

Dimensional Crossover in Quantum Antiferromagnets

Sudip Chakravarty

Department of Physics and Astronomy, University of California at Los Angeles, Los Angeles, California 90095-1547

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The dimensional crossover in a spin- S nearest-neighbor Heisenberg antiferromagnet is discussed as it is tuned from a two-dimensional square lattice, of lattice spacing a , towards a spin chain by varying the width L_y of a semi-infinite strip $L_x \times L_y$. For integer spins and arbitrary L_y , and for half integer spins with L_y/a an arbitrary even integer, explicit analytical expressions for the zero temperature correlation length and the spin gap are given. For half integer spins and L_y/a an odd integer, it is argued that the $c = 1$ behavior of the $SU(2)_1$ Wess-Zumino-Witten fixed point is squeezed out as the width $L_y \rightarrow \infty$; here c is the conformal charge. The results specialized to $S = \frac{1}{2}$ are applied to spin-ladder systems. [S0031-9007(96)01673-0]

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One-dimensional quantum antiferromagnets have many unusual properties. For example, nearest-neighbor Heisenberg spin chains with half-integer spins are gapless, but those with integer spins are generically gapped [1]. Many properties such as these can be understood from the correspondence of the spin chain to a $(1 + 1)$ -dimensional $O(3)$ nonlinear σ model, augmented by a term in the action that contributes a phase factor $e^{i\theta Q}$ to the path integral where $\theta = 2\pi S$; S is the spin and Q is an integer winding number. For integer spins, $\theta = 0 \pmod{2\pi}$, the phase factor is unity, but for half-integer spins $\theta = \pi \pmod{2\pi}$, it is $(-1)^Q$. This leads to the crucial difference between the integer and the half-integer spins. Although the existence of the gap in the model with $\theta = 0$ can be seen in a variety of ways [2], the model with $\theta = \pi$ is more subtle [3]. For $\theta = \pi$, the short distance behavior is dominated by two weakly interacting goldstone modes. These are correctly described by the perturbative renormalization group analysis that is impervious to the existence of the θ term. In the language of conformal field theory, the system is in the proximity of an infrared unstable fixed point corresponding to conformal charge $c = 2$. At short distances, there is no distinction between integer and half-integer spins, and the system appears gapful. However, on longer scales the $\theta = \pi$ model flows to $k = 1$ $SU(2)$ Wess-Zumino-Witten model [$SU(2)_1$ WZW], corresponding to a $c = 1$ massless theory. Indeed all critical theories in two dimensions must belong to a conformally invariant fixed point.

The two-dimensional square-lattice, nearest-neighbor Heisenberg antiferromagnet is entirely different. It is rigorously known that the ground state is Néel ordered for $S \geq 1$ [4], but no such proofs exist for $S = 1/2$. Nonetheless, the numerical evidence for an ordered ground state for $S = \frac{1}{2}$ is strong [5]. Moreover, the assumption of an ordered ground state has yielded predictions [6] that are confirmed in neutron scattering experiments [7]. Henceforth, I shall assume that this is also a solved problem, and the correct low energy theory is a $(2 + 1)$ -dimensional

$O(3)$ nonlinear σ model, which is in the broken symmetry phase in its ground state [6]. (The possible existence of topological terms was considered and discarded by a number of authors [8].) The corresponding elementary excitations are weakly interacting Goldstone modes, that is spin waves. This low energy, long wavelength model is essentially geometrical and is almost entirely determined by symmetry [9] regardless of whether or not the magnitude of the spin is large. The two needed phenomenological constants are the spin wave velocity and the spin stiffness constant. In principle, experiments can determine these constants, and there is no need to rely on a presumed large- S expansion.

It is an intriguing question to ask how a two-dimensional system would evolve if we began with a strip $L_x \times L_y$ and continuously tuned the system by varying the width L_y , with L_x kept infinitely large. Would it approach the one-dimensional limit, and if so, how would we recover the sensitivity to the topological angle θ ? This would be of only theoretical, albeit considerable interest, if it were not for experiments on spin ladders [10] in which $S = \frac{1}{2}$ systems of varying width are explored. The purpose of the present paper is an attempt to clarify this crossover and to determine the evolution of the excitation spectrum.

It has been argued [11,12] that spin ladders correspond to an effective $(1 + 1)$ -dimensional $O(3)$ nonlinear σ model with the θ parameter given by $\theta = 2\pi n_l S$, where n_l is the number of legs. Thus for $S = \frac{1}{2}$, the system is gapful for even-leg ladders and gapless for odd-leg ladders in accord with experiments [10]. There are complimentary theoretical and numerical approaches to the ladder systems that are outside the scope of the reasoning in this paper [13]. However, the crossover problem stated above has not been fully elucidated, although it was anticipated [12] that, when approached along the sequence of even-leg ladders, the gap must collapse exponentially with the increasing width of the system. In the present paper I shall show precisely how this happens

and derive a formula that can be checked. At first sight the approach to the two-dimensional limit along the odd sequence appears to be simple because they are gapless. However, this is not so because the two-dimensional problem, which is insensitive to topology, is described by two Goldstone modes; it cannot be a straightforward extension of the $c = 1$ fixed point of the $SU(2)_1$ WZW model.

The Euclidean action of the $O(N)$ quantum nonlinear σ model, in which one of the dimensions is singled out and is of finite extent L , is

$$\frac{S}{\hbar} = \frac{\rho_s^0}{2\hbar} \int_0^{\beta\hbar} d\tau \int d^{d-1}x \times \int_0^L dx_1 \left[(\partial_\mu \hat{\Omega})^2 + \frac{1}{c^2} \left(\frac{\partial \hat{\Omega}}{\partial \tau} \right)^2 \right], \quad (1)$$

where the index μ runs over all the spatial dimensions, 1 through d . The extent of the imaginary time dimension, $\beta\hbar$, tends to infinity as the temperature $T = 1/k_B\beta$ tends to zero. We shall impose a periodic boundary condition along the direction 1; the remaining spatial directions will be assumed to be infinite in extent. The staggered order parameter field of the antiferromagnet, $\hat{\Omega}$, is an N -component unit vector field, which is a function of $(\tau, x_1, x_2, \dots, x_d)$; the spin- S antiferromagnet corresponds to $N = 3$. The parameter ρ_s^0 is the bare spin stiffness constant at the spatial cutoff Λ^{-1} of the model, and the parameter c is the spin wave velocity on the same scale. I shall focus on the zero temperature behavior and report results of a ‘‘Lorentz’’ invariant analysis; therefore, the spin wave velocity will not renormalize.

The action at $T = 0$ is interesting. The extents in all directions, except x_1 , are infinite; along x_1 we have a periodic boundary condition. The physical problem at $T = 0$ is, therefore, isomorphic to a problem at finite ‘‘temperature,’’ where the temperature-like variable is $\varepsilon_L = \hbar c/L$. With proper identifications of the parameters, it is *identical* to that solved in Ref. [6]. Let us define two dimensionless bare coupling constants:

$$g_0 = \frac{\hbar c \Lambda^{d-1}}{\rho_s^0}, \quad (2)$$

$$\varepsilon_L^0 = \frac{\hbar c \Lambda^{d-2}}{L \rho_s^0}.$$

The energy-like parameter ε_L^0 plays the role of the dimensionless temperature-like coupling constant in Ref. [6], and g_0 is the same as that defined previously.

The renormalization group equations can be simply read off from Ref. [6]. The crossover phase diagram, in $d = 2$, constructed from these equations is shown in Fig. 1, merely for orientation. The three distinct regions had to be renamed, as the present analysis corresponds to $T = 0$. The regions previously named ‘‘renormalized classical,’’ ‘‘quantum critical,’’ and ‘‘quantum disordered’’ are now renamed to be ‘‘dimensionally reduced,’’ ‘‘critical spin liquid,’’ and ‘‘gapped spin liquid,’’ respectively. With simple transcriptions, the physical pictures of the crossover boundaries are the same as before. The analy-

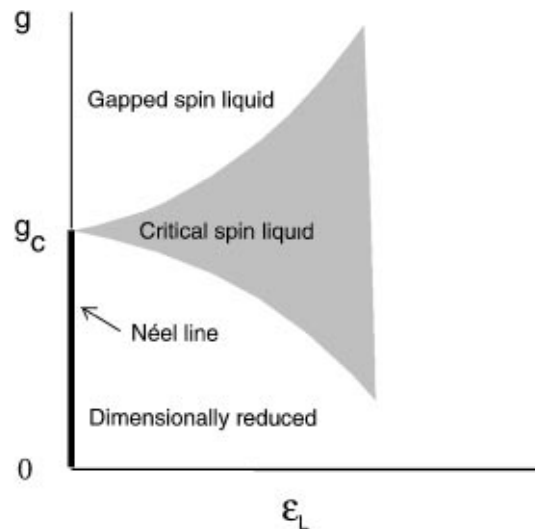


FIG. 1. The crossover phase diagram in $d = 2$.

ses of the gapped and critical spin liquid regimes are exceedingly complex and are beyond the scope of the present paper.

The region of the phase diagram for which we can make precise predictions is the dimensionally reduced region. In this region, the system is in the Néel ordered state when $L = \infty$, or $\varepsilon_L = 0$. When $L \neq \infty$, the system is equivalent to a dimensionally reduced effective $(1 + 1)$ -dimensional model with no long range order. This can be seen from the renormalization group equations [6]. At first, with increasing length scale, g rapidly decreases and ε_L increases slowly, that is, the system appears more and more ordered. Subsequently, ε_L increases rapidly, but g decreases very slowly, thereby breaking up the order at longer length scales and resulting in the reduction from $(2 + 1)$ to $(1 + 1)$ dimensions. The effective coupling constant to be used in the $(1 + 1)$ -dimensional model is easily calculated to be

$$\frac{1}{\varepsilon_{\text{eff}}} = \frac{L}{\hbar c} \rho_s \left[1 + \frac{\hbar c}{2\pi L \rho_s} \ln(\Lambda L) \right], \quad (3)$$

where ρ_s is the fully renormalized macroscopic spin stiffness constant at $T = 0$ of the square-lattice spin- S antiferromagnetic Heisenberg model ($L_x = \infty, L_y = \infty$) [14]. This definition can be made more explicit if we recall that $\rho_s = JS^2 Z_{\rho_s}$ and $\hbar c = 2\sqrt{2}JSaZ_c$, where J is the exchange constant, a is the lattice spacing; Z_{ρ_s} and Z_c are the renormalization factors [15]. We can now write

$$\varepsilon_{\text{eff}} = \frac{2}{S} \left[\left(\frac{Z_{\rho_s}}{\sqrt{2}Z_c} \right) \frac{L}{a} + \frac{1}{\pi S} \ln(\Lambda L) \right]^{-1}. \quad (4)$$

Therefore, for large (L/a) the input bare coupling constant to the effective $(1 + 1)$ -dimensional model is greatly reduced from its value $(2/S)$ of a spin chain. This is due to increased order at short distances, concomitant of the quasi two-dimensional nature of the model with finite width L .

For integer spins and for even-leg ladders with half-integer spins the description of the dimensional crossover is conceptually complete. The system is massive and its mass gap should be calculated with the effective coupling derived above. I shall make more precise predictions later. The case of odd-leg ladders with half-integer spins requires further clarification. Because all possible topological terms were dropped in the $(2 + 1)$ -dimensional model, the masslessness of the dimensionally reduced system could not be recovered. Even in the presence of sufficiently strong local Néel order, the proof of the nonexistence of the topological term in $d = 2$ is correct strictly when the number of spins along both L_x and L_y are even. For an odd number of rows along L_y , but $L_x = \infty$, a topological term $2\pi i S Q$ remains [8]. If we wish, we can rewrite it as $2\pi i S Q n_l$ by realizing that the topological angle is only defined modulo 2π . It has been never fully explained why this odd-chain case is physically irrelevant; in fact it is not, as we shall see. Imagine that we include such a term in our action [16]. For finite L , this should, in principle, render the model massless in the sense of $c = 1$, not in the sense of a Goldstone phase. However, the $c = 1$ behavior will be difficult to see when L/a is large. The reason is that the effective coupling constant derived in Eq. (4) will be very small, and the perturbative renormalization group, which is impervious to the topological term, will be valid up to very long distances until the running coupling constant becomes of order unity for the system to crossover to $c = 1$ $SU(2)_1$ WZW model. [The crossover length scale will be of the order of the correlation length given below in Eq. (8).] Thus the region in which the $c = 1$ behavior is seen is squeezed out as $L \rightarrow \infty$, and all we see is the Goldstone phase. Conversely when L/a is of order unity, the $c = 1$ feature should be visible. It is important to keep in mind that the $\theta = \pi$ model itself is not conformally invariant in $(1 + 1)$ dimensions; it has a nontrivial β function and an associated mass gap.

Using Ref. [6] it is possible to write down by inspection the expression for the correlation length ξ in our $O(3)$ model defined on a strip for which $L_x = \infty$, $L_y = L$. It is important to note that the dimensionally reduced effective $(1 + 1)$ -dimensional model has ‘‘Lorentz’’ invariance; integrating out the L_y modes does not destroy the proportionality between the imaginary time and the L_x directions. There is, therefore, one and only one correlation length [17]. The result for ξ is

$$\xi = \sqrt{32} e^{\pi/2} (2\pi C) \left(\frac{\hbar c}{2\pi \rho_s} \right) \exp\left(\frac{2\pi \rho_s L}{\hbar c} \right) \times \left[1 - A \left(\frac{\hbar c}{2\pi \rho_s L} \right) + O\left(\frac{\hbar c}{2\pi \rho_s L} \right)^2 \right]. \quad (5)$$

From strong coupling simulations, the quantity $2\pi C$ was estimated in Ref. [6] to be between 0.01 and 0.013. This makes the overall numerical prefactor between 0.27 and 0.35. Since then an asymptotically exact expression has been derived [18], and the exact prefactor is known to

be $e/8 \approx 0.34$. In addition, the constant which was previously known to be only of order unity is determined to be $A = \frac{1}{2}$.

It is interesting to rewrite Eq. (5) in terms of the Josephson correlation length of the $L = \infty$ $(2 + 1)$ -dimensional $O(3)$ nonlinear σ model [6], which is given by $\xi_J = \hbar c / \rho_s$. This length separates the short distance critical behavior from the long distance Goldstone behavior. In terms of ξ_J the correlation length takes the simple finite-size scaling form

$$\xi = \frac{e}{8} \left(\frac{\xi_J}{2\pi} \right) e^{2\pi L / \xi_J} \left[1 - \frac{1}{2} (\xi_J / 2\pi L) + O(\xi_J / 2\pi L)^2 \right]. \quad (6)$$

For spin- S square-lattice Heisenberg antiferromagnet, ξ_J is given by [15]

$$\xi_J = \left(\frac{2\sqrt{2}Z_c}{SZ_{\rho_s}} \right) a. \quad (7)$$

Because of Lorentz invariance, the spin gap Δ is simply $\Delta = \hbar c / \xi$. Note again that the spin wave velocity does not renormalize, and this relation does not have any corrections (cf. below). Specializing to $S = \frac{1}{2}$, we get

$$(\xi/a)_{\frac{1}{2}} = 0.499 e^{0.682(L/a)} [1 - 0.734(a/L)], \quad (8)$$

$$(\Delta/J)_{\frac{1}{2}} = 3.347 e^{-0.682(L/a)} [1 - 0.734(a/L)]^{-1}. \quad (9)$$

The field theory analysis presumes that a continuum theory is applicable in both directions, and therefore the expressions in Eqs. (8) and (9) cannot be accurate for $(L/a) \sim 1$. Moreover, these expressions, obtained with a periodic boundary condition, are likely to be different from those obtained from other boundary conditions, such as the open boundary condition, especially when $(L/a) \sim 1$. Nonetheless if we take $L/a = 4$ corresponding to four-leg ladders, we get $(\Delta/J)_{\frac{1}{2}} = 0.268$ and $(\xi/a)_{\frac{1}{2}} = 6.23$. For $L/a = 6$ we get $(\Delta/J)_{\frac{1}{2}} = 0.064$ and $(\xi/a)_{\frac{1}{2}} = 26.2$.

To compare, numerical results, with open boundary condition along L_y , are available for $L/a = 4$ and 6. According to Ref. [19], we have, for $L/a = 4$, $(\Delta/J)_{\frac{1}{2}} = 0.190$, and $(\xi/a)_{\frac{1}{2}} = 5-6$. According to Ref. [20], we have, for $L/a = 4$, $(\Delta/J)_{\frac{1}{2}} = 0.160$, and $(\xi/a)_{\frac{1}{2}} = 10.3$. From the same work, we have, for $L/a = 6$, $(\Delta/J)_{\frac{1}{2}} = 0.055$. The value for the correlation length for $L/a = 6$ is not given explicitly. However, a simple extrapolation yields a value close to 30. From Ref. [21], we have, for $L/a = 4$, $(\Delta/J)_{\frac{1}{2}} = 0.17$; for $L/a = 6$, $(\Delta/J)_{\frac{1}{2}} = 0.05$.

Note that the gaps should be inversely proportional to the correlation lengths, where the proportionality constant is $\hbar c$, where c is the *two*-dimensional spin wave velocity, which is unrenormalized to the accuracy of the present calculation. This proportionality is automatically satisfied for the analytical expressions given in this paper and should be a good check on the numerical work.

Based on the simple observation that at $T = 0$ the spin- S square-lattice Heisenberg model of finite width can

be mapped onto a $(2 + 1)$ -dimensional $O(3)$ nonlinear σ model with a finite dimension, I have provided a theory for crossover in spin ladders. Explicit analytical expressions for the correlation length and the spin gap were obtained by transcribing the results in Ref. [6]. The agreement with numerical calculations is very good considering the difference in the boundary conditions employed. The analytical expressions show precisely that the crossover to the two-dimensional limit is approached exponentially as the number of legs in the ladder system is increased. The extension of the present theory to anisotropic coupling and to finite temperature should be straightforward. I hope to return to these extensions in the future.

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