A difference in the properties of one-dimensional antiferromagnets with integer and half-integer spins

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It is shown explicitly that, despite the existence of logarithmic divergences in the perturbation theory, a one-dimensional antiferromagnet with $S = 1/2$ is equivalent at large scales to a system of free bosons.

1. One of the most interesting phenomena which has been studied in magnetism in recent years is the fundamental dependence of the behavior of one-dimensional Heisenberg antiferromagnets on the parity of the doubled spin. This dependence was originally predicted by Haldane.[1] According to Haldane's hypothesis, antiferromagnets with integer values of S remain in a paramagnetic state even at absolute zero, while for antiferromagnets with half-integer values of S the point $T = 0$ serves as a critical point, and at it we have a quantum-mechanical analog of a (Berezinskiǐ-) Kosterlitz-Thouless phase. Haldane's hypothesis has now been verified both by the results of numerical simulations[2] and by measurements of the magnetic characteristics of the quasi-one-dimensional compound $Ni(C_2H_8N_2)_2NO_2(ClO_4)$ ($S = 1$).[3] On the theoretical side, most of the work has invoked the analogy with field theory. At the semiclassical ($S \gg 1$) level, for example, it has been established[4,5] that a 1D Heisenberg antiferromagnet is equivalent to the $O(3)$ σ model with an additional topological θ-term with a coefficient $\theta = 2\pi S$. For integer values of S we have $\theta = O(\text{mod } 2\pi)$; the topological term is not important; and, as we know from the exact solution,[6] quantum fluctuations lead in the σ model to a dynamic generation of mass (i.e., to a gap in the spectrum of excitations). At half-integer values of $S[\theta = \pi(\text{mod } 2\pi)]$, the σ model has a critical point; i.e., the growth of fluctuations comes to a halt, and there is a critical behavior, characteristic of a Kosterlitz-Thouless phase.

2. In this letter we will attempt to explain the difference in the properties of 1D antiferromagnets with integer and half-integer values of S, without appealing to the analogy with the θ-model. Specifically, we will discuss an $S = 1/2$ antiferromagnet. The basic idea of our approach is to explicitly incorporate in the one-particle formalism the difference between the order parameter in an antiferromagnet and a unit vector; in other words, we bring into the discussion the additional internal degree of freedom, of the Ising type, which an antiferromagnet has. This additional degree of freedom is associated with the circumstance that for $S = 1/2$ the resultant spin of two neighbors (the ferromagnetism vector), $\mathbf{M}_{2l} = \mathbf{S}_{2l} + \mathbf{S}_{2l+1}$, can take on two values: $M = 1$ and $M = 0$. Correspondingly, the square of the antiferromagnetism vector, i.e., the operator $\mathbf{L}_{2l} = \mathbf{S}_{2l+1}$, takes on the two values 0 and 3. All four states of M can be described by the one-particle formalism if the operators M and L are associated with three boson fields, rather than two, as in the semiclassical treatment. The explicit transformation for making the switch to such bosons is

$$M_z = a^+a - b^+b, \qquad M_+ = \sqrt{2}\,(a^+c - c^+b), \qquad M_- = \sqrt{2}\,(c^+a - b^+c)$$
$$L_z = -(c^+U + Uc), \qquad L_+ = \sqrt{2}\,(a^+U + Ub), \qquad L_- = \sqrt{2}\,(b^+U + Ua), \tag{1}$$

where $U = (1 - a^+a - b^+b - c^+c)^{1/2}$. Physical states at a site of the "double lattice" correspond to the vacuum and to three states with a single excitation, of any type. In the physical subspace, the commutation relations $[M_iM_j] = i\epsilon_{ijk}M_k$, $[L_iL_j] = i\epsilon_{ijk}M_k$, $[M_iL_j] = i\epsilon_{ijk}L_k$ hold, along with the condition that the length of the vector part of the order parameter, $M^2 + L^2 = 3$ is fixed. Furthermore, M does indeed take on the values 0 and 1: $M^2 = 2(a^+a - b^+b - c^+c)$. The matrix elements for transitions between physical and nonphysical states are zero, so transformation (1) may be regarded as exact at $T = 0$. By using it we can express the original spins, S_{2l} and S_{2l+1}, in terms of bosons and therefore represent the antiferromagnet as a system of three interacting Bose fields. The choice of four physical states of M_{2l} means that each of the spins S_{2l}, S_{2l+1} is described by one of the spinors φ, $\tilde{\varphi}$, where $(1 = 2l$, $2 = 2l + 1)$

$$\varphi_1 = \begin{pmatrix} |a_1\rangle \\ \frac{1}{\sqrt{2}}(|0_1\rangle + |c_1\rangle) \end{pmatrix} \quad \tilde{\varphi}_1 = \begin{pmatrix} \frac{1}{\sqrt{2}}(|0_1\rangle - |c_1\rangle) \\ |b_1\rangle \end{pmatrix},$$
$$\varphi_2 = \begin{pmatrix} -|a_2\rangle \\ \frac{1}{\sqrt{2}}(|0_2\rangle - |c_2\rangle) \end{pmatrix} \quad \tilde{\varphi}_2 = \begin{pmatrix} \frac{1}{\sqrt{2}}(|0_2\rangle + |c_2\rangle) \\ -|b_2\rangle \end{pmatrix}. \tag{2}$$

Here $|0\rangle$, $|a\rangle$, $|b\rangle$, and $|c\rangle$ represent the vacuum and the states with a single excited boson of a certain type. The terms $S_{2l}S_{2l-1} = 1/2(S_{2l} + S_{2l-1})^2 - 3/4$ introduce a nonlocal nature in the Bose Hamiltonian; in these terms, the interacting spins belong to neighboring sites in the lattice coarsened by a factor of two. The redundancy of the description of the states of the resultant spin, $M = S_{2l} + S_{2l-1}$, makes it possible to incorporate, in a unique way, the interaction of the vector and scalar (a real scalar) parts of the order parameter, after we use the components of the spinors to construct four wave functions ψ which give a complete description of the states $\tilde{M}$ and after we eliminate from the boson Hamiltonian the terms which contribute zero when applied to any of the ψ. We choose these wave functions to be

$$\psi_1^1 = \frac{1}{\sqrt{2}}(\varphi_1^{(1)}\tilde{\varphi}_2^{(1)} + \tilde{\varphi}_1^{(1)}\varphi_2^{(2)})$$
$$\psi_1^0 = \frac{1}{\sqrt{2}}[(\varphi_1^{(1)}\tilde{\varphi}_2^{(2)} + \varphi_1^{(2)}\tilde{\varphi}_2^{(1)}) + (\tilde{\varphi}_1^{(1)}\varphi_2^{(2)} + \tilde{\varphi}_1^{(2)}\varphi_2^{(1)})]$$
$$\psi_1^{-1} = \frac{1}{\sqrt{2}}(\varphi_1^{(2)}\tilde{\varphi}_2^{(2)} + \tilde{\varphi}_1^{(2)}\varphi_2^{(2)}) \tag{3}$$
$$\psi_0 = \frac{1}{2}[(\varphi_1^{(1)}\tilde{\varphi}_2^{(2)} - \varphi_1^{(2)}\tilde{\varphi}_2^{(1)}) - (\tilde{\varphi}_1^{(1)}\varphi_2^{(2)} - \tilde{\varphi}_1^{(2)}\varphi_2^{(1)})],$$

where $\varphi_1 \equiv \varphi_{2l}$, $\varphi_2 \equiv \varphi_{2l-1}$, and the superscripts in parentheses specify the upper and lower components of the spinors.

The modified Bose analog of the spin Hamiltonian $H = \Sigma_l S_l S_{l+1}$ is written as the sum $H = H_{ab} + H_c + H^c_{ab}$, where the first term is the boson version of Hamiltonian of a system with a vector order parameter. After we diagonalize the quadratic form $(a, b \to p, q)$ and take the long-wavelength limit, this Hamiltonian becomes

$$H_{ab} = \sum_k |k| \sqrt{2} (q_k^+ q_k + p_k^+ p_k) + \frac{2}{N} \sum_{k_i} \phi [q_1^+ q_2^+ q_3 q_4 + p_3^+ p_4^+ p_1 p_2 + q_1^+ q_2^+ p_3^+ p_4^+$$

$$+ q_3 q_4 p_1 p_2 + 2(q_1^+ q_2^+ p_3^+ q_4 + p_1 p_2 q_3 p_4^+ - q_1^+ p_2 q_3 q_4 - p_3^+ p_4^+ q_2^+ p_1) - 4 q_1^+ p_2 q_3 p_4^+], \quad (5)$$

where

$$\phi = \frac{\sqrt{2}}{16} g_0 \frac{|k_1||k_2| - k_1 k_2}{(|k_1 k_2 k_3 k_4|)^{1/2}}, \quad g_0 = \frac{1}{2\sqrt{2}}.$$

The interaction of the excitations of the p and q types increases with increasing scale: In the one-loop approximation we have $g = g_0/1 - g_0/2\pi|\ln k|$. We would naturally expect that this growth would lead to a dynamic generation of mass, as in the σ model. The second term, H_c, originally corresponded to an Ising model with $S = 1/2$ in a transverse field. In the modified version, the quadratic form in H_c becomes

$$H_c^{(2)} = \frac{1}{2} \left\{ \sum_k c_k^+ c_k - \frac{\cos 2k}{2} (c_k^+ c_{-k}^+ + c_k c_{-k}) \right\}; \quad (6)$$

in other words, the seed spectrum of excitations of type c contains two Goldstone models at $k = 0$ and at the boundary of the Brillouin zone in the doubled lattice, $k = \pi/2$. Separating out the low-energy regions, and diagonalizing the quadratic part of the Hamiltonian, we find an expression which is precisely the same as (4), except that ϕ has the opposite sign. In this case, therefore, the coupling constant demonstrates a *zero-charge behavior*, and the seed rigidity of the spin waves is not disrupted by fluctuations.

The last term describes the interaction of the subsystems with the vector and scalar parts of the order parameter. A calculation shows that the corresponding coupling constant *does not undergo a logarithmic renormalization*; in other words, at large scales the gap excitations of types a and b differ from the gapless excitations of type c, and we arrive at a critical theory specified by H_c. The central charge C has twice the value (two Goldstone bosons) in the Ising model; i.e., we have $C = 1$, as for free bosons, in agreement with the result of Ref. 7.

3. On the basis of this analysis of antiferromagnets with $S = 1/2$ we could suggest that the difference between Heisenberg antiferromagnets with integer and half-integer values of S stems from a difference in the parity of the number of states of the ferromagnetism vector $M = S_1 + S_2$. For integer values of S, a complete description of the states of M in terms of one-particle excitations would require the introduction of $(2S + 1)^2 - 1$, i.e., an even number, bosons. As we are assuming here, these bosons will be either gap bosons or bosons coupled in pairs by a logarithmically growing interaction, so as a result all of the excitations will be gap excitations. For half-integer values of S, in contrast, the number of bosons required is an odd number, and after they are combined in pairs we are left with one extra boson, which determines the low-energy properties of the antiferromagnet. Just what happens at the integrable points for generalized models requires a separate study.

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