A LETTERS JOURNAL EXPLORING THE FRONTIERS OF PHYSICS

Finite-Size Scaling for the Two-Dimensional Frustrated Quantum Heisenberg Antiferromagnet

To cite this article: H. J. Schulz and T. A. L. Ziman 1992 *EPL* **18** 355

EUROPHYSICS LETTERS 21 February bis 1992
Europhys. Lett., 18 (4), pp. 355-360 (1992)

Finite-Size Scaling for the Two-Dimensional Frustrated Quantum Heisenberg Antiferromagnet.

H. J. SCHULZ (*) and T. A. L. ZIMAN (**)
(*) *Laboratoire de Physique des Solides* (§), *Université Paris-Sud 91405 Orsay, France*
(**) *Department of Physics and Astronomy, University of Delaware Newark, DE 19716*

(received 14 January 1992; accepted 4 February 1992)

PACS. 75.10J – Heisenberg and other quantized localized spin models.
PACS. 75.40M – Numerical simulation studies.

Abstract. – Using results for the 4×4 and 6×6 lattice, we produce the first finite-size scaling analysis of the frustrated Heisenberg model in two dimensions. The results indicate a continuous phase transition from the ordered phase into an intermediate phase without long-range magnetic order, as for the $(2+1)$-dimensional nonlinear sigma-model. The intermediate phase is stable for $0.4 < J_2/J_1 < 0.65$ and exhibits either dimerization or broken chiral symmetry. The transition to the collinear phase at $J_2/J_1 \simeq 0.65$ is apparently of first order.

The two-dimensional spin-(1/2) Heisenberg antiferromagnet is the basis for the theoretical understanding of the insulating phase of $La_{2-x}Sr_xCuO_4$ and other copper-oxide–based high-T_c superconducting materials [1]. Using quantum Monte Carlo [2, 3], series expansion [4], and finite-size diagonalization [5-8] methods, it is by now well established that this model has an antiferromagnetically ordered ground state. The calculated staggered magnetization, $m_0 \approx 0.6\mu_B$, is in close agreement with experimental findings on La_2CuO_4.

One of the most intriguing properties of the copper-oxide–based compounds is the rapid suppression of antiferromagnetism upon doping. This has led to the suggestion that the resulting conducting state might be unusual and different from the usual Fermi liquid [9]. Within the Heisenberg model, antiferromagnetism can be destabilized by introducing frustration into the model, *e.g.*, by a second–nearest-neighbor antiferromagnetic interaction [10] (though this most likely does not represent the effect of doping to its full extent):

$$H = J_1 \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + J_2 \sum_{\langle i,j' \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_{j'} . \tag{1}$$

Here $\boldsymbol{S}_i$ are spin-(1/2) operators ($\boldsymbol{S}_i \cdot \boldsymbol{S}_i = 3/4$) at lattice site i, and $\langle i,j \rangle$, $\langle i,j' \rangle$ mean summation over first- and second-neighbor pairs on a square lattice. For simplicity we shall

(§) Laboratoire associé au CNRS.

put $J_1 = 1$ in the following. Increasing J_2 destabilizes the antiferromagnetic state, and a variety of novel states have been hypothesized to exist for $J_2 \approx 0.5$: dimerized (or spin-Peierls) [11, 8], twisted (spiral incommensurate) [12, 13], or chiral (parity breaking) [14, 15]. In particular, due to the possibility of fractional statistic excitations («anyons»), the chiral state has raised considerable interest. In the frustrated model Monte Carlo methods are difficult to apply owing to sign problems, whereas series expansion results depend on the state one expands around [4], and variational methods [10] cannot provide unbiased results. Finite-size studies have so far been limited to clusters of 16 or 20 sites [5, 6, 8], and therefore a reliable extrapolation to the thermodynamic limit is impossible. We here report for the first time results of the diagonalization of clusters up to 36 (6×6) sites. This allows us to perform a finite-size scaling analysis, which is expected to provide unbiased results. In particular, using the known finite-size properties of quantum antiferromagnets [16], we obtain the fundamental parameters of the antiferromagnetic state (order parameter m, spin wave velocity c, and stiffness constant ρ_s). We find that the vanishing of the antiferromagnetism is qualitatively similar to the phase transition of the (2 + 1)-dimensional nonlinear sigma-model. On the other hand, we also obtain new information on possible unusual ordered states: in particular, our analysis indicates the existence of an intermediate phase without long-range order in the range $0.4 < J_2 < 0.65$, with either dimerization or chiral symmetry breaking in this state.

To obtain the ground state of the 6×6 cluster (with periodic boundary conditions), we use the full space group symmetry: reflections on the horizontal, vertical, and diagonal axis, and translations. In addition spin rotation around the x-axis by 180° ($S_z \to - S_z$) is used. The size of the Hilbert space then is 15 804 956, and there are approximately $1.17 \cdot 10^9$ nonzero matrix elements. Eigenvalues and vectors are obtained using a Lanczos method, implemented by the Harwell library routine EA15 which performs extensive convergence checks and thus avoids unnecessary iterations. We have a typical accuracy of 10^{-6} for energy eigenvalues, and of 10^{-4} for expectation values. Our program runs on a Cray-2. The (gigantic) matrix cannot be kept in memory, and therefore is read in from disk piece by piece whenever needed. In favourable circumstances ($J_2 = 0$) the ground state can be found in about 40 min CPU time, but determination of excited states can take several hours.

The energy of the ground state (E_0) and of certain excited states as a function of J_2 is shown in fig. 1. In particular, for $J_2 = 0$ one has $E_0 = -24.4394$. For small J_2 the ground state

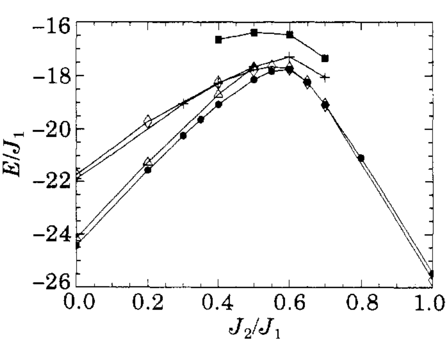

Fig. 1.

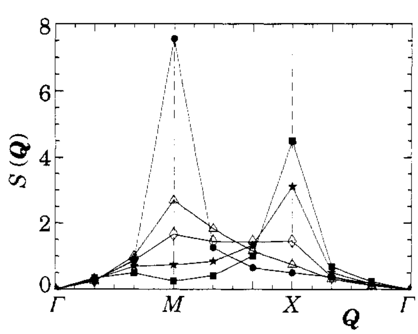

Fig. 2.

Fig. 1. – Energies of different eigenstates of the 6×6 cluster as a function of J_2/J_1: the fully symmetric (A_1) state (●), the B_1 state (◇), the A_2 state (■), the A_1 state at $\boldsymbol{Q} = (0, \pi)$ (+), and the lowest triplet state at $\boldsymbol{Q} = (\pi, \pi)$ (△). Unless stated otherwise all states are at $\boldsymbol{Q} = 0$.

Fig. 2. – Magnetic structure factor, as obtained from the 6×6 cluster, in the Brillouin zone for $J_2/J_1 = 0$ (●), 0.55 (△), 0.6 (◇), 0.65 (★), 1 (■). The points Γ, M, X are $\boldsymbol{Q} = 0$, $\boldsymbol{Q}_0$, $\boldsymbol{Q}_1$, respectively.

is completely symmetric under all symmetry operations. However, for $J_2 > 0.6$, the ground state has B_1 symmetry (odd under reflection on the diagonal). At first sight, this could be taken as a sign of a first-order phase transition. However, one should notice that for large J_2 the 6×6 system consists of two weakly coupled 18-site clusters. By general arguments, the ground state of each of these clusters is odd under symmetry operations exchanging two sublattices [5] ([1]), which means that for sufficiently large J_2 the 6×6 cluster *must* have B_1 symmetry. We here find the transition to occur at $J_2 = 0.6$. In order to avoid spurious first-order transitions to appear in our results, we will in the following always evaluate expectation values in the fully symmetric state.

In fig. 2 we show the equal-time correlation function (magnetic structure factor)

$$S(\boldsymbol{Q}) = \frac{1}{N} \sum_{i,j} \exp[i\boldsymbol{Q}(\boldsymbol{R}_i - \boldsymbol{R}_j)] \langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle, \tag{2}$$

calculated for the 6×6 cluster (N is the total number of spins). The figure clearly shows a change from predominant antiferromagnetism at small J_2 to ordering at $\boldsymbol{Q}_1 = (\pi, 0)$ («collinear state») at larger J_2. More quantitative results can be obtained considering the quantity $M_N^2(\boldsymbol{Q}) = S(\boldsymbol{Q})/N$ (fig. 3) which is normalized so that in the thermodynamic limit it tends to the square of the order parameter if there is magnetic ordering at some wave vector, and that it scales like $1/N$ in a magnetically disordered phase. In particular, using the finite-size properties of the antiferromagnet [16], one has (at $\boldsymbol{Q}_0 = (\pi, \pi)$) $M_N^2 = m^2 + 1.2416\kappa_1^2/\sqrt{N}$, where the staggered magnetization is $m_0 = 2\mu_B m$, and for the infinite system κ_1 gives the amplitude of the diverging matrix element of the spin operator between the ground state and single magnon states for $\boldsymbol{Q} \approx \boldsymbol{Q}_0$. The results for the staggered magnetization obtained using the 4×4 and 6×6 clusters are shown in fig. 4. For $J_2 = 0$, we obtain $m_0 = 0.553\mu_B$, about 10% lower than current estimates. With increasing J_2 m_0 decreases and vanishes in a second-order fashion at a critical value of $J_{2c} \approx 0.4$. This critical value is quite close to series expansion results [4]. A critical value $J_{2c} \approx 0.4$ is also consistent with our results for the gap Δ_T between the ground state and the triplet excited state at $\boldsymbol{Q}_0$. From ref. [16] one expects $\Delta_T = \Delta_{T\infty} + \text{const}/N$, where ideally in an antiferromagnet $\Delta_{T\infty} = 0$. From the data in fig. 1 and corresponding results for the 4×4 system, we find $\Delta_{T\infty} = 0.05$ for $J_2 = 0$, 0.2, but $\Delta_{T\infty} = 0.09$, 0.16 for $J_2 = 0.4$, 0.5, *i.e.* the ideal antiferromagnetic scaling $\Delta_{T\infty} = 0$ is rather badly violated for $J_2 \geqslant 0.4$, consistent with the absence of antiferromagnetic order in that region. Obviously, a precise determination of J_{2c} from the extrapolated value of $\Delta_{T\infty}$ is not possible.

The spin wave velocity can be obtained from the finite-size formula for the ground-state energy per site $E_0(N)/N = e_\infty - 1.4372c/N^{3/2}$. An alternative method for calculating the spin-wave velocity, using the scaling of the excited states [16], was less successful because of large-amplitude subleading corrections. For $J_2 = 0$ we find $c = 1.45J_1$, close to, but somewhat lower than, the spin-wave result $c_{sw} = 1.65J_1$ ([2]). With increasing J_2 c decreases somewhat but goes to a nonzero constant as $J_2 \to J_{2c}$. Finally, the stiffness constant can be obtained from $\rho_s = m^2 c/(2\kappa_1^2)$ ([3]), and is also shown in fig. 4. The «critical» behaviour, namely m, $\rho_s \to 0$,

---

([1]) We are grateful to D. Poilblanc for pointing this out.

([2]) Using 6×4 and 6×6 clusters, we find $m_0 = 0.588\mu_B$ and $c = 1.64J_1$, very close to results obtained by other methods. However, the 6×4 cluster does not have the full lattice rotation symmetry, and therefore cannot be used for nonzero J_2, where states with broken rotation symmetry (*e.g.* collinear) play an important role.

([3]) The value found at $J_2 = 0$ is about a factor two lower than other estimates (ref. [1, 17]). Alterna-

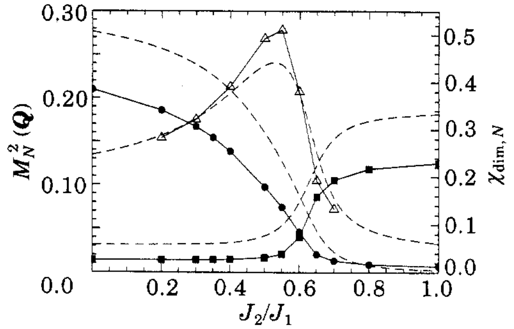

Fig. 3.

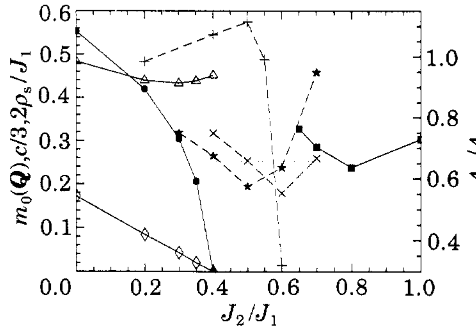

Fig. 4.

Fig. 3. – The correlation function $M_N^2(\boldsymbol{Q})$ for $N = 36$ and $\boldsymbol{Q} = (\pi, \pi)$ (●), and for $\boldsymbol{Q} = (\pi, 0)$ (■), and $\chi_{\mathrm{dim},N}$ for $N = 36$ (△). Full lines are guides to the eye, dashed lines are the corresponding results for the 4×4 cluster. For better comparison, $\chi_{\mathrm{dim},36}$ has been multiplied by a factor $9/4$.

Fig. 4. – The parameters of the nonlinear sigma-model as obtained from finite-size scaling: order parameters $m_0(\boldsymbol{Q})$ for the antiferromagnetic (●) and collinear state (■), spin wave velocity c (△), and spin wave stiffness ρ_s (◇). The order parameters are in units of μ_B, c and ρ_s in units of J_1. Also shown are the scaled gap ratios for state of B_1 (+), A_1 (★), and A_2 (×) symmetry.

$c \to$ const as $J_2 \to J_{2c}$, is in qualitative agreement with the predictions of the nonlinear sigma-model [1].

For large J_2, fig. 2 and 3 strongly suggest the existence of a collinearly ordered magnetic state, as also obtained from spin-wave theory [12]. The low-energy excitations of this state are spin-waves with a linear dispersion relation, and we therefore use the same finite-size scaling as for the staggered magnetization parameter. As seen in fig. 4, the resulting collinear order parameter is approximately constant for $J_2 \geqslant 0.65$: $m_0(\boldsymbol{Q}_1) \approx 0.3\mu_B$. On the other hand, for $J_2 = 0.6$ the data of fig. 3 already extrapolate to a negative value of $m^2(\boldsymbol{Q}_1)$, indicating that the collinear state has vanished extremely rapidly at a critical value $J_{2c} \approx$ $\approx 0.6 \dots 0.65$, probably in a first-order transition.

What is the nature of the ground state in the intermediate region $0.4 < J_2 < 0.65$? One suggested possibility is a twisted (or spiral) state [12, 13]. In that case, one would expect maxima in the magnetic structure factor at some incommensurate wave vector. Figure 2 shows $S(\boldsymbol{Q})$ along high-symmetry directions of the Brillouin zone. In no case, not even in the vicinity of $J_2 = 0.5$, is there a peak away from (π, π) or $(\pi, 0)$. The present results thus provide no evidence for a twisted phase (4).

Another possible state in the intermediate region is the dimerized (or spin-Peierls) state characterized by an order parameter

$$O_r^{\mathrm{dim}} = \boldsymbol{S}_r \cdot [(-1)^x \boldsymbol{S}_{r+\hat{x}} + i(-1)^y \boldsymbol{S}_{r+\hat{y}}], \tag{3}$$

which has been suggested previously from a large-N expansion [11]. The corresponding susceptibility $\chi_{\mathrm{dim},N} = \langle | \sum_r O_r^{\mathrm{dim}} / N |^2 \rangle$ is shown in fig. 3 for the 4×4 and 6×6 clusters. The data in fig. 3 are scaled so that in a state with only short-range order, the curves for 4×4 and

---

tively, one can use $\rho_s = c^2/(L^2 \Delta_T)$ [16], which leads to $\rho_s = 0.2J_1$ at $J_2 = 0$. However, one then finds severe finite-size corrections for $J_2 \to J_{2c}$.

(4) The gap-scaling analysis (see below) does not favour a twisted phase either.

for 6×6 should be identical, whereas for a long-range ordered state the 6×6 results should be larger than the 4×4 results by a factor $9/4$. As one sees, the data provide no strong evidence for spin-Peierls order: in most cases 4×4 and 6×6 are identical to within a few percent, and only for $J_2 = 0.55$ is there a noticeable increase by about 20%, much smaller than the factor $9/4$ expected for an ordered state.

An alternative possibility to check the existence of ordered states from finite-size calculations is provided by energy gaps between the ground state and excited state of appropriate symmetry. In particular, at a critical point, $\Delta_L \propto 1/L$, whereas in an ordered phase $\Delta_L \propto \exp[-L/\xi]$, and in a disordered state $\Delta_L \rightarrow$ const (L is the *linear* dimension of the system). The dimerized state breaks translational symmetry, and consequently the gap with the lowest state of A_1 symmetry (even under all reflections) and wave vector $(0, \pi)$ is expected to vanish in the thermodynamic limit if this type of symmetry breaking exists. We have calculated this energy level for the 6×6 cluster (fig. 1) ([5]), and fig. 4 shows the corresponding ratio Δ_6/Δ_4. In the region between the Néel and the collinear state this ratio is smaller than $2/3$, indicating that a dimerized state is indeed stable. This conclusion, has, however, to be taken with some caution: the dimerized state also breaks lattice rotation symmetry, and therefore the gap between the ground state and the lowest state of B_1 symmetry should also vanish. As shown in fig. 4, for $J_2 < 0.6$ the corresponding ratio is considerably bigger than $2/3$, indicating a state without long-range dimer order, contrary to the conclusion from the A_1 gap. These conflicting results may possibly be related to the fact that for $J_2 > 0.6$ the B_1 state becomes the ground state, and one then would trust the A_1-gap more ([6]). The rapid decrease of the B_1-gap ratio at $J_2 = 0.6$ is obviously related to the change of symmetry of the ground state discussed above, and in our opinion cannot be taken as indicating any type of ordering.

Finally, let us turn to the chiral state, characterized by the parity-breaking order parameter

$$O_r^{\mathrm{ch}} = \boldsymbol{S}_r \cdot (\boldsymbol{S}_{r+\hat{x}} \times \boldsymbol{S}_{r+\hat{y}}). \tag{4}$$

As discussed in a recent paper [18], it is important to consider linear combinations of this operator adapted to the lattice symmetry. According to those calculations, performed on the 4×4 cluster, the most promising candidate for an ordered state has A_2 symmetry (odd under all reflections). The corresponding gap ratio is shown in fig. 4. We observe that for $0.5 \leqslant J_2 \leqslant 0.7$ this ratio is smaller than $2/3$, indicating *a state with long-range chiral order*. The interval of stability roughly, but not completely, agrees with the region where our finite-size scaling results indicate the absence of any magnetic ordering ($0.4 < J_2 < 0.65$). This difference of course may well be due to finite-size effects. It would clearly be interesting to investigate the existence of a chiral state further, *e.g.*, by calculating the corresponding order parameter susceptibility. Unfortunately, O^{ch} is a rather complicated operator, which makes the calculation of correlation functions extremely time-consuming, and therefore for the moment it has not been possible to perform this calculation.

In conclusion, we have investigated a frustrated quantum antiferromagnet using finite-size scaling between 4×4 and 6×6 clusters. We have obtained the parameters

---

([5]) Due to the lower symmetry, in this case the size of the Hilbert space and the number of nonzero matrix elements double.

([6]) More generally speaking, one might question the validity of gap scaling when the ground states for the 4×4 and 6×6 clusters have different symmetry. We note, however, that in the interesting region $J_2 \leqslant 0.7$ the B_1 state is lower than the fully symmetric state by at most $0.002 J_1$, and therefore we do not believe this to be a problem.

(staggered magnetization, spin wave velocity and stiffness constant) determining the low-energy behaviour of the antiferromagnetic state as a function of frustration. The antiferromagnetic state vanishes for $J_2 \approx 0.4$, whereas for $J_2 \geqslant 0.65$ another magnetically ordered state appears. In the intermediate region, no evidence for long-range twist order is found, whereas both a dimerized or a chiral state are compatible with our data. We expect that in the thermodynamic limit one of these two possibilities is realized. The close vicinity of the two types of order suggests that small changes in the Hamiltonian can be sufficient to change the ground-state symmetry. We emphasize that both our determination of the parameters of the antiferromagnetic state and our results for different states in the region of intermediate J_2 rely heavily on the variation of physical properties with increasing system size. We therefore expect our results to be more reliable than those of previous finite-size studies which are based on only one system size, usually the 4×4 cluster.

* * *

We thank L. PIERRE for suggesting an important improvement in our programs. Computing time was made available by the scientific committee of Centre de Calcul Vectoriel pour la Recherche (CCVR), Palaiseau, France. We are especially grateful to the technical staff of CCVR for efficient help with various computing problems.

REFERENCES

[1] CHAKRAVARTY S., NELSON D. and HALPERIN B. I., *Phys. Rev. Lett.*, **60** (1988) 1057; CHAKRAVARTY S.,HALPERIN B. I. and NELSON D., *Phys. Rev. B*, **39** (1989) 2344.
[2] REGER J. D. and YOUNG A. P., *Phys. Rev. B*, **37** (1988) 5978; GROSS M., SANCHEZ-VELASCO E. and SIGGIA E., *Phys. Rev. B*, **39** (1989) 2484.
[3] DING H.-Q. and MAKIVIĆ M. S., *Phys. Rev. Lett.*, **64** (1990) 1449.
[4] GEL'FAND M. P., SINGH R. R. P. and HUSE D. A., *Phys. Rev. B*, **40** (1989) 10801; GEL'FAND M. P., *Phys. Rev. B*, **42** (1990) 8206.
[5] OITMAA J. and BETTS D. D., *Can. J. Phys.*, **56** (1978) 897.
[6] DAGOTTO E. and MOREO A., *Phys. Rev. Lett.*, **63** (1989) 2148.
[7] FIGUEIRIDO F. *et al.*, *Phys. Rev. B*, **41** (1989) 4619.
[8] SINGH R. R. P. and NARAYANAN R., *Phys. Rev. Lett.*, **65** (1990) 1072.
[9] ANDERSON P. W., *Science*, **235** (1987) 1196.
[10] INUI M., DONIACH S. and GABAY M., *Phys. Rev. B*, **38** (1988) 6631; DONIACH S. *et al.*, *Europhys. Lett.*, **6** (1988) 663.
[11] READ N. and SACHDEV S., *Phys. Rev. Lett.*, **62** (1989) 1694; **66** (1991) 1773.
[12] CHANDRA P. and DOUCOT B., *Phys. Rev. B*, **38** (1988) 9335; CHANDRA P., COLEMAN P. and LARKIN A., *Phys. Rev. Lett.*, **64** (1990) 88.
[13] GABAY M. and HIRSCHFELD P. J., *Physica C*, **162** (1989) 823.
[14] KALMEYER V. and LAUGHLIN R. B., *Phys. Rev. Lett.*, **59** (1987) 2095.
[15] WEN X. G., WILCZEK F. and ZEE A., *Phys. Rev. B*, **39** (1989) 11413.
[16] NEUBERGER H. and ZIMAN T. A. L., *Phys. Rev. B*, **39** (1989) 2608.
[17] SINGH R. R. P. and HUSE D. A., *Phys. Rev. B*, **40** (1989) 7247.
[18] POILBLANC D. *et al.*, *Phys. Rev. B*, **43** (1991) 10970.