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Symmetry breaking and finite size scaling in antiferromagnets

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Résumé. — Nous montrons que l'analyse du comportement à taille finie du modèle sigma non linéaire quantique O(3)/O(2) adapté aux antiferromagnétiques justifie l'existence d'une tour d'états excités proposée pour la première fois par Anderson pour expliquer la brisure de symétrie des antiferromagnétiques quantiques dans la limite thermodynamique. Nous donnons également les formules de taille finie pour l'énergie du fondamental et pour la valeur moyenne dans le vide du paramètre d'ordre.

Abstract. — We show that the finite size scaling analysis of the quantum non linear sigma model O(3)/O(2) associated with antiferromagnets justifies the existence of the tower of excited states first proposed by Anderson to explain the symmetry breaking of quantum antiferromagnets in the thermodynamical limit. Finite size formulas for the ground state energy and for the ground state expectation value of the order parameter are explicitly given.

1. Introduction.

The most famous model for discussing the Spontaneous Symmetry Breaking (SSB) mechanism in condensed matter physics is the ferromagnetic Heisenberg model. However, ferromagnetism is almost unique since the order parameter is a constant of the motion. As a consequence, the ground state is exactly known and is rotationally degenerate: it coincides with the classical vacuum. In the ferromagnetic state, the symmetry is spontaneously broken by choosing a particular ground state among the set of degenerate ones.

In the antiferromagnetic model on the square lattice, the order parameter is not a constant of the motion. For any value N^d of the number of spins, the ground state is non degenerate and

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is a singlet for the rotation group. In the thermodynamical limit, there is long range order in the ground state for $S \geq 1$ [1, 2], a result which is believed to hold even for spin one half [3]. In quantum systems, the fact that there is long range order does not necessarily imply that there is symmetry breaking with a non vanishing expectation value of the order parameter. However, in antiferromagnets, we expect the rotational symmetry to be broken in a "semi-classical" Néel state. In contrast with ferromagnets, it could seem difficult to understand how there can be SSB when the ground state is non-degenerate. However, it has been recognized for many years by Anderson that the symmetry breaking mechanism involves a whole tower of low-lying excited states that should collapse, in the infinite volume limit, onto the true ground state of the theory [4]. Since these states are not in general rotationally invariant, nothing prevents that some combination of them, which for large N will persit a very long time, explicitly breaks rotational symmetry. The relevance of the tower of state has recently received renewed interest in discussing symmetry breaking in exact diagonalizations of finite systems [5].

This picture is not particular to antiferromagnets but is common to many other quantum systems which have a non conserved order parameter. As a prototypical example is the quantum lattice rotator model. This model turns out to be equivalent, when there is long range order, to the antiferromagnetic Heisenberg model, provided one is concerned with the lowest part of the spectrum [3]. One may thus learn about the SSB mechanism in antiferromagnets by studying that of the rotator model. The advantage of the latter model is that since it possesses a classical counterpart with a well defined Lagrangian, its quantization *via* the functional integral is straightforward. Therefore, the SSB mechanism can be investigated by the standard methods of relativistic quantum field theory.

In this paper we obtain the low energy spectrum of antiferromagnets which follows from a finite size scaling analysis of the non linear sigma model O(3)/O(2) which is the field theory associated with the rotator model. More precisely, as our principal result, we confirm the existence of a tower of state which contains a large number of finite dimensional representations of the total angular momentum that collapse onto the ground state as $1/N^2$ when there is SSB in the thermodynamical limit. In addition, we give the finite size scaling for both the ground state energy and the ground state expectation value of the order parameter which can be compared with numerical computations.

2. The quantum lattice rotator model.

It has been shown that when the net magnetization vanishes, the long distance physics of antiferromagnets with local Néel correlations is described by the O(3)/O(2) quantum non linear sigma (NLσ) model [3]. Let us recall that this field theory is only obtained by means of coherent spin states which makes its derivation non trivial [6]. On the other hand, the rotator model gives a natural way to cast the partition function into a functional integral. The lattice regularized version of the NLσ model is therefore that of quantum rotators interacting with nearest neighbour interaction. A way to understand this result is to imagine that after a sufficiently large number of iterations of some Renormalization Group transformation (by blocking, say) the Heisenberg system becomes equivalent, at some scale Λ^{-1}, to N^d quantum rotators with Hamiltonian in spatial dimension d:

$$H_N = \frac{1}{2}\,\Lambda^{-d}\left[\sum_x \frac{L(x)^2}{\chi\Lambda^{-2d}} + \rho\sum_{x,\mu}|\delta_\mu\Omega(x)|^2\right]\,, \tag{1}$$

where Ω is the orientation of a rotator and where $L(x)$ and χ are its angular and inertia momenta. Finally, ρ is a stiffness constant. On a Bravais lattice with basis n_μ, $\mu = (1,..,d)$, the expression for the potential term reads:

$$|\delta_\mu \Omega(x)|^2 = \Lambda^2 \ |\Omega(x + n_\mu \Lambda^{-1}) - \Omega(x)|^2 \tag{2}$$

Note that Λ^{-1} is the lattice spacing of the rotator model which is not simply related to the lattice constant of the Heisenberg model. The total angular momentum $L_{\rm T} = \sum_x L(x)$ commutes with Hamiltonian (1) and is a constant of the motion, a fact which is reminiscent of rotational invariance. From the classical point of view, the ground state of (1) is obtained with $L_{\rm T} = 0$ and $\Omega(x) = \Omega_0$ and is degenerate. However, since the order parameter $\Omega_{\rm T} = N^{-d}\sum_x \Omega(x)$ does not commute with H_N and is not a conserved quantity, these classical states are not stable under quantum corrections. The true quantum ground state of (1) is of a totally different nature: it is non degenerate and rotationally invariant [4]. As is the case for the antiferromagnetic Heisenberg model, it is thus difficult to imagine how the rotational symmetry can be broken.

However, as is well known, one expects that for suitable values of the parameters entering in (1), the rotational symmetry will be broken in the $N \rightarrow \infty$ limit. Arguments leading to the above conclusion rely on the mechanism of SSB which is familiar to quantum field theoreticians. In the infinite volume limit, the symmetry is broken at the classical level by choosing a particular classical ground state. Quantum corrections are then taken into account in a semi-classical loopwise expansion of the O(3)/O(2) NLσ model. Then, depending on the values of the couplings and on the dimension d, the semi-classical ground state may retain its symmetry breaking nature or not. In real systems, large but finite, this semi-classical SSB mechanism does not give an intuitive insight into the mechanism that, at the quantum level, allows the symmetry to be broken.

Let us see qualitatively what we expect to happen. Consider Hamiltonian (1). When $\rho\chi$ is small, we expect that, at any scale larger that some finite value ξ, the rotators will be decoupled. The effective Hamiltonian will consist in $\sim (N\Lambda^{-1}/\xi)^d$ independent rotators with an inertia of order $1 + O(1/N)$. Thus, there will be a gap in the spectrum and no symmetry breaking. However, for a sufficiently large value of $\rho\chi$, the individual rotators are tightly bounded so that, at large scale, the whole system behaves as a single rotator with effective inertia $\chi_{\rm eff} \propto N^d$. Therefore, the system will be described by the effective Hamiltonian:

$$H_{\rm eff} = E_{0N} + 1/2 \ \frac{L_{\rm T}^2}{\chi_{\rm eff}} \tag{3}$$

It describes the angular part of the fluctuations of $\Omega_{\rm T}$, whose modulus is equal, at leading order in N, to some field renormalization $Z^{1/2}$. With the eigenstates of (3), we can form a continuous set of rotationally degenerate semiclassical wave packets:

$$|\varphi_N> = \sum_{l,m} c_{lm} |l, m> \ , \tag{4}$$

in which $\Omega_{\rm T}$ has a definite orientation. Of course, these states are not eingenstates of (1) but in the infinite volume limit they will be (quasi) degenerate with the true ground state of the theory, and one may expect that any infinitesimal symmetry breaking perturbation localizes the system into one of these states. It is important to notice that for such a phenomenon to occur, it is necessary that there exists a whole tower of states which contains, when $N \rightarrow \infty$, an infinite number of finite dimensional representations of the rotation group in order to fix the orientation of $\Omega_{\rm T}$ with no uncertainty.

As seen, the possibility of SSB in the $N \rightarrow \infty$ limit relies on the properties on the low-lying spectrum of Hamiltonian (1) for a large but finite system. In the following, we shall investigate the finite size properties of (1) by means of the NLσ model.

3. The quantum non linear sigma model.

Finite temperature and ground state properties of the rotator model can be investigated by means of the imaginary time Feynman path integral. Correlation functions and thermodynamical quantities can be evaluated by functional averaging with Boltzmann weight $\omega_N = e^{-S_N}$ where S_N is the Euclidean action associated with Hamiltonian (1):

$$S_N = \frac{1}{2}\,\Lambda^{-d} \int_0^{\beta} d\tau \left[\chi \sum_x \left|\frac{\partial \Omega}{\partial \tau}\right|^2 + \rho \sum_{x,\mu} |\delta_\mu \Omega|^2 \right] \tag{5}$$

Now $\Omega\,(x,\tau)$ is a classical variable subject to the constraint $|\Omega|^2 = 1$. Action (5) is nothing but a lattice regularization of the O(3)/O(2) NLσ model in $d+1$ dimensions. This theory is renormalizable in a double expansion in $\epsilon = d-1$ and in the coupling constant. We thus expect that the long distance, long wavelength properties of (5) are described by the continuous O(3)/O(2) NLσ model with action:

$$S = \frac{\rho}{2c} \int_0^{\beta c} dt \int_{L^d} d^d x \ \left[\, |\partial_t \Omega|^2 + |\partial_\mu \Omega(x)|^2 \right] \ , \tag{6}$$

where we have rescaled the time dimension with the dimensionful spin wave velocity $c = \sqrt{\rho/\chi}$ and where the linear size of the system is $L = N\Lambda^{-1}$ When β and N goes to infinity, the latter model is known to have a phase transition, analogous to that of the $d+1$ classical ferromagnet, from disordered to ordered phase with SSB characterized by $< \Omega(x,\tau) >= Z^{1/2}\hat{\Omega}_0$, where $\hat{\Omega}_0$ is some unit vector and $Z < 1$. Therefore, for suitable values of the coupling ρ/c, and for $d > 1$, there is SSB for the rotator model (1) at zero temperature when $N \to \infty$. In this phase, according to the Goldstone theorem, there are two massless modes, with a long wavelength relativistic spectrum $\omega_k = ck$. Being granted that there exist parameters for which there is SSB when $N \to \infty$ one can investigate the finite size properties of (1) in this regime by means of the field theory (5).

3.1 RENORMALIZATION. — The renormalization group properties of (5) or equivalently of (6) stem only from the ultraviolet or short distance behaviour. They are insensitive to the presence of the infrared cut-off L or βc. The one loop recursion relation for the coupling entering (6) is [3]:

$$\frac{\partial g}{\partial \lambda} = (1-d)g + g^2 \frac{K_d}{2} \ , \tag{7}$$

where $g = (c/\rho)\Lambda^{d-1}$ is the dimensionless coupling and $K_d^{-1} = 2^{d-1}\pi^{d/2}\Gamma(d/2)$. The spin wave velocity does not renormalize, as is the case for both L and βc. The scaling equations for the dimensionless "slab thicknesses" in both space and "time" directions, N and $T = \beta c \Lambda^{-1}$, are trivial since they follow from dimensional analysis:

$$\frac{\partial N}{\partial \lambda} = -N \tag{8}$$

$$\frac{\partial T}{\partial \lambda} = -T. \tag{9}$$

At T and N equal to infinity, apart from the $g = 0$ fixed point, there is a nontrivial fixed point $g = g^* = 2(d-1)/K_d$ for $d > 1$ which governs the phase transition from an ordered phase at small g to a quantum disordered phase for larger $g > g^*$.

Equation (7) has solution with:

$$g(\lambda) = \frac{g_0 \mathrm{e}^{-(d-1)\lambda}}{1 - \frac{g_0}{g^*}(1 - \mathrm{e}^{-(d-1)\lambda})}, \tag{10}$$

where g_0 is the value of the coupling at the scale of the lattice spacing Λ^{-1} The last equation defines three regimes for the asymptotic large λ behaviour:

-when $g_0 < g^*$, $g(\lambda)$ behaves as $g(\lambda) = \mathrm{e}^{-(d-1)\lambda} g_0/(1 - g_0/g^*) + O(\mathrm{e}^{-2(d-1)\lambda})$ as λ is very large. As seen, $g(\lambda)$ flows toward the trivial infrared fixed point $g = 0$ which ensures the existence of a well defined spin wave phase with long wavelength renormalized coupling:

$$\left(\frac{\rho}{c}\right)_{\mathrm{R}} = \Lambda^{d-1} \lim_{\lambda \to \infty} \frac{\mathrm{e}^{(1-d)\lambda}}{g(\lambda)} \tag{11}$$

In two dimensions, this defines the Josephson correlation length:

$$\xi_{\mathrm{J}} = \left(\frac{c}{\rho}\right)_{\mathrm{R}}, \tag{12}$$

that separates the long-distance spin wave behaviour from the critical regime.

-When $g_0 = g^*$, the system is scale invariant and we have of course $g(\lambda) = g^*$.

-Finally, for $g_0 > g^*$, there exists a length scale $\mathrm{e}^{\lambda_{\max}} = ((g_0 - g^*)/g_0)^{-1/(d-1)}$ above which the recursion equation (7) ceases to be satisfied. This defines the correlation length in the disordered phase: $\xi \sim \Lambda^{-1} \mathrm{e}^{\lambda_{\max}}$ For length scale λ such that $1 \ll \lambda \ll \lambda_{\max}$ the system is critical and we have $g(\lambda) \sim g_0$ as long as λ is not too large.

4. Finite size scaling.

4.1 THE TOWER OF STATE. — We now consider a finite lattice with $1 \ll N \ll \beta$. Starting with action (5), one can integrate out all the spatial degrees of freedom until one arrives at an effective one dimensional action S_{eff}. Clearly, we end up with a quantum mechanical effective problem with effective Hamiltonian describing the lowest part of the spectrum of (1). We expect of course that this effective Hamiltonian is given by (3) when $g_o < g^*$. To this end one has to iterate the recursion relations $\lambda \sim \ln N$ times until the spatial part of (5, 6) vanishes. Since the theory is renormalizable, we should end up with an effective one-dimensional action of the same form as the time dependent part of (5) and hence with a one-body quantum rotator model. Let us do this at one loop order.

In order to integrate out the spatial degrees of freedom, it is convenient to introduce the following decomposition for the fluctuations: $\Omega(x,t) = R(x,t)\Omega(t)$ where $R(x,t)$ is in the coset O(3)/O(2). We have, $R(x,t) = \exp(t_a \zeta^a(x,t))$ where the t_a's are generators in LieO(3) - LieO(2) and the fields $\zeta^a(x,t)$ are subject to the constraint: $\int_{L^d} \mathrm{d}^d x \;\; \zeta^a(x,t) = 0$ in order that the Fourier components $\zeta^a(k,\omega)$ do not contain the quantum mechanical mode $k = 0$. Expanding R to order ζ^2 and integrating over ζ in (5), we obtain at leading order in N:

$$S_{\mathrm{eff}} = \beta c \Lambda \sum_k \sqrt{\Delta_0(k)} + \frac{1}{2} (\Lambda L)^d \left(\frac{N^{1-d}}{\Lambda c g(\ln N)}\right) \int_0^\beta dt \left|\frac{\partial \Omega}{\partial t}\right|^2, \tag{13}$$

where $g(\ln N)$ is the dimensionless coupling, solution of the scaling equation (7) at scale $\lambda = \ln N$. In the first term of (13), which is the one loop quantum correction to the classical ground state energy, $\Delta_0(k)$ is the inverse lattice bare propagator. On the square lattice $\Delta_0(k) = 2(2 - \sum_\mu \cos k_\mu n_\mu)$, the sum being performed over the first Brillouin zone of the lattice.

Action (13) defines the effective quantum Hamiltonian H_{eff} of Equation (3) with:

$$E_{0N} = c\Lambda \sum_k \sqrt{\Delta_0(k)}\,, \tag{14}$$

and

$$\chi_{\text{eff}} = (\Lambda L)^d \left(\frac{N^{1-d}}{\Lambda c g(\ln N)}\right) \tag{15}$$

One may wonder how equations (14) and (15) are modified by the inclusion of higher order loop corrections. For χ_{eff}, since the theory is renormalizable, these corrections only affect, to leading order in $1/N$, the scaling equation (10) that defines $g(\lambda)$ and therefore the value of the physical renormalized parameter $(\rho/c)_{\text{R}}$. On the other hand, while our one loop calculation cannot calculate the exact value for the ground state energy per spin, e_N, the difference $\delta_N = e_\infty - e_N$ is given at the leading order in $1/N$ by the one loop result:

$$\delta_N = \Lambda c \left(\int \frac{\mathrm{d}^d k}{(2\pi)^d} \sqrt{\Delta_0(k)} - \frac{1}{N^d} \sum_k \sqrt{\Delta_0(k)}\right) \tag{16}$$

The reason for this is that the leading $1/N$ behaviour of δ_N depends only on $|\partial\Delta_0(k)/\partial k^2|_{k=0}$, which does not renormalize since c does not renormalize.

We now focus on the $d = 2$ case. Our first finite size formula for the ground state energy is:

$$\delta_N = \Lambda c \, \frac{\delta}{N^3}\,, \tag{17}$$

where δ is a numerical constant which depends on the lattice [7, 8]. On the square lattice we have $\delta = 1.438$.

Let us look now at the asymptotic behaviour for χ_{eff}. Here again we have to distinguish between three cases:

- when $g_0 < g^*$, we have from (11):

$$\chi_{\text{eff}} = \chi_{\text{R}} \, N^2\,, \tag{18}$$

where $\chi_{\text{R}} = \Lambda^{-2}(\rho/c^2)_R$. This is the scaling expected from our qualitative discussion in section 2.

Therefore, the expression of the energy for the first excited states of (1) is:

$$E_{l,m} = E_{0N} + \frac{l(l+1)}{2\chi_{\text{R}} N^2}\,. \tag{19}$$

For $l \leq \sqrt{N}$, the latter equation defines a tower of states that collapses onto the ground state faster than the first magnon states (whose energy scales as $1/N$).

- When $g_0 = g^*$, the system is at its critical point and one has $\chi_{\text{eff}} = N\chi^*$. The predicted scaling for the tower of state is:

$$E_{l,m} = E_{0N} + \frac{l(l+1)}{2\chi^* N} \tag{20}$$

In this case, the tower of state collapses onto the ground state together with the first magnon states since the system is critical. Note that this result is independent of the dimension d.

- Finally, for $g_0 > g^*$, it is tempting to extend our analysis when $N \ll \Lambda\xi$. In this region, one should observe the critical scaling (20) with $\chi^* \rightleftharpoons \chi_0$. However for larger values of N, the low g expansion which is at the basis of (13) fails. We expect that, in this region, the low lying states consist in massive vector like excitations [9].

4.2 THE MAGNETIZATION. — As seen from (13), the first excited states of (1) are described by the effective Hamiltonian (3) that describes the orientation of the order parameter Ω_{T} with wave functions $Y_{lm}(\theta,\phi)$, where θ,ϕ are the polar angles . For $l<\sqrt{N}$, the modulus of Ω_{T} is fixed, at leading order in $1/N$, to a constant value $Z^{1/2}<1$ in the subspace of the tower of state (19) (in fact, for finite N, we may have different values of $Z_{N,l,m}$ in each state (l,m) of the tower of state. However, we expect (but we have no proof) that $Z_{N,l,m}=Z+O(1/\sqrt{N})$). Here $Z^{1/2}$ is the field renormalization constant calculated in the $N\to\infty$ limit of the NLσ model with renormalized coupling (11). It is given by:

$$Z \;=\; \lim_{\beta,N\to\infty} \;<{\Omega_{\mathrm{T}}}^2>_{\beta,N} \;, \tag{21}$$

which is the ground state expectation value of the order parameter. Let us now investigate the finite size scaling of:

$$Z_N \;=\; <{\Omega_{\mathrm{T}}}^2>_{\beta,N} \tag{22}$$

We obtain at one loop order:

$$Z_N \;=\; 1 \;-N^{d-1}g(\ln N)\;\frac{1}{N^d}{\sum_k}' \frac{1}{\sqrt{\Delta_0(k)}}\;, \tag{23}$$

where ${\sum_k}'$ is the sum over the Brillouin zone of the lattice except $k=0$ and $g(\ln N)$ is given again by (7). In dimension $d=2$, when $g_0<g^*$, Z_N has a non vanishing value when $N\to\infty$ given at one loop by:

$$Z \;=\; 1 \;-\xi_{\mathrm{J}}\Lambda\int_0^{2\pi}\frac{\mathrm{d}^2k}{(2\pi)^2}\,\frac{1}{\sqrt{\Delta_0(k)}}\;, \tag{24}$$

where ξ_{J} is given by (12). For finite N, Z_N is known to satisfy the scaling equation [10]:

$$Z_N \;=\; Zf\left(\frac{\xi_{\mathrm{J}}}{N\Lambda^{-1}}\right)\;, \tag{25}$$

where f is a function that can be obtained from the low g perturbative expansion. Using (25) it is easy to obtain:

$$f\left(\frac{\xi_{\mathrm{J}}}{N\Lambda^{-1}}\right) \;=\; 1-\xi_{\mathrm{J}}\Lambda\left[\frac{1}{N^2}{\sum_k}'\frac{1}{\sqrt{\Delta_0(k)}} \;-\int_0^{2\pi}\frac{\mathrm{d}^2k}{(2\pi)^2}\,\frac{1}{\sqrt{\Delta_0(k)}}\right] \tag{26}$$

At leading order in N we have:

$$Z_N \;=\; Z\left(1-\gamma\;\frac{\xi_{\mathrm{J}}\Lambda}{N}\right)\;, \tag{27}$$

where γ depends on the lattice [7] and is given by:

$$\gamma \;=\; \lim_{N\to\infty} N\left(\;\frac{1}{N^2}{\sum_k}'\frac{1}{\sqrt{\Delta_0(k)}} \;-\int_0^{2\pi}\frac{\mathrm{d}^2k}{(2\pi)^2}\,\frac{1}{\sqrt{\Delta_0(k)}}\right) \tag{28}$$

On the square lattice we have: $\gamma=-0.6208$.

5. Symmetry breaking and concluding remarks.

We have shown that, when $g_o < g^*$, there exists a tower of state which contains $l \sim \sqrt{N}$ representations of the rotation group SO(3) and collapses onto the ground state faster than any other excited states. To break the symmetry, the orientation of the order parameter has to be fixed. In a large system, it is possible to superimpose the $\sim \sqrt{N}$ states of the tower of state to obtain a wave packet in which Ω_T has a definite orientation. In this symmetry breaking state, the mean value of Ω_T will be equal to $Z^{1/2}\hat{\Omega}_o + O(1/N)$, where $\hat{\Omega}_o$ is some unit vector, with uncertainty of order $O(1/N)$ [11]. In real systems, large but finite, we are lead to imagine that the environment acts on the system as a perturbation with energy scale T_o of order $1/\chi N^2 \ll T_o \ll c/N$ which mixes the first excited states and allows for SSB. Numerical methods could provide a test for this scenario.

All our finite size formulas may be applied to the non frustrated antiferromagnetic model since its low energy physics is identical to that of the rotator model provided there is sufficiently Néel order. If one sees, by some exact diagonalization method, the tower of state described by (3) with the correct degeneracy and scaling, at least for $l \ll \sqrt{N}$ and if the scalings (18), (19) and (27) are observed one will be able to conclude that there is SSB in the thermodynamical limit. In addition, the long distance spin wave phase will be well described by the non linear σ model with long wavelength renormalized couplings ρ_R and c that can be obtain directly from exact diagonalization methods with the help of (18) and (19). To conclude let us recall that the key ingredient that allowed us to draw a consistent picture of the finite size behaviour of the antiferromagnetic model was the existence of a renormalizable relativistic quantum field theory that describes its low energy physics. The same work can be done on the more controversial frustrated antiferromagnetic model on the triangular lattice. In this case, the long distance physics is expected to be described by a NLσ model with an order parameter in SO(3). We expect that in this case the effective Hamiltonian that describes the tower of state will be that of a quantum symmetric top instead of a rotator [12]. The observation of a corresponding tower of state in exact diagonalization will give evidence for symmetry breaking with Néel order [5].

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