Many-body spin Berry phases emerging from the $\pi$-flux state: antiferromagnetic/valence-bond-solid competition

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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 (AF) 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 AF monopoles with VBS cores, and reproduces Haldane’s hedgehog Berry phases. The theory readily generalizes to $\pi$-flux states for all $D$.

Our understanding on quantum critical points [1]/phases [2] in $D=2+1$ antiferromagets, and the issue of deconfinement therein have recently undergone a rapid sequence of developments. Competition between antiferromagnetic (AF) 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 AF 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 AF and VBS orders, which lead 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 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 AF order near the singular core. Meanwhile, in the discussions which follow, the system takes advantage of the inherent AF-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 AF-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 $Z_2$ vortices. Close inspection of the lattice model shows that these defects have an AF 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 AF 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 Haldane’s Berry phase starting from the $\pi$-flux state.

Continuum fermion model The $\pi$-flux hopping Hamiltonian on a two dimensional square lattice is $H_\pi = \sum_{i,\mu,\sigma} t_{\mu,i}^c \bar{T}_\mu c_{i\sigma}$, where $T_\mu$ with $\mu=x,y$ generates translation by one site. The $\pi$-flux condition imposes the anticommutation relation $\{T_x, T_y\} = 0$, which immediately leads to the spinon’s dispersion $E(k) = \pm t \sqrt{\cos^2 k_x + \cos^2 k_y}$ with Dirac nodes at $k = (\frac{\pi}{2}, \pm \frac{\pi}{2})$. It is convenient to group together the four cites 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].

![FIG. 1. Lattice used to derive continuum Dirac theory](image)

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 spacetime conventions) $\mathcal{L} = i \bar{\Psi} \not\partial \Psi$, where the slash indicates the contraction with the gamma matrices $\gamma_0 = \sigma_0 \otimes \sigma_z$, $\gamma_1 = -\sigma_0 \otimes \sigma_z$, $\gamma_2 = \sigma_y \otimes \sigma_y$. Here the first (second) matrix within a direct product determines the block structure (the matrix elements within the cells). Hermele et al have recently shown 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 AF 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 term $\mathcal{H}_{\text{SDW}} = \sum M(-1)^{\tau_i}(c^\dagger_\sigma \sigma \epsilon_{\sigma \epsilon_{\sigma \sigma}} + \text{h.c.})$, which appears to be in accord with angular resolved photoemission experiments on cuprate Mott insulators [10]. Being interested in extracting the dependence of the effective action and possible Berry phase terms on the Néel unit director $\mathbf{n}$, we make in $\mathcal{H}_{\text{SDW}}$ the generalization $\mathbf{\sigma} \rightarrow \mathbf{n} \cdot \mathbf{\sigma}$, which is physically a potential energy term imposing the generation of AF spin moment with the space-time-dependent orientation $\mathbf{n}(\tau, x, y)$. In the continuum limit this becomes the mass term $\mathcal{L}_\text{AF} = im_{\text{AF}}(\mathbf{n} \cdot \mathbf{\sigma})\Psi$. 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 “$\gamma_5$’s”), we have two generators of chiral transformations at our disposal, $\gamma_3 = \sigma_x \otimes \mathbf{1}$ and $\gamma_5 = \sigma_z \otimes \mathbf{1}$, 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 $\overline{\Psi}\gamma_3\Psi$ and $\overline{\Psi}\gamma_5\Psi$ each amount to breaking lattice translational symmetry by introducing band alternations $t \rightarrow t + (-1)^{x+y}$ in the horizontal ($\mu = x$) and vertical ($\mu = y$) directions. A crucial observation here is that the SDW and the two VBS ordering potentials $\overline{\Psi}Q_1\Psi$ and $\overline{\Psi}Q_2\Psi$ all belong to the family of chirally rotated mass terms $\mathcal{L}_\text{chiral} \propto i\overline{\Psi}Q^a(\alpha, \beta)\otimes \gamma_5\Psi$ ($Q^a = n \cdot \sigma$, i.e. they transform into one another by suitable chiral transformations. Finally we mention that in the 4D irreducible representation we have another possible mass term [11] $\overline{\Psi}\gamma_3\gamma_5\Psi$ which has relevance to chiral spin liquids (see footnote [21]). We do not retain this P- and T-violating term.

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

$$\mathcal{L}^\text{eff}_{\text{VBS}} = i\overline{\Psi}[\partial_T + m\sqrt{V}_{(2+1)}]\Psi,$$

(1)

where $V_{(2+1)} = v_1\sigma_x + v_2\sigma_y + v_3\sigma_z + i\gamma_3v_4 + i\gamma_5v_5$, and $v_{(2+1)} \equiv (v^1, \ldots, v^5)$ is a five component unit vector. The first three components comprise a vector $v_{\text{AF}} \equiv (v^1, v^2, v^3)$ 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 $v_{(2+1)}$, to yield an effective action which contains a new Berry phase term. Central to this feat is the following relation [12,13] satisfied by the Dirac operator $D[v_{(2+1)}] = i\partial_T + im\sqrt{V}_{(2+1)}$ and its hermitian conjugate,

$$D^\dagger D = -\partial_T^2 + m^2 - m\sqrt{V}_{(2+1)}.$$

(2)

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

$$\delta S_{\text{eff}} = -\text{tr} \left[ \frac{1}{-\partial_T^2 + m^2 - m\sqrt{V}_{(2+1)}} \partial_D^\dagger \partial_D \right].$$

(3)

It is easy to see that a nonlinear sigma (NL$\sigma$) model $S_{\text{NLaf}} = \frac{\pi i}{2}\oint d^2x \partial_\mu \mathbf{P}(v_{(2+1)})^2$ arises, with $\mathbf{g}$ a nonuniversal coupling constant. Less trivial is an imaginary contribution to eq. (3), $\delta S^\text{BP}^\text{2+1}_{\text{BP}}$, which we pick up at third order in powers of $\sqrt{V}_{(2+1)}$. As is usual with Wess-Zumino type terms, one recovers the action $S^\text{BP}^\text{2+1}_{\text{BP}}$ from its variation $\delta S^\text{BP}^\text{2+1}_{\text{BP}}$ with the aid of an auxiliary variable $t \in [0, 1]$ which smoothly sweeps the extended function $v_{(2+1)}(t, x_\mu)$ between its two asymptotics, a fixed value at $t = 0$, say $(0, 0, 0, 0, 1)$, and the physical value at $t = 1$, $v_{(2+1)}(x_\mu)$. The result is

$$S^\text{BP}^\text{2+1}_{\text{BP}} = \frac{-2\pi i e_{abcd}^{\text{eff}}}{\text{Area}(S^4)^2} \int_0^1 dt d^2x \sqrt{\gamma} \partial_T v^a \partial_\mu v^b \partial_\nu v^c \partial_\nu v^d \partial_T v^e,$$

(4)

where $\text{Area}(S^4) = \frac{2\pi^2}{(12)} = \frac{\pi}{3}\pi^2$. Topologically, this is $\frac{i2\pi}{\text{Area}(S^4)}$ times the winding number which counts the number of times the compactified “space-time” $(t, x_\mu)$ isomorphic to $S^3 \times S^1 \sim S^4$ wraps around the target space (also $S^4$) for $v_{(2+1)}(t, x_\mu)$. It is important not to confuse this action with Hopf or Chern-Simons terms, which have been studied extensively in the context of chiral spin systems [14] and are strongly tied to the dimensionality $D=2+1$. Indeed, as we now show, the foregoing readily generalizes to theories of AF-VBS competition in arbitrary space-time dimensions $D=d+1$, where for each $d$ we find topological terms that are generalized versions of $S^\text{BP}^\text{2+1}_{\text{BP}}$. We will return to the physical contents for the specific case of $D=2+1$ later.

**AF-VBS competition for general $D$** Our detour starts by mentioning a generic property of Clifford algebras [15] which lies behind this generalization. **Property:** Let $n$ be the number of matrices spanning the algebra $\{\gamma_i, \gamma_j\} = 2\delta_{ij}(i, j = 1, \ldots, n)$. Representations for this algebra can be realized by a set of $2^n \times 2^n$ 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 AF-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 anticommutivity among the generators of translation $\{\mathbf{T}_l, \mathbf{T}_m\} = 0$ for $l \neq m(l, m = 1, \ldots, d)$. 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 applies 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 $\mathcal{L}_F^{d+1} = i \bar{\Psi} [\partial + V_{(d+1)}] \Psi$, 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 $\gamma_0, \ldots, \gamma_d$, 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 mathematical property aforementioned 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 $\mathcal{D}[v_{(d+1)}]$ obeys eqs. (2) and (3), in which the replacement $v_{(2+1)} \rightarrow v_{(d+1)}$ 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 models within the context of $D=2+1$ quantum chromodynamics [19], where current algebras similar to those which determine the conformal field theory contents of the WZW model were derived. We need be aware though, of theprivellaged role of dimensionality $D=1+1$ for which thecoupling constant becomes dimensionless. Hence theintriguing possibility of a nontrivial infrared fixed point isunresolved, and warrants further study from the viewpointof exotic quantum spin systems.

We now let an anisotropic term favoring the AF sector, e.g. of the form $-\alpha^2 \cos^2 \phi$ with $\alpha > 0$, take us away from theisotropic regime. In contrast to similar models in theirreducible representation [20], here there are no topologicallyconserved fermionic currents which forbids changes inthe Skyrmion number [21]. Finding Berry phases accompanying such processes requires us to extract the dependence of eq. (4) on $n$, which proceeds in two steps. We first integrate over theauxiliary variable $t$. We use without loss of generality theparametrization $v^1 = \sin(t\phi)\pi_1$, $v^2 = \sin(t\phi)\pi_2$, $v^3 = \sin(t\phi)\pi_3$, $v^4 = \sin(t\phi)\pi_4$, and $v^5 = -\cos(t\phi)$, where $\phi = (\pi_1, \ldots, \pi_4)$ is a four component unit vector. The resulting Lagrangian density is

$$\mathcal{L} = \frac{1}{2g} \left[ \sin^2 \phi (\partial_\mu \pi)^2 + (\partial_\mu \phi)^2 \right] + i \theta q_{txy} + \mathcal{L}_{\text{anis}}, \quad (6)$$

where $\theta = \pi(1 - \frac{2}{3} \cos \phi + \frac{1}{3} \cos 3\phi)$, $q_{txy} \equiv \frac{1}{4\pi^2} e^{-|\mathbf{n}|^2} \partial_\tau \pi^a \partial_x \pi^b \partial_y \pi^c \partial^d \pi^d$, 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 $\phi = 0$. When the phase field $\phi$ is locked at a constant value—corresponding to fixing the bond alteration strength in the vertical direction relative to the magnitude of the remaining four components of $\mathbf{v}$, this reduces to the $D=2+1$ $O(4)$ nonlinear sigma model with a $\theta$-term [12]. (This intermediate model should thus be relevant to spin systems with anisotropic bond alternation [22,23].) Going on to the second step, we now parametrize the components of $\pi$ as $\pi^1 = \sin \phi \mathbf{n}^1$, $\pi^2 = \sin \phi \mathbf{n}^2$, $\pi^3 = \sin \phi \mathbf{n}^3$, $\pi^4 = -\cos \phi$. The Berry phase term can now be recast in a way which explicitly depends on monopole-like configurations [24]. The
result, obtained by integrating by parts, is
\[ \mathcal{L}_{BP} = -\frac{i}{2}(2\phi - \sin 2\phi)(1 - \frac{9}{8}\cos \varphi + \frac{1}{8}\cos 3\varphi)\rho_m, \] (7)
where \( \rho_m = \partial_r(\frac{1}{2\pi n^a n^b \partial_r n^c} + \text{c.p.}) \) 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.
\[ \int d\mathbf{r} d\mathbf{x} d\mathbf{y} \rho_m = \Delta \Omega_{xy}. \]

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

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 \( \mathcal{L}_{anis} \), 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 \( S^1_{BP} = 1 \), 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 \( \varphi \) by \( \frac{\pi}{2} \) (keeping \( \phi \) fixed). Either way the Berry phase shifts by \( \frac{\pi}{2} \Delta \Omega_{xy} \). In this way, we find that in order to have AF monopoles with VBS cores having the same orientation for all four sites sharing the plaquette, we must have
\[ S^{a}_{BP} = e^{i\frac{\pi}{2} \Delta \Omega_{xy}}, \quad S^{b}_{BP} = e^{i\pi \Delta \Omega_{xy}}, \quad S^{a}_{BP} = e^{i\frac{\pi}{2} \Delta \Omega_{xy}}, \quad S^{b}_{BP} = e^{i\pi \Delta \Omega_{xy}}. \]

This method also applies to the case where the VBS state is favored in the bulk, where one recovers the Berry phase for the AF core in the VBS vortex [7,25], \( \frac{1}{2}(-1)^{x+y+z} \), 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 AF and VBS orders provides a natural framework for studying effective theories which incorporates defects and their Berry phases in \( D=2+1 \) antiferromagnets. We have also demonstrated that the same methods also offers a framework to explore exotic Berry phases in \( D=3+1 \) spin systems as well.

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