PHYSICAL REVIEW B VOLUME 40, NUMBER 16 1 DECEMBER 1989

Spin-wave velocity and susceptibility for the two-dimensional Heisenberg antiferromagnet

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(Received 20 December 1988)

The two physical parameters needed to specify the long-wavelength properties of a spin-$\frac{1}{2}$ quantum antiferromagnet are determined numerically. The fluctuation-induced renormalization of the stiffness constant differs by 40% from the expansion results of Oguchi, necessitating a corresponding adjustment in the value of the exchange deduced from the measured correlation length.

It has been established numerically[1,2] and by other means[3] that the two-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet on a square lattice has a conventionally ordered ground state. The staggered magnetization Ω is in fact 60% of its classical value.[1-3] The long-range order, together with the probable absence of any topological term,[4] makes the nonlinear σ model (NLσ) a highly plausible representation of the antiferromagnet.[5] There are then two nontrivial parameters to be determined which completely fix the long-wavelength properties of the model and allow comparison with experiment, namely the uniform field susceptibility χ and the stiffness constant ρ. Their bare values enter the NLσ model as

$$\mathcal{H}_{\mathrm{NL}\sigma}=\int\left[\frac{\mathbf{m}^2}{2\chi_0}+\tfrac{1}{2}\rho_0(\nabla\boldsymbol{\Omega})^2\right], \tag{1}$$

where $\boldsymbol{\Omega}$ is normalized to $\boldsymbol{\Omega}^2=1$ and $\mathbf{m}$ is the magnetization density.

We noted in a previous publication[2] that knowledge of the Heisenberg ground-state energy as a function of lattice size (L by L sites, L even) and the total spin S suffices to determine χ and ρ by the following asymptotic formula for the energy per site:

$$E=E_0-\frac{1.437c_s}{L^3}+\frac{S(S+1)}{2\chi L^4}+\cdots , \tag{2}$$

where the spin-wave velocity $c_s^2=\rho/\chi$.[6,7] To make the various terms plausible, we note that S should appear as $S(S+1)$ on quantum mechanical grounds and the factors of L in the last term give the proper limit for L large, S/L^2 small but nonzero. The dominant finite-size effects involve the renormalized spin-wave velocity since it is only the long-wavelength modes that sense the presence of boundaries. The numerical coefficient, 1.437, is universal and was found by linearizing the Heisenberg Hamiltonian and computing the spin-wave energy exactly on a series of $L\times L$ lattices. The linearization is not quantitatively valid for the smaller scales but serves to smoothly cut off the large wave numbers in the sum over the Brillouin zone which do not contribute to the leading L dependence anyway.

Our data, determined by the von Neumann–Ulam method of Ref. 2, are given in Table I and plotted in Figs. 1 and 2. Our units are defined by

$$\mathcal{H}_{\mathrm{Heis}}=J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j , \tag{3}$$

where the sum runs over all nearest-neighbors pairs of sites $\langle ij\rangle$ and the $\mathbf{S}_i$ are Pauli matrices. For the quantum numbers S in (2) we use physical units, i.e., S can assume any integer value $\leq L^2/2$. To present our results in a convention free manner, we divide out the spin-wave values of

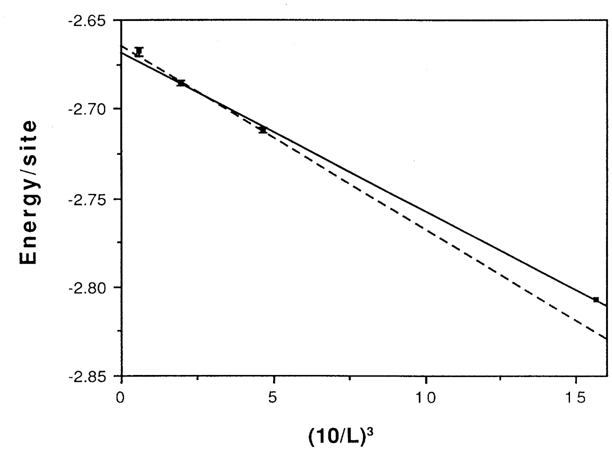

FIG. 1. Ground-state energy, $S=0$, per site vs $(10/L)^3$ in units of J. The solid line has a slope of -8.85×10^{-3} and an intercept of -2.669 ± 0.0011 (statistical error only). To assess systematic errors we show a fit (dashed line) omitting the 4×4 point which gave an intercept of -2.665 ± 0.002 and a slope of -1.03×10^{-2}.

TABLE I. Ground-state energies for the Hamiltonian (3) in units of J as a function of total spin S on $L\times L$ square lattices. The error bars represent sampling errors only. The energies given to 10 places were determined by direct iteration of the Hamiltonian and are exact.

S	Energy
	4×4
0	−2.807 120 802
1	−2.662 471 218 1
2	−2.379 421 995 9
3	−1.959 134 393 3
4	−1.404 319 875 8
5	−0.716 549 565 6
6	0.088 562 172 233
7	1.000 000 000 0
8	2.000 000 000 0
	6×6
0	−2.7120 ± 0.0013
1	−2.6839 ± 0.0005
2	−2.6202 ± 0.0002
4	−2.4026 ± 0.0010
6	−2.0685 ± 0.0006
	8×8
0	−2.6860 ± 0.0015
2	−2.6590 ± 0.0006
4	−2.5905 ± 0.0030
6	−2.4719 ± 0.0020
12	−1.9032 ± 0.0007
30	+1.503 595 830 8
	12×12
0	−2.6680 ± 0.0026
4	−2.648 08 ± 0.0030
8	−2.591 ± 0.006
16	−2.391 ± 0.004
24	−2.052 ± 0.003

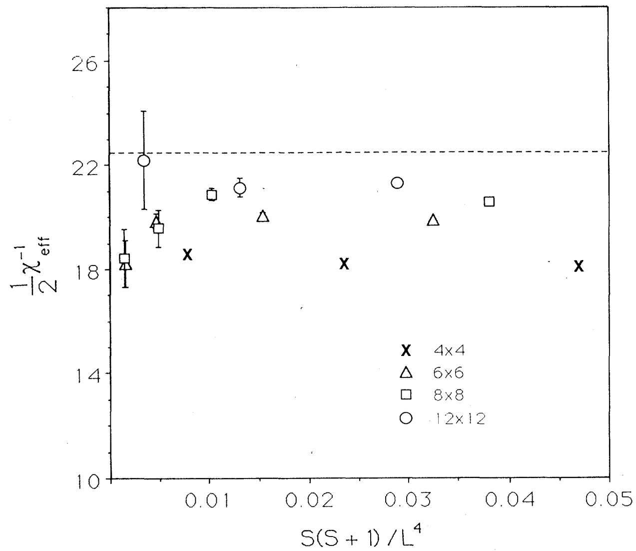

FIG. 2. A plot of the scaled energy difference, $L^4[E(S,L)-E(0,L)]/S(S+1)\equiv\frac{1}{2}\chi_{\mathrm{eff}}^{-1}$, vs $S(S+1)/L^4$ for the data in Table I. The ordinate is scaled as suggested by Eq. (2). The abscissa is essentially the squared magnetization density, and the four tabulated values of L are represented by distinct symbols. The statistical error bars are large for small S since nearly equal energies are being subtracted, but are negligible for abscissa $\gtrsim 0.01$. Since the 6×6 and 8×8 points for abscissa $\lesssim 0.01$ are possibly systematically low because of incomplete relaxation and the data for given L is otherwise independent of abscissa; we have done the extrapolation to infinite L using just the points between 0.01 and 0.02. The dashed line represents this value which also appears in Eq. (4).

c_s and χ:

$$c_s/(4\sqrt{2}J)=Z_c=1.18\pm 0.10\,,\qquad 32J\chi=Z_\chi=0.71\pm 0.04\,. \tag{4}$$

The error bars represent sampling errors plus our estimation of the systematic errors. The latter are particularly large for c_s since we took the average of the slopes in Fig. 1.[8] For χ, we took the data for χ_{eff}^{-1} in Fig. 2 and plotted it separately against both $1/L$ and $1/L^2$. The points did not display a clear preference for either power law, so we quote the average of the two with a standard deviation equal to their difference. To obtain a χ smaller than we quote would require extrapolating with a power of $1/L$ less than one, which is precluded since (2) is analytic in $1/L$.

It is interesting to note that the S dependence in (2) works remarkably well for all spins. There is no noticeable slope in Fig. 2, and Fig. 3 plots the 4×4 data out to the maximum spin possible. In addition we find, from the difference of $S=0$ and 30 (two spins reversed from fully polarized) for the 8×8 lattice, an effective $Z_\chi=0.867\pm 0.001$. This all accords well with a simple classical calculation at zero temperature which predicts that the energy is quadratic in the magnetization until it saturates.

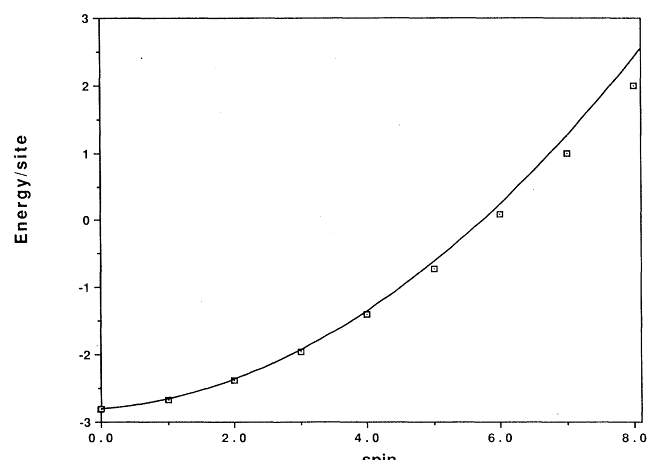

FIG. 3. Energy per site as a function of S for the 4×4 lattice. The solid curve is $c\,S(S+1)$ with c fit to the first two points. Note that $S=8$ represents a fully ferromagnetically polarized system.

Oguchi[9] has computed the $O(1/S)$ corrections to spin-wave theory and finds for $S=\frac{1}{2}$

$$Z_c = 1.158\,,\qquad Z_\chi = 0.449\,. \tag{5}$$

The velocity factor agrees well, but the susceptibility does not. The nature of the deviation suggests that the S^{-1} series for χ has important oscillations, which is not too surprising since $S=\frac{1}{2}$ is hardly small. Our result is closer to spin-wave theory and confirms the tendency noted in Ref. 10 for the one-hole energies also, that the semiclassical limit works remarkably well for $S=\frac{1}{2}$.

At present, there is a reasonably well-known value of ρ from the correlation length in La_2CuO_4 which yields J after correction by the factor $Z_c^2 Z_\chi = 1.0 \pm 0.20$ from (4) rather than 0.602 from (5). (A value of $Z_c^2 Z_\chi$ greater than one is curious but not excluded by any rigorous argument we are aware of. Using just the solid line in Fig. 1 would imply $Z_c^2 Z_\chi = 0.84$.) We find from Ref. 11, $J \sim 750$ K. Another determination of J from light scattering requires very different corrections and gave a somewhat larger J.[12] It does not appear excluded that direct measurements of c_s and χ will someday be available and permit a more accurate comparison with the Heisenberg model.

Note added in Proof. Since this paper was submitted, two more accurate Green's function-Monte Carlo studies became available which gave slightly better energies but a comparable value of Z_c.[13] There is significant disagreement with the series estimate of $Z_\chi = 0.52 \pm 0.03$ in Ref. 14 and also with Ref. 15.

M.G. and E.S.-V. were supported in part by National Science Foundation Grant No. PHY-87-15272 and E.D.S. acknowledges support from National Science Foundation Grant No. DMR-83-14625, Department of Energy Grant No. DEACO2-83-ER13044, and the Guggenheim Foundation.

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