Order – Disorder Transition in a Two-Layer Quantum Antiferromagnet

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Abstract

We have studied the antiferromagnetic order – disorder transition occurring at $T = 0$ in a 2-layer quantum Heisenberg antiferromagnet as the inter-plane coupling is increased. Quantum Monte Carlo results for the staggered structure factor in combination with finite-size scaling theory give the critical ratio $J_c = 2.51 \pm 0.02$ between the inter-plane 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 $\sigma$-model. The susceptibility is found to exhibit quantum critical behavior at temperatures significantly higher than the correlation length.
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 \(\sigma\)-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 \[1–4\]. In order to test these predictions, it is useful to compare them with exact numerical results for some appropriate model. The 2-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

\[
\hat{H} = J_1 \sum_{a=1,2} \sum_{\langle i,j \rangle} \vec{S}_{a,i} \cdot \vec{S}_{a,j} + J_2 \sum_i \vec{S}_{1,i} \cdot \vec{S}_{2,i}
\]

(1)

where \(\langle i, j \rangle\) is a pair of nearest-neighbors on a square lattice, and \(\vec{S}_{a,i}\) is a spin-\(\frac{1}{2}\) operator at site \(i\) in plane \(a\). With the inter-plane 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 \(\sigma\)-model. In their study of this model, Chakravarty et al. \[3\] 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 \(\xi\) diverges as \(e^{2\pi \rho s/T}\), where \(\rho s\) 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 $g_c$, $\rho_s$ vanishes and the QC regime extends down to $T = 0$, whereas for $g \neq g_c$ there is a cross-over 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 cross-over from the QC regime to a “local moment” (LM) regime.

The 3D nonlinear $\sigma$-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 $\sigma$-model description is valid at the critical point [6].

Chubukov et al. [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 2-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 2-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 $[\sum_{a,i} S_{a,i}^z = 0]$ 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 result 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

$$S_1(L) = \frac{1}{L^2} \sum_{i,l} \langle S_{1,i+l}^z S_{1,l}^z \rangle (-1)^{l_x+l_y}$$  \hspace{1cm} (2)

and the full two-plane staggered structure factor

$$S_2(L) = \frac{1}{2L^2} \sum_{i,l} \langle [S_{1,i+l}^z - S_{2,i+l}^z][S_{1,l}^z - S_{2,l}^z] \rangle (-1)^{l_x+l_y}.$$  \hspace{1cm} (3)

In addition we have evaluated the corresponding staggered susceptibilities $\chi_1$ and $\chi_2$, with

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

and a similar expression for $\chi_2$.

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

$$m_n(L) = \sqrt{3S_n(L)/nL^2}.$$  \hspace{1cm} (5)

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

$$C_1(\vec{r}) = \langle S_{1,i+r}^z S_{1,i}^z \rangle (-1)^{r_x+r_y}$$  \hspace{1cm} (6a)

$$C_2(\vec{r}) = \langle ([S_{1,i+r}^z - S_{2,i+r}^z][S_{1,i}^z - S_{2,i}^z] \rangle (-1)^{r_x+r_y}$$  \hspace{1cm} (6b)

should have the form
\[ C_n(r) = m_n^2 + b_n r^{-(1+n)}, \]  

which gives for the sublattice magnetization

\[ m_n^2(L) = m_n^2(\infty) + k_n(1/L)^{1-\eta}. \]  

Exactly at the critical point, we expect that \( \eta \) is equal to the 3D Heisenberg exponent \( \eta \approx 0.03 \) \cite{18}. Hence, we have fit our results for \( m_n^2 \) to (8) with this \( \eta \). 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 \( m_2^2 \). Fig. 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 \( \xi \) 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

\[ \gamma_S = \nu(1 - \eta) \]  

(9a)

\[ \gamma_\chi = \nu(2 - \eta). \]  

(9b)

For a quantity \( A \) which diverges as \( j^{-\gamma_A} \), finite-size scaling \cite{19} relates the value \( A_L \) for a finite system to the infinite-size value \( A_\infty \) according to

\[ A_L(j) = A_\infty(j)f[\xi_\infty(j)/L]. \]  

(10)

Eqs. (9) and (10) give for the size-dependence of \( S_n(L) \) and \( \chi_n(L) \) at the critical point:

\[ S_n(L, j = 0) \sim L^{1-\eta} \]  

(11a)

\[ \chi_n(L, j = 0) \sim L^{2-\eta}. \]  

(11b)

Fig. 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 $\nu$ agrees with its expected 3D Heisenberg value $\nu \approx 0.70$ \cite{L}, one can use the scaling relation \eqref{eq:scaling} for $j > 0$. Graphing $A_L(j)j^{\gamma A}$ versus $Lj^{\nu}$ for various $J$ and $L$ should produce points collapsed onto a single curve. This is indeed the case for $S_n$ and $\chi_n$ if $J_c \approx 2.50$. The best over-all results are obtained with $J_c = 2.51$, in good agreement with the results for $m_1$. Fig. 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 ($J_c = 2.56$) \cite{F}.

We now discuss some finite-temperature results for systems close to criticality. For the single-plane Heisenberg model, QC behavior has been observed for the uniform susceptibility at temperatures $0.35 < T/J_1 < 0.55$ \cite{E, F}. For the 2-layer model with $J \approx J_c$, one would expect the cross-over from the LM regime to the QC regime to occur at a higher temperature, since the thermal fluctuations are reduced by the strong coupling between the planes.

Chubukov et al. \cite{E} carried out $\frac{1}{N}$ expansions of the non-linear $\sigma$-model and obtained the temperature dependence of a number of observables. Their result for the uniform magnetic susceptibility is (for $N = 3$)

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

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 $c$. Fig. 4 shows numerical results for the $q = 0$ susceptibility

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

for $L=10$. The size-dependence of $\chi_u$ 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 $c = 2.39 \pm 0.02$, in units of $J_1 a/\hbar$ [$a$ is the lattice constant].
The inverse correlation length is predicted to be a linear function of the temperature: \[ (3) \]

\[ \xi^{-1} = 1.0791 \times 2 \ln \left( \frac{\sqrt{5} + 1}{2} \right) \frac{T}{c} - \frac{4\pi \rho_s}{3\sqrt{5}c}. \] (14)

In order to extract \( \xi \), we fit the correlation function \( C_1(\vec{r}) \), Eq. \((10a)\), 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. \([20]\). In Fig. 5, \( L = 10 \) and \( L = 24 \) results for \( \xi^{-1} \) at \( J = 2.5 \) and 2.6 are graphed along with the predicted form \((14)\) for \( \rho_s = 0 \) and \( c = 2.39 \). In view of the susceptibility results one would expect \((14)\) to apply for \( T \lesssim 0.9 \), which is clearly not the case. It appears that a cross-over from the LM regime occurs around \( T = 0.6 \). Below this temperature the \( J = 2.6 \) results are close to the predicted form. For \( J = 2.5 \) the correlation length grows faster than \( 1/T \) in the regime studied, suggesting that this coupling is slightly lower than the critical coupling. Larger systems at lower temperatures have to be studied in order to determine the \( T \to 0 \) behavior of \( \xi \) more precisely.

In conclusion, we have studied the order – disorder transition of a 2-layer Heisenberg antiferromagnet using a quantum Monte Carlo technique \([9,10]\). The critical ratio between the inter-plane and in-plane coupling constants was determined to be \( 2.51 \pm 0.02 \). 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 \( T \lesssim 0.9 J_1 \), in agreement with predictions \([2,3]\) for the 2+1-dimensional nonlinear \( \sigma \)-model. The predicted linear behavior of the inverse correlation length applies only for \( T \lesssim 0.6 J_1 \).

For the single-plane 2D Heisenberg model, the uniform susceptibility has a roughly linear temperature dependence for \( 0.35 \lesssim T \lesssim 0.55 \) \([2,3]\). However, a regime where \( \xi^{-1} \) has the \( T \) dependence predicted for the quantum critical regime has not been observed \([13,21]\). The results presented here indicate that the uniform susceptibility exhibits the predicted linear behavior at temperatures significantly higher than the correlation length. Hence, it
appears that the susceptibility exhibits quantum critical behavior well beyond the cross-over boundaries defined by the behavior of the correlation length.

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FIGURES

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.

FIG. 2. Size dependence of $S_1$ (open squares), $S_2$ (solid squares), $\chi_1$ (open circles), and $\chi_2$ (solid circles) at $J = 2.5$. The solid and dashed lines have slopes $1 - \eta = 0.97$, and $2 - \eta = 1.97$, respectively.

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, $f(x \rightarrow 0) \sim x^{1-\eta}$.

FIG. 4. The uniform susceptibility 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 solid lines are of the predicted form, Eq. (14) with $\rho_s = 0$ and $c = 2.39$. 