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Quantum phase transitions in bilayer SU(N) antiferromagnets

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We present a detailed study of the destruction of SU(N) magnetic order in square lattice bilayer antiferromagnets using unbiased quantum Monte Carlo numerical simulations and field theoretic techniques. We study phase transitions from an SU(N) Néel state into two distinct quantum disordered "valence-bond" phases: a valence-bond liquid (VBL) with no broken symmetries and a lattice-symmetry-breaking valence-bond solid (VBS) state. For finite interlayer coupling, the cancellation of Berry phases between the layers has dramatic consequences on the two phase transitions: the Néel-VBS transition is first order for all $N \geqslant 5$ accesible in our model, whereas the Néel-VBL transition is continuous for $N = 2$ and first order for $N \geqslant 4$; for $N = 3$ the Néel-VBL transition show no signs of first-order behavior.

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The study of quantum phase transitions is an exciting field at the forefront of theoretical condensed-matter physics.[1] The nature of a particular quantum phase transition is governed by properties that affect long-distance physics, such as broken symmetries, topological order, and the presence of Berry phases, and is generally insensitive to microscopic details. Quantum magnets provide the richest examples of quantum phase transitions because they possess internal symmetries in addition to the usual lattice and time-reversal symmetries and because they often have nontrivial Berry phases in their long wavelength descriptions.[2] The most popular internal symmetry group in condensed matter is the SU(N) group. Initial interest was focused on SU(2), and the case of $N > 2$ was introduced purely as a theoretical tool to access the analytically solvable $N \to \infty$ limit.[3,4] However, in the ensuing years it has come to be recognized that SU(N) systems with $N > 2$ *but finite* are interesting in their own right, since they serve to model a number of physical systems ranging from spin-orbit coupled solid-state materials[5] to ultracold atoms in optical lattice potentials.[6] While the ground states of SU(N) spin models in one-dimensional chains are relatively well understood,[7,8] two-dimensional phases[9–11] and their associated phase transitions are only poorly understood.

In this work we address the destruction of the SU(N) symmetry-breaking Néel order in the two-dimensional bilayer system shown in Fig. 1(a). In the bilayer geometry the Berry phases cancel between the two layers in the continuum limit, allowing access to the phase transitions of interest without the additional complication of quantum interference effects. We have studied the properties of the phase transitions from Néel order to two different types of paramagnetic states, the valence-bond liquid (VBL) and the valence-bond solid (VBS) [see Figs. 1(b) and 1(c)]. The Néel-VBL transition for $N = 2$ has been studied extensively[12–15] and is well known to be continuous in the O(3) universality class. Here we address the fate of this transition when $N > 2$. We find that a simple Landau mean-field theory predicts a discontinuous Néel-VBL transition for $N > 2$ and a continuous transition for $N = 2$. Using unbiased quantum Monte Carlo simulations, we confirm the expectations of the Landau theory, except for $N = 3$, where we find no evidence for a first-order transition. We show that if this transition is continuous, its universality class should be identified with a critical point in the compact CP^2 model.[16,17] The Néel-VBS transition in the single-layer model has been predicted[18] and numerically found to be continuous and in the universality class of the *noncompact* CP^{N-1} model for all N.[19–21] We show that remarkably the Néel-VBS transition, characterized by the same broken symmetries, becomes first order in the bilayer geometry for all N studied here (our model gives us access to $N \geqslant 5$), a striking consequence of the cancellation of Berry phases between layers.

Bilayer model. Our SU(N) symmetric model is defined with a local Hilbert space of N states on each site of the bilayer square lattice illustrated in Fig. 1(a). We label these states as $|\alpha\rangle$ with $1 \leqslant \alpha \leqslant N$. We adopt the representation used previously in both analytic[3,4,22] and numerical[21,23,24] works on bipartite lattices, where the sublattice-A states transform under rotations with the fundamental representation of SU(N) [generated by the $N^2 - 1$ matrices T^a], and the B sublattice states transform with the conjugate of this representation. We consider two different SU(N) invariant interaction: between sites i and j on the same sublattice $\Pi_{ij} \equiv \sum_a T_i^a T_j^a$ and between sites on opposite sublattices $P_{ij} \equiv \sum_a T_i^a T_j^{*a}$. Using these interactions, we define a model SU(N) symmetric bilayer system as follows:

$$H_{\text{bil}} = -\frac{J_1}{N}\sum_{\langle ij\rangle} P_{ij} - \frac{J_2}{N}\sum_{\langle\langle ij\rangle\rangle} \Pi_{ij} - \frac{J_\perp}{N}\sum_{[ij]} P_{ij}, \qquad (1)$$

where $\langle ij\rangle$ denotes nearest neighbors in the square lattice layers, $\langle\langle ij\rangle\rangle$ denotes next nearest neighbors in the square lattice layers, and $[ij]$ denotes interlayer bonds, as illustrated in Fig. 1(a). The J_1 term by itself gives the familiar single-layer SU(N) antiferromagnet, which is Néel ordered for $N \leqslant 4$ and VBS ordered for $N \geqslant 5$. Adding a J_2 term to the J_1 model favors the Néel state, causing the Néel-VBS transition to move to arbitrary large N as J_2 is increased.[21] Finally, when the $J_\perp$ term is made large enough, it always favors the formation of a VBL by forcing the formation of local singlets [see Fig. 1(b)]. The model bilayer antiferromagnet, Eq. (1), reduces to the familiar SU(2) bilayer model for $N = 2$ and $J_2 = 0$.

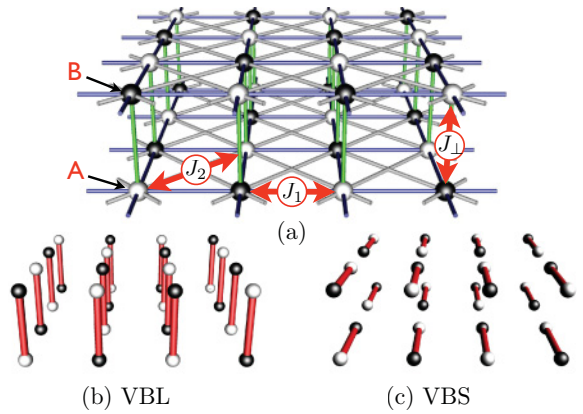

FIG. 1. (Color online) (a) Bilayer geometry: The white (black) sites are the A(B) sublattice on which spins transform as the fundamental (conjugate) representation of SU(N). J_1 connects nearest neighbors in the plane, J_2 connects next nearest neighbors in the plane, and $J_\perp$ connects sites on different layers. Panels (b) and (c) show cartoon product wave functions of local singlets for the VBL and VBS states. In reality, the ground state is a strongly interacting superposition of all valence-bond coverings. The ground state nevertheless (b) preserves all symmetries for the VBL, but (c) breaks lattice symmetry (as shown) for the VBS. In this Rapid Communication, we provide a detailed study of the Néel-VBL and Néel-VBS quantum phase transitions.

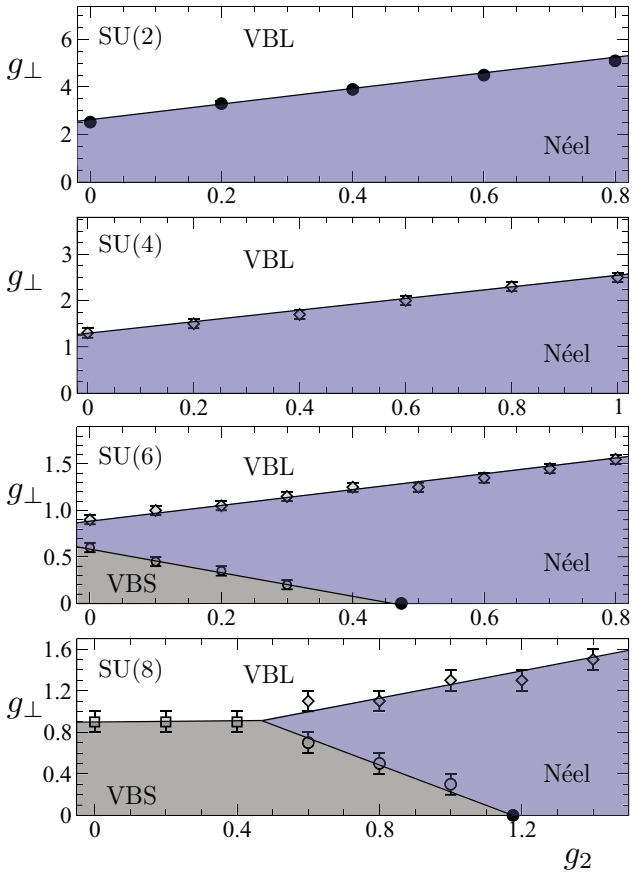

FIG. 2. (Color online) Phase diagram of the model $H_{\rm bil}$ defined in Eq. (1) for SU(2), SU(4), SU(6) and SU(8) symmetry in the plane of $g_2 \equiv J_2/J_1$ and $g_\perp \equiv J_\perp/J_1$. The unfilled symbols are locations of first order phase transitions, Néel-VBL (diamonds), Néel-VBS (circles) and VBS-VBL (squares). The solid black circles mark continuous transitions. For SU(2), the line of Néel-VBL critical points shown are in the universality class of the O(3) non-linear $\sigma-$model. For SU(6) and SU(8) the Néel-VBS transitions shown are in the universality class of the non-compact CP^{N-1} models (with $N = 6,8$ respectively). Solid lines and shaded regions are guides to the eye.

Since $H_{\rm bil}$ satisfies Marshall's sign criteria, it can be simulated using unbiased quantum Monte Carlo methods on large lattices of linear dimension L with $2 \times L \times L$ sites and at finite-temperature T using the stochastic series expansion method with loop updates .[25–27] Néel order is detected by the existence of a nonzero spin stiffness $\rho_s = T\langle W^2\rangle$ in the limit of $L \to \infty$, where W is the spatial winding number of the world lines.[27] Likewise, long-range order in the correlation function $N^2 C_V(\mathbf{r},\tau) = \langle P_{\mathbf{0},\mathbf{0}+\mathbf{x}}(0) P_{\mathbf{r},\mathbf{r}+\mathbf{x}}(\tau)\rangle - \langle P_{\mathbf{0},\mathbf{0}+\mathbf{x}}(0)\rangle^2$ signals spontaneous translational symmetry breaking, that is, the onset of VBS order. All the VBS ordering studied in our bilayer system is of the columnar type [at momentum $(\pi,0)$] and is in phase between the layers [see Fig. 1(c)]. We define $O^2_{\rm VBS}$ in the usual way as the long-distance limit of the VBS correlation function. Finally, an absence of both long-range Néel and VBS orders indicates the formation of a VBL state. Using these tests for the three phases, Néel, VBS, and VBL, we have computed the $T = 0$ phase diagram in the $g_\perp - g_2$ plane ($g_\perp \equiv J_\perp/J_1$, $g_2 \equiv J_2/J_1$) for each $N \leqslant 10$. For $N \leqslant 4$, the model Eq. (1) has only two phases: Néel and VBL [Fig. 1(b)]. For $N \geqslant 5$, the model admits in addition a VBS phase [Fig. 1(c)]. Phase diagrams for the bilayer model, Eq. (1), for SU(2), SU(4), SU(6), and SU(8) symmetry are shown in Fig. 2. These four cases contain all the types of phase diagrams we have encountered in our study with $N \leqslant 10$. We now turn to the main focus of our paper, a detailed analysis of the nature of the Néel-VBL and Néel-VBS phase transitions that appear in these phase diagrams for each N.

Néel-VBL. First, we analyze the transition between the Néel state and the featureless fully symmetric valence bond liquid [a cartoon of the VBL state is illustrated in Fig. 1(b)]. The Néel-VBL transition in the bilayer model for $N = 2$ and $J_2 = 0$ has been studied extensively.[12–15] In the special case of $N = 2$ the order parameter describing the SU(2) symmetry breaking can be written as an O(3) vector. The absence of Berry phases in the bilayer geometry then allows for the description of the critical point in terms of the well-known O(3) nonlinear σ model.[2] This simple mapping has no known generalization for $N > 2$. For general N, the simplest description of the Néel-VBL phase transition is found by writing a Landau theory for the order parameter of the SU(N) antiferromagnet. Such a description contains both the Néel and VBL phases, since the VBL is featureless and can be thought of simply as a phase in which the SU(N) order parameter is quantum disordered. The appropriate order parameter is an $N \times N$ traceless Hermitian matrix, $Q_{\alpha\beta}$, which transforms as $Q \to UQU^\dagger$ under SU(N) rotation. In our model, Eq. (1), such a matrix can be constructed microscopically from a local operator defined as, $\hat{Q}_{\alpha\beta}(i) \equiv |\alpha\rangle_i\langle\beta|_i - 1/N$ on the A sublattice and $\hat{Q}_{\alpha\beta}(i) \equiv |\beta\rangle_i\langle\alpha|_i - 1/N$ on the B sublattice. We can now coarse grain this local operator to obtain the order parameter, $\mathbb{Q}$, and write down a Landau theory action, which being SU(N) invariant must

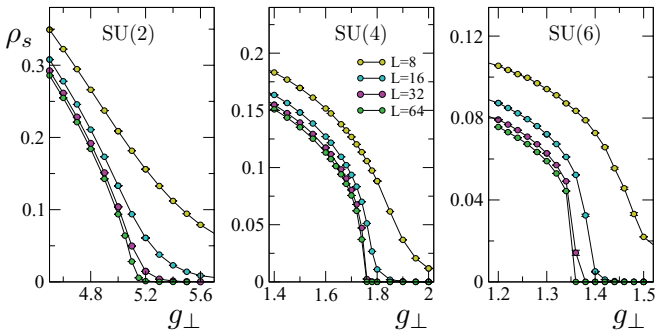

FIG. 3. (Color online) Néel-VBL: The spin stiffness ρ_s close to the Néel-VBL transition for SU(2), SU(4), and SU(6). The SU(2) transition is continuous and in the O(3) universality class. The quantity ρ_s for SU(4) and SU(6) show signs of steplike behavior. Close to the step we find double-peaked histograms (see Fig. 4) characteristic of a first-order transition. The Néel-VBL transition shows such first-order behavior for all $N \geqslant 4$. The parameters used are $g_2 = 0.8$ for SU(2), $g_2 = 0.4$ for SU(4), and $g_2 = 0.6$ for SU(6). The legend shows the value of L; we have set $J_1\beta = L$ everywhere.

consist of traces of powers of $\mathbb{Q}$.

$$S_L = \alpha_L \mathrm{Tr}(\mathbb{Q}^2) + \beta_L \mathrm{Tr}(\mathbb{Q}^3) + \gamma_L \mathrm{Tr}(\mathbb{Q}^4). \qquad (2)$$

Once the order parameter acquires an expectation value, we can do an SU(N) rotation to obtain a diagonal form for $Q_{\alpha\beta} = m(\delta_{\alpha 1}\delta_{\beta 1} - \delta_{\alpha\beta}/N)$, which is the analog of a "collinear" magnet and the quantity m is the condensate. If we now substitute the diagonal form for $\mathbb{Q}$ in S_L we can see that generally cubic terms in m are present in the action for $N > 2$. In the mean-field approach for $N > 2$ such terms will render the phase transition first order, very much like the first-order nematic-isotropic transition in liquid crystals.[28] When $N = 2$, it is easy to see that $\mathrm{Tr}(\mathbb{Q}^3)$ evaluates to zero and does not give rise to a cubic m term, making a continuous transition possible. Indeed by identifying $n_x = (Q_{12} + Q_{21})/2$, $n_y = (Q_{12} - Q_{21})/2i$, $n_z = Q_{11}$, and including gradient terms in the action, we arrive at the well-known O(3) σ model for the $\vec{n} = (n_x, n_y, n_z)$ order parameter.

Consistent with the above Landau theory we confirm from our numerical simulations (see Figs. 3, 4, and 5) that the

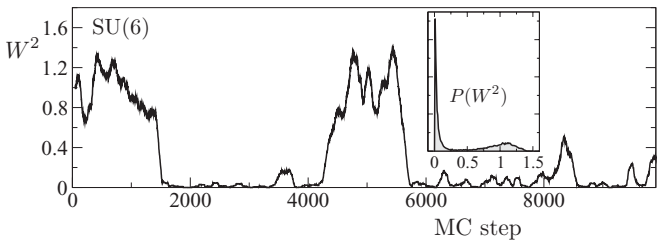

FIG. 4. Néel-VBL: Hysteresis and double-peaked histograms at a first-order Néel-VBL transition in the SU(6) bilayer. In the main frame we show a sample Monte-Carlo history of the binned squared spatial winding number, W^2, which shows clear evidence for metastability. The inset shows a histogram for the same quantity, with clear double-peaked structure. This behavior is found only very close to the transition and for sufficiently large volumes, providing unambiguous evidence for a first-order transition. Here it is shown for $L = 32$, $g_2 = 0.6$, and $g_\perp = 1.36$.

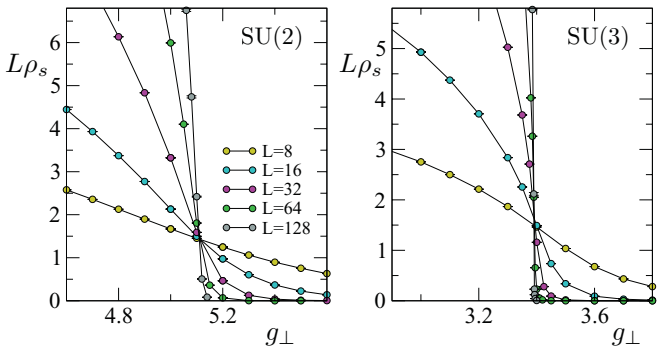

FIG. 5. (Color online) Néel-VBL: Crossings of the fluctuations of the spatial winding number at the Néel-VBL transition for SU(2) and SU(3). In both cases up to sizes of $L = 128$ we see good evidence for a nice crossing, indicating a continuous transition. No evidence for first-order behavior was found in these two cases.

Néel-VBL phase transition is continuous for $N = 2$ [and in the O(3) universality class] and first order for $N \geqslant 4$. The first-order transitions get progressively weaker as N is lowered. Indeed for $N = 3$ we find no evidence for a discontinuous transition up to $L \leqslant 128$[17] (see Fig. 5). If the SU(3) Néel-VBL transition is continuous, what is the continuum field theoretic description? Does the field theory admit a critical fixed point? The continuum description of the Néel-VBL phase transition in our SU(N) bilayer Hamiltonian is a CP^{N-1} field theory with a *compact* U(1) gauge field. In order to make this connection, we introduce N complex numbers z_α with the constraint $\sum_\alpha |z_\alpha|^2 = 1$[22] and use them to rewrite $Q_{\alpha\beta} = z^*_\alpha z_\beta - \delta_{\alpha\beta}/N$. This representation has a well-known U(1) gauge redundancy, which can be made explicit with the introduction of a gauge field a_μ in the long wavelength effective action, the famous CP^{N-1} model description,

$$S = \int d^2x d\tau \left[\frac{1}{g} |(\partial_\mu - i a_\mu) z_\alpha|^2 + F_{\alpha\beta} F_{\alpha\beta} \right], \qquad (3)$$

where $F_{\alpha\beta} = \partial_\alpha a_\beta - \partial_\beta a_\alpha$ is the electromagnetic tensor. Following previous work on quantum antiferromagnets,[29,30] it is clear that in order for the above field theory to possess the VBL state of the bilayer system when $J_\perp \gg J_1, J_2$, the gauge field a_μ must be *compact*. The Higgs phase with z_α condensed corresponds to a phase with SU(N) symmetry breaking, and we identify this phase with the Néel phase. On the other hand, in the phase where z_α is massive, the photon mode gets confined because of the compactness of the gauge field and Polyakov's mechanism of monopole proliferation, resulting in a simple fully gapped paramagnet, which we identify with the VBL phase, Fig. 1(b). Thus the SU(N) Néel-VBL transition in our bilayer can be described in the continuum limit by the Higgs "confined phase" transition in the *compact* CP^{N-1} theory. Recent work[16] has found that a lattice discretization of the compact CP^{N-1} field theory has a continuous transition for $N = 2,3$ and a first-order transition for $N \geqslant 4$. Remarkably, this is in full agreement with our findings here for the SU(N) bilayer, strengthening the evidence for our identification of a continuous transition between Néel and VBL for $N = 3$. A detailed study of critical singularities of the SU(3) Néel-VBL fixed point will be presented elsewhere.

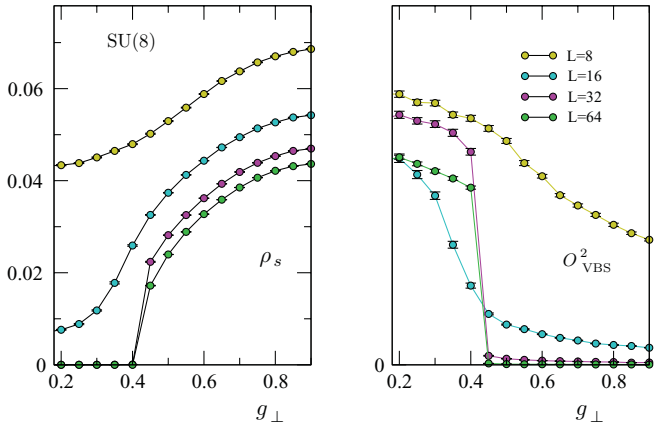

FIG. 6. (Color online) Néel-VBS: First-order nature of the Néel-VBS transition in the two-dimensional square lattice bilayer. Both $O^2_{\rm VBS}$ and ρ_s show evidence for steplike behavior at the same $g_\perp$. Close to the jump we find the same kind of double-peaked behavior in ρ_s that is illustrated in Fig. 4. Here we have shown sample data for $N = 8$ and $g_2 = 0.8$. Similar behavior is found for all N studied here.

Néel-VBS. We now turn to the transition between the Néel and translational symmetry breaking valence-bond solid state [the VBS state is illustrated in Fig. 1(c)]. For a single layer the Néel-VBS transition in the model defined by Eq. (1) was found to be continuous[21] as predicted by the "deconfined" field theoretic arguments.[18] While it is clear that the Néel and VBS phases are individually stable to a small but finite $g_\perp$, the interlayer coupling is expected to be strongly relevant at the fixed point of decoupled deconfined quantum critical points. What is the fate of the Néel-VBS transition in the bilayer geometry? From a theoretical point of view, in the bilayer geometry the cancellation of Berry phases negates the quantum interference effects that are crucial to the deconfined quantum criticality scenario.[18] In the absence of such effects one expects the restoration of the conventional Landau paradigm, where the direct transition between two symmetry-breaking states is necessarily first order independent of the value of N. Indeed as illustrated in Fig. 6 from our QMC simulations we find that the Néel-VBS phase transition is always first order in the bilayer geometry. In our model we only have access to this transition for $N \geqslant 5$ and in these cases we always find a first-order transition. This is a remarkable effect since the phase transition in the single layer and in the bilayer is in both cases between the same two phases, that is, characterized by exactly the *same sets* of broken symmetries and in the same spatial dimension. The difference in the long-distance physics between the bilayer and single layer, much like the Haldane gap in one dimension, is purely due to the presence (cancellation) of the Berry phases in the single (bilayer) systems.

In conclusion we have presented a detailed analysis of two sets of quantum phase transitions in bilayer SU(N) spin systens: First, we have studied the fate of the popular[12–15] bilayer SU($N = 2$) Néel-VBL transition for the case $N > 2$, and second, we have studied the fate of the SU(N) Néel-VBS deconfined critical point[18,21] for a single layer in the bilayer geometry. We have found that the $N = 2$ continuous Néel-VBL phase transition remains continuous for $N = 3$ (in the universality class of the compact CP^2 model[16]), becoming first order for $N \geqslant 4$, and that the cancellation of Berry phases in the bilayer geometry restores Landau's paradigm for the Néel-VBS transition, resulting in a first-order phase transition between two phases with distinct broken symmetries.

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