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Sine-Gordon theory of the non-Néel phase of two-dimensional quantum antiferromagnets

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We examine a recently developed sine-Gordon model description of the non-Néel phase of quantum antiferromagnets on two-dimensional bipartite lattices. Using a spatial dimensionality $d=1+\epsilon$ expansion we argue that the model always scales to its strong-coupling limit and displays spin-Peierls or valence-bond-solid order. The structure of the theory in this strong-coupling limit bears a remarkable resemblance to a fermionic large-N limit of the nearest-neighbor SU(N) antiferromagnet.

The recent discovery of high-temperature superconductivity[1] has led to renewed interest in the properties of non-Néel phases of two-dimensional quantum antiferromagnets. This is motivated in part by the suggestion of Anderson[2] that novel properties of such phases may be linked to the appearance of high-temperature superconductivity.

In a recent series of papers,[3-6] Read and Sachdev have considered two-dimensional antiferromagnets which have a two-sublattice Néel state as their classical ground state. Following a suggestion by Haldane,[7] they considered the effect of instantons (hedgehogs) and their associated Berry phases in the non-Néel phase of such antiferromagnets. They argued that close to the transition to the Néel phase, the instanton effects led to the following effective sine-Gordon theory for the long-wavelength ($\gg\xi$, the spin-correlation length) properties of the spin-disordered state of *any* such antiferromagnet:[5]

$$Z=\int \mathcal{D}\chi \exp(-S_{\rm sG}),$$
$$S_{\rm sG}=\int_0^{c\beta}\frac{d\tilde{\tau}}{a}\left\{\frac{K}{2}\left[\sum_{\langle s,t\rangle}(\chi_s-\chi_t)^2+\sum_s a^2\left(\frac{\partial\chi_s}{\partial\tilde{\tau}}\right)^2\right]-y\sum_s\cos(\chi_s-\pi S\zeta_s)\cdots\right\}, \quad (1)$$

where τ is the Matsubara time, c is a velocity which becomes the spin-wave velocity in the Néel phase, $\tilde{\tau}=c\tau$, a is the lattice spacing, β is the inverse temperature, S is the magnitude of the spin at each lattice site, and K and y are dimensionless coupling constants.[4,5] The sine-Gordon field χ_s has space-time coordinates $(\mathbf{R}_s,\tilde{\tau})$, where the $\mathbf{R}_s$ are located at the centers of the plaquettes of the lattice of spins. The ζ_s are a set of fixed numbers determined by the lattice structure: For the case of the square lattice they take the values 0,1,2,3 on the four dual sublattices W,X,Y,Z (the lattice of spins is made up of sublattices A and B; see Fig. 1). The ellipse at the end of Eq. (1) indicate additional terms involving cosines of multiples of $(\chi_s-\pi S\zeta_s)$: for simplicity we will neglect these terms in the initial discussion. All of the remaining discussion will focus on the case of the square lattice; other bipartite lattices can be treated similarly. It is clear from the structure of $S_{\rm sG}$ on the square lattice that the results are a function of $2S(\mathrm{mod}4)$. We will explicitly present the results for the most important case of $S=\frac{1}{2}$; the generalization of the calculations to $2S(\mathrm{mod}4)\neq 1$ is straightforward and the results will be indicated later.

An important property of $S_{\rm sG}$ is that, *in the absence of dynamical symmetry breaking,* all physically measurable correlation functions are invariant under the full space group of the square lattice (we will find later in this paper that such a dynamical breaking of the square lattice symmetry in fact occurs for all non-even-integer S). The choice of the ζ_s does not explicitly break the symmetry between the sublattices. To demonstrate this we need the mapping between correlation functions of χ to those of the spin operators $\mathbf{S}(\mathbf{r})$ of the antiferromagnet.[4,5] Let $\mathcal{R}$ denote the coordinates of the centers of the links of the square lattice; then, for $\mathcal{R}$ on any horizontal link,

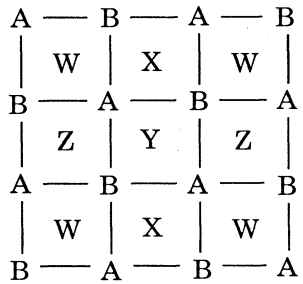

FIG. 1. The two sublattices A,B of the square lattice and the four sublattices W,X,Y,Z of the dual lattice.

$$\left\langle \mathbf{S}\left(\mathcal{R}+\frac{\hat{x}}{2}\right)\cdot\mathbf{S}\left(\mathcal{R}-\frac{\hat{x}}{2}\right)\right\rangle = C_1 + C_2(-1)^{\mathcal{R}_x+\mathcal{R}_y-1/2}\left\langle \chi\left(\mathcal{R}+\frac{\hat{y}}{2}\right)-\chi\left(\mathcal{R}-\frac{\hat{y}}{2}\right)\right\rangle, \tag{2}$$

while, for $\mathcal{R}$ on a vertical link,

$$\left\langle \mathbf{S}\left(\mathcal{R}+\frac{\hat{y}}{2}\right)\cdot\mathbf{S}\left(\mathcal{R}-\frac{\hat{y}}{2}\right)\right\rangle = C_1 + C_2(-1)^{\mathcal{R}_x+\mathcal{R}_y+1/2}\left\langle \chi\left(\mathcal{R}+\frac{\hat{x}}{2}\right)-\chi\left(\mathcal{R}-\frac{\hat{x}}{2}\right)\right\rangle, \tag{3}$$

where C_1 and C_2 are two link-independent constants which are determined by microscopic details of the physics. The expectation values of the $\mathbf{S}(\mathbf{r})$ on the left-hand sides of Eqs. (2) and (3) are clearly physically measurable. Let us now consider different elements of the square lattice space group: (a) the physics is clearly invariant under all translations which preserve the W,X,Y,Z sublattices; (b) the χ fields transform nontrivially under transitions that interchange the sublattices; e.g., under translation in which $W,X,Y,Z \rightarrow X,W,Z,Y$ we have

$$\chi \rightarrow \pi S - \chi . \tag{4}$$

The right-hand sides of Eqs. (2) and (3) remain invariant after we account for the change in sign of the $(-1)^{\mathcal{R}_x+\mathcal{R}_y\pm 1/2}$ factors. Note that this particular transformation also interchanges sublattices A,B. (c) Under rotations about any point of the A sublattice by the angle $n\pi/2$ (n integer), the χ fields transform as

$$\chi \rightarrow \chi - nS\pi , \tag{5}$$

which leaves the correlation functions in Eqs. (2) and (3) invariant. The same transformation about a point on the B sublattice yields $\chi \rightarrow \chi + nS\pi$.

The invariances under other elements of the square lattice space group can be verified in a similar manner.

The mapping between sine-Gordon models and interface-roughening problems[8] is useful in visualizing the physics of S_{sG}. The field χ_s can be considered as the displacement of a three-dimensional interface. The preferred values of χ_s are, however, dependent upon the sublattice location: interface pinning potential has minima at $\chi_s = 2n_s\pi + \pi S\zeta_s$ where the n_s are arbitrary integers.

Reference 4 considered the properties of S_{sG} in the small y limit and found that for $2S(\mathrm{mod}4)\neq 0$, the uniform χ state was *unstable* to a spontaneous lattice symmetry breaking and the appearance of spin-Peierls order. In this paper we shall reach an identical conclusion using a more general renormalization-group-based analysis of S_{sG}. As is the case with the usual sine-Gordon model which has $\zeta_s = 0$ on every site, a renormalization-group transformation can be performed in spatial dimensions $d = 1+\epsilon$ for small values of y and ϵ.[9,10] It is necessary to consider a unit cell of four plaquettes with the fields χ_W, χ_X, χ_Y, and χ_Z on their respective sublattices. We expand the partition function in powers of y (Ref. 9) and integrate out fluctuations in χ_W, χ_X, χ_Y, and χ_Z over the momentum shell $\Lambda e^{-l} < |\mathbf{k}|, \tilde{\omega} < \Lambda$, where Λ is an upper cutoff for the momentum $\mathbf{k}$ and "frequency" $\tilde{\omega}$. After reexponentiating the series and rescaling, we obtain, for small y and ϵ, the following renormalization-group equations:

$$\begin{aligned} \frac{dy}{dl} &= (2+\epsilon-\alpha K^{-1})y + \cdots , \\ \frac{dK^{-1}}{dl} &= -\epsilon K^{-1} - \beta K^{-3}y^2 - \cdots , \end{aligned} \tag{6}$$

where α,β are positive constants. These equations are identical in form to those obtained with the ordinary sine-Gordon model with $\zeta_s = 0$;[9] to this order in y the only effect of nonzero values of ζ_s are changes in the numerical values of α and β. The most notable feature of these equations is that for all initial values of K and y there is a runaway flow towards large y. The action acquires many additional cosine terms under renormalization but it is clear that none of them alter the instability towards strong coupling.[10]

We physically interpret the flow to strong coupling[10] as signaling the dominance of the on-site potentials in controlling the fluctuations of χ; the χ fields fluctuate in the small neighborhood of a *fixed* minimum of a potential with terms involving the cosines of sums over multiples of $\chi_s - \pi S\zeta_s$. (In the language of the interface-roughening problem this is equivalent to stating that the interface is *smooth*.) We begin by considering the simplest such potential: We examine S_{sG} in the large-y limit, ignoring the effect of the cosines of multiple angles. The on-site potential energy is minimized by the choice

$$\chi_s = \chi_s^0 \equiv \frac{\pi\zeta_s}{2} + 2n_s\pi , \tag{7}$$

for $S = \frac{1}{2}$ and any set of integers n_s. We expect χ_s to fluctuate in a small neighborhood of χ_s^0. By inserting these values of χ_s into Eqs. (2) and (3) we find that *any* choice of the integers n_s (including the spatially uniform one) *spontaneously breaks at least the lattice rotation symmetry in the values of* $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$. The values of the n_s will be determined by minimizing corrections to the energy to zeroth and first order in $1/y$; we examine these corrections in the following paragraphs.

To zeroth order in $1/y$, we may neglect fluctuations of χ_s about χ_s^0. The preferred n_s configurations are obtained by minimizing the energy

$$E_1(\{n_s\}) = \frac{Kc}{2a}\sum_{\langle s,t\rangle}(\chi_s^0 - \chi_t^0)^2 . \tag{8}$$

This is equivalent to maximizing the number of links with phase slip $|\chi_s^0 - \chi_t^0| = \pi/2$. It is impossible, however, to eliminate links with phase slip $|\chi_s^0 - \chi_t^0| = 3\pi/2$. The minima of E_1 are obtained by placing *exactly one* $3\pi/2$ phase slip on every elementary loop of the dual lattice. We show examples of two such configurations in Fig. 2.

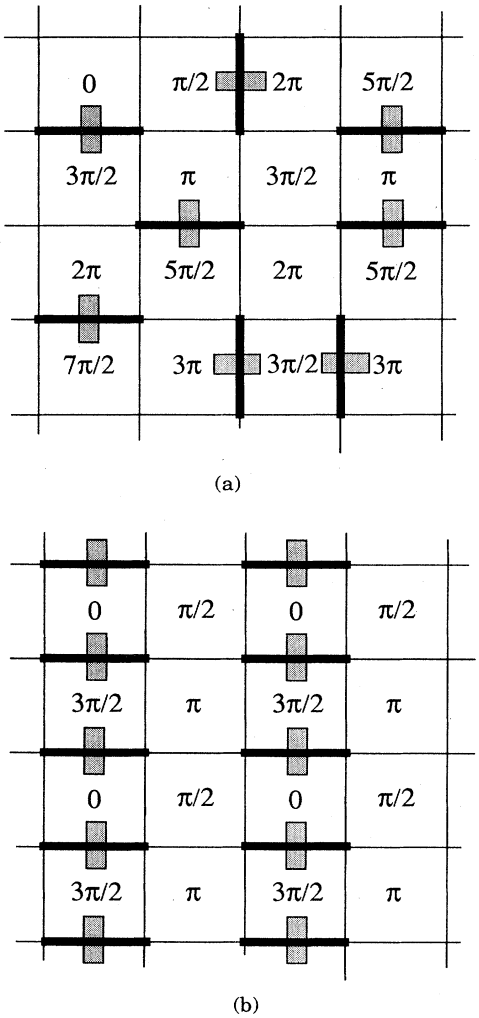

FIG. 2. (a),(b) Two configurations of χ_s^0 which minimize the energy E_1. The shaded boxes denote links of the dual lattice which have a phase slip of $3\pi/2$; all other links have a $\pi/2$ phase slip. The darkened lines of the lattice of spins are conjugate to the $3\pi/2$ phase slips and denote links of the lattice which have values of $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ which differ from those on the thin lines. (b) One of four spin-Peierls states which are global minima of S_{sG}.

We also note from Eqs. (2) and (3) that the values of $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ on bonds intersecting a $3\pi/2$ phase slip will differ from those intersecting a $\pi/2$ phase slip; we refer to the bonds conjugate to a $3\pi/2$ phase slip as "dimers." The condition of one $3\pi/2$ phase slip per loop is easily seen to translate into the condition that the dimers are nonintersecting and close packed. There is thus a remarkable connection between the minima of E_1 and the large-N fermionic mean-field solution of the nearest-neighbor SU(N) antiferromagnet;[3,11] in the latter case the minima of the energy consisted of nearest-neighbor dimers of singlet bonds.

As was the case with the large-N antiferromagnet,[3] it is necessary to consider fluctuation corrections to determine the n_s configurations which are the true global minima of the energy. Expanding S_{sG} to second order in χ_s-χ_s^0 and evaluating the resulting Gaussian functional integral, we find the following corrections to the energy at order $1/y$:

$$E_2(\{n_s\}) = E_2^0 - \frac{cK^2}{2ay} \sum_s \sum_{\langle s,t\rangle\langle s,u\rangle} (\chi_s^0 - \chi_t^0)(\chi_s^0 - \chi_u^0) , \tag{9}$$

where E_2^0 is a constant independent of the n_s and the sum over t and u extends over all the near neighbors of s. A simple calculation shows that E_2 is minimized by the dimer configuration shown in Fig. 2(b) and the three other configurations related to it by the square lattice symmetry. This result is again identical with that obtained in the fermion large-N theory.[3] Thus, our final result is that the ground state of S_{sG} is fourfold degenerate due to spontaneous lattice-symmetry breaking.

We now discuss the effect of adding additional terms to S_{sG}. It is clear that terms which are cosine of simple multiples of $\chi_s - \pi S \zeta_s$ on a single site will only affect the strength of the Gaussian fluctuations but not qualitatively change the form of the results above. Terms involving sums and differences of multiples of $\chi_s - \pi S \zeta_s$ on different sites could possibly change the allowed values of χ_s^0 but it is unlikely that they will reduce the lattice symmetry breaking.

The extension of these results to other values of $2S$(mod 4) is straightforward. The case $2S$(mod4)=3 is very similar to the $S=\frac{1}{2}$ analysis discussed above; we find a fourfold degenerate columnlike spin-Peierls state as the global ground state. For $2S$(mod4)=2, the allowed values of χ_s^0 are $2n_s\pi$ on sublattices W, Y and $(2n_s+1)\pi$ on sublattices X,Z: After minimizing the fluctuations we obtain a twofold degenerate linelike spin-Peierls state as the global ground state.[3,4] Finally for $2S$(mod4)=0, S_{sG} is identical to the usual sine-Gordon model[9] and there is no dynamical symmetry breaking; the χ fluctuations are massive, leading to valence-bond-solid order.[4,5,12]

This paper has examined a previously developed sine-Gordon model for the disordered phase of quantum antiferromagnets on bipartite lattices in two dimensions. We have shown that under renormalization the model scales to a strong-coupling limit whose structure is very similar to the fermion large-N limit of a nearest-neighbor SU(N) antiferromagnet. The scaling to strong coupling is intimately linked to the absence of a rough phase in the three-dimensional interface-roughening problem. In the strong-coupling limit, for $2S$(mod4)$\neq$0, the system is unstable to the formation of a strongly dimerized spin-Peierls state which spontaneously breaks the group of lattice rotations; breakdown of additional symmetries is also possible.

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