Evidence for a phase transition in the zero-temperature anisotropic two-dimensional Heisenberg antiferromagnet

T. Barnes, D. Kotchan, and E. S. Swanson
Department of Physics, University of Toronto, 60 St. George Street, Toronto, Ontario, Canada M5S 1A7
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We describe a Monte Carlo study of the ground state of of the two-dimensional anisotropic Heisenberg antiferromagnet. Values of the energy per spin and the rms $\hat{z}$-staggered magnetization are determined for a range of transverse couplings. At zero temperature the isotropic point $g=1$ apparently separates two phases having nonzero and zero $\hat{z}$-staggered magnetization for $g<1$ and $g>1$, respectively. This may imply that the *isotropic* Heisenberg antiferromagnet is unsuitable as a model of the precursor insulators of the high-temperature superconductors. We also compare our results with previous conjectures regarding the ground state of the anisotropic system.

I. INTRODUCTION

Perhaps the most interesting development in high-temperature superconductivity since its discovery[1] is the observation of antiferromagnetic spin alignment in the copper-oxygen planes.[2–4] This has stimulated intense interest in the spin ordering of the two-dimensional Hubbard and Heisenberg models, as these are believed to describe the superconductors in certain limits.[5] The undoped precursor insulators such as La_2CuO_4 have one unpaired valence electron per CuO_2 site (a "half-filled band") but these materials are not metallic because the large on-site Coulomb repulsion U elevates the unfilled levels to relatively high energies. Such a system is known as a Mott-Hubbard insulator; a model system of this type is described by the Heisenberg Hamiltonian

$$H=\sum_{\langle i,j\rangle}\mathbf{S}^i\cdot\mathbf{S}^j\ . \tag{1}$$

This Hamiltonian may be derived from the half-filled Hubbard model in the limit of large on-site Coulomb repulsion, which is believed to be appropriate for the high-temperature superconductors.

Recent results suggest that (1) is gapless[6–10] (which has been conjectured on theoretical grounds by analogy with one-dimensional systems[11,12] and has a ground-state energy per spin on an $L\times L$ square lattice of $E_0/L^2=-0.67$ (Refs. 7–20) in the bulk limit. Most studies have also found evidence for long-range antiferromagnetic spin order in the ground state, as has been observed in the precursor insulators, although one (Ref. 18) suggests that there might be no such order (see Table I). A determination of this long-range spin order is of particular interest because of suggestions that it can quantitatively explain the Cu^{2+} moment suppression observed in the insulators.[13] The Mermin-Wagner theorem[21] however makes this problematical.

The actual value of the staggered magnetization for the Heisenberg Hamiltonian (1) ground state is not well established, due to the difficulty of extrapolating to infinite lattices from systems of moderate size or to zero temperature from finite-T results. In an attempt to clarify the properties of the ground state of the isotropic Heisenberg Hamiltonian (1), in particular the staggered magnetization, we have carried out measurements on the anisotropic system defined by

$$H=\sum_{\langle i,j\rangle}S_z^iS_z^j+g\,(S_x^iS_x^j+S_y^iS_y^j)\ . \tag{2}$$

We define the antiferromagnetic alignment through an rms $\hat{z}$ ground-state staggered magnetization

$$\mathbf{N}_z\equiv(\langle\psi_0|N_z^2|\psi_0\rangle)^{1/2}\ , \tag{3}$$

where the $\hat{z}$ component of the staggered magnetization operator is

$$N_z\equiv\frac{1}{L^2}\sum_i(-1)^{i_x+i_y}2S_z^i\ . \tag{4}$$

With this normalization allowed values are between $\mathbf{N}_z=1$ for a Néel state and $\mathbf{N}_z=0$ for a state with no long-range $\hat{z}$ spin antialignment. This $\mathbf{N}_z$ at isotropy (assuming an isotropic ground state as well) takes values which are $2/\sqrt{3}$ larger than the conventional definition of the staggered magnetization used for example by Reger and Young.[14] A summary of $\mathbf{N}_z$ estimates on an infinite square lattice with our normalization is given in Table I.

II. METHOD

We employed a Hamiltonian Monte Carlo algorithm[29] which was previously applied to the isotropic system,[7] and in the present work certain improvements were incorporated which decreased the statistical errors.[30] We studied the system with g values from 0.4 to 1.4 on square lattices of side $L=4$, 6, and 8, and a few additional measurements were carried out with $L=10$ and 12. The Euclidean time step size h_τ was usually taken to be $0.2/L^2$, with occasional tests at $0.1/L^2$. The guidance matrix $r_{ss'}$ was of the form (2.48) of Ref. 30 with $r=g/2$ and $c=0.27$, except at $g=0.4$ where a perturbative form de-

TABLE I. Summary of $\mathbf{N}_z$ estimates on an infinite square lattice.

$\mathbf{N}_z$	Method	Reference
0.49	finite-lattice	22
0.464	variational	23
0.441	perturbative	24
0.429	Monte Carlo, fit 1	18
0.418	perturbative	25
0.396	var. and finite-lattice	15
0.361	perturbative	13
0.350	spin-wave	26
0.35	Monte Carlo	14
0.34	Monte Carlo	19
0.33	Monte Carlo	20
0.29	finite-lattice	9
0.283	variational	27
0.21	finite-lattice	28
0.0	Monte Carlo, fit 2	18

rived from the $O(g^4)$ expansion of ψ_0 and Eq. (2.36) of Ref. 30 was used. We measured the energy and the staggered magnetization [using the Feynman-Hellmann theorem through Eq. (2.58) of Ref. 30] with $\tau_2=\tau_1+1.0$ for a range of τ_1 values between 0.8 and 4.4 to confirm that the results had converged to within our statistical errors. The number of configurations generated varied with the coupling constant; for $0.8<g\leq 1.0$ it was 2^{14} for $L=4$ and 6 and 2^{16} for $L=8$. For $g=1.05$ and 1.1 we reduced the $L=8$ runs to 2^{15} configurations. Other g values had smaller associated statistical errors, so we usually employed only 2^{12} configurations. The exceptions were g and $L=0.8$ and $8(2^{16})$, 1.2, and $6(2^{14})$, and 1.0 and $12(2^{16})$ with the corresponding number of configurations in parentheses. We also tested the effect of starting the walks from two different initial configurations, a Néel state and a "triplet dimer" state, which have $\mathbf{N}_z=1$ and $\mathbf{N}_z=0$, respectively. The triplet dimer state is defined by

$$S_z(\mathbf{n})=\frac{(-1)^{\text{int}(n_x/2)+n_y}}{2} . \tag{5}$$

Typically the Néel initial state gave smaller errors for $g<1$ and the triplet dimer gave smaller errors for $g>1$. Since the simulations using different initial states converged to a limiting value of $\mathbf{N}_z$ from different extremes it was possible to check convergence in Euclidean time by inspection.

Most of the numerical work was done on the Caltech "hypercube," a concurrent computation computer whose use was pioneered by the Caltech Concurrent Computation Program (CCCP) group. This machine was built by NCUBE and consists of 512 separate processors or "nodes" which are capable of executing code independently or communicating if necessary. Applications of the hypercube to various scientific and engineering problems have been reviewed by the CCCP group.[31] A single node operates at about $\frac{1}{3}$ the speed of a microVAX and is capable of running programs of sizes up to 256 Kbytes. On concurrent computation machines one often must compromise between partitioning a program into small and large components; small components maximize concurrent execution on individual nodes whereas large ones reduce the amount of internode communication required. In this regard the Monte Carlo algorithm employed here was particularly well suited to the hypercube architecture. The algorithm is CPU intensive but has very modest memory requirements and was therefore easily accommodated on a single node. It was thus possible to generate configurations on a single node without requiring internode communication during execution. The hypercube operating system transfers information to and from the individual nodes, so that no special programming knowledge was required beyond that needed to collect information from all nodes at the end. Typical execution times to generate 2^{16} configurations with $\tau_1=4.4$ on 256 nodes were 14 minutes on $L=6$ and 32 minutes on $L=8$.

III. RESULTS

Our results for E_0/L^2 and $\mathbf{N}_z$ are shown in Tables II and III and in Figs. 1 and 2, respectively. In our discussion of these results it will be useful to distinguish a weak-coupling region $0\leq g<0.8$, a transition region $0.8\leq g\leq 1.0$ and a strong-coupling region $g>1.0$. The energies are quoted to three places and have estimated errors of ± 0.0005 for $L=4$ and 6 and ± 0.001 for $L=8$, 12, and ∞. The staggered magnetization measurements have rather uncertain systematic errors, especially in the tran-

TABLE II. Ground-state energy per spin on the $L\times L$ lattice.

g	$L=4$	6	8	12	∞
0.40	−0.528				
0.60	−0.562				
0.80	−0.618	−0.609	−0.608		−0.607
0.85	−0.637	−0.623	−0.622		−0.620
0.90	−0.657	−0.640	−0.637		−0.634
0.95	−0.678	−0.658	−0.656		−0.653
1.00	−0.702	−0.679	−0.673	−0.670	−0.669
1.05	−0.726	−0.702	−0.698		−0.694
1.10	−0.750	−0.726	−0.721		−0.717
1.20	−0.801	−0.778	−0.773		−0.769
1.40	−0.906	−0.882	−0.877		−0.873

TABLE III. The rms $\hat{z}$-staggered magnetization $\mathbf{N}_z$ on the $L \times L$ lattice.

g	$L=4$	6	8
0.40	0.96		
0.60	0.91		
0.80	0.79	0.83	0.82
0.85	0.74	0.77	0.80
0.90	0.69	0.71	0.72
0.95	0.66	0.63	0.64
1.00	0.61	0.52	0.39
1.05	0.57	0.44	0.33
1.10	0.55	0.39	0.30
1.20	0.50	0.34	0.24
1.40	0.45	0.29	0.21

sition region. This region is especially problematic because the statistical errors are typically larger here, and convergence to a large τ_1 limit is not always monotonic. We estimate the total error in $\mathbf{N}_z$ to be about ± 0.005, ± 0.02, and ± 0.03 for $L=4$, 6, and 8, respectively, although this error may be somewhat larger in the transition region.

First we consider the energy per spin. The infinite lattice estimate is obtained from an extrapolation of the 4×4 and 8×8 data assuming an asymptotic approach of the form $e_0 + c/L^3$. While this apparently works very well for $g \geq 1$, convergence is actually faster for $g < 1$, and hence our estimated infinite-lattice energies for $g < 1$ may be systematically too negative by ≈ 0.001–0.002.

In the weak coupling and transition regions the infinite-lattice energy per spin closely follows the $O(g^4)$ perturbative result[32,33]

$$e_0(g) \equiv \lim_{L\to\infty} \frac{E_0(g)}{L^2} = -\tfrac{1}{2} - \tfrac{1}{6}g^2 + \tfrac{1}{1080}g^4 + O(g^6) , \qquad (6)$$

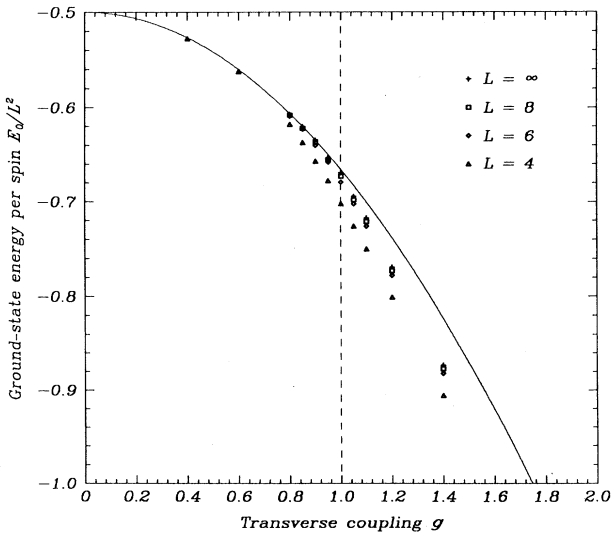

FIG. 1. Energy per spin vs transverse coupling.

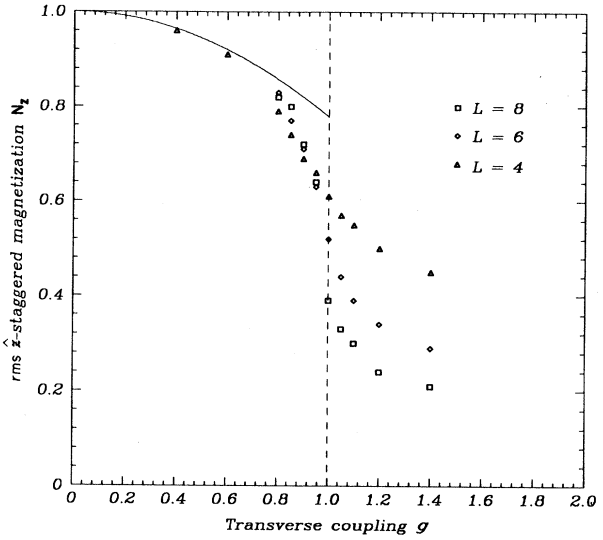

FIG. 2. The rms $\hat{z}$-staggered magnetization vs transverse coupling.

which is also shown in Fig. 1. At the isotropic point $g=1$ our estimate of the energy per spin is

$$e_0(1.0) = -0.669 \pm 0.001 . \qquad (7)$$

This is somewhat less negative than our previous estimate of -0.672 ± 0.001;[7] the improved result (7) followed from the use of the "triplet dimer" initial configuration and from the smaller weight factor variance which resulted from discarding the transition weight, as described in Ref. 30. The $L=6$ and $L=8$ isotropic energies were both found to be about 0.002 higher than previously estimated in Ref. 7; these and an $L=12$ measurement were combined to give (7). The $g=1$ energies for $L=4$, 8, and 12 and the infinite-lattice estimate are all equal to recent variational results[34] to within one of our standard deviations. An independent high-statistics measurement on the $L=16$ lattice[35] using 384 K random walks at $\tau_1 = 5.0$ gave $e_0(1) = -0.668$ with an error of perhaps 0.002, consistent with (7).

In the strong-coupling limit $g \to \infty$ the Heisenberg $e_0(g)$ should approach g times the XY-model ground-state energy per spin. In practice we find that $e_0(g)$ is approximately linear in g for $g \geq 1$, with a slope of $de_0/dg = -0.48$ near the isotropic point (at $g=1.05$), which has increased to $de_0/dg = -0.52$ at $g=1.3$ The measured slope appears consistent with an approach to the XY result of -0.55 (Refs. 19 and 36) as g goes to infinity.

The staggered magnetization $\mathbf{N}_z(g)$ for $L=4$, 6, and 8 is shown in Fig. 2 and Table III. In the weak-coupling region the larger finite-lattice results are consistent both with the $O(g^2)$ perturbation series

$$\mathbf{N}_z(g) = 1 - \tfrac{2}{9}g^2 + O(g^4) \qquad (8)$$

and with the recent proof that such order exists at least for $g < 0.52$.[37] In the transition region $0.8 \leq g \leq 1.0$ a

rapid decrease of $\mathbf{N}_z(g)$ is evident, which becomes more pronounced as L increases. Our strong-coupling staggered-magnetization measurements ($g>1$) are consistent with an approach to $\mathbf{N}_z(g)=0$ as c/L, with a slightly delayed onset ($L\geq 6$) for the smallest value of g studied above isotropy, $g=1.05$. Marcu and Schmatzer[38,39] similarly found $\mathbf{N}_z=0$ far in the XY region.

The $g=1$ measurements were found to have especially large statistical errors and slow convergence in Euclidean time. The $L=4$ value for $\mathbf{N}_z$ is consistent with the Lanczos result of 0.6072 (Refs. 8 and 10) and $L=6$ is consistent with other Monte Carlo results which use the Suzuki-Trotter formula.[14,18] The $L=8$ measurement however appears anomalously low, with 0.49 a more typical value for Suzuki-Trotter simulations. This discrepancy may be a statistical fluctuation, but it appears more likely to be a systematic error, and it is obviously important to reconcile these results. A significant bias in our random walk algorithm could have arisen from too few configurations or insufficient Euclidean time evolution, which will be investigated. The Suzuki-Trotter method may have an important systematic error due to a delayed approach to asymptotic values as a function of the step number m; this can lead to overestimates of the staggered magnetization.[38–40] We have not attempted to extrapolate to a unique infinite-lattice value for $\mathbf{N}_z$ at $g=1$ because of these uncertainties and because our $g\neq 1$ measurements suggest that $\mathbf{N}_z$ may actually be undefined at isotropy. We shall review the evidence for this in the next section.

IV. DISCUSSION

From these results it appears probable that $g=1$ is a critical point that separates two phases having finite ($g<1$) and zero ($g>1$) long range $\mathbf{N}_z$ order. The possibility of various types of singular behavior in this system at $T=0$ has been the subject of recent speculation. Huse suggests that the total staggered magnetization should approach a finite $g=1$ limit from $g<1$ as $c_0+c_1(1-g^2)^{1/2}$,[13] and that the rms transverse components are zero in the bulk limit for all $g<1$.[41] Affleck expects a transition from the Néel phase to a strong coupling phase at some finite value of the transverse coupling g.[11,42] Tang and Hirsch[8] conjectured a discontinuous jump from a finite expectation value of $\mathbf{N}_z$ at $g=1$ to zero for $g>1$ (and perhaps to $\langle\psi_0|\mathbf{N}^2|\psi_0\rangle=0$ as well) based on their study of the distribution of staggered magnetization for 18- and 26-spin systems with $g=\frac{9}{11}$, 1, and $\frac{11}{9}$. Finally, Liang, Doucot and Anderson[16] speculated that the isotropic model might be close to criticality because their RVB variational calculations found nearly equal expected energies for $\mathbf{N}_z$-ordered and -disordered trial states.

The nature of the suggested transition is not unambiguously determined with present statistics; three possibilities consistent with our data are shown schematically in Fig. 3. The curves are shown with finite slope as $g\rightarrow 1_-$ only for ease of visualization, as we have no reason to exclude an infinite slope.

A type 1 [Fig. 3(a)] transition is a monotonic, continuous decrease of the long-range order to zero at the isotropic point. Although this behavior has received little support in the literature, for completeness we include it as a possibility which is not inconsistent with our Monte Carlo data.

The type-2 [Fig. 3(b)] transition, which has a unique, finite value for $\mathbf{N}_z$ at isotropy, is the behavior conjectured by Tang and Hirsch.[8] They speculate that the ground-

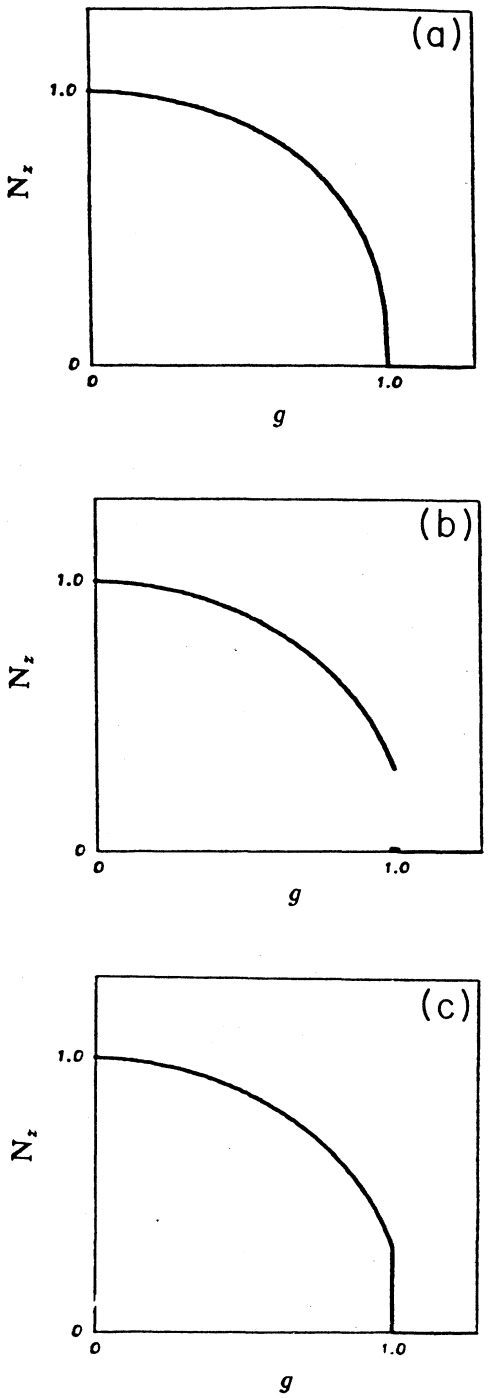

FIG. 3. Possible forms of the rms $\hat{z}$-staggered magnetization.

state expectation value of $\mathbf{N}^2$ might also discontinuously go to zero in the XY phase. A measurement of the transverse staggered magnetization near $g=1$ would be a useful test of this second conjecture.

A closely related transition (type 3 [Fig. 3(c)]) which is instead characterized by an undefined $\mathbf{N}_z$ at isotropy might arise in the following manner. Assuming that the isotropic model is gapless, the ground-state is degenerate and the corresponding staggered magnetization could depend on the particular linear combination of ground states chosen. This type of transition appears to us the most plausible explanation of our Monte-Carlo results.

An important feature of type-3 behavior is that it implies that an attempt to extract a unique value for $\mathbf{N}_z$ at isotropy on an infinite lattice is ill motivated. Specification of a unique ground state would require an additional constraint, provided for example by boundary conditions or an infinitesimal external field.[42] Finite-lattice and Monte-Carlo studies implicitly introduce such a constraint, namely that the infinite-lattice ground state is isotropic. Our limiting value for $\mathbf{N}_z$ as $g \rightarrow 1_-$ of ≈ 0.5 (Fig. 2) can be compared with their isotropic results (Table I) after it is divided by $\sqrt{3}$. Type-3 behavior would also explain the findings of Liang, Doucot, and Anderson, as it implies that e_0 is independent of $\mathbf{N}_z$ at isotropy within the ensemble of degenerate ground states. We emphasize that a jump in $\mathbf{N}_z$ need not imply that the total staggered magnetization is undefined; there could be a constraint on the degenerate states such that $\mathbf{N}^2$ has a well-defined expectation value at $g=1$. A compensating jump in the transverse staggered magnetization would be required, and the transition thus might be second order despite a discontinuous change in the orientation of the rms $\mathbf{N}$.[43]

The order of a zero-temperature phase transition is defined in terms of singular behavior of the ground-state energy per spin $e_0(g)$ or its derivatives at the critical coupling. To show the behavior of $e_0(g)$ near isotropy we display the inferred slope $\Delta e_0/\Delta g$ on an infinite lattice in Fig. 4. A first-order phase transition corresponds to a jump in Fig. 4, a second-order transition to a discontinuous slope in the figure, and so forth. Perturbative weak-coupling [de_0/dg of Eq. (6)] and XY strong-coupling limits are shown as continuous curves, and a theoretical $g=1$ slope of $2e_0(1)/3=-0.446$ which follows from an assumed isotropic ground state is also indicated. Although rapid variation of de_0/dg is evident near $g=1$, the nature of the transition is not clear in this data.

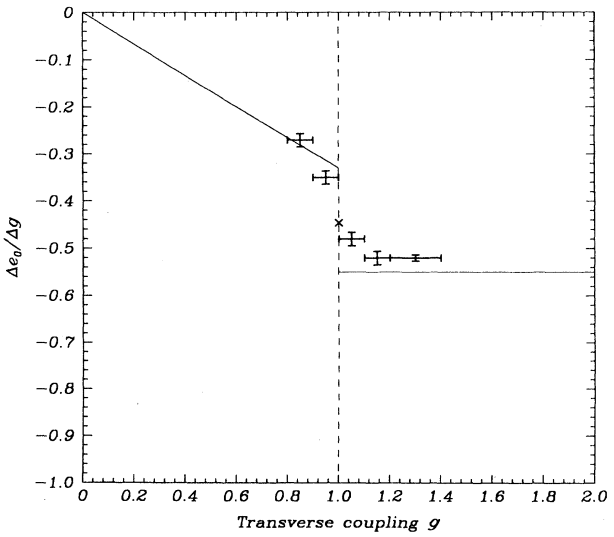

FIG. 4. Slope of the energy per spin versus transverse coupling.

Of course our measurements do not eliminate the possibility of a rapidly varying but nonsingular $\mathbf{N}_z(g)$, and a more accurate determination of properties of the system near isotropy would be of great interest. Future studies might attempt to resolve the order of the suggested phase transition through more accurate measurements of $e_0(g)$ on large lattices. A study of the finite-size dependence of the staggered susceptibility might also be of interest in this regard. A determination of the g dependence of the transverse staggered magnetization would be especially useful in distinguishing between the various transitions which have been suggested. Finally, measurements of the spin-spin correlation function near isotropy would be useful because the singularities of nearest-neighbor (i,j) correlations are simply related to those of $e_0(g)$ through the identities

$$\langle \psi_0(g)|S_z^i S_z^j|\psi_0(g)\rangle = \frac{1}{2}\left[e_0 - g\frac{\partial e_0}{\partial g}\right], \tag{9}$$

and

$$\langle \psi_0(g)|S_x^i S_x^j|\psi_0(g)\rangle = \frac{1}{4}\frac{\partial e_0}{\partial g}. \tag{10}$$

These could provide an independent check of singular behavior extracted from $e_0(g)$. The large distance correlation is also of interest in that it is related to the $\hat{z}$-staggered magnetization through

$$\mathbf{N}_z^2 = \langle (-1)^{n_x+n_y} C_z(\mathbf{n})\rangle_{\mathbf{n}}, \tag{11}$$

where $C_z(\mathbf{n})$ is defined by

$$C_z(\mathbf{n}) \equiv \langle \psi_0|2S_z(\mathbf{m})2S_z(\mathbf{m}+\mathbf{n})|\psi_0\rangle. \tag{12}$$

Assuming that the isotropic Heisenberg antiferromagnet is indeed a boundary between phases having different long-range spin alignment, it is probably unsuitable as a model of magnetism in the precursor insulators. The physics of the isotropic model and its response to various perturbations is presumably strongly dependent on the existence of these two adjacent phases, and this feature is not shared with the precursor insulators. As the long-range spin order observed in the insulators is dominantly planar, a more realistic model should incorporate this anisotropy. The isotropic Hubbard model is similarly unrealistic in not providing a preferred spin orientation, and it may be advisable to incorporate anisotropic spin interactions in that model as well.

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