PHYSICAL REVIEW B VOLUME 48, NUMBER 17 1 NOVEMBER 1993-I

Spin stiffness in frustrated antiferromagnets

B. W. Southern* and A. P. Young

Physics Department, University of California, Santa Cruz, California 95064

(Received 8 July 1993)

The classical antiferromagnetic Heisenberg model on the triangular lattice is studied using Monte Carlo techniques. The behavior of the antiferromagnetic structure factor, antiferromagnetic correlation length, and spin stiffness at low temperatures is consistent with recent low-temperature renormalization-group predictions based on a nonlinear sigma model (NLσ) description of the system. Our results support the validity of the NLσ model approach to the study of frustrated systems.

The nature of the ordering in frustrated magnetic systems is a topic of considerable interest. The classical Heisenberg model on the triangular lattice with antiferromagnetic couplings is perhaps the simplest example of such a frustrated system. The ground state has three sublattices with a *noncollinear* arrangement of the spins on each triangle and hence the local order parameter is a rotation matrix. This suggests that this model belongs to a different universality class from the corresponding model on bipartite lattices where there is no frustration and the order parameter corresponds to a unit vector. Dombre and Read[1] have mapped the continuum version of the model on to a nonlinear sigma model (NLσ) and Azaria *et al.*[2–4] have used renormalization-group (RG) techniques to study the correlation length and effective long-wavelength spin stiffness of this NLσ at low temperatures. These calculations and also those of Apel *et al.*[5] indicate that the symmetry of the model is dynamically enlarged at a zero-temperature critical fixed point and belongs to the $N = 4$ Wilson-Fisher universality class of the $O(N)/O(N-1)$ NLσ model. Due to the fact that the local order parameter is similar to a rigid body, there are three spin stiffness coefficients ρ_1, ρ_2, ρ_3 which describe how the system responds to twists about three mutually orthogonal directions in spin space. Azaria *et al.*[3,4] obtained the two-loop recursion equations which describe the effect of thermal fluctuations on these stiffness coefficients as well as the correlation length to two-loop order.

In this paper, we study the classical Heisenberg antiferromagnet on the triangular lattice using both Monte Carlo techniques and high-temperature series expansions. In particular, we study the temperature dependence of the structure factor $S(\mathbf{Q})$ at the antiferromagnetic ordering wave vector $\mathbf{Q}$ and the antiferromagnetic correlation length ξ for systems of linear size $L = 30$ to $L = 240$, as well as the dependence of the spin stiffness coefficients ρ_1, ρ_2, ρ_3 on system size at low temperatures. Our results are in excellent agreement with the predictions of Azaria *et al.*[3,4] for the dependence of the spin stiffness on the lattice size and are consistent with the predicted temperature dependence of the correlation length.

We consider the classical Heisenberg model on a triangular array of L^2 sites with the Hamiltonian

$$H = \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j \quad , \tag{1}$$

where $\mathbf{S}_i$ is a three component unit vector at each site, the sum is over nearest-neighbor pairs (each distinct pair counted once), and the interaction J has been set to unity. The structure factor $S(\mathbf{q})$ is defined by

$$S(\mathbf{q}) = \frac{1}{L^2} \sum_{i,j} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \quad , \tag{2}$$

where $\langle \cdots \rangle$ denotes a thermal average and $\mathbf{q}$ is a wave vector in the first Brillouin zone. The classical ground state is a coplanar arrangement in which the three spins on each triangle are oriented at 120° with respect to one another. This corresponds to ordering at the zone corner wave vector $\mathbf{Q} = (4\pi/3, 0)$ in units where the lattice spacing is unity. The antiferromagnetic correlation length ξ can be obtained from the structure factor using the Ornstein-Zernicke form

$$S(\mathbf{q}) = \frac{S(\mathbf{Q})}{1 + \xi^2 (\mathbf{q} - \mathbf{Q})^2} \quad , \tag{3}$$

which is valid for $\mathbf{q}$ near the ordering wave vector.

Our Monte Carlo program uses a heat bath algorithm[6] to update the spin directions and all thermal averages are replaced by time averages. For the largest value of $L = 240$ we discard the first 2×10^4 time steps and perform averages over the next 2×10^5 steps. Figures 1 and 2 show the structure factor $S(\mathbf{Q})$ and the square of the correlation length ξ^2, respectively, as a function of temperature T for various system sizes. Both quantities increase by two orders of magnitude as the temperature T decreases from 0.4 to 0.3. Kawamura and Miyashita[7] observed a sharp peak in the specific heat at $T \sim 0.33$ and estimated the correlation length to be 20–30 lattice spacings at this temperature. Our results confirm this estimate and also show that the correlation increases dramatically below this temperature.

The two-loop renormalization-group (RG) calculation of Azaria *et al.*[3] for the corresponding NLσ model predicts the following form for the correlation length (in units of the lattice spacing) at low temperatures:

$$\xi = C_\xi (T/B)^x \exp(B/T), \tag{4}$$

where C_ξ is an unknown constant and $B = 2\pi(\frac{2+\pi}{8})\sqrt{3} = 6.994$. The exponent x has the value 1/2, the same as for the $O(N)$ vector model with $N = 4$, and is to be

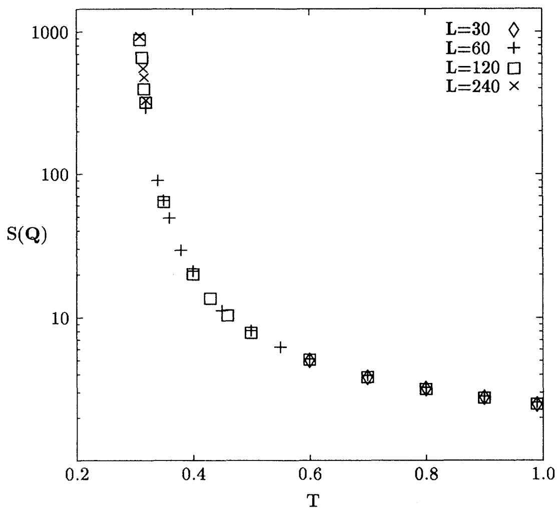

FIG. 1. A semilogarithmic plot of the structure factor at the antiferromagnetic ordering wave vector, $S(\mathbf{Q})$, as a function of temperature T for system sizes $L = 30, 60, 120, 240$.

compared with the value of unity[8] for the $O(3)$ vector model. The structure factor $S(\mathbf{Q})$ is proportional to $\xi^{2-\eta}$ at low temperatures and, although $\eta = 0$ at the fixed point, finite temperature corrections yield a temperature dependent prefactor. We use the following form:

$$S(\mathbf{Q}) = C_S (T/B)^y \exp(2B/T), \tag{5}$$

where C_S is an unknown constant and the value of y can be determined from the $2 + \epsilon$ expansion for η. Azaria *et al.*[9] have recently calculated η for this model and using their results we find $y = 5$. For the $O(3)$ model on bipartite lattices where the order parameter is a unit vector, this exponent has the value[8] 4.

In order to make a better comparison of our Monte Carlo results with the expected behavior, we have also derived the high-temperature series for $S(\mathbf{Q})$ and ξ^2 up

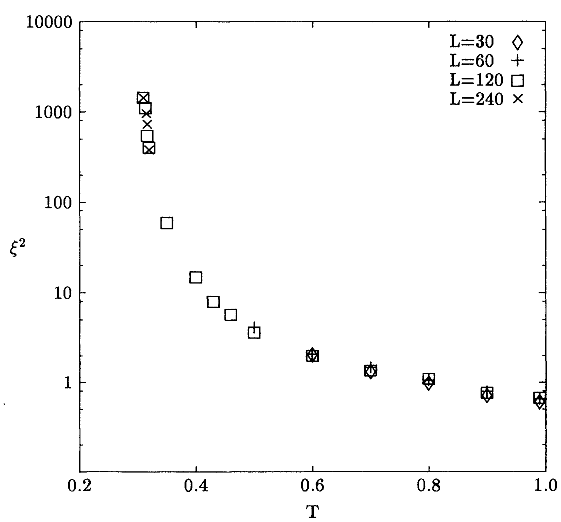

FIG. 2. A semilogarithmic plot of the square of the antiferromagnetic correlation length as a function of temperature T for system sizes $L = 30, 60, 120, 240$.

TABLE I. Coefficients in the high-temperature series of the antiferromagnetic structure factor and the square of the antiferromagnetic correlation length. We write each quantity as $\sum_n a_n (1/T)^n$ and the table gives the coefficients a_n.

n	$S(\mathbf{Q})$	ξ^2
0	1.000 000 000 00	0.000 000 000 00
1	1.000 000 000 00	0.250 000 000 00
2	0.333 333 333 33	0.250 000 000 00
3	0.155 555 555 56	0.094 444 444 44
4	0.051 851 851 85	0.027 777 777 78
5	0.011 781 305 11	0.017 760 141 09
6	0.013 850 676 07	0.006 237 507 35
7	-0.009 934 548 30	-0.002 126 200 27
8	0.016 812 444 59	0.004 975 728 56

to eighth order in $1/T$. We have used the diagrammatic results of Stanley[11] and the coefficients are tabulated in Table I. Figures 3 and 4 show plots of $T \ln S(\mathbf{Q})$ vs T and $T \ln(4T\xi^2)$ vs T, respectively. The Monte Carlo data have been fitted to the predicted forms in (4) and (5) and these curves are indicated by the solid lines. We have assumed the predicted values for B, x, and y to obtain estimates for the constants C_S and C_ξ. We find the surprisingly small values $C_S = (1.3 \pm 0.1)10^{-10}$ and $C_\xi = (3.1 \pm 0.1)10^{-8}$. Very small prefactors for the correlation length have also been found for another model with the same symmetry.[10] Also shown in Figs. 3 and 4 are a few Padé approximants $[N/M]$ to each curve using our high-temperature series coefficients. The Monte Carlo results are consistent with both the low-temperature predictions of Azaria *et al.*[3] and with the high-temperature series. Note the rapid crossover in behavior at $T \sim 0.32$. Because of this, if we had no information about the low-

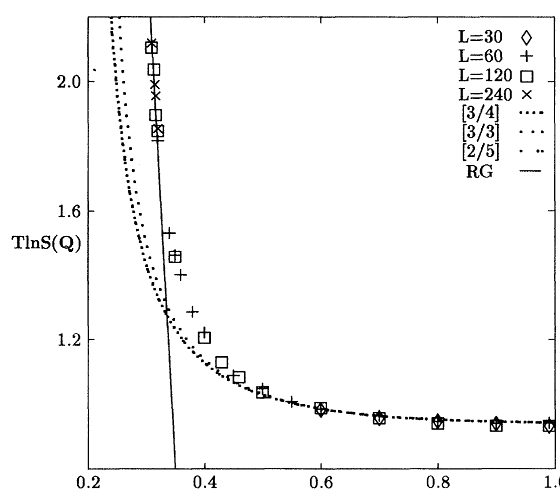

FIG. 3. $T \ln S(\mathbf{Q})$ as a function of temperature T. The Monte Carlo data for different system sizes are indicated by the symbols. The solid line is a fit to the low-T RG predictions (Ref. 3) and the dotted lines represent Padé approximants to the function using the high-temperature series coefficients in the table. $[N/M]$ denotes the ratio of a polynomial of order N in the numerator to one of order M in the denominator.

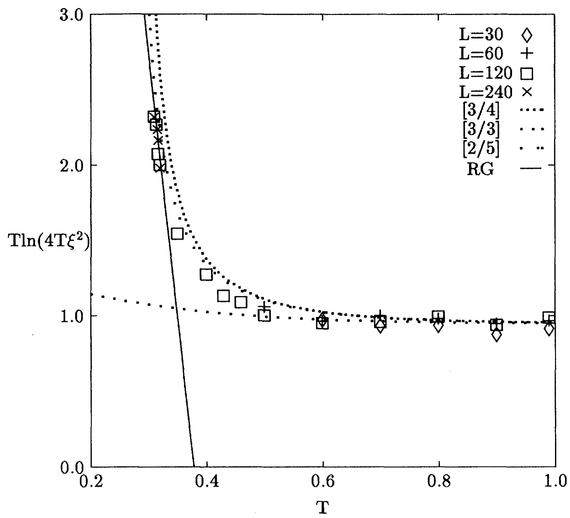

FIG. 4. $T\ln(4T\xi^2)$ as a function of temperature T. The notation is the same as that in Fig. 3.

T limit from the RG study of the NLσ model,[3] but only had available the Monte Carlo data and the series (which can be trusted only at temperatures where the different Padés agree), one would greatly underestimate the value of the coefficient B in the exponential in Eqs. (4) and (5). Conversely, one could argue that while our results are *consistent* with the value of B obtained theoretically,[3] they do not *demonstrate* that this is the correct value. However, we shall present below much more convincing evidence which supports the RG analysis based on the NLσ model.[2–4] Our results are rather insensitive to the values of the exponents, x and y, in the power law prefactors in Eqs. (4) and (5).

The most convincing evidence for the validity of the NLσ model RG treatment is provided by the size dependence of the spin stiffness at low temperatures. The spin stiffness tensor is given by the second derivative of the free energy with respect to the twist angle about a particular direction in spin space. In order to measure the three principal stiffness coefficients $\rho_\alpha(\alpha=1,2,3)$ we define the following set of vectors:

$$\begin{aligned}\hat{\mathbf{n}}_1 &= (\mathbf{S}_A+\mathbf{S}_B-2\mathbf{S}_C)/|\mathbf{S}_A+\mathbf{S}_B-2\mathbf{S}_C|,\\ \hat{\mathbf{n}}_2 &= (\mathbf{S}_A-\mathbf{S}_B)/|\mathbf{S}_A-\mathbf{S}_B|,\\ \hat{\mathbf{n}}_3 &= \hat{\mathbf{n}}_1\times\hat{\mathbf{n}}_2,\end{aligned} \tag{6}$$

where $\mathbf{S}_A, \mathbf{S}_B, \mathbf{S}_C$ are the magnetizations on the three sublattices, A, B, and C. These vectors are orthonormal when the system is in the ground state. Applying a twist to every spin pair about each of these axes by an angle $\Delta\theta_{ij}=\frac{\Theta}{L}\hat{\mathbf{e}}_{ij}\cdot\hat{\mathbf{u}}$ and evaluating the second derivative of the free energy with respect to Θ at $\Theta=0$ yields the following form for the stiffness coefficients:

$$\rho_\alpha = -\frac{2}{\sqrt{3}L^2}\sum_{\langle i,j\rangle}(\hat{\mathbf{e}}_{ij}\cdot\hat{\mathbf{u}})^2\langle S_i^\beta S_j^\beta + S_i^\gamma S_j^\gamma\rangle - \frac{2}{\sqrt{3}L^2T}\left\langle\left(\sum_{\langle i,j\rangle}(\hat{\mathbf{e}}_{ij}\cdot\hat{\mathbf{u}})[S_i^\beta S_j^\gamma - S_i^\gamma S_j^\beta]\right)^2\right\rangle \tag{7}$$

where $\alpha=1,2,3$ and α,β,γ are to be taken in cyclic order. Here S_i^α denotes the component of the spin at site i in the $\hat{\mathbf{n}}_\alpha$ direction, $\hat{\mathbf{e}}_{ij}$ are unit vectors along neighboring bonds, and $\hat{\mathbf{u}}$ is the direction along the lattice of the twist. All stiffnesses have been normalized by the unit cell area in order to allow direct comparison of our results with those of the NLσ model calculations.

Both ρ_1 and ρ_2 correspond to twists about axes in the plane of the ordering whereas ρ_3 measures the stiffness about an axis perpendicular to this plane. As T approaches zero, we obtain the values $\rho_3=2\rho_1=2\rho_2=\sqrt{3}/2$ in agreement with the microscopic values of the NLσ model.[1,5] At any finite temperature T, the stiffnesses are zero on scales large compared with the correlation length. However, on length scales smaller than the correlation length, the local spin stiffness is nonvanishing at low temperatures. Azaria *et al.*[4] have made detailed predictions for the dependence of these stiffnesses on the linear size of the system when $1\ll L\ll\xi$. In our notation, the RG equations of Azaria *et al.* for the stiffnesses are

$$\begin{aligned}\frac{d\rho_1}{d\ln L} &= -t\left(1-\frac{1}{2}\lambda\right)-\left(\frac{t^2}{\rho_1}\right)\left(\frac{5}{8}\lambda^2-\frac{3}{2}\lambda+1\right),\\ \frac{d\rho_3}{d\ln L} &= -t\left(\frac{1}{2}\lambda^2\right)-\left(\frac{t^2}{\rho_1}\right)\left(\frac{1}{8}\lambda^3\right),\end{aligned} \tag{8}$$

where $t=T/2\pi$, $\lambda=\rho_3/\rho_1$, and $\rho_2=\rho_1$. Since our Monte Carlo results indicate that the correlation length ξ is about 40 lattice spacings at $T=0.32$ and increases dramatically below this temperature, we have measured the stiffnesses at $T=0.2$ for system sizes ranging from $L=12$ to $L=180$. The results for the three stiffness coefficients and the average stiffness $\bar{\rho}=\sum_\alpha\rho_\alpha/3$ are shown in Fig. 5. The solid curves are obtained using our measured values of the ρ_α at $L=12$ and numerically integrating Eqs. (8) to $L=180$. The agreement is excel-

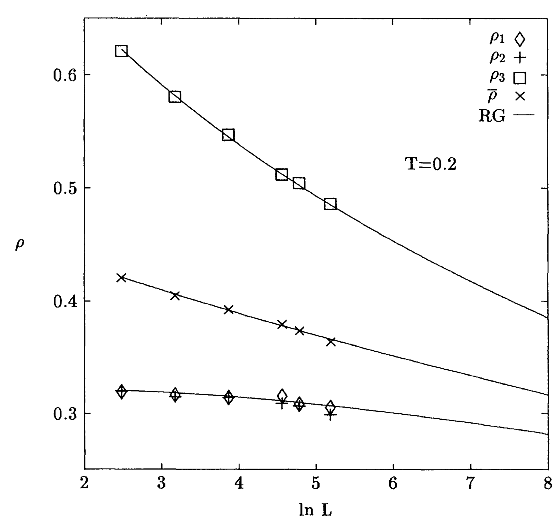

FIG. 5. The three spin stiffness coefficients ρ_1,ρ_2,ρ_3 plotted as a function of $\ln L$ for system sizes $L=12$ to $L=180$ at $T=0.2$. The solid lines are the low-T RG predictions, obtained by integrating Eqs. (8) from $L=12$, as discussed in the text, and $\bar{\rho}$ is the average stiffness.

lent. The fact that the ρ_α converge towards each other (faster than either of them tends to zero) as L increases indicates that the zero-temperature critical behavior is described quite accurately by the NLσ model and that the symmetry is indeed enlarged to $O(4)$ at the zero-temperature fixed point.

To conclude we have studied the low-temperature behavior of the classical Heisenberg antiferromagnet on the triangular lattice. We find a rapid crossover in behavior at around $T = 0.32$ which is clearly shown in Figs. 3 and 4. This may be related to the vortices which Kawamura and Miyashita[7] have shown exist in the model. According to linear spin wave theory the vortices interact logarithmically so, by analogy with the Kosterlitz-Thouless theory of the two-dimensional XY model, they[7] proposed that there might be a finite transition temperature at about $T = 0.3$. However, in contrast to the XY model, spin wave interactions here give a finite correlation length even without topological defects. It therefore seems more likely to us that the interaction between vortices will only be logarithmic up to a finite distance ξ. If so, there will be some free vortices at any temperature and hence the transition will be at $T_c = 0$. It is, nonetheless, possible that the rapid crossover in Figs. 3 and 4 may be due to a sudden increase in the number of free vortices. While our simulations *by themselves* do not conclusively rule out a transition at a nonzero temperature, the data for the spin stiffnesses in Fig. 5 is in excellent agreement with the predictions of the NLσ model, which neglects vortices and hence predicts $T_c = 0$. We feel that this excellent agreement supports the validity of the NLσ model approach to the study of frustrated systems.

This work was supported by NSF under Grant No. DMR 911576, the Organized Research Unit in Non-Linear Science at the University of California Santa Cruz (UCSC), and the Natural Sciences and Engineering Research Council of Canada. B.W.S. would like to thank the Physics Department at UCSC for their kind hospitality. We should also like to thank T. Jolicoeur for helpful correspondence and for bringing Ref. 10 to our attention.

*Permanent address: Department of Physics, University of Manitoba, Winnipeg, Manitoba, Canada R3T 2N2.

[1] T. Dombre and N. Read, Phys. Rev. B **39**, 6797 (1989).

[2] P. Azaria, B. Delamotte, and T. Jolicoeur, Phys. Rev. Lett. **64**, 3175 (1990).

[3] P. Azaria, B. Delamotte, and D. Mouhanna, Phys. Rev. Lett. **68**, 1762 (1992).

[4] P. Azaria, B. Delamotte, T. Jolicoeur, and D. Mouhanna, Phys. Rev. B **45**, 12 612 (1992).

[5] W. Apel, M. Wintel, and H.U. Everts, Z. Phys. B **86**, 139 (1992).

[6] J.A. Olive, A.P. Young, and D. Sherrington, Phys. Rev. B **34**, 6341 (1986).

[7] H. Kawamura and S. Miyashita, J. Phys. Soc. Jpn. **53**, 4138 (1984); H. Kawamura and M. Kikuchi, Phys. Rev. B **47**, 1134 (1993).

[8] S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. B **39**, 2344 (1989).

[9] P. Azaria, B. Delamotte, F. Delduc, and T. Jolicoeur (unpublished).

[10] S. Caracciolo, R.G. Edwards, A. Pelissetto, and A.D. Sokal (unpublished).

[11] H.E. Stanley, Phys. Rev. **158**, 537 (1967).