Order-Disorder Transition in a Two-Layer Quantum Antiferromagnet

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We have studied the antiferromagnetic order-disorder transition occurring at $T = 0$ in a two-layer quantum Heisenberg antiferromagnet as the interplane coupling is increased. Finite-size scaling of quantum Monte Carlo results for the staggered structure factor gives the critical ratio $J_c = 2.51 \pm 0.02$ between the interplane and in-plane coupling constants. The critical behavior is consistent with the 3D classical Heisenberg universality class. Results for the uniform magnetic susceptibility and the correlation length at finite temperature are compared with recent predictions for the (2+1)-dimensional nonlinear σ model.

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It was recently suggested [1–5] that the unusual normal-state magnetic properties of the high-T_c superconducting cuprates are characteristic of two-dimensional (2D) quantum antiferromagnets close to the critical point of a zero-temperature order-disorder transition, with the disordered phase having a gap towards spin excitations. It has been argued that the physics of such antiferromagnets is described by the nonlinear σ model in 2+1 dimensions [6]. Studies of this field theory based upon a $1/N$ expansion have resulted in detailed predictions for the behavior of near-critical systems [1–5]. In order to test these predictions, it is useful to compare them with exact numerical results for some appropriate model. The two-layer Heisenberg antiferromagnet can be tuned through an order-disorder transition by varying the coupling between the planes [7,8], and constitutes an ideal system for such comparisons. In this Letter, the $T = 0$ order-disorder transition and the finite-temperature "quantum critical" regime of this model are studied using a modification of the Handscomb quantum Monte Carlo algorithm [9,10]. Details of this work will be presented elsewhere [11].

The model we study is defined by the Hamiltonian

$$\hat{H} = J_1 \sum_{a=1,2} \sum_{\langle i,j \rangle} \mathbf{S}_{a,i} \cdot \mathbf{S}_{a,j} + J_2 \sum_i \mathbf{S}_{1,i} \cdot \mathbf{S}_{2,i}, \qquad (1)$$

where $\langle i,j \rangle$ is a pair of nearest neighbors on a square lattice, and $\mathbf{S}_{a,i}$ is a spin-$\frac{1}{2}$ operator at site i in plane a. With the interplane coupling $J_2 = 0$, the independent planes have long-range order at $T = 0$ [12], and the spectrum is gapless. For a large ratio $J = J_2/J_1$, there is a tendency for neighboring spins in adjacent planes to form singlets. There is a gap for spin-1 excitations and no long-range order. A series expansion calculation by Hida gave a critical coupling $J_c = (J_2/J_1)_c = 2.56$ [7]. A Schwinger boson mean-field calculation by Millis and Monien, on the other hand, resulted in $J_c = 4.48$ [8].

The coupling ratio J is analogous to the coupling g of the (2+1)-dimensional nonlinear σ model. In their study of this model, Chakravarty *et al.* [6] identified three regimes in the T-g plane. For $g < g_c$ there is long-range antiferromagnetic order at $T = 0$. At low temperatures, in the so-called renormalized classical (RC) regime, the correlation length ξ diverges as $e^{2\pi\rho_s/T}$, where ρ_s is the spin stiffness. For $g > g_c$, there is an excitation gap and the correlation length is constant in the low-temperature "quantum disordered" (QD) regime. For $g \approx g_c$, $\xi \sim T^{-1}$ in the high-temperature "quantum critical" (QC) regime. Exactly at g_c, ρ_s vanishes and the QC regime extends down to $T = 0$, whereas for $g \neq g_c$ there is a crossover to either the RC or the QD regime as the temperature becomes low enough for the deviation from g_c to be sensed. On the lattice, the spins become effectively decoupled as $T \to \infty$ and there is a high-temperature crossover from the QC regime to a "local moment" (LM) regime.

The 3D nonlinear σ model is the appropriate continuum field theory for the phase transition of the 3D classical Heisenberg model. The $T = 0$ transition of 2D quantum antiferromagnets is therefore expected to belong to the universality class of that model, provided that the σ-model description is valid at the critical point [6].

Chubukov and co-workers [2,3] showed that close to criticality, many physical observables depend in a universal manner on a few model-dependent parameters. Once these parameters are determined, the temperature dependence of, e.g., the wave-vector and frequency dependent magnetic susceptibility is known for temperatures $T \lesssim J_1$.

Quantum Monte Carlo studies have confirmed that the 2D Heisenberg model has long-range order at $T = 0$ [12]. The low-temperature behavior is consistent with the predictions for the RC regime [13,14]. It has been argued that this model is close enough to criticality to exhibit QC behavior for $0.35 \lesssim T/J_1 \lesssim 0.55$ [2,3]. However, this regime is narrow, making it difficult to verify the predicted behavior. Introducing frustrating interactions reduces the long-range order and widens the QC regime. Unfortunately, frustrated quantum models are difficult to study numerically, due to "sign problems" which arise in Monte Carlo algorithms [15]. The two-layer model (1) does not have this problem, and can be tuned through the critical point by varying J_2/J_1.

In order to determine the critical ratio $J_c = (J_2/J_1)_c$

of the two-layer model, and to investigate its $T = 0$ critical behavior, we have carried out quantum Monte Carlo simulations of periodic lattices with $2L^2$ spins, with $L = 4, 6, 8, 10$. In order to obtain essentially ground state results we chose an inverse temperature $\beta = 48$, which for the system sizes studied is sufficient for all calculated quantities to have saturated at their $T = 0$ values. Monte Carlo moves necessary to ensure ergodicity in the subspace with zero total magnetization $[\sum_{a,i} S^z_{a,i} = 0]$ were carried out. We have also investigated the finite temperature properties for various values of J near J_c. In these finite-temperature simulations, Monte Carlo moves changing the total magnetization were carried out. Systems with L up to 24 at $T/J_1 \geq 0.3$ were studied [16]. For small systems we have checked simulation results against exact diagonalization data. At higher temperatures our results are in good agreement with series expansion results recently obtained by Singh and Sokol [17].

We have calculated the in-plane staggered structure factor for coupled $L \times L$ planes

$$S_1(L) = \frac{1}{L^2}\sum_{i,l}\langle S^z_{1,i+l}S^z_{1,l}\rangle(-1)^{l_x+l_y} \tag{2}$$

and the full two-plane staggered structure factor

$$S_2(L) = \frac{1}{2L^2}\sum_{i,l}\langle [S^z_{1,i+l} - S^z_{2,i+l}][S^z_{1,l} - S^z_{2,l}]\rangle(-1)^{l_x+l_y}. \tag{3}$$

In addition we have evaluated the corresponding staggered susceptibilities χ_1 and χ_2, with

$$\chi_1(L) = \frac{1}{L^2}\sum_{i,l}\int_0^\beta d\tau\langle S^z_{1,i+l}(\tau)S^z_{1,l}(0)\rangle(-1)^{l_x+l_y} \tag{4}$$

and a similar expression for χ_2.

Two possible order parameters of the phase transition are the sublattice magnetizations m_1 and m_2 of a single plane and the whole system, respectively. These can be defined in terms of the structure factors as

$$m_n(L) = \sqrt{3S_n(L)/nL^2}. \tag{5}$$

For $J \leq J_c$ the asymptotic $T = 0$ spin-spin correlation functions

$$C_1(\mathbf{r}) = \langle S^z_{1,i+r}S^z_{1,i}\rangle(-1)^{r_x+r_y}, \tag{6a}$$

$$C_2(\mathbf{r}) = \langle [S^z_{1,i+r} - S^z_{2,i+r}][S^z_{1,i} - S^z_{2,i}]\rangle(-1)^{r_x+r_y} \tag{6b}$$

should have the form

$$C_n(r) = m_n^2 + b_n r^{-(1+\eta)}, \tag{7}$$

which gives for the sublattice magnetization

$$m_n^2(L) = m_n^2(\infty) + k_n(1/L)^{1-\eta}. \tag{8}$$

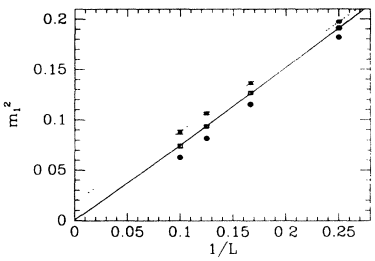

FIG. 1. The sublattice magnetization m_1 versus $1/L$ for $J = 2.4$ (solid squares), $J = 2.5$ (open squares), and $J = 2.6$ (solid circles). The dashed and solid curves are least squares fits of the form given by Eq. (8) with $\eta = 0.03$ for $J = 2.4$ and 2.5, respectively.

Exactly at the critical point, we expect that η is equal to the 3D Heisenberg exponent $\eta \approx 0.03$ [18]. Hence, we have fit our results for m_n^2 to (8) with this η. For m_1^2 the Monte Carlo results agree well with this form for all $L \geq 4$, whereas $L \geq 6$ is needed to obtain good fits to the results for m_2^2. Figure 1 shows $m_1^2(L)$ versus $1/L$ for $J = 2.4$, 2.5, and 2.6, along with least-squares fits of (8) to the $J = 2.4$ and 2.5 data. At $J = 2.5$ the extrapolated values of $m_1(\infty)$ and $m_2(\infty)$ are both zero within statistical errors, indicating that the critical ratio is close to 2.5.

Define a reduced coupling $j = (J - J_c)/J_c$. As $j \to 0$ from above, the correlation length ξ diverges as $j^{-\nu}$, and the staggered structure factors and susceptibilities diverge as $j^{-\gamma_S}$ and $j^{-\gamma_\chi}$, respectively. These exponents are related according to

$$\gamma_S = \nu(1 - \eta), \tag{9a}$$

$$\gamma_\chi = \nu(2 - \eta). \tag{9b}$$

For a quantity A which diverges as $j^{-\gamma_A}$, finite-size scaling [19] relates the value A_L for a finite system to the infinite-size value A_∞ according to

$$A_L(j) = A_\infty(j)f[\xi_\infty(j)/L]. \tag{10}$$

Equations (9) and (10) give for the size dependence of $S_n(L)$ and $\chi_n(L)$ at the critical point:

$$S_n(L, j = 0) \sim L^{1-\eta}, \tag{11a}$$

$$\chi_n(L, j = 0) \sim L^{2-\eta}. \tag{11b}$$

Figure 2 shows results for $\ln(S_n)$ and $\ln(\chi_n)$ versus $\ln(L)$ at $J = 2.5$. If Eqs. (11) hold, the data should fall onto straight lines with slopes $1-\eta$ and $2-\eta$, respectively. All of the S_1 results agree well with this form, whereas the other quantities agree within statistical errors for $L \geq 6$.

In order to test whether the exponent ν agrees with its expected 3D Heisenberg value $\nu \approx 0.70$ [18], one can use the scaling relation (10) for $j > 0$. Graphing $A_L(j)j^{\gamma_A}$ versus Lj^ν for various J and L should produce points collapsed onto a single curve. This is indeed the case for S_n and χ_n if $J_c \approx 2.50$. The best overall results are

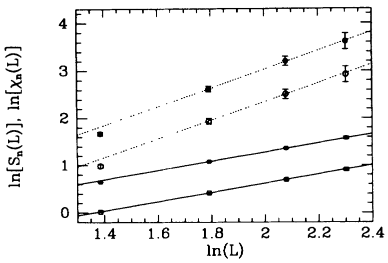

FIG. 2. Size dependence of S_1 (open squares), S_2 (solid squares), χ_1 (open circles), and χ_2 (solid circles) at $J = 2.5$. The solid and dashed lines have slopes $1 - \eta = 0.97$, and $2 - \eta = 1.97$, respectively.

obtained with $J_c = 2.51$, in good agreement with the results for m_1. Figure 3 displays results for S_1 using $\nu = 0.70, \eta = 0.03$, and $J_c = 2.51$ for various J and L. Based on the appearance of such graphs with various assumptions for J_c, and the results for m_1 displayed in Fig. 1, we estimate the critical coupling and its error limits to be $J_c = 2.51 \pm 0.02$. This is only slightly lower than Hida's series expansion result ($J_c = 2.56$) [7].

We now discuss some finite-temperature results for systems close to criticality. For temperatures $T \ll J_2$, the planes are strongly coupled, and the high-energy "optical" excitations do not affect the low-energy physics. There is therefore effectively only 1 degree of freedom per chemical unit cell, and a description in terms of the (2+1)-dimensional nonlinear σ model is expected to be valid [8].

Chubukov *et al.* [3] carried out $\frac{1}{N}$ expansions of the nonlinear σ model and obtained the temperature dependence of a number of observables. Their result for the uniform magnetic susceptibility is (for $N = 3$)

$$\chi_u = \frac{\sqrt{5}}{\pi c^2} \ln\Big(\frac{\sqrt{5}+1}{2}\Big)\Big(\frac{8\pi}{15}\rho_s + 0.7937T\Big), \qquad (12)$$

where c is the spin-wave velocity. Hence, at the critical coupling, where $\rho_s = 0$, the susceptibility graphed versus the temperature should produce a straight line with intercept zero and a slope which depends only on c. Figure 4 shows numerical results for the $q = 0$ susceptibility per unit cell

$$\chi_u = \frac{\beta}{L^2} \sum_{i,j} \langle [S^z_{1,i} + S^z_{2,i}][S^z_{1,j} + S^z_{2,j}] \rangle \qquad (13)$$

for $L = 10$. The size dependence of χ_u is very weak for $L \geq 10$ at the temperatures studied. For $J = 2.5$ a least-squares fit to the $T \leq 0.9$ results gives an intercept close to zero. The slope of the line gives $c = 1.69 \pm 0.02$ in units of $J_1 a/\hbar$ [a is the lattice constant], which within statistical errors is equal to the single-plane spin-wave velocity [20]. On the other hand, spin-wave theory for the two-layer system with $J = 2.5$ gives $c = 1.97$ [this includes a renormalization factor $Z_c = 1.094$ calculated to order $1/S$].

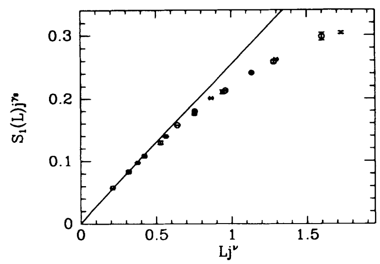

FIG. 3. Finite-size scaling of S_1 with $J_c = 2.51$ and 3D Heisenberg exponents. Open squares are for $J = 2.55$, solid squares for $J = 2.60$, open circles for $J = 2.70$, solid circles for $J = 2.75$, and crosses for $J = 2.80$. The solid curve is the asymptotic form for the scaling function, $f(x \to 0) \sim x^{1-\eta}$.

The nonlinear σ-model prediction for the inverse correlation length is also a linear function of the temperature [3]:

$$\xi^{-1} = 1.0791 \times 2 \ln\Big(\frac{\sqrt{5}+1}{2}\Big)\frac{T}{c} - \frac{4\pi\rho_s}{3\sqrt{5}c}. \qquad (14)$$

In order to extract ξ, we fitted the correlation function $C_1(\mathbf{r})$, Eq. (6a), to the form $C_1(r) = Ae^{-r/\xi}r^{-(1+\eta)}$ with $\eta = 0.03$. We have taken the effects of the periodic boundaries into account analogously [11] to the proposal for 1D systems in Ref. [21]. In Fig. 5, $L = 10$ and $L = 24$ results for ξ^{-1} at $J = 2.5$ and 2.6 are graphed along with the predicted form (14) for $\rho_s = 0$ and $c = 1.69$, shown as a solid line. A crossover from the high-temperature behavior appears to take place around $T = 0.6$, below which the T dependence is approximately linear. For $J = 2.5$ the intercept is negative, indicating that this is below the critical coupling. For $J = 2.6$, the intercept is close to zero, but the slope does not agree with the predicted value at the critical point for the c used. For comparison we also show as the dashed line in Fig. 5 the form (14) using the spin-wave theory result $c = 1.97$. Clearly, a more accurate calculation of the spin-wave velocity for the two-layer system is needed in order to determine the relative accuracies of the prefactors of the forms (12) and (14). It should be noted that for a single plane, Monte

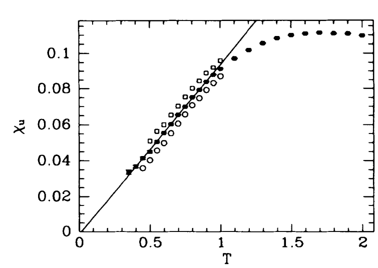

FIG. 4. The uniform susceptibility per unit cell versus the temperature for $L = 10$ at $J = 2.4$ (open squares), $J = 2.5$ (solid squares), and $J = 2.6$ (open circles). The line is a least squares fit to the $T \leq 0.9$, $J = 2.5$ data.

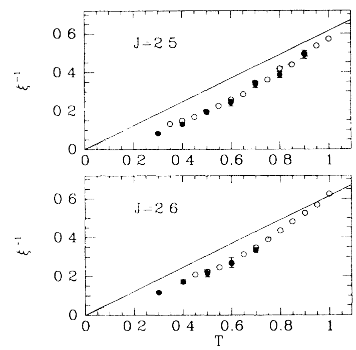

FIG. 5. The inverse correlation length for $L = 10$ (open circles) and $L = 24$ (solid circles) versus the temperature for $J = 2.5$ and $J = 2.6$. The lines are the predicted form, Eq. (14) with $\rho_s = 0$ and $c = 1.69$ (solid lines), and $c = 1.97$ (dashed lines).

Carlo results [13] for the uniform susceptibility are in agreement with Eq. (12), although only over a narrow temperature regime [2,3], whereas the inverse correlation length is not accurately described by Eq. (14) [13,22].

In conclusion, we have studied the order-disorder transition of a two-layer Heisenberg antiferromagnet using a modification of Handscomb's quantum Monte Carlo technique [9,10]. The critical ratio between the interplane and in-plane coupling constants was determined to be 2.51 ± 0.02. The $T = 0$ critical behavior is consistent with the transition belonging to the universality class of the 3D classical Heisenberg model. At finite temperature we have studied the uniform magnetic susceptibility and the correlation length. Close to criticality the susceptibility is a linear function of the temperature for $T \lesssim 0.9J_1$, in agreement with predictions [2,3] for the (2+1)-dimensional nonlinear σ model. The inverse correlation length shows a linear behavior for $T \lesssim 0.6J_1$. However, the ratio of the linear coefficients of χ_u and ξ^{-1} does not have its predicted value, however. As also appears to be the case for the single-plane Heisenberg model [2,3,13,22] the uniform susceptibility exhibits quantum critical behavior well beyond the crossover boundaries defined by the behavior of the correlation length.

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