RAPID COMMUNICATIONS

PHYSICAL REVIEW B **74**, 140407(R) (2006)

Effective field theory with a θ-vacua structure for two-dimensional spin systems

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(Received 13 June 2006; revised manuscript received 12 September 2006; published 27 October 2006)

We construct a nonlinear σ (NLσ) model description of (2+1)-dimensional [(2+1)D] antiferromagnetic spin systems, by coupling together spin chains via interchain exchange terms. Our mapping incorporates methods developed recently by ourselves and by Senthil and Fisher, which aim at describing competition between antiferromagnetic and valence-bond-solid orders in quantum magnets. The resulting (2+1)D O(4) NLσ model contains a topological θ term whose vacuum angle θ varies continuously with δ, the bond-alternation strength of the interchain interaction. This implies that the θ-vacua structure for this NLσ model can be explored by tuning δ in a suitable 2D spin system, which is strongly reminiscent of the situation for 1+1 antiferromagnetic spin chains with bond alternation.

DOI: 10.1103/PhysRevB.74.140407 PACS number(s): 75.10.Jm, 73.43.Nq, 74.20.Mn, 75.10.Pq

The semiclassical description of antiferromagnetic (AF) spin chains in terms of an O(3) nonlinear σ (NLσ) model provides a simple and yet powerful format for detecting quantum exotica in one dimension (1D).[1] In this language one exercises special care to keep track of possible "θ terms,"[2] which introduce complex-number-valued weights, and hence nontrivial quantum interference among configurations into the partition function $Z[\boldsymbol{n}]=\int\mathcal{D}\boldsymbol{n}\, e^{-(S_{NL\sigma}+S_\theta)}$. The θ-term action is $S_\theta=i\theta\mathcal{Q}_{\tau x}$, where the winding number $\mathcal{Q}_{\tau x} \equiv 1/4\pi\int d\tau dx \boldsymbol{n}\cdot\partial_\tau\boldsymbol{n}\times\partial_x\boldsymbol{n}$ probes the global topology of the unit Néel vector $\boldsymbol{n}$'s space-time configuration. The presence of S_θ has profound consequences;[3] in particular a continuous quantum phase transition is encountered when the vacuum angle θ traverses the value $\theta=\pi$ modulo 2π. Following the success in discriminating between the spectral properties of integer and half-integer spin systems,[1] this framework was applied to bond-alternating AF spin chains,[4] with the Hamiltonian $H=\Sigma_i J[1-(-1)^i\delta]\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1}$. Here θ was found to depend on the bond-alternation strength δ as $\theta=2\pi S(1-\delta)$. Sweeping δ through the interval $[-1,1]$ would therefore enable one to probe the entire θ-vacua structure, in which process the system will undergo $2S$ successive quantum phase transitions between different valence-bond-solid (VBS) states, as later verified numerically.[5] Variants of this mapping technique are now incorporated routinely to determine the global phase diagram of 1D and quasi-1D AF systems.

The present study addresses the question of whether there exists a class of bulk 2D spin systems that can also be described in terms of a NLσ model exhibiting a nontrivial θ-vacua structure. This is in part motivated by recent interest in exotic phase transitions in 2D AFs, e.g., between 2D VBS states.[6] We will show that certain inter-VBS transitions in 2D can indeed be described by a NLσ model with a θ term, albeit on the target manifold O(4). [Observe that four is the required number of components for constructing the winding number $\mathcal{Q}_{\tau xy}$ (defined later), which is the (2+1)D analog of $\mathcal{Q}_{\tau x}$.]

Earlier searches for novel Berry phase effects in 2D AFs were carried out in the framework of the (2+1)D O(3) NLσ model,[1,7,8] and showed that singular hedgehog events leave behind Berry phase factors that drive the system into a VBS paramagnet.[7,9] An alternative strategy is to drop the O(3) description where the amplitude of the AF order parameter is kept fixed, and instead use a composite five-component order parameter explicitly accounting for the competition between the three AF and two (horizontal and vertical) VBS components. Previously we found[10] that the (2+1)D O(5) NLσ model derived in this spirit from competing orders inherent in the Marston-Affleck π-flux state contains a new Wess-Zumino (WZ) term, which reproduces the hedgehog Berry phase factors in certain limits. We also observed that "freezing" the fluctuating VBS amplitude along one of the two spatial directions, thereby reducing the number of effective components to four, will turn our effective O(5) action into a (2+1)D O(4) NLσ model with a θ term. This leads us to an intriguing possibility which we take up below: that a θ-vacua structure may arise out of a 2D spin system sustaining an AF-VBS competition with a strong spatial anisotropy, such as may be realized in a stack of coupled 1D spin chains with sufficient competing orders along the intrachain direction.

To further exploit this possibility, we make a suitable extension of Senthil and Fisher's recent work[11] motivated along similar lines, which takes as its point of departure Wess-Zumino-Witten (WZW) models, i.e., 1D systems conveniently equipped (see below) with the desired intrachain AF-VBS competition. These authors demonstrate that coupling the WZW models uniformly along a transversal direction indeed yields an O(4) model at $\theta=\pi$. Our objective of exposing the θ-vacua structure in its entirety prompts us to a search for spin interactions that can sweep θ away from this value. Guided by analogy with the spin chain counterpart,[4] we show in the following that (1) adding on a bond-alternating component to the interchain interaction does just such a job, and (2) extracting such a correction to the vacuum angle involves a crucial intermediate step, consisting of identifying and integrating out high-frequency modes.

We first collect features of the level-1 SU(2) WZW model relevant to our study. In the spin chain context, this system simply describes the quantum criticality arising from competing AF and VBS orders.[10–12] This becomes transparent when the SU(2)-valued WZW field g is written in terms of a unit four-vector ϕ_α ($\alpha=0,1,2,3$), viz., $g=\phi_0+i\boldsymbol{\phi}\cdot\boldsymbol{\sigma}$, where $\boldsymbol{\phi}\equiv(\phi_1,\phi_2,\phi_3)$. Indeed non-Abelian bosonization techniques can be employed to check that ϕ_0 and $\boldsymbol{\phi}$ each correspond in spin language to the dimer (VBS) order parameter $(-1)^i\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}\rangle$, and the Néel vector $\boldsymbol{n}(x)$.[13] As a functional of the composite AF-VBS order parameter ϕ_α, the WZW action becomes an O(4) NLσ model with a WZ term,

$$\mathcal{S}[\phi_\alpha] = \frac{1}{8\pi}\int d\tau\, dx[(\partial_\tau \phi_\alpha)^2 + (\partial_x \phi_\alpha)^2] + \Gamma[\phi_\alpha], \quad (1)$$

where the WZ functional is

$$\Gamma[\phi_\alpha] = \frac{i\epsilon^{abcd}}{\pi}\int_0^1 dt \int d\tau\, dx\ \phi_a \partial_t \phi_b \partial_\tau \phi_c \partial_x \phi_d. \quad (2)$$

The extra parameter $t \in [0,1]$ is a complication common to all WZ-type terms; its purpose here is to locally frame the three-dimensional "area" on the surface of the hypersphere S_3 swept out by the map $(x,\tau) \in S_2 \to \phi_\alpha \in S_3$. We record two properties of $\Gamma[\phi_\alpha]$ which we incorporate below. First, the change under a slight deformation of the configuration $\phi_\alpha \to \phi_\alpha + \delta\phi_\alpha$ can be written as a local functional (i.e., one without t):

$$\delta\Gamma[\phi_\alpha(\tau,x)] = \frac{i\epsilon^{abcd}}{\pi}\int d\tau\, dx\ \phi_a \delta\phi_b \partial_\tau \phi_c \partial_x \phi_d + O(\delta\phi_\alpha^2). \quad (3)$$

Second, since $\Gamma[\phi_\alpha]$ is linear in all four components of the vector ϕ_α, simultaneously flipping any three will induce a sign change. In particular,

$$\Gamma[\phi_0, -\boldsymbol{\phi}] = -\Gamma[\phi_0, \boldsymbol{\phi}]. \quad (4)$$

Following Ref. 11 we now stack our 1D $\phi_\alpha(\tau,x)$ chains along a second (y) spatial direction. We include a bond alternation δ in the interchain coupling, anticipating its contribution to the θ term. As seen below, the interchain interaction $\mathcal{S}_\perp = \int d\tau H_\perp$ that generates our θ vacua bears the form

$$H_\perp = -\int dx \sum_y \{J_\perp[1 + (-1)^y \delta]\boldsymbol{N}(x,y) \cdot \boldsymbol{N}(x,y+1) + J_\perp[1 - (-1)^y \delta] N_0(x,y) N_0(x,y+1)\}, \quad (5)$$

with $J_\perp > 0$, and $N_\alpha(x,y) = (N_0(x,y), \boldsymbol{N}(x,y)) \equiv (\phi_0(x,y) + a(-1)^y l_0(x,y), (-1)^y \boldsymbol{\phi}(x,y) + a\boldsymbol{l}(x,y))$ (a is the lattice constant). Here a small and rapidly fluctuating component $l_\alpha(x,y) = (l_0(x,y), \boldsymbol{l}(x,y))$, to be eventually integrated out, has been added on top of the slowly varying field $\phi_\alpha(x,y)$. This plays a role analogous to that of the uniform magnetization $\boldsymbol{L}$ in the 1D problem (the subdominant fluctuation in that case), which needed to be integrated out in order to arrive at the final effective action.[1] The SU(2) symmetry of the WZW field g imposes the constraint $N_\alpha N_\alpha = N_0^2 + \boldsymbol{N}^2 \equiv 1$, which implies that $\phi_\alpha l_\alpha = 0$. The form of $H_\perp$ dictates how the slow and rapid modes of the WZW fields on adjacent chains are to align. The slow fluctuations consist of a staggered alignment of $\boldsymbol{\phi}(x,y)$ fields and a columnar alignment of $\phi_0(x,y)$ fields along the y direction.[11] This is consistent with our previous work, which suggested that an intrinsic competition between 2D AF and columnar dimer states exists in the vicinity of the π-flux state.[10] As for the rapidly varying modes, the vector

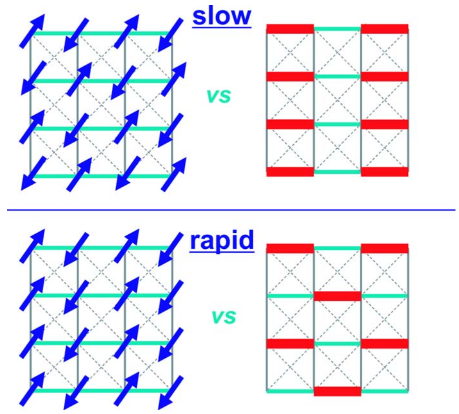

FIG. 1. (Color online) Slowly and rapidly fluctuating degrees of freedom, expressed in terms of competing AF and VBS ordering tendencies. The rapid modes are integrated out to derive an effective action for the slow modes. Crossed lines indicate the presence of a frustrating exchange discussed later in the text.

$\boldsymbol{l}(x,y)$ tends to pile up in a ferromagnetic fashion, while the component l_0 corresponds to a staggered VBS configuration. This situation is depicted in Fig. 1. Later we will return to the issue of how these relate to a real spin system.

Our goal below is to extract an effective theory for $\phi_\alpha(\tau,x,y)$. Readers familiar with Haldane's mapping for AF spin chains[7] may find what follows more tractable by keeping in mind the set of correspondences between the 1D and 2D cases, displayed in Table I. In the last row, the winding number $\mathcal{Q}_{\tau xy} \equiv \frac{1}{2\pi^2}\int d\tau\, dx\, dy\, \epsilon^{abcd}\phi_a \partial_\tau \phi_b \partial_x \phi_c \partial_y \phi_d$, associated with the homotopy $\Pi_3(S_3)$, enters into the θ term for the (2+1)D O(4) NLσ model.

We now proceed to the continuum approximation. We begin by carrying out the y summation over the WZ functionals with the help of Eqs. (3) and (4):

$$\sum_y \Gamma[\phi_0 + a(-1)^y l_0, (-1)^y \boldsymbol{\phi} + a\boldsymbol{l}] = \sum_y (-1)^y \Gamma[\phi_\alpha] + \frac{ia}{\pi}\epsilon^{abcd}\sum_y \int d\tau\, dx\ \phi_a l_b \partial_\tau \phi_c \partial_x \phi_d. \quad (6)$$

The alternating series in the last line is converted into an integral[11] $\Sigma_y(-1)^y \Gamma[\phi_\alpha(y)] \sim \frac{1}{2}\int dy \partial_y \Gamma[\phi_\alpha] = -i\pi \mathcal{Q}_{\tau xy}$. Next we turn to the interchain term $H_\perp$, which contains two contributions $H_{\perp 1}$ and $H_{\perp 2}$, where $H_{\perp 1} = -\int dx\, J_\perp \Sigma_y N_\alpha(y) N_\alpha(y+1)$, and $H_{\perp 2} = -\int dx\, J_\perp \delta \Sigma_y (-1)^y [N_0(y) N_0(y+1) - \boldsymbol{N}(y) \cdot \boldsymbol{N}(y$

TABLE I. Correspondence with Haldane's mapping in 1D.

1D [O(3)]	2D [O(4)]
$\boldsymbol{n}(\tau,x) + (-1)^x a/s\boldsymbol{L}(\tau,x)$	$\phi_\alpha(\tau,x,y) + a(-1)^y l_\alpha(\tau,x,y)$
$iS\omega[\boldsymbol{n}(\tau,x)]$	$\Gamma[\phi_\alpha(\tau,x,y)]$
$i\delta\omega[\boldsymbol{n}] = i\int d\tau\, \boldsymbol{n} \cdot \delta\boldsymbol{n} \times \partial_\tau \boldsymbol{n}$	Eq. (3)
$\omega[-\boldsymbol{n}] = -\omega[\boldsymbol{n}]$	Eq. (4)
$S_\theta = i\theta\mathcal{Q}_{\tau x}$	$S_\theta = i\theta\mathcal{Q}_{\tau xy}$

+1)]. Here we have suppressed the explicit dependence on x for brevity. The continuum forms of these interactions (discarding oscillatory contributions) read

$$H_{\perp 1} \sim \int dx\, dy \left(\frac{J_\perp}{2} a (\partial_y \phi_\alpha)^2 + 2 J_\perp a l_\alpha^2 \right) \tag{7}$$

and

$$H_{\perp 2} \sim 2 J_\perp \delta a \int dx\, dy\, l_\alpha \partial_y \phi_\alpha. \tag{8}$$

Finally we integrate over l_α, by collecting terms from Eqs. (6)–(8), and completing the square with respect to l_α. Dropping a higher-order derivative term and carrying out a suitable rescaling, our effective action reads

$$\mathcal{S}_{eff}[\phi_\alpha(\tau,x,y)] = -i\pi(1-\delta)\mathcal{Q}_{\tau xy} + \int d^3x \frac{1}{2g}\left(\frac{1}{v}(\partial_\tau \phi_\alpha)^2 + v(\partial_x \phi_\alpha)^2 + v(1-\delta^2)(\partial_y \phi_\alpha)^2 \right), \tag{9}$$

where the velocity v and the coupling constant g depend on parameters of the original Hamiltonian. The main findings here are (1) the dependence of the vacuum angle on the bond-alternation parameter $\theta = \pi(1-\delta)$, and (2) the factor $(1-\delta^2)$ that enters the coefficient for the interchain kinetic energy, both of which coincide with known results[4] for the $S=1/2$ bond-alternated spin chain. In particular the vacuum angle $\theta=\pi$ (corresponding to $\delta=0$) lies at the point in parameter space where the "strong" and "weak" vertical bonds are interchanged. To strengthen the analogy we can generalize to arbitrary S, by starting with the level $2S$ WZW model. Repeating the mapping procedure then gives $\theta = 2\pi S(1-\delta)$, an exact reproduction of the 1D result mentioned earlier.

The parallelism discussed above naturally leads us to adopt the physical picture established within the spin chain context, and associate the $\theta = \pi (\mathrm{mod}\, 2\pi)$ points with phase transitions between different (vertical) VBS ground states. In the presence of an AF-favoring anisotropy, one can seek some support for this expectation by invoking the meron gas expansion[2,14] described for the case $\theta=\pi$ in Ref. 11. Extending this to arbitrary θ results in an effective sine-Gordon type theory of the form

$$\mathcal{S}_{meron}[\varphi] = \int d\tau\, dx\, dy \left(K(\partial_\mu \varphi)^2 - \lambda_1 \cos\frac{\theta}{2} \cos\varphi - \lambda_2 \cos\theta \cos 2\varphi + \cdots \right). \tag{10}$$

In the above, each harmonic [proportional to $\cos(n\varphi)$] represents the process associated with single merons $(n=1)$, doubled merons $(n=2)$, etc. When $\theta \neq \pi$ $(\delta \neq 0)$, the $\cos\varphi$ term is the most relevant (provided the fugacity expansion is valid) and picks out a unique ground-state value for φ with (depending on θ) either $e^{i\varphi}=1$ or $e^{i\varphi}=-1$. Resorting to the symmetry analysis of Senthil and Fisher,[11] one finds that this corresponds to a vertical VBS state that simply follows the externally imposed bond-alternation pattern. The special role

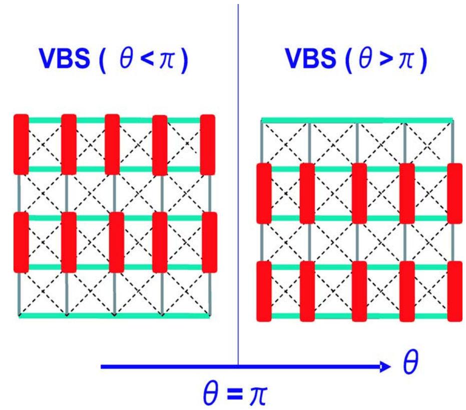

FIG. 2. (Color online) The proposed θ-vacua structure in the presence of AF-favoring anisotropy as applied to the case of $S=1/2$.

of the $\theta=\pi$ point manifests itself here in the vanishing of the $\cos\varphi$ term and all other odd harmonics. Here the doubled meron term $\cos 2\varphi$ becomes dominant, leading to doubly degenerate ground states satisfying $e^{i\varphi}=\pm i$.[11] Hence, tracing the change of θ through $\theta=\pi$ shows that the system switches at this point between two vertical VBS states, corresponding to $e^{i\varphi}=1$ and $e^{i\varphi}=-1$ (Fig. 2).

While the foregoing establishes a link (together with a qualitative physical picture) between 2D spin systems and the (2+1)D O(4) NLσ model with a tunable θ term, mapping out the precise phase diagram of the latter, especially near $\theta=\pi$, calls for further investigations, e.g., through numerical schemes similar to those that have been applied to the (1+1)D O(3) NLσ model with a θ term.[15] Another obvious question to address is the circumstances under which the above physics is likely to emerge in actual spin systems. Since 2D AFs have much stronger tendencies toward Néel ordering than in 1D, one would generally expect an AF phase to intervene between different VBS phases.[16] A partial clue toward resolving this issue lies in the mapping process itself; it is clear that the system consistent with the preceding derivation must have the l_α modes as the chief rapid fluctuations. With the introduction of a frustrating diagonal exchange, configurations such as depicted in the lower half of Fig. 1 would start to have significant weight, thus weakening the AF dominance. Frustrated anisotropic spin systems with external bond alternation are therefore likely places to seek realizations. (Similar situations may also arise by projecting 3D frustrated magnets such as studied in Ref. 17 onto an effective model of coupled chains.) If a direct inter-VBS transition is observed with an appropriate amount of frustration—perhaps supplemented with additional perturbations—our results suggest that such points are described by the strong-coupling regime of our effective theory at $\theta=\pi$. Thus, although considerably fragile in nature compared to the 1D case, we believe our model should have relevance to actual frustrated magnets.

We close with two additional clarifying remarks. (1) Readers can check that various aspects of θ-term physics familiar from 1D will find incarnations in our (2+1)D problem. To name one, the θ term for an open spin chain contains a boundary contribution that induces an edge state with fractional spin.[18] This would correspond here to spin-chain-like channels localized to the upper and lower ends of our system. (2) Mathematically our prescriptions rest on rather general relations between θ terms and WZ terms,[19] and are hence readily generalized to arbitrary dimensions. A 3D system with a θ-vacua structure can be derived by repeating the above steps in one dimension higher, where the appropriate starting point would now be the (2+1)D O(5) model that we found in Ref. 12. The latter contains the WZ term [compare with Eq. (2)] $\Gamma^{2+1}[\boldsymbol{\phi}_{\rm VBS},\boldsymbol{\phi}_{\rm AF}] = -i\frac{3}{4\pi}\int_0^1 dt \int d\tau\, dx\, dy\, \epsilon^{abcde}\phi_a\partial_t\phi_b\partial_\tau\phi_c\partial_x\phi_d\partial_y\phi_e$, where the VBS sector of the five-component composite order parameter $\boldsymbol{\phi}_{\rm VBS}$ consists of two components. Stacking up the 2D systems along a third (z) direction, we obtain in the absence of bond alternation a Berry phase term, $i\pi\mathcal{Q}_{\tau xyz}$, where $\mathcal{Q}_{\tau xyz} = \frac{3}{8\pi^2}\int d\tau\, dx\, dy\, dz\, \epsilon^{abcde}\phi_a\partial_\tau\phi_b\partial_x\phi_c\partial_y\phi_d\partial_z\phi_e$. This is a NL$\sigma$ model with $\theta=\pi$, this time in (3+1)D and taking values on the manifold O(5). Here again, adding on an interplanar bond alternation would shift the value of θ, with the point $\theta=\pi$ (invariant under $\mathcal{Q}_{\tau xyz}\to -\mathcal{Q}_{\tau xyz}$) playing a special role. Such theories may well capture new physics in 3D magnets.

In summary we have proposed that direct transitions among VBS states in anisotropic 2D AF systems can in certain cases be described in terms of the θ-vacua structure of the (2+1)D O(4) NLσ model, in much the same way that inter-VBS transitions in spin chains have been understood using the θ term of the (1+1)D O(3) NLσ model. We suggested that realizations may be found in anisotropic frustrated magnets.

We thank M. Kohno and C. Yasuda for fruitful discussions. This work was supported in part by a Grant-in-Aid for Scientific Research (C) No. 10354143 from the Ministry of Education, Culture, Sports, Science and Technology of Japan.

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