Large-N Expansion for Frustrated Quantum Antiferromagnets

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A large-N expansion technique based on symplectic [Sp(N)] symmetry for frustrated magnetic systems is proposed and applied to the square-lattice quantum antiferromagnet with first-, second-, and third-neighbor antiferromagnetic coupling. In addition to disordered states similar to those in unfrustrated systems, phases with incommensurate coplanar spin correlations and unconfined bosonic spinons are found. The occurrence of "order from disorder" is discussed. Neither chirally ordered nor spin-nematic states are found.

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Recently, there has been much activity aimed at understanding quantum antiferromagnetism, in particular states not having long-range order in the spins, especially in two spatial dimensions and in frustrated systems. Resonanting valence bonds[1] provide one way of looking at such problems. Renormalization-group treatments based on a nonlinear sigma (NLσ) model description of the ordered phase indicate[2] that a transition to a state with no long-range order can occur in spatial dimensions $d>1$ when quantum fluctuations are strong enough. Large-N techniques[3] suggest[4,5] that some unfrustrated systems develop spin-Peierls order or a valence-bond-solid (VBS) state[6] when not Néel ordered, depending on the value of the spin at each site.[7] In frustrated systems, magnetic order may be induced by quantum fluctuations when the classical system would have a degenerate ground state[8] ("order from disorder"). "Chiral"[9] and "spin-nematic"[10] order are two proposals for states without magnetic order. Numerical[11] and series[12] work on a model with first- and second-neighbor coupling and spin $\frac{1}{2}$ suggests that the disordered state at intermediate coupling has columnar spin-Peierls order as suggested by the authors for unfrustrated systems.[4,5]

In this paper we provide a systematic analytic technique for frustrated and doped antiferromagnets (AFMs) by introducing a new large-N expansion based on symplectic symmetry. The method is applied to square-lattice models with first-, second-, and third-neighbor antiferromagnetic coupling and phase diagrams are obtained (see Figs. 1–3). The nature of the disordered phases is explored via a mapping to lattice gauge theories, which exhibit new behavior when incommensurate spin correlations are present; in particular, unconfined spin-$\frac{1}{2}$ bosonic spinons[1] are possible for all values of the on-site spin. Exotic states[8,9] are absent, at least in the large-N limit.

Large-N methods based on the SU(N) generalization of the SU(2) AFM have been successfully applied[3–5] to unfrustrated AFMs by exploiting the two-sublattice (labeled A, B) structure of the model. "Spins" placed on sublattice A form an irreducible representation of SU(N), while those on B form the conjugate representation; this ensures both that a classical Néel state exists and that it is possible to make an SU(N) singlet from a pair of such sites. In particular, totally symmetric representations can be formed[3] by placing n_b bosons created by $b_{i\alpha}^\dagger$ ($\alpha=1,\ldots,N$) on sites $i\in A$ and created in the conjugate representation $\bar{b}_j^{\dagger\alpha}$ on sites $j\in B$. The operator $b_{i\alpha}^\dagger\bar{b}_j^{\dagger\alpha}$ creates an SU(N) singlet pair of bosons (a valence bond). The antiferromagnetic coupling $-(b_{i\alpha}^\dagger\bar{b}_j^{\dagger\alpha})(b_i^\beta\bar{b}_{j\beta})$ is the analog of $S_i\cdot S_j$ (plus a constant) and tries to maximize the number of valence bonds between the two sites. Sites on the same sublattice may have the ferromagnetic coupling $-(b_{i\alpha}^\dagger b_{i'}^\alpha)(b_{i'\beta}^\dagger b_i^\beta)$;[3] reversing the sign disfavors ferromagnetism rather than favoring antiferromagnetism. The two couplings are equivalent only for SU(2).

In a frustrated AFM, the two-sublattice structure does not exist and we must place the same representation at every site. For SU(2), valence-bond operators can be rewritten $\varepsilon^{\sigma\sigma'}b_{i\sigma}^\dagger b_{j\sigma'}^\dagger$ ($\varepsilon^{\sigma\sigma'}=-\varepsilon^{\sigma'\sigma}$ and $\varepsilon^{\uparrow\downarrow}=1$). This generalizes to the symplectic group Sp(N) of $2N\times2N$ unitary matrices U such that $\mathcal{J}^{\alpha\beta}b_{i\alpha}^\dagger b_{j\beta}^\dagger$ is invariant under $b\to Ub$ (independently of whether b is Bose or Fermi), where $\mathcal{J}^{\alpha\alpha'}=\mathcal{J}_{\alpha\alpha'}=\delta^{mm'}\varepsilon^{\sigma\sigma'}$, $\alpha\equiv(m,\sigma)$, $m=1,\ldots,N$ [Sp(1)$\cong$SU(2)].

In a Hubbard or t-J model, which introduces holes into the AFM, the hopping term transfers spin from site to site and so resembles the ferromagnetic coupling. Thus in SU(N) models with conjugate representations on neighboring sites there is no simple SU(N)-invariant hopping term for $N>2$; if instead one chooses all sites with the same representation, hopping can be included but not antiferromagnetic exchange. Our symplectic approach allows inclusion of both exchange and hopping for all N. In particular, using fermions with Sp(N) indices for spins and bosons for holes, the large-N limit justifies the decoupling of Ref. 13 and produces superconductivity; phase separation into an insulating AFM and hole-rich superconductor is also present. Details will be given elsewhere.

In this paper we study AFMs where the Hamiltonian contains only antiferromagnetic couplings as described above. The order-parameter manifold and the NLσ models for the magnetically ordered states can be determined along the lines of previous work.[4,14,15] For a collinear ordered state (i.e., a Néel state with two sublattices), the B sublattice has its spin $\langle b_a^\dagger S^a_{\alpha\beta} b^\beta \rangle$ [S_a is a generator of Sp(N) opposite in sign to that on A and the order parameter is a point in the manifold $M_{\rm coll} = {\rm Sp}(N)/{\rm U}(1)\times{\rm Sp}(N-1)$; for $N=1$ we recover CP^1 (the unit sphere, S^2). We note that $\pi_2(M_{\rm coll})=Z$, the group of integers, so that topologically stable point defects in spacetime (hedgehogs) exist for all N when $d=2$, while $\pi_1=0$ so there are no line defects. For a noncollinear AFM, spins at different sites are not aligned, and the order-parameter manifold enlarges to $M_{\rm noncoll}={\rm Sp}(N)/Z_2\times{\rm Sp}(N-1)$. This generalizes the result for $N=1$, SO(3)$\cong$SU(2)/Z_2 pointed out previously.[14,15] For $M_{\rm noncoll}$, $\pi_2=0$ but $\pi_1=Z_2$, so there are line defects in spacetime (vortex world lines) for $d=2$ in this case.

We shall study AFMs at zero temperature defined by the Hamiltonian

$$H=-\sum_{i,p,\eta_p}\frac{J_p}{N}(\mathcal{J}^{\alpha\beta}b^\dagger_{i\alpha}b^\dagger_{i+\eta_p,\beta})(\mathcal{J}_{\gamma\delta}b_i^\gamma b^\delta_{i+\eta_p})\,, \qquad (1)$$

where i runs over sites of a square lattice, and η_p over first-, second-, and third-neighbor vectors for $p=1,2,3$. The bosons satisfy the constraint $b_\alpha^\dagger b^\alpha = n_b$ at each site ($n_b=2S$ for $N=1$). The large-N limit is taken with n_b/N fixed[3,5] and the resulting saddle-point equations expressed in terms of the bond fields $Q_p=\langle \mathcal{J}^{\alpha\beta}b^\dagger_{i\alpha}b^\dagger_{i+\eta_p,\beta}\rangle/N$, a Lagrange multiplier, $i\lambda=\bar\lambda$, which enforces the constraint. The phases with long-range magnetic order (LRO) require the additional variable[16] $x^\alpha=\langle b^\alpha\rangle/\sqrt{N}$ and thus break global Sp(N) symmetry. For large n_b/N, the saddle-point equations reduce to those obtained in the classical limit ($n_b\to\infty$, N fixed), which in turn have the same form for all N. Thus the $n_b\to\infty$, $N\to\infty$ limits commute and the large-n_b/N limit of our results reproduces the classical limit of H at $N=1$. We have solved numerically the saddle-point equations as a function of n_b/N, J_2/J_1, and J_3/J_1 at $T=0$ with up to two sites per unit cell and sixteen variational parameters; wave-vector-dependent susceptibilities were calculated at representative points to verify stability.

For $J_3=0$ the phase diagram is shown in Fig. 1. For small N/n_b we find two phases with LRO: (i) For small J_2/J_1 we have $Q_1\neq Q$, $Q_2=Q_3=0$, the ordering wave vector is at (π,π) and the phase is the analog of the Néel state in SU(N) systems. (ii) For large J_2/J_1, the classical limit[12] has independent Néel order on each of the A and B sublattices; quantum fluctuations, which are automatically included in the present approach, cause the Néel order parameters to align (order from disorder) leading to LRO at $(\pi,0)$ (with $Q_2\neq 0$, $Q_{1,x}\neq 0$, $Q_{1,y}=0$, $Q_3=0$) or at $(0,\pi)$. The transition from LRO at (π,π)

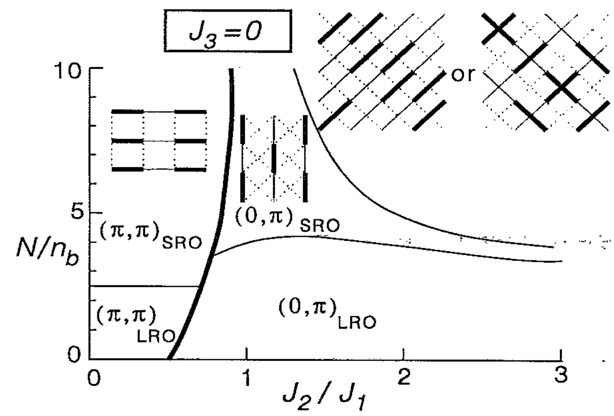

FIG. 1. Ground states of H for $J_3=0$ as a function of J_2/J_1 and N/n_b [$n_b=2S$ for Sp(1)$\cong$SU(2)]. Thick (thin) lines denote first- (second-) order transitions at $N=\infty$. Phases are identified by the wave vectors at which they have magnetic long-range order (LRO) or short-range order (SRO). The links with $Q_p\neq 0$ in each SRO phase are shown. The large N/n_b, large J_2/J_1 has the two sublattices decoupled at $N=\infty$; each sublattice has Néel-type SRO. Spin-Peierls order at finite N for odd n_b is illustrated by the thick, thin, and dotted lines. The (π,π) SRO and the "decoupled" states have line-type (Ref. 5) spin-Peierls order for $n_b=2$(mod4) and are VBS for $n_b=0$(mod4). The $(0,\pi)$ SRO state is a VBS for all even n_b.

to LRO at $(\pi,0)$ or $(0,\pi)$ is first order even for $N/n_b\neq 0$. This disagrees with Ref. 17 which finds a "spin liquid" phase exists at arbitrarily small N/n_b near $J_2/J_1=0.5$. While we agree that quantum fluctuations are very important in a "fan" emanating from $J_2/J_1=0.5$, $N/n_b=0$, we find that these fluctuations just reinforce the classical order—another example of order from disorder. The spin-wave stiffness of both LRO phases, which is typically of order $N(n_b/N)^2$, is reduced to a positive value of order $N(n_b/N)$ at or close to the phase boundary.

For larger N/n_b, both LRO phases undergo continuous (at $N=\infty$) transitions (Fig. 1) to the corresponding short-range-ordered (SRO) phases with no gapless excitations, unbroken Sp(N) symmetry ($x^\alpha=0$) but the same spatial distribution of the Q_p, and the accompanying broken rotational symmetry of the lattice. The transition line from LRO to SRO at (π,π) is independent of J_2/J_1, but this is surely an artifact of the large-N limit. Finite-N fluctuations should be stronger as J_2/J_1 increases, causing the boundary to bend a little downwards to the right. The $(\pi,0)$ or $(0,\pi)$ SRO phase breaks the lattice symmetry $x\leftrightarrow y$. For J_2/J_1 and N/n_b both large, we have an additional "decoupled" state ($Q_2\neq 0$, $Q_1=Q_3=0$) where Q_p is nonzero only for sites on the same sublattice. This state does not break any lattice symmetry. Fluctuations can induce further breaking of lattice symmetry in all of these SRO phases and will be considered later.

For $J_3 \neq 0$, it is known that the classical magnet has incommensurate helical order with noncollinear LRO.[12] Our phase diagram for a small value of N/n_b [$N/n_b=1$, Fig. 2(a)] is similar to the classical one and displays two new LRO phases: (i) A (1,0) helix with ordering at $\pm(q,\pi)$ with $Q_{1,x} \neq Q_{1,y} \neq 0$, $Q_{2,x+y}=Q_{2,y-x}\neq 0$, $Q_{3,x} \neq 0$, and $Q_{3,y}=0$; the degenerate (0,1) helix is obtained by the mapping $x \leftrightarrow y$. (ii) A (1,1) helix with ordering at $\pm(q,q)$ with $Q_{1,x}=Q_{1,y}\neq 0$, $Q_{2,x+y}\neq 0$, $Q_{2,y-x}=0$, and $Q_{3,x}=Q_{3,y}\neq 0$; this is degenerate with a $(1,-1)$ helix.[18] The wave vector q varies smoothly from 0 to π and is continuous across second-order phase boundaries [Fig. 2(a)]. In contrast to the classical limit,[12] for N/n_b finite it requires a finite J_3 to induce helical order; the first-order transition from (π,π) to $(\pi,0)$ order persists for small J_3.

As before, as N/n_b is increased, the Sp(N) symmetry is restored and the LRO phases become the corresponding SRO phases; any broken discrete lattice symmetries remain. Figure 2(b) shows the phase diagram for $N/n_b=5$. Note that global broken symmetries in states with SRO at $(0,\pi)$ and (q,π) are identical and are only distinguished by a nonzero value of Q_3 in the (q,π) phase. In the absence of any further fluctuation-driven lattice symmetry breaking (see below), the transition between SRO at $(0,\pi)$ and (q,π) is an example of a *disorder line.*[19]

Figure 3 shows the transition from LRO to SRO as a function of N/n_b for $J_3 \neq 0$. An intermediate state in which Sp(N) symmetry is only partially restored (spin nematic[10]) does not appear in the large-N limit; a $d=1+\epsilon$ expansion of similar NLσ models[2] also does not show any tendency towards such ordering. The Q_p variables can all be chosen real in all the phases, indicating the absence of chiral[9] order. Note also that the commensurate states squeeze out the incommensurate phases as N/n_b increases. We expect that this suppression of incommensurate order by quantum fluctuations is a general feature of frustrated AFMs.

We next consider finite-N, nonperturbative, topological effects in the SRO states. In the collinear states, this can be done along the lines of previous work.[5]

(i) (π,π).—The field-theory description is almost identical to the SU(N) case.[5] Berry phases for spacetime instanton point defects in a compact U(1) gauge theory lead to spin-Peierls order of column (shown in Fig. 1) or line type (not shown) for $n_b=1,3$(mod4) and 2, respectively, or a featureless VBS state for $n_b=0$(mod4), throughout the (π,π) SRO phase. The "spinon" excitations (b_α) are permanently confined. Numerical[11] and series analysis[12] appear to find columnar spin-Peierls order for $J_3=0$, $N=1$, $n_b=1$, and $J_2/J_1\approx\frac{1}{2}$; this is consistent with our results if the (π,π) LRO to SRO boundary moves down and bends downwards with increasing J_2/J_1 at finite N, as predicted above.

(ii) "Decoupled" state.—We can apply the previous analysis to each sublattice separately, giving, e.g., for $n_b=1$(mod4), the type of spin-Peierls correlations shown in Fig. 1. There is a total of $4\times 4=16$ states for this case but coupling between the sublattices will reduce this to 8 states, all of one of the two types shown. For $n_b=2$(mod4), there will be $2\times 2/2=2$ states, and for $n_b=0$(mod4), just 1.

(iii) $(0,\pi)$.—This is an intermediate case where the J_2 and J_1 compete. Despite the presence of three nonzero Q's in the unit cell of 1 site, there remains an unbroken U(1) gauge symmetry for slowly varying transformations close to $(0,\pi)$ as can be seen from the absence of odd rings in the $Q\neq 0$ links in Fig. 1. The low-energy theory is again a compact U(1) gauge theory and possesses instantons which are the remnants of hedgehogs in the LRO phase and sit naturally on the horizontal links where $Q_{1,x}=0$. Calculation either in the LRO or SRO states gives Berry phases $i\pi n_b R_x$, where R_x is the integer x coordinate of the left end of the link. Analysis of the sine-Gordon model[5] resulting from duality in this case leads to spin-Peierls order of the type shown in Fig. 1 for n_b odd, and a VBS state for n_b even.

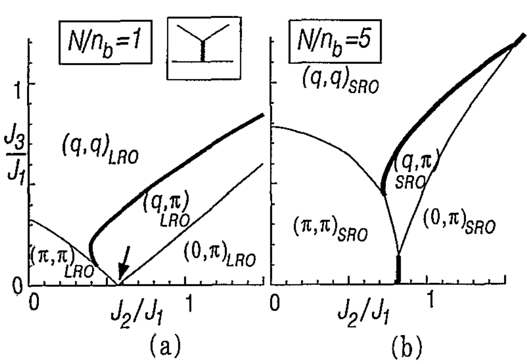

FIG. 2. As in Fig. 1 but as a function of J_2/J_1 and J_3/J_1 for (a) $N/n_b=1$ and (b) $N/n_b=5$. Inset in (a): The region at the tip of the arrow magnified by 20. A direct first-order transition from (π,π) LRO to $(0,\pi)$ LRO occurs up to $J_3/J_1=0.005$.

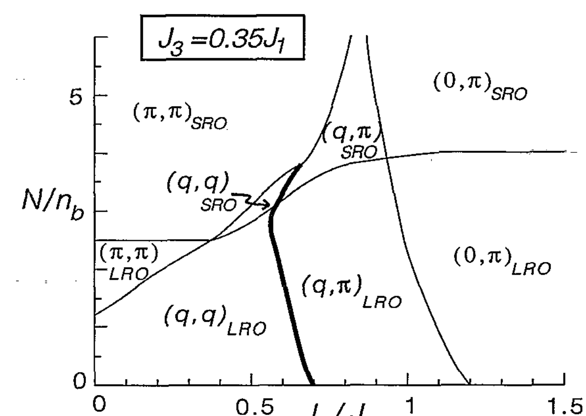

FIG. 3. As in Fig. 1 but for $J_3/J_1=0.35$.

Combined with the choice $(0,\pi)$ or $(\pi,0)$ this gives degeneracies 2,4,2,4 for $n_b = 0,1,2,3(\mathrm{mod}4)$. All the spin-Peierls states found can be understood as dimer packings of valence bonds arranged to maximize the amount of possible resonance and so gain energy from the links with nonzero Q_p. This picture also suggests that in the decoupled state resonance using J_1 will favor the configurations with parallel dimers on the two sublattices.

Fluctuations in the incommensurate SRO states are of a radically different nature. Consider, e.g., the (q,q) SRO state at a point close to its phase boundary to (π,π) SRO. The two states differ by small nonzero values of $Q_{2,x+y}Q_3$ in the (q,q) phase. These fields transform as charge-2 Higgs scalars on the links under the slowly varying U(1) gauge transformation of the (π,π) phase. In the (q,q) state the scalar fields can form vortices with flux quantum π: Instantons can change this flux by 2π, so only a Z_2 quantum number is topologically stable,[20] in agreement with the analysis of the LRO phase. The $d+1=3$ charge-2 scalar, compact $U(1)$ gauge theory can display a variety of phases:[21] (i) A Higgs phase in which the vortices are suppressed. The b^a quanta carry charge 1 and are unconfined.[22] These bosonic spin-$\frac{1}{2}$ spinons occur for all n_b. Gauge excitations have a gap. There is no breaking of lattice symmetries beyond those found at $N=\infty$. However, with periodic boundary conditions the ground state has an additional factor-of-4 degeneracy for all n_b: The additional states are obtained by changing the sign of all Q_p fields cut by a loop wrapped around the system.[20] This phase is expected to survive in our phase diagram at finite N. (ii) A confinement phase with proliferation of vortices and instantons, confinement of spinons, and a gap towards gauge excitations controlled by the instanton density.[23] A plausible scenario is that this phase in fact coincides with the (π,π) SRO phase and possesses spin-Peierls order. (iii) Additional intermediate phases driven by the Berry phases of the instantons and vortices—this possibility is under investigation. Similar considerations also apply to the (π,q) SRO phase. Numerical analysis of H for $N=1$ (Ref. 24) to search for these incommensurate phases would be useful.

This paper has presented a systematic analysis of frustrated quantum AFMs which displays clearly the crossover from the known classical limit to the quantum disordered phases.

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