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Thermodynamic parameters of the $T=0$, spin-$\frac{1}{2}$ square-lattice Heisenberg antiferromagnet

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Transverse susceptibility ($\chi_\perp$), spin stiffness constant (ρ_s), spin-wave velocity (c_s), staggered magnetization (M^+), and the ground-state energy (E_0) of the $T=0$, spin-$\frac{1}{2}$ square-lattice Heisenberg antiferromagnet are estimated by expansions around the Ising limit. Extrapolations of the series, which take into account the leading singular behavior, give $Z_\chi(=8\chi_\perp J)=0.52\pm0.03$, $Z_{\rho_s}(=4\rho_s/J)=0.72\pm0.04$, $Z_{c_s}(=c_s/\sqrt{2}J)=1.18\pm0.02$, $2M^+=0.605\pm0.015$, and $4E_0/J=-2.6785\pm0.0010$. The extrapolations are aided by universal amplitude ratios, whose values can be obtained exactly from the spin-wave theory.

The discovery of "two-dimensional" antiferromagnetism in a number of "high-T_c" materials has generated a lot of theoretical interest. A host of numerical studies[1] have presented strong evidence in favor of a zero-temperature ordered state for the square lattice $S=\frac{1}{2}$ Heisenberg antiferromagnets. A continuum theory has been developed[2] to address the growth of the two-dimensional correlation length above the three-dimensional ordering temperature.[3] The parameters entering such a description are the spin stiffness constant (ρ_s), the transverse susceptibility ($\chi_\perp$) and the sublattice magnetization (M^+), which can, in principle, be obtained from an underlying microscopic model. If one assumes, for example, that the square-lattice Heisenberg model with only nearest-neighbor exchange J is a good representation for the physics at the time and length scales of the experiments, then the various parameters ρ_s/J, $J\chi_\perp$, and M^+ are uniquely determined. The interrelation between the parameters is important as some combinations of them control not only the growth of equilibrium correlation length but also the low-temperature dynamics in these systems.[4,5] It is important to realize, however, that these quantities are not universal and would change if one was to add, for example, a small second-neighbor interaction. Nevertheless, certain suitably scaled dimensionless quantities will remain universal [see Eq. (5)].

The original determination of these parameters comes from the order $1/S$ expansion of the spin-wave theory.[1(a)] Recent numerical studies, with varying degrees of accuracy, have shown that the spin-wave estimates are accurate to better than 10%, except perhaps for $\chi_\perp$ and ρ_s. It is standard to quote $\chi_\perp$ in terms of multiplicative renormalization of the classical ($S=\infty$) answer ($\chi_\perp J=\frac{1}{8}Z_\chi$). The estimates for Z_χ have been higher than the spin-wave estimate of 0.448 and have ranged between 0.523[5-7] and 0.74.[1(d)] We are not aware of any previous direct estimate of ρ_s.

The purpose of this paper is twofold. We develop for the first time expansions for $\chi_\perp$ and ρ_s in the variable $(J_\perp/J_\parallel)$, where $J_\perp$ is the exchange perpendicular to the direction of ordering and $J_\parallel$ the exchange along it. To estimate ρ_s, the Ising axis is gradually rotated in space in order to calculate the energy of an imposed twist. The details of this ρ_s expansion and its analysis will be discussed elsewhere.[8] We also extend the existing series for the sublattice magnetization and ground-state energy to order $(J_\perp/J_\parallel)^{10}$. Previously, the series were known[9] to order $(J_\perp/J_\parallel)^6$. The motivation for extending the series for M^+ comes from the surprisingly rapid apparent convergence of the magnetization series in order $(J_\perp/J_\parallel)^6$, when the singularity of the form $[1-(J_\perp/J_\parallel)^2]^{1/2}$ is removed by going to a new variable δ given by[1(b)]

$$1-\delta=[1-(J_\perp/J_\parallel)^2]^{1/2}. \tag{1}$$

We find that the next two terms in the δ series actually increase, thus indicating that the apparent convergence seen in the shorter series[1(b)] was spurious. The net effect of these terms is to lower the estimate for M^+, thus bringing it closer to the spin-wave estimate.[1]

In order to extrapolate the $\chi_\perp$ series reliably, we have to consider the singular parts of $\chi_\perp$ and M^+ in the variable $(1-J_\perp/J_\parallel)$ in some detail. Since these singularities are caused by Goldstone modes and not by critical fluctuations, one expects the associated exponents to be given exactly by the spin-wave value.[1] Thus, if we write

$$M^+=M_0+M_{\rm sing},\quad \chi_\perp=\chi_\perp^0+\chi_{\rm sing}, \tag{2}$$

then the singular parts $M_{\rm sing}$ and $\chi_{\rm sing}$ vanish as $[1-(J_\perp/J_\parallel)^2]^{1/2}$ as $J_\perp/J_\parallel\to1$. Since the Goldstone mode is a long wavelength property one also expects that once the appropriate dimensional parameters are scaled out, one should be left with universal amplitudes independent of short distance properties such as spin, etc. More precisely, one expects that

$$M^+=M_0(1+At),\quad \chi_\perp=\chi_\perp^0(1+Bt), \tag{3}$$

where A and B are universal and the scale for the anisotropy variable t is set by the spin S through the relation

$$t=\theta(S)[1-(J_\perp/J_\parallel)^2]^{1/2}, \tag{4}$$

where $\theta(S)$ goes as S^{-1} as $S\to\infty$.[1] Thus, the quantity

$$R=\frac{M_{\rm sing}/M_0}{\chi_{\rm sing}/\chi_\perp^0}, \tag{5}$$

should be a universal independent of S. In the $S \to \infty$ limit the spin-wave theory gives $R=1$.[1]

The series are analyzed in two different ways. One is employing the change-of-variables technique of Huse,[1(b)] the other using a method that allows us to enforce the ratio R to be one. The agreement between the estimates is excellent and gives us further confidence in our extrapolations.

We consider the Hamiltonian

$$H=\sum_{\langle ij\rangle}[J_{\parallel}S_i^zS_j^z+J_{\perp}(S_i^xS_j^x+S_i^yS_j^y)]+H\sum_i S_i^x \,, \qquad (6)$$

where the sum $\langle ij\rangle$ runs over nearest-neighbor pairs of the square lattice. The Heisenberg model is given by $J_{\parallel}=J_{\perp}=J$. The series is developed by the method of Singh, Gelfand, and Huse.[10] The sublattice magnetization is given by

$$M^+=\langle S_0^z\rangle \,, \qquad (7)$$

while the susceptibility $\chi_{\perp}$ is obtained through the ground-state energy, via the relation

$$E(H)=E_0-\tfrac{1}{2}\chi_{\perp}H^2+\cdots \,. \qquad (8)$$

The expansions are $(x=J_{\perp}/J_{\parallel})$ (quoting six significant digits)

$$2M^+=1-\tfrac{2}{9}x^2-\tfrac{8}{225}x^4-0.0189426x^6-0.0148858x^8-0.00875382x^{10}-\cdots \,, \qquad (9a)$$

$$4E_0/J=-2-\tfrac{2}{3}x^2+0.0\dot{0}3\dot{7}x^4-0.00632628x^6-0.00330085x^8-0.00124740x^{10}-\cdots \,, \qquad (9b)$$

and

$$\tfrac{1}{2}\chi_{\perp}J=+\tfrac{1}{8}-\tfrac{1}{6}x+0.17708\dot{3}x^2-0.1898\dot{1}4\dot{8}x^3+0.191761x^4-0.196579x^5+0.197934x^6-0.201447x^7+\cdots \,. \qquad (9c)$$

As argued earlier, the quantities M^+, E_0, and $\chi_{\perp}$ have singularities at the Heisenberg point $(x=1)$. The form of these singularities is known exactly from the spin-wave theory to be of the type $(1-x^2)^{m+1/2}$ with $m=0,1,2,\cdots$ for M^+ and $\chi_{\perp}$, and $m=1,2,3,\cdots$ for E_0. We wish to incorporate this knowledge in our extrapolations. One way of doing this is to go to the variable δ defined in Eq. (1). In this variable the Heisenberg point $(\delta=1)$ is free of singularities. However, this is achieved at the cost of bringing other unphysical singularities in the complex plane closer to the origin. The magnetization series in δ becomes (quoting four significant digits)

$$M^+=1-\tfrac{4}{9}\delta+0.08\delta^2-0.009319\delta^3-0.04642\delta^4+0.08257\delta^5+\cdots \,. \qquad (10)$$

Although, the first three terms in this series are decreasing in magnitude, the next two are increasing. Thus, this series may be divergent at $\delta=1$. This can happen because going to the variable δ maps a region of the negative x^2 axis $(-x^2<3)$ within unit distance of the origin on the negative δ axis. Hence, the physical singularity at $\delta=1$ may no longer be the closest one to the origin. The resulting series can nevertheless be summed through Padé approximants. Ignoring the direct summation, the Padé estimates for the five term series lie between 0.610 and 0.624.

Here we will use a different method for summing these series, where the convergence is controlled by the physical singularity. Thus, so long as the amplitude for the higher-order singularities, such as $(1-x^2)^{5/2}$, etc., are not anomalously large, the extrapolation will converge rapidly and in a predictable way. We perform partial sums, S_N, for the series in Eq. (9). Then, asymptotically (as $N\to\infty$)

$$S_N \approx S_\infty+\frac{C}{(N+\alpha)^\lambda} \,, \qquad (11)$$

where S_∞ is the sum of the infinite series and C is related to the amplitude of the leading singularity which is of the form $(1-x)^\lambda$. The parameter α depends on the amplitude of the next to leading singularity which is of the form $(1-x)^{\lambda+1}$. We plot S_N vs $1/(N+\alpha)^\lambda$ and by adjusting α try to get the points to lie in a straight line. Thus, we can extrapolate to determine both S_∞ and C. The uncertainty in estimating S_∞ should be of order $1/N^{\lambda+2}$.

Using the criteria of least squares, the best fits are obtained for $\alpha=0.7$ in case of M^+ and $\alpha=0.35$ in case of E_0. The plots are shown in Figs. 1 and 2. We estimate

$$2M^+=0.605\pm0.015, \quad 4E_0/J=-2.6785\pm0.0010 \,. \qquad (11a)$$

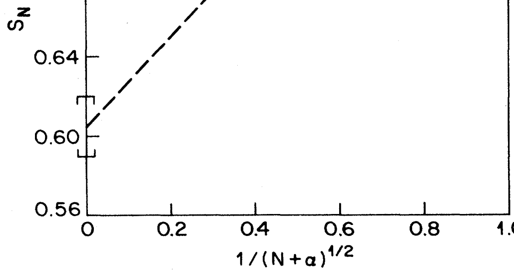

FIG. 1. Plots of partial sums S_N vs $1/\sqrt{N+\alpha}$ for the magnetization series in Eq. (9a). The filled circles correspond to $\alpha=0$ and the open circles to $\alpha=0.7$. The dashed line is a least-squares fit to the points. The estimated uncertainties are shown by brackets.

Setting $\theta(S=\frac{1}{2})$ equal to unity, the amplitude A in Eq. (3) is estimated to be

$$A=0.66\pm0.13\,. \tag{11b}$$

Here the uncertainties are set by extrapolating with $\alpha=0$. These numbers compare very favorably with the Monte Carlo estimates of Reger and Young,[1(c)] who find $2M^+=0.60\pm0.04$ and $4E_0/J=-2.680\pm0.002$. The energy estimates are also consistent with the best variational bounds of Liang *et al.*[1(e)] who find $4E_0/J \leq -2.6752\pm0.0016$.

The $\chi_\perp$ series is dominated by a simple pole at $x=-1$, which corresponds to the *staggered perpendicular* susceptibility. It is essential to remove this singularity before further analysis. This is done by going to a new variable z given by

$$z=2x/(1+x)\,. \tag{12}$$

The resulting series is

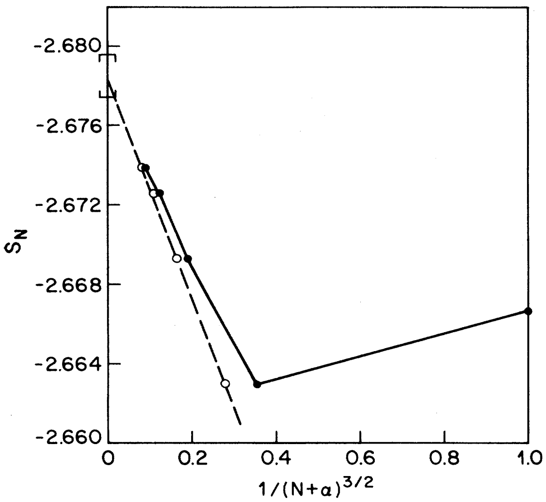

FIG. 2. Plots of partial sums S_N, as in Fig. 1, for the Energy series in Eq. (9b). The open circles are for $\alpha=0.35$.

$$\frac{1}{2}\chi_\perp J=\frac{1}{8}-\frac{1}{12}z+0.002\,604\,1\dot{6}z^2-0.000\,289\,352z^3 -0.000\,818\,749z^4-0.000\,836\,162z^5-0.000\,730\,472z^6-0.000\,615\,089z^7-\cdots\,. \tag{13}$$

The change of variables in Eq. (12) enhances the amplitude of the $(1-x^2)^{3/2}$ singularity by a factor of 4 relative to the amplitude for the $(1-x^2)^{1/2}$ singularity. This would suggest that in an extrapolation of the type used for E_0 and M^+ the α needed may be much larger. Furthermore, the amplitude for all higher-order singularities, such as $(1-x^2)^{5/2}$, is enhanced even more. This makes the above extrapolation procedure less reliable. Hence, we supplement the above method by the restriction that the estimates for $\chi_\perp$ and its amplitude for the square-root singularity should lead to the universal amplitude ratio R in Eq. (5) equal to unity. We choose α such that this constraint is met (see Fig. 3). This leads to the estimate

$$\frac{1}{2}\chi_\perp J=0.0328\pm0.0015\,. \tag{14}$$

Alternatively, we can use the change-of-variables method discussed earlier. Since that method eliminates all singularities at the Heisenberg point, it is not affected by large amplitudes for higher-order singularities. Hence, one might expect it to do relatively better in this case. Going to a new variable δ defined by

$$1-\delta=(1-z)^{1/2}, \tag{15}$$

and constructing Padé approximants, we estimate $\frac{1}{2}\chi_\perp J=0.0322\pm0.0010$. Here the uncertainties reflect the spread in the Padé estimates. Thus, we take our final estimate for $\chi_\perp$ to be

$$\frac{1}{2}\chi_\perp J=0.0325\pm0.0015\,. \tag{16}$$

To compare with other answers, note that

$$Z_\chi=8\chi_\perp J=0.52\pm0.03\,. \tag{17}$$

This number is remarkably close to that obtained by random-phase approximation[7] and the Schwinger boson mean-field theory.[5] By a similar analysis of the ρ_s series[8] the renormalization of the spin stiffness constant is estimated to be

$$Z_{\rho_s}=0.72\pm0.04\,. \tag{18}$$

Furthermore, the ratio of the series for ρ_s and $\chi_\perp$ lead to the estimate for the renormalization of spin-wave velocity

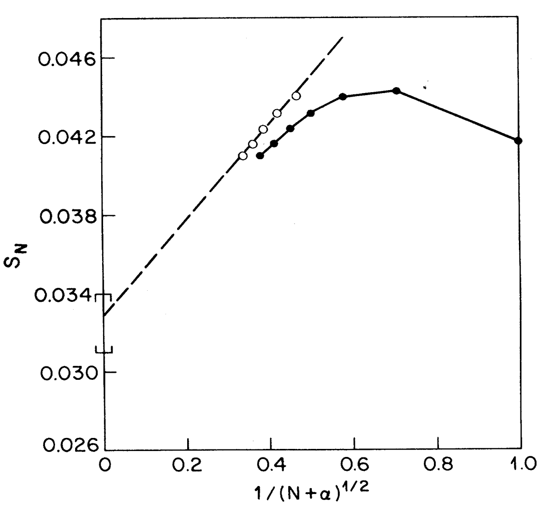

FIG. 3. Plots of partial sums S_N, as in Fig. 1 for the $\chi_\perp$ series in Eq. (13). The open circles are for $\alpha=1.65$. This value of α is chosen to get the amplitude ratio R in Eq. (5) equal to unity.

to be

$$Z_{c_s}=(Z_{\rho_s}/Z_\chi)^{1/2}=1.18\pm 0.02\,. \qquad (19)$$

Thus, although our estimates for Z_χ and Z_{ρ_s} differ from the order $1/S$ spin-wave values by more than 10%, the estimate for Z_{c_s} is quite close to it.

The idea of universal amplitude ratios[11] suggests that the $1/L$ correction to $\chi_\perp$ should be as large as that for M^+. This should be taken into account when extrapolating results of finite-size calculations.[1(d)]

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