Intertwining Topological Order and Broken Symmetry in a Theory of Fluctuating Spin-Density Waves

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Phys. Rev. Lett. **119**, 227002 — Published 29 November 2017

DOI: 10.1103/PhysRevLett.119.227002

Intertwining topological order and broken symmetry in a theory of fluctuating spin density waves

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(Dated: October 30, 2017)

The pseudogap metal phase of the hole-doped cuprate superconductors has two seemingly unrelated characteristics: a gap in the electronic spectrum in the 'anti-nodal' region of the square lattice Brillouin zone, and discrete broken symmetries. We present a SU(2) gauge theory of quantum fluctuations of magnetically ordered states which appear in a classical theory of square lattice antiferromagnets, in a spin density wave mean field theory of the square lattice Hubbard model, and in a $\mathbb{CP}^1$ theory of spinons. This theory leads to metals with an antinodal gap, and topological order which intertwines with the observed broken symmetries.

A remarkable property of the pseudogap metal of the hole-doped cuprates is that it does not exhibit a 'large' Fermi surface of gapless electron-like quasiparticles excitations, *i.e.* the size of the Fermi surface is smaller than expected from the classic Luttinger theorem of Fermi liquid theory [1]. Instead it has a gap in the fermionic spectrum near the 'anti-nodal' points ($(\pi, 0)$ and $(0, \pi)$) of the square lattice Brillouin zone. Gapless fermionic excitations appear to be present only along the diagonals of the Brillouin zone (the 'nodal' region). One way to obtain such a Fermi surface reconstruction is by a broken translational symmetry. However, there is no sign of broken translational symmetry over a wide intermediate temperature range [2], and also at low temperatures and intermediate doping [3], over which the pseudogap is present. With full translational symmetry, violations of the Luttinger theorem require the presence of topological order [4–6].

A seemingly unrelated property of the pseudogap metal is that it exhibits discrete broken symmetries, which preserve translations, over roughly the same region of the phase diagram over which there is an antinodal gap in the fermionic spectrum. The broken symmetries include lattice rotations, interpreted in terms of an Ising-nematic order [7–10], and one or both of inversion and time-reversal symmetry breaking [11–16]. Luttinger's theorem implies that none of these broken symmetries can induce the needed fermionic gap by themselves.

The co-existence of the antinodal gap and the broken symmetries can be explained by intertwining them [17–19], *i.e.* by exploiting flavors of topological order which are tied to specific broken symmetries. Here we show that broken lattice rotations, inversion, and time-reversal appear naturally in several models appropriate to the known cuprate electronic structure.

We consider quantum fluctuations of magnetically ordered states found in two different computations: a classical theory of frustrated, insulating antiferromagnets on the square lattice, and a spin density wave theory of metallic states of the square lattice Hubbard model. The types of magnetically ordered states found are sketched in Fig. 1a. The quantum fluctuations of these states are described by a SU(2) gauge theory, and this leads to the loss of magnetic order, and the appearance of phases with topological order and an anti-nodal gap in the fermion spectrum. We find that the topological order intertwines with precisely the observed broken discrete symmetries, as shown in Fig. 1b. We further show that the same phases are also obtained naturally in a $\mathbb{CP}^1$ theory of bosonic spinons supplemented by Higgs fields conjugate to long-wavelength spinon pairs.

Magnetic order: We examine states in which the electron spin $\hat{\boldsymbol{S}}_i$ on site i of the square lattice, at position $\boldsymbol{r}_i$, has the expectation value

$$\left\langle \hat{\boldsymbol{S}}_i \right\rangle = N_0 \left[\cos\left(\boldsymbol{K}\cdot\boldsymbol{r}_i\right)\cos(\theta)\,\hat{\boldsymbol{e}}_x + \sin\left(\boldsymbol{K}\cdot\boldsymbol{r}_i\right)\cos(\theta)\,\hat{\boldsymbol{e}}_y + \sin(\theta)\,\hat{\boldsymbol{e}}_z\right]. \tag{1}$$

The different states we find are (see Fig. 1a) (D′) a Néel state with collinear antiferromagnetism at wavevector (π, π), with $\boldsymbol{K} = (\pi, \pi)$, $\theta = 0$; (A′) a canted state, with (π, π) Néel order co-existing with a ferromagnet moment perpendicular to the Néel order, with $\boldsymbol{K} = (\pi, \pi)$, $0 < \theta < \pi/2$, (B′) a planar spiral state, in which the spins precess at an incommensurate wavevector $\boldsymbol{K}$ with $\theta = 0$; (C′) a conical spiral state, which is a planar spiral accompanied by a ferromagnetic moment perpendicular to the plane of the spiral [20] with $\boldsymbol{K}$ incommensurate, $0 < \theta < \pi/2$.

First, we study the square lattice spin Hamiltonian with near-neighbor antiferromagnetic exchange interactions $J_p > 0$, and ring exchange K [21–25]:

$$\mathcal{H}_J = \sum_{i<j} J_{ij}\,\hat{\boldsymbol{S}}_i\cdot\hat{\boldsymbol{S}}_j + 2K \sum_{\substack{k\;\;\ell\\ j\,\square\, i}} \Big[(\hat{\boldsymbol{S}}_i\cdot\hat{\boldsymbol{S}}_j)(\hat{\boldsymbol{S}}_k\cdot\hat{\boldsymbol{S}}_\ell) + (\hat{\boldsymbol{S}}_i\cdot\hat{\boldsymbol{S}}_\ell)(\hat{\boldsymbol{S}}_k\cdot\hat{\boldsymbol{S}}_j) - (\hat{\boldsymbol{S}}_i\cdot\hat{\boldsymbol{S}}_k)(\hat{\boldsymbol{S}}_j\cdot\hat{\boldsymbol{S}}_\ell)\Big]. \tag{2}$$

$J_{ij} = J_p$ when i, j are p'th nearest neighbors, and we only allow J_p with $p = 1, 2, 3, 4$ non-zero. The classical ground states are obtained by minimizing $\mathcal{H}_J$ over the set of states in Eq. (1); results are shown in Fig. 2a-c. We find the states A′, B′, C′, D′, all of which meet

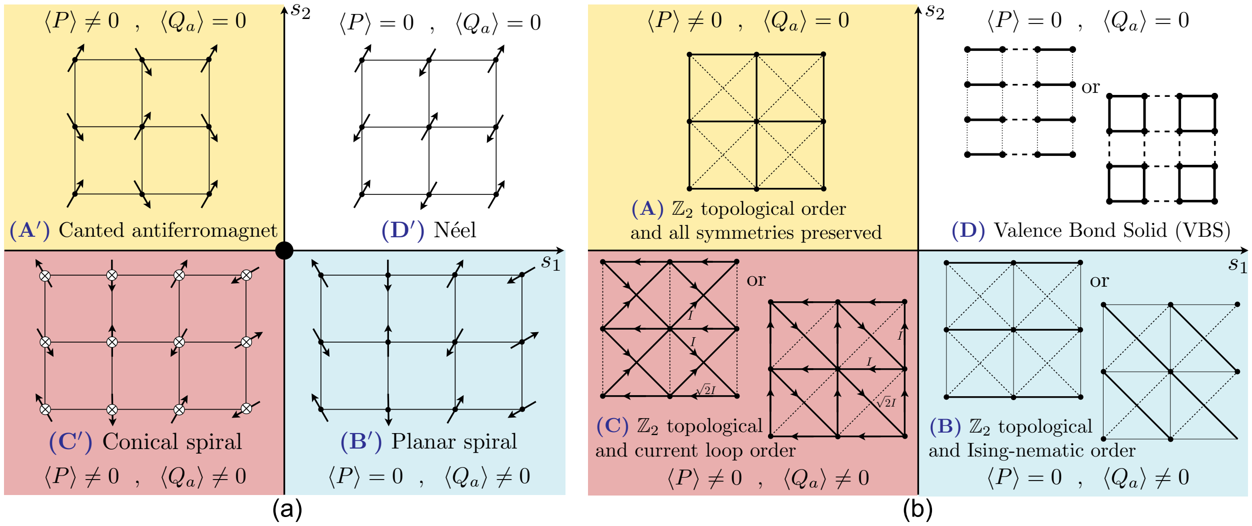

FIG. 1. (a) Schematics of the magnetically ordered states obtained in the classical antiferromagnet, and in the spin density wave theory of the Hubbard model. (b) Corresponding states obtained after quantum fluctuations restore spin rotation symmetry. Phase D has U(1) topological order in the metal, but is unstable to the appearance of VBS order in the insulator. The crossed circles in phase C′ indicate a canting of the spins into the plane. The labels s_1, s_2, P, Q_a refer to the $\mathbb{CP}^1$ theory: the phases in (a) are obtained for small g, and those in (b) for large g.

at a multicritical point, just as in the schematic phase diagram in Fig. 1a. A semiclassical theory of quantum fluctuations about these states, starting from the Néel state, appears in Supplemental Material A [27].

For metallic states with spin density wave order [28–31], we study the Hubbard model

$$\mathcal{H}_U = -\sum_{i<j,\alpha} t_{ij} c_{i,\alpha}^\dagger c_{j,\alpha} - \mu \sum_{i,\alpha} c_{i,\alpha}^\dagger c_{i,\alpha} + U \sum_i \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} \tag{3}$$

of electrons $c_{i,\alpha}$, with $\alpha = \uparrow,\downarrow$ a spin index, $t_{ij} = t_p$ when i,j are p'th nearest neighbors, and we take t_p with $p = 1,2,3,4$ non-zero. U is the on-site Coulomb repulsion, and μ is the chemical potential. The electron density, $\hat{n}_{i,\alpha} \equiv c_{i,\alpha}^\dagger c_{i,\alpha}$, while the electron spin $\hat{\boldsymbol{S}}_i \equiv (1/2) c_{i,\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{i,\beta}$, with $\boldsymbol{\sigma}$ the Pauli matrices. We minimized $\mathcal{H}_U$ over the set of free fermion Slater determinant states obeying Eq. (1), while maintaining uniform charge and current densities; results are illustrated in Fig. 2d-f, and details appear in Supplemental Material B [27]. Again, note the appearance of the magnetic orders A′, B′, C′, D′, although now these co-exist with Fermi surfaces and metallic conduction.

SU(2) gauge theory: We describe quantum fluctuations about states of $\mathcal{H}_U$ obeying Eq. (1) by transforming the electrons to a rotating reference frame by a SU(2) matrix R_i [36]

$$\begin{pmatrix} c_{i,\uparrow} \\ c_{i,\downarrow} \end{pmatrix} = R_i \begin{pmatrix} \psi_{i,+} \\ \psi_{i,-} \end{pmatrix}, \qquad R_i^\dagger R_i = R_i R_i^\dagger = \mathbb{1}. \tag{4}$$

The fermions in the rotating reference frame are spinless 'chargons' ψ_s, with $s = \pm$, carrying the electromagnetic charge. In the same manner, the transformation of the electron spin operator $\hat{\boldsymbol{S}}_i$ to the rotating reference frame is proportional to the 'Higgs' field $\boldsymbol{H}_i$ [36],

$$\boldsymbol{\sigma} \cdot \boldsymbol{H}_i \propto R_i^\dagger \, \boldsymbol{\sigma} \cdot \hat{\boldsymbol{S}}_i \, R_i. \tag{5}$$

The new variables, ψ, R, and $\boldsymbol{H}$ provide a formally redundant description of the physics of $\mathcal{H}_U$ as all observables are invariant under a SU(2) gauge transformation V_i under which

$$\begin{array}{c} R_i \to R_i \, V_i^\dagger \\ \boldsymbol{\sigma} \cdot \boldsymbol{H}_i \to V_i \, \boldsymbol{\sigma} \cdot \boldsymbol{H}_i \, V_i^\dagger \end{array} \quad \begin{pmatrix} \psi_{i,+} \\ \psi_{i,-} \end{pmatrix} \to V_i \begin{pmatrix} \psi_{i,+} \\ \psi_{i,-} \end{pmatrix}, \tag{6}$$

while c_i and $\hat{\boldsymbol{S}}_i$ are gauge invariant. The action of the SU(2) gauge transformation V_i, should be distinguished from the action of global SU(2) spin rotations Ω under which

$$\begin{array}{c} R_i \to \Omega \, R_i \\ \boldsymbol{\sigma} \cdot \hat{\boldsymbol{S}}_i \to \Omega \, \boldsymbol{\sigma} \cdot \hat{\boldsymbol{S}}_i \, \Omega^\dagger \end{array} \quad \begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix} \to \Omega \begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix}, \tag{7}$$

while ψ and $\boldsymbol{H}$ are invariant.

In the language of this SU(2) gauge theory [36, 37], the phases with magnetic order obtained above appear when both R and $\boldsymbol{H}$ are condensed. We may choose a gauge in which $\langle R\rangle \propto \mathbb{1}$, and so the orientation of the $\boldsymbol{H}$ condensate is the same as that in Eq. (1),

$$\langle \boldsymbol{H}_i \rangle = H_0 \Big[\cos(\boldsymbol{K}\cdot\boldsymbol{r}_i)\cos(\theta)\, \hat{\boldsymbol{e}}_x + \sin(\boldsymbol{K}\cdot\boldsymbol{r}_i)\cos(\theta)\, \hat{\boldsymbol{e}}_y + \sin(\theta)\, \hat{\boldsymbol{e}}_z \Big]. \tag{8}$$

We can now obtain the phases of $\mathcal{H}_U$ with quantum fluctuating spin density wave order, (A,B,C,D) shown in

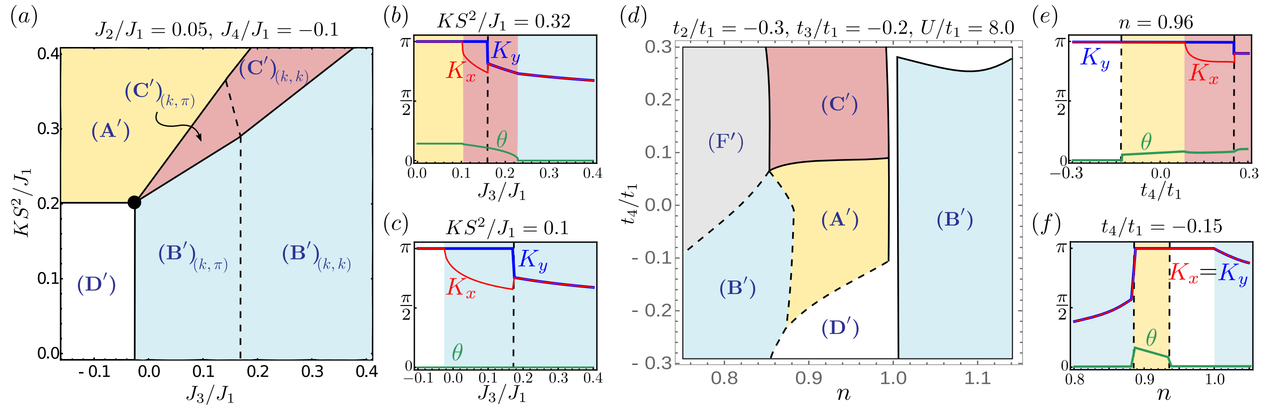

FIG. 2. (a) Phase diagram of $\mathcal{H}_J$, for a spin S model in the classical limit $S \to \infty$, exhibiting all phases of Fig. 1a. The subscript of the labels (B′) and (C′) indicates the wavevector $\boldsymbol{K} = (K_x, K_y)$ of the spiral. Note that the phases A′, C′, B′, D′ meet at a multicritical point, just as in Fig 1a. (b) and (c) show K_x, K_y, and the canting angle θ along two different one-dimensional cuts of the phase diagram in (a). The phase diagram resulting from the spin-density wave analysis of the Hubbard model (3) can be found in (d). Besides an additional ferromagnetic phase, denoted by (F′), we recover all the phases of the classical phase diagram in (a). Part (e) and (f) show one-dimensional cuts of the spin-density wave phase diagram. In all figures, solid (dashed) lines are used to represent second (first) order transitions.

Fig. 1b, in a simple step: the quantum fluctuations lead to fluctuations in the orientation of the local magnetic order, and so remove the R condensate leading to $\langle R \rangle = 0$. The Higgs field $\boldsymbol{H}_i$ retains the condensate in Eq. (8) indicating that the magnitude of the local order is non-zero. In such a phase, spin rotation invariance is maintained with $\langle \hat{\boldsymbol{S}} \rangle = 0$, but the SU(2) gauge group has been 'Higgsed' down to a smaller gauge group which describes the topological order [17, 38–42]. The values of θ and $\boldsymbol{K}$ in phases (A,B,C,D) obey the same constraints as the corresponding magnetically ordered phases (A′, B′, C′, D′). In phase D, the gauge group is broken down to U(1), and there is a potentially gapless emergent 'photon'; in an insulator, monopole condensation drives confinement and the appearance of VBS order, but the photon survives in a metallic, U(1) 'algebraic charge liquid' (ACL) state [43] (which is eventually unstable to fermion pairing and superconductivity [44]). The remaining phases A,B,C have a non-collinear configuration of $\langle \boldsymbol{H}_i \rangle$ and then only $\mathbb{Z}_2$ topological order survives [17]: such states are ACLs with stable, gapped, 'vison' excitations carrying $\mathbb{Z}_2$ gauge flux which cannot be created singly by any local operator. Phase A breaks no symmetries, phase B breaks lattice rotation symmetry leading to Ising-nematic order [17, 38], and phase C has broken time-reversal and mirror symmetries (but not their product), leading to current loop order [45]. All the 4 ACL phases (A,B,C,D) may also become 'fractionalized Fermi liquids' (FL*) [4, 5] by formation of bound states between the chargons and R; the FL* states have a Pauli contribution to the spin susceptibility from the reconstructed Fermi surfaces.

The structure of the fermionic excitations in the phases of Fig. 1b, and the possible broken symmetries in the $\mathbb{Z}_2$ phases, can be understood from an effective Hamiltonian for the chargons. As described in Supplemental Material C [27], a Hubbard-Stratonovich transformation on $\mathcal{H}_U$, followed by the change of variables in Eqs. (4) and (5), and a mean field decoupling leads to

$$\mathcal{H}_\psi = -\sum_{i<j,s} t_{ij} Z_{ij} \psi^\dagger_{i,s} \psi_{j,s} - \mu \sum_{i,s} \psi^\dagger_{i,s} \psi_{i,s} - \sum_{i,s,s'} \boldsymbol{H}_i \cdot \psi^\dagger_{i,s} \boldsymbol{\sigma}_{ss'} \psi_{i,s'} \,. \tag{9}$$

The chargons inherit their hopping from the electrons, apart from a renormalization factor Z_{ij}, and experience a Zeeman-like coupling to a local field given by the condensate of $\boldsymbol{H}$: so the Fermi surface of ψ reconstructs in the same manner as the Fermi surface of c in the phases with conventional spin density wave order. Note that this happens here even though translational symmetry is fully preserved in all gauge-invariant observables; the apparent breaking of translational symmetry in the Higgs condensate in Eq. (8) does not transfer to any gauge invariant observables, showing how the Luttinger theorem can be violated by the topological order [4–6] in Higgs phases. However, other symmetries are broken in gauge-invariant observables: Supplemental Material C [27] examines bond and current variables, which are bilinears in ψ, and finds that they break symmetries in the phases B and C noted above.

$\mathbb{CP}^1$ **theory:** We now present an alternative description of all 8 phases in Fig. 1 starting from the popular $\mathbb{CP}^1$ theory of quantum antiferromagnets. In principle (as we note below, and in Supplemental Material D [27]) this theory can be derived from the SU(2) gauge theory above [46] after integrating out the fermionic chargons, and representing R in terms of a bosonic spinon field z_α

by

$$R_i = \begin{pmatrix} z_{i,\uparrow} & -z_{i,\downarrow}^* \\ z_{i,\downarrow} & z_{i,\uparrow}^* \end{pmatrix}, \qquad |z_{i,\uparrow}|^2 + |z_{i,\downarrow}|^2 = 1. \tag{10}$$

However, integrating out the chargons is only safe when there is a chargon gap, and so the theories below can compute critical properties of phase transitions only in insulators.

We will not start here from the SU(2) gauge theory, but present a direct derivation from earlier analyses of the quantum fluctuations of a $S = 1/2$ square lattice antiferromagnet near a Néel state, which obtained the following action [47] for a $\mathbb{CP}^1$ theory over two-dimensional space ($r = (x, y)$) and time (t)

$$\mathcal{S} = \frac{1}{g} \int d^2 r dt \, |(\partial_\mu - i a_\mu) z_\alpha|^2 + \mathcal{S}_B. \tag{11}$$

Here μ runs over 3 spacetime components, and a_μ is an emergent U(1) gauge field. The local Néel order $\boldsymbol{n}$ is related to the z_α by $\boldsymbol{n} = z_\alpha^* \boldsymbol{\sigma}_{\alpha\beta} z_\beta$ where $\boldsymbol{\sigma}$ are the Pauli matrices. The U(1) gauge flux is defined modulo 2π, and so the gauge field is compact and monopole configurations with total flux 2π are permitted in the path integral. The continuum action in Eq. (11) should be regularized to allow such monopoles. $\mathcal{S}_B$ is the Berry phase of the monopoles [48–50]. Monopoles are suppressed in the states with $\mathbb{Z}_2$ topological order [17, 38], and so we do not display the explicit form of $\mathcal{S}_B$.

The phases of the $\mathbb{CP}^1$ theory in Eq. (11) have been extensively studied. For small g, we have the conventional Néel state, D$'$ in Fig. 1a, with $\langle z_\alpha \rangle \neq 0$ and $\langle \boldsymbol{n} \rangle \neq 0$. For large g, the z_α are gapped, and the confinement in the compact U(1) gauge theory leads to valence bond solid (VBS) order [49, 50], which is phase D in Fig. 1b. A deconfined critical theory describes the transition between these phases [51].

We now want to extend the theory in Eq. (11) to avoid confinement and obtain states with topological order. In a compact U(1) gauge theory, condensing a Higgs field with charge 2 leads to a phase with deconfined $\mathbb{Z}_2$ charges [52]. Such a deconfined phase has the $\mathbb{Z}_2$ topological order [17, 38–42] of interest to us here. So we search for candidate Higgs fields with charge 2, composed of pairs of long-wavelength spinons, z_α. We also require the Higgs field to be spin rotation invariant, because we want the $\mathbb{Z}_2$ topological order to persist in phases without magnetic order. The simplest candidate without spacetime gradients, $\varepsilon_{\alpha\beta} z_\alpha z_\beta$ (where $\varepsilon_{\alpha\beta}$ is the unit antisymmetric tensor) vanishes identically. Therefore, we are led to the following Higgs candidates with a single gradient ($a = x, y$)

$$P \sim \varepsilon_{\alpha\beta} z_\alpha \partial_t z_\beta \quad , \quad Q_a \sim \varepsilon_{\alpha\beta} z_\alpha \partial_a z_\beta \,. \tag{12}$$

These Higgs fields have been considered separately before. Condensing Q_a was the route to $\mathbb{Z}_2$ topological order in Ref. 38, while P appeared more recently in Ref. 53.

	$\mathcal{T}$	T_x	I_x	$R_{\pi/2}$
z_α	$\varepsilon_{\alpha\beta} z_\beta$	$\varepsilon_{\alpha\beta} z_\beta^*$	z_α	z_α
Q_x	Q_x	Q_x^*	$-Q_x$	Q_y
Q_y	Q_y	Q_y^*	Q_y	$-Q_x$
P	$-P$	P^*	P	P

TABLE I. Symmetry signatures of various fields under time reversal ($\mathcal{T}$), translation by a lattice spacing along x (T_x), reflection about a lattice site with $x \to -x$, $y \to y$ (I_x), and rotation by $\pi/2$ about a lattice site with $x \to y$, $y \to -x$ ($R_{\pi/2}$).

The effective action for these Higgs fields, and the properties of the Higgs phases, follow straightforwardly from their transformations under the square lattice space group and time-reversal: we collect these in Table I. From these transformations, we can add to the action $\mathcal{S} \to \mathcal{S} + \int d^2 r dt \, \mathcal{L}_{P,Q}$

$$\begin{aligned} \mathcal{L}_{P,Q} &= |(\partial_\mu - 2ia_\mu)P|^2 + |(\partial_\mu - 2ia_\mu)Q_a|^2 \\ &\quad + \lambda_1 P^* \, \varepsilon_{\alpha\beta} z_\alpha \partial_t z_\beta + \lambda_2 Q_a^* \varepsilon_{\alpha\beta} z_\alpha \partial_a z_\beta + \text{H.c.} \\ &\quad - s_1 |P|^2 - s_2 |Q_a|^2 - u_1 |P|^4 - u_2 |Q_a|^4 \, , + \ldots \end{aligned} \tag{13}$$

where we do not display other quartic and higher order terms in the Higgs potential.

For large g, we have $\langle z_\alpha \rangle = 0$, and can then determine the spin liquid phases by minimizing the Higgs potential as a function of s_1 and s_2. When there is no Higgs condensate, we noted earlier that we obtain phase D in Fig. 1b. Fig. 1b also indicates that the phases A,B,C are obtained when one or both of the P and Q_a condensates are present. This is justified in Supplemental Material D [27] by a computation of the quadratic effective action for the z_α from the SU(2) gauge theory: we find just the terms with linear temporal and/or spatial derivatives as would be expected from the presence of P and/or Q_a condensates in $\mathcal{L}_{P,Q}$.

We can confirm this identification from the symmetry transformations in Table I:
(A) There is only a P condensate, and the gauge-invariant quantity $|P|^2$ is invariant under all symmetry operations. Consequently this is a $\mathbb{Z}_2$ spin liquid with no broken symmetries; it has been previously studied by Yang and Wang [53] using bosonic spinons.
(B) With a Q_a condensate, one of the two gauge-invariant quantities $|Q_x|^2 - |Q_y|^2$ or $Q_x^* Q_y + Q_x Q_y^*$ must have a non-zero expectation value. Table I shows that these imply Ising-nematic order, as described previously [17, 38, 54]. We also require $\langle Q_x \rangle \langle Q_y^* \rangle$ to be real to avoid breaking translational symmetry.
(C) With both and P and Q_a condensates non-zero we can define the gauge invariant order parameter $O_a = P Q_a^* + P^* Q_a$ (again $\langle P \rangle \langle Q_a^* \rangle$ should be real to avoid translational symmetry breaking). The symmetry transformations of O_a show that it is precisely the 'current-loop' order parameter of Ref. 19: it is odd under reflection and time-reversal but not their product.

A similar analysis can be carried out at small g, where z_α condenses and breaks spin rotation symmetry. The structure of the condensate is determined by the eignmodes of the z_α dispersion in the A,B,C,D phases, and this determines that the corresponding magnetically ordered states are precisely A′,B′,C′,D′, as in Fig. 1a.

We have shown here that a class of topological orders intertwine with the observed broken discrete symmetries in the pseudogap phase of the hole doped cuprates. The same topological orders emerge from a theory of quantum fluctuations of magnetically ordered states obtained by four different methods: the frustrated classical antiferromagnet, the semiclassical non-linear sigma model, the spin density wave theory, and the $\mathbb{CP}^1$ theory supplemented by the Higgs fields obtained by pairing spinons at long wavelengths. The intertwining of topological order and symmetries can explain why the symmetries are restored when the pseudogap in the fermion spectrum disappears at large doping.

We thank A. Chubukov, A. Eberlein, D. Hsieh, Yin-Chen He, B. Keimer, T. V. Raziman, T. Senthil, and A. Thomson for useful discussions. This research was supported by the NSF under Grant DMR-1664842 and the MURI grant W911NF-14-1-0003 from ARO. Research at Perimeter Institute is supported by the Government of Canada through Industry Canada and by the Province of Ontario through the Ministry of Research and Innovation. SS also acknowledges support from Cenovus Energy at Perimeter Institute. MS acknowledges support from the German National Academy of Sciences Leopoldina through grant LPDS 2016-12.

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