

Quantum critical behavior in a two-layer antiferromagnet

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We analyze quantum Monte Carlo data in the vicinity of the quantum transition between a Néel state and a quantum paramagnet in a two-layer, square-lattice spin- $\frac{1}{2}$ Heisenberg antiferromagnet. The real-space correlation function and the universal amplitude ratio of the structure factor and the dynamic susceptibility show clear evidence of quantum critical behavior at low temperatures. The numerical results are in good quantitative agreement with $1/N$ calculations for the $O(N)$ nonlinear σ model. A discrepancy, reported earlier, between the critical properties of the antiferromagnet and the σ model is resolved. We also discuss the values of prefactors of the dynamic susceptibility and the structure factor in a single-layer antiferromagnet at low T .

The two-layer, square-lattice spin- $\frac{1}{2}$ Heisenberg antiferromagnet has recently attracted some attention for a number of reasons. It has been proposed that its properties should help explain neutron-scattering, photoemission, and relaxation rate data in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (YBCO) and $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ (Bi-2212) cuprate superconductors.^{1,2} On the theoretical side, it is among the simplest, two-dimensional (2D) Heisenberg spin systems which display a quantum phase transition between a Néel state and a quantum paramagnet.² Quantum Monte Carlo (QMC) simulations on this model do not suffer from a sign problem, making it possible to obtain precision data on the critical properties of the quantum transition. It therefore constitutes an attractive setting for testing our understanding of transitions in two-dimensional Heisenberg spin systems. This is particularly important as there are conflicting reports on the observation of quantum-critical behavior in a single-layer antiferromagnet.³⁻⁸

A popular approach for the analysis of the collective properties of two-dimensional, square-lattice antiferromagnets has been to model the long-wavelength, long-time spin fluctuations in terms of those of the $O(3)$ nonlinear σ model.^{3,4} The main difference between the antiferromagnet and the σ model is that the microscopic action for the former contains Berry phases, associated with the commutation relations between different components of the Heisenberg spins. The Berry phases, however, cancel between the two sublattices for smooth spin configurations.⁹ For the two-layer antiferromagnet there should be a further cancellation between the two layers, which should occur even for singular saddle points (pairs of “hedgehogs” on the two layers) of the effective action. There are, therefore, strong theoretical reasons for believing that the quantum transitions in the two-layer antiferromagnet and the σ model should be in the same universality class.

In a recent paper¹⁰ reporting QMC results on the two-layer antiferromagnet near the critical point, it was found

that while the measurements were qualitatively consistent with the predictions of the σ model, there was a discrepancy in a coefficient in the temperature (T) dependence of the correlation length (ξ). The origin of this discrepancy was not understood, and it was not clear whether the theoretical picture based on the σ model should be questioned.

In this paper, we reexamine this issue by improving the accuracy of the numerical calculations, and performing a more detailed analysis of the data. As shown below, we now find complete consistency between the measured universal critical properties of the two-layer antiferromagnet and the σ model, and understand the origin of the earlier discrepancy.¹⁰ For comparison, we will also present some additional data on the correlation function in a single-layer antiferromagnet at low temperatures, when the system is in the renormalized-classical regime.

We start by presenting some analytical results. Consider the spin-correlation function in real space, $G(r)$, where $(-1)^r G(r)$ is the Fourier transform of the static structure factor,

$$S(k) = T \sum_{\omega_m} \chi(k, \omega_m), \quad (1)$$

where χ is the dynamic susceptibility, and ω_m is a Matsubara frequency. Here and below we set $k_B = \hbar = 1$. Results for $\chi(k, \omega_m)$ in the quantum-critical region have been presented in Ref. 4 — using these results, we obtain at the critical coupling, but T finite,

$$G(r) = \frac{1}{3} N_0^2 \left(\frac{3T}{2\pi\rho_s} \right)^{1+\eta} \int dx \Xi(x) J_0\left(\frac{xrT}{c}\right). \quad (2)$$

Here x is a rescaled momentum, J_0 is a Bessel function, c is the spin-wave velocity, and ρ_s and N_0 are spin stiffness and sublattice magnetization, respectively, measured just away

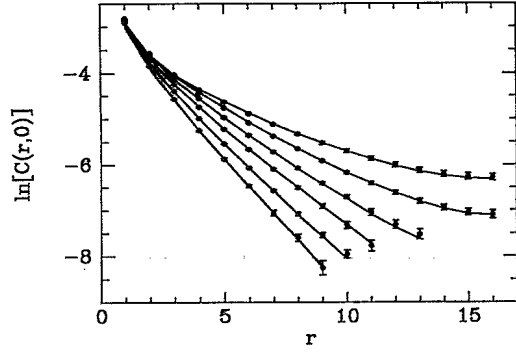


FIG. 1. QMC results for the staggered spin-correlation function $G(\vec{r}) = (-1)^r \langle (S_{1,r}^z - S_{2,r}^z)(S_{1,0}^z - S_{2,0}^z) \rangle$ (the indices 1,2 refer to the two planes) along $\vec{r} = (r, 0)$, for an interplane coupling $J_2 = 2.55J_1$ at temperatures $T = 0.3 - 0.8J_1$ (the top curve is for $T = 0.3J_1$). The solid curves are fits to $G(r) + G(L-r)$, with $G(r)$ given by (2).

from the critical point on the ordered side—the ratio $N_0^2/\rho_s^{1+\eta}$ remains finite upon approaching criticality. Finally, $\Xi(x)$ is the universal crossover function, which we have computed in a $1/N$ expansion for the $O(N)$ σ model for $0 < x < 5$ (in Ref. 4, this function was computed only in the limits of small and large x). We found that to the accuracy needed here, $\Xi(x)$ to order $O(1/N)$ can be modeled by the same functional form as in the $N = \infty$ result,

$$\Xi(x) = \frac{1 + 2n_x}{2\sqrt{x^2 + m^2}}, \quad (3)$$

where $n_x = (\exp\sqrt{x^2 + m^2} - 1)^{-1}$ is a Bose function, but with $m \approx 1.04$ instead of the $N = \infty$, $m_0 = 2\ln[(\sqrt{5} + 1)/2] = 0.9624$. The difference between the $1/N$ result for Ξ , extended to the physical case of $N = 3$, and Eq. (3) is less than 1% for $x < 2$ and does not exceed 2% for larger x . This form of Ξ indeed implies that the argument of the Bessel function can be rewritten as $1.04xr/\xi$ ($\xi^{-1} = mT/c$).

The two terms in (3) yield the same exponential decay of the spin correlations at large distances, but with different prefactors. The term without a Bose function is a purely quantum contribution, which yields $r^{-1}e^{-r/\xi}$, while the integration over x in the second term in (3) yields a classical result $(r/\xi)^{-1/2}e^{-r/\xi}$. In the earlier report, the QMC data near the critical point were fitted using only the first quantum contribution to $G(r)$ at large distances.¹⁰ Meanwhile, we have checked that the dominant contribution to $S(k)$ in (1) actually comes from the few first terms in the frequency sum. Consequently, the piece in $G(r)$ associated with the classical fluctuations is at least as important as the piece related to quantum fluctuations. Moreover, as the QMC data were obtained for finite-size systems, we found it useful to extract the correlation length from the fit to the functional form of $G(r)$ at moderate distances of 5–10 lattice spacings. At such distances, $G(r)$ is not necessary well approximated by the exponential form, and one should use the full Eq. (2) for numerical comparisons.

The advantage of introducing the correlation length into the argument of the Bessel function is that Eq. (2) no longer contains the spin-wave velocity which in a two-layer system is not known precisely.¹¹ Once ξ is obtained from the fit to

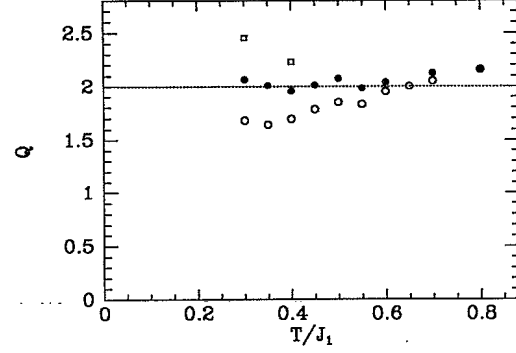


FIG. 2. QMC results for the universal parameter ratio $Q = \xi^{-1}(T/\chi_u)^{1/2}$ for the interplane couplings $J_2/J_1 = 2.50$ (open circles), 2.55 (solid circles), and 2.60 (open squares). The dashed line is the prediction for the quantum-critical regime.

the QMC data, one can use the QMC results for the uniform susceptibility (χ_u) and compute the dimensionless ratio $Q(T) = \xi^{-1}(T/[\chi_u(T)])^{1/2}$. It is predicted⁴ that at the critical point, $Q(T)$ takes a T -independent universal value—using the result for χ_u we obtain $Q \approx 1.92m = 2.0$ (at $N = \infty$, $Q = 1.64$). Away from the critical point, we expect that as $T \rightarrow 0$, Q vanishes as $\sim \exp(-2\pi\rho_s/T)$ on the Néel ordered side, and Q diverges as $\sim \exp(\Delta/2T)$ on the quantum-disordered side (Δ is the spin gap).

For the numerical calculations we have used a variant of the Handscomb QMC technique.¹² All results for two coupled layers shown here are for systems with $2 \times L \times L$ spins with $L = 32$. For a single layer, we discuss results for systems of size 64×64 .

The QMC data for $G(r)$ in the two-layer model at a near critical $J_2/J_1 = 2.55$ (Refs. 13,10,14) are presented in Fig. 1 (J_2 and J_1 are inter and intralayer exchange integrals, respectively). We fitted the data for $G(r)$ to Eq. (2) with ξ and the prefactor as the fitting parameters. We then used the QMC results for the uniform susceptibility¹⁰ and obtained $Q(T)$. The results, along with results for systems just above ($J_2/J_1 = 2.6$) and below ($J_2/J_1 = 2.5$) the critical point, are shown in Fig. 2. The results are in good accord with the theoretical predictions discussed above. At the critical point

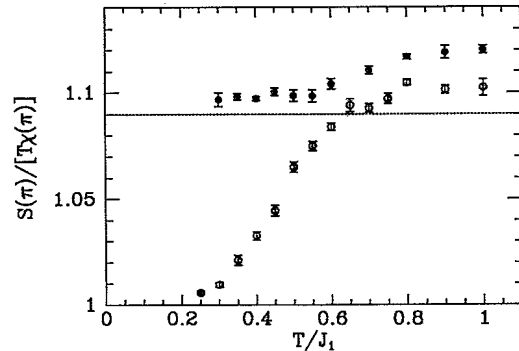


FIG. 3. QMC results for the universal ratio $S(\vec{\pi})/[T\chi(\vec{\pi})]$ for a single plane (open circles), and two coupled planes with $J_2/J_1 = 2.55$ (solid circles). The dashed line is the prediction for the quantum-critical regime.

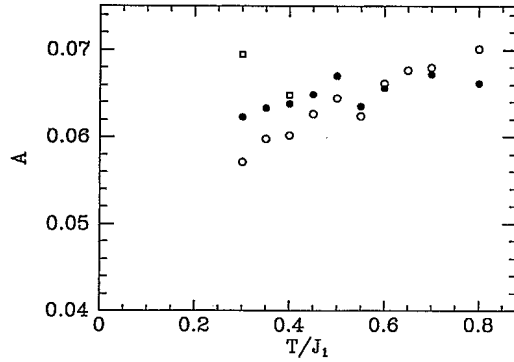


FIG. 4. QMC results for the prefactor, A , in the correlation function for interplane couplings $J_2/J_1=2.50$ (open circles), 2.55 (solid circles), and 2.60 (open squares).

$J_2/J_1=2.55$, Q changes little with temperature below $T \sim 0.5J_1$ and remains close to the theoretical prediction, $Q=2.0$ (i.e., $\xi^{-1}=1.04T/c$) down to the lowest temperature studied. To the best of our knowledge, this is the first observation of the *universal* quantum-critical behavior of the correlation length in 2D magnets.

Another interesting dimensionless ratio of the quantum-critical region is $W(T) \equiv S(\pi)/T\chi(\pi,0)$.⁷ On the ordered side, as $T \rightarrow 0$, $W \rightarrow 1$ as only the first term in the frequency sum in (1) is important in this classical regime. At the critical point we, however, have to perform the full frequency summation. Using the $1/N$ results of Ref. 4, we find $W \approx 1.05m = 1.09$. The QMC results for the ratio are shown in Fig. 3. We see that at the transition point, W is T independent and its value is close to the predicted one down to the lowest temperatures studied. Notice that earlier studies⁷ have found the same value of W in a single-layer antiferromagnet, but at relatively high temperatures, $T > 0.6J_1$, when nonuniversal corrections to χ and S are relevant, and one can only hope that they are canceled out in the ratio $S/T\chi$.

The prefactor $A = N_0^2(J_1/2\pi\rho_s)(T/2\pi\rho_s)^\eta$ extracted from the fits to the correlation function is shown in Fig. 4. We see that $A \approx 0.063$ is almost T independent, as it should be given that η is very small. This prefactor can also be extracted from the product $V(T) \equiv S(\pi)\chi_u(T)$ which again does not contain the spin-wave velocity. In the $1/N$ expansion,⁴ we obtain $V(T) = 1.7A$. Averaging the QMC data for V at $T = 0.3J_1 - 0.5J_1$, we obtain $V \approx 0.107$ which yields $A = 0.063$ in complete agreement with the above result.

Finally, we extracted m and A directly from the fit of the QMC data to Eq. (3). We used $c = 1.8J_1$ which is the average of $c = 1.7J_1$ and $1.9J_1$ obtained from the fits to the data for the uniform susceptibility¹⁰ and $S(k)/T\chi(k,0)$ at $k \leq \pi$,¹⁵ respectively. Using m and A as fitting parameters, we obtained $A = 0.063$ and $m = 1.02$, again very close to the theoretical prediction. The A factor was also extracted from QMC calculations of the static structure factor $S(\pi)$. At the lowest available $T \sim 0.3J_1$, we obtained using $c = 1.8J_1$, $A = 0.063$, in complete agreement with the above results.

For comparison, we also discuss some low-temperature data for a single-layer antiferromagnet, particularly for the prefactor of the correlation function. At low enough temperatures, the physics of a single-layer antiferromagnet is gov-

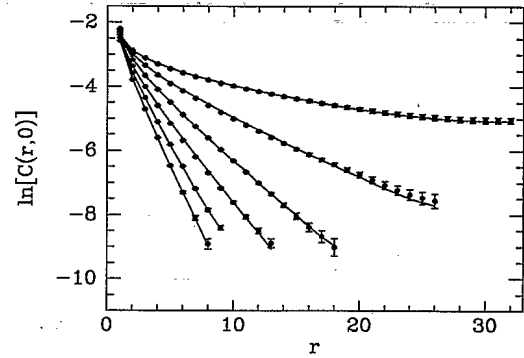


FIG. 5. QMC results for the spin-correlation function $C(\vec{r}) = (-1)^r \langle S_z^r S_z^0 \rangle$ along $\vec{r} = (r,0)$ for a single-layer antiferromagnet at temperatures $T = 0.3 - 0.8J_1$ (the top curve is for $T = 0.3J_1$). The solid curves are fits to $G(r) + G(L-r)$, with $G(r)$ given by (4).

erned by thermal, classical fluctuations. The $N = \infty$ result for Ξ is now *qualitatively* wrong, as the $1/N$ corrections are logarithmically divergent, and the series for the $1/N$ terms gives rise to an extra power of T in the structure factor. The real-space correlator $G(r)$ now has the form

$$G(r) = Z_N \frac{N_0^2 T}{\rho_s} \left(\frac{(N-2)T}{2\pi\rho_s} \right)^{1/(N-2)} \times \int dx x f(x/m) J_0\left(\frac{xrT}{c}\right), \quad (4)$$

where $f(y)$ is a universal scaling function ($f(0)=1$), and Z_N is the overall renormalization factor. The behavior of $f(y)$ at large y is rather complex, but we actually need to know $f(y)$ only for $y = O(1)$ as the momentum integration in (4) is confined to $x \sim m$. For such y , virtually all $1/N$ corrections to the mean-field expression $f(x/m) = (x^2 + m^2)^{-1}$ can be absorbed into the renormalization of the mass,⁴ so that for practical purposes we again can use the mean-field functional dependence of f . This is consistent with the earlier analysis of Tyc *et al.*,¹⁶ who introduced a semiphenomenological one-parameter scaling form for $f(y)$. For $y = O(1)$, this scaling form is well approximated by the mean-field expression. The prefactor Z_N was obtained analytically to first order in $1/N$.¹⁷ To estimate Z_3 , we assume that the $1/N$ corrections collapse into a single exponent (this is known to be true for the correlation length¹⁸). We then obtain

$$Z_N = \left(\frac{\Gamma(1/3)\Gamma(7/6)}{\Gamma(2/3)\Gamma(5/6)} \right)^{3/(N-2)} \frac{2^{(2-N)}}{\Gamma[1+1/(N-2)]}. \quad (5)$$

To first order in $1/N$, we have $Z_N = 1 + 0.188/N$,⁴ while for $N=3$, we have $Z_3 \approx 2.15$, which is larger than the first-order result but still substantially smaller than the previous estimate of Tyc *et al.*,¹⁶ $Z_3 \approx 6.63$.

The QMC data for the real-space correlation function and their fit to the Eq. (4) are shown in Fig. 5. There is no need to exclude the spin-wave velocity, as in a single-layer antiferromagnet c and other input parameters are known to high accuracy.¹⁹ The mass extracted from the fit at low temperatures agrees well with the results of other nu-

merical studies²⁰ and with the theoretical formula for the classical region,^{3,18} though perfect agreement with the theory is reached at ρ_s slightly smaller than $0.18J$. The prefactor is now $A = (N_0^2/2\pi\rho_s)[Z_3(T/2\pi\rho_s)]$, i.e., it should decrease linearly with T . The A inferred from the fit indeed decreases with T , though there are not enough points at low T to obtain the T dependence. The value of A at the lowest temperature in the simulations, $T=0.3J_1$ is $A=0.07$, while from the theoretical formula we obtain $A \approx 0.05$. This indicates that the actual value of Z_3 is probably about 40% higher than in (5). Another way to find A is to consider the ratio $X = S(\pi)J_1^2/(T\xi)^2 = N_0^2Z_3J_1^2/(2\pi\rho_s^2)$. The QMC result for this ratio is $X \approx 1.34$ at $T=0.3J_1$, while the theory gives $X=0.98$, which is again less by about 40%.

To summarize, in this paper we presented the first numerical evidence for the universal quantum-critical behavior of the correlation length in a 2D antiferromagnet near the criti-

cal point *at low temperatures*. We compared the results for the universal parameter ratios $\xi^{-1}/(T\chi_u)^{1/2}$ and $S(\pi)/[T\chi(\pi,0)]$ with QMC data, and in both cases obtained good agreement with the theory based on the $O(3)$ σ model. The prefactor A extracted from the fit is nearly T independent which agrees with the theoretical prediction $A \propto T^\eta$. For comparison, we also presented data for the correlation function of a single-layer antiferromagnet at low T . We found good agreement with the theoretical result for the correlation length in the renormalized-classical region, but the prefactor in the correlation function disagrees with the classical formula by about 40%.

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