Universal Quantum-Critical Dynamics of Two-Dimensional Antiferromagnets

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The universal dynamic and static properties of two-dimensional antiferromagnets in the vicinity of a zero-temperature phase transition from long-range magnetic order to a quantum-disordered phase are studied. Random antiferromagnets with both Néel and spin-glass long-range magnetic order are considered. Explict quantum-critical dynamic scaling functions are computed in a $1/N$ expansion to two-loop level for certain nonrandom, frustrated square-lattice antiferromagnets. Implications for neutron scattering experiments on the doped cuprates are noted.

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Recently, there have been a number of fascinating and detailed experiments [1-3] on layered antiferromagnets (AFMs) close to a zero-temperature (T) phase transition at which magnetic long-range order (LRO) vanishes. The most prominent among these are the cuprates [1,2], which, upon doping with a small concentration of holes, lose their long-range Néel order and undergo a transition to a $T=0$ phase with magnetic, long-range spin-glass order; at a larger doping there is presumably a second transition to a quantum-disordered (QD) ground state. There have also been low-T experiments on layered AFMs on frustrated lattices [3], which have at most a small ordering moment. A remarkable feature of the measured dynamic susceptibilities of these AFMs is that the overall frequency scale of the spin excitation spectrum is given simply by the absolute temperature. In particular, it appears to be independent of all microscopic energy scales, e.g., an antiferromagnetic exchange constant.

In this paper, we show that this anomalous dynamics is a very general property of finite-T, "quantum-critical" (QC) [4] spin fluctuations near the initial onset of a $T=0$ QD phase. We present the first calculation of universal, QC dynamic scaling functions in $2+1$ dimensions; these will be calculated for a model system—nonrandom, frustrated two-dimensional Heisenberg AFMs with a vector order parameter. Quenched randomness will be shown to be a relevant perturbation to the clean system, and must be included in any comparison with experiments. Scaling forms for the dynamic susceptibility in random AFMs will be presented, and exponent (in)equalities will be discussed.

QC dynamic scaling functions can also be studied in other dimensions. In $1+1$ dimensions the exact scaling functions can be obtained by a simple argument based on conformal invariance [5]; most $(3+1)$-dimensional models are in the upper-critical dimension and we expect the scaling functions to be the free-field type with logarithmic corrections. This leaves $2+1$ dimensions, which is studied here for the first time in the context of AFMs; however, our results are more general, and should also be applicable to other phenomena like the superconductor-insulator transition [6].

Most of our discussion will be in the context of the following quantum AFMs:

$$\mathcal{H}=\sum_{i,j} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j\,, \tag{1}$$

where $\mathbf{S}_i$ are quantum spin operators on the sites i of a two-dimensional lattice, and the J_{ij} are a set of possibly random, short-range antiferromagnetic exchange interactions. The lightly doped cuprates are insulating at $T=0$, suggesting a model with completely localized holes. A specific form of $\mathcal{H}$ with frustrating interactions was used by Gooding and Mailhot [7] and yielded reasonable results on the doping dependence of the $T=0$ correlation length. Models with mobile holes have also been considered [8] and the results will be noted later.

Two different classes of ground states of $\mathcal{H}$ can be distinguished: (i) states with magnetic LRO $\langle\mathbf{S}_i\rangle=\mathbf{m}_i$ and (ii) QD states which preserve spin-rotation invariance $\langle\mathbf{S}_i\rangle=0$. Further, we will distinguish between two different types of magnetic LRO: (A) Néel LRO in which case $\mathbf{m}_i\sim e^{i\vec{Q}\cdot\mathbf{R}_i}$ with $\vec{Q}$ the Néel ordering wave vector and (B) spin-glass LRO in which case $\mathbf{m}_i$ can have an arbitrary dependence on i, specific to the particular realization of the randomness. The lower critical dimension of the Heisenberg spin glass [9] may be larger than 3—in this case the spin-glass LRO will not survive to any finite T, even in the presence of a coupling between the layers. This, however, does not preclude the existence of spin-glass LRO at $T=0$.

Consider now a $T=0$ phase transition between the magnetic LRO and the QD phases, induced by varying a coupling constant g (dependent on the ratios of the J_{ij} in $\mathcal{H}$) through a critical value $g=g_c$, where there is a diverging correlation length $\xi\sim|g-g_c|^{-\nu}$. For Néel LRO, $1/\xi$ is the width of the peak in the spin structure factor at the ordering wave vector $\vec{Q}$. For spin-glass LRO, there is no narrowing of the structure factor, and ξ is instead a correlation length associated with certain four-spin correlation functions [9]. At finite T we can define a thermal length $\xi_T\sim T^{-1/z}$ (z is the dynamic critical exponent) which is the scale at which deviations from

$T=0$ behavior are first felt. The QC region is defined by the inequality $\xi_T < \xi$ (Fig. 1); in this case the spin system notices the finite value of T *before* becoming sensitive to the deviation of g from g_c, and the dynamic spin correlations will be found to be remarkably universal.

We consider first the case (A)—a phase transition from Néel LRO to a QD phase; such transitions can occur for both random and nonrandom $\mathcal{H}$. At $T=0$ the static spin susceptibility χ will have a divergence at $g=g_c$ and wave vector $\vec{q}=\vec{Q}$: $\chi(\vec{q}=\vec{Q},\omega=0) \sim |g-g_c|^{-\gamma}$ with $\gamma=(2-\eta)\nu$. The form of the $(\vec{q},\omega,T)$-dependent susceptibility in the QC region can be obtained simply by finite-size scaling: ξ_T acts as a finite size in the imaginary-time direction for the quantum system at its critical point [4,6] and hence implies the scaling form

$$\chi(\vec{q},\omega) = \frac{a_1}{T^{(2-\eta)/z}} \Phi\left(\frac{a_2|\vec{q}-\vec{Q}|}{T^{1/z}}, \frac{\hbar\omega}{k_B T}\right), \tag{2}$$

where a_1, a_2 are nonuniversal constants, and Φ is a universal, complex function of both arguments. The deviations from quantum criticality lead to an additional dependence of Φ on ξ_T/ξ: This number is small in the QC region and has been set to 0. Also of experimental interest is the local dynamic susceptibility $\chi_L(\omega) = \int d\vec{q}\,\chi(\vec{q},\omega) \equiv \chi_L' + i\chi_L''$, with real (imaginary) part χ_L' (χ_L'') [note $d\vec{q} \equiv d^2q/4\pi^2$]. As $\chi' \sim |\vec{q}-\vec{Q}|^{-2+\eta}$ for $|\vec{q}-\vec{Q}| \gg \omega^{1/z}, T^{1/z}$, the real part of the $\vec{q}$ integral is dominated by its singular piece only if $\eta<0$. However, χ_L'' will involve only on-shell excitations, and the imaginary part of the $\vec{q}$ integral is expected to be convergent in the ultraviolet for both signs of η. Thus the leading part of χ_L'' will always obey the scaling form

$$\chi_L''(\omega) = a_3|\omega|^{\mu} F(\hbar\omega/k_B T), \tag{3}$$

with

$$\mu = \eta/z, \tag{4}$$

$F(y) = y^{-\mu} \int d\vec{x}\,\mathrm{Im}\Phi(\vec{x},y)$ a universal function, and a_3 a nonuniversal number. χ_L' also has a part obeying an identical scaling form which is dominant only if $\eta<0$. As we expect $\chi_L'' \sim \omega$ for small ω, we have the limiting forms

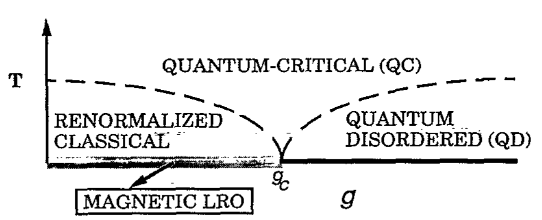

FIG. 1. Phase diagram of $\mathcal{H}$ (after Ref. [4]). The magnetic LRO can be either spin-glass or Néel type, and is present only at $T=0$. The boundaries of the QC region are $T \sim |g-g_c|^{z\nu}$. For nonrandom $\mathcal{H}$ which have commensurate, collinear, Néel LRO for $g<g_c$, all of the QD region ($g>g_c$) has spin-Peierls order at $T=0$—this order extends to part of the QD region at finite T.

$F \sim \mathrm{sgn}(y)|y|^{1-\mu}$ for $y \ll 1$ and $F \sim \mathrm{sgn}(y)$ for $y \gg 1$. Note that all the nonuniversal energy scales only appear in the prefactor a_3 and the frequency scale in F is determined solely by T.

Now we consider the other case (B)—the transition from spin-glass LRO to a QD phase. We do not expect singular behavior as a function of $\vec{q}$ because the spin-condensate $\mathbf{m}_i$ is a random function of i; therefore the scaling form (2) will *not* be obeyed. However, the local susceptibility $\chi_L(\omega_n) \equiv \int_0^{1/k_BT} d\tau\, e^{i\omega_n\tau} C(\tau)$, $C(\tau) = \langle\overline{\mathbf{S}_i(0)\cdot\mathbf{S}_i(\tau)}\rangle$ [where ω_n (τ) is a Matsubara frequency (time) and the bar represents average over sites i], will be quite sensitive to spin-glass LRO. In the spin-glass phase at $T=0$, $\lim_{\tau\to\infty} C(\tau) = \overline{\mathbf{m}_i^2} > 0$ [9]. In the QD phase, numerical studies of random, spin-$\frac{1}{2}$ AFMs [10] suggest that at $T=0$, $C(\tau) \sim 1/\tau^{1-\alpha}$, $\alpha>0$, for large τ. At the critical point $g=g_c$ and $T=0$, we therefore expect the intermediate scaling behavior with $C(\tau) \sim 1/\tau^{1+\mu}$, $\chi_L' \sim \chi_L'' \sim |\omega|^{\mu}$, and $-1<\mu<0$. In the QC region the scaling form (3) for χ_L continues to be valid, despite the inapplicability of (2). The limiting forms for F are as in (A), although the value μ is different: The Edwards-Anderson order parameter obeys $\overline{\mathbf{m}_i^2} \sim |g-g_c|^{\beta}$ for $g<g_c$; connecting the form of χ_L in the spin-glass phase to the critical point, we get

$$\mu = -1 + \beta/z\nu. \tag{5}$$

We now consider various model systems for which exponents and/or scaling functions have to be computed.

We consider first a transition from Néel LRO to a QD phase in a nonrandom spin-$\frac{1}{2}$ square lattice AFM with, e.g., first- (J_1) and second- (J_2) neighbor interactions [11,12]. As has been discussed in great detail elsewhere [12], spin-Peierls order appears in the QD phase in this case (and in all other nonrandom AFMs with commensurate, collinear, Néel LRO). We now argue that the two-spin, QC dynamic scaling functions are not sensitive to the spin-Peierls fluctuations, and one may use an effective action for only the Néel order. It was found in the large-M calculations for SU(M) AFMs that the asymptotic decay of the spin-Peierls correlations is governed by a scale ξ_{SP}, which is much larger (for M large) than the scale ξ governing the decay of the Néel order [12,13]. The two scales are related by $\xi_{\mathrm{SP}} = \xi^{4M\rho_1}$, where ρ_1 is a critical exponent given by $\rho_1 = 0.062296$ to leading order in $1/M$ [13]. Fisher [14] has noted that this is reminiscent of three-dimensional statistical models with a "dangerously irrelevant" perturbation; e.g., the $d=3$ classical XY model with a cubic anisotropy [15] has a phase transition in the pure XY class, but the "irrelevant" cubic anisotropy becomes important in the low-T phase at distances larger than ξ_{XY}^{ψ} ($\psi>1$). By analogy, we may conclude that the spin-Peierls fluctuations are irrelevant at the critical fixed point governing the quantum phase transition, and relevant only at the strong-coupling fixed point which governs the nature of the QD phase.

It has been argued in Ref. [4] that the dynamics of the Néel order parameter is well described by an O(3) nonlinear sigma (NLσ) model in the renormalized classical region (Fig. 1). The gist of the above arguments is that this mapping continues to be valid in the QC region—but not any further into the QD phase. We have computed properties of the QC region by a $1/N$ expansion on a O(N) NLσ model:

$$S_{\hat{n}}=\frac{1}{2g}\int d\tau\, d^2r\left[(\nabla\hat{n})^2+\frac{1}{c^2}\left(\frac{\partial\hat{n}}{\partial\tau}\right)^2\right],\quad \hat{n}^2=1\,, \tag{6}$$

where $\hat{n}$ is a real N-component spin field, and c is a spin-wave velocity. The saddle-point equations of the large-N expansion [16] were solved and the correlation functions were shown to satisfy the scaling forms (2),(3) to order $1/N$ (two-loop level). We determined the values of $\Phi(x,y)$ for real frequencies y by analytically continuing the Feynman graphs and subsequently numerically evaluating the integrals. The numerical computations required the equivalent of 40 h of vectorized supercomputer time.

Our results for ImΦ and F for $N=3$ are summarized in Figs. 2 and 3. The transition has the exponent $z=1$ which fixes the constant $a_2=\hbar c/k_B$ in Eq. (2). We normalized $\Phi(x,y)$ such that $\partial\Phi^{-1}/\partial x^2|_{0,0}=1$. Analytic forms for Φ can be obtained in various regimes. We have

$$\mathrm{Re}\Phi^{-1}=C_Q^{-2}+x^2+\cdots,\quad x,y\text{ small}. \tag{7}$$

The universal number C_Q, to order $1/N$, is

$$C_Q^{-1}=\Theta(1+0.22/N),\quad \Theta=2\ln[(1+\sqrt{5})/2]\,. \tag{8}$$

ImΦ has a singular behavior for x,y small: $\mathrm{Im}\Phi(x=0,y)\sim\exp(-3\Theta^2/2|y|)/N$ while $\mathrm{Im}\Phi(y<x)\sim y\times\exp(-3\Theta^2/2|x|)/N$. With either x or y large, Φ has the form

$$\Phi=D_Q(x^2-y^2)^{-1+\eta/2}+\cdots,\qquad D_Q=1-0.3426/N\,. \tag{9}$$

The exponents μ,η have the known [17] expansion $\mu=\eta=8/(3\pi^2N)-512/(27\pi^4N^2)>0$. The scaling function for the local susceptibility, $F(y)$, has the limiting forms

$$F(y)=\begin{cases}\mathrm{sgn}(y)\dfrac{0.06}{N}|y|^{1-\eta}, & y\ll 1,\\[2ex] \mathrm{sgn}(y)\dfrac{D_Q}{4}\dfrac{\sin(\pi\eta/2)}{\pi\eta/2}, & y\gg 1.\end{cases} \tag{10}$$

As η is small, F is almost linear at small y. At $N=\infty$, $F=\mathrm{sgn}(y)\theta(|y|-\Theta)/4$.

We now study $\mathcal{H}$ with quenched randomness. The simplest model adds a small fluctuation in the J_1 bonds of the J_1-J_2 model above; i.e., $J_1\to J_1+\delta J_1$ where δJ_1 is random, with rms variance $\ll J_1$, ensuring that a Néel-LRO to QD transition will continue to occur. However, the transition will not be described by the "pure" fixed point as $\nu_{\mathrm{pure}}=0.705\pm0.005$ [18] and thus violates the bound $\nu>2/d=1$ required of phase transitions in random systems [19]. At long wavelengths we expect the spin fluctuations to be described by the NLσ model, $S_{\hat{n}}$ [Eq.(6)], with random, space-dependent, but time-independent, couplings g,c. A soft-spin version of $S_{\hat{n}}$ with random couplings in $d=4-\epsilon-\epsilon_\tau$ space dimensions and ϵ_τ time dimensions has been examined in a double expansion in ϵ,ϵ_τ [20]. The expansion is poorly behaved, and for the case of interest here ($N=3$, $\epsilon=1$, $\epsilon_\tau=1$) the random fixed point has the exponent estimates $\eta=-0.17$, $z=1.21$, $\nu=0.64$, $\mu=-0.15$. Note that (i) μ,η are negative, unlike the pure fixed point, and (ii) ν is smaller than $2/d$, suggesting large higher-order corrections.

Consider next a $\mathcal{H}$ on the square lattice with only J_1

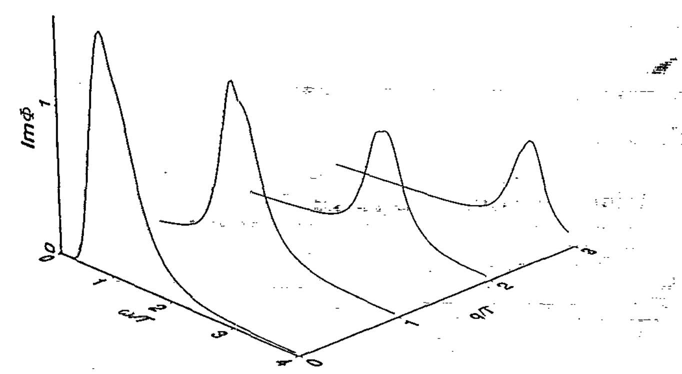

FIG. 2. The imaginary part of the universal susceptibility in the QC region, Φ, as a function of $x=\hbar cq/k_BT$ and $y=\hbar\omega/k_BT$ for a nonrandom square lattice AFM which undergoes a $T=0$ transition from Néel-LRO to a QD phase. The results have been computed in a $1/N$ expansion to order $1/N$ and evaluated for $N=3$. The two-loop diagrams were analytically continued to real frequencies and the integrals then evaluated numerically. The shoulder on the peaks is due to a threshold towards three-spin-wave decay.

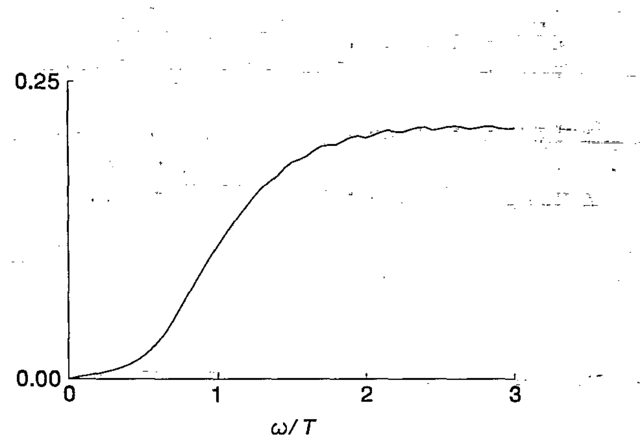

FIG. 3. The imaginary part of the universal local susceptibility, F, for the same model as in Fig. 2. We have $F(y)=y^{-\mu}\int d\bar{x}\,\mathrm{Im}\Phi(\bar{x},y)$. The oscillations at large y are due to a finite step size in the momentum integrations.

couplings, but with a small concentration of static, spinless holes on the vertices; this model will display a Néel-LRO to QD transition at a critical concentration of holes. In the coherent-state path-integral formulation of the pure model, each spin contributes a Berry phase which is almost completely canceled in the continuum limit between the contributions of the two sublattices [21]. The model with holes will have large regions with unequal numbers of spins on the two sublattices: Such regions will contribute a Berry phase which will almost certainly be relevant at long distances. Therefore the field theory of Ref. [20] is not expected to describe the Néel-LRO to QD transition in this case. A cluster expansion in the concentration of *spins* has recently been carried out by Wan, Harris, and Adler [22], and yields the exponents $\eta=-0.6$, $z=1.7$, $\nu=0.8$, $\mu=-0.35$. Note again that $\mu,\eta<0$, although the violation of $\nu>2/d$ suggests problems with the series extrapolations.

Finally, we have also considered [8] the consequences of mobile holes in a nonrandom AFM. The spin waves and holes were described by the Shraiman-Siggia [23] field theory. Integrating out the fermionic holes led to a spin-wave self-energy $\Sigma_{\hat{n}} \sim a_1|\vec{q}-\vec{Q}|^2+a_2\omega_n^2+\cdots$, ($a_1,a_2$ constants) at $g=g_c$, $T=0$; nonanalytic $|\omega_n|$ terms appear only with higher powers of $|\vec{q}-\vec{Q}|,\omega_n$ indicating that the Néel-LRO to QD transition has the same leading critical behavior as that in the undoped, nonrandom J_1-J_2 model above. The exponents and scaling functions are identical, but the corrections to scaling are different.

To conclude, we discuss implications for neutron scattering experiments in the doped cuprates [1,2]. The significant low-T region with a T-independent width of the spin structure factor indicates that the experiments can only be in the QC region (Fig. 1) of a $T=0$ transition from spin-glass LRO to QD: The diverging spin-glass correlation length will then not be apparent in the two-spin correlations. The numerical results of Ref. [7] also indicate that, in the absence of a coupling between the planes, a spin-glass phase will appear at any nonzero doping. The experimental χ_L'' has been fitted with a form $I(|\omega|)F(\hbar\omega/k_BT)$ [1] which is compatible with the theoretical QC result (3) if $I\sim|\omega|^\mu$. A fit with this form for I in $La_{1.96}Sr_{0.04}CuO_4$ yielded $\mu=-0.41\pm0.05$ with all the predicted points within the experimental error bars [24]. As it appears that only random models have $\mu<0$, it is clear that the effects of randomness are experimentally crucial, confirming the theoretical prediction of their relevance. Further theoretical work on the QC dynamics of random quantum spin models is clearly called for.

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