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Broken symmetry in antiferromagnets

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Abstract. We discuss limitations of the conventional 'broken symmetry' picture of the Heisenberg antiferromagnet. The exact results on the ground state of the linear chain and of the three-dimensional Hamiltonian do not show a 'degeneracy of the vacuum'. With the help of a solvable model it is shown that the correlations in the ground state may have the Néel character, as revealed by the neutron experiments, even though the ground state is quite different from the Néel states. There is no Goldstone mode in the linear chain. The spin of the antiferromagnetic spin wave is $\frac{1}{2}$. But the physical states have a doublet of the spin waves which could be regarded as degenerate states of spin 1 and spin 0. The fermionic character is suppressed and the bosonic character revealed, as in the decolouring phenomena in quantum field theory. It is plausible that in the three-dimensional case also there is no Goldstone mode.

Keywords. Broken symmetry; antiferromagnets; ground state; excitation spectrum.

1. Introduction

In the condensed matter problems treated by quantum mechanics, broken symmetry is of common occurrence. The fundamental interaction between the constituent nuclei and electrons is the coulomb interaction, which is rotationally and translationally invariant. But the ground state of a quantum many-particle system often lacks rotational as well as translational invariance. At the lowest temperature most condensed systems form solid crystals which do not possess full continuous translational symmetry or rotational symmetry. Crystals are invariant under discrete translation groups and point groups. A Heisenberg ferromagnet is described by a rotationally invariant Hamiltonian, but the ordered state shows directionality.

The Hamiltonian may have other more sophisticated symmetries like the gauge symmetry, and the ground state may break gauge invariance. The superconductor as well as the superfluid liquid He^4 breaks the gauge symmetry. The superfluid phases of He^3 and liquid crystals display complicated broken symmetry phases. Sophisticated mathematical techniques are currently being explored to tackle the broken symmetry problems. For example, Sen (1978) has proposed to treat He^4 by fibre bundles, the broken symmetry operations acting on the base space of the Hilbert bundle. Mermin (1979) and Michel (1980) have discussed the application of homotopy groups to liquid He^3 and liquid crystals.

Associated with broken symmetry there is the Goldstone mode, an excitation branch that starts with a zero frequency excitation (Goldstone 1961; Lange 1966). Phonons in a solid and spin waves in an isotropic ferromagnet are examples of Goldstone modes. Other examples are given by Anderson (1963) and Wagner (1966). In the symposium celebrating fifty years of Bose Statistics, Sinha (1975) summarized the results on boson excitation modes in condensed systems. In that article he follows the conventional point of view of the broken symmetry in antiferromagnets. Here we would like to discuss the more recent results specifically on antiferromagnets and show that the problem is not yet fully understood.

2. Phenomenology of an antiferromagnet

We consider the Heisenberg Hamiltonian for an antiferromagnet

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{1}$$

The exchange constant J is positive. The spins $\mathbf{S}_i$ are distributed over a lattice. The angular bracket $\langle \quad \rangle$ around i, j indicates that the summation goes over the nearest neighbours in the lattice. For simplicity, we shall restrict our discussion to spin $\frac{1}{2}$ only, $|\mathbf{S}_i| = \frac{1}{2}$. This is the 'extreme quantum' case.

If J were negative, we would have the ferromagnetic situation. The ground state of aligned spins can then be easily written down. By contrast, the ground state wavefunction of the antiferromagnetic Hamiltonian cannot be written down explicitly.

Similarly the partition function and the free energy cannot be exactly computed for the Hamiltonian (1) for the ferro-or antiferromagnetic situation. One resorts to some approximation like that of the molecular field. In the ferromagnet the molecular field is uniform. In the antiferromagnet it is assumed to be oscillatory. Consider a bipartite lattice, one that can be broken up into two sublattices such that the nearest neighbours of one sublattice lie on the other. The antiferromagnetic molecular field orients the two sublattices in opposite directions. In a linear chain, for example, the even sites point up and the odd sites point down, or vice versa. The problem is reduced to a calculation of two effectively ferromagnetic sublattices and the molecular field has to be calculated self-consistently. Thus the calculation of susceptibility (van Vleck 1941) shows that there exists a critical temperature

$$T_c = \tfrac{2}{3} JzS(S+1)/k_B, \tag{2}$$

where z is the coordination number of the lattice. The susceptibility is found to have a maximum and a cusp at T_c. Above T_c it obeys the Curie–Weiss law. Below T_c the parallel susceptibility falls off to zero and the perpendicular susceptibility remains constant and equal to the value at T_c. The susceptibility of a polycrystalline sample, obtained by averaging over the parallel and the perpendicular values, falls below the maximum and approaches a constant value as the temperature goes to absolute zero. Experimental data are in qualitative agreement with these results. Susceptibility obeys Curie–Weiss law at high temperature, goes through a maximum and shows strong anisotropy effects at low temperature. Actually the transition temperature is slightly below the temperature of the maximum of the susceptibility (Fisher 1962). Its order of magnitude is given by (3).

The neutron diffraction experiments on antiferromagnets are supposed to give the 'spin arrangements'. Thus in a typical antiferromagnet MnO, the spins in single [111] plane are parallel but in adjacent [111] planes they are antiparallel.

The success of the thermodynamic calculations and the results of the neutron experiments are taken to mean that the Néel states—up spins on one sublattice and down spin on the other of a bipartite lattice—are good approximations to the ground state.

The classical spin wave theory is based on this picture; the Holstein–Primakoff transformations are applied to each sublattice to get the excitation spectrum. The low lying states, the so-called spinwaves, have the energy dispersion relation

$$\omega \sim k \tag{3}$$

for small wave vector k.

Of course, the Néel states are not even eigenstates of the Hamiltonian (1) and break the rotational and translational symmetry. Anderson (1952, 1964) provides two arguments for the broken symmetry situation. First, one may assume that a small amount of anisotropy energy is present to hold the spins constant in the z-direction; one then examines if the required anisotropy is infinitesimally small and allows smooth passage to the isotropic limit. Secondly, one may suppose that the spin wave theory really starts from 'wave-packets' of states, chosen in such a way that the z component of the total spin is roughly constant. Inquiry into the properties of the longest wavelength spin waves shows that the energy required to form such a packet is infinitesimal, of order $1/N$, where N is the number of atoms in the lattice. This energy is small. An equivalent result of experimental interest is that the time required for the total spin to drift around from one orientation to another essentially different one, is of order N and thus extremely large. Neutron diffraction pictures are possible because the time the neutron takes to sample the spins is small compared with the turn-over time.

We shall comment on the question of anisotropy below. With respect to the spin arrangements, we shall show that a different interpretation without broken symmetry is possible.

3. Exact results for the ground state

Several exact results are known about the ground state of the Heisenberg Hamiltonian (1). For the linear chain

$$H = 2J \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} \tag{4}$$

(N even; periodic boundary conditions $N+1 \equiv 1$) solved by the Bethe (1931) ansatz, Hulthen (1938) showed that the ground state has spin 0 and is unique. The total spin and its z-component

$$\mathbf{S} = \sum_{i=1}^{N} \mathbf{S}_i, \qquad S_z = \sum_{i=1}^{N} S_i^z, \tag{5}$$

are both constants of motion. Hulthen's calculation shows that the ground state occurs in the $S_z = 0$ subspace. The uniqueness follows from the fact that the choice of the wavevectors in the Bethe ansatz is unique.

For the three-dimensional Heisenberg Hamiltonian these results are generalized by Peierls and Marshall (1955) and Lieb *et al* (1961). Consider the relation

$$\mathbf{S}^2 = \left(\sum_{i=1}^{N} \mathbf{S}_i \right)^2 = \sum_{i=1}^{N} \mathbf{S}_i^2 + 2 \sum_{i<j}^{1,N} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{5}$$

or

$$2 \sum_{i<j}^{1,N} \mathbf{S}_i \cdot \mathbf{S}_j = \mathbf{S}^2 - \sum_{i=1}^{N} \mathbf{S}_i^2. \tag{6}$$

Since $S^2 = S(S+1)$ has values $S = 0, 1, 2, \ldots$ (N even), the eigenvalues of the left side of (6) are arranged in the order of an increasing sequence. The ground state belongs to $S = 0$. This ground state wavefunction can be shown to be not orthogonal to that of the Heisenberg Hamiltonian (1), which consequently must also have $S = 0$ ground state. Peierls and Marshall have shown the non-degeneracy of the ground state. It is shown that all the $\binom{N}{N/2}$ states in the $S_z = 0$ subspace occur in the ground state. Then their coefficients with a factor taken out are found to be all positive. Hence the spin 0 ground state is unique. There is no 'degeneracy of the vacuum'.

We must now consider the results of neutron scattering experiments. We note that the neutron scattering is determined by correlation functions (van Hove 1954). The pictures of the spin pattern are pictorial representations of the correlation functions. What can be inferred about the ground state wave function from these pictures? We may turn the question around and ask specifically: Is it possible that the ground state wavefunction is rather complicated but the correlation functions have the simple Néel structure?

The space-time correlation functions $\langle S^z_{i+n}(t)\, S^z_i(0) \rangle$ have only been numerically studied (Carboni and Richards 1969). Because of the difficulty in getting the normalization of wavefunction in the Bethe ansatz, the static correlation function $\langle S^z_i S^z_{i+n} \rangle$ has not been calculated for the linear chain. Only $\langle S^z_i S^z_{i+1} \rangle$ is exactly known, as it is related to the ground state energy. From numerical computations (Bonner and Fisher 1964) it has been estimated that there is no long range order

$$\lim_{n \to \infty} \langle S^z_i S^z_{i+n} \rangle = 0. \tag{7}$$

The short range order oscillates in sign, thus we have

$$\begin{aligned} 4\langle S^z_1 S^z_2 \rangle &= \langle \sigma^z_1 \sigma^z_2 \rangle = -0{\cdot}591, \\ 4\langle S^z_1 S^z_3 \rangle &= \langle \sigma^z_1 \sigma^z_3 \rangle = 0{\cdot}25, \\ 4\langle S^z_1 S^z_4 \rangle &= \langle \sigma^z_1 \sigma^z_4 \rangle = -0{\cdot}19, \\ 4\langle S^z_1 S^z_5 \rangle &= \langle \sigma^z_1 \sigma^z_5 \rangle = 0{\cdot}15, \end{aligned} \tag{8}$$

and so on.

An even clearer picture emerges from a study of a Hamiltonian for which the ground state can be explicitly written down (Majumdar and Ghosh 1969; Majumdar 1970). This is

$$H_A = 2J \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+2} \tag{9}$$

with periodic boundary conditions ($N+1 \equiv 1$, $N+2 \equiv 2$). Consider the states

$$\begin{aligned} \phi_1 &= [1, 2]\,[3, 4]\,[5, 6] \ldots [N-1, N], \\ \phi_2 &= [2, 3]\,[4, 5]\,[6, 7] \ldots [N, 1], \end{aligned} \tag{10}$$

where

$$[m, n] = \alpha(m)\,\beta(n) - \beta(m)\,\alpha(n)$$

is the usual singlet spin combination of up-spin function α and down-spin function β. By direct calculation

$$H_A \phi_1 = -\tfrac{3}{4} NJ \phi_1, \qquad H_A \phi_2 = -\tfrac{3}{4} NJ \phi_2, \tag{11}$$

and the ground state energy can be shown to be $-\frac{3}{4}NJ$. We have here a case of degenerate vacuum that breaks the translation symmetry. If T is a translation operator for unit displacement, we have

$$T\phi_1 = \phi_2, \qquad T\phi_2 = \phi_1. \tag{12}$$

Hence we can construct two ground state functions which diagonalise the translational operator T

$$\phi^+ = \frac{1}{\sqrt{2}}(\phi_1 + \phi_2), \qquad \phi^- = \frac{1}{\sqrt{2}}(\phi_1 - \phi_2), \tag{13}$$

with

$$T\phi^+ = \phi^+, \qquad T\phi^- = -\phi^-. \tag{14}$$

The correlation functions can be calculated exactly. For ϕ^+ we get table 1. Similar results hold for ϕ^-. Notice that for any finite N the order quickly settles down to an alternating function—exactly what is expected from the Néel states—although the ground state wavefunction is very different. The long range order is evanescent, and as $N \to \infty$ only the nearest neighbour order remains non-vanishing and antiferromagnetic. The model in that limit represents a quantum spin liquid.

We conclude that the observation of Néel type correlations does not say much about the ground state wavefunction and does not require broken symmetry in the ground state.

Turning to the question of anisotropy we note first that the Néel states are indeed the lowest states of the Ising model, an extremely anisotropic situation. But we can generate a more general Hamiltonian with Néel states as ground states. Start from the ferromagnetic Hamiltonian in one dimension

$$H_F(-J, -\Delta) = \sum_{i=1}^{N} [-J S_i^z S_{i+1}^z - \tfrac{1}{2}\Delta(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)], \tag{15}$$

($J > 0, \Delta > 0$). The ground state is the fully aligned state. First, we rotate every alternate spin by an angle π about the z axis:

$$S_i^x \to -S_i^x, \quad S_i^y \to -S_i^y, \quad S_i^z \to S_i^z.$$

We get

$$H_F(-J, \Delta) = \sum_{i=1}^{N} [-J S_i^z S_{i+1}^z + \tfrac{1}{2}\Delta(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)]. \tag{16}$$

Table 1. Spin correlations for ϕ^+.

No. of spins	10	12	∞
$\langle \sigma_1^z \sigma_2^z \rangle$	−0·467	−0·516	−0·5
$\langle \sigma_1^z \sigma_3^z \rangle$	−0·067	0·030	0
$\langle \sigma_1^z \sigma_4^z \rangle$	0·067	−0·030	0
$\langle \sigma_1^z \sigma_5^z \rangle$	−0·067	0·030	0
$\langle \sigma_1^z \sigma_6^z \rangle$	0·067	−0·030	0
$\langle \sigma_1^z \sigma_7^z \rangle$		0·030	0

Next we rotate every alternate spin by an angle π about the x-axis:

$$S_i^x \to S_i^x, \quad S_i^y \to -S_i^y, \quad S_i^z \to -S_i^z.$$

We thus arrive at the antiferromagnetic Hamiltonian

$$H_A(J,\Delta) = \sum_{i=1}^{N} [J S_i^z S_{i+1}^z + \tfrac{1}{2}\Delta(S_i^+ S_{i+1}^+ + S_i^- S_{i+1}^-)]. \tag{17}$$

Since either the even or the odd spins can be rotated, we generate the two Néel states by the above process. That these are the ground states can be seen by direct calculation too, as the terms involving Δ vanish when acting on these Néel states. Equation (17) is a special case of the XYZ Hamiltonian (Baxter 1972)

$$H_{XYZ} = \sum_{i=1}^{N} [J_x S_i^x S_{i+1}^x + J_y S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z] \tag{18a}$$

$$= \sum_{i=1}^{N} [J_z S_i^z S_{i+1}^z + \tfrac{1}{4}(J_x - J_y)(S_i^+ S_{i+1}^+ + S_i^- S_{i+1}^-)$$
$$+ \tfrac{1}{4}(J_x + J_y)(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)]. \tag{18b}$$

The longitudinal anisotropy is put to zero, $J_x = -J_y$, and only the transverse anisotropy is kept in (17).

The result can be generalised to three dimensions (Bose *et al* 1984). In a bipartite lattice of two sublattices A and B the Hamiltonian

$$H_A(J,\Delta) = \sum_{\substack{\langle i\in A, \\ j\in B\rangle}} [J S_i^z S_j^z + \tfrac{1}{2}\Delta(S_i^+ S_j^+ + S_i^- S_j^-)] \tag{19}$$

has the Néel states as ground states. With sufficiently strong anisotropy one can thus force the ground state to have the Néel form but this fact has little bearing on the isotropic situation of equation (1).

4. Excitation spectrum and spin of the antiferromagnetic spin wave

The excitation spectrum calculated from the spin wave theory by Anderson (1952) is

$$\hbar\omega = 2J|\sin k|. \tag{20}$$

The spectrum is thus linear as $\omega \to 0$, $k \to 0$, and this has been interpreted as the Goldstone boson mode (Sinha 1975). Notice the characteristic double periodicity of the spectrum. However, the degeneracy of the spectrum is not correct. A careful examination of the derivation shows that the spectrum is correct in the limit $S \to \infty$; this is confirmed by numerical calculation on short chains (Jain *et al* 1975).

Continuing the Bethe ansatz calculations des Cloizeaux and Pearson (1962) have constructed the exact excitation spectrum of spin 1 states to be

$$\hbar\omega = \pi J|\sin q|, \tag{21}$$

where the wavevector q is measured from that of the ground state (the wavevector of the ground state is 0 if N is of the form $4j$ and π if N is of the form $4j+2$ where j is an integer). Notice that the spectrum is doubly periodic here also. Experimentally, neutron scattering on dichlorobis (pyridine) copper II (CPC) confirms the existence of a branch of the form (21) (Endoh *et al* 1974).

The calculation of des Cloizeaux and Pearson is not strictly rigorous but depends on a guess of the distribution of the wavevectors of the Bethe ansatz. From numerical calculations Fazekas and Sueto (1976) and Sueto (1976) have pointed out that a branch of $S = 0$ states is degenerate with the $S = 1$ states of (21).

Takahasi (1971) and Woynarovich (1982) have reanalyzed the Bethe ansatz equations and made an exact calculation of the excited state spectrum possible. From a different point of view—that of Yang Baxter equations—Faddeev and Takhtajan (1983) have arrived at the same conclusions. The low lying states are now reinterpreted as follows. The low lying excitation is a doublet of spin-$\frac{1}{2}$ spin waves with the dispersion law

$$\varepsilon_d = \pi J \sin k, \quad 0 \leqslant k \leqslant \pi. \tag{22}$$

The excitation is a kink rather than an ordinary particle. The quasimomentum of an individual kink runs through the half zone. The ground state however has momentum 0 or π according as $N = 4j$ or $4j+2$, respectively. This will reproduce the double periodicity. The kinks are localizable objects and there are no bound states of kinks.

The spin of antiferromagnetic spin wave is $\frac{1}{2}$. All physical states have, however, even number of spin waves. The doublet of spin states can be looked upon a singlet $S = 0$ state and a triplet $S = 1$ state degenerate with each other. The fermionic nature of the spectrum is suppressed and the bosonic nature is perceived. This feature of the excitation is similar to the phenomenon of decolouring in quantum field theory. The excitation spectrum is not just that of a Goldstone boson.

The excitation spectrum of the Hamiltonian (9) is not exactly known. Because the symmetry broken is a discrete translational symmetry there is no logical necessity of a Goldstone mode. Approximate calculations have been done by Majumdar *et al* (1972) and Shastry and Sutherland (1981). Both groups have found a spin 1 branch and a spin 0 branch which can be thought of as a bound state branch of antiferromagnetic spin waves of spin 1. Shastry and Sutherland have also argued that there may be a gap in the excitation spectrum. The only exact information available is from numerical computations on chains of length up to $N = 12$. The question of the gap cannot be settled. There are $S = 1$ and $S = 0$ states, nearly degenerate and forming a doubly periodic spectrum. The $S = 0$ states lying partly below the $S = 1$ states may give rise to bound states. But the numerical results cannot rule out a complete degeneracy of the $S = 1$ and $S = 0$ states in the $N \to \infty$ limit and the decolouring phenomenon in the Hamiltonian (9) as well.

The excitation spectrum of the Hamiltonian $H_A(J, \Delta)$ for $J = \Delta$ is $\omega \sim k^2$ as $\omega \to 0$, $k \to 0$ in one as well as three dimensions. This is, of course, the ferromagnetic spectrum appearing unchanged under the canonical transformation. There is no Goldstone mode associated here.

5. Conclusion

In the one-dimensional antiferromagnetic models there is no evidence of broken symmetry or Goldstone modes. It appears likely that the same results are valid in three dimensions for the Hamiltonian (1). But the nature of long range order in the three-dimensional ground state of the Hamiltonian (1), if it exists, remains unclear. We have here concentrated on the spin $\frac{1}{2}$ extreme quantum limit only. For larger spins Anderson's broken symmetry picture and the spin wave calculations based on it still probably provide good physical descriptions of the experimental phenomena.

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