

# Universal scaling of the Néel temperature of near-quantum-critical quasi-two-dimensional Heisenberg antiferromagnets

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We use a quantum Monte Carlo method to calculate the Néel temperature  $T_N$  of weakly coupled  $S=1/2$  Heisenberg antiferromagnetic layers consisting of coupled ladders. This system can be tuned to different two-dimensional scaling regimes for  $T > T_N$ . In a single-layer mean-field theory,  $\chi_s^{2D}(T_N) = (z_2 J')^{-1}$ , where  $\chi_s^{2D}$  is the exact staggered susceptibility of an isolated layer,  $J'$  the interlayer coupling, and  $z_2=2$  the layer coordination number. With a renormalized  $z_2$ ,  $z_2 \rightarrow k_2 z_2$ , we find that this relationship applies not only in the renormalized-classical regime, as shown previously, but also in the quantum-critical regime and part of the quantum-disordered regime. The renormalization is nearly constant;  $k_2 \approx 0.65-0.70$ . We also study other universal scaling functions.

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Antiferromagnets with effectively low dimensionality, consisting of weakly coupled chains [quasi-one-dimensional (quasi-1D)] or layers (quasi-2D), offer unique opportunities to study quantum mechanical collective behavior. A multitude of quasi-1D and quasi-2D antiferromagnetic compounds have been discovered, or deliberately designed, and they exhibit a wide range of ordered and disordered phases. At the same time, new and improved experimental techniques enable increasingly sophisticated studies of their properties. It is thus possible to test in detail microscopic quantum spin models and theoretical quantum many-body concepts, such as quantum-critical scaling.<sup>1</sup> Motivation for studying these systems often come from phenomena directly associated with low dimensionality. Real materials, however, almost always have some 3D couplings that cannot be completely ignored at low temperatures. The ways in which these couplings change the physics, e.g., leading to phase transitions or dimensional crossovers,<sup>2</sup> are also governed by the physics of the 1D or 2D units. Studies of 3D effects can therefore also provide important insights.

The Néel temperature in systems of coupled antiferromagnetic layers was studied earlier by Lines using Green's functions.<sup>3</sup> More recently, Sengupta *et al.* used a QMC method to study  $T_N$  and the dimensional crossover in the specific heat.<sup>4</sup> Yasuda *et al.* calculated  $T_N$  more systematically at very small ratio  $J'/J$  of the inter- and intralayer couplings, for  $S=1/2$  as well as higher spins.<sup>5</sup>

Previous work focused on spatially isotropic layers. In this paper we investigate  $T_N$  of a quasi-2D  $S=1/2$  Heisenberg model consisting of layers of coupled ladders. In the absence of interlayer couplings, the Mermin-Wagner theorem dictates that the system can have long-range order only at  $T=0$ .<sup>6</sup> The 2D Heisenberg model with spatially isotropic nearest-neighbor couplings  $J$  has an ordered ground state.<sup>7,8</sup> At low temperatures, in the renormalized classical (RC) regime, its spin correlation length is exponentially divergent.<sup>8</sup> Systems with a coupling pattern favoring formation of nearest-neighbor singlets,<sup>9</sup> e.g., coupled two-leg ladders,<sup>10</sup> can be tuned through a quantum phase transition into a quantum disordered (QD) state. This  $T=0$  transition and its associated  $T > 0$  quantum-critical (QC) scaling regime have been

studied in detail, using field-theoretical approaches<sup>11</sup> and quantum Monte Carlo (QMC) simulations.<sup>10,12,13</sup>

Our motivation to study the coupled-ladder system comes from recently proposed scaling functions relating  $T_N$  and various 2D and 3D staggered susceptibilities.<sup>14,15</sup> We focus in particular on interladder couplings for which the system is near-quantum-critical in the absence of interlayer couplings. This system is also relevant to layered cuprates. Recent neutron scattering studies show a universal magnetic response in  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$  and  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ ,<sup>16</sup> which can be explained by the coupled spin ladders near the quantum critical point. Our main finding is that two of the scaling functions are almost constant and do not change appreciably between the RC and QC regimes. In particular, the coordination number renormalization introduced by Yasuda *et al.* changes from  $k_2 \approx 0.65$  in the RC regime<sup>5</sup> to  $k_2 \approx 0.68$  in the QC regime. This minute change implies that the Néel ordering takes place almost exactly at the same temperature at which the planes start to correlate appreciably, and that these correlations are almost completely governed by the magnitude of the static staggered susceptibility of the planes. The nature of the fluctuations, RC or QC (for which the dynamic susceptibilities are completely different<sup>11</sup>), does not play a major role.

In a single-layer mean-field theory (also referred to as RPA),<sup>17</sup> the 3D couplings of a layer  $l=0$  are taken into account by a static staggered magnetic field arising from the ordered moments of the two adjacent planes  $l = \pm 1$ . The self-consistent Néel temperature is then obtained by solving the equation

$$\chi_s^{2D}(T_N) = (z_2 J')^{-1}, \quad (1)$$

where  $z_2=2$  is the layer coordination number and  $\chi_s^{2D}$  is the staggered susceptibility of a single layer, the  $T$  dependence of which is known from studies of the quantum nonlinear  $\sigma$  model. In the RC regime,  $T < 4\pi\rho_s$ ,<sup>8</sup>

$$\chi_s^{2D}(T) \propto T e^{4\pi\rho_s/T}, \quad (2)$$

where  $\rho_s$  is the spin stiffness. Using numerically exact QMC results for  $\chi_s^{2D}$  and  $T_N$ , Yasuda *et al.*<sup>5</sup> found that the mean-

field expression (1) accurately captures the  $J'/J \ll 1$  dependence of  $T_N$ , if  $z$  is replaced by a renormalized coordination number  $z_2 k_2$ :

$$\chi_s^{2D}(T_N) = (k_2 z_2 J')^{-1}. \quad (3)$$

Moreover, the renormalization,  $k_2 \approx 0.65$ , was found to be independent on the spin  $S$ . This intriguing result prompted Hastings and Mudry to carry out a detailed renormalization group (RG) study of the anisotropic  $O(N)$  nonlinear sigma model.<sup>14</sup> Instead of a constant coordination number renormalization, they argued that the quantity

$$F_1 = (k_2 z_2)^{-1} = J' \chi_s^{2D} \quad (4)$$

is a universal function of  $x = c[T_N \xi^{2D}(T_N)]^{-1}$  when  $J'/J \ll 1$ . Here  $\xi^{2D}$  is the correlation length of a single isolated layer and  $c$  the spin wave velocity. They concluded that the reason for the near constant  $k_2$  is that the single layer is in the RC regime for all  $S$  at low  $T$ , whence  $x$  is exponentially small and  $F_1(x \rightarrow 0)$  is constant. In the QC and QD regimes  $F_1$  should approach other constant values. A quantity involving the susceptibility  $\chi(\mathbf{Q})$  of the full 3D system at wave-vector  $\mathbf{Q} = (\pi, \pi, 0)$  was also introduced

$$F_2 = J' \chi(\pi, \pi, 0). \quad (5)$$

To leading order in an  $1/N$  approximation, Praz *et al.*<sup>15</sup> found that  $F_2 = 1/4$  in all regimes when  $J'/J \rightarrow 0$ . This prediction should be easier to test experimentally because it involves only properties of the actual quasi-2D system. They also proposed a third universal quantity

$$F_3 = J' S(\pi, \pi, 0) T_N^{-1}, \quad (6)$$

where  $S(\mathbf{Q})$  is the static spin structure factor. This function was shown to distinguish between the RC, QC, and QD regimes already at the  $N = \infty$  level.

Since the  $J'/J \rightarrow 0$  values of  $F_1$ ,  $F_2$ , and  $F_3$  were evaluated at the  $N = \infty$  level or including only order- $1/N$  corrections, significant higher-order corrections to these results were expected.<sup>15</sup> Unbiased numerical results would therefore be useful. The previous QMC results by Yasuda *et al.* for  $k_2 = [2F(x \rightarrow 0)]^{-1}$  in the RC regime,  $k_2 \approx 0.65$ ,<sup>5</sup> falls between the  $N = \infty$  and  $1/N$  values;  $k_2 = 1/2$  and  $1.01$ .<sup>15</sup>  $F_2$  and  $F_3$  have not yet been calculated in the RC regime, and none of the predictions have been tested against numerical results in the QC and QD regimes. The universal constants could be very useful for extracting interlayer couplings experimentally.

In the coupled-ladder system, the individual layers can be tuned through a quantum-critical point. We can thus obtain numerical results for  $F_1$ – $F_3$  in all three 2D temperature regimes. The Hamiltonian we study is

$$H = J_1 \sum_{\langle i,j \rangle_1} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle i,j \rangle_2} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{\langle i,j \rangle_3} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (7)$$

where  $\langle i,j \rangle_1$  denotes a pair of nearest-neighbor spins in the same ladder,  $\langle i,j \rangle_2$  in different ladders of the same layer, and  $\langle i,j \rangle_3$  in adjacent layers. For simplicity, we define the coupling ratios  $q = J_2/J_1$  and  $\alpha = J'/J_1$ .

The quantum phase transition of the single layer ( $J' = 0$ )

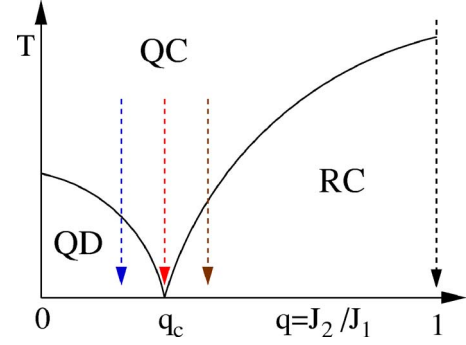


FIG. 1. (Color online) Quantum regimes for a 2D layer of coupled ladders with interladder coupling  $q$ . The curves indicate crossover temperatures. We study  $T > 0$  properties of a quasi-2D system (coupled layers) with  $q$  at and close to the 2D critical point  $q_c$  and at the isotropic point  $q = 1$ .

has been studied by Matsumoto *et al.*<sup>10</sup> The critical coupling  $q_c = 0.31407(5)$ . The  $T > 0$  crossovers for an isolated layer are shown schematically in Fig. 1. In the limit  $\alpha \rightarrow 0$ , the quantum-critical coupling of the quasi-2D system approaches  $q_c$  of the single layer. In our study we focus on values of  $q$  close to the 2D quantum-critical point, choosing  $q = 0.25, 0.30, 0.31407 = q_c$ , and  $0.33$ . We also consider the previously studied case  $q = 1$ ,<sup>5</sup> to calculate also  $F_2$  and  $F_3$  deep inside the RC regime. We have obtained results for  $\alpha$  in the range  $10^{-3}$  to 1.

We use the stochastic series expansion (SSE) QMC method<sup>18</sup> to study periodic lattices with  $L_x L_y L_z$  spins, with  $L_x = L_y = L$  up to 128. To take into account, at least partially, the fact that  $\xi_{x,y} \gg \xi_z$  when  $\alpha \ll 1$ , we use aspect ratios  $L/L_z$  up to 16. To determine the Néel temperature, we use the finite-size scaling of the spin stiffness constants  $\rho_s^\mu$  in the three different directions,  $\mu = x, y, z$ , of the spatially anisotropic lattice. This approach was previously taken in Ref. 4. For fixed aspect ratio, the stiffness at  $T_N$  should scale as  $L^{-1}$ . We thus locate the point at which  $L\rho_\mu(T)$  becomes asymptotically size-independent (extrapolating crossing points for different size  $L$  to  $L \rightarrow \infty$ ). For  $q = 1$ , we use  $T_N$  from Ref. 5. For the calculations of the 2D staggered susceptibility  $\chi_s^{2D}(T)$  we have used  $L$  up to 800.

The  $\alpha$  dependence of the Néel temperature for the different  $q$  values is shown on a log-log scale in Fig. 2. When  $q < q_c$ , there is a minimum value  $\alpha_c$  of the inter-layer coupling below which the system cannot order— $\alpha_c(q)$ , where  $q < q_c$ , is the line of 3D quantum-critical points and  $\alpha_c(q_c) = 0$ . In our results for  $q > q_c$  we see a downturn of  $T_N$  as  $\alpha$  decreases, reflecting the 3D quantum-critical point. From our limited low- $T_N$  data we can only roughly extract two points on the critical line;  $\alpha_c(q = 0.30) \approx 0.001$  and  $\alpha_c(q = 0.25) \approx 0.006$ .

For  $q > q_c$  we can solve the mean-field equation (1) with the RC form (2) of the correlation length, giving, to leading order in  $\alpha$ ,

$$T_N(\alpha) \propto -[\ln(\alpha)]^{-1}. \quad (8)$$

As shown in Fig. 2, for  $q = 1$  this form does not yet apply at  $\alpha = 10^{-3}$ , but it should be the correct form for  $\alpha \rightarrow 0$ .

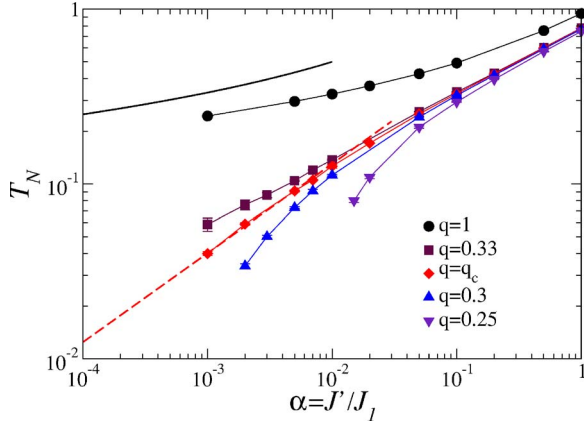


FIG. 2. (Color online) Néel temperature vs interlayer coupling at different interladder couplings  $q$ . The  $q=1$  results are from Ref. 5. The solid (black) and dashed (red) lines show the expected  $\alpha \rightarrow 0$  forms in the RC and QC regimes.

Yasuda *et al.* presented an empirical formula that works well also at higher  $\alpha$ .<sup>5</sup> For  $q=0.33$  we should also approach the RC form when  $\alpha \rightarrow 0$ , but here we instead observe an almost perfect power law in the whole range of  $\alpha \geq 10^{-3}$ . However, the exponent is not the one expected in the QC scaling regime (discussed further below), and we expect the behavior to eventually cross over to the log form.

In the QC regime, the 2D staggered susceptibility takes an asymptotic  $T \rightarrow 0$  power-law form,

$$\chi_s^{2D}(T) \propto T^{-2+\eta}, \quad (9)$$

where  $\eta \approx 0.038$  (Ref. 19) is the correlation function exponent of the 3D  $O(3)$  universality class. Using this form in the mean-field equation (11) we get a corresponding power-law behavior of  $T_N$ ;

$$T_N(\alpha) \propto \alpha^{1/(2-\eta)}. \quad (10)$$

In Fig. 2 we can see that this quasi-2D quantum-critical form accurately describes the results for  $q=q_c$  below  $\alpha \approx 10^{-2}$ . For larger  $\alpha$ ,  $T_N$  is still in the high-temperature regime where the behavior is influenced by nonuniversal lattice effects.<sup>8,11</sup> The two  $q$  values close to  $q_c$ , for which the reduced coupling  $|g-g_c|/g_c \approx 0.05$ , are already too far from the critical point to observe any distinct (asymptotic-form) QC behavior before the crossovers occur.

Following Ref. 5, we study the coordination number renormalization

$$k_2(\alpha) = [2\alpha\chi_s^{2D}(T_N)]^{-1} = (2F_1)^{-1}. \quad (11)$$

In Fig. 3 we show our QMC results for the staggered susceptibility of the isolated 2D layers. Using these results and the  $T_N$  data shown in Fig. 2, we obtain the results for  $k_2$  shown in the upper panel of Fig. 4. For  $q=1$ , Yasuda *et al.* found  $k_2 \approx 0.65$  for  $\alpha < 0.1$ .<sup>5</sup> We here show  $q=1$  results obtained with their listed  $T_N$  values and our own results for  $\chi_s^{2D}$ . The resulting  $k_2$  agree with the previous results. Surprisingly, we hardly see any change in  $k_2$  when going to the near-critical systems, except some small differences when  $\alpha > 0.1$ . At lower  $\alpha$ ,  $k_2$  is only a few percent larger for

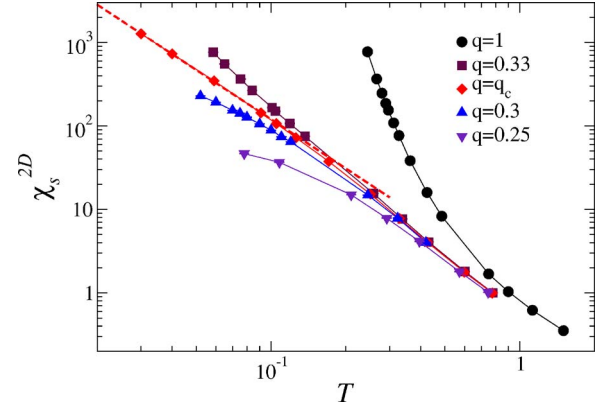


FIG. 3. (Color online) Staggered susceptibility  $\chi_s^{2D}$  vs temperature for 2D systems composed of coupled two-leg ladders with different interladder coupling ratios  $q$ . The dashed line shows the asymptotic QC power-law behavior, Eq. (10).

$q \approx q_c$  than at  $q=1$ ;  $k_2(q_c) \approx 0.68$ . Even for our  $q < q_c$  points,  $k_2$  remains close to this value, even though  $T_N$  is seen crossing over into QD behavior in Fig. 2. For the lowest  $\alpha$  considered for  $q=0.25$  and  $0.30$  we see a slight increase in  $k_2$ , but the effect is barely statistically significant. Note that for  $q < q_c$ ,  $k_2$  is not defined for  $\alpha < \alpha_c(q)$ .

In the RG study by Praz *et al.*,<sup>15</sup> different expressions for  $F_1(k_2)$  were obtained in saddle-point approximations for the RC, QC, and QD regimes. No numerical values were given, however, except for  $k_2=1/2$  in the RC regime. Corrections to the constant behavior were expected (and calculated to order

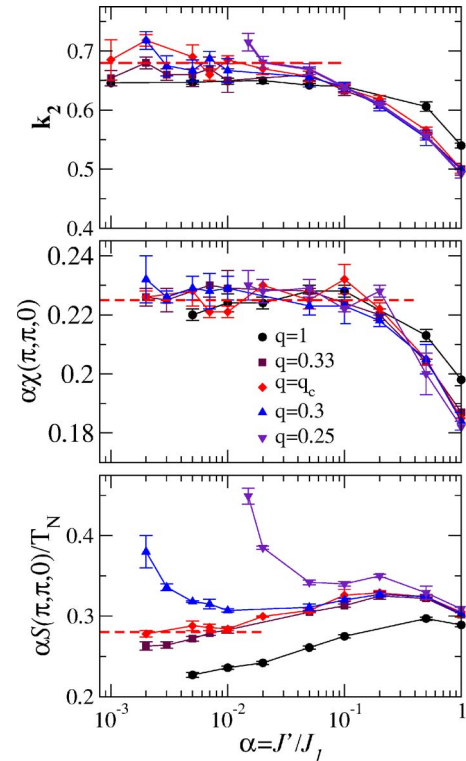


FIG. 4. (Color online) Coupling dependence of the quantities (4)–(6). The horizontal dashed lines show our extracted values for the QC regime.

$1/N$  in the case of the RC regime, then giving  $k_2=1.01$ ). Furthermore, significantly different constants were expected for the three regimes. The near constant  $k_2 \approx 0.65-0.70$  we find here for such a wide range of  $q$  values, spanning all three temperature regimes, is thus quite remarkable.

We now turn to the second scaling function, Eq. (5). As seen in the middle panel of Fig. 4, we obtain an almost constant  $F_2 = \alpha\chi(\pi, \pi, 0) \approx 0.22-0.23$  for all  $q$  and for a wide range of  $\alpha$ . In the  $N=\infty$  approximation,  $F_2=1/4$  in all three temperature regimes,<sup>15</sup> remarkably close to what we find here. However, also in this case the actual values in the RC, QC, and QD regimes were expected to differ markedly once  $1/N$  and higher corrections are included.

The third scaling function, Eq. (6), distinguishes between the RC, QC, and QD regimes already at the  $N=\infty$  level.<sup>15</sup> In the RC regime  $S(\mathbf{Q})=T\chi(\mathbf{Q})$  to leading order<sup>8</sup> and thus  $F_3 = F_2 = 1/4$ . Our results for the RC regimes ( $q=1$ ), shown in the bottom panel of Fig. 4, are slightly lower than the predicted value for  $\alpha < 0.1$ . There is also still a decreasing trend as  $\alpha$  decreases and we cannot reliably extract the asymptotic constant RC value (for  $\alpha=10^{-3}$  our calculations for  $q=1$  are not completely size converged and we therefore do not show them here). For  $q=0.33$ , which also should give RC behavior for  $\alpha \rightarrow 0$ , the results are still quite far from the  $q=1$  curve for all  $\alpha$ , but the decreasing trend is consistent with the same asymptotic value. For  $F_3$  we also see clear differences in behavior in the three regimes. There are distinct crossovers from QC to RC or QD behavior. The results for  $q=q_c$ , 0.30, and 0.33 all fall on the same universal QC curve for  $\alpha$  down to  $\approx 0.05$ , below which the  $q=0.25$  curve splits off. The  $q=q_c$  and 0.3 curves coincide to even lower  $\alpha$ . The asymptotic value at  $q_c$  is  $\approx 0.27$ . For  $q < q_c$  we expect a

divergence at  $\alpha_c(q)$ , as  $S(\pi, \pi, 0)$  must converge to a constant when  $q < q_c$  and  $T_N \rightarrow 0$ . We see clear signs of this divergence.

In conclusion, we have presented results for the quantities  $\alpha\chi_s^{2D} \equiv 1/2k_2$ ,  $\alpha\chi(\pi, \pi, 0)$ , and  $\alpha S(\pi, \pi, 0)/T$ , at  $T=T_N$  for a quasi-2D system of coupled ladders. For weak interlayer coupling,  $\alpha \rightarrow 0$ , these quantities have been predicted to take different universal constant values in the RC, QC, and QD regimes.<sup>14,15</sup> We have investigated the dependence on  $\alpha$  for  $10^{-3} \leq \alpha \leq 1$ , with the goal of extracting the constants and investigate the  $\alpha > 0$  corrections. We find a remarkably stable value of the coordination number renormalization  $k_2$  and  $\alpha\chi(\pi, \pi, 0)$ : For  $\alpha < 0.1$  they are almost independent on  $\alpha$  and do not change appreciably between the RC, QC, and QD regimes. Significant differences in the three regimes were anticipated based on the previous RG study of the nonlinear  $\sigma$  model by Praz *et al.*<sup>15</sup> Only in  $\alpha S(\pi, \pi, 0)$  do we see distinct differences. It would be useful to extend the calculations to still lower interlayer couplings, but reaching significantly below  $\alpha=10^{-3}$  with QMC requires prohibitively large lattices.

The almost constant  $F_1$  and  $F_2$  imply that the correlations between layers is predominantly governed by the magnitude of the static staggered susceptibility of the layers. The range of temperatures for which the system is 3D critical is almost negligible, regardless of the nature of the 2D fluctuations—RC or QC—that initially lead to correlations between the layers.

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