Quantum phase transitions around the staggered valence-bond solid

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Quantum Phase Transitions around the Staggered Valence Bond Solid

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Motivated by recent numerical results, we study the quantum phase transitions between Z_2 spin liquid, Néel ordered, and various valence bond solid (VBS) states on the honeycomb and square lattices, with emphasis on the staggered VBS. In contrast to the well-understood columnar VBS order, the staggered VBS is not described by an XY order parameter with Z_N anisotropy close to these quantum phase transitions. Instead, we demonstrate that on the honeycomb lattice, the staggered VBS is more appropriately described as an O(3) or CP(2) order parameter with cubic anisotropy, while on the square lattice it is described by an O(4) or CP(3) order parameter.

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I. INTRODUCTION

Exotic criticality, in particular transitions which violate the Landau rules for continuous phase transitions, is now believed to be possible and perhaps even prevalent at quantum critical points. The best-studied example of such phenomena is the "Deconfined Quantum Critical Point" (DQCP) between the columnar valence bond solid ($c-$VBS, Fig. 2*a*, Fig. 3*b*) and Néel ordered antiferromagnet, in simple unfrustrated geometries such as the square and honeycomb lattices. An intuitive understanding of this transition is available through the topological defects of these phases. Coming from the antiferromagnetic state, one can regard the transition as the proliferation of the skyrmion of the Néel order parameter[1,2], which destroys the Néel order. It simultaneously creates valence bond solid order, because the skyrmion carries the same quantum number as $c-$VBS[3,4] on both the honeycomb and the square lattices. In this picture, we can view the skyrmion as a boson, and the $c-$VBS order simply corresponds to the superfluid phase of the skyrmion boson. Although this skyrmion boson is not precisely a conserved particle, it is expected that at the deconfined quantum critical point, the skyrmions is fully conserved in the long wavelength limit. Hence it is reasonable to describe the $c-$VBS with an XY order parameter, whose anisotropies become irrelevant at the critical point. This is a specific *embedding* of the discrete $c-$VBS order parameter in a larger XY (U(1)) order parameter space. A consequence of the irrelevance of anisotropy in this XY space is that the $c-$VBS order is "unified" with plaquette VBS order, such that both types of states are nearly degenerate near the critical point. A similar picture can be applied to the transition between the Z_2 spin liquid phase and the $c-$VBS, where the XY order parameter is the vison field in the Z_2 spin liquid. This picture has been confirmed with quantum Monte Carlo simulation on the $J-Q$ spin models with multi-spin interactions, and it was clearly shown that the U(1) symmetry of the $c-$VBS order parameter is fully restored at the critical point between Néel and $c-$VBS[5].

The staggered VBS ($s-$VBS) is another very natural pattern on both the honeycomb and the square lattices (Fig. 2*b*, Fig. 3*c*), and quite distinct from the $c-$VBS. However, so far there has been no theory describing the transition from magnetic ordered phases or spin liquid to the $s-$VBS. The difference between the $c-$VBS and $s-$VBS is hinted at by their vortices. It was noticed that a vortex of $c-$VBS always carries an unpaired spinon, thus the proliferation of $c-$VBS vortices will lead to magnetic order. However, in Fig. 1 it is clearly shown that the vortex of $s-$VBS is completely featureless, hence the transition into magnetic order cannot be driven by these vortices. Therefore a completely different theory is needed to describe the $s-$VBS and its quantum phase transitions.

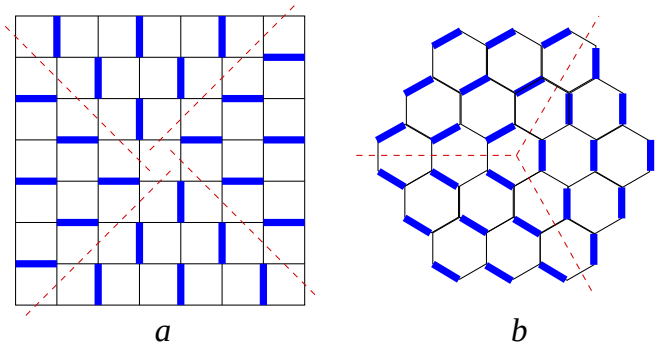

FIG. 1: The Z_4 vortex and Z_3 vortex of $s-$VBS on the square and honeycomb lattice, the vortex core is featureless.

It was proposed that for spin-1/2 systems on the honeycomb lattice, the quantum fluctuations tend to melt the incommensurate spin spiral order, and induce a $s-$VBS[6]. Also, phase diagrams involving the $s-$VBS have been proposed in many recent numerical works. For instance, exact diagonalization of the J_1-J_2 Heisenberg model on the honeycomb lattice found a gapped liquid phase between the Néel order and $s-$VBS[7], and a similar phase diagram of this model including the liquid phase and the $s-$VBS was later confirmed with variational methods[8]. Strong tendency towards the $s-$VBS was also verified by functional renormalization group studies on

the same model[9]. On the square lattice, exact diagonalization of the $J-Q$ model[10] suggests that the Néel order can have direct transition into both $c-$VBS and $s-$VBS. QMC of a modified $J-Q$ model on the square lattice also revealed a direct transition between Néel order and $s-$VBS (although it was found to be first order in this case)[11].

These numerical results strongly suggest that the $s-$VBS is a very important competing order on the honeycomb lattice and square lattice. In this paper we develop a theory of phase transitions to/from the $s-$VBS. Put simply, the main result of our analysis is that the appropriate embedding for the $s-$VBS order parameter is into a vector (O(n)) or complex projective (CP(n)) space, both very different from the XY order parameter of the $c-$VBS case. In the main text, we propose effective field theories for several quantum critical points neighboring the $s-$VBS phase, which expose these embeddings. As in the original proposal for the DQCP, these are strongly coupled field theories in 2+1 dimensions, so some of their properties cannot be established conclusively from analytics (we discuss in the main text what can be inferred from the renormalization group literature). However, a robust prediction of the proposed field theories is that, like in the Néel–$c-$VBS problem, the embedding into a larger order parameter space unifies $s-$VBS order with other competing orders, all of which should be present in low energy fluctuations in the vicinity of the quantum critical points. The nature of the competing order(s) is determined from our analysis. For instance, at the transition between the $s-$VBS and a Z_2 spin liquid, the competing order is of four-sublattice plaquette VBS type (Fig. 2c). Other cases are described in the main text. The presence of such competing orders at low energies is testable in numerics or experiment.

The remainder of the paper is organized as follows. In sections II and III, we discuss the theory describing the phase transition between the Z_2 spin liquid and various VBS orders, including the $s-$VBS. In section IV, this theory is extended to the transition between the (easy-plane) Néel order and $s-$VBS. We conclude with some general remarks in Sec. V.

II. ODD Z_2 GAUGE FIELD ON THE HONEYCOMB LATTICE

In this section we begin by considering the simplest candidate for the fully gapped spin liquid state observed in recent numerics on the honeycomb lattice[7,8,12], which is the Z_2 spin liquid. Although honeycomb lattice is a bipartite lattice, the effective spin Hamiltonian of the Hubbard model at intermediate t/U regime is rather complicated[13], thus the spin ground state can be very different from the semiclassical Néel order. Theoretical proposals of Z_2 spin liquid (as well as its generalized versions) on the honeycomb lattice have been made[14–19]. We will study the transition between the Z_2 liquid phase and different types of VBS orders using an effective Z_2 gauge theory on the honeycomb lattice, and eventually in this way connect to the $s-$VBS state. To perform the analysis, we will work with a lattice Z_2 gauge theory, which is particularly convenient. One may wonder whether this is a sufficient and general starting point, correct for all possible Z_2 spin liquid states, since many distinct such states are possible using the projective symmetry group analysis of candidate wavefunctions (see, e.g. Wen's analysis of the square lattice[20]). The answer is, we believe, yes, since our analysis of the lattice gauge theory in fact rests only on three key assumptions, which are true for all fully gapped symmetric Z_2 spin liquids: (1) the Z_2 state supports "visons" (Z_2 vortices), which have a mutual statistics angle of π with respect to elementary spin-1/2 spins; (2) the Z_2 state preserves all the lattice symmetries; and (3) there is a gap to all excitations in the spin liquid state. Thus we believe the results of the following analysis are generally true for transitions from arbitrary gapped Z_2 spin liquids to VBS states.

To understand the meaning of the Ising gauge theory, consider constructing VBS ordered states as the limit of "hard dimers", in which precisely one dimer (spin singlet) is attached to each site. The dimer constraint is translated into the Gauss law constraint in the gauge field language: $\vec{\nabla}\cdot\vec{e}=\eta_i$, and $\eta_i=\pm 1$ on two different sublattices. Now if the U(1) gauge symmetry is broken down to Z_2, we need to introduce a Z_2 electric field $\sigma^x_{ij}=(-1)^{n_{ij}}$ on every link ($n_{ij}=0,1$ denotes the absence and presence of dimer), and the gauge constraint becomes

$$\prod_{\text{links round site } i}\sigma^x_{ij}=-1. \tag{1}$$

With this Z_2 gauge constraint, we can write down the simplest Z_2 gauge theory on the honeycomb lattice as follows:

$$H=\sum_{\hexagon}-K\prod_{\text{links in }\hexagon}^{6}\sigma^z_{ij}-\sum_{i,j}h\sigma^x_{ij}+\cdots. \tag{2}$$

The first term is a sum of the ring product of the Z_2 gauge field σ^z_{ij} in every hexagon, and the second term is a Z_2 "string tension". The ellipses include other interaction terms between Z_2 electric field.

When the K term dominates everything else in Eq. 2, the system is in the deconfined phase of the Z_2 gauge theory, with topological degeneracy. When h or other interaction terms between σ^x dominate K, the system enters the confined phase. In order to analyze the confined phase, it is convenient to go to the dual picture of the Z_2 gauge theory. Dual variables τ^z and τ^x are defined on the dual lattice sites $\bar{m}$, which are located at the center of the hexagons (Fig. 2a):

$$\sigma^x_{ij}=-\tau^z_{\bar{p}}\tau^z_{\bar{q}},\quad \bar{p}\text{ and }\bar{q}\text{ share link }ij,$$

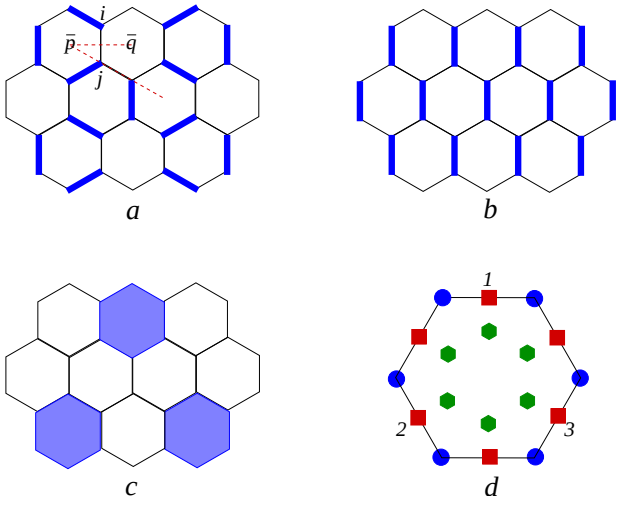

FIG. 2: (a), $c-$VBS order. $\bar{p}$ and $\bar{q}$ are the dual triangular lattice sites. We consider the nearest and 2nd neighbor hopping for vison (vortex). (b), the $s-$VBS pattern, realized when $h/8 < J < h$ in the dual Ising Hamiltonian Eq. 9. (c), the four sublattice plaquette order, realized when $w > 0$ in Eq. 13. (d), the vison (vortex) Brillouin zone. For weak 2nd neighbor vison (vortex) hopping, the minima of band structure are located at the corner of the BZ (circles); with intermediate 2nd neighbor hopping, there are three inequivalent minima located at the center of the edges of BZ (square); There are six inequivalent incommensurate minima with strong 2nd neighbor hopping (hexagon).

$$\prod_{\text{links around } \bar{p}}^{6} \sigma^z_{ij} = \tau^x_{\bar{p}}. \tag{3}$$

Introduction of τ^z_i automatically solves the odd Z_2 gauge constraint Eq. 1. Now the Hamiltonian becomes an *antiferromagnetic* transverse field Ising model on the dual triangular lattice:

$$H = \sum_{\bar{p}} -K\tau^x_{\bar{p}} + \sum_{\bar{p},\bar{q}} J_{\bar{p},\bar{q}}\tau^z_{\bar{p}}\tau^z_{\bar{q}} \tag{4}$$

For nearest neighbor sites $\bar{p}, \bar{q}$, $J_{\bar{p},\bar{q}} = h$. When $J_{\bar{p},\bar{q}}$ dominates K, $\tau^z_{\bar{p}}$ takes on a non-zero expectation value forming some pattern which optimizes the $J_{\bar{p},\bar{q}}$ term. The non-zero "condensate" of τ^z signals that the Z_2 gauge theory has entered the confined phase.

The pattern of order in $\tau^z_{\bar{p}}$ depends upon the detailed form of $J_{\bar{p},\bar{q}}$. This can be analyzed by treating $\tau^z_{\bar{p}}$ as a "soft" scalar field taking all possible real values, rather than the integers ± 1; this approximation describes well the critical region in which fluctuations on short time scales render the average of τ^z non-integral. Then, the quadratic form defined by $J_{\bar{p},\bar{q}}$ can be diagonalized in wavevector space and generically has multiple minima in its Brillouin zone. Physically the eigenvalues of this quadratic form define the dispersion relation of visons in the Z_2 phase. On entering the confined phase, the location of these minima determines the VBS pattern. Notice that the physical VBS order parameter should always be a bilinear of $\langle\tau^z\rangle$, since under transformation $\tau^z \to -\tau^z$ the physical quantity σ^x is unchanged. In the following we will discuss four types of VBS patterns on the honeycomb lattice.

A. $c-$VBS order

Now let us take the simplest case, with nonzero $J_{\bar{p},\bar{q}}$ only between nearest neighbor dual sites $\bar{p}, \bar{q}$. Taking $h > 0$, the model becomes the nearest neighbor frustrated quantum Ising model with transverse field. This model was studied in Ref.[21]. Solving the band structure of τ^z, we find two inequivalent minima at the corners of the vison BZ: $\vec{Q} = (\pm\frac{4\pi}{3}, 0)$. Expanding τ^z at these two minima, we obtain a complex local order parameter ψ:

$$\tau^z \sim \psi e^{i\frac{4\pi}{3}x} + \psi^* e^{-i\frac{4\pi}{3}x}. \tag{5}$$

The low energy physics of visons should be fully characterized by ψ.

Under discrete lattice symmetry, ψ transforms as

$$\begin{aligned}
T_1 &: x \to x+1, \quad \psi \to e^{i\frac{4\pi}{3}}\psi, \\
T_2 &: x \to x+\frac{1}{2}, \; y \to y+\frac{\sqrt{3}}{2}, \quad \psi \to e^{i\frac{2\pi}{3}}\psi, \\
\mathrm{P}_y &: x \to -x, \quad \psi \to \psi^*, \\
\mathrm{P}_x &: y \to -y, \quad \psi \to \psi, \\
\mathrm{T} &: t \to -t, \psi \to \psi^*, \\
\mathrm{R}_{\frac{2\pi}{3}} &: \psi \to \psi.
\end{aligned} \tag{6}$$

$\mathrm{R}_{\frac{2\pi}{3}}$ is the rotation by $2\pi/3$ around the center of hexagon.

The transformations in Eq. 6 determine that the low energy Lagrangian for ψ reads

$$L = |\partial_\mu\psi|^2 + r|\psi|^2 + u|\psi|^4 + w(\psi^6 + \psi^{*6}), \tag{7}$$

i.e. The condensation of ψ is described by a $3d$ XY transition with Z_6 anisotropy. The physical VBS order parameter V should be a bilinear of ψ, *i.e.* $V \sim \psi^2$. It is straightforward to check that V transforms in the same way as the columnar VBS order parameter on the honeycomb lattice. Notice that on the honeycomb lattice the $c-$VBS and the $\sqrt{3}\times\sqrt{3}$ plaquette order have the same symmetry, hence the condensate of ψ can be either the $c-$VBS or the plaquette order depending on the sign of w. Recently this plaquette order has been observed with exact diagonalization on frustrated spin models on the honeycomb lattice[22]. The Z_6 anisotropy introduced by the w term in Eq. 7 is an irrelevant perturbation at the 3d XY fixed point.

If we approach this transition from the $c-$VBS side of the phase diagram, this transition can be interpreted as a

proliferation of the vortex of ψ *i.e.* double vortex of VBS order paramter V, while the single vortex of V is still gapped. In fact, the single vortex core of the $c-$VBS is attached with a spinon (analogous to the square lattice case discussed in Ref.[23]), proliferation of single vortex will lead to a spinon condensate, which corresponds to certain spin order. However, if the spinon gap is finite, the finite temperature thermal fluctuation can proliferate the single vortex. Therefore although the quantum phase transition is driven by double vortices, the finite temperature phase transition is still driven by single vortex, hence at finite temperature the Z_6 anisotropy of Eq. 7 becomes the Z_3 anisotropy, and there is no algebraic Kosterlitz-Thouless phase at finite temperature. This is a key difference between our current case and a physical transverse field frustrated quantum Ising model, where a finite temperature algebraic phase is expected[21].

B. $s-$VBS order and four-fold plaquette order

Now we modify the Z_2 gauge theory in Eq. 2 by turning on the interaction between Z_2 electric field σ^x on second nearest neighbor links:

$$H_J = \sum_{\text{2nd neighbor links}} J\sigma^x_{ij}\sigma^x_{kl}. \tag{8}$$

In the dual theory this electric field interaction becomes a next nearest neighbor hopping of τ^z, and the full dual Hamiltonian reads

$$H = \sum_{\bar{p}} -K\tau^x_{\bar{p}} + \sum_{<\bar{p},\bar{q}>} h\tau^z_{\bar{p}}\tau^z_{\bar{q}} + \sum_{\ll\bar{p},\bar{q}\gg} J\tau^z_{\bar{p}}\tau^z_{\bar{q}}. \tag{9}$$

The vison minima $(\pm\frac{4\pi}{3}, 0)$ are stable with $J/h < 1/8$. When $1/8 < J/h < 1$, the minima of the vison band structure are shifted to three inequivalent points on the edges of BZ (Fig. 2*d*):

$$\begin{aligned}
\vec{Q}_1 &= (0, \frac{2\sqrt{3}\pi}{3}),\\
\vec{Q}_2 &= (-\pi, -\frac{\sqrt{3}\pi}{3}),\\
\vec{Q}_3 &= (\pi, -\frac{\sqrt{3}\pi}{3}).
\end{aligned} \tag{10}$$

Notice that $-\vec{Q}_a$ are equivalent to $\vec{Q}_a$ in the BZ.

Now three low energy modes can be defined by expanding τ^z at momenta $\vec{Q}_a$:

$$\tau^z \sim \sum_a \varphi_a \; e^{i\vec{Q}_a\cdot\vec{r}}. \tag{11}$$

Since $\vec{Q}_a$ and $-\vec{Q}_a$ are equivalent, all three fields φ_a are real. Under lattice symmetry, φ_a transform as

$$\begin{aligned}
T_1 &: \varphi_1 \to \varphi_1, \quad \varphi_2, \varphi_3 \to -\varphi_2, -\varphi_3,\\
T_2 &: \varphi_1, \varphi_2 \to -\varphi_1, -\varphi_2, \quad \varphi_3 \to \varphi_3,\\
\mathrm{P}_y &: \varphi_1 \to \varphi_1, \quad \varphi_2, \varphi_3 \to \varphi_3, \varphi_2,\\
\mathrm{P}_x &: \varphi_1 \to \varphi_1, \quad \varphi_2, \varphi_3 \to \varphi_3, \varphi_2,\\
\mathrm{T} &: \varphi_a \to \varphi_a,\\
\mathrm{R}_{\frac{2\pi}{3}} &: \varphi_1 \to \varphi_2, \; \varphi_2 \to \varphi_3, \; \varphi_3 \to \varphi_1.
\end{aligned} \tag{12}$$

Now the symmetry allowed Lagrangian for φ_a up to the quartic order reads

$$L = \sum_a (\partial_\mu \varphi_a)^2 + r\varphi_a^2 + u(\sum_a \varphi_a^2)^2 + w(\sum_a \varphi_a^4). \tag{13}$$

This is an O(3) model with cubic anisotropy. There are two possible types of condensates of φ_a:

(*i*) When $w > 0$, the condensate $\langle\vec{\varphi}\rangle$ are along the diagonal directions, and there are in total four independent states with $\langle\vec{\varphi}\rangle \sim (1,1,1)$, $(-1,-1,1)$, $(-1,1,-1)$, $(1,-1,-1)$. According to the transformation of $\vec{\varphi}$, these four states correspond to the four-sublattice plaquette phase (Fig. 2*c*).

(*ii*) When $w < 0$, the condensate $\langle\vec{\varphi}\rangle$ has three fold degeneracy: $\langle\vec{\varphi}\rangle \sim (1,0,0)$, $(0,1,0)$ and $(0,0,1)$. These three condensates break the rotation symmetry of the lattice, but they do not break the translation symmetry. This is again because physical order parameters are bilinears of φ_a, hence they are insensitive to the sign change of φ_a under translation. These three states correspond precisely to the three $s-$VBS pattern. Unlike the $c-$VBS, the $s-$VBS is no longer described by an XY order parameter, and the phase transition is not driven by vortex-like VBS defect.

The universality class of Eq. 13 was studied extensively with $\epsilon = 4 - d$ expansion[24]. The results is that the O(3) Heisenberg fixed point is not stable. For $w > 0$ the transition is controlled by a stable cubic fixed point with nonzero fixed point values w^* and u^*. This case corresponds to the transition between the Z_2 spin liquid and the four-sublattice plaquette phase described above. For $w < 0$, which corresponds to the transition to the $s-$VBS phase, there is instead a run-away flow, which most likely implies a first order transition. But if w is small enough, for numerical simulations on finite system the transition between Z_2 spin liquid and $s-$VBS will be similar to the $3d$ O(3) transition.

Although we chose a specific vison hopping model Eq. 9 to obtain the vison band structure, the three minima $\vec{Q}_a$ in the BZ are stable against any symmetry allowed perturbations on Eq. 9. This is because no linear spatial derivative terms are allowed in Eq. 13 by transformations Eq. 12. Thus there are only two ways to destabilize the minima in the BZ: (*1*). the current minima will be replaced by a new set of minima through a first order transition, like the transition between $c-$VBS and $s-$VBS at $J/h = 1/8$; (*2*). the sign of the spatial derivative

terms in Eq. 9 changes through a second order Lifshitz transition. The second situation will lead to the incommensurate VBS order, which will be discussed in the next subsection.

C. incommensurate VBS

In Eq. 9, if $J/h > 1$, the vison band structure has six inequivalent incommensurate minima $\vec{Q}_a$ in its BZ (Fig. 2*d*). Since $\vec{Q}_a$ and $-\vec{Q}_a$ are no longer equivalent, the low energy vison modes are described by three *complex* fields φ_a:

$$\tau^z \sim \sum_a \left(\varphi_a e^{i\vec{Q}_a\cdot\vec{r}} + \varphi_a^* e^{-i\vec{Q}_a\cdot\vec{r}}\right). \quad (14)$$

Under lattice symmetries, these vison fields transform as

$$\begin{aligned} T_1 &: \varphi_a \to e^{i\vec{Q}_{a,x}x}, \\ P_y &: \varphi_1 \to \varphi_1, \quad \varphi_2,\varphi_3 \to \varphi_3,\varphi_2, \\ P_x &: \varphi_1 \to \varphi_1^*, \quad \varphi_2,\varphi_3 \to \varphi_3^*,\varphi_2^*, \\ T &: \varphi_a \to \varphi_a^*, \\ R_{\frac{2\pi}{3}} &: \varphi_1 \to \varphi_2,\ \varphi_2 \to \varphi_3,\ \varphi_3 \to \varphi_1. \end{aligned} \quad (15)$$

The field theory describing φ_a is

$$\begin{aligned} L &= \sum_a |\partial_\mu \varphi_a|^2 + r|\varphi_a|^2 + u(\sum_a |\varphi_a|^2)^2 + w(\sum_a |\varphi_a|^4) \\ &+ v_1|\varphi_1|^2|\varphi_2|^2|\varphi_3|^2 + v_2(\varphi_1^2\varphi_2^2\varphi_3^2 + H.c.) + \cdots \end{aligned} \quad (16)$$

When $\vec{\varphi}$ condenses, the system exhibits incommensurate VBS order. Since incommensurate VBS order has yet to be observed numerically, we will not explore this phase or the corresponding transitions further.

D. A quantum dimer model

In addition to the numerical works introduced in section I, a recent QMC simulation discovered a gapped liquid phase in the SU(4) Hubbard model on the honeycomb lattice. In those simulations, this liquid phase appeared between the semimetal phase and $c-$VBS phase, and SU(4) Néel order was completely absent[25]. Since all the gapped liquids observed numerically are adjacent to VBS phases, it is natural to approach the gapped liquid phase starting with dimer (spin singlet) basis. In this subsection we write down a quantum dimer model which realizes part of the physics discussed above.

The standard quantum dimer model (QDM) on the honeycomb lattice has been studied carefully in the past[26]:

$$H_0 = H_t + H_v$$

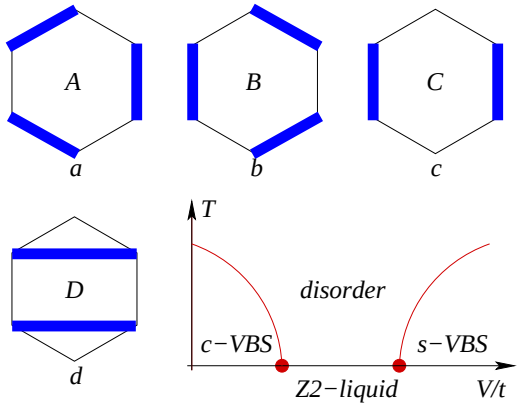

FIG. 3: $(a)-(d)$, the dimer patterns involved in the quantum dimer model Eq. 17 and Eq. 19. e, phase diagram of the quantum dimer model tuned with V/t, with the presence of H_1 in Eq. 19.

$$= -t\ (|A\rangle\langle B| + |B\rangle\langle A|) + V\ (|A\rangle\langle A| + |B\rangle\langle B|) \quad (17)$$

$|A\rangle$ and $|B\rangle$ are dimer configurations depicted in Fig. 3*a*, *b*. This model can be mapped to a compact U(1) gauge theory in the standard way:

$$\vec{e}_{ij} = \vec{v}\cdot n_{ij}, \quad H_t \sim -t\cos(\vec{\nabla}\times\vec{a}). \quad (18)$$

Here $n_{ij} = 0, 1$ is the dimer density on each link (i, j), $\vec{v}$ is a unit vector defined on each link, and it always points from sublattice A to B on the honeycomb lattice. $\vec{e}$ and $\vec{a}$ are electric field and gauge vector potential respectively. Due to the confinement of compact U(1) gauge theory in two dimensions[27], the system is gapped and VBS ordered throughout the phase diagram, except for the isolated gapless RK point at $V = t$. There is thus no stable gapped liquid phase in this phase diagram[26]. Therefore in order to understand the gapped liquid phase around VBS phases on the honeycomb lattice, a modified QDM is needed.

First of all, we notice that all the gapped liquid phases observed numerically only occur at intermediate J_2/J_1 or t/U (Ref.[7,8,25]). In this regime, there must be a considerable probability for dimers to form not only between nearest neighbor sites but also between next nearest neighbor sites. Then, in addition to the standard QDM Eq. 17, we turn on the following dimer flipping term:

$$H_1 = -\tilde{t}\ (|C\rangle\langle D| + |D\rangle\langle C|). \quad (19)$$

$|C\rangle$ and $|D\rangle$ are dimer configurations in Fig. 3*c*, *d*. This term breaks the U(1) gauge symmetry of the original QDM down to Z_2 gauge symmetry, because it annihilates two electric flux quanta along the same direction. An alternative way of understanding this Z_2 effect is by noticing that annihilating configuration $|C\rangle$ is equivalent to hopping two unit U(1) gauge charges, hence H_1 is

equivalent to the following term at low energy:

$$H_1 \sim -\cos(2\nabla_\mu \phi - 2a_\mu). \quad (20)$$

Here $\exp(i\phi)$ creates a unit gauge charge. When ϕ condenses, it breaks the U(1) gauge symmetry down to Z_2. As an analogue, the triangular lattice QDM can also be viewed as a square lattice QDM with extra diagonal dimers, which also breaks the U(1) gauge symmetry down to Z_2.

The term H_1 can drive the system into a Z_2 liquid phase on the honeycomb lattice. In the presence of nonzero H_1, a possible schematic phase diagram for the QDM is shown in Fig. 3*e*. The Z_2 liquid phase intervenes between the $c-$VBS and $s-$VBS phases. The nature of the phase transitions in this phase diagram have been discussed in subsection IIA and IIB.

The transition between the Z_2 liquid phase and the $c-$VBS can also be more intuitively understood as follows: The $c-$VBS is a confined phase of the compact U(1) gauge field, where the triple-monopole of the compact U(1) gauge field leads to the following height field theory in the dual theory:

$$L_h = (\partial_\mu h)^2 - g\cos(6\pi h), \quad (21)$$

where height field h is defined as $\vec{e} = \hat{z} \times \vec{\nabla} h$, and $\exp(i2\pi h)$ creates a flux quantum of the compact U(1) gauge field $\vec{a}$. The vertex operator $-g\cos(6\pi h)$ has three independent minima $h = 0,\ \pm 1/3$, which corresponds to the three fold degenerate $c-$VBS phase. In the Z_2 liquid phase, since the U(1) gauge symmetry is broken down to Z_2, there are stable π-flux excitations of the U(1) gauge field. Hence the triple-monopole of the U(1) gauge field corresponds to creating/annihilating six π-flux. If we describe the transition in terms of these π-flux excitations, the field theory takes exactly the same form as Eq. 7.

At the transition between the $c-$VBS and Z_2 liquid phase, based on the well-known critical exponent of the 3d XY fixed point obtained from various methods[24], we predict the anomalous dimension of the $c-$VBS order parameter to be $\eta_V = 1.47$ (much larger than the ordinary Wilson-Fisher transitions). Also, close to this transition, the $c-$VBS order parameter scales as $\langle V \rangle \sim (r_c - r)^\beta$, with $\beta = 0.83$. These predictions can be checked numerically.

III. ODD Z_2 GAUGE THEORY ON THE SQUARE LATTICE

Now we switch gears to the odd Z_2 gauge theory on the square lattice. Again we want to discuss the phase transition from the Z_2 liquid phase to both $c-$VBS and $s-$VBS. The odd Z_2 gauge theory is dual to a transverse field quantum Ising model on the dual square lattice (Fig. 4*a*). Unlike the honeycomb lattice case, now the dual quantum Ising model has to apparently break the lattice symmetry in any specific gauge choice. The correct lattice symmetry transformation for the dual vison field τ^z must be combined with a nontrivial Z_2 gauge transformation, *i.e.* τ^z carries a projective representation of the symmetry group. The dual quantum Ising model has to be invariant under the projective symmetry group (PSG).

We consider the following Hamiltonian for the dual Ising model:

$$H = \sum_{\bar{p}} -K\tau^x_{\bar{p}} + \sum_{<\bar{p},\bar{q}>} J_{\bar{p},\bar{q}}\tau^z_{\bar{p}}\tau^z_{\bar{q}} + \sum_{\bar{p},\bar{q}} J'_{\bar{p},\bar{q}}\tau^z_{\bar{p}}\tau^z_{\bar{q}}. \quad (22)$$

J and J' denote the nearest and fourth nearest neighbor Ising couplings. J and J' are chosen to be positive on all the solid bonds, but negative on all the dashed bonds in Fig. 4*a*. The Hamiltonian of Eq. 22 with the current choice of gauge is invariant under the PSG of τ^z. Notice that 2nd nearest neighbor Ising couplings are entirely prohibited by the PSG.

If $J'/J < 0.0858$, there are two inequivalent minima in the vison band structure, located at $\vec{Q} = (0, \pm\frac{\pi}{2})$. Again we can expand τ^z at these two minima as

$$\tau^z \sim \varphi e^{i\frac{\pi}{2}y} + \varphi^* e^{-i\frac{\pi}{2}y}. \quad (23)$$

The PSG for φ reads

$$\begin{aligned}
\mathrm{T}_x &: x \to x+1, \quad \varphi \to e^{i\frac{\pi}{4}x}\varphi^*, \\
\mathrm{T}_y &: y \to y+1, \quad \varphi \to e^{-i\frac{\pi}{4}x}\varphi^*, \\
\mathrm{P}_y &: x \to -x, \quad \varphi \to \varphi, \\
\mathrm{P}_x &: y \to -y, \quad \varphi \to \varphi, \\
\mathrm{P}_{x+y} &: x \to y,\ y \to x, \quad \varphi \to i\varphi^*. \quad (24)
\end{aligned}$$

Notice that the reflection P_x and P_y are site-centered reflection of the dual lattice (bond-centered reflection of the original lattice). The PSG allowed field theory for φ reads

$$L = |\partial_\mu \varphi|^2 + r|\varphi|^2 + g|\varphi|^4 + w(\varphi^8 + \varphi^{*8}). \quad (25)$$

The gauge invariant physical order parameters are

$$\begin{aligned}
c-\mathrm{VBS}_x &: e^{i\frac{\pi}{4}}\varphi^2 + e^{-i\frac{\pi}{4}}\varphi^{*2}, \\
c-\mathrm{VBS}_y &: e^{-i\frac{\pi}{4}}\varphi^2 + e^{i\frac{\pi}{4}}\varphi^{*2}. \quad (26)
\end{aligned}$$

The quantum phase transition between the Z_2 liquid and the $c-$VBS is a $3d$ XY transition, since the Z_8 anisotropy in Eq. 25 is highly irrelevant at the $3d$ XY fixed point. This result is consistent with previous studies on fully frustrated Ising model on the cubic lattice[28,29].

When $J'/J > 0.0858$, the minima of the vison band structure are shifted to four other inequivalent momenta in the BZ:

$$Q_1 = (0,0), \quad Q_2 = (0,\pi),$$

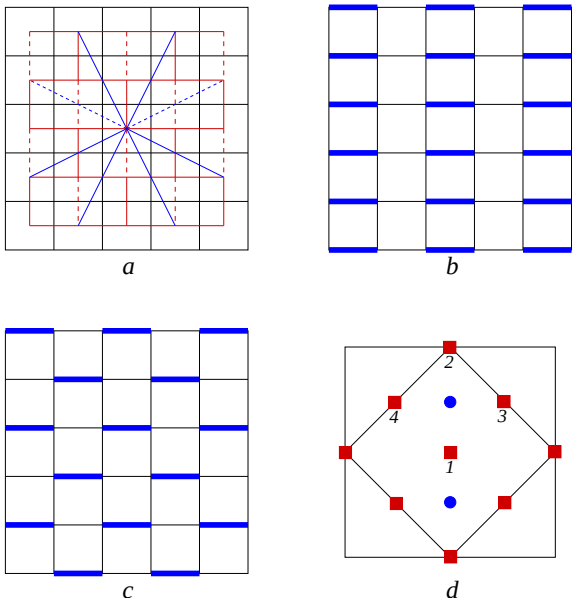

FIG. 4: (a), the dual square lattice. The vison (vortex) hopping on the dashed bonds are negative. (b), (c), the $c-$VBS and $s-$VBS patterns. (d), the vison (vortex) Brillouin zone. When the nearest neighbor vison (vortex) hopping is dominant, there are two inequivalent minima located at $(0, \pm\frac{\pi}{2})$ (circles); when the 4th neighbor hopping is dominant, there are four inequivalent minima described by Eq. 27.

$$Q_3 = (\frac{\pi}{2}, \frac{\pi}{2}), \quad Q_4 = (-\frac{\pi}{2}, \frac{\pi}{2}). \tag{27}$$

We denote the low energy vison modes at these four momenta by φ_a with $a = 1 \cdots 4$. Notice all these four modes are real fields, because Q_a are equivalent to $-Q_a$.

The PSG action on φ_a reads

$$\begin{aligned}
\mathrm{T}_x &: \varphi_1 \to \varphi_2, \quad \varphi_2 \to \varphi_1, \quad \varphi_3 \to \varphi_4, \quad \varphi_4 \to -\varphi_3, \\
\mathrm{T}_y &: \varphi_1 \to \varphi_2, \quad \varphi_2 \to -\varphi_1, \quad \varphi_3 \to \varphi_4, \quad \varphi_4 \to \varphi_3, \\
\mathrm{P}_y &: \varphi_1 \to \varphi_1, \quad \varphi_2 \to \varphi_2, \quad \varphi_3 \to \varphi_4, \quad \varphi_4 \to \varphi_3, \\
\mathrm{P}_x &: \varphi_1 \to -\varphi_2, \quad \varphi_2 \to -\varphi_1, \quad \varphi_3 \to \varphi_3, \quad \varphi_4 \to \varphi_4, \\
\mathrm{P}_{x+y} &: \varphi_1 \to \varphi_3, \quad \varphi_3 \to \varphi_1, \quad \varphi_2 \to \varphi_4, \quad \varphi_4 \to \varphi_2.
\end{aligned} \tag{28}$$

It is straightforward to show that these four vison minima actually describe the $s-$VBS pattern on the square lattice. By using the PSG transformations above, we find that fields transforming as the $s-$VBS order parameters are

$$\begin{aligned}
s-\mathrm{VBS}_x &: \varphi_1^2 - \varphi_2^2, \\
s-\mathrm{VBS}_y &: \varphi_3^2 - \varphi_4^2.
\end{aligned} \tag{29}$$

Applying the PSG to obtain a general invariant field theory, we find, up to quartic order the Lagrangian

$$\begin{aligned}
L &= \sum_a (\partial_\mu \varphi_a)^2 + r\varphi_a^2 + u(\sum_a \varphi_a^2)^2 \\
&+ w(\sum_a \varphi_a^4) + v(\varphi_1^2 + \varphi_2^2)(\varphi_3^2 + \varphi_4^2)
\end{aligned} \tag{30}$$

The location of vison band structure minima is stable, since no linear spatial derivative terms are allowed in this field theory. The first line of this equation describes an O(4) theory, which is very different from the effective XY theory in the $c-$VBS case. The second line of Eq. 30 breaks this O(4) symmetry down to $Z_4 \times Z_4 \times Z_2$. When $v > 0$, $w < 0$, the visons condense in a way that yields $s-$VBS order. However, according to the high order ϵ expansion in Ref.[30], both v and w are relevant perturbations at the 3d O(4) universality class. This likely indicates the lack of a direct continuous Z_2 spin liquid to s-VBS transition (though a weakly first-order transition would be possible).

IV. MAGNETIC ORDER – VBS TRANSITIONS

The phase transition between the standard collinear ordered antiferromagnet and the $c-$VBS phase is described by the theory of deconfined criticality, with the critical effective field theory being the noncompact CP(1) model[1,2]. This deconfined phase transition is realized in the $J-Q$ model on the square lattice with both two spin and four spin interactions[3132]. Recent exact diagonalization simulation of the same model (with full parameter space of $J-Q$)[10] and QMC on a modified $J-Q$ model[5] discovered that there can also be a direct transition between the Néel and $s-$VBS order, and this transition is what we will try to understand in this section.

To simplify this problem, we turn on an easy plane anisotropy on the spin system. Now the spin-1/2 problem is equivalent to a hard-core boson model at half-filling, and the Néel order is mapped to the superfluid phase of the boson system. It is well-known that the hard-core boson problem is dual to its vortex theory, where vortices are bosons hopping on the dual lattice sites, with coupling to a dynamical U(1) gauge field, this U(1) gauge field is precisely the dual of the Goldstone mode of the superfluid phase. Because the boson is half-filled, a vortex will see a $\pi-$flux through each of the dual plaquettes.

Previous studies showed that if the nearest neighbor vortex hopping is considered in the dual Hamiltonian, the transition between superfluid (Néel order) and $c-$VBS may be described as the condensation of vortices[33,34]. In the follows we will see that if further neighbor vortex hoppings are taken into account, the superfluid (Néel order) to $s-$VBS transition can also be understood as vortices condensing in its BZ, just like the vison theory in the previous sections.

For instance, on both the honeycomb and square lattice, in order to describe the $s-$VBS phase, we only need

to turn on exactly the same further neighbor vortex hopping as the previous vison theories in section II and III. The PSG of the vortices is almost identical to that of the visons in the previous sections, thus we will not write it down explicitly. The main differences between the vortex theory and vison theory are, (*1*) the vortex is described by a complex boson instead of real boson, (*2*) the vortex is coupled to a dynamical U(1) gauge field, (*3*) physical order parameters should be U(1) gauge invariant.

We summarize our results here:

(*i*) on the honeycomb lattice, with 2nd neighbor vortex hopping, the vortex band structure can have minima located at the three momenta in Eq. 10, the low energy vortex mode at each momentum is described by a complex boson field φ_a. The transition between the superfluid (magnetic order) and the $s-$VBS is described by the CP(2) theory with cubic anisotropy:

$$\begin{aligned} L &= \sum_{\alpha=1}^{3} |(\partial_\mu - iA_\mu)\varphi_\alpha|^2 + r|\varphi_\alpha|^2 + g(\sum_\alpha |\varphi_\alpha|^2)^2 \\ &+ \sum_\alpha u|\varphi_\alpha|^4 + \cdots \end{aligned} \tag{31}$$

When $u < 0$ and $r < 0$, only one of the vortex modes is condensed, which corresponds to the $s-$VBS order. Although φ_a is a complex field, its condensate has no gapless Goldstone mode, due to its coupling to U(1) gauge field A_μ. It is unclear whether cubic anisotropy is relevant or not at this CP(2) quantum critical point. The scaling dimension of the cubic anistropy can be calculated systematically with the standard $1/N$ expansion.

(*ii*) on the square lattice, the transition between the superfluid (magnetic order) and the $s-$VBS is described by the CP(3) theory with anisotropies that break the SU(4) symmetry down to $(\mathrm{U}(1))^4$ and discrete interchange symmetries between φ_a:

$$\begin{aligned} L &= \sum_{\alpha=1}^{4} |(\partial_\mu - iA_\mu)\varphi_\alpha|^2 + r|\varphi_\alpha|^2 + g(\sum_\alpha |\varphi_\alpha|^2)^2 \\ &+ \sum_\alpha u|\varphi_\alpha|^4 + v(|\varphi_1|^2 + |\varphi_2|^2)(|\varphi_3|^2 + |\varphi_4|^2) + \end{aligned} \tag{32}$$

φ_α are four low energy vortex modes at the four momenta in Eq. 27. When $u < 0$, $v > 0$ the condensate of φ_a corresponds to the $s-$VBS order. The $s-$VBS order parameters are

$$\begin{aligned} s-\mathrm{VBS}_x &: |\varphi_1|^2 - |\varphi_2|^2, \\ s-\mathrm{VBS}_y &: |\varphi_3|^2 - |\varphi_4|^2. \end{aligned} \tag{33}$$

Here there are two quartic anisotropies, though again their scaling behavior at the CP(3) point needs to be addressed by further calculations.

It was shown in Ref.[23] that the Z_4 vortex of $c-$VBS has to carry a spinon. However, in Fig. 1 we illustrated that there is no spinon attached to the Z_4 vortex of the $s-$VBS, thus the $s-$VBS to magnetic order transition should not be induced with Z_4 vortex proliferation. This difference can be understood with the $s-$VBS order parameters in Eq. 33: the flux of the U(1) gauge field in Eq. 32 carries spin (since A_μ is the dual of Goldstone mode associated with S^z conservation), while the Z_4 vortex of $s-$VBS is simply a vortex surrounded by φ_1, φ_3, φ_2 and φ_4 condensate cyclicly, thus no gauge flux is attached with this vortex core. In fact, the U(1) gauge flux corresponds to the "skyrmion" type of defect of the CP(2) and CP(3) manifold. Thus to induce a magnetically ordered phase, we need to condense the more complicated skyrmion defect of the $s-$VBS order.

V. SUMMARY AND OUTLOOK

In this work we studied the quantum transitions from the Z_2 spin liquid and magnetically ordered phases to different types of VBS orders, with the focus on the staggered VBS. Although the $s-$VBS and $c-$VBS have the same degeneracy, the low energy field theories describing these two cases close to the transitions are very different. In our current work we only considered the case of transitions from magnetically ordered phases with easy plane anisotropy, while a description for the SU(2) invariant case is still needed. We will leave this case to future study. Moreover, even in the easy plane case, the field theories we obtained are not well-studied, and the effects of anisotropies on their critical properties (and indeed stability of the latter) deserve more detailed study.

The formalisms we used in this work, namely the odd Z_2 gauge theory, the dual vortex theory, and quantum dimer model, are all theories for strongly coupled systems, *i.e.* the electric charge excitations of this system were ignored completely. However, the deconfined quantum criticality theory can also be formulated in the weak coupling limit, as it can be interpreted as the phase transition between five competing mass gap order parameters of Dirac fermion[35]. The Dirac fermion will generate a topological Wess-Zumino-Witten (WZW) term for these competing orders[36,37], and physically the WZW term attaches a spin-1/2 degree of freedom to each vortex core of the $c-$VBS. Fermions on both honeycomb lattice, and square lattice with $\pi-$flux through every plaquette have Dirac fermion in the band structure, and in both cases the Néel and $c-$VBS are five competing order parameters with a WZW term[38].

Unlike the $c-$VBS, the $s-$VBS does not generate a Dirac mass gap for either honeycomb or square lattice $\pi-$flux state, thus the standard calculation used in Ref.[36,37] does not lead to a WZW term between $s-$VBS and Néel order. This observation also suggests that the $s-$VBS and $c-$VBS are fundamentally different, which echoes the results obtained in our current paper. In the future, it would be very meaningful to also pursue a weak coupling version of the theory for quantum phase transitions with $s-$VBS using fermion band structure.

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