Impurity spin texture at a deconfined quantum critical point

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The spin texture surrounding a non-magnetic 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.

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.

Some of these experiments have focused on the effects of non-magnetic impurity atoms which give rise to a missing-spin defect in strongly correlated Mott insulators. Due to the uncompensated Berry phase associated with such a missing moment, it induces a non-trivial 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. These experiments have motivated several theoretical studies of such physics—these include calculations of such impurity effects in antiferromagnets, superconductors, as well as at a quantum phase transition (QPT) signalling the destruction of antiferromagnetism.

In this Letter, we use impurities to theoretically probe a class of unconventional QPTs between an antiferromagnetic phase with long range Néel order and a phase with Valence Bond Solid (VBS) order in square lattice $S = 1/2$ magnets. Using an extension of the Sandvik-Evertz valence bond projector loop Quantum Monte Carlo (QMC) technique that two of us have developed recently, we access the total spin 1/2 doublet ground state of the system with a missing-spin defect and compute the spin texture induced by this impurity at these Néel-VBS transitions. We find that this spin texture does not obey the universal scaling form expected to hold at scale-invariant quantum critical points. Furthermore, by identifying the actual logarithmic form of the impurity scaling violations, we argue that the data does not support a first order transition.

Much of our interest in the Néel-VBS transition of square lattice antiferromagnets stems from the seminal work of Senthil et al. who argued that this QPT is generically continuous, and admits a natural description in terms of ‘deconfined’ strongly interacting $S = 1/2$ spinon excitations rather than the order parameter fields of conventional Landau theory—in this sense, it falls outside the well-known Landau classification of phase transitions, which predicts a first-order QPT. Numerical evidence for this theoretical proposal of ‘deconfined criticality’ is mixed: while Sandvik and Melko and Kaul see an apparently continuous transition consistent with deconfined criticality in a microscopic S=1/2 spin model, Jiang et al. provide a detailed analysis consistent with the competing scenario of a conventional weakly-first order transition.

Our identification of logarithmic violations of impurity scaling at these Néel-VBS transitions should be contrasted with the near-perfect scaling collapse we observe for the spin texture at a different conventional $T = 0$ critical point between a Néel ordered antiferromagnet and a quantum paramagnet without spontaneous VBS order. These results are expected to yield important clues about the correct theory of these unconventional Néel-VBS transitions.

We focus here on two putative realizations of deconfined criticality corresponding to the Hamiltonians $\mathcal{H}_{\text{Q2}}$ and $\mathcal{H}_{\text{Q3}}$ defined by Sandvik and coworkers:

$$\mathcal{H}_{\text{Q2}} = -J \sum_{\langle ij \rangle} \vec{P}_{ij} - Q \sum_{\langle ij \rangle \langle kl \rangle} \vec{P}_{ij} \vec{P}_{kl}$$

$$\mathcal{H}_{\text{Q3}} = -J \sum_{\langle ij \rangle} \vec{P}_{ij} - Q \sum_{\langle ij \rangle \langle kl \rangle \langle rs \rangle} \vec{P}_{ij} \vec{P}_{kl} \vec{P}_{rs}$$

Here, $P_{ij} = 1/4 - S_i \cdot S_j$, $\langle ij \rangle$ refers to a nearest neighbour (n.n.) bond on the square lattice connecting sites.
i and j, and \( \langle ij \rangle (kl) \) refer to two (three) adjacent parallel n.n. bonds. As a foil of the unconventional physics of these JQ models, we also study a coupled spin-dimer Hamiltonian \( H_{J,J'} \) with antiferromagnetic n.n. Heisenberg exchange couplings \( J \) for all vertical bonds, and \( J (J') \) for even (odd) columns of horizontal bonds [17]. These models capture two different mechanisms for destabilizing the Néel ordered antiferromagnet: while large values of \( Q \) favour a VBS phase in the \( JQ_2 \) and \( JQ_3 \) models, large values of \( J' \) drive the system to a quantum paramagnetic state that has 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 have adapted [10] the valence bond projector loop-QMC method [9] to enable an efficient computation of the properties of ground states with \( S_{tot} = 1/2 \), and \( S_{tot}^z \) fixed from the outset to be either +1/2 or −1/2. This extension of the projector algorithm performs as well in the \( S_{tot} = 1/2 \) sector as the original algorithm does in the singlet sector. Using this modified algorithm, we study the \( S_{tot}^z = S_{tot}^z = 1/2 \) ground states \( |G \rangle \) of periodic systems with a missing spin at \( r = 0 \) at the Néel-VBS transitions in \( H_{JQ_2} \) (at \( q_c \approx (Q|J)_c/(Q|J)_c + 1) \approx 0.962 \) and \( H_{JQ_3} \) (at \( q_c \approx 0.603 \) [12], and at the Néel-paramagnet transition of \( H_{J,J'} \) (at \( (J'/J)_c \approx 1.9006 \) [17].

The total \( S^z = 1/2 \) carried by the ground state spreads out throughout the sample to form the impurity-induced spin texture \( \Phi(r) = \langle G|S^z(r)|G \rangle \). This texture is expected to have a smooth uniform part \( \Phi^u(r) \), and a Néel component \( \Phi^a(r) \) that alternates in sign between the two sublattices of the square lattice.

If the QPT in question obeys standard scaling theory, one expects [8, 18] \( \Phi^u(r) = \frac{1}{L^{(3+\eta)/2}} f^u(r/L) \) and \( \Phi^a(r) = \frac{1}{L^{(3+\eta)/2}} f^a(r/L) \), where \( \eta \) is the bulk anomalous exponent associated with the Néel order parameter, and \( f^u \) and \( f^a \) are the scaling forms for the uniform and alternating signals.

Earlier work [8] has validated this scaling ansatz for the conventional Néel-paramagnet QPT by studying two coarse-grained fields (representing the uniform and alternating signals) obtained from the computed texture \( \Phi(r) \) by a specific choice of coarse-graining procedure. Although straightforward to implement, such a procedure is somewhat ad-hoc, and depends on the choice of coarse-graining prescription.

Here we finesse this difficulty by noting that the Fourier transform \( S_z(k) = \sum_r \Phi(r) \exp(i k \cdot r) \) (with \( k = 2 \pi m/L \) and \( m = (m_x,m_y) \) with integers \( m_x/m_y = 0, 1, \ldots L - 1 \) is expected to have two peaks, one at \( k = 0 \) with magnitude constrained to be 1/2, and the second one at \( k = Q = (\pi, \pi) \) reflecting the tendency to Néel order. The standard scaling ansatz [8, 18] implies that these peaks should satisfy the scaling laws

\[
S_z(q) = g_0(Lq) \quad \text{for} \quad |q| \ll \pi/2
\]

\[
S_z(Q + q) = L^{(3-\eta)/2} g_Q(Lq) \quad \text{for} \quad |q| \ll \pi/2 \quad (1)
\]

The advantage of this new \( k \) space formulation is clear: one may unambiguously test for scaling by simply examining the computed \( S_z(k) \) for \( k \) in the vicinity of \( k = Q \). In particular, the data for \( S_z(q) \) at the transition point computed from samples of varying size \( L \) must fall on top of each other for \( |q| \ll \pi/2 \). This is a completely unbiased test of scaling as it does not need any a priori estimate of the bulk anomalous exponent \( \eta \) for the Néel order parameter, nor does it rely on a specific coarse-graining procedure to define the scaling components of the texture.

Our first inklings that standard scaling does not work at these Néel-VBS transitions comes from the computed values of \( |S_z(q)| \) shown in Fig[1] and Fig[2] for \( q = 2 \pi m/L \) with \( |m| \ll L/2 \) (in practice, we focus on \( |m| \lesssim L_{min}/12 \) and average over all \( m \) that correspond to a given \( |m| \)).

FIG. 1: \( k \) dependence of \( |S_z(k)| \) near the \( k = 0 \) and \( k = Q \) peaks at the (a) Néel-paramagnet and (b)-(c) Néel-VBS transitions. Values of the bulk exponent \( \eta \) were taken from Ref. [8] for the Néel-paramagnet transition and from Ref. [12] for the Néel-VBS transitions. Solid lines in a) are fits to power-law forms obtained by using the value \( \eta \approx 0.44 \pm 0.02 \) for the impurity exponent, consistent with the estimate in Ref[3].
Larger values of $L$ are seen to yield a systematically larger value of $|S_z|$ at the same $|\mathbf{m}|$. This behaviour at the Néel-VBS transitions is in clear violation of the scaling form Eq. (4) this should be contrasted with the excellent scaling observed at the conventional Néel-paramagnet critical point of the $J - J'$ 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 wavevector, $\mathbf{k} = \mathbf{Q}$, focusing on the $L$ dependence at the Néel-VBS transition point in both $JQ$ models. We find no evidence of any double-peak structure for the histogram of $|S_z(\mathbf{Q})|$ at these Néel-VBS transitions, implying that the first order jump in the order parameter, if any, is immeasurably small even at sizes as large as $L = 96$. Furthermore, we confirm that the computed values obey the power-law scaling $|S_z(\mathbf{Q})| \sim L^{(3-\eta)/2}$ quite well at both Néel-VBS transitions, with the anomalous exponents $\eta_{JQ_3} \approx 0.33$ and $\eta_{JQ_2} \approx 0.35$ taken from Refs. 12, 13. Our results for the $J - J'$ 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 8.

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 $|\mathbf{m}|$ small but non-zero (we focus on $|\mathbf{m}| \leq L_{\text{min}}/12$ and average over all $\mathbf{m}$ that correspond to a given $|\mathbf{m}|$) — again, larger $L$ give larger values of $|S_z(\mathbf{m})|$ for the same non-zero $|\mathbf{m}|$ (Fig. 1 and Fig. 2). This is again underlined by the excellent scaling collapse exhibited by the corresponding quantities computed at the Néel-paramagnet quantum critical point of the $J - J'$ model (Figures 1 and 2).

![FIG. 2: 1/L dependence of $|S_z(\mathbf{Q} + 2\pi \mathbf{m}/L)|/L^{(3-\eta)/2}$ and $|S_z(2\pi \mathbf{m}/L)|$ for small $|\mathbf{m}|$ at the Néel-VBS and Néel-Paramagnet transitions. All horizontal lines are guides to the eye that indicate the expected behaviour if scaling was perfectly obeyed, and values of $\eta$ are the same as in Fig. 1.](image1)

![FIG. 3: Logarithmically modified scaling collapse of $S_z(\mathbf{k})$ near $\mathbf{k} = 0$ at the Néel-VBS transition, with $l_0 = 5 \pm 1$ ($l_0 = 12 \pm 1$) for the $JQ_2$ ($JQ_3$) model.](image2)
We are thus led to conclude that although the Néel-VBS transition is continuous, the theory of deconfined criticality needs to be modified in order to account for these logarithmic corrections. This conclusion underscores the utility of impurity physics as a probe of complex strongly-correlated states of many-body systems. An interesting follow-up would be to use the same probe at non-zero temperature above the QPT and test for violations of scaling predictions for the impurity susceptibility.

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FIG. 4: Logarithmically modified scaling collapse of $S_z(\mathbf{k})$ near $\mathbf{k} = \mathbf{Q}$ at the Néel-VBS transition, with $l_0 = 0.75 \pm 0.2$ ($l_\mathbf{Q} = 1.5 \pm 0.5$) for the $JQ_2$ ($JQ_3$) model.

signal? This is best addressed by asking if the computed spin texture satisfies some suitably modified scaling laws. To explore this, we first note that the absence of any power-law prefactor to $g_0$ in the scaling ansatz Eq. [11] reflects the conservation of total spin and the specific power of $L$ that multiplies $g_0$ reflects the presence of power-law Néel order at criticality, while the scaling argument $L_\mathbf{Q}$ of both functions follows simply from the statement that $L$ is the only length scale of relevance to the long-distance physics at a scale invariant critical point.

This form of the scaling argument can break down if the effective low-energy theory has a term which is marginally irrelevant for the long-distance physics, and renormalizes to zero slowly. This can introduce an additional length scale, and give rise to logarithmic violations of scaling. Indeed, signatures of such logarithmic drifts have been recently seen by Sandvik in his analysis of the bulk Néel-VBS transitions [19].

This motivates us to ask if the computed spin texture obeys a modified scaling form (for $|\mathbf{q}| \ll \pi/2$)

$$S_z(\mathbf{q}) = g_0(L\mathbf{q}/\log(L/l_0))$$

$$S_z(\mathbf{Q} + \mathbf{q}) = L^{(3-\eta)/2}g_0(L\mathbf{q}/\log(L/l_\mathbf{Q}))$$

(2)

where $l_0$ and $l_\mathbf{Q}$ are related to the additional non-universal length scale introduced by the slow vanishing of a marginally irrelevant term in the effective Hamiltonian. As is clear from Figs [4][11] the answer is yes: this modified scaling law gives an extremely good account of our results.

These logarithmic violations of scaling are at odds with predictions of the theory of deconfined criticality [18]. However, given the absence of any clear signal for phase-coexistence at the transition point, one cannot simply ascribe these violations to the presence of an immeasurably weak first-order jump in the order parameters. We are thus led to conclude that although the Néel-VBS transition is continuous, the theory of deconfined criticality needs to be modified in order to account for these logarithmic corrections. This conclusion underscores the utility of impurity physics as a probe of complex strongly-correlated states of many-body systems. An interesting follow-up would be to use the same probe at non-zero temperature above the QPT and test for violations of scaling predictions for the impurity susceptibility.

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