Scaling in the Fan of an Unconventional Quantum Critical Point

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We present results of extensive finite-temperature Quantum Monte Carlo simulations on a SU(2) symmetric $S = 1/2$ quantum antiferromagnet with a four-spin interaction [Sandvik, Phys. Rev. Lett. 98, 227202 (2007)]. Our simulations, which are free of the sign-problem and carried out on lattices containing in excess of $1.6 \times 10^5$ spins, indicate that the four-spin interaction destroys the Néel order at an unconventional $z = 1$ quantum critical point, producing a valence-bond solid paramagnet. Our results are consistent with the ‘deconfined quantum criticality’ scenario.

Research into the possible ground states of SU(2) symmetric quantum antiferromagnets has thrived over the last two decades, motivated to a large extent by the undoped parent compounds of the cuprate superconductors. In these materials, the Cu sites can be well described as doped parent compounds of the cuprate superconductors. In recent work [Senthil et al., Phys. Rev. Lett. 98, 227202 (2007)], the possibility of a direct continuous Néel-VBS transition was proposed. The natural field theoretic description of this ‘deconfined quantum critical point’ is written in terms of certain fractionalized fields that are confined on either side of the QCP and become ‘deconfined’ precisely at the critical point. As is familiar from the general study of QCPs, these fractional excitations are expected to influence the physics in a large fan-shaped region that extends above the critical point at finite-$T$. (see Fig. 1).

It is clearly of great interest to find models that harbor a direct Néel-VBS QCP and that can be studied without approximation on large lattices. Currently, the best candidate is the ‘JQ’ model, introduced by Sandvik [6], which is an $S = 1/2$, SU(2) invariant antiferromagnet with a frustrating four-spin interaction,

$$H_{JQ} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - Q \sum_{\langle jkl \rangle} (\mathbf{S}_j \cdot \mathbf{S}_l - \frac{1}{4}) (\mathbf{S}_k \cdot \mathbf{S}_l - \frac{1}{4}),$$

where $J$, $Q$, and $z = 1$ are coupling constants.

The inset shows how the frustrating $Q$ term is written in terms of bonds on a plaquette. Using a $T = 0$ projector Quantum Monte Carlo (QMC) method on lattices sizes up to $32 \times 32$ [7], Sandvik showed that the four-spin interaction destroys Néel order and produces a VBS phase at $J/Q \sim 0.04$. Close to this critical value of $J/Q$, scaling in the spin and dimer correlation functions suggests a continuous transition with anomalous dimensions of the Néel and VBS order parameters equal, with a common value $\eta = 0.26(3)$. In this Letter, we explore the candidate Néel-VBS QCP in the full $T - J/Q$ phase diagram on large lattices using a complementary finite-$T$ QMC technique, the Stochastic Series Expansion (SSE) method with directed loops [7]. The SSE QMC allows access to the physically important quantum critical fan (see Fig. 1), and admits high-accuracy estimates for the spin stiffness, $\rho_S$, and the uniform susceptibility, $\chi_u$. The
scaling of these observables provides strong evidence for a continuous $z = 1$ transition in the JQ model.

**Basis and Sign of Matrix Elements:** A priori, it is unclear that SSE simulations of $H_{Q}$ are free of the notorious sign-problem: a fluctuating sign in the weights used in the QMC sampling. In the SSE, finding an orthogonal basis in which all off-diagonal matrix elements of the Hamiltonian are non-positive solves the sign-problem. A simple unitary transformation on the basis used here, it is easy to measure the correlation functions by Fourier transformation at equal correlation functions by Fourier transformation at equal

**Numerical Results:** Using the SSE QMC, we studied various physical observables in the JQ model on finite-size lattices of linear dimension $L$ (with number of spins $N_{\text{spin}} = L^2$). Particular attention was paid to the scaling of the spin stiffness $\rho_s = \partial^2 E_0/\partial \phi^2$ ($E_0$ is the energy and $\phi$ is a twist in the boundary conditions) and the uniform spin susceptibility $\chi_u = (<(\sum_i S_i^z)^2>)/TN_{\text{spin}}$. In the $S^z$ basis used here, it is easy to measure the correlation functions $C_\phi(r, \tau) = <S^z(r, \tau)S^z(0, 0)>$ and $C_{\phi}(r, \tau) = <[S^z(r, \tau)S^z(r+\hat{\mathbf{x}}, \tau)][S^z(0, 0)S^z(\hat{\mathbf{x}}, 0)>]$. While $C_\phi$ is the correlation function of the Néel order parameter, the VBS order is indicated by $C_{\phi}^v$, which is the correlation function of the composite operator $S^z(r)S^z(r+\hat{\mathbf{x}})$, receiving contribution from both the standard VBS order parameter $\chi_N = <\langle S^z(0, 0)S^z(\hat{\mathbf{x}}, 0)>/>N_{\text{spin}}$ and $\chi_N$ is the anomalous dimension of the Néel field.

**Figure 2:** (color online) $T \to 0$ converged Néel (main) and VBS (inset) order parameters as a function of $1/L$. Dashed lines are quadratic fits that illustrate the finite condensate in the ordered phases. The solid (red) line is a fit to the form $y = c_1 x^{c_2}$ (illustrated for $J/Q = 0.040$), where $c_2 = z + \eta_N$ is expected at the critical coupling. In fitting to the nine $L$ values for each $J/Q$, we find a minimum in the chi-squared value (per degree of freedom) of 3.1 for $J/Q = 0.040$, with $c_2 \approx 1.35(1)$. For $J/Q = 0.038$, the chi-squared value is 3.9, with $c_2 \approx 1.37(1)$. All other $J/Q$ produce much larger chi-square (greater than 10).

**Figure 3:** (color online) Criticality of the Néel field at $J = 0.038$: collapse of the Néel structure factor ($S_N$) and susceptibility ($\chi_N$) with $z = 1$ and $\eta_N = 0.35$, determining the universal functions $\chi_N(x)$ (for (up to non-universal scale factors) on the $x$ and $y$ axes). The only fit parameter for both $S_N$ and $\chi_N$ is $\eta_N$, the anomalous dimension of the Néel field.
(b) the collapse of both $S_N$ and $\chi_N$ takes place over two and a half orders of magnitude of $LT$ with only one common fit parameter, $\chi_N$; both facts give us confidence in our estimate. The critical scaling of $C_V$ is more complicated; due to the aforementioned mixing-in of two order parameters, $C_V$ is expected to receive two independent power-law contributions. Indeed, it is difficult to disentangle these individual contributions on the limited range of lattices sizes available, precluding us from verifying the proposal [8] that $\eta_N = \eta_N$.

We now turn to an analysis of the scaling properties of $\chi_u$ and $\rho_s$ in the hypothesized quantum critical fan region of Fig. 4, $\chi_u$ and $\rho_s$, being susceptibilities of conserved quantities have no anomalous scaling dimension, and hence at finite-$T$ and $L$ in the proximity of a scale-invariant critical point, assuming hyper-scaling:

$$\rho_s(T, L, J) = \frac{T}{L^{d-2}} \mathbb{V} \left( \frac{L^2 T}{c} g L^{1/\nu} \right),$$

$$\chi_u(T, L, J) = \frac{1}{T L^d} \mathbb{Z} \left( \frac{L^2 T}{c} g L^{1/\nu} \right),$$

where $g \propto (J - J_c)/J_c$. At criticality ($g = 0$), it is easy to see that $\mathbb{V}(x \rightarrow 0, 0) = A_p(x)$ and $\mathbb{Z}(x \rightarrow \infty, 0) = A_x x^{d/z}$, where $\mathbb{V}(x, y)$ and $\mathbb{Z}(x, y)$ are universal scaling functions and $A_p, A_x$ are universal amplitudes of the quantum critical point; $c$ is a non-universal velocity.

At criticality and $L \rightarrow \infty$, one can show from Eq. (3) that $\chi_u = \frac{A_u}{\nu} T^{d/z} - 1$; i.e. for a $z = 1$ transition, $\chi_u$ should be $T$-linear and have a zero intercept on the $y$-axis at $T = 0$ [10]. In Fig. 4, $\chi_u$ data for an $L = 128$ system is presented. Within our error bars, this data is $L \rightarrow \infty$ converged for the region of $T$ shown; at smaller $T$ the finite-size gap causes an exponential reduction in $\chi_u$. The inset shows how the extracted value of the $y$-intercept, $a$ (from a fit to the form $a + bT$), changes sign as the coupling is tuned, consistent with $0.36 \leq J_c \leq 0.40$ and demonstrating to high precision the $z = 1$ scaling.

Turning to study Eqs. (2,3) further, one may hold the first argument of the universal functions fixed by setting $L = 1/T$ (assuming $z = 1$ as indicated above). In order to achieve this, we performed extensive simulations on lattices sizes up to $L = 1/T = 64$, illustrated in Fig. 5. According to Eqs. (2,3), data curves for $L\rho_s$ and $L\chi_u$ plotted versus $J$ should show a crossing point with different $L$ precisely at $J_c$. We find that for relatively large sizes ($32 \leq L \leq 64$) the crossing point converges quickly in the interval $0.038 \leq J \leq 0.040$. The insets show the data collapse when the $x$-axis is re-scaled to $g L^{1/\nu}$ (with $\nu = 0.68$). We note that with the inclusion of small sub-leading corrections (of the form $a_u L^c$), the crossing point and data collapse of $\rho_s$ and $\chi_u$ can be made consistent, at the expense of two more fit parameters, even for much smaller system sizes than illustrated [9]. In contrast to the U(1) symmetric JK model [11], where the absence of a $T$-linear $\chi_u$ and a crossing in the data for $\rho_s L$ cast doubt on its interpretation as a $z = 1$ QCP, the present data for this SU(2) symmetric model gives strong support for a $z = 1$ QCP between $0.038 \leq J \leq 0.040$.

Finally, we hold the second argument of the scaling functions [Eqs. (2,3)] constant by tuning the system to $g = 0$. One then expects a data collapse for $\rho_s / T$ and $L\chi_u$ when they are plotted as a function of $L^2 T$ (with $z = 1$). Fig. 5 shows this collapse for simulations carried out with extremely anisotropic arguments $LT$, varying over almost three orders of magnitude. There is an excellent data collapse over 8 orders of magnitude of the range of $J/Q$.
and J/Q interaction: the deconfined quantum criticality scenario [4], in rough currently available for a continuous Néel-VBS transition. It is interesting to compare our results to the only theoretical behavior on the relatively large length scales studied here. We have found no evidence for double-peaked distributions, indicating an absence of this sort of first-order behavior associated with the QCP, which the Néel-VBS transition is described by the non-compact CP^1 field theory. All of the qualitative observations above, including an unusually large η_N [13] agree with the predictions of this theory. Indeed, our estimate of η_N ≈ 0.35 [Fig. 3] is in remarkable numerical agreement with a recent field-theoretic computation [14] of this quantity, which finds η_N = 0.3381. With regard to other detailed quantitative comparisons, we have provided the first step by computing many universal quantities, \( \chi(x), \chi_S(x), \chi(0), \chi(x,0), \text{ and } A_p/\chi \approx 0.075 \) [Fig. 6] in the JQ model. Analogous computations in the CP^1 model, although currently unavailable [15] are highly desirable to further demonstrate that the JQ model realizes this new and exotic class of quantum criticality.

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The expected asymptotes (see text) are plotted as dashed lines \( \chi(x,0) = A_p/x \) and \( \chi(x,0) = A_p x^{d/z} \). From fits to the data, we find \( A_p/\chi(c) = 0.041(4) \) and \( A_p/\chi = 0.37(3) \), allowing us to estimate a universal model-independent number associated with the QCP, \( A_p\sqrt{\chi(c)} \approx 0.075(4) \).

**Discussion:** In this paper we have presented extensive data for the SU(2) symmetric JQ model which indicates that the Néel order (present when \( J > Q \)) is destroyed at a continuous quantum transition as \( Q \) is increased [3]. In the finite-\( T \) quantum critical fan above this QCP, scaling behavior is found that confirms the dynamic scaling exponent \( z = 1 \) to high accuracy. The anomalous dimension of the Néel field at this transition is determined to be \( \eta_N \approx 0.35(3) \), almost an order of magnitude more than its value of 0.038 [12] for a conventional \( O(3) \) transition. For sufficiently large values of \( Q \) we find that the system enters a spin-gapped phase with VBS order. To the accuracy of our simulations, our results are fully consistent with a direct continuous QCP between the Néel and VBS phases, with a critical coupling between \( J/Q \approx 0.038 \) and \( J/Q \approx 0.040 \). Although our finite size study cannot categorically rule out a weak first-order transition, we have found no evidence for double-peaked distributions, indicating an absence of this sort of first-order behavior on the relatively large length scales studied here. It is interesting to compare our results to the only theory currently available for a continuous Néel-VBS transition: the deconfined quantum criticality scenario [4], in which the Néel-VBS transition is described by the non-compact CP^1 field theory.

![Fig. 6: Scaling of \( \chi(c) \) and \( \rho_s \) at \( J = 0.038 \approx J_c \), with \( z = 1 \) and \( d = 2 \). These plots are the universal functions \( \chi(x,0) \) and \( \chi(x,0) \) up to the non-universal scale factor \( c \) on the \( x \)-axis. The expected asymptotes (see text) are plotted as dashed lines \( \chi(x,0) = A_p/x \) and \( \chi(x,0) = A_p x^{d/z} \). From fits to the data, we find \( A_p/\chi(c) = 0.041(4) \) and \( A_p/\chi = 0.37(3) \), allowing us to estimate a universal model-independent number associated with the QCP, \( A_p\sqrt{\chi(c)} \approx 0.075(4) \).](image-url)

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