Spontaneous Symmetry Breaking in Quantum Frustrated Antiferromagnets

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We show that the spontaneous symmetry breaking mechanism in quantum antiferromagnets is due to the collapse, in the thermodynamical limit, of an infinite set of excited states onto the ground state. We characterize both the nature and the scaling of the relevant tower of states for the quantum antiferromagnet on the triangular lattice. Comparison with recent numerical results for the $S = 1/2$ case gives strong support for the existence of long range order in this system.

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Despite many theoretical and numerical studies, the nature of the order of the 2D quantum $S = 1/2$ antiferromagnetic Heisenberg model on the triangular lattice (AFT model) at $T = 0$ is still very much debated. Whereas various exotic states have been proposed [1–4], results from renormalization group and large-N expansion conclude stability of the semiclassical Néel ground state for a sufficiently large value of the spin S [5,6]. This conclusion is highly questionable for finite value of S and in particular for $S = 1/2$ because of strong frustration effects in this system. In fact one must have recourse to numerical methods and the only known results for $S = 1/2$, obtained by exact diagonalization on finite lattices, have led to contradictory conclusions when extrapolated to the thermodynamical limit [7–9]. Thus there is up to now no definitive conclusion about the existence of long range order in the $S = 1/2$ AFT model. The main problem is to understand—and thus to characterize—the mechanism of spontaneous symmetry breaking (SSB) that occurs in the thermodynamical limit. The difficulty lies in the fact that for any finite size antiferromagnetic system, the ground state, contrary to ferromagnets, is believed to be a singlet, rotationally invariant, and nondegenerate. Anderson was the first to point out that the SSB mechanism involves in fact a whole tower of low-lying excited states that collapse, in the infinite volume limit, onto the ground state [10]. Since these states are in general not rotationally invariant, they can sum up to a nontrivial state in which the spins point in a definite direction with a Néel-like order. For large systems, this state can persist a very long time and justifies the usual semiclassical picture of SSB. Thus to be able to conclude about SSB in antiferromagnets from finite size data, one needs not only reliable predictions for the leading scaling behavior of ground state quantities but also to characterize the nature and the scaling of the low-lying excited states responsible for SSB. To this end, we need the effective theory that describes the low energy sector of the original Heisenberg model and which, contrary to the semiclassical spin wave theory, preserves rotational symmetry. We derive this theory in the large S limit, keeping in mind that renormalization group arguments will allow us to extend our results to finite values of the spin S.

The quantum tops model.—The Hamiltonian of the quantum AFT model for N^2 spins is

$$H = J \sum_{\langle x,y\rangle} \mathbf{S}(x)\cdot\mathbf{S}(y)\,, \tag{1}$$

where $J > 0$, $\mathbf{S}^2 = S(S+1)$, and $[S^i(x), S^j(y)] = i\delta_{xy}\epsilon^{ijk}S^k(x)$. The sum in (1) is performed over all nearest neighbors of the triangular lattice.

The Hamiltonian (1) is invariant under both the action of the usual O(3) group of spin rotations and of the discrete C_{3v} group of the triangular lattice. Accordingly, the system can be split into three sublattices with spins $\mathbf{S}_1, \mathbf{S}_2$, and $\mathbf{S}_3$, defined on each triangular elementary cell.

We now introduce on each cell the following fields:

$$\begin{aligned} \mathbf{J} &= \mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3\,,\\ \boldsymbol{\phi}_1 &= \frac{3}{\sqrt{2}S}\left[-\frac{\sqrt{3}+1}{2}\mathbf{S}_1 + \frac{\sqrt{3}-1}{2}\mathbf{S}_2 + \mathbf{S}_3\right],\\ \boldsymbol{\phi}_2 &= \frac{3}{\sqrt{2}S}\left[\frac{\sqrt{3}-1}{2}\mathbf{S}_1 - \frac{\sqrt{3}+1}{2}\mathbf{S}_2 + \mathbf{S}_3\right],\\ \boldsymbol{\phi}_3 &= \boldsymbol{\phi}_1 \wedge \boldsymbol{\phi}_2\,, \end{aligned} \tag{2}$$

such that $\mathbf{J}$ and the "staggered magnetization" $(\boldsymbol{\phi}_1, \boldsymbol{\phi}_2)$ span the unit and two-dimensional irreducible representations of C_{3v}.

Classically, $\mathbf{J}$ has a vanishing expectation value in the ground state which leads to the well-known 120° structure. In this case $(\boldsymbol{\phi}_1, \boldsymbol{\phi}_2, \boldsymbol{\phi}_3)$ is an orthonormal frame, i.e., a rigid body, and is taken as the order parameter. Furthermore, it can be shown that, in the long distance limit, the classical AFT model is equivalent to a system of interacting symmetric tops, the symmetry of the tops being a consequence of the original C_{3v} invariance of (1). It is then natural to expect that, when S is sufficiently large, the low energy effective Hamiltonian for the quantum AFT model will be that of quantum symmetric tops.

Quantum mechanically, the components of $\mathbf{J}$ on a fixed orthonormal basis $\mathbf{x}^i$, $J_L^i = \mathbf{J} \cdot \mathbf{x}^i$, $i = 1,2,3$, act as generators of O(3) left rotations:

$$[J_L^i, J_L^j] = i\epsilon^{ijk} J_L^k \ , \ \ [J_L^i, \phi_a^j] = i\epsilon^{ijk}\phi_a^k, \ \ a = 1,2,3 \ . \tag{3}$$

The commutators and the products of the ϕ_a^i's are less trivial but they simplify in the large S limit to

$$[\boldsymbol{\phi}_a^i, \boldsymbol{\phi}_b^j] = O(J/S), \quad \boldsymbol{\phi}_a \cdot \boldsymbol{\phi}_b = \delta_{ab} + O(J/S) \ . \tag{4}$$

To go further, we need the components of $\mathbf{J}$ with respect to the $\boldsymbol{\phi}_a$'s, $J_{aR} = \mathbf{J} \cdot \boldsymbol{\phi}_a$ which in the large S limit obey the commutation relations

$$\begin{aligned} [J_{aR}, J_{bR}] &= -i\epsilon_{abc} J_{cR} + O(J/S) \ , \\ [J_{aR}, \phi_b^i] &= -i\epsilon_{abc}\phi_c^i + O(J/S) \ . \end{aligned} \tag{5}$$

We see that the J_{aR}'s act as generators of O(3) right rotations that mixes the $\boldsymbol{\phi}_a$'s together. When $J \ll S$, the commutators (3) to (5) become exact and we recognize the algebra of a quantum top.

The low energy, long distance effective Hamiltonian of (1) is now obtained, as usual, by taking the continuum limit. Substituting in (1) the spin operators by their expression in terms of $\mathbf{J}$ and $(\boldsymbol{\phi}_1, \boldsymbol{\phi}_2, \boldsymbol{\phi}_3)$, we obtain the following Hamiltonian when $S \gg 1$ [11]:

$$H_N(x) = \int_{N^2} d^2x \left[\frac{1}{2\chi_1} \mathbf{J}^2(x) + \left(\frac{1}{2\chi_3} - \frac{1}{2\chi_1} \right) J_{3R}^2(x) + p_1\{[\nabla\boldsymbol{\phi}_1(x)]^2 + [\nabla\boldsymbol{\phi}_2(x)]^2\} + p_3[\nabla\boldsymbol{\phi}_3(x)]^2 \right] . \tag{6}$$

H_N is the Hamiltonian of N^2 quantum symmetric tops with principal axes $\boldsymbol{\phi}_1(x)$, $\boldsymbol{\phi}_2(x)$, and $\boldsymbol{\phi}_3(x)$ and angular momentum $\mathbf{J}(\mathbf{x})$. In Eq. (6), (χ_1, χ_1, χ_3) are the principal inertia momenta of the tops, and $(p_1, p_1, p_3) \propto S^2$ are stiffness constants. In addition to the global rotational O(3) symmetry, Hamiltonian (6) is invariant under the action of the O(2) right group generated by $J_{3RN} = \int_{N^2} J_3(x)$. This O(2) invariance reflects the original C_{3v} symmetry of the triangular lattice. Its continuous character is an artifact of the continuous limit.

The quantum phase transition.—Let us now qualitatively discuss the behavior of this system according to the values of the coupling constants entering in (6). When $p\chi$ is small, we expect that, at large scale the tops are almost decoupled. At these scales, the system consists in independent tops with inertia momenta of order $1+O(1/N)$. There is a gap in the spectrum and no symmetry breaking. For sufficiently large value of $p\chi$, the individual tops are tightly bound so that, at large scale, the whole system behaves as a single top with effective inertia momentum $\propto N^2$. Therefore there is no gap and the system exhibits long range order. Since we expect a phase transition between these two regimes, there should exist, in the Heisenberg system, a critical value S_c above which it is ordered.

To investigate this quantum phase transition we need the partition function $Z_N = \mathrm{Tr}(\exp -\beta H_N)$ in the limit where $\beta \to \infty$. As usual, Z_N can be expressed as a functional integral:

$$Z_N = \int DR(x,\tau) e^{-S_{N,\beta}} \tag{7}$$

with

$$S_{N,\beta} = -\frac{1}{2} \int_0^\beta d\tau \int_{N^2} d^2x \{ \mathrm{Tr}[P_0(R^{-1}\partial_0 R)^2 + P_\perp (R^{-1}\partial_i R)^2] \}. \tag{8}$$

which is the action of the O(3)$\otimes$O(2)/O(2) quantum nonlinear sigma (NLσ) model [5,12]. In Eqs. (7) and (8), $R(x,\tau) = (\boldsymbol{\phi}_1, \boldsymbol{\phi}_2, \boldsymbol{\phi}_3)$ is a SO(3) matrix; $\partial_\mu = (\partial_0, \partial_i) = (\partial/\partial\tau, \partial/\partial x_i)$; $i = 1,2$; and $P_\mu = \mathrm{diag}(p_{1\mu}, p_{1\mu}, p_{3\mu})$, $\mu = 0, \perp$ are diagonal matrices which contain the coupling constants. Whereas the $p_\perp$'s can be identified with the stiffness constants appearing in (6), the p_0's are related to the inertia momenta by $\chi_a = -\mathrm{Tr}(P_0 T_a^2)$ where $T_a \in \mathrm{Lie[SO(3)]}$. When β and N go to infinity there is a phase transition as one varies the P_μ's. The recursion equations for these parameters have been given in [5]. They admit a nontrivial ultraviolet fixed point, P_μ^*. The critical surface associated to this fixed point divides a disordered phase, at small S, from an ordered phase with SSB at large S. In this Néel phase, action (8) describes three interacting massless modes (spin waves) with bare velocities $c_1 = c_2 = \sqrt{(p_{1\perp} + p_{3\perp})/\chi_1}$, $c_3 = \sqrt{2p_{1\perp}/\chi_3}$. Their low energy physics is governed by the trivial infrared fixed point at $S = \infty$ so that they are infrared free. At long distance the spin wave spectrum is $\omega_a = \bar{c}_a k, a = 1,2,3$, where the $\bar{c}_a$'s are the velocities renormalized by quantum fluctuations. It is important to notice that in the spin wave phase all models with $S > S_c$ have the same long distance behavior governed by the infrared fixed point at $S = \infty$. This justifies *a* *posteriori* the large S limit used in (6) for all systems with $S > S_c$.

The tower of states and the spontaneous symmetry breaking.—Since one is not able to calculate precisely S_c for the AFT model (6), the relevant question is to characterize the low-lying spectrum of (1) that should be observed in finite systems when there is SSB in the thermodynamical limit. We want therefore the effective Hamiltonian for the *first* excited states. It is convenient to work with the path-integral formulation of the theory. The idea is to integrate out in (8) the spatial degrees of freedom, i.e., the $k \neq 0$ modes, to obtain an effective action at the scale N for the $k = 0$ mode. From this action follows the one body effective Hamiltonian. To do this we split up the field $R(x,\tau)$ in (8) into $R_0(\tau)\exp\phi(x,\tau)$ where $R_0(\tau)$ and $\phi(x,\tau)$ represent the $k = 0$ and $k \neq 0$ modes, respectively. By expanding R to order ϕ^2 and by integrating out ϕ in (8), we find, after some algebra, at leading order in N the Hamiltonian of a single symmetric top:

$$H_{\text{eff}}(N) = E_{0N} + \frac{1}{N^2}\left[\frac{\mathbf{J}_N^2}{2\chi_1(N)} + \left(\frac{1}{2\chi_3(N)} - \frac{1}{2\chi_1(N)}\right)(J_{3RN})^2\right] , \tag{9}$$

where

$$E_{0N} = \frac{1}{2}[c_3(N) + 2c_1(N)] \sum k \tag{10}$$

is the leading quantum correction to the classical ground state energy. The Hamiltonian (9) describes the angular part of the fluctuations of the total order parameter $\boldsymbol{\phi}_{aN} = \int_{N^2} \boldsymbol{\phi}_a(x)$, $a = 1,2,3$, whose modulus is equal, at leading order in N, to its infinite volume limit. $\mathbf{J}_N$ and J_{3RN} are respectively the total angular momentum and its projection on the symmetric axis $\boldsymbol{\phi}_{3N}$. Finally, $c_a(N)$ and $\chi_a(N)$, $a = 1,2,3$, are the renormalized values of the spin wave velocities and inertia momenta at scale N. We are now in a position to discuss the properties of the tower of states according to the spin S.

When the system has long range order, i.e., when $S > S_c$, both $c_a(N)$ and $\chi_a(N)$ have finite limits, $\overline{c}_a$ and $\overline{\chi}_a$, when $N \to \infty$. The energy of the first excited states of (6) is

$$E_{j,m_L,m_R} = E_{0N} + \frac{1}{N^2}\left[\frac{j(j+1)}{2\overline{\chi}_1} + \left(\frac{1}{2\overline{\chi}_3} - \frac{1}{2\overline{\chi}_1}\right) m_R^2\right] , \tag{11}$$

where $j(j+1), m_L$, and m_R are the eigenvalues of $\mathbf{J}_N^2$, J_{ZN}, and J_{3RN}, respectively. For each value of j, there are $(2j+1)^2$ eigenstates with degeneracy $2(2j+1)$. Apart from these states, the other low energy modes of (6) have $k \neq 0$ and are the first magnon states which scale as $1/N$. Thus, there are $j_{\max} \sim \sqrt{N}$ states in (11) that collapse onto the ground state, when $N \to \infty$, faster than the first magnons and which define the relevant tower of states. With these states one can form the symmetry breaking Néel state in which the order parameter has a nonzero mean value with an uncertainty of order $\sim 1/\sqrt{N}$. Of course, this state being not an eigenvector of (11) has a finite lifetime of order $\sim \sqrt{N}$. Because of the long range order, the system develops a macroscopic collective variable with a "mass" of order N^2 which is localized in the infinite volume limit.

At the critical point $S = S_c$, the system becomes Lorentz invariant when $N \to \infty$: $c_a(N) \to c^*$ [5]. In addition we have $\chi_a(N) \to \chi^*/N$ as follows from simple dimensional analysis. The predicted scaling for the tower of state changes drastically:

$$E_{j,m_L,m_R} = E_{0N} + \frac{1}{N}\frac{j(j+1)}{2\chi^*} . \tag{12}$$

At this point the tower of states collapses onto the ground state *together* with the first magnon states. This is completely consistent with the fact that the theory is critical. This result is independent of the space dimension.

To complete our discussion, we need the leading finite size corrections for the ground state observables: e_N, the total energy per spin, and the mean value of the total order parameter $(\boldsymbol{\phi}_{1N}, \boldsymbol{\phi}_{2N}, \boldsymbol{\phi}_{3N})$. We find for the ground state energy

$$e_N = e_\infty - \frac{\delta}{2N^3}(\overline{c}_3 + 2\overline{c}_1) , \tag{13}$$

where δ is a numerical constant which depends on lattice. As discussed above, the order parameter is the rotation matrix $R(x,\tau) = (\boldsymbol{\phi}_1, \boldsymbol{\phi}_2, \boldsymbol{\phi}_3)$. As a consequence of the O(2) right symmetry the fields $\boldsymbol{\phi}_1$ and $\boldsymbol{\phi}_2$ renormalize with the same constant and we have $\langle(\boldsymbol{\phi}_{1N})^2\rangle = \langle(\boldsymbol{\phi}_{2N})^2\rangle = M_N^2$ while $\langle(\boldsymbol{\phi}_{3N})^2\rangle = \kappa_N^2$. We find for the leading finite size correction of M_N and κ_N

$$M_N = M_\infty\left(1 - \frac{\gamma}{2N}\left[\frac{1}{\overline{\chi}_1\overline{c}_1} + \frac{1}{\overline{\chi}_3\overline{c}_3}\right]\right) , \tag{14}$$

$$\kappa_N = \kappa_\infty\left(1 - \frac{\gamma}{N\overline{\chi}_1\overline{c}_1}\right) , \tag{15}$$

where γ depends on the lattice.

While the scaling given by Eqs. (13), (14), and (15) constitutes the standard test for long range order in the ground state, the observation of the tower of state (11) with the predicted degeneracy and scaling provides a test which involves a *whole set* of low lying excited states. Since it is deeply related to the mechanism of SSB, it constitutes a richer and more effective test for long range order.

Let us now return to the $S = 1/2$ AFT model. From Eqs. (2) we identify M_N in (14) with the sublattice magnetization and κ_N in (15) with the helicity operator as defined for example in [13]. Numerical results obtained for the ground state quantities e_N, M_N, and κ_N for different lattices up to 27 sites have led to contradictory conclusions [7–9]. Very recently, extended numerical results have been obtained by exact diagonalization on lattices up to 36 sites [14]. The authors have identified a whole set of low lying excited states that constitute the tower of state (11) but they did not observe the correct degeneracy associated to a symmetric top. This is probably due to the small size of the sample. However, they found $(2j+1)^2$ states for each value of the spin j and the predicted scaling $\sim 1/N^2$ for SSB as given by (11). This rules out the possibility that the $S = 1/2$ AFT model is at a critical point as it was suggested in [15] and gives strong support for the existence of a Néel ground state in the thermodynamical limit.

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