Jolicoeur[5] suggest that the transition in frustrated antiferromagnets could be first order. The only evidence so far of the continuous nature of this transition is the apparent continuity of thermodynamic quantities and the absence of hysteresis.[3,6,7] Many examples exist, however (see Ref. 13), where the weak first-order nature of a transition could not be detected in this way. A more precise tool we now have to identify the order of the transition is the Binder cumulant[14] defined by

$$U_L^{(B)}=1-\frac{\langle E^4 \rangle_L}{3\langle E^2 \rangle_L^2} \ . \tag{6}$$

This variable has a minimum as a function of temperature, and, when extrapolated to the thermodynamic limit $L\rightarrow\infty$, the value of this minimum is $(U_L^{(B)})_{\min}=\frac{2}{3}$ for a continuous transition but is smaller for a first-order transition. If it is a weak first-order transition, $(U_L^{(B)})_{\min}$ will be close to $\frac{2}{3}$. From this we see that the possibility that a transition is very weakly first order can never be completely ruled out on the basis of finite-size simulation results.[15]

Figure 2 shows the scaling of $(\frac{2}{3}-U_L^{(B)})$ as a function of $1/L^3$. By performing such a scaling analysis we assume a first-order transition.[13,14] The extrapolated value we find is $U_\infty^{(B)}=0.666\,66(1)$, which is not different from $\frac{2}{3}$ within error. Thus we conclude that the transition is likely continuous.

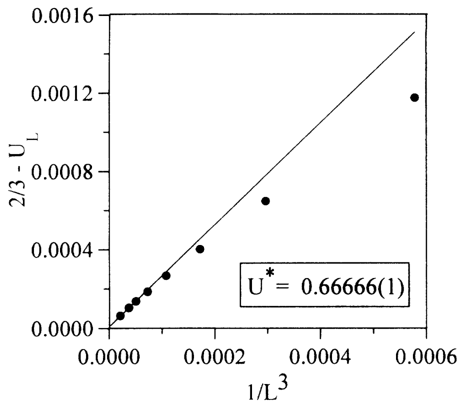

FIG. 2. Scaling of the energy-cumulant minimum with the inverse volume. Only the three largest lattice sizes ($L=27$, 30, and 36) are used in the fit.

C. Estimation of the critical exponents

We estimated the exponents in two different ways. First we looked at the scaling of the maxima of some thermodynamic variables.[12] This required that the simulation temperatures be close enough to the maximum to get reliable results. Since different variables order at different temperatures for finite-size lattices, simulations at many temperatures were necessary, especially for the smaller lattices. The second approach was to consider the scaling of these variables at the estimated transition temperature.[16] It is important to note, however, that the values of the exponents obtained from these different methods are consistent with each other.

1. Estimation of the critical exponents from the scaling of maxima

The following scaling relations were used for the evaluation of the critical exponents γ and ν:

$$\left[\frac{\partial}{\partial K}[\ln(\langle m\rangle)]\right]_{\max}=\frac{\langle mE\rangle}{\langle m\rangle}-\langle E\rangle\sim L^{1/\nu} ,$$
$$\left[\frac{\partial}{\partial K}[\ln(\langle m^2\rangle)]\right]_{\max}=\frac{\langle m^2E\rangle}{\langle m^2\rangle}-\langle E\rangle\sim L^{1/\nu} , \quad (7)$$
$$(\chi')_{\max}=KL^3[\langle m^2\rangle-\langle m\rangle^2]\sim L^{\gamma/\nu} .$$

In these expressions K is the inverse temperature and E is the internal energy. The maximum of the thermodynamic derivative, $(dU_L/dK)_{\max}$, was also considered but the large fluctuations associated with this quantity made the extraction of reliable estimates of ν difficult. The same functions were used for the calculation of the chiral exponents in which m is replaced by κ. Table II presents the values of the exponents obtained from the scaling of the maxima of these functions.

2. Estimation of the critical exponents from scaling at T_c

The transition temperature for both the chiral and the magnetic transitions was assumed to be $T_c=0.9577(2)$.

TABLE II. Estimates of the magnetic and chiral critical exponents resulting from the scaling of the maxima of different thermodynamic variables. The quoted susceptibilities are the ones defined according to Eq. (7). The asterisk indicates that the fits were done excluding the smallest lattice size $L=12$.

Variable	Exponent	Value
$\partial[\ln\langle m\rangle]/\partial K$	ν	0.59(1)*
$\partial[\ln\langle m^2\rangle]/\partial K$	ν	0.59(1)*
χ'	γ/ν	2.21(3)
$\partial[\ln\langle\kappa\rangle]/\partial K$	ν_κ	0.60(1)*
$\partial[\ln\langle\kappa^2\rangle]/\partial K$	ν_κ	0.605(15)*
χ'_κ	γ_κ/ν_κ	1.36(3)

Scaling of the various functions that appear in Eq. (7), evaluated at T_c, was performed. We also considered the scaling of the magnetic and chiral order parameters $\langle m\rangle$ and $\langle\kappa\rangle$ at $T=T_c$, which are of the form

$$\langle m\rangle_c\sim L^{-\beta/\nu} ,$$
$$\langle\kappa\rangle_c\sim L^{-\beta_\kappa/\nu_\kappa} . \quad (8)$$

In addition, the chiral and magnetic susceptibilities defined by

$$\chi=KL^3\langle m^2\rangle ,$$
$$\chi_\kappa=KL^3\langle\kappa^2\rangle , \quad (9)$$

were also evaluated. In these expressions, we assume $\langle m\rangle\sim 0$ and $\langle\kappa\rangle\sim 0$, which should be the case at T_c. When computing the value of $\langle m\rangle$ in the simulation we take, in fact, the absolute value of the order parameter.[12] We considered the two definitions of the susceptibility, Eqs. (7) and (9), as in Ref. 12.

The scaling of some thermodynamic functions at T_c is presented in Figs. 3 and 4. Estimated exponent values are given in Table III. The errors were estimated by tak-

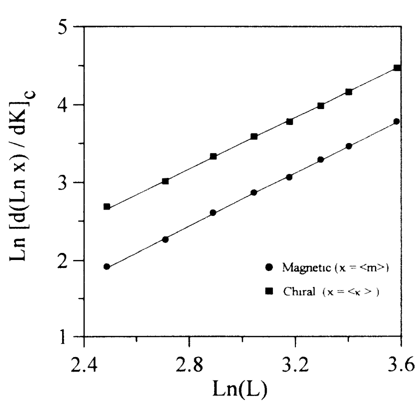

FIG. 3. Log-log plot of the logarithmic derivatives of the chiral and magnetic order parameters as a function of lattice size L at the estimated transition temperature $T_c\sim 0.9577$. The resulting values of the critical exponents are $\nu=0.587(5)$ and $\nu_\kappa=0.605(6)$. The resulting fit for the magnetic exponent takes account of all the lattice sizes, whereas the one for the chiral exponent excludes the smallest lattice size $L=12$.

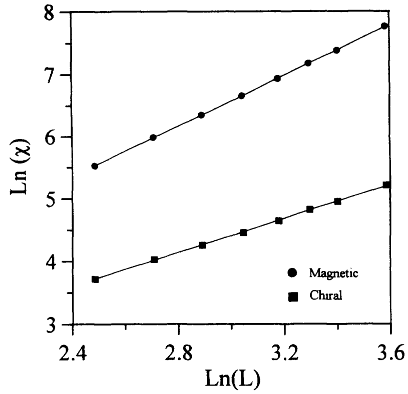

FIG. 4. Log-log plot of the magnetic and chiral susceptibilities [Eq. (9)] as a function of L at the estimated transition temperature $T_c=0.9577$. The fits include all the lattice sizes and the resulting values of the critical exponents are $\gamma/\nu=2.033(5)$ and $\gamma_\kappa/\nu_\kappa=1.354(11)$.

ing account of the uncertainties in the values of the quantities as well as in the critical temperature (i.e., exponents were estimated also from results at $T=0.9575$ and 0.9579). In order to investigate possible corrections to scaling due to L being too small, fits were also done without values from the smallest lattice sizes: a significant effect was found only in the case of ν_κ. As can be seen, the values are consistent with each other except for the magnetic susceptibility where we observe large differences between the estimates obtained from the scaling of χ and χ'. Such differences were also observed by Peczak, Ferrenberg, and Landau[16] for the classical Heisenberg ferromagnet although they were much less pronounced in that case. However, no differences were found between the estimates of γ_κ/ν_κ obtained from the scaling of χ_κ and χ'_κ. Note that the exponent ratios given in Table III are consistent with those of Table II. For our final estimate of γ/ν, we took the value obtained from the scaling of χ at T_c. This definition corresponds to the one used by Kawamura. The corresponding values

TABLE III. Estimates of the magnetic and chiral critical exponents obtained from the scaling of the thermodynamic variables at the estimated critical temperature $T_c=0.9577(2)$. The quoted errors take account of the errors in the simulation values and in the critical temperature. The asterisk indicates that the fits were done excluding the smallest lattice size $L=12$.

Variable	Exponent	Value
$\partial[\ln(\langle m\rangle)]/\partial K$	ν	0.587(9)
$\partial[\ln(\langle m^2\rangle)]/\partial K$	ν	0.585(8)
χ'	γ/ν	2.23(3)
χ	γ/ν	2.033(19)
$\langle m\rangle$	β/ν	0.486(12)
$\partial[\ln(\langle\kappa\rangle)]/\partial K$	ν_κ	0.605(12)*
$\partial[\ln(\langle\kappa^2\rangle)]/\partial K$	ν_κ	0.611(11)*
χ'_κ	γ_κ/ν_κ	1.355(20)
χ_κ	γ_κ/ν_κ	1.35(4)
$\langle\kappa\rangle$	β_κ/ν_κ	0.823(20)

are in agreement with the one obtained in Ref. 6. The most striking result from these simulations is the apparent inequality of the exponents ν and ν_κ. The hyperscaling relations

$$\alpha=2-\nu d\ , \qquad \alpha=2-\nu_\kappa d \tag{10}$$

when applied to the chiral and the magnetic exponents imply $\nu=\nu_\kappa$ if $T_c^{(m)}=T_c^{(\kappa)}$. The values reported by Kawamura[2] are $\nu=0.59(2)$ and $\nu_\kappa=0.60(3)$ and thus, within the error bars, these two values are effectively equal. The values we finally quote from our simulations are $\nu=0.586(8)$ and $\nu_\kappa=0.608(12)$. These values are in agreement with those of Kawamura but they are marginally different from each other. In order to obtain these estimates and the uncertainties associated with them we assume $T_c^{(\kappa)}\equiv T_c^{(m)}=0.9577(2)$. However, the error related to the chiral transition temperature is much larger. If this uncertainty is used to estimate the error in the chiral exponent one has $\nu_k=0.608(36)$. But by doing so we implicitly assume that the two transitions occur at different temperatures. The reason for this possible inequality of the exponents ν and ν_k requires better understanding before any clear conclusions can be drawn. Corrections to scaling are also possible, which biased our estimates because of the small lattices considered in the simulations. However, these results do not rule out the possibility that the two transitions occur at different temperatures so close that we cannot distinguish them within the precision of these simulations.

In Table III we present no estimate of the α exponent. This exponent is associated with the scaling of the specific heat according to the expression

$$C_v \sim a + bL^{\alpha/\nu}\ . \tag{11}$$

The large fluctuations in our results for C_v and the small value of α prevent a direct evaluation of this critical ex-

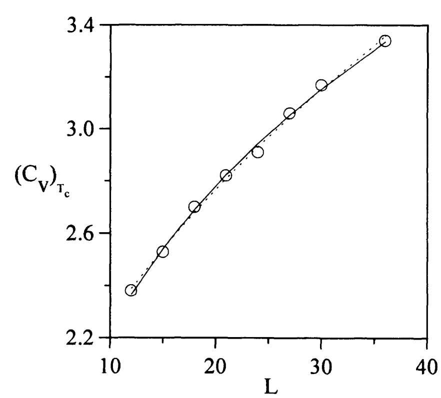

FIG. 5. Scaling of the specific heat at T_c as a function of lattice size L. The different curves are obtained by fitting the data according to Eq. (11) with an exponent α/ν set equal to the extreme values reported by Ref. 2, i.e., $\alpha=0.16$ (continuous curve) and $\alpha=0.32$ (hatched curve). The corresponding values of the fitting parameters a and b are $a=-0.44$, $b=1.44$ for $\alpha=0.16$, and $a=1.19$, $b=0.31$ for $\alpha=0.32$.

TABLE IV. Comparison of the critical exponents obtained from this work with those of Refs. 3, 6, and 7.

Exponent	This study	Ref. 3	Ref. 6	Ref. 7
α		0.24(8)		
β	0.285(11)	0.30(2)	0.289(10)	0.28(2)
ν	0.586(8)	0.59(2)	0.585(9)	0.59(1)
γ	1.185(3)	1.17(7)	1.176(20)	1.25(3)
β_κ	0.50(2)	0.55(4)		
ν_κ	0.608(12)	0.60(3)		
γ_κ	0.82(4)	0.72(8)		

ponent. If we assume a value of $\alpha=0.24(8)$, as quoted in Ref. 3, and fit the results of $(C_v)_{T=T_c}$ or of $(C_v)_{\max}$ [both should scale according to Eq. (11)], the curve obtained is consistent with our data. If now we set α to the extreme values that this estimate allows, namely $\alpha=0.16$ or $\alpha=0.32$, and do the same exercise, the resulting fits are again quite good. Figure 5 shows the graph obtained for $(C_v)_{T=T_c}$ assuming these extreme values. The only alternative is the use of scaling relations, but, as we have seen, the use of the hyperscaling relation to estimate α implies two different values of this exponent since we have $\nu\neq\nu_\kappa$. If we apply these hyperscaling relations to the chiral exponents we get $\alpha=0.18$ and for the magnetic exponent $\alpha=0.24$. Both values are within the errors of the quoted value of Kawamura but, as seen on Fig. 5, our specific heat data cannot discriminate between these possibilities.

Table IV presents the results of our simulations (those obtained at T_c) compared with those of Refs. 3, 6, and 7. Our values of the magnetic exponents are in close agreement with those of Ref. 6, which use also a histogram Monte Carlo technique with scaling at T_c. The only other results on the chiral exponents are those of Kawamura, who uses the "data collapsing" method. Our values agree with those of Kawamura within error margins.

IV. CONCLUSION

We have reported the results of extensive histogram Monte Carlo simulations of the antiferromagnetic Heisenberg model on a hexagonal lattice for which *both* magnetic and chiral order parameters were measured. The transition temperatures of the magnetic and chiral orderings were determined by the highly accurate "cumulant crossing" method and we find that, within errors, the two transitions occur at the same temperature $T_c=0.9577(2)$. This is in agreement with less accurate results reported by Kawamura. The order of the transition was also studied by considering scaling of the Binder cumulant and we conclude that the transition is likely continuous. The sets of exponents obtained from this analysis (see Table IV) agree with results from previous works. However, our values may suggest that $\nu\neq\nu_\kappa$. This surprising result was also observed for the *XY* model on a stacked triangular lattice, for which the difference between these exponents is even greater[17] and where the chiral and magnetic transitions also appear to occur at the same temperature.

Although our results generally support the conjecture by Kawamura of a new chiral universality class for the frustrated Heisenberg model, the possibility of a very weak first-order transition, with a set of effective critical exponents,[15] cannot be excluded from available simulation results. Conclusions regarding the simultaneous ordering of both magnetic and chiral degrees of freedom are complicated by the possibility that these two transitions are "decoupled,"[8] each with its own characteristic length scale, so that it is not necessary to have $\nu=\nu_\kappa$. We know of no physical reason why the two transitions should occur at the same temperature; indeed, a two-step process for frustrated spin systems has recently been proposed.[18] It appears that further information from simulations on the critical behavior of this system must await the advent of much improved algorithms for the treatment of frustrated vector spin systems.

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