Spin gap and symmetry breaking in CuO_2 layers and other antiferromagnets

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We discuss the possibility of magnetically disordered ground states in antiferromagnets and argue that a variety of systems, including the CuO_2 layers in the high-T_c superconductors, should have either a spontaneously broken symmetry or else gapless excitations. Models which may have unbroken symmetry and a gap, possibly including the honeycomb-lattice $s=\frac{1}{2}$ antiferromagnet, are also discussed.

I. INTRODUCTION

Lieb, Schultz, and Mattis (LSM) proved[1] a remarkable theorem in 1961, which states that the $s=\frac{1}{2}$ antiferromagnetic periodic chain of length L has a low-energy excitation of $O(1/L)$. Very recently it was observed[2] that this theorem can be trivially extended to arbitrary *half-odd-integer* spin but not to integer spin, thus suggesting a difference between these two cases which was first pointed out by Haldane.[3] In fact, this theorem implies[2] that for half-integer spin, in the infinite length limit, either the ground state is degenerate or else there are gapless excitations. In the former case this ground-state degeneracy is likely to be the result of a spontaneously broken symmetry. A unique ground state with a gap is impossible for half-integer spin. By contrast it *can* occur for integer spin as was proved rigorously by constructing a solvable model.[4]

Lieb, Schultz, and Mattis[1] also pointed out that their theorem could be extended to higher dimension. We wish to give a somewhat more detailed discussion of this extension and draw some (nonrigorous) conclusions from it. Besides extending it to higher dimension, we will also discuss its extension to include phonons (Heisenberg-Peierls model). Another extension is to SU(n) generalizations of the usual SU(2) spin systems. In fact, the theorem appears to be remarkably insensitive to details of the Hamiltonian, due to its essentially topological nature. In the case of ordinary SU(2) antiferromagnets, it works whenever the total spin per unit cell is half-odd-integer. Thus, for example, it works for half-odd-integer spin on an arbitrary Bravais lattice (in which the unit cell contains a single spin). These cases include the two-dimensional triangular and square lattices, discussed by Anderson and co-workers[5] in the context of "resonating valence bonds." The theorem fails for a half-odd-integer spin chain with alternating interaction strength, or for a half-odd-integer spin honeycomb-lattice antiferromagnet, since there are two spins per unit cell in these cases. Indeed a solvable spin-$\frac{3}{2}$ honeycomb-lattice model was studied[4,6] which was proved to have exponentially decaying correlation functions and a unique ground state, and appears very likely to have a gap.

In the case of realistic Heisenberg Hamiltonians, a very powerful theorem of Dyson, Lieb, and Simon,[7] together with its extension to two dimensions,[8] prove that the ground state is Néel ordered for bipartite lattices and sufficiently large spin. For the square, cubic, or honeycomb lattice this theorem applies for spin $s\geq 1$ (the triangular lattice is not bipartite).

Haldane developed an approximate mapping of the large-s antiferromagnet onto the σ model, valid in any dimension.[3] We use this to show the tendency towards Néel order for larger spin, based on renormalization group ideas. This suggests that there should be a phase transition from a Néel ordered to disordered state as a function of the spin-wave coupling constant g which decreases with increasing s and also depends on the strength of next-nearest-neighbor couplings.[9] In general, frustrating spin-couplings tend to increase the spin-wave coupling constant and thus to increase the strength of disordering fluctuations. Naively, the σ-model mapping seems to suggest that the disordered phase should have a unique ground state and a gap, analogous to the high-temperature phase of a classical ferromagnet in one higher dimension. However, the Lieb-Schultz-Mattis theorem[1] implies that this cannot be the case in general. In one dimension this difficulty is removed by the inclusion of a topological term in the σ model.[9] While a topological term also exists in the two-dimensional case, it is unclear whether it plays a role. Indeed, the σ-model mapping, while generally valid in the weak coupling Néel-ordered phase right up to the critical point, may break down in the strong-coupling phase in some cases. Thus while a transition out of the Néel phase should occur for sufficiently strong spin-wave coupling, it is unclear what the strong coupling phase is. The Lieb-Schultz-Mattis theorem gives valuable information about the possibilities.

The rigorous results on Néel order[7,8] imply that, in the case of Heisenberg antiferromagnets on bipartite lattices, only for $s=\frac{1}{2}$ is there a chance of a "fluctuation-dominated" ground state. For the square lattice, if the ground state is not Néel ordered (finite-size calculations[10] suggest that it is) then the Lieb-Schultz-Mattis theorem suggests that either translational symmetry is broken, leading to a doubling of the unit cell, as in the spin-Peierls phase, or else there are gapless excitations. Only the $s=\frac{1}{2}$ honeycomb lattice seems to be a candidate for an experimentally realizable higher-dimensional extension of the Haldane phase,[3] characterized by a unique ground state and a gap.

The outline of this paper is as follows. In the next section we will review the Lieb-Schultz-Mattis theorem and discuss its extension to higher dimension and to include phonons. In Sec. III we will take up the issue of Néel order versus disorder, by considering the large-s mapping onto the nonlinear σ model. In Sec. IV we will give some further discussion of the implication of these results to triangular-lattice antiferromagnets and to the high-T_c superconductors.

II. THE LIEB-SCHULTZ-MATTIS THEOREM

Consider the $s=\frac{1}{2}$ Heisenberg antiferromagnet on a periodic chain of length L even.

$$H=\sum_i \mathbf{S}_i\cdot\mathbf{S}_{i+1} .$$

We wish to prove that there is a low-energy excitation of $O(1/L)$. We may assume that the ground state $|\psi_0\rangle$ is unique, since otherwise the result would be trivially true. In fact, a rigorous proof of uniqueness exists in this case and most others of interest.[11] The proof of a low-energy excitation[1] proceeds by constructing a state $|\psi_1\rangle$ which has low energy, i.e., $\langle\psi_1|(H-E_0)|\psi_1\rangle=O(1/L)$, and which is orthogonal to the ground state. $|\psi_1\rangle$ is constructed by making a unitary transformation on $|\psi_0\rangle$, namely a slowly varying rotation about the z axis:

$$|\psi_1\rangle=U|\psi_0\rangle ,\qquad U\equiv\exp\left[i(2\pi/L)\sum_n nS_n^z\right] . \tag{1}$$

This state has low energy because, for large L, the relative rotation of two neighboring sites is $O(1/L)$. Requiring the relative rotation between the Lth and 1st sites to be small fixed the overall coefficient in the exponent in U. Noting that

$$\exp(i\theta S^z)S^+\exp(-i\theta S^z)=\exp(i\theta)S^+$$

we see that

$$\langle\psi_1|(H-E_0)|\psi_1\rangle=\frac{1}{2}\left[[\exp(i2\pi/L)-1]\times\sum_i\langle S_i^+S_{i+1}^-\rangle+\text{H.c.}\right] .$$

Since the ground state is unique it must be isotropic, implying

$$\langle S_i^+S_{i+1}^-\rangle=\langle S_i^-S_{i+1}^+\rangle .$$

Thus

$$\langle\psi_1|(H-E_0)|\psi_1\rangle=[\cos(2\pi/L)-1]\sum_i\langle S_i^+S_{i+1}^-\rangle .$$

Since $S_i^+S_{i+1}^-$ is a bounded operator,

$$\langle\psi_1|(H-E_0)|\psi_1\rangle=O(1/L) .$$

In fact, we have

$$\langle\psi_1|(H-E_0)|\psi_1\rangle=[\cos(2\pi/L)-1]2E_0/3 ,$$

where E_0 is the ground-state energy.

Of course, merely constructing a low-energy state proves nothing; it might become equal to the ground state as $L\to\infty$. To complete the proof, we must show that this does not happen. This can be done by showing that $|\psi_1\rangle$ is orthogonal to $|\psi_0\rangle$. This is true because $|\psi_1\rangle$ has momentum π relative to the ground state, and thus must be orthogonal due to our uniqueness assumption which implies that $|\psi_0\rangle$ is a momentum eigenstate. To calculate the momentum of $|\psi_1\rangle$, we must calculate the effect on U of a translation by one site:

$$U\to TUT^{-1}=\exp\left[i(2\pi/L)\sum_{n=1}^{L-1}nS_{n+1}^z+LS_1^z\right]$$
$$=U\exp\left[-i(2\pi/L)\sum_{n=1}^{L}S_n^z\right]\exp(i2\pi S_1^z) .$$

The ground state has spin 0 since it is unique, and thus the first exponential gives one

$$U|\psi_0\rangle\to U\exp(i2\pi S_1^z)|\psi_0\rangle .$$

Finally since S_1^z has eigenvalues $\pm\frac{1}{2}$,

$$TU|\psi_0\rangle=-UT|\psi_0\rangle .$$

Thus there is a low-energy state of momentum π, relative to the ground state. This proof extends immediately[2] to arbitrary half-odd-integer s but fails in the integer-s case. The reason is that $\exp(i2\pi S_1^z)$ is ±1 for integer or half-odd integer s, respectively, and so the momentum is zero or π, respectively. In the former case it cannot be proved that $|\psi_1\rangle$ is orthogonal to $|\psi_0\rangle$. This appears not to be a mere technicality but to cut to the heart of the difference between integer and half-odd integer spin, using as it does the fact that half-odd integer wave functions change sign under 2π rotations.

In the half-odd integer case, the proof can easily be extended to much more general Hamiltonians. Anisotropic and non-nearest-neighbor interactions can be added. The fact that $|\psi_1\rangle$ has low energy is true for essentially *any* reasonable Hamiltonian, and the fact that the momentum is π did not use any property of the Hamiltonian at all, except that translation by one site is a symmetry. (This latter property would fail with alternating interactions.) Of course, the assumption of a unique ground state can fail for some Hamiltonians (for example ferromagnetic ones), in which case, while there *is* a low-energy state (another ground state), it does not necessarily have momentum π.

Of course, even if the finite-chain ground state is unique, the infinite length ground state may not be. For the Hamiltonian

$$H=\sum_i(\mathbf{S}_i\cdot\mathbf{S}_{i+1}+\tfrac{1}{2}\mathbf{S}_i\cdot\mathbf{S}_{i+2}) , \tag{2}$$

the finite-chain ground state is twofold degenerate, the two ground states differing by translation by one site. These two ground states correspond to pairs of nearest-neighbor valence bonds.[12,4] It is believed[13] that this twofold degeneracy persists for a finite range of second nearest-neighbor coupling, over some of which the *finite* chain presumably has a unique ground state. In this situation, the ground state of a large finite chain is essentially the symmetric combination of the two infinite-chain ground states. The low-energy excited state is the antisymmetric combination. The overlap of the two different pure states and hence the splitting of the finite chain eigenstates is $O[\exp(-\text{const}\times L)]$. This low-energy state has momentum π relative to the ground state. One expects a finite gap to all other states, as $L\rightarrow\infty$. This has been proven rigorously[4] for the solvable model of Eq. (2).

In the case of the Heisenberg Hamiltonian, the Bethe ansatz solution shows that the ground state is unique but the dispersion relation for one-particle excitations is

$$E\propto|\sin k| .$$

This vanishes at $k=\pi$, as required by the LSM theorem.

The LSM theorem seems to imply that half-odd integer antiferromagnets are generically in a gapless nondegenerate phase or else have broken translational symmetry.

Let us now consider higher-dimensional generalizations of the LSM theorem. Consider first a half-odd integer s Heisenberg model on a square lattice of length L and width M with periodic boundary conditions. Let us again attempt to construct a low-energy state, orthogonal to the ground state.[1] We may again consider making slowly varying rotations of definite momentum. Suppose we use a unitary operator of momentum $(\pi,0)$:

$$U\equiv\exp\left[i(2\pi/L)\sum_{\mathbf{x}}XS^z_{\mathbf{x}}\right]$$

(the coordinates are integers). We may bound the energy of $U|\psi_0\rangle$ as before. There is no increase in energy for the vertical bonds and each of the LM horizontal bonds has an increase in energy of $O(1/L^2)$. Thus the energy is $O(M/L)$. This is a low-energy state for a strip with $L\gg M$. In particular it gives a zero-energy state for an infinite strip.

However, we must ask if $U|\psi_0\rangle$ is orthogonal to the ground state. We may calculate the momentum of U as before. We find

$$TUT^{-1}=U\exp\left[-i(2\pi/L)\sum_{\mathbf{x}}S^z_{\mathbf{x}}\right]\exp\left[i2\pi\sum_{y}S^z_{(1,y)}\right] .$$

As before, we may assume that the ground state has total spin zero. The second exponential contains the total z component of spin on the first column. This will be an integer or half-odd integer according to whether M is even or odd, respectively. Thus the theorem works if and only if the number of rows, M, is odd.

This result is certainly much less complete than in the one-dimensional case. The energy is only small if the strip is much longer than it is wide, and furthermore, the number of rows must be odd. We hasten to observe that the result *does* hold with periodic boundary conditions, and that requiring an odd number of rows does not cause any obvious pathologies, since the total number of *sites* is even.

There is another respect in which the result is less complete in two dimensions. To actually prove rigorously the existence of ground-state degeneracy or zero gap, we constructed[2] a slow-energy state spread over a region of length l in a chain of length $L\gg l$, with energy $O(1/l)$. This was done by the same procedure, introducing a slow twist over a portion of the chain. In two dimensions, although we *could* twist over only a portion of each row, we find it necessary to twist *all* rows, i.e., the excitation fills the whole width of the lattice. The problem is that, in principle, such a spread out excitation might become completely unobservable for the infinite system without necessarily implying ground-state degeneracy. An example of such an excitation would be a spin wave of momentum $k_y=0$. This would be no more observable in an infinite lattice than a photon with wavelength equaling the size of the universe.

However, we regard this as a technical limitation not a fundamental one for the following reason. In a physically sensible model, if there are $k_y=0$ spin waves, there are also spin waves with k_y close to zero. By forming a linear combination of these states, we can always obtain a localized low-energy state. On the other hand, if the low-energy $k_y=0$ state is *not* accompanied by other nearby low-energy states, then it should indicate ground-state degeneracy. Likewise, if the state only existed for an odd number of rows, we would again expect broken symmetry. One might be happier if the state could be found for an $L\times L$ lattice. However, we expect that the energy gap should *decrease* not increase, if we increase the width from M $(\ll L)$ to L. While this argument has not been made rigorous, we can think of no physical counter examples. Of course, this may simply reflect a lack of imagination.

We feel that this theorem, incomplete though it is, *does* imply essentially the same result as in one dimension. Namely, either there are gapless excitations of momentum $(0,\pi)$ in the infinite area limit, or else broken translational symmetry. In any event, any approximate solution of the model must pass the test of having a low-energy state for a long strip with an odd number of rows.

Let us now consider other lattices. The theorem can be extended immediately to a cubic lattice in three dimensions. The energy is $O(A/L)$ where A is the area and L the length. This state has low energy for a very long box. The proof also works for a triangular lattice in two dimensions since an odd number of rows is again consistent with periodic boundary conditions. The proof goes through exactly as before. We may again choose the rotation at location $\mathbf{x}$ to be $(2\pi/L)x$, where the x axis lies along a lattice row. There is now a contribution to the energy of $O(1/L^2)$ from all three types of bonds, again giving a total energy of $O(M/L)$. It was crucial that we could choose an odd number of rows consistently with periodic boundary conditions. Note that the fact that the triangular lattice is not bipartite plays no role here. In fact, it is more natural to take an odd number of rows in this case. For a square lattice, an odd number of rows would force a seam into the Néel state. (Of course this is not a problem for our arguments since the Néel phase has broken translational symmetry.) For the triangular lattice, an odd number of rows is consistent with a tripartite ordered state, provided that that number is divisible by three. Now consider the honeycomb lattice with half-odd integer spin. We may again consider making a rotation whose magnitude varies with distance along a lattice row. But in this case, it is not possible to have an odd number of rows consistent with periodic boundary conditions. This follows because there are two inequivalent types of rows and neighboring rows are not connected by primitive translations. Indeed an $s=\frac{3}{2}$ model was constructed which can be proven to have exponential decaying correlation functions[4] and a unique ground state[6] and appears to have a gap.

Let us now consider the extension of the theorem beyond Hamiltonians containing only spin variables. We may easily generalize it to a Heisenberg-Peierls model in which the magnetic interaction strength between two neighboring spins, J_{ij}, depends in some way on the distance between them, the displacement of each spin from its equilibrium position being treated as a quantum variable. The proof proceeds exactly as before. The unitary transformation has no effect on the phonon degrees of freedom. The excitation energy for a chain is given by

$$\langle \psi_1 | (H-E_0) | \psi_1 \rangle = [\cos(2\pi/L)-1] \times \sum_i \langle J_{i,i+1} S_i^+ S_{i+1}^- \rangle ,$$

and so should be $O(1/L)$. The theorem was also extended to chains with SU(n) generalizations of SU(2) spin variables on the sites.[2] The extension of these cases to higher dimension goes exactly the same way as for SU(2). A large-n limit of the square lattice SU(n) Heisenberg model was solved recently,[14] and that solution was consistent with our conclusion, namely translational symmetry was broken in the ground state.

We have *not* been able to extend the proof to itinerant electron models although we expect that the result holds in those cases as well. Field theory analysis of one-dimensional models suggests that in the phase in which both the spin and charge excitations have a gap, there is a broken translational symmetry. The large-n solution[14] of the Hubbard-Heisenberg model on a square lattice is also consistent with the general conclusion.

III. σ-MODEL MAPPING

The one-dimensional Heisenberg model does not display Néel order even at $T=0$, due to infrared-singular quantum fluctuations. (This is the quantum version of the Mermin-Wagner theorem,[15] known in field theory as Coleman's theorem.[16]) On the other hand, in two dimensions Néel order is possible in the ground state, although not inevitable. A nice way of understanding these issues is to make a mapping of the spin system onto the nonlinear σ model.[3,17,9]

In the one-dimensional case, this can be done[17,9] by combining pairs of neighboring spins to define the field and rotation generators of the σ model:

$$\boldsymbol{\varphi}(2n+\tfrac{1}{2}) \equiv (\mathbf{S}_{2n}-\mathbf{S}_{2n+1})/2\sqrt{s(s+1)} ,$$

$$\mathbf{l}(2n+\tfrac{1}{2}) \equiv (\mathbf{S}_{2n}+\mathbf{S}_{2n+1})/2 .$$

$\boldsymbol{\varphi}$ and $\mathbf{l}$ are then assumed to be slowly varying on the scale of the lattice spacing; we are keeping only momentum modes near zero and π, the two low-energy regions for an antiferromagnet. In the large-s continuum limit, $\boldsymbol{\varphi}$ and $\mathbf{l}$ obey the commutation relations and constraints of the σ model:

$$[l^a(x),\varphi^b(y)] = i\varepsilon^{abc}\varphi^c(x)\delta(x-y) ,$$

$$[l^a(x),l^b(y)] = i\varepsilon^{abc}l^c(x)\delta(x-y) ,$$

$$[\varphi^a(x),\varphi^b(y)] = i\varepsilon^{abc}l^c(x)\delta(x-y)/s(s+1) \to 0 ,$$

$$\boldsymbol{\varphi}\cdot\mathbf{l}=0 ,$$

$$\boldsymbol{\varphi}^2 = 1-\mathbf{l}^2/s(s+1) \to 1 .$$

Ignoring higher derivitive terms, the Hamiltonian density becomes

$$\mathcal{H}/v = (g/2)[l+(\theta/4\pi)(d\boldsymbol{\varphi}/dx)]^2 + (1/2g)(d\boldsymbol{\varphi}/dx)^2 ,$$

with velocity, coupling constant, and topological angle

$$v=2\sqrt{s(s+1)},\quad g=2/\sqrt{s(s+1)},\quad \theta=2\pi\sqrt{s(s+1)} .$$

The corresponding Lagrangian density is

$$\mathcal{L} = (1/2g)(\partial_\mu\boldsymbol{\varphi})^2 + (\theta/4\pi)\boldsymbol{\varphi}\cdot(\partial_\mu\boldsymbol{\varphi}\times\partial_\nu\boldsymbol{\varphi})\varepsilon^{\mu\nu} .$$

θ multiplies the topological term which is always i times an integer, the winding number, for a smooth configuration in Euclidean space. Thus θ is a periodic variable, and the different behavior for s integer or half-integer can be explained. For $\theta=0$, s integer, we simply have the Lagrangian describing the continuum limit of a <u>*two-dimensional*</u> classical ferromagnet, with temperature $g=2/\sqrt{s(s+1)}$. For large s the coupling constant is weak and we may do perturbation theory. This is done by assuming that $\boldsymbol{\varphi}$ has an expectation value, corresponding to Néel order. The perturbative spectrum consists of two Goldstone bosons. The leading infrared divergences of σ-model perturbation theory would correspond to standard spin-wave perturbation theory based on the Holstein-Primakoff approximation. However, we find that the coupling grows with increasing length scale (or decreasing energy scale):

$$dg/d\ln L = g^2/2\pi .$$

This suggests that the symmetry is not really spontaneously broken, and that there is a finite correlation length of order

$$\xi \approx \exp[\pi\sqrt{s(s+1)}] ,$$

and a corresponding gap $\Delta \approx v/\xi \approx s\exp[-\pi\sqrt{s(s+1)}]$. This behavior corresponds to the fact that the critical temperature of the two-dimensional classical ferromagnet is zero, and there is an exponentially large correlation length at low temperatures.

The behavior of the $\theta=\pi$ σ model is less familiar, but there appears to be unbroken symmetry with a (non-Goldstone) massless sector.

All of this holds for arbitrarily large s. We may also add a second nearest-neighbor coupling. This modifies the σ model coupling constant to[9]

$$g=2/[\sqrt{s(s+1)}\sqrt{1-4J_2}] .$$

A frustrating coupling ($J_2>0$) tends to increase the σ-

model coupling, disfavoring the Néel-ordered state.

We may attempt to repeat the above procedure in higher dimension. The validity of the σ-model mapping in higher dimension was pointed out in Ref. 3. Consider first the simplest case of a square lattice in two dimensions. The natural extension of the above approach is to define continuum limit variables on every fourth plaquette. We may define a σ-model field, the order parameter

$$\boldsymbol{\varphi}(2x+\tfrac{1}{2},2y+\tfrac{1}{2})\equiv(\mathbf{S}_{2x,2y}-\mathbf{S}_{2x+1,2y}-\mathbf{S}_{2x,2y+1}+\mathbf{S}_{2x+12,y+1})/4\sqrt{s(s+1)}\ .$$

We may also define the continuum rotation generator, related to the conjugate momentum for $\boldsymbol{\varphi}$, as

$$\mathbf{l}(2x+\tfrac{1}{2},2y+\tfrac{1}{2})\equiv(\mathbf{S}_{2x,2y}+\mathbf{S}_{2x+1,2y}+\mathbf{S}_{2x,2y+1}+\mathbf{S}_{2x+1,2y+1})/4\ .$$

$\boldsymbol{\varphi}$ and $\mathbf{l}$ again obey the correct commutation relations and constraints for large s. However, a difference emerges from the one-dimensional case. To converse the number of degrees of freedom, we must define two other fields:

$$\mathbf{A}_x(2x+\tfrac{1}{2},2y+\tfrac{1}{2})\equiv(\mathbf{S}_{2x,2y}-\mathbf{S}_{2x+1,2y}+\mathbf{S}_{2,2y+1}-\mathbf{S}_{2x+1,2y+1})/4[s(s+1)]^{1/4}\ ,$$

$$\mathbf{A}_y(2x+\tfrac{1}{2},2y+\tfrac{1}{2})\equiv(\mathbf{S}_{2x,2y}+\mathbf{S}_{2x+1,2y}-\mathbf{S}_{2x,2y+1}-\mathbf{S}_{2x+1,2y+1})/4[s(s+1)]^{1/4}\ .$$

Treating all these fields as slowly varying, $\boldsymbol{\varphi}$, $\boldsymbol{l}$, $\mathbf{A}_x$, and $\mathbf{A}_y$ correspond to the Fourier modes of the spin operators, $\mathbf{S}$, with momentum near (π,π), $(0,0)$, $(\pi,0)$, and $(0,\pi)$, respectively. $\boldsymbol{l}$ generates rotations of the $\mathbf{A}_i$ as well as of $\boldsymbol{\varphi}$. In the continuum limit $\boldsymbol{\varphi}$ commutes with the $\mathbf{A}_i$:

$$[\varphi^a(\mathbf{x}),A_x^b(\mathbf{y})]=i\varepsilon^{abc}A_y^c(\mathbf{x})\delta(\mathbf{x}-\mathbf{y})/\sqrt{s(s+1)}\to 0\ ,$$

$$[\varphi^a(\mathbf{x}),A_y^b(\mathbf{y})]=i\varepsilon^{abc}A_x^c(\mathbf{x})\delta(\mathbf{x}-\mathbf{y})/\sqrt{s(s+1)}\to 0\ .$$

On the other hand, the $\mathbf{A}_i$ have a nonzero commutator:

$$[A_y^a(\mathbf{x}),A_x^b(\mathbf{y})]=i\varepsilon^{abc}\varphi^c(\mathbf{x})\delta(\mathbf{x}-\mathbf{y})\ ,$$

$$[A_x^a(\mathbf{x}),A_x^b(\mathbf{y})]=[A_y^a(\mathbf{x}),A_y^b(\mathbf{y})]=i\varepsilon^{abc}l^c(\mathbf{x})\delta(\mathbf{x}-\mathbf{y})/\sqrt{s(s+1)}\to 0\ .$$

All four fields are exactly mutually orthogonal. They also obey the constraint

$$\boldsymbol{\varphi}^2=1-l^2/s(s+1)-\mathbf{A}_x^2/\sqrt{s(s+1)}-\mathbf{A}_y^2/\sqrt{s(s+1)}\to 1\ .$$

The two additional fields that we have been forced to introduce do not seem to have any obvious interpretation in the σ model. Making a gradient expansion, we now find the Hamiltonian density:

$$\mathcal{H}/v=(g/2)l^2+(1/2g)(\nabla\boldsymbol{\varphi})^2+\tfrac{1}{2}\mathbf{A}_x^2+\tfrac{1}{2}\mathbf{A}_y^2\ ,$$

where $g=2/\sqrt{s(s+1)}$, $v=4\sqrt{s(s+1)}$. Once again, g will increase with a frustrating second-nearest-neighbor coupling. Temporarily ignoring the extra fields, let us consider the σ model alone. We now have a continuum version of the *three*-dimensional classical ferromagnet at temperature g. Thus there should be a phase transition at some finite value of g (or order one). This can be seen, for example, from the $(2+\varepsilon)$ expansion of the σ model.[18] The fixed point at couplings of order ε presumably persists up to three dimensions. In the weak coupling phase, there is Néel order and two Goldstone bosons.

Let us now consider the affect of the additional fields in the weak coupling phase. Choosing $\langle\varphi^a\rangle=\delta^{a3}$, the commutation relations become, to leading order in $1/s$.

$$[A_x^1(\mathbf{x}),A_y^2(\mathbf{y})]=-[A_x^2(\mathbf{x}),A_y^1(\mathbf{y})]=-i\delta(\mathbf{x}-\mathbf{y})\ ,$$

with the other commutators lower order. Thus (A_x^1,A_y^2) and $(A_x^2,-A_y^1)$ define two field-conjugate momentum pairs, while A_x^3 and A_y^3 are classical fields. In this approximation, the extra fields are decoupled and massive. Thus the low-energy sector in the Néel phase consists only of the Goldstone bosons as expected. Once again, the Goldstone modes, with momentum near (π,π) and (0,0), are those obtained from standard spin-wave theory. The extra fields $\mathbf{A}_i$, with momentum near $(\pi,0)$ and $(0,\pi)$, do not affect the leading infrared behavior of perturbation theory, or, presumably the existence of a critical point. However, it is much less obvious what role these extra fields may play in the strong-coupling phase.

Based on the LSM theorem and our experience with the one-dimensional case, it seems likely that the nature of the strong-coupling phase depends radically on whether the spin is integer or half-odd integer. In the former case a unique ground state with a gap may occur, corresponding to the disordered phase of a classical three-dimensional ferromagnet. However, in the half-odd integer case, this is inconsistent with the LSM theorem. Instead there is presumably either a breaking of the symmetry of translation by one site, or else a unique ground state with vanishing gap. The former case corresponds to some two-dimensional generalization of the dimerized phase. The lattice translational symmetry is broken but not the spin-rotational symmetry. In the latter case we can imagine (at least) two possibilities. One is that there is a gapless pseudo-Fermi surface and effectively massless free fermions as in the resonating valence bond model discussed by Anderson and collaborators.[5] Another possibility is that the gap vanishes only at discrete points in momentum space, probably (0,0), $(0,\pi)$, $(\pi,0)$, and (π,π). In this case, there is likely to be a $(2+1)$-dimensional field theory description of the gapless sector. It is possible that the Hopf topological term of the $(2+1)$-dimensional σ model[19] appears. On the other hand, if there is a gapless Fermi surface in the strong-coupling phase, then a $(2+1)$-dimensional field theory is *not* the correct description, since for such a field theory the gap would only vanish at discrete points in momentum space.

In the large-n limit of the Heisenberg model,[14] we

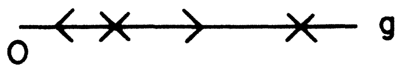

FIG. 1. The proposed renormalization group flow diagram for $d \geq 2$ antiferromagnets subject to the LSM theorem.

found a dimerized ground state, although a nondegenerate ground state with the gap vanishing at discrete points in momentum space, represented another locally stable state of slightly higher energy. (For the Heisenberg-Hubbard model, the latter state became the ground state for a range of parameters and a ground state with a gapless Fermi surface also occurred away from half-filling.)

In renormalization group language, there is an infrared unstable fixed point corresponding to the Néel ordering transition, as a function of g (which can be controlled by varying s or a second-nearest-neighbor coupling). For integer s the flow on the strong-coupling side is to some short-range (nonuniversal) fixed point. For half-odd-integer s the flow is to some other attractive fixed point (see Fig. 1), or else to some short-range (nonuniversal) dimerized phase.

The above discussion was given for a square lattice, but very similar results would immerge for *any* bipartite lattice in any dimension greater than one. In the continuum limit, the σ-model fields $\boldsymbol{\varphi}$ and $\boldsymbol{I}$ would arise together with a lattice-dependent number of additional fields, which would be massive in the Néel phase. A transition out of the Néel phase should be generic for sufficiently small s or large second-nearest-neighbor coupling. This is the analogue of the fact that a classical ferromagnet has a finite-temperature transition for any dimension greater than two. In cases where the LSM theorem applies, the strong-coupling phase should be either dimerized or gapless; in other cases it may be a short-range nondegenerate phase with a gap.

There does not appear to be any simple way of estimating the critical value of s at which the Néel transition occurs for various lattice types. The critical coupling in the σ model is nonuniversal and regularization dependent. The most useful result, in this regard, is the rigorous theorem of Dyson, Lieb, and Simon,[7] which shows that there is Néel order for the Heisenberg Hamiltonian and any $s \geq 1$, for most lattice types.

IV. DISCUSSION

Let us summarize our main conclusions. In any dimension greater than one and any lattice type, there should be a critical coupling separating the Néel phase from a strong-coupling phase, where the σ-model coupling constant decreases as $1/s$ but increases with a frustrating second-nearest-neighbor spin coupling. In cases where the LSM theorem does not apply, namely where the spin per unit cell is integer, a unique ground state with a gap may occur. Where the LSM theorem *does* apply, we expect the strong-coupling phase to have either broken translational symmetry or else gapless excitations. In the latter case, these may either be on a Fermi surface, or at the discrete points $(0,0)$, $(0,\pi)$, $(\pi,0)$, and (π,π) only.

What are the prospects for testing these predictions? Numerical work on finite two-dimensional lattices is certainly one possibility. In the one-dimensional case it was necessary to go[20] to spin-1 chains of length 30 to show fairly convincingly the existence of a gap, although the experts now generally agree that a sufficiently sophisticated analysis of a chain of 16 sites might really have been enough.

The solvable $s=\frac{3}{2}$ honeycomb-lattice model of Refs. 4 and 6 provides an example of the strong-coupling phase with a unique ground state and (presumably) a gap.

Most interesting is the possibility of experimentally observing the strong-coupling phase in a quasi-two-dimensional (or three-dimensional) antiferromagnet. Nature restricts us, more or less, to pure nearest-neighbor Heisenberg Hamiltonians. The powerful results of Dyson, Lieb, and Simon[7] show that the critical value of s is less than one. It may be less than $\frac{1}{2}$ also, meaning that even the $s=\frac{1}{2}$ case is Néel ordered. This could depend on lattice type, of course. The $s=\frac{1}{2}$ square lattice is subject to the LSM theorem and so should have a broken translational symmetry or zero gap in the strong-coupling phase. We might expect quantum fluctuations to be even stronger for the $s=\frac{1}{2}$ honeycomb lattice, since the number of nearest neighbors is only three. For this case the strong-coupling phase may have a unique ground state with a gap.

Let us summarize the situation for the triangular lattice antiferromagnets. A tripartite magnetically ordered state is a possibility. The Dyson, Lieb, Simon theorem[7] has not been extended to tripartite lattices, so no rigorous results are known on this ordered state. The σ-model mapping could presumably be carried out, and one would expect order for sufficiently large spin, and disordered phases for small enough spin and large enough frustrating second-nearest-neighbor couplings. Since the LSM theorem applies for half-odd-integer s, the strong-coupling phase should have either broken translational symmetry or vanishing gap in this case. An interesting variational ground-state wave function for the $s=\frac{1}{2}$ triangular case was recently discussed by Kalmeyer and Laughlin,[21] based on Laughlin's fractional quantum Hall effect wave function.[22] They used a boson representation for the spin variables with an infinite hard-core repulsion. An empty or occupied site corresponds to $S_z=-\frac{1}{2}$ or $\frac{1}{2}$, respectively. In the boson representation, U becomes

$$U=\exp\left[i(2\pi/L)\sum_j x_j\right] .$$

The energy is $O(M/L)$ as can be seen by applying U to the boson hopping term, representing the S^+S^- couplings. Under a translation by one site, each x_j is increased by 1 (or decreased by $L-1$ if $x=L$). The total number of bosons is $LM/2$ so $U\rightarrow -U$ for M odd. Thus this excited state has momentum $(\pi,0)$ relative to the ground state.

The CuO_2 planes in La_2CuO_4 (and also in $YBa_2Cu_3O_x$ for some values of x) are probably well described by the

Heisenberg model. An orthorhombic distortion of the lattice has been observed.[23] However, apparently the square Cu plaquettes of the tetragonal phase are simply tilted into a rhombus with no breaking of the translational symmetry in the effective two-dimensional Heisenberg model. Néel order has also been observed.[24,25] However, it is not clear if the two-dimensional planes would order at $T=0$ or if the observed ordering is entirely due to interplane coupling. Some experimental observations relevant to this question are presented in Ref. 26. In the latter case the material may be well described by a disordered $s=\frac{1}{2}$ square lattice ground state. The LSM theorem should then imply either broken translational symmetry or vanishing gap. Apparently, no indications of broken translational symmetry *in the effective Heisenberg model* have been observed. If the gap vanishes linearly at discrete points in momentum space, as in a relativistic $(2+1)$-dimensional quantum field theory, then the specific heat would be quadratic at low T. On the other hand, if the gap vanishes linearly on a Fermi surface then the specific heat would be linear at low T.

Note added in proof. Since submitting this paper, we have received a number of related preprints. Experimental[27] and theoretical[28] evidence that the two-dimensional square lattice $s=\frac{1}{2}$ Heisenberg model Néel orders at $T=0$ has been given. The effects of the Hopf invariant in the σ-model representation of the large-s limit of half-integers s antiferromagnets have been discussed.[29]

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