

## Many-Body Spin Berry Phases Emerging from the $\pi$ -Flux State: Competition between Antiferromagnetism and the Valence-Bond-Solid State

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We uncover new topology-related features of the  $\pi$ -flux saddle-point solution of the  $D = 2 + 1$  Heisenberg antiferromagnet. We note that symmetries of the spinons sustain a built-in competition between antiferromagnetic (AFM) and valence-bond-solid (VBS) orders, the two tendencies central to recent developments on quantum criticality. An effective theory containing an analogue of the Wess-Zumino-Witten term is derived, which generates quantum phases related to AFM monopoles with VBS cores, and reproduces Haldane's hedgehog Berry phases. The theory readily generalizes to  $\pi$ -flux states for all  $D$ .

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Our understanding on quantum critical points [1] or phases [2] in  $D = 2 + 1$  antiferromagnets, and the issue of deconfinement therein have recently undergone a rapid sequence of developments. Competition between antiferromagnetic (AFM) and valence-bond-solid (VBS)-like fluctuations constitute the basic premises for much of these activities. These theories have brought into wide recognition the relevance of monopole defects of the AFM order-parameter and, in particular, the nontrivial Berry phase factors [3,4] associated with such objects. Here, with these new perspectives, we revisit the Berry phase effect [5] in states emerging from the  $\pi$ -flux saddle-point solution of the Heisenberg antiferromagnet [6], a popular point of departure for studying undoped and lightly doped cuprate Mott insulators. We find that their topological properties are rather rich. Among our findings are (1) a *chiral* symmetry of the  $\pi$ -flux Dirac fermion relating the AFM and VBS orders, which leads us to a natural framework for studying their mutual competition, (2) a low energy effective theory with a novel many-spin Berry phase term for which the contributions from a *composite* defect (see below) reproduce the monopole Berry phases, (3) a natural extension of such a framework to arbitrary dimensions with possible relevance to higher dimensional spin liquids.

It is worth digressing on the second point before proceeding to the more technical aspects. An important feature of monopole excitations is the energy cost due to the rapid modulation of the AFM order near the singular core. Meanwhile, in the discussions which follow, the system takes advantage of the inherent AFM-VBS competition and saves energy by escaping into a local VBS state at the defect cores. Such physics share in spirit with work by Levin and Senthil [7], who study AFM-VBS competition starting from the VBS side. In that work, the four-state clock ordering of the VBS state is disordered through the introduction of  $Z_4$  vortices. Close inspection of the lattice model shows that these defects have an AFM core, as opposed to conventional vortices with featureless singular cores; hence their condensation leads to the Néel state.

Likewise, it is natural to expect a VBS core to be present in a hedgehog-like configuration of the AFM order parameter, the condensation of which would give way to a VBS state. Indeed we will see that incorporation of this feature is essential in recovering the hedgehog Berry phases [3,4] starting from the  $\pi$ -flux state.

*Chiral structure of  $\pi$ -flux state.*—The  $\pi$ -flux hopping Hamiltonian on a two dimensional square lattice is  $\mathcal{H}_\pi = \sum_{i,\mu,\sigma} t c_{i\sigma}^\dagger \mathbf{T}_\mu c_{i\sigma}$ , where  $\mathbf{T}_\mu$  with  $\mu = x, y$  generates translation by one site. The  $\pi$ -flux condition imposes the anticommutation relation  $\{\mathbf{T}_x, \mathbf{T}_y\} = 0$ , which immediately leads to the spinon's dispersion  $E(\mathbf{k}) = \pm t \sqrt{\cos^2 k_x + \cos^2 k_y}$  with Dirac nodes at  $\mathbf{k} = (\frac{\pi}{2}, \pm \frac{\pi}{2})$ . It is convenient to group together the four sites sharing a unit plaquette (Fig. 1) into components (with spin indices) of a Dirac spinor,  $\Psi = (\psi_{1\sigma}, \psi_{2\sigma}, \psi_{3\sigma}, \psi_{4\sigma})$  [8].

To fix the representation of the Dirac gamma matrices, we account for the  $\pi$ -flux condition by assigning negative hopping integrals  $-t$  to links residing on every other horizontal rows; all other links have positive hopping integrals,  $+t$ . Linearizing around the nodes, we arrive at the Dirac action (hereafter we employ Euclidean space-time conventions)  $\mathcal{L} = i\bar{\Psi}\not{\partial}\Psi$ , where the slash indicates the contraction with the gamma matrices  $\gamma_0 = \tau_0 \otimes \tau_z$ ,  $\gamma_1 = -\tau_0 \otimes \tau_x$ ,  $\gamma_2 = \tau_y \otimes \tau_y$ . Here the first (second) ma-

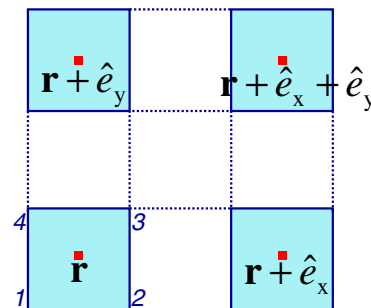


FIG. 1 (color online). Lattice used to derive continuum Dirac theory.

trix within a direct product determines the block structure (the matrix elements within the cells).

A recent study indicates that the algebraic spin liquid described by the  $\pi$ -flux Hamiltonian is stable against monopoles, at least for large  $N$  [2]. We now move away from this critical phase by supplementing the theory with mass terms so that the system can acquire AFM order. Indeed, earlier works on the  $\pi$ -flux state show [9] that a substantial improvement on the variational energy is achieved by adding on a spin density wave (SDW) term  $\mathcal{H}_{\text{SDW}} = \sum_i M(-1)^{i_x+i_y} c_{i\alpha}^\dagger (\sigma_z)_{\alpha\beta} c_{i\beta}$ , which appears to be in accord with angular resolved photoemission experiments on cuprate Mott insulators [10]. With the aim of extracting the dependence of the effective action with possible Berry phase terms on the Néel unit director  $\mathbf{n}$ , we make in  $\mathcal{H}_{\text{SDW}}$  the generalization  $\sigma_z \rightarrow \mathbf{n} \cdot \boldsymbol{\sigma}$ . Physically this potential energy term imposes the generation of an AFM spin moment with a space-time-dependent orientation  $\mathbf{n}(\tau, x, y)$ , and yields in the continuum limit the mass term  $\mathcal{L}_{\text{AFM}} = im_{\text{AFM}} \bar{\Psi}(\mathbf{n} \cdot \boldsymbol{\sigma})\Psi$ . Next, we recall [8,11] that in contrast to usual irreducible representations for Dirac fermions in  $D = 2 + 1$  where the notion of chirality is absent (no “ $\gamma_5$ ”), we have *two* generators of chiral transformations at our disposal,  $\gamma_3 = \tau_z \otimes \tau_y$  and  $\gamma_5 = \tau_x \otimes \tau_y$  which anticommute mutually as well as with the space-time components  $\gamma_0, \gamma_1$ , and  $\gamma_2$ . One reads off from the explicit matrix elements that the effects of chiral mass terms proportional to  $\bar{\Psi}\gamma_3\Psi$  and  $\bar{\Psi}\gamma_5\Psi$  each amount to breaking lattice translational symmetry by introducing bond alternations  $t \rightarrow t + (-1)^{i_\mu} \delta t$  in the horizontal ( $\mu = x$ ) and vertical ( $\mu = y$ ) directions. A crucial observation here is that the SDW and the two VBS ordering potentials  $i\bar{\Psi}Q\Psi$ ,  $\bar{\Psi}\gamma_3\Psi$  and  $\bar{\Psi}\gamma_5\Psi$  ( $Q \equiv \mathbf{n} \cdot \boldsymbol{\sigma}$ ) all belong to the family of chirally rotated mass terms  $\mathcal{L}_{\text{chiral}} \propto i\bar{\Psi}Qe^{i(\alpha\gamma_3+\beta\gamma_5)\otimes Q}\Psi$  ( $\alpha, \beta \in \mathbf{R}$ ); i.e., they transform into one another by suitable chiral transformations. The 4D representation also allows for an alternative class of mass term [11],  $\bar{\Psi}\gamma_3\gamma_5\Psi$ . There the parity anomalies responsible for Chern-Simons terms do not cancel between the two nodes (i.e., a chiral spin liquid [12]), and take us out of the manifold of  $T$ -invariant states. We do not retain this term.

*Bosonization.*—The preceding implies that the spontaneous breaking of the chiral symmetry present in the  $\pi$ -flux state can lead to AFM or VBS orders, depending on the chiral angles  $\alpha$  and  $\beta$  [13]. This has motivated us to study the AFM-VBS competition in terms of the following theory with a generalized mass term (equivalent to  $\mathcal{L}_{\text{chiral}}$ ),

$$\mathcal{L}_{\text{F}}^{2+1} = i\bar{\Psi}[\not{\partial} + mV_{(2+1)}]\Psi, \quad (1)$$

where  $V_{(2+1)} \equiv v^1\sigma_x + v^2\sigma_y + v^3\sigma_z + i\gamma_3v^4 + i\gamma_5v^5$ , and  $\mathbf{v}_{(2+1)} \equiv (v^1, \dots, v^5)$  is a five component unit vector. The first three components comprise a vector  $\mathbf{v}_{\text{AFM}} \equiv (v^1, v^2, v^3)$  which is parallel to  $\mathbf{n}$  and in competition with a VBS-like order parameter ( $v^4, v^5$ ). We now show that this theory can be “bosonized” in terms of  $\mathbf{v}_{(2+1)}$ , to

yield an effective action which contains a new Berry phase term. Central to this feat is the following relation [14,15] satisfied by the Dirac operator  $\mathcal{D}[\mathbf{v}_{(2+1)}] = i\not{\partial} + imV_{(2+1)}$  and its Hermitian conjugate,

$$\mathcal{D}^\dagger \mathcal{D} = -\partial^2 + m^2 - m\not{\partial}V_{(2+1)}, \quad (2)$$

which enables one to rewrite the variation of the fermionic determinant  $S_{\text{eff}} = -\text{ln det} \mathcal{D}[\mathbf{v}_{(2+1)}]$  into a form suitable for generating a derivative expansion:

$$\delta S_{\text{eff}} = -\text{Tr} \left[ \frac{1}{-\partial^2 + m^2 - m\not{\partial}V_{(2+1)}} \mathcal{D}^\dagger \delta \mathcal{D} \right]. \quad (3)$$

It is easy to see that a nonlinear sigma ( $\text{NL}\sigma$ ) model  $S_{\text{NL}\sigma} = \frac{1}{2g} \int d^3x (\partial_\mu \mathbf{v}_{(2+1)})^2$  arises, with  $g$  a nonuniversal coupling constant. Less trivial is an imaginary contribution to Eq. (3),  $\delta S_{\text{BP}}^{2+1}$ , which we pick up at third order in powers of  $\not{\partial}V_{(2+1)}$ . As is usual with Wess-Zumino type terms, one recovers the action  $S_{\text{BP}}^{2+1}$  from its variation  $\delta S_{\text{BP}}^{2+1}$  with the aid of an auxiliary variable  $t \in [0, 1]$  which smoothly sweeps the extended function  $\mathbf{v}_{(2+1)}(t, x_\mu)$  between its two asymptotics, a fixed value at  $t = 0$ , say  $(0,0,0,0,1)$ , and the physical value at  $t = 1$ ,  $\mathbf{v}_{(2+1)}(x_\mu)$ . The result is

$$S_{\text{BP}}^{2+1} = \frac{-2\pi i \epsilon_{abcde}}{\text{Area}(S^4)} \int_0^1 dt \int d^3x v^a \partial_t v^b \partial_\tau v^c \partial_x v^d \partial_y v^e, \quad (4)$$

where  $\text{Area}(S^4) = \frac{2\pi^{5/2}}{\Gamma(\frac{5}{2})} = \frac{8}{3}\pi^2$ . Topologically, this is  $-i2\pi$  times the winding number which counts the number of times the compacted “space-time”  $\{(t, x_\mu)\}$  isomorphic to  $S^3 \times S^1 \sim S^4$  wraps around the target space (also  $S^4$ ) for  $\mathbf{v}_{(2+1)}(t, x_\mu)$ . We stress that this term differs in origin from Hopf or Chern-Simons terms arising in the context of chiral spin systems [12], which are strongly tied to the dimensionality  $D = 2 + 1$ . Indeed, as we now show, the foregoing readily generalizes to theories of AFM-VBS competition in arbitrary space-time dimensions  $D = d + 1$ , where for each  $d$  we find topological terms that are generalized versions of  $S_{\text{BP}}^{2+1}$ . We will return to the physical contents for the specific case of  $D = 2 + 1$  later.

*AFM-VBS competition for general  $D$ .*—Our detour starts by mentioning a generic property of Clifford algebras [16] which lies behind this generalization. *Property:* Let  $n$  be the number of matrices spanning the algebra  $\{\gamma_i, \gamma_j\} = 2\delta_{ij}$  ( $i, j = 1, \dots, n$ ). Representations for this algebra can be realized by a set of  $2^p \times 2^p$   $\gamma_i$  matrices where either  $n = 2p$  or  $n = 2p + 1$ . To see why this goes hand in hand with the construction of a fermionic theory describing AFM-VBS competition let us consider a  $\pi$ -flux state on a  $d$ -dimensional hypercubic lattice. The latter, in analogy with the  $D = 2 + 1$  case, is defined by the anticommutativity among the generators of translation  $\{\mathbf{T}_l, \mathbf{T}_m\} = 0$  for  $l \neq m$  ( $l, m = 1, \dots, d$ ). This gives rise to Dirac nodes within the Brillouin zone. (For  $d = 1$ , where there are no

notions of flux-lines which pierce plaquettes, it suffices to simply start with a free tight-binding model which gives rise to massless Dirac fermions. The arguments below apply for this case as well.) In going to the continuum language, Dirac spinors are constructed by dividing all lattice sites into cells consisting of  $2^d$  sites. The Dirac matrices  $\gamma_\mu$  are therefore  $2^d \times 2^d$  matrices. Meanwhile, what we wish to construct is a fermionic theory of the form  $\mathcal{L}_F^{d+1} = i\bar{\Psi}[\not{\partial} + V_{(d+1)}]\Psi$ , where notations are obvious extensions from those used in the  $D = 2 + 1$  case. The number of Dirac matrices required for this purpose is  $2d + 1$ ,

there being in addition to the  $d + 1$  space-time components  $\gamma_0, \dots, \gamma_d$ , a total of  $d$  chiral matrices ( $\gamma_5$ s), each standing for the directions available for dimerization. We see that this fits in nicely with the aforementioned mathematical property when we put  $p = d$ . (It is also straightforward to work out an explicit derivation of  $\mathcal{L}_F^{d+1}$  starting from the lattice theory.)

The Dirac operator  $D[\mathbf{v}_{(d+1)}]$  obeys Eqs. (2) and (3), in which the replacement  $\mathbf{v}_{(2+1)} \rightarrow \mathbf{v}_{(d+1)}$  is to be made. Carrying out the derivative expansion as before we obtain the low energy effective theory which is an  $O(3 + d)$  NL $\sigma$  model supplemented with the topological term

$$S_{\text{BP}}^{d+1} = \frac{-2\pi i}{\text{Area}(S^{d+2})} \int_0^1 dt \int d^{d+1}x \epsilon_{\alpha_1 \dots \alpha_{d+3}} v^{\alpha_1} \partial_t v^{\alpha_2} \partial_\tau v^{\alpha_3} \partial_{x_1} v^{\alpha_4} \dots \partial_{x_d} v^{\alpha_{d+3}}. \quad (5)$$

For  $D = 1 + 1$  ( $d = 1$ ), the isotropic  $O(4)$  theory with the partition function  $Z[\mathbf{v}_{(1+1)}] = \int D\mathbf{v}_{(1+1)} e^{-(S_{\text{NL}\sigma} + S_{\text{BP}}^{1+1})}$  has been identified (e.g., [14,17]) with the  $SU(2)_1$  Wess-Zumino-Witten (WZW) model, the fixed point theory for the  $S = 1/2$  Heisenberg antiferromagnet [18]. It is instructive to analyze the effect of introducing different types of anisotropy between the AFM and dimer sectors in this model [17], breaking down the symmetry to  $O(3) \times Z_2$  or lower (the appearance of  $Z_2$  is a remnant of the underlying lattice). First, the effective theory for the AFM limit reduces at the semiclassical level to the  $O(3)$  NL $\sigma$  model at topological angle  $\theta = \pi$ , as originally proposed by Haldane [3]. Taking the opposite limit with complete dimerization makes the kinetic and Berry phase terms of the  $O(3)$  AFM sector vanish, reflecting the quenching of the spin moment. An intermediate situation arises when the anisotropy modulates in space, physically corresponding to a distribution of nonmagnetic impurities. This induces  $S = 1/2$  moments in the background of a singlet state, whose spin Berry phases are responsible for novel power-law correlations. The isotropic (WZW) point may be viewed in light of this picture as the case where the anisotropy acquires a temporal dependence as well. The main insight gained from these examples is how the interplay between AFM (spin-moment generating) and dimer (spin-moment quenching) ordering tendencies determines the Berry phase, which in turn acts back on the ordering of the system. Turning to higher dimensions, three dimensional spin liquid systems which may be realized in frustrated magnets have lately received considerable interest, where again subtle Berry phase effects due to monopole configurations can be present [19]. We believe our approach as applied to the  $D = 3 + 1$  case could provide a new route to capture the topological properties of such systems, wherein the novel Berry phase term  $S_{\text{BP}}^{3+1}$  would play a key role.

*Monopoles and Berry phases.*—Returning now to  $D = 2 + 1$ , the theory at the  $O(5)$ -symmetric point enjoys its role as a higher dimensional analogue of the WZW model in the sense detailed above. Indeed, a similar parallelism was substantiated within the context of  $D = 2 + 1$  quan-

tum chromodynamics [20]. The case  $D = 1 + 1$  is however unique in that the coupling constant is dimensionless, and the reappearance of this model here motivates further studies of possible infrared fixed points from the viewpoint of exotic quantum spin systems. We now let an anisotropic term favoring the AFM sector, e.g., of the form  $-\alpha \mathbf{v}_{\text{AFM}}^2$  with  $\alpha > 0$ , take us away from the isotropic regime. (This term may be conveniently introduced within a 5-component Ginzburg-Landau theory such as in Ref. [21]. The spatial structure of hedgehog excitations discussed below can also be analyzed by resorting to this framework.) In contrast to similar models in the *irreducible* representation [22], here there are no topologically conserved fermionic currents which forbid changes in the Skyrmion number  $\mathcal{Q}_{xy} = \frac{1}{4\pi} \int dx dy \mathbf{n} \cdot \partial_x \mathbf{n} \times \partial_y \mathbf{n}$ . Finding Berry phases accompanying such processes requires us to extract the dependence of Eq. (4) on  $\mathbf{n}$ , which proceeds in two steps. We first integrate over the auxiliary variable  $t$ . We use without loss of generality the parametrization  $v^1 = \sin(t\varphi)\pi^1$ ,  $v^2 = \sin(t\varphi)\pi^2$ ,  $v^3 = \sin(t\varphi)\pi^3$ ,  $v^4 = \sin(t\varphi)\pi^4$ , and  $v^5 = -\cos(t\varphi)$ , where  $\boldsymbol{\pi} = (\pi^1, \dots, \pi^4)$  is a four component unit vector. The resulting Lagrangian density is

$$\mathcal{L} = \frac{1}{2g} [\sin^2 \varphi (\partial_\mu \boldsymbol{\pi})^2 + (\partial_\mu \varphi)^2] + i\theta q_{\tau xy} + \mathcal{L}_{\text{anis}}, \quad (6)$$

where  $\theta = \pi(1 - \frac{9}{8} \cos \varphi + \frac{1}{8} \cos 3\varphi)$ ,  $q_{\tau xy} \equiv \frac{1}{2\pi^2} \epsilon_{abcd} \pi^a \partial_\tau \pi^b \partial_x \pi^c \partial_y \pi^d$ , and  $\mathcal{L}_{\text{anis}}$  is the anisotropy term. Notice that the first and third terms vanish, as they must, under the spin-moment quenching condition  $\varphi = 0$ . Locking the phase field  $\varphi$  at a constant value, i.e., fixing the bond alternation strength along one of the spatial directions yields the  $D = 2 + 1$   $O(4)$  NL $\sigma$  model with a  $\theta$  term [14]. (This intermediate model should thus be relevant to spin systems with anisotropic bond alternation [23,24].) Going on to the second step, we now parametrize the components of  $\boldsymbol{\pi}$  as  $\pi^1 = \sin \phi n^1$ ,  $\pi^2 = \sin \phi n^2$ ,  $\pi^3 = \sin \phi n^3$ ,  $\pi^4 = -\cos \phi$ . The Berry phase term can now be recasted in a way which explicitly depends on monopole-

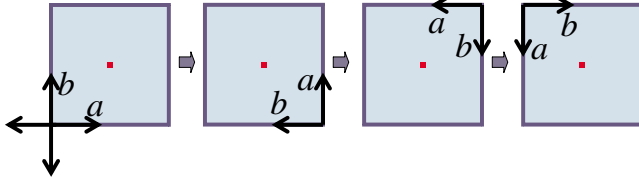


FIG. 2 (color online). Sequence of  $\frac{\pi}{2}$  rotations around a dual site which simultaneously rotates the direct sites and the VBS order parameter.

like configurations [25]. The result, obtained by integrating by parts, is

$$\mathcal{L}_{\text{BP}} = -\frac{i}{2}(2\phi - \sin 2\phi)\left(1 - \frac{9}{8}\cos\phi + \frac{1}{8}\cos 3\phi\right)\rho_m, \quad (7)$$

where  $\rho_m = \partial_\tau \left(\frac{\epsilon_{abc}}{4\pi} n^a \partial_x n^b \partial_c n^c\right) + \text{cyc. perm.}$  is the monopole charge density. Integrating  $\rho_m$  over a space-time region surrounding the center of the monopole event gives the change in the Skyrmion number between the two time-slices before and after occurrence of the event, i.e.,  $\int d\tau dx dy \rho_m = \Delta Q_{xy}$ .

A spatially modulated pattern in the monopole Berry phase [3,4] arises from this term in the following way. At each lattice site there is a competition between spin momentum generation and a local  $Z_4$ -valued VBS order. While the bulk favors the former due to the presence of  $\mathcal{L}_{\text{anis}}$ , the latter emerges locally when a monopole happens to be centered at that particular site. We may choose this VBS core to be represented, e.g., at sublattice 1 in Fig. 1 by the combination  $\varphi = \frac{\pi}{2}$  and  $\phi = 0$ , which implies, according to Eq. (7), that  $S_{\text{BP}}^1 = 1$ , with the superscript standing for the sublattice index. We then go around the plaquette counterclockwise as depicted in Fig. 2, which simultaneously rotates the orientation of the VBS order parameter by 90 degrees increment. Noting that the orientation of the ‘‘VBS clock’’ is specified by the angle  $\phi - \varphi$ , we must correct for this by also incrementing  $\phi$  by  $-\frac{\pi}{2}$  (while keeping  $\varphi$  fixed) or  $\phi$  by  $\frac{\pi}{2}$  (keeping  $\varphi$  fixed). Either way the Berry phase shifts by  $\frac{\pi}{2}\Delta Q_{xy}$ . In this way, we find that in order to have AFM monopoles with VBS cores having the same orientation for all four sites sharing the plaquette, we must have  $S_{\text{BP}}^2 = e^{i\pi/2\Delta Q_{xy}}$ ,  $S_{\text{BP}}^3 = e^{i\pi\Delta Q_{xy}}$ ,  $S_{\text{BP}}^4 = e^{i3\pi/2\Delta Q_{xy}}$ .

This method also applies to the case where the VBS state is favored in the bulk, where one recovers the Berry phase for the AFM core in the VBS vortex [7,26],  $\frac{1}{2}(-1)^{i_x+i_y}\omega$ , where  $\omega$  is the solid angle subtended by the spin. In addition, the framework can be extended to make it applicable for studying *staggered* flux states. In this sense, our method is capable of ‘‘generating’’ a rich variety of spin Berry phase effects.

In summary, we have shown that the  $\pi$ -flux state perturbed by competing AFM and VBS orders provides a

natural framework for studying effective theories which incorporate defects and their Berry phases in  $D = 2 + 1$  antiferromagnets. We have also demonstrated that the same methods also offer a framework to explore exotic Berry phases in  $D = 3 + 1$  spin systems as well.

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