Dimerized Phase and Transitions in a Spatially Anisotropic Square Lattice Antiferromagnet

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We investigate the spatially anisotropic square lattice quantum antiferromagnet. The model describes isotropic spin-1/2 Heisenberg chains (exchange constant J) coupled antiferromagnetically in the transverse (J_{\perp}) and diagonal (J_{\times}) , with respect to the chain, directions. Classically, the model admits two ordered ground states—with antiferromagnetic and ferromagnetic interchain spin correlations—separated by a first-order phase transition at $J_{\perp} = 2J_{\times}$. We show that in the quantum model this transition splits into two, revealing an intermediate quantum-disordered columnar dimer phase, both in two dimensions and in a simpler two-leg ladder version. We describe quantum-critical points separating this spontaneously dimerized phase from classical ones.

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An interplay between geometric frustration and guantum fluctuations is at the heart of intensive current investigations into the nature of possible SU(2)-invariant Mott insulators and quantum phase transitions. The absence of any "natural" small parameter, however, makes a traditional perturbative approach difficult. Aside from direct numerical attacks involving exact diagonalization and quantum Monte-Carlo techniques, this feature forces one to extend the parameter space of frustrated magnetic models and explore various "corners" of the resulting phase diagram in the hope of gaining new insights into the physically relevant region of system's parameters. In this Letter, we explore a simple spatially anisotropic frustrated spin model which allows the application of powerful analytical methods borrowed from one dimension.

The model we consider-the spatially anisotropic lattice antiferromagnet-is a square quasi-onedimensional generalization of the well-studied square lattice antiferromagnet with frustrating antiferromagnetic exchange along diagonals, also known as the $J_1 - J_2$ model. It describes a collection of antiferromagnetic spin -S chains with exchange constant J running along horizontal (chain) direction. The chains are interacting with their nearest neighbors via weak antiferromagnetic spin exchange in the transverse (J_{\perp}) and diagonal (J_{\times}) , with respect to the chain, directions. Recently this model was investigated by Nersesyan and Tsvelik (NT) [1] who predicted a novel RVB-like phase with deconfined massive spinons at the special ratio of microscopic exchange constants: $J_{\perp} = 2J_{\times} \ll J$. We shall comment on this work and subsequent numerical investigations [2,3] at the end of our Letter. Let integer index n numerate sites along the chain while index m numerates chains. Then the Hamiltonian is $H = \sum_{m} H_{m}^{(0)} +$ V, where $H_m^{(0)}$ is the standard Heisenberg Hamiltonian of the *m*-th chain and the interchain interaction reads

$$V = \sum_{n,m} \{ J_{\perp} S^a_{n,m} S^a_{n,m+1} + J_{\times} \sum_{q=\pm 1} S^a_{n,m} S^a_{n+q,m+1} \}.$$
 (1)

Here a = x, y, z is the vector index over which implicit summation is implied. The classical $(S = \infty)$ phase diagram is simple: for $J_{\perp} > 2J_{\times}$ ordering of the spins in the transverse to chain direction is antiferromagnetic (AFM phase), whereas for $J_{\perp} < 2J_{\times}$ it is ferromagnetic (FM phase); spins order antiferromagnetically along chains. In the isotropic $J_1 - J_2$ model these orderings correspond to the Néel and four-sublattice phases, respectively. The line $J_{\perp} = 2J_{\times}$ describes a first-order transition between these two phases. Along this line the interchain interaction can be written in a more suggestive form

$$V_{\times} = \sum_{n,m} J_{\times} (S^a_{n,m} + S^a_{n+1,m}) (S^a_{n,m+1} + S^a_{n+1,m+1}).$$
(2)

Our goal is to understand the phase diagram of the quantum S = 1/2 model in the limit of weak interchain couplings $J_{\perp}, J_{\times} \ll J$. Taking the continuum limit along the chain direction (x = na, a is the lattice spacing), the spin operator is decomposed as

$$S_{n,m}^{a} \to a[J_{m,R}^{a}(x) + J_{m,L}^{a}(x) + (-1)^{n}N_{m}^{a}(x)]$$
 (3)

in terms of chiral components $J_{m,R/L}^a$ of the uniform spin magnetization of the *m*-th chain, and the staggered spin magnetization N_m^a (scaling dimension 1/2). The uniform spin magnetization $J_m^a = J_{m,R}^a + J_{m,L}^a$ is the conserved spin current (scaling dimension 1) and a generator of O(3) spin rotations. The two fields in (3) are connected via the following operator product expansion (OPE)

$$J^{a}_{R/L}(x,\tau)N^{b}(x',\tau') = \frac{\overline{\pm i\delta^{ab}\epsilon(x',\tau') + i\epsilon^{abc}N^{c}(x',\tau')}}{4\pi[\upsilon(\tau-\tau') \mp i(x-x')]}$$
(4)

Here the upper/lower signs on the right hand side apply for the right/left (R/L) moving currents, respectively, and $v = \pi J a/2$ is the spin velocity. Of major importance is the appearance of the staggered *dimerization* operator ϵ (scaling dimension 1/2). It is the continuum limit of the lattice operator involving the scalar product of two neighboring spins, $\epsilon_m(x) \sim (-1)^n S_{n,m}^a S_{n+1,m}^a$.

The spin algebra encoded in (4) and well-known OPE of the chiral components of the spin current [4] follow from the fact that the Hamiltonian density of the isolated Heisenberg chain is described by the $SU_1(2)$ WZW model perturbed by a marginally irrelevant backscattering term $[g_{bs} = O(J)]$

$$\mathcal{H}_{m}^{(0)} = \frac{2\pi\nu}{3} (J_{m,R}^{a} J_{m,R}^{a} + J_{m,L}^{a} J_{m,L}^{a}) - g_{bs} J_{m,R}^{a} J_{m,L}^{a}.$$
 (5)

The c-functions appearing in the OPE above are just the Green's functions of right- and left-moving fermions which are governed by the Hamiltonian (5) with $g_{bs} = 0$.

Having exposed the structure of the unperturbed theory, we now turn to the interchain interaction (1). Its continuum low-energy Hamiltonian density contains all terms allowed by the symmetries of the lattice model (these include reflection with respect to transverse direction and translation by one lattice constant)

$$\mathcal{V} = \sum_{m} g_1 N_m^a N_{m+1}^a + g_2 J_m^a J_{m+1}^a + g_3 a^2 \partial_x N_m^a \partial_x N_{m+1}^a + g_4 \epsilon_m \epsilon_{m+1}$$
(6)

Here ∂_x denotes derivative with respect to x and the bare coupling constants follow from substituting (3) in (1)

$$g_1 = (J_{\perp} - 2J_{\times})a, \qquad g_2 = (J_{\perp} + 2J_{\times})a,$$

 $g_3 = \frac{J_{\perp}a}{2}, \qquad g_4 = 0.$ (7)

The scaling dimensions of the first, second, and third interaction terms in (6) are one, two, and three, respectively. The last term (scaling dimension 1) is included here because it respects the symmetries of the lattice model (1). Although its bare coupling constant is zero, quantum fluctuations can (and will) generate some finite g_4 .

At this level the phase diagrams of the quantum model, (6) with $g_4 = 0$, and classical one, (1) with $S = \infty$, are identical. As long as $J_{\perp} \neq 2J_{\times}$, (6) is dominated by the strongly relevant interaction of staggered magnetizations which drives the system into one of the classically ordered phases: AFM for $g_1 > 0$ and FM for $g_1 < 0$.

However, the transitional region $J_{\perp} \approx 2J_{\times}$ requires a closer look because there the amplitudes of the both relevant terms are zero. To begin, let us fine tune to the point $g_1 = 0$. On the lattice this corresponds to (2), whose continuum limit is given by (6) with $g_1 = g_4 = 0$,

$$\mathcal{V}_{\times} = \sum_{m} g_2 J_m^a J_{m+1}^a + g_3 a^2 \partial_x N_m^a \partial_x N_{m+1}^a.$$
(8)

The situation is now apparently controlled by the marginally relevant $(g_2 > 0)$ current-current interaction 127202-2 which seems to suggest that the strongly irrelevant g_3 term does not play any role. Recall that the (Kac-Moody) algebra of spin currents $J_{R/L}^a$ is closed in the sense that OPE of two like currents produces another current of the same chirality [4]. Thus \mathcal{V}_{\times} with $g_3 = 0$ will "reproduce" itself in every order of the expansion in powers of the coupling constant g_2 . This peculiar behavior is destroyed by $g_3 \neq 0$ (or any other equally or even more irrelevant term). To see so, we expand the partition function to second order in \mathcal{V}_{\times} . As follows from the discussion above, one should concentrate on the *cross-term* ($\propto g_2g_3$)

$$\int_{x,\tau}\int_{x',\tau'}J^a_m(x',\,\tau')\partial_xN^b_m(x,\,\tau)J^a_{m+1}(x',\,\tau')\partial_xN^b_{m+1}(x,\,\tau).$$

Applying the OPE (4) to the same-chain operators at nearby points, differentiating the c-function prefactors with respect to x and performing elementary integration over the relative coordinates, one obtains a *relevant* correction to the Hamiltonian of the same form as (6). The coefficients in (7) are thereby replaced by

$$g_1 = \left(J_\perp - 2J_\times + \frac{2J_\times^2}{\pi^2 J}\right)a, \qquad g_4 = -\frac{3J_\times^2 a}{\pi^2 J}, \qquad (9)$$

while two other couplings $g_{2,3}$ remain unchanged. Exactly the same result (9) can be obtained by performing the standard renormalization group (RG) analysis of (5) and (6). There one obtains five coupled nonlinear differential equations for g_{1-4} and g_{bs} . In the transitional region, corresponding to $g_{1,4} = O(J_{\times}^2/J) \ll J_{\times}$, RG equations decouple and admit a simple analytical solution, which reproduces (9), for ℓ of the order 1 (here ℓ parametrizes the short-distance cutoff: $a_{\ell} = a_0 e^{\ell}$). Our derivation of the renormalized coupling constants is very similar in spirit to the recent calculation of second-order corrections to coupling constants of two relevant and competing interactions in the extended Hubbard model [5].

What are the phases of \mathcal{V} with relevant couplings given by (9)? We begin our analysis by studying two coupled chains, that is, frustrated spin ladder (m = 1, 2in (6)). Hamiltonian density of the ladder $\mathcal{H}_{\text{ladder}} =$ $\mathcal{H}_1^{(0)} + \mathcal{H}_2^{(0)} + \mathcal{V}$ can be recast as a theory of four massive real (Majorana) fermions, see Ch. 21 of [4],

$$\mathcal{H}_{\text{ladder}} = \sum_{a=1}^{4} \left(-\frac{iv}{2} \xi_R^a \partial_x \xi_R^a + \frac{iv}{2} \xi_L^a \partial_x \xi_L^a \right) - im_t \sum_{a=1}^{3} \xi_R^a \xi_L^a - im_s \xi_R^4 \xi_L^4 + \delta \mathcal{H}_{\text{marg}}$$
(10)

where $\delta \mathcal{H}_{marg}$, originating from g_{bs} in (5) and g_2 in (6), describes residual *marginal* interactions between Majorana fermions

$$\delta \mathcal{H}_{\text{marg}} = \frac{g_{-}}{4} \left(\sum_{a=1}^{3} \xi_{R}^{a} \xi_{L}^{a} \right)^{2} - \frac{g_{+}}{2} \sum_{a=1}^{3} \xi_{R}^{a} \xi_{L}^{a} \xi_{R}^{a} \xi_{L}^{a} \xi_{R}^{4} \xi_{L}^{4}, \quad (11)$$

with $g_{\pm} = g_2 \pm g_{\rm bs}$. Ignoring $\delta \mathcal{H}_{\rm marg}$, the first three 127202-2

Majorana fermions form a triplet with the mass

$$m_t = \frac{\lambda^2 (g_1 - g_4)}{2\pi a} = \frac{\lambda^2}{2\pi} \left(J_\perp - 2J_\times + \frac{5J_\times^2}{\pi^2 J} \right), \tag{12}$$

whereas the fourth fermion $\xi_{R/L}^4$ is a singlet with

$$m_s = -\frac{\lambda^2 (3g_1 + g_4)}{2\pi a} = -\frac{3\lambda^2}{2\pi} \Big(J_\perp - 2J_\times + \frac{J_\times^2}{\pi^2 J} \Big).$$
(13)

Both masses receive *finite* logarithmic corrections from $\delta \mathcal{H}_{marg}$ which we omit in the following. Here $\lambda \sim 1$ is the expectation value of the charge operator which multiplies abelian bosonization expressions for the staggered magnetization and dimerization operators [6]

$$\mathbf{N}_{m} = \frac{\lambda}{\pi a} (\cos\sqrt{2\pi}\theta_{m}, \sin\sqrt{2\pi}\theta_{m}, -\sin\sqrt{2\pi}\varphi_{m}),$$

$$\boldsymbol{\epsilon}_{m} = \frac{\lambda}{\pi a} \cos\sqrt{2\pi}\varphi_{m}.$$
(14)

The Hamiltonian (10) predicts *two* transitions [7] which happen when one of the renormalized masses becomes zero.

(i) $m_t = 0$: at this point triplet excitations become gapless. Integrating out massive fermion ξ^4 , we find that $\mathcal{H}_{\text{ladder}}$ is the Hamiltonian of the $SU_2(2)$ WZW model with central charge c = 3/2. The nature of the transition is determined by the sign of remaining marginal coupling $g_2 - g_{\text{bs}}$. Its positive initial value implies marginally relevant flow to the strong coupling, and hence, first-order phase transition. For the negative initial value one obtains marginally irrelevant flow of the coupling constant to zero, and hence, second-order transition.

(ii) $m_s = 0$: singlet excitations become massless. This is a continuous Z_2 (Ising) transition.

Properties of the various phases are most conveniently understood from the bosonized form of the *relevant* part of interchain interaction (6), \mathcal{V}_{rel} , which corresponds to mass terms in (10). In terms of symmetric and antisymmetric combinations of bosonic fields on two chains, $\varphi_{\pm} = (\varphi_1 \pm \varphi_2)/\sqrt{2}$ (and similarly for θ_{\pm}) it reads

$$\mathcal{V}_{\rm rel} = \frac{\lambda^2}{2(\pi a)^2} [2g_1 \cos\sqrt{4\pi}\theta_- + (g_1 + g_4) \cos\sqrt{4\pi}\varphi_- - (g_1 - g_4) \cos\sqrt{4\pi}\varphi_+]$$
(15)

Depending on the ratio g_1/g_4 four phases are possible:

(a) $g_1 \rightarrow -\infty$ is the Haldane (effective spin-1 chain) phase; $m_t < 0$, $m_s > 0$ and $\varphi_+ = \sqrt{\pi}/2$, $\theta_- = 0$. Interchain spin correlations are ferromagnetic. This is the ladder analog of the classical FM phase.

(b) $g_1 \rightarrow +\infty$ is the rung-singlet phase; $m_t > 0$, $m_s < 0$ and $\varphi_+ = 0$, $\theta_- = \sqrt{\pi}/2$. Here interchain spin correlations are antiferromagnetic, which corresponds to the classical AFM phase.

(c) $g_4 \rightarrow -\infty$ is the columnar dimer phase (DC); $m_{s,t} > 0$ and $\varphi_+ = 0$, $\varphi_- = 0$. 127202-3 (d) $g_4 \rightarrow +\infty$ is the staggered dimer phase (DS); $m_{s,t} < 0$ and $\varphi_+ = \sqrt{\pi}/2$, $\varphi_- = \sqrt{\pi}/2$.

The last two phases are spontaneously dimerized and do not have classical prototypes. Using (14) we find that both dimerized phases break translational symmetry (along the chain direction) but their ordering patterns are different. In the DC phase $\langle \epsilon_1 \rangle = \langle \epsilon_2 \rangle$, which describes *columnar dimer* long-range order. In the DS phase $\langle \epsilon_1 \rangle = -\langle \epsilon_2 \rangle$, which makes it the *staggered dimer* state. Observe that microscopic couplings (9) choose *columnar dimer* as the intermediate phase between the Haldane and rung-singlet phases of the frustrated ladder.

This feature was missed by [8,9] who described $J_{\perp} =$ $2J_{\times}$ point of the lattice ladder by (8) with $g_3 = 0$. Our analysis shows that multicritical point where chains are coupled only by the marginal current-current interaction requires additional fine tuning of both g_1, g_4 (equally, of m_s, m_t) to zero. A more detailed understanding can be gained by considering the model $g_2 > 0$ and exponen*tially* small relevant couplings $g_{1,4}$ (more specifically $1/|\ln g_{1,4}| \ll g_2$)-though this is not realized by the lattice model. In this case the NT analysis[1] can be taken over, treating $g_{1,4}$ as small perturbations. A semiclassical analysis for $g_{1,4} = 0$ shows that the NT model has a manifold of ground states in which minima of type (a) and (b) above -, i.e., Haldane and rung-singlet states-are degenerate. Perturbing with (15) above *splits* the *energy densities* of these two degenerate states, so that the $g_4 =$ $3g_1$ becomes a first-order transition line (dashed line through the origin in Fig. 1). Furthermore, the spinons of the NT phase correspond to domain walls between these two coexisting states. Remembering that the finite length spin chains in the Haldane phase are characterized by spin-1/2 end states, the spinons become physically transparent as mobile versions of these. Away from the first-order line, such spinons are therefore *confined* (i.e. cost an energy linear in system size), due to the energy cost to create a domain of the disfavored phase. Thus although it does not occur in the lattice model studied



FIG. 1. Phase diagram of the frustrated ladder. Line AB marks the parameters corresponding to the lattice model.

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here, the NT state and its spinons can exist as a first-order line in a generalized ladder model.

Having understood the ladder, we tackle the full twodimensional problem. We treat the relevant interchain interactions $g_{1,4}$ (taking $g_{2,3} = 0$) using a self-consistent mean-field approximation[10,11]. Assuming symmetry breaking along z direction,

$$\mathcal{V} = -z(|g_1|\langle N_m^z \rangle N_m^z + |g_4|\langle \boldsymbol{\epsilon}_m \rangle \boldsymbol{\epsilon}_m) \qquad (16)$$

where we used $\langle N_{m+1}^z \rangle = \pm \langle N_m^z \rangle$ for g_1 negative (positive), and z = 2 is the number of neighboring chains. Using (14) and bosonized form of $\mathcal{H}_m^{(0)}$ (with $g_{\rm bs} = 0$), rescaling euclidian time $\tau = y/v$ and introducing dimensionless euclidian distance r = (x, y)/a, we arrive at the following single-chain sine-Gordon action

$$S_{\rm mf} = \int d^2r \left[\frac{1}{2} (\nabla_r \varphi)^2 - p \sin\sqrt{2\pi}\varphi - q \cos\sqrt{2\pi}\varphi \right]$$
(17)

where dimensionless parameters

$$p \equiv \frac{z\lambda^2|g_1|}{\pi^2 v} \langle \sin\sqrt{2\pi}\varphi \rangle, \quad q \equiv \frac{z\lambda^2|g_4|}{\pi^2 v} \langle \cos\sqrt{2\pi}\varphi \rangle \quad (18)$$

are effective staggered magnetization and dimerization fields, respectively. These averages are found by differentiating the free energy density $F(p, q) = -\ln Z/V$, Z = $\text{Tr}(e^{-S_{\text{mf}}})$ with respect to p and q, respectively. Clearly from (17), the mean-field free energy can depend on p, qonly through $\kappa = \sqrt{p^2 + q^2}$. One can therefore take $F(p, q) = F(0, \kappa)$ and take advantage of exact results for the standard sine-Gordon action[12]. In particular $dF/d\kappa = -c_1\kappa^{1/3}$, where the numerical constant c_1 follows from equations (10-14) of ref.[12]

$$c_1 = \frac{\tan(\pi/6)}{3} \left(\frac{2\Gamma(1/6)}{\sqrt{\pi}\Gamma(2/3)}\right)^2 \left(\frac{\pi\Gamma(3/4)}{2\Gamma(1/4)}\right)^{4/3}.$$
 (19)

Thus our self-consistent equations

$$\langle \sin\sqrt{2\pi}\varphi \rangle = \frac{c_1 p}{\kappa^{2/3}}, \langle \cos\sqrt{2\pi}\varphi \rangle = \frac{c_1 q}{\kappa^{2/3}}$$
 (20)

become simple algebraic ones. They predict two transitions, at $g_1 = \pm |g_4|$, where both order parameters $(N_m^z, \epsilon_m \sim p, q)$ are nonzero. This makes them *first-order* transitions - the first-order nature may be an artifact of the mean-field approximation. These two transitions separate three phases, indicated in Fig. 2. For $|g_1| > |g_4|$, $p \neq 0, q = 0$, so the system is AFM or FM, depending on the sign of g_1 . For $|g_1| < |g_4|$, one finds the columnar dimer phase (rather than staggered since $g_4 < 0$). Note that obtained phase diagram (Fig. 2) is in qualitative agreement with that of the ladder, which provides a posteriori support of our mean-field treatment. Moreover, it agrees very well with the phase diagram of the lattice model (1) obtained in the exact diagonalization study [3]. We should add that DC phase was not observed in density matrix renormalization group study [2], pre-



FIG. 2. Phase diagram of the two-dimensional model. Solid (dashed) lines denote phase boundaries of the quantum (classical) model.

sumably due to strong finite-size effects at small J_{\perp}/J . Now, since exactly this type of dimer ordering is known to take place in the spatially isotropic $J_1 - J_2$ model [13], it is natural to conclude that the DC phase found here extends all way up to $J_{\perp} = J$.

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