Impurity spin texture at a deconfined quantum critical point

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The spin texture surrounding a nonmagnetic impurity in a quantum antiferromagnet is a sensitive probe of the novel physics of a class of quantum phase transitions between a Néel ordered phase and a valence-bond solid phase in square lattice S=1/2 antiferromagnets. Using a newly developed T=0 quantum Monte Carlo technique, we compute this spin texture at these transitions and find that it does *not* obey the universal scaling form expected at a scale invariant quantum critical point. We also identify the precise logarithmic form of these scaling violations. Our results are expected to yield important clues regarding the probable theory of these unconventional transitions.

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I. INTRODUCTION

A particularly elegant strategy in the study of strongly correlated materials exploits the presence of small concentrations of well-characterized impurities in an otherwise pure sample. Each impurity acts more or less independently of the others to alter the state of the system around it, and these impurity-induced charge and spin textures can then be picked up by nuclear magnetic resonance (NMR) or scanning tunneling microscopy experiments. As these local responses are characteristic signatures of the underlying low-temperature state, such experiments provide a valuable window to the underlying physics, especially if the state in question has strong correlations but no obvious charge or spin order.¹

Some of these experiments² have focused on the effects of nonmagnetic impurity atoms which give rise to a missingspin defect in strongly correlated Mott insulators. Due to the uncompensated Berry phase associated with such a missing moment,³ it induces a nontrivial pattern of spin density around it, and a direct signature of this spin texture can be obtained by analyzing the pattern of Knight shifts in NMR experiments. Other experiments have also studied such effects in cuprate high- T_c superconductors.⁴ These experiments have motivated several theoretical studies of such physics—these include calculations of such impurity effects in antiferromagnets,⁵ superconductors,⁶ as well as at a quantum phase transition (QPT) signaling the destruction of antiferromagnetism.⁷

Here, we use impurities to theoretically probe a class of unconventional QPTs between an antiferromagnetic phase with Néel order and a phase with valence-bond solid (VBS) order in square lattice S=1/2 magnets. Using a recent extension⁸ of the valence-bond projector loop quantum Monte Carlo (QMC) technique,⁹ we access the total spin-1/2 doublet ground state of the system with a missing-spin defect and compute the induced spin texture at these Néel-VBS transitions.

We use this texture to carefully check for signs of phase coexistence that would signal first-order Néel-VBS transitions and find no such signatures (see Appendix). Although this indicates that these transitions are continuous, we find that the spin texture at these QPTs *does not* obey the universal scaling form expected to hold at any continuous transition described by a scale-invariant quantum critical theory. Furthermore, we find that this failure of scaling cannot be attributed to conventional finite-size corrections but instead represents logarithmic violations of standard quantum critical scaling. These logarithmic violations of scaling at the Néel-VBS QPTs are in stark contrast to the near-perfect scaling collapse we observe for the spin texture at a conventional QPT between a Néel ordered antiferromagnet and a quantum paramagnet *without* spontaneous VBS order. Our results thus demonstrate that although the Néel-VBS QPT is continuous on the square lattice, the critical theory is characterized by logarithmic violations of scaling.

This is extremely significant since the field-theoretical work of Senthil et al.¹⁰ argues that this Neel-VBS QPT can be generically continuous and admits a natural description in terms of "deconfined" S=1/2 spinon excitations of a noncompact CP^1 (NCCP¹) field theory rather than the order parameter fields of conventional Landau theory, which generically predicts a first-order QPT. This "deconfined criticality" scenario has been challenged by Kuklov et al. who argue¹¹ that lattice regularizations of the $NCCP^1$ field theory themselves exhibit no second-order transitions. This contradicts Motrunich and Vishwanath,¹² who conclude in favor of a generic second-order transition in a lattice regularized version of the $NCCP^1$ field theory. Early numerical evidence from microscopic spin models did not resolve this fieldtheoretical controversy since Sandvik¹³ and Melko and Kaul¹⁴ found an apparently continuous transition consistent with deconfined criticality in two S=1/2 spin models while Jiang et al.¹⁵ found a weakly first-order transition in one of these models. However, more recent work of Sandvik and collaborators has convincingly demonstrated the secondorder nature of the Neel-VBS transition in the same models:^{16,17} this is consistent with our own findings.

Our study of impurity properties demonstrates that this continuous transition has logarithmic violations of scaling *that are not predicted by the NCCP*¹ field theory, at least within standard approximate analytical treatments.¹⁸ Remarkably, this recent work of Sandvik¹⁷ also finds similar logarithmic violations of scaling, but in very different, *bulk* physical quantities.



FIG. 1. (Color online) Main figures: **k** dependence of $|S_z(\mathbf{k})|$ at the Néel-VBS transition in the JQ_2 and JQ_3 models, and the Néelparamagnet transition in the JJ' model **k** near $\mathbf{k}=\mathbf{Q}$ (right panels) and $\mathbf{k}=0$ (left panels). Values of the bulk exponent η were taken from Ref. 7 (Ref. 16) for the Néel-paramagnet (Néel-VBS) transitions. Lines passing through the JJ' model data are fits to power-law forms $(|\mathbf{q}|L/2\pi)^{-(3-\eta+\eta')/2}$ for $|S_z(\mathbf{Q}+\mathbf{q})|L^{-(3-\eta)/2}$ (right panel) and $(|\mathbf{q}|L/2\pi)^{-(\eta'/2)}$ for $|S_z(\mathbf{q})|$ (left panel), obtained by using the common value $\eta' \approx 0.44 \pm 0.02$ for this "impurity exponent," consistent with the estimate in Ref. 7. Insets: $|S_z(\mathbf{Q}+2\pi\mathbf{m}/L)|/L^{(3-\eta)/2}$ and $|S_z(2\pi\mathbf{m}/L)|$ for small $|\mathbf{m}|$ versus 1/L at these transitions.

II. MODELS AND METHODS

We focus here on two putative realizations^{13,16} of deconfined criticality corresponding to the Hamiltonians

$$\mathcal{H}_{JQ2} = -J\sum_{\langle ij\rangle} P_{ij} - Q\sum_{\langle ij\rangle\langle kl\rangle} P_{ij}P_{kl}$$

and

$$\mathcal{H}_{JQ3} = -J\sum_{\langle ij\rangle} P_{ij} - Q\sum_{\langle ij\rangle\langle kl\rangle\langle rs\rangle} P_{ij}P_{kl}P_{rs}$$

defined by Sandvik and co-workers. Here, $P_{ij}=1/4-\mathbf{S}_i\cdot\mathbf{S}_j$, $\langle ij \rangle$ refers to a nearest-neighbor (nn) bond on the square lattice connecting sites *i* and *j*, and $\langle ij \rangle \langle kl \rangle \langle (ij \rangle \langle kl \rangle \langle rs \rangle)$ refer to two (three) adjacent parallel nn bonds. As a foil of the unconventional physics of these JQ models, we also study a coupled spin-dimer Hamiltonian $\mathcal{H}_{JJ'}$ with antiferromagnetic nn Heisenberg exchange couplings J for all vertical bonds and J(J') for even (odd) columns of horizontal bonds.¹⁹ These models capture different mechanisms for destabilizing the Néel order while large values of Q favor a VBS phase in the JQ_2 and JQ_3 models, large values of J' drive the system to a quantum paramagnetic state with no spontaneous symmetry breaking.

In order to study the impurity physics at these transitions, one needs to access the total spin-1/2 doublet ground state of an $L \times L$ periodic system with one missing site (periodic boundary conditions fix *L* to be even). We do this using a recently developed modification⁸ of the valence-bond projector loop-QMC method,⁹ and focus on the $S_{tot}=S_{tot}^{z}=1/2$



FIG. 2. (Color online) Logarithmically modified scaling collapse of $S_z(\mathbf{k})$ near $\mathbf{k}=\mathbf{0}$ (left panel) and near $\mathbf{k}=\mathbf{Q}$ (right panel) at the Néel-VBS transition, with $l_0=5\pm 1$, $l_0=0.75\pm 0.2$ for the JQ_2 model, and $l_0=12\pm 1$, $l_{\mathbf{Q}}=1.5\pm 0.5$ for the JQ_3 model.

ground state $|G\rangle$ of periodic systems with a missing spin at $\mathbf{r}=0$ at the Néel-VBS transitions in \mathcal{H}_{JQ2} , at $q_c \equiv (Q/J)_c/[(Q/J)_c+1] \approx 0.962$, and \mathcal{H}_{JQ3} (at $q_c \approx 0.603$),¹⁶ and at the Néel-paramagnet transition of $\mathcal{H}_{JJ'}$ [at $(J'/J)_c \approx 1.9096$].¹⁹

The total $S^z = 1/2$ carried by the ground state spreads out throughout the sample to form the impurity-induced spin texture $\Phi(\mathbf{r}) = \langle G | S^z(\mathbf{r}) | G \rangle$. This texture is expected to have a smooth uniform part $\Phi^u(\mathbf{r})$ and a Néel component $\Phi^n(\mathbf{r})$ that



FIG. 3. (Color online) Histograms of $|D| = \sqrt{D_x^2 + D_y^2}$ [with $D_x^2 = \sum_{ij} \gamma_i \gamma_j \langle (\vec{S}_i \cdot \vec{S}_{j+\hat{x}}) \langle \vec{S}_j \cdot \vec{S}_{j+\hat{x}} \rangle \rangle$ where γ_i is +1(-1) if the *x* coordinate of site *i* is even (odd), and similarly for D_y^2] and $|M| = \sqrt{m^2} [m^2 \equiv \sum_{ij} \eta_i \eta_j \langle \vec{S}_i \cdot \vec{S}_j \rangle$, with η_i equal to +1(-1) for *i* belonging to the A(B) sublattice] for a periodic boundary condition defect free JQ_2 and JQ_3 models with $L_x = L_y = 80$. Also shown is the histogram of $\langle S_z(\mathbf{k} = \mathbf{Q}) \rangle$ in periodic boundary condition samples with one site missing and $L_x = L_y = 80$ for both the JQ_2 and JQ_3 models.



FIG. 4. (Color online) [(a) and (b)] Attempts at collapsing the **k**=**0** Fourier peak of the spin texture in the JQ_2 model assuming a standard finite-size correction to the scaling argument give very large values for the best-fit microscopic length: $l_0^p \ge 100$ and small values of the power $p \approx 0.25$. (c) This is equivalent to saying that the best collapse is obtained with a nonstandard argument. (d) The quality of collapse obtained by assuming logarithmic violations of standard scaling is equally good if not better. See text for details.

alternates in sign between the two sublattices of the square lattice. The Fourier transform

$$S_z(\mathbf{k}) = \sum_{\mathbf{r}} \Phi(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r}),$$

defined for wave vectors $\mathbf{k}=2\pi\mathbf{m}/L$ [where $\mathbf{m}\equiv(m_x,m_y)$ with $m_{x/y}=0,1,\ldots,L-1$], is thus expected to have two peaks, one at $\mathbf{k}=0$ of magnitude 1/2, and the other at $\mathbf{k}=\mathbf{Q}\equiv(\pi,\pi)$ reflecting the tendency to Néel order.

A first-order transition would imply that the distribution of $|S_z(\mathbf{Q})|$ has a double-peak structure signaling phase coexistence. Although we look for such signatures in $|S_z(\mathbf{Q})|$ and other observables such as the valence-bond solid order parameter and spin correlations at wave vector \mathbf{Q} for both JQ_2 and JQ_3 models, we see absolutely no such evidence of firstorder behavior (see Appendix), which leads us to conclude that these Néel-VBS transitions are continuous. If these continuous transitions obeys standard scaling theory, one expects^{7,18}

$$\Phi^{u}(\mathbf{r}) = \frac{1}{L^{2}} f^{u}(\mathbf{r}/L),$$
$$\Phi^{n}(\mathbf{r}) = \frac{1}{L^{(1+\eta)/2}} f^{n}(\mathbf{r}/L),$$

where η is the bulk anomalous exponent associated with the Néel order parameter, and f^{u} and f^{n} are the scaling forms for

the uniform and alternating signals. Earlier work⁷ has validated this scaling ansatz for the conventional Néelparamagnet QPT by studying two coarse-grained fields (representing the uniform and alternating signals) obtained from the computed texture $\Phi(\mathbf{r})$. Although straightforward to implement, this procedure depends on an *ad hoc* coarsegraining prescription.

Here we finesse this difficulty by noting that standard scaling arguments^{7,18} also imply

$$S_{z}(\mathbf{q}) = g_{0}(L\mathbf{q}) \quad \text{for } |\mathbf{q}| \ll \pi/2,$$

$$S_{z}(\mathbf{Q} + \mathbf{q}) = L^{(3-\eta)/2} g_{\mathbf{Q}}(L\mathbf{q}) \quad \text{for } |\mathbf{q} \ll \pi/2$$
(1)

in Fourier space. The advantage of this formulation is clear: one may *unambiguously test for scaling by simply examining* the computed $S_z(\mathbf{k})$ for \mathbf{k} in the vicinity of $\mathbf{k} = \mathbf{Q}$ and $\mathbf{k} = 0$. In particular, the data for $S_z(\mathbf{q})$ at the transition point computed from samples of varying size *L* must fall on top of each other for $|\mathbf{q}| \ll \pi/2$. This unbiased test of scaling does not need any *a priori* estimate of the bulk anomalous exponent η for the Néel order parameter nor does it rely on a specific coarsegraining procedure.

III. RESULTS AND DISCUSSION

Our first inkling that standard scaling does not work at these Néel-VBS transitions comes from the computed values



FIG. 5. (Color online) [(a) and (b)] Attempts at collapsing the $\mathbf{k}=\mathbf{Q}$ Fourier peak of the spin texture in the JQ_2 model assuming a standard finite-size correction to the scaling argument give very large values for the best-fit microscopic length: $l_0^0 \ge 100$ and small values of the power $p \approx 0.2$. (c) This is equivalent to saying that the best collapse is obtained with a nonstandard argument. (d) The quality of collapse obtained by assuming logarithmic violations of standard scaling is equally good if not better. See text for details.

of $|S_z(\mathbf{q})|$ shown in Fig. 1 for $\mathbf{q}=2\pi\mathbf{m}/L$ with $|\mathbf{m}| \ll L/2$.²⁰ Larger values of *L* are seen to yield a systematically larger value of $|S_z|$ at the same $|\mathbf{m}|$. This behavior at the Néel-VBS transitions is in clear violation of the scaling form Eq. (1); this should be contrasted with the excellent scaling observed at the conventional Néel-paramagnet critical point of the *JJ'* model. Given the unbiased nature of this test of scaling, we consider this rather strong evidence for violation of impurity scaling properties at these Néel-VBS transitions in the *JQ*₂ and *JQ*₃ models.

Next, we analyze the Bragg peak at the antiferromagnetic wave vector, $\mathbf{k} = \mathbf{Q}$, focusing on the L dependence at the Néel-VBS transition points. We find that the peaks values obey the power-law scaling $|S_{\tau}(\mathbf{Q})| \sim L^{(3-\eta)/2}$ quite well for both models with the anomalous exponents $\eta_{JQ_3} \approx 0.33$ and $\eta_{JQ_2} \approx 0.35$ taken from Refs. 14 and 16. Our results for the JJ' model are also consistent with the power-law scaling $|S_z(\mathbf{Q})| \sim L^{(3-\eta)/2}$ with the known value of $\eta \approx 0.04$ for the Néel-paramagnet QPT.⁷ However, violations of impurity scaling in the staggered component of the texture at the Néel-VBS transitions become evident when one tests for scaling collapse at $\mathbf{k}=\mathbf{Q}+2\pi\mathbf{m}/L$ with $|\mathbf{m}| \ll L/2$.²⁰ In contrast to the excellent scaling collapse found at the Néelparamagnet QPT of the JJ' model, larger L again yield larger values of $|S_{z}(\mathbf{k})|$ for the same nonzero $|\mathbf{m}|$ at the Neel-VBS transitions (Fig. 1).

Can conventional finite-size corrections account for these violations? To address this, we note that the scaling functions

 $g_{0/\mathbf{Q}}$ have a dimensionless argument **m**, implying that finitesize corrections should be incorporated by modifying their argument to read $\mathbf{m}[1+(l_{0/\mathbf{Q}}/L)^p]$, where the positive power p controls the approach to the scaling regime when L becomes much larger than the microscopic length scale $l_{0/\mathbf{Q}}$. When we attempt to collapse data by including finite-size corrections in this manner, we find (see Appendix) that this only works for unphysically large best-fit values for the length scales $l_{0/\mathbf{Q}}^p \gtrsim 100$ and small powers $p \sim 0.2-0.6$ (depending on which JQ model and which peak).

We are thus forced by the data to consider a scaling argument of the form \mathbf{m}/L^p with small $p \sim 0.2-0.6$, which has no known basis in the theory of phase transitions. However, for such small p, this form is essentially indistinguishable from *logarithmic violations* of impurity scaling with scaling argument $\mathbf{m}/\log(L/l_{0/\mathbf{Q}})$. Such logarithmic violations are wellknown consequences of a marginally irrelevant perturbation of the critical fixed point. Furthermore, such logarithmic violations have been observed at the bulk Neel-VBS transitions in impurity-free systems in the recent work¹⁷ of Sandvik.

We therefore ask if the computed spin texture obeys a modified scaling form

$$S_{z}(\mathbf{q}) = g_{0}[L\mathbf{q}/\log(L/l_{0})],$$

$$S_{z}(\mathbf{Q} + \mathbf{q}) = L^{(3-\eta)/2}g_{\mathbf{Q}}[L\mathbf{q}/\log(L/l_{\mathbf{Q}})]$$
(2)

for $|\mathbf{q}| \ll \pi/2$, where l_0 and $l_{\mathbf{Q}}$ now represent the additional nonuniversal length scale introduced by the slow vanishing



FIG. 6. (Color online) [(a) and (b)] Attempts at collapsing the $\mathbf{k}=0$ Fourier peak of the spin texture in the JQ_3 model assuming a standard finite-size correction to the scaling argument give very large values for the best-fit microscopic length: $l_0^p \ge 100$ and small values of the power $p \approx 0.6$. (c) This is equivalent to saying that the best collapse is obtained with a nonstandard argument. (d) The quality of collapse obtained by assuming logarithmic violations of standard scaling is equally good if not better. See text for details.

of some marginally irrelevant operators. As is clear from Fig. 2, the answer is yes: this modified scaling law gives an extremely good account of our results.

We are thus led to conclude that although the Néel-VBS transition is continuous, the critical theory has logarithmic violations of scaling. This conclusion underscores the utility of impurity physics as a probe of complex strongly correlated states of many-body systems and raises interesting questions regarding the correct field theoretical description of such critical points. An interesting follow up would be to use the same probe at nonzero temperature above the QPT and test for related violations of scaling in the impurity susceptibility.

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APPENDIX

This detailed appendix addresses two important concerns that could potentially arise regarding the conclusions reached in the preceding sections. First, are there other interpretations of the results of our numerical simulations, that could, in particular, point toward a first-order transition? To address this, we note that firstorder transitions are caused by a direct coexistence between two phases at the transition point, which reflects itself in the existence of double-peaked distributions of order parameters and related quantities at the transition. We have looked very carefully in the transition region for such signatures in histograms of the square of the Néel order parameter, again for a pure system, as well as the Fourier component of the impurity spin texture at the antiferromagnetic ordering wave vector for a system with one nonmagnetic impurity.

This extensive data set is presented in Fig. 3. Based on this evidence, we simply do not find any such signature of phase coexistence although we study large systems with state-of-the-art numerical techniques. As a result, we just cannot conclude in favor of a first-order transition.

Second, it is natural to wonder if the lack of scaling seen in the critical spin texture at the Néel-VBS transition (Fig. 1) can be interpreted as strong but ordinary finite-size corrections to conventional critical scaling, instead of a logarithmic violation of standard scaling?

This is much more subtle: as is well-known, standard scaling theory requires that the argument of the scaling functions, g_0 and $g_{\mathbf{Q}}$ in Eq. (1) of our paper, be dimensionless. The standard scaling argument $\mathbf{m}=\mathbf{q}\cdot L/2\pi$ indeed has this property. Therefore, if there are any standard power-law finite-size corrections to scaling, they should take the form



FIG. 7. (Color online) [(a) and (b)] Attempts at collapsing the $\mathbf{k}=\mathbf{Q}$ Fourier peak of the spin texture in the JQ_3 model assuming a standard finite-size correction to the scaling argument give very large values for the best-fit microscopic length: $l_0^p \ge 100$ and small values of the power $p \approx 0.3$. (c) This is equivalent to saying that the best collapse is obtained with a nonstandard argument. (d) The quality of collapse obtained by assuming logarithmic violations of standard scaling is equally good if not better. See text for details.

 $\mathbf{m}(1+l_{0/Q}^p/L^p)$, where the power p is positive and $l_{0/Q}$ is a microscopic length scale beyond which finite-size corrections become small in the vicinity of the particular Fourier peak. In other words the data at different L and various **m** should saturate to an L-independent value which defines the scaling function of **m** with the power p controlling how quickly it saturates to this function of **m** once L is much bigger than $l_{0/Q}$.

However, when this standard "finite-size corrections to conventional scaling" ansatz is used, the data fail to collapse with reasonable values for the microscopic length $l_{0/Q}$. We illustrate this in Figs. 4(a), 4(b), 5(a), 5(b), 6(a), 6(b), 7(a), and 7(b), where we see that any attempts at collapsing the data with this ansatz lead to *unphysically large* best-fit values of $l_{0/Q}^p \gtrsim 100$ and very small best-fit values of $p \sim 0.2-0.6$ (depending on which JQ model and which peak). Thus, as mentioned in our earlier discussion, any attempts at using finite-size corrections to model the data leads us instead to a very nonstandard form of scaling argument of the type \mathbf{m}/L^p with small $p \sim 0.2-0.6$ [see Figs. 4(c), 5(c), 6(c), and 7(c)],

which has no known basis in the theory of continuous phase transitions.

Faced with this behavior, we note that a small power $p \sim 0.2-0.6$ and a logarithm are hard to tell apart without access to unfeasibly large sizes. Furthermore, a scaling argument of the form $\mathbf{m}/\log(L/l_{0/Q})$ admits a well-known theoretical interpretation in terms of logarithmic violations of impurity scaling known to arise when marginally irrelevant operators are present at a fixed point.

We therefore check for scaling collapse using an argument $\mathbf{m}/\log(L/l_{0/Q})$, and, as mentioned in the earlier discussion, observe that it gives rise to very good scaling collapse with very reasonable values for the microscopic length $l_{0/Q}$ [see Figs. 2, 4(d), 5(d), 6(d), and 7(d) included here].

Thus, our conclusion in favor of a continuous transition with logarithmic violations of standard scaling is, in fact, the most conservative and unbiased finding possible given the numerical data at hand, and given standard theoretical inputs from the theory of phase transitions.

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- ²⁰In practice, we focus on $|\mathbf{m}| \leq L_{\min}/12$ and average over all \mathbf{m} that correspond to a given $|\mathbf{m}|$.