Series investigations of magnetically disordered ground states in two-dimensional frustrated quantum antiferromagnets

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An extensive series-expansion study of the square-lattice, spin-$\frac{1}{2}$ Heisenberg antiferromagnet with nearest- and second-neighbor couplings has been carried out to investigate the nature of the ground state for $J_2/J_1 \approx \frac{1}{2}$. In agreement with an earlier numerical study along similar lines, we find that the magnetically disordered phase exhibits columnar spontaneous dimerization, but the magnitude of such order may not be as large as had been suggested previously. Although the magnetically disordered phase is not critical, it appears to have both spin-spin and energy-energy correlations of range greater than a few lattice spacings. The possibility of "spin-nematic" order, as proposed by Chandra, Coleman, and Larkin, has not been directly ruled out, but the balance of circumstantial evidence weighs against it in this system.

I. INTRODUCTION

Consider the question of $T=0$ order in the square-lattice, spin-$\frac{1}{2}$ quantum Heisenberg antiferromagnet with nearest- and second- (i.e., nearest-diagional-) neighbor interactions,

$$\mathcal{H} = \sum_{\mathrm{NN}} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\mathrm{2NN}} \mathbf{S}_i \cdot \mathbf{S}_j \ , \tag{1.1}$$

also known as the "J_1-J_2" model. (We have set $J_1 \equiv 1$ for convenience.) Classically, $J_2 = \frac{1}{2}$ is a point of infinite degeneracy, separating a two-sublattice Néel phase, for $J_2 < \frac{1}{2}$, from a four-sublattice Néel phase, for $J_2 > \frac{1}{2}$. For J_2 not too close to $\frac{1}{2}$,[1] and especially for $J_2 = 0$,[2] there is convincing numerical evidence that even for $S = \frac{1}{2}$ quantum spins the character of the ground state is faithfully described by spin-wave theory, that is, the classical ground state gives a qualitatively correct picture of the quantum ground state. For $J_2 \approx \frac{1}{2}$, say $0.35 \lesssim J_2 \lesssim 0.65$, much numerical evidence, as well as spin-wave theory itself,[3] indicates that the ground state is not simply a quantum-renormalized version of the corresponding classical ground state. The character of the ground-state order in this case has been the subject of a remarkable variety of proposals, including (i) complete disorder, with a gap, i.e., a "spin-liquid" or "short-range resonating valence bond" phase,[4] (ii) spontaneous dimerization in a particular "columnar" pattern, with fourfold degeneracy and a gap,[5] and (iii) "spin-nematic" order, in which the system lacks any sublattice magnetization, but, nonetheless, has long-range order in, say, $\mathbf{S}_{\mathbf{r}} \times \mathbf{S}_{\mathbf{r}+\hat{\mathbf{y}}}$.[6] The J_1-J_2 model thus serves as a testing ground for current theories of exotic behavior in quantum many-body systems. (Of course, the absence of, say, spin-nematic order in the J_1-J_2 model does not rule out its existence in nature.) The model also poses a challenge for numerical studies, which have so far proven unable to conclusively establish the nature of the ground state for $J_2 \approx \frac{1}{2}$. The present work substantially advances the numerical attack on the J_1-J_2 model, providing new, direct evidence in favor of spontaneous dimerization (and, necessarily, against disorder), and also offering circumstantial evidence against spin-nematic order.

The standard numerical method for elucidating ground-state properties, namely, finite-cluster diagonalization, suffers from substantial finite-size and boundary effects for the clusters up to size $N=20$ that have been examined. Indeed, two cluster-diagonalization studies, those of Dagotto and Moreo,[1] and Figueirido *et al.*,[7] which employ different approaches in the analysis of the data, reach opposite conclusions regarding the tendencies towards both collinear order in the four-sublattice Néel phase and columnar dimerization in the magnetically disordered phase, with the former authors in favor and the latter opposed on both counts.[8] We should also note that the increase in the magnitude of the "twist order parameter" of Ref. 1 for $0.50 \lesssim J_2 \lesssim 0.57$ on going from $N=16$ to 20, which one might take as evidence in favor of spin-nematic order,[6] really shows that the lattices used are too small to draw definitive conclusions: on general grounds, one expects any order parameter to asymptotically decrease with increasing N towards its value on the infinite system.[9]

Because the finite-cluster studies are not entirely conclusive, it is sensible to try alternate numerical approaches to shed more light on the problem. In an earlier work,[10] henceforth denoted I, a method of $T=0$ series expansions (high-order, nondegenerate perturbation theory about explicitly dimerized models) was applied to the J_1-J_2 model, and also to models with third-neighbor interactions, and it was concluded that the magnetically disordered phase was spontaneously dimerized. However, as noted by Kivelson,[11] the degree of dimerization suggested by the series expansions is so large, roughly half of the maximum value possible, that one might expect all correlations to be quite short-ranged[12] and, hence, the finite-cluster studies to *clearly* indicate that di-

merization. Even if the correlations are not very short ranged one might still expect strong long-range order to be reflected in strong local order in finite systems. It is thus difficult to understand the results of Figueirido *et al.*[7] given the estimates of the spontaneous dimerization in I (and vice versa). This observation, as well as the recent suggestion of spin-nematic order in the J_1-J_2 model, motivated the present work.

The outline of the paper is as follows. In Sec. II, we review the expansion method and discuss the calculated two-point correlations, and particularly the magnetic phase boundaries, for five choices of the unperturbed Hamiltonian, of which only two had been studied in I. The phase diagrams might, on the face of it, appear to support the notion of a spin-liquid phase, and contradict the conclusions of I. Various scenarios for the resolution of this apparent inconsistency are outlined, and tested in the remainder of Sec. II, and in the sections that follow. In Sec. III the ground-state energy series (obtained to at least one order higher than in I) are analyzed, and shown to be more consistent with columnar spontaneous dimerization than with disorder. More direct evidence for dimerization comes from a calculation of the susceptibility to columnar dimerization, described in Sec. IV. Section V summarizes the results of the preceding sections. The evidence pertaining to the possible existence of spin-nematic order, both from the two-point correlations and the ground-state energies, is presented; we conclude, while leaving some room for doubt, that spin-nematic order is not present in the J_1-J_2 model. We also suggest, based on evidence from several of the series expansions, that there are a variety of correlations in the non-Néel phase which, though not long ranged, never become very short ranged either; this is what one would expect, in light of the discussion regarding the finite-cluster studies, above.

II. TWO-POINT CORRELATIONS

A. Background

For any nearest-neighbor dimer covering of the square lattice $\mathcal{D}$ one can define a two-parameter family of "dimerized J_1-J_2" models, via

$$\mathcal{H}=\sum_{(i,j)\in\mathcal{D}}\mathbf{S}_i\cdot\mathbf{S}_j+\lambda\left[\sum_{\substack{\mathrm{NN}\\(i,j)\notin\mathcal{D}}}\mathbf{S}_i\cdot\mathbf{S}_j+J_2\sum_{\mathrm{2NN}}\mathbf{S}_i\cdot\mathbf{S}_j\right]. \tag{2.1}$$

For any $\mathcal{D}$, one recovers (1.1) when $\lambda=1$, while at $\lambda=0$ (and any J_2) (2.1) is trivially solvable. The value of extending the J_1-J_2 model to (2.1) is that for any value of J_2 one can construct power series expansions in λ for a variety of quantities, particularly ground-state expectation values and $T=0$ susceptibilities.

The first step in such calculations is to specify the "unperturbed" Hamiltonian, by choosing a dimer covering. We will consider the five periodic dimer coverings displayed in Fig. 1; of these, the "columnar" and "staggered" ones were already considered in I. (The present selection of dimer coverings was not entirely arbitrary, as will become evident later.) Expansions for the ground-state two-point correlations, $S(\mathbf{r})\equiv\langle\mathbf{S}_{(0,0)}\cdot\mathbf{S}_{\mathbf{r}}\rangle$, and energy per spin E, were carried out to orders λ^5 and λ^6, respectively, by the cluster method of Singh, Gelfand, and Huse.[13] Most of the technical details are described at length elsewhere;[14] the principle innovation developed for the present calculations was in improved graph enumeration algorithm, which could be readily adapted to more complicated dimer coverings than those treated in I. The connected graphs needed for the expansions starting from the columnar, staggered, checkerboard, herringbone, and striped coverings number 1245, 1295, 1188, 548, and 4434, respectively.

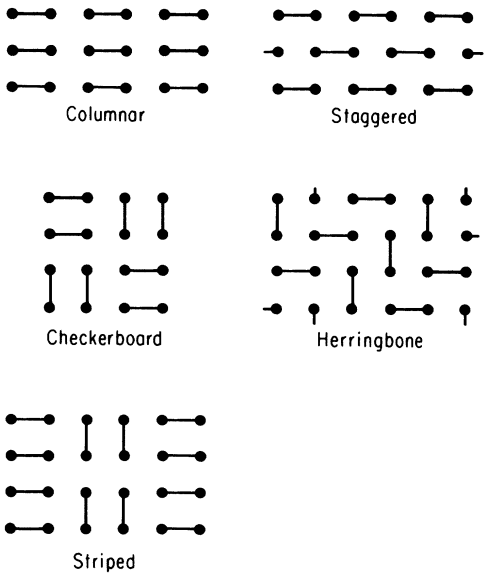

FIG. 1. Dimer coverings of the square lattice, used to define the dimerized J_1-J_2 models treated in this work.

B. Magnetic phase diagrams

Let us now discuss some results of the calculations of $S(\mathbf{r})$. The magnetic phase diagrams, estimated by the same procedure as in I, are displayed in Fig. 2. Several features are immediately evident. First, for the staggered and herringbone dimer coverings, there is always a magnetic phase transition between $\lambda=0$ and 1; while in the columnar, checkerboard, and striped cases, there is a range of J_2 where analytic continuation to the uniformly coupled J_1-J_2 model, at $\lambda=1$, seems possible. (One should note that nonmagnetic continuous transitions, and any first-order transitions, cannot be detected by inspection of the series for the two-point correlations and hence are not displayed in Fig. 2.) A reasonable guess, based on the five available examples, is that *infinitely* many dimer coverings will lack a magnetic phase transition for $J_2\approx\frac{1}{2}$, namely, all those in the zero-winding-number sector of the Rokhsar-Kivelson hard-core dimer gas model.[15] Does this prove that the magnetically disordered phase of the J_1-J_2 model lacks any particular pattern of spontaneous dimerization? The answer is that while the magnetic phase diagrams are consistent with a disordered phase,

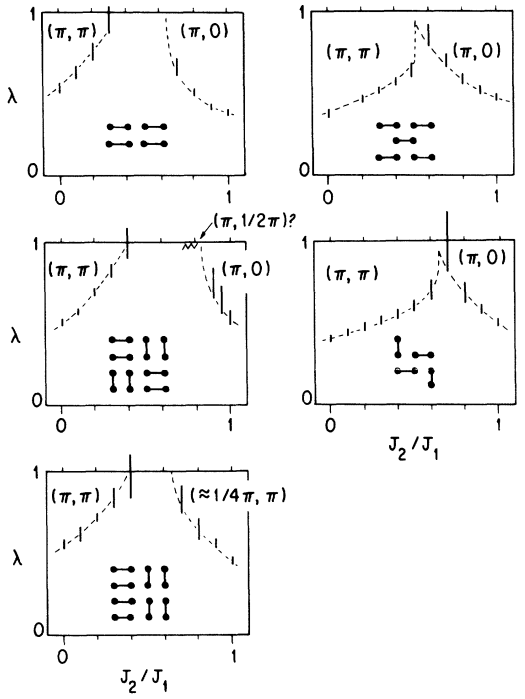

FIG. 2. Magnetic phase diagrams associated with the five dimer coverings in Fig. 1. The solid vertical segments indicate the confidence limits of the magnetic critical points at the indicated wave vectors; the dashed lines serve to guide the eye. Note that the diagrams for both the staggered and herringbone coverings exhibit rather asymmetric bicritical points, while the others lack any magnetic instability for some range of J_2. The transitions denoted by $(\approx\frac{1}{4}\pi,\pi)$ for the striped covering are to an apparently incommensurate phase; the ordering wave vector moves towards $(\frac{1}{4}\pi,\pi)$ as $J_2\to\infty$. The interval $0.7\lesssim J_2\lesssim 0.8$ for the checkerboard dimerization, indicated on the figure, shows strong short-range ordering (or, possibly, an instability very near $\lambda=1$) at the wave vectors close to $(\pi,\frac{1}{2}\pi)$; but this is presumably preempted by another transition (see Sec. IV).

they do not imply one. (Indeed, to the extent that the magnetic phase diagrams support the notion that the hard-core quantum dimer gas[15] accurately represents the low-energy physics of the J_1-J_2 model, they also provide support for columnar spontaneous dimerization, since the dimer gas model is now believed to exhibit such ordering in the relevant parameter range.[16]) Let us turn the question around, and ask, if there *is* columnar spontaneous dimerization, what does that imply that we might test numerically?

C. Tests of columnar spontaneous dimerization

(1) If one starts at $\lambda=0$ with the columnar pattern, the nearest-neighbor correlations at $\lambda=1$ should remain of that character: if the dimer covering couples (0,0) to (1,0), then at λ_1 one should have

$$\langle \mathbf{S}_{(1,0)}\cdot\mathbf{S}_{(2,0)}\rangle-\langle \mathbf{S}_{(0,0)}\cdot\mathbf{S}_{(1,0)}\rangle>0\ , \tag{2.2}$$

and so forth. This issue was investigated in I; the spontaneous dimerization estimated by Padé approximants was quite large, and easily distinguished from zero. However, one might doubt the accuracy of the numerical extrapolations, thus motivating the second test.

(2) If one starts at $\lambda=0$ with any pattern other than columnar, the nearest-neighbor correlations at $\lambda=1$ should also exhibit columnar spontaneous dimerization. This is a trivial restatement of our working hypothesis. However, it is not always possible to test this by the series method—if any phase transition intervenes between $\lambda=0$ and $\lambda=1$, the correlations at $\lambda=1$ cannot be reliably estimated even from series of arbitrary length. Thus it is clearly pointless to examine the correlations for the staggered and herringbone coverings.

For the checkerboard covering, it is also impossible to analytically continue from $\lambda=0$ to a spontaneously columnar-dimerized phase, as one sees by the following argument. At $\lambda=1$, the columnar-dimerized ground state is fourfold degenerate, while at $\lambda=1^-$, it should be evident from Fig. 3 that the fourfold degeneracy is reduced to twofold. However, at $\lambda=0$ the ground state is nondegenerate. Thus at least one phase transition must be present between $\lambda=0$ and 1^-. (At $\lambda=1$ itself there is necessarily a first-order transition if the ground state is spontaneously dimerized; see the discussion in Sec. IV of I.) If there is only one transition, it may be first order or continuous; in the latter case, symmetry considerations

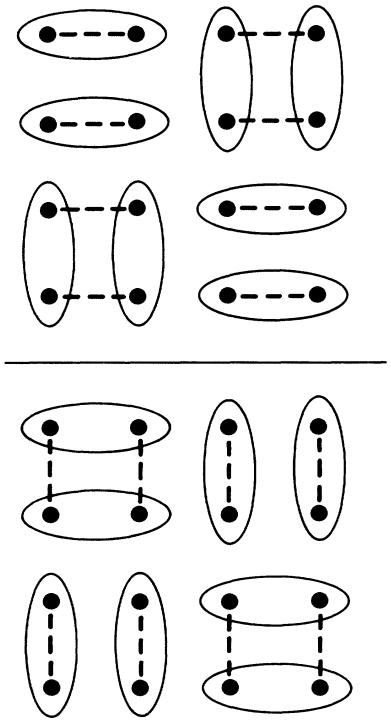

FIG. 3. The two parts of this figure represent the same set of spins, with the dashed lines indicating the nearest-neighbor pairs with the largest values of $-\langle \mathbf{S}_i\cdot\mathbf{S}_j\rangle$, for two of the four possible spontaneously columnar-dimerized ground states. These states remain degenerate even when the Hamiltonian is slightly dimerized in the checkerboard pattern, with the stronger bonds indicated by the ovals.

suggest it should lie in the universality class of the classical three-dimensional Ising transition.

Note that for most dimer coverings, including the striped pattern, the fourfold degeneracy in the columnar-dimerized phase is completely lifted at $\lambda=1^-$, and hence no transition need intervene between $\lambda=0$ and 1^-—although one might, regardless.

In summary, as a test of columnar spontaneous dimerization we should study the nearest-neighbor correlation series extrapolated to $\lambda=1$, starting from the striped pattern; the results will be discussed later in this section. The discussion above also suggests two further tests.

(3) In the simplest scenario, the ground-state energies extrapolated to $\lambda=1$ in the magnetically disordered regime should be the same for the columnar and striped patterns. The checkerboard pattern should yield rather different extrapolated energies, but the character of that difference will depend on the nature of the intervening phase transition. A first-order transition might be expected to yield energy estimates that are too high (as appears to happen in the J_1-J_3 model, for the staggered pattern[10]), while a continuous transition might be reflected in a large fraction of defective Padé approximants, with poles on the real axis between $\lambda=0$ and $\lambda=1$. The analysis of the energy series will be deferred to Sec. III; let us note here only that neither of these two reasonable expectations concerning the energies for the checkerboard pattern is entirely fulfilled.

(4) Assuming there is a single, continuous transition from onefold to twofold ground-state degeneracy for the checkerboard pattern, we should be able to calculate a series expansion for an appropriate susceptibility that diverges at that transition. Such a calculation is described in detail in Sec. IV.

D. Nearest-neighbor correlations

Let us address point (2) above, and turn to the numerical results for the nearest-neighbor correlations starting from the striped covering. There are six distinct nearest-neighbor correlations, indicated in Fig. 4(a); let us denote the corresponding values of $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ by $S^{(1)}(\lambda)$ through $S^{(6)}(\lambda)$. What does the assumption of columnar dimerization at $\lambda=1$ tell us about the $S^{(i)}(1)$? Unfortunately the situation is complicated by the fact that two of the four possible columnar-dimerized states remain degenerate to first order in $(1-\lambda)$ (although this will not persist in higher orders, unlike the case of the checkerboard pattern, because no symmetry demands it), so it is difficult to determine *a priori* which of the two the striped pattern will evolve towards. If the columnar pattern of Fig. 4(b) is the result, then one expects

$$S^{(1)}(1)=S^{(3)}(1) , \tag{2.3a}$$

$$S^{(4)}(1)=S^{(5)}(1)=S^{(6)}(1) , \tag{2.3b}$$

$$S^{(1)}(1)<S^{(2)}(1),\ S^{(4)}(1) , \tag{2.3c}$$

while if that of Fig. 4(c) is the result,

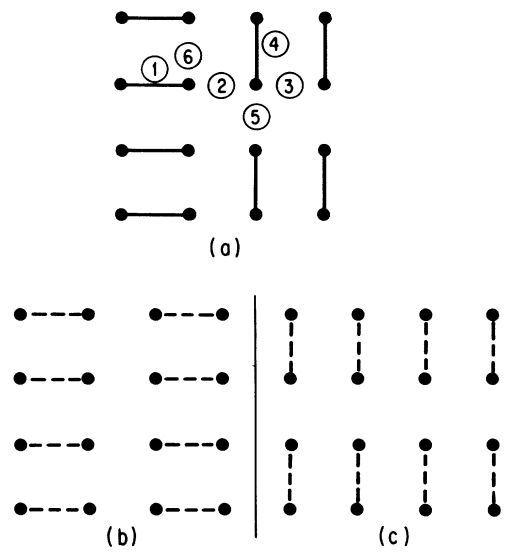

FIG. 4. In (a), the encircled numbers label the six distinct nearest-neighbor correlations in the striped-dimerized J_1-J_2 model. The two patterns of columnar spontaneous dimerization that might arise at $\lambda=1$ are shown in (b) and (c), with the dashed lines indicating the nearest-neighbor pairs with the largest $-\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$.

$$S^{(4)}(1)=S^{(6)}(1) , \tag{2.4a}$$

$$S^{(1)}(1)=S^{(2)}(1)=S^{(3)}(1) , \tag{2.4b}$$

$$S^{(4)}(1)<S^{(5)}(1),S^{(1)}(1) . \tag{2.4c}$$

Of course, if the ground state is, instead, a spin liquid, one would expect to find

$$S^{(1)}(1)=S^{(2)}(1)=\cdots=S^{(6)}(1) . \tag{2.5}$$

To what extent are any of these expectations fulfilled? The results at $J_2=0.5$ are typical: For $S^{(1)}$, $S^{(2)}$, and $S^{(3)}$, the few nondefective Padé approximants in each case vary widely at $\lambda=1$, so it is not possible to estimate them with any confidence. For the others, the estimates are

$$8S^{(4)}(1)\approx -2.5 , \tag{2.6a}$$

$$8S^{(5)}(1)\approx -0.3 , \tag{2.6b}$$

$$8S^{(6)}(1)\approx -1.0 , \tag{2.6c}$$

with uncertainties of ± 0.1 in each case determined by the consistency of the nondefective Padés. Certainly one cannot claim that (2.6) is entirely consistent with either (2.3), (2.4), or (2.5). Our preferred interpretation is that (2.6) is most consistent with (2.4), but the extrapolated series underestimate the difference between $S^{(i)}(0)$ and $S^{(i)}(1)$ in every case. [Note that $8S^{(4)}(0)=-3$, while $S^{(5)}(0)=S^{(6)}(0)=0$.] If the variation of the nearest-neighbor correlations with λ is similarly underestimated for the columnar covering, the estimates of the degree of columnar spontaneous dimerization given in I are too large. Of course this discussion is rather speculative; what is clear is that the estimates of the nearest-neighbor

correlations, for both the columnar and striped coverings, do not by themselves offer a convincing case for columnar spontaneous dimerization.

E. Intermediate-range magnetic order

Let us assume, for the purposes of this subsection, that the magnetically disordered phase is spontaneously dimerized, and ask now what is the range of the two-point correlations in the J_1-J_2 model when the system lacks Néel order. To investigate this, it is appropriate to consider only the series for the columnar covering, since, as argued earlier, all others except the striped have a phase transition between $\lambda=0$ and 1 for all J_2. Moreover, the striped covering shows a first magnetic instability, for all $J_2 \geq 0.7$ (calculations have been done for J_2 as large as 5), at $\mathbf{q} \approx (\frac{1}{4}\pi, \pi)$; this is clearly not indicative of the ordering at $\lambda=1$, and fairly substantial correlations of that type persist into the magnetically disordered phase. Thus it seems that only the columnar covering might offer reliable insights into the two-point correlations.

One finds that the wave vector with the longest-range correlations switches abruptly from (π,π) to $(\pi,0)$ between $J_2=0.5$ and 0.6; see the series in Table I. The quantities $\hat{S}(\mathbf{q})$ and $\hat{M}(\mathbf{q})$ given there are the zeroth and second radial moments of the correlations at wave vector $\mathbf{q}$, that is

$$\hat{S}(\mathbf{q}) = \sum_{\mathbf{r}} \mathbf{S}(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} , \tag{2.7}$$

and

$$\hat{M}(\mathbf{q}) = \sum_{\mathbf{r}} \mathbf{S}(\mathbf{r}) r^2 e^{i\mathbf{q}\cdot\mathbf{r}} . \tag{2.8}$$

For most $\mathbf{q}$, the coefficients in these series are irregular in sign and/or small; the preferred $\mathbf{q}$ are readily found by inspection.

To characterize the range of the preferred correlations, one may study the length ξ defined by $\xi^2(\mathbf{q}) = 2\hat{M}(\mathbf{q})/\hat{S}(\mathbf{q})$; the factor of 2 is included so that $\xi((\pi,q_y))=1$ at $\lambda=0$. At $J_2=0.5$, $\xi((\pi,\pi)) \approx 4$ and at $J_2=0.6$, $\xi((\pi,0)) \approx 7$. Both of these estimates are, of course, for $\lambda=1$, and the associated uncertainties are quite large, at least 30%.

To investigate the crossover between (π,π) and $(\pi,0)$ quasiordering in more detail, the correlations have been calculated at $J_2=0.55$. In this case there is no obvious choice for a preferred wave vector. We estimate $\xi((\pi,0)) \approx 3$, which is probably the longest spin-spin correlation length for this value of J_2.

To recapitulate, it seems likely that substantial antiferromagnetic correlations extend over several lattice spacings in the magnetically disordered phase of the J_1-J_2 model, except perhaps for a narrow region close to $J_2=0.55$.

III. GROUND-STATE ENERGIES

Here we address the third point in Sec. II C, and discuss the ground-state energies extrapolated to $\lambda=1$ in the magnetically disordered regime for the columnar, checkerboard, and striped coverings. The Padé approximants are displayed in Fig. 5 for $0.3 \leq J_2 \leq 0.8$ at intervals of 0.1; also shown are upper and lower bounds on the energies determined by diagonalization of a 16-site cluster with free boundaries[10] and a 20-site cluster with periodic boundaries.[1] For the columnar covering at $0.4 \leq J_2 \leq 0.7$, the energy series were calculated to seventh order, and the [2/5], [3/4], [4/3], and [5/2] approximants, which use all the terms, are denoted by arrows in the figure. (These expansions involved a total of 7242 connected clusters.) There are several observations to be made regarding Fig. 5.

(i) At $J_2=0.3$ and 0.8, the magnetic phase transitions are clearly evident in the large spread in the approximants displayed. Approximants are not displayed only because they fall outside the limits of the graph, or because they are defective; in either case the missing points may also be taken as evidence for an intervening phase transition. It is quite surprising, then, that the approximants for the columnar and striped patterns at $J_2=0.7$ appear to be very well behaved. This suggests that the magnetically disordered phase extends past $J_2=0.7$, and the estimates of the relevant phase boundaries, as shown in Fig. 2, are inaccurate; however, one might conclude, alternatively, that a phase transition does not necessarily affect the convergence of (sufficiently low-order) energy approximants. We favor the latter suggestion in this case, since the series extrapolations on which the phase diagrams are based seem quite convincing.

(ii) For $J_2=0.4$, 0.5, and 0.6, safely inside the magnetically disordered regime, the energy approximants for the columnar covering are reasonably clustered and clearly indicative of an extrapolated energy that lies between the indicated upper and lower bounds. The approximants for

TABLE I. Coefficients in the expansion of the zeroth ($\hat{\mathbf{S}}$) and second ($\hat{\mathbf{M}}$) radial moments of the two-point correlations at wave vectors (π,π) and $(\pi,0)$, for $J_2=0.5$ and 0.6.

	$J_2=0.5$				$J_2=0.6$			
n	$4\hat{\mathbf{S}}((\pi,\pi))$	$4\hat{\mathbf{M}}((\pi,\pi))$	$4\hat{\mathbf{S}}((\pi,0))$	$4\hat{\mathbf{M}}((\pi,0))$	$4\hat{\mathbf{S}}((\pi,\pi))$	$4\hat{\mathbf{M}}((\pi,\pi))$	$4\hat{\mathbf{S}}((\pi,0))$	$4\hat{\mathbf{M}}((\pi,0))$
0	6	3	6	3	6	3	6	3
1	3	1.5	3	25.5	1.8	−2.7	4.2	29.7
2	1.125	3.375	−2.625	37.3125	−0.6	−1.83	0.24	61.86
3	2.031 25	7.640 63	−3.0625	6.984 37	0.987	4.4935	0.133	73.2215
4	0.571 45	5.313 31	−3.144 69	−40.7156	−0.609 51	−1.847 62	−1.115 96	69.6838
5	1.975 41	8.289 22	−0.341 93	−74.6100	1.271 93	1.587 43	−0.021 07	49.3266

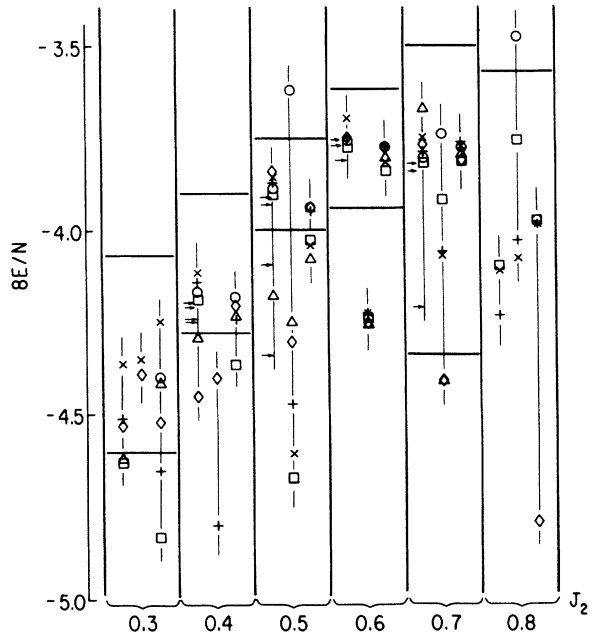

FIG. 5. Ground-state energies per spin, extrapolated to $\lambda=1$ by Padé approximants, for $0.3 \le J_2 \le 0.8$ at intervals of 0.1, from expansions about the columnar, checkerboard, and striped dimer coverings (for which the results are displayed from left to right at each J_2, with thin vertical lines to guide the eye). Each symbol denotes a different approximant, namely, the [2/2] (□), [3/2] (+), [2/3], (×), [3/3] (○), [4/2] (◇), and [2/4] (△), except that the arrows used to denote all approximants $[L/M]$ for which $L+M=7$. Note that $[L/M]$ indicates the approximant composed of an order L polynomial divided by an order M polynomial, and that to construct such an approximant one requires an expansion to order λ^{L+M}. The solid horizontal line segments indicate upper and lower bounds, described in the text.

the striped covering, while not quite as well behaved (particularly at $J_2=0.5$), are consistent with the hypothesis that the columnar and striped coverings should yield the same (and correct) energies when the series are extrapolated to $\lambda=1$, because there are no intervening singularities in either case.

(iii) For the checkerboard covering and $J_2=0.4$ and 0.5, the energy approximants are ill behaved: in the first case most are defective and in the second they are nondefective but widely spread. At $J_2=0.6$, they are strikingly *convergent,* but to an energy that is below the lower bound and clearly distinguishable from the results for the columnar and striped coverings. One sees that the approximants are again ill behaved for $J_2 \ge 0.7$.

It is not entirely clear what to conclude from these data. If the approximants at $J_2=0.6$ were as poorly convergent as those at all other values of J_2, one would have clear evidence for a continuous phase transition intervening between $\lambda=0$ and $\lambda=1$ in the magnetically disordered regime, where the two-point correlations show no hint of an instability. Despite the anomaly at $J_2=0.6$, this still seems to be the most likely state of affairs, particularly in light of the results in the following section.

In summary, Fig. 5 is largely consistent with the scenario described in point (3) of Sec. II C, and thus lends support to the notion that the magnetically disordered phase is spontaneously dimerized in the columnar pattern. The energies for the checkerboard covering seem to indicate a continuous symmetry-breaking transition; let us attempt to study this transition directly.

IV. SUSCEPTIBILITY TO COLUMNAR DIMERIZATION

We now address point (4) of Sec. II C. It should be apparent from Fig. 3 that an appropriate order parameter for the (hypothetical) phase transition is

$$\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle|_{(i,j)\in\mathcal{D},\,\mathbf{r}_i-\mathbf{r}_j=\pm\hat{x}} - \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle|_{(i,j)\in\mathcal{D},\,\mathbf{r}_i-\mathbf{r}_j=\pm\hat{y}} , \tag{4.1}$$

and the field conjugate to this, which we may denote $\mathcal{H}_2$, is defined simply by taking (4.1), stripping the angular brackets, and summing over all dimers in the checkerboard covering. We will investigate the possibility that this (lattice) rotational symmetry of the checkerboard-dimerized J_1-J_2 model is spontaneously broken by calculating a series expansion for the susceptibility with respect to the field $\mathcal{H}_2$. Thus, we consider an extension of the dimerized J_1-J_2 model (2.1), namely,

$$\mathcal{H}=\mathcal{H}_0+\lambda\mathcal{H}_1+\mu\mathcal{H}_2 , \tag{4.2}$$

where $\mathcal{H}_0$ and $\mathcal{H}_1$ denote the "unperturbed" and "perturbing" parts of the Hamiltonian that were written out fully in (2.1). The susceptibility of interest is

$$\chi_2 \equiv -\lim_{N\to\infty} N^{-1}\partial^2\langle \mathcal{H} \rangle/(\partial\mu)^2|_{\mu=0} , \tag{4.3}$$

for which the expansion in λ is calculated by performing a two-variable expansion of the ground-state energy per site, in λ and μ, and picking out the terms that are of second order in μ. The connected clusters for this expansion are, fortunately, the same ones that were employed in the expansions for the two-point correlations.

It is clear that the zero-order term in the expansion for χ_2 is identically zero. Furthermore, the coefficient of λ^1 in the expansion is also zero for any J_2, for the same reason that this coefficient vanishes in the expansion for the ground-state energy. Thus, the connected clusters that allowed for the calculation of six nonzero terms in the expansions for the two-point correlations only yield four nonzero terms in the expansions for χ_2. As the results for χ_2 were not entirely unambiguous, as will be seen shortly, the calculations were extended to order λ^6; a total of 6110 connected clusters needed to be considered at that order.

Table II displays the coefficients in the expansion of χ_2 for several values of J_2. Note that at $J_2=0.5$, 0.6, and 0.7, the coefficients are all positive and increase with order. At $J_2=0.4$, positivity still holds but the last term is slightly less than the preceding one. The data is qualitatively consistent with the existence of a continuous rotational-symmetry breaking transition for those J_2 that lack a magnetic transition for $0<\lambda<1$. [Since the

TABLE II. Coefficients in expansion for the susceptibility to lattice-rotational-symmetry breaking for the checkerboard-dimerized J_1-J_2 model. (The coefficients of λ^0 and λ^1 vanish for all J_2.)

n	$J_2=0$	$J_2=0.4$	$J_2=0.5$	$J_2=0.6$	$J_2=0.7$	$J_2=1$
2	0.75	0.33	0.281 25	0.255	0.251 25	0.375
3	1.5	0.612	0.457 03	0.336 75	0.255 09	0.281 25
4	1.418 40	0.987 23	0.814 75	0.655 75	0.532 59	0.624 57
5	−0.203 70	1.102 59	1.027 12	0.870 22	0.694 22	0.846 25
6	−3.120 15	0.900 53	1.176 48	1.205 36	1.082 71	1.503 98

checkerboard-dimerized model may have a (π,π) instability for $J_2=0.4$—see Fig. 2—a nondivergent χ_2 for $J_2=0.4$ would not be in contradiction with the hypothesis of columnar spontaneous dimerization.] A precise determination of the critical λ values, however, is not possible. Indeed, it is not entirely clear that $\lambda_c<1$ even for $J_2=0.5$ or 0.6: the standard ratio plots, of the ratio of adjacent coefficients c_n/c_{n-1} versus $1/n$, cannot be extrapolated to $1/n=0$ with any confidence, and there is no hope at all of checking if the critical points are classical, $d=3$ Ising transitions, as anticipated. Certainly one may conclude that the critical points are not close to $\lambda=0$. If one believed they exist for $J_2=0.5$ or 0.6—and the results of Sec. III, in conjunction with the monotonicity of the series coefficients offer a strong case in their favor—then they are probably in the range $0.75<\lambda<1$, and thus every point in the magnetically disordered phase of the J_1-J_2 model would be close to a model with a divergent energy-energy correlation length.

V. RECAPITULATION AND DISCUSSION

Numerical evidence from series expansions for two-point correlations, for the ground-state energy, and for a novel susceptibility suggests that the magnetically disordered regime of the J_1-J_2 model is not fully disordered, but, rather, is spontaneously dimerized in a columnar pattern, as had been predicted by Read and Sachdev.[5] It is possible, though by no means certain, that the degree of such dimerization is much less than one would estimate on the basis of expansions about the columnar-dimer covering; one should note that the magnitude of "column-state order parameter" calculated by Dagotto and Moreo for small clusters[1] is consistent with the dimerization estimates reported in I. With rather more confidence, we may state that substantial magnetic correlations extend over distances of several lattice spacings through nearly all of the magnetically disordered phase; energy-energy correlations are likely to be reasonably long ranged, as well. One might speculate that this last result accounts for the large overlap, found by Figueirido *et al.*,[7] between the exact ground state of 16-site clusters and trial spin-density-wave states even well inside the magnetically disordered phase.

We should not give the impression here that the results of series expansions are entirely clear cut. Indeed, the present calculations, particularly of the energy, have some peculiar features that are not at all understood (see Sec. III). However, the consistency of a wide variety of results with the hypothesis of spontaneous dimerization is most appealing.

Let us now address the issue of spin-nematic order in the J_1-J_2 model. First we should consider whether spontaneous dimerization is incompatible with spin-nematic order. Since $(\mathbf{S}_1\times\mathbf{S}_2)^2=\frac{1}{2}(\frac{3}{4}+\mathbf{S}_1\cdot\mathbf{S}_2)$, it is apparent that dimerization works against spin-nematic ordering at the shortest length scales. Note, however, that even in a fully columnar-dimerized state, with the dimer configuration shown in Fig. 1, there are strong short-range spin-nematic correlations associated with $\mathbf{S}_\mathbf{r}\times\mathbf{S}_{\mathbf{r}+\hat{\mathbf{y}}}$; it seems conceivable that such vectors might develop long-range order as λ is increased from zero, even if the dimerization persists.

A good way to address this issue numerically would be to calculate series expansions, starting from the columnar covering, for the quantities $Q(\mathbf{r})=\langle(\mathbf{S}_0\times\mathbf{S}_{\hat{\mathbf{y}}})\cdot(\mathbf{S}_\mathbf{r}\times\mathbf{S}_{\mathbf{r}+\hat{\mathbf{y}}})\rangle$. One could then investigate the question of long-range order by examining radial moments of these correlations, just as the two-point correlations were analyzed. Unfortunately, it turns out that the connected clusters that were used for all the calculations so far are not suitable for expansions of $Q(\mathbf{r})$. The appropriate set of clusters seems to be rather difficult to construct; worse yet, some fairly large clusters are needed for even low-order calculations (e.g., 12-spin clusters appears in third order, whereas for the other calculations the largest clusters at that order have 8 spins). Consequently, this approach to the problem was not carried further.

The only avenue remaining is to consider the implications of spin-nematic order for the quantities that have already been calculated. Let us consider, in particular, the expansions about the columnar covering. The appearance of long-range spin-nematic order at $\lambda_n(J_2)$ might be evident in (i) the ground-state energy, for which the extrapolations via Padé approximants to $\lambda=1$ should generally be rendered unreliable by the phase transition, and (ii) in the two-point correlations, which should hint at substantial short-range correlations at wave vectors consistent with noncollinear ordering [and particularly not (π,π) or $(\pi,0)$]. That neither of these expectations is fulfilled may be taken as circumstantial evidence against the existence of spin-nematic order, despite the fact that the spin-nematic order parameter calculated by Dagotto and Moreo[1] for finite periodic clusters increases with lattice size (on going from 16 to 20 sites) for $0.50\lesssim J_2\lesssim 0.57$. It may not be entirely coincidental that this interval is precisely where the series calculations in-

dicate a switch-over from (π,π) to $(\pi,0)$ as the wave vector at which correlations are strongest.

A final note: A recent calculation by Singh and Narayanan[17] for the J_1-J_2 model on the 16-site cluster at nonzero temperatures (by full diagonalization of the Hamiltonian) also concludes that columnar dimerization seems to be preferred over spin nematicity in the magnetically disordered phase.

Note added in proof. The picture presented in the spin-wave calculation of Ref. 3 may require reconsideration even at large S; see Ref. 18.

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