Quantum Critical Scaling in a Moderately Doped Antiferromagnet

Alexander Sokol
Department of Physics and Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801-3080
and L.D. Landau Institute, Moscow, Russia

Rodney L. Glenister and Rajiv R. P. Singh
Department of Physics, University of California, Davis, California 95616
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Using high temperature expansions for the equal time correlator $S(q)$ and static susceptibility $\chi(q)$ for the t-J model, we present evidence for quantum critical (QC), $z=1$, behavior at intermediate temperatures in a broad range of t/J ratio, doping, and temperatures. We find that the dynamical susceptibility is very close to the universal scaling function computable for the asymptotic QC regime, and that the dominant energy scale is temperature. Our results are in excellent agreement with measurements of the spin-echo decay rate, $1/T_{2G}$, in La_2CuO_4, and provide qualitative understanding of both $1/T_1$ and $1/T_{2G}$ nuclear relaxation rates in doped cuprates.

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Recent interest in the doped antiferromagnets is related to the problem of high temperature superconductivity. While the magnetic behavior of the parent insulating compound, La_2CuO_4, can be described in terms of the $S=1/2$ Heisenberg model with the dominant interaction being the in-plane nearest-neighbor exchange coupling $J\simeq 1500$ K, current understanding of the doped materials is far from complete. The consensus on the details of the microscopic model which would quantitatively describe the magnetic properties over the entire doping range from the insulator to the fully doped compounds has yet to be reached.

Recently, significant progress has been made in understanding the low energy spin dynamics of these systems from a scaling and renormalization group point of view. As shown by Chakravarty, Halperin, and Nelson [1], the spin dynamics of an insulator, such as La_2CuO_4, is well described by the quantum nonlinear sigma (QNLσ) model. In the case when the average sublattice magnetization is present at $T=0$, the low temperature renormalized classical (RC) phase is characterized by an exponentially increasing antiferromagnetic correlation length, $\xi/a\sim\exp(2\pi\rho_s/T)$, where a is the lattice constant and ρ_s spin stiffness (below we assume the units where $\hbar=k_B=a=1$). Beyond the critical point, i.e., when the ground state does not possess Néel order, the quantum disordered (QD) phase has a finite ξ at $T=0$.

Another aspect of the phase diagram of Ref. [1], which did not attract much attention until the recent work of Sachdev and Ye [2], and Chubukov and Sachdev [3], is the quantum critical (QC) region, where in the leading order $\xi\sim 1/T$ [1]. Only at the critical point, i.e., at the boundary between the zero temperature Néel and disordered phases, QC behavior holds down to $T=0$. In this case ρ_s vanishes so that the model does not possess any energy scale, which thus is set by the temperature. For doped antiferromagnets, the possibility of $z=1$ criticality has been first pointed out in Ref. [2].

Although for small temperatures a fine tuning of the model parameters to the critical point is necessary to have the QC phase with $\xi\sim c/T$, the range of parameters where it exists rapidly widens as the temperature increases (c is the spin wave velocity). While in the continuum QNLσ model the quantum critical behavior persists for arbitrarily high temperature, on the lattice the range of its applicability is necessarily limited from above, i.e., quantum critical regime is intermediate between low and high temperatures. It has been argued in Ref. [3] that the region of its applicability in the 2D $S=1/2$ Heisenberg model exists around $T\sim 0.5J$ and that small doping should lead to a decrease in ρ_s, thus extending the temperature range of QC behavior.

Recently, it has been shown by Pines and one of us (A.S.) [4], using purely scaling considerations, that the experimental data of [5–8] on the nuclear magnetic relaxation rates $1/T_1$ and $1/T_{2G}$ in the superconducting cuprates imply a QC behavior at high temperatures over an unexpectedly broad doping range. This indicates that the high energy spin waves may survive even substantial doping, which would have important implications for superconductivity.

In view of the above discussion, we present a study of the moderately doped 2D t-J model using the high temperature series expansion approach [9]. We find that the spin dynamics at intermediate temperatures is described by universal scaling functions which agree well with those calculated for the QNLσ model in the quantum critical regime. While the overall prefactors are not in such good quantitative agreement, and appear to be affected by the lattice corrections, we should emphasize that the agreement for the scaling functions and various dimensionless ratios is quite striking.

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The nearest-neighbor version of the t-J model is described by the Hamiltonian

$$\hat{H} = -t\sum_{\langle ij\rangle} P(c_{i\sigma}^{\dagger}c_{j\sigma} + \text{H.c.})P + J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j. \quad (1)$$

(P is the projection operator prohibiting double occupancy.) The 10-term series in $\beta \equiv 1/T$ for the equal time correlation function, $S(\mathbf{q})$, and static susceptibility, $\chi(\mathbf{q})$, has been generated for arbitrary t/J, number of electrons per unit cell $\rho = 1-x$, as well as for arbitrary $\mathbf{q}$. The substitution of the expansion variable $w = \tanh(\beta/\beta_0)$, which eliminates the influence of any singularities outside the stripe $|\text{Im}\beta| < \pi\beta_0/2$, has been applied in order to improve the convergence; several different values of β_0 have been used and the consistency of the approximations have been checked. Although our qualitative results hold for a broad range of t/J ratio, we chose to present our data for one particular value of t/J=1 because the accuracy improves for smaller t/J.

Our first important result is that in a broad range of the doping x, temperature, and t/J ratio, $S(\mathbf{q})$ and $\chi(\mathbf{q})$ near $\mathbf{Q} = (\pi,\pi)$ are well described by the following scaling expressions:

$$S(\mathbf{q}) = S_Q\hat{S}_m(\tilde{q}\xi_m), \quad \chi(\mathbf{q}) = \chi_Q\hat{\chi}_m(\tilde{q}\xi_m'), \quad (2)$$

where $\tilde{\mathbf{q}} = (q_x-\pi, q_y-\pi)$, $\hat{S}_m$ and $\hat{\chi}_m$ are *universal* scaling functions, while S_Q, χ_Q, ξ_m, ξ_m' depend on T, x, and t/J. We define $\hat{S}_m(\kappa)$ and $\hat{\chi}_m(\kappa)$ so that $\hat{S}_m(0) = \hat{\chi}_m(0) = 1$ and $d^2\hat{S}_m/d\kappa^2|_{\kappa=0} = d^2\hat{\chi}_m/d\kappa^2|_{\kappa=0} = -2$. In this case, ξ_m and ξ_m' correspond to the "second moment" definition of the correlation length for $S(\mathbf{q})$ and $\chi(\mathbf{q})$, respectively. Gradual character of deviation from the universal behavior described by Eq. (2) does not allow us to define an unambiguous boundary at which Eq. (2) fails. For t/J=1, the approximate range where the scaling behavior holds well is $T = 0.6J$–J, $x = 0\%-15\%$; more detailed discussion will be given in a subsequent publication [10].

The scaling functions $\hat{S}_m$ and $\hat{\chi}_m$ are computable in the QNLσ model. We observe that the $1/N$ calculation of Ref. [3] indicates negligible $1/N$ corrections to $\hat{\chi}_m$ and $\hat{S}_m$ in the QC regime (note that $1/N$ corrections to the prefactors and ξ are not negligible). Therefore, we can safely use scaling functions calculated for $N=\infty$, which we plot in Fig. 1 along with our data. We find that calculated $\hat{S}_m$ and $\hat{\chi}_m$ are very close to those obtained from the collapsed data for the t-J model (Fig. 1). Further, in the asymptotic QC regime, $1/N$ calculation predicts that $\hat{\chi}_m(\kappa)$ is nearly Lorentzian, while $\hat{S}_m(\kappa)$ is larger than Lorentzian for any given κ. On the other hand, in the asymptotic RC regime, $\hat{S}_m(\kappa)$ and $\hat{\chi}_m(\kappa)$ coincide and both are nearly Lorentzian. We therefore conclude that the scaling functions of Eq. (2) indicate quantum critical behavior in the t-J model at moderate temperatures.

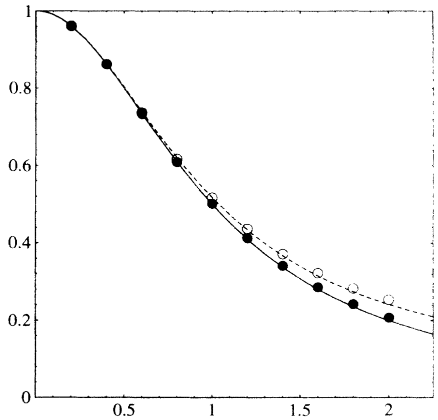

FIG. 1. Universal scaling functions $\hat{\chi}(\kappa)$ (● and solid line) and $\hat{S}(\kappa)$ (○ and dashed line). Symbols are obtained by collapsing our numerical data for the t-J model. Lines show analytical predictions for the $O(N)$ QNLσ model; results of Ref. [3] indicate that there is virtually no dependence on N for $N \geq 3$. Note that the lines are universal scaling predictions rather than fits.

We now turn to the dynamical properties. Since

$$S(\mathbf{q}) = T\frac{1}{\pi}\int d\omega\, g(\omega/T)\,\frac{\chi''(\mathbf{q},\omega)}{\omega},$$
$$\chi(\mathbf{q}) = \frac{1}{\pi}\int d\omega\,\frac{\chi''(\mathbf{q},\omega)}{\omega}, \quad (3)$$

where $g(\zeta) = \frac{1}{2}\zeta/\tanh\left(\frac{1}{2}\zeta\right)$, the ratio $S(\mathbf{q})/T\chi(\mathbf{q})$ reflects the frequency distribution of the spectral weight at $\mathbf{q}$. We find that for zero doping this ratio at $\mathbf{q} = (\pi,\pi)$ varies less than 1% in the range $T = 0.6J$–J and is in excellent agreement with the $O(N)$ sigma model calculation of Ref. [3]:

$$\frac{S_Q}{T\chi_Q} \simeq \begin{cases} 1.10 \pm 0.02 \text{ (Heisenberg model)}, \\ 1.09(N=3) \text{ and } 1.08(N=\infty); \end{cases} \quad (4)$$

in the asymptotic RC regime, this ratio would be equal to unity. In the doped case, the ratio somewhat increases, up to 1.16 for 15% doping at $T = J$. This increase may be caused by a broad electron-hole continuum, which does not significantly modify $\chi''(\mathbf{q},\omega)$ for small frequencies, but can yield significant contribution to the ratio because $g(\zeta)$ is large for $\zeta \gg 1$.

Another universal quantity which may be temperature independent only when $\bar{\omega} \sim T$, i.e., in the case of QC behavior, is $1 - \xi_m/\xi_m'$. For the insulator, this quantity indeed has less than 7% variation in the range $T = 0.6J$–J. The comparison to $O(N)$ calculations of Ref. [3] for the asymptotic QC regime of the QNLσ model yields

$$1 - \frac{\xi_m}{\xi_m'} \simeq \begin{cases} 0.042 \pm 0.003 \text{ (Heisenberg model)}, \\ 0.043(N=3) \text{ and } 0.035(N=\infty). \end{cases} \quad (5)$$

In the doped case, ξ_m/ξ_m' becomes 10% smaller at $T =$

$0.6J$, a decrease that may also be caused by the electron-hole continuum; it remains nearly doping independent at $T = J$.

On the basis of the above arguments, we conclude that the dynamical susceptibility of the t-J model can be written as

$$\chi(\mathbf{q},\omega) = \chi_Q \hat{\chi}\left(\tilde{q}\xi, \frac{\omega}{\bar{\omega}}\right), \tag{6}$$

where to the leading order $\bar{\omega} \sim T$. In addition, in the asymptotic QC regime of the QNLσ model, not only Eq. (6) holds, but it is also expected that $\chi_Q \sim \xi^{2-\eta}$, where the critical exponent η is nearly zero and can be neglected, and $1/\xi \sim T$. We first calculate χ_Q/ξ^2 by generating 9-term series directly for this quantity and find that for $T = 0.6J$–J it varies not more than 16%, compared to far greater (nearly by the factor of 5 in the undoped case) change in χ_Q and ξ^2 separately.

We now turn to the temperature dependence of ξ and evaluate it by generating 9-term series for $\xi T^{1/2}$ and 10-term series for S_Q and $\chi_Q T$. $\xi^{-1}(T,x)$ for $t/J = 1$ is plotted as a function of temperature in Fig. 2. As one can see, in a broad range of doping and temperature ξ^{-1} is nearly linear in T with doping independent slope. As shown by Chakravarty [11], one would expect the temperature dependence to be of the form

$$\frac{1}{\xi} \sim \frac{bT}{c} - C(x)\,T^{1-1/\nu} \tag{7}$$

with the critical exponent $\nu \sim 0.7$. The second term varies slowly as a function of temperature over the interval of comparisons and provides a doping dependent intercept for nearly linear $\xi^{-1}(T)$. We note, however, that the slope of $\xi^{-1}(T)$ determined from the numerical data differs nearly by the factor of 2 from the value calculated using Eq. (7) with $T = 0$ value of c and $b \simeq 0.8 - 1$ determined in Refs. [1,3,12]. We conjecture that the difference is caused by the lattice corrections above $T = 0.6J$. Indeed, ξ for the Heisenberg model is quite close to the value given by Eq. (7) at $T = 0.6J$ [3] and the deviation occurs only at higher temperatures. On the other hand, our data unambiguously show that such corrections do not modify universal scaling functions of Eqs. (2) and (6). Note that were the spin waves absorbed by the electron-hole background in this doping range, $1/\xi^2$ and not $1/\xi$ would be linear in temperature [13,14]. Further, in the t-J model $1/\xi^2$ and not $1/\xi$ is linear in temperature for $T \gg J$. The measurements of Ref. [15] also indicate linear $\xi^{-1}(T,x)$ with nearly doping independent slope.

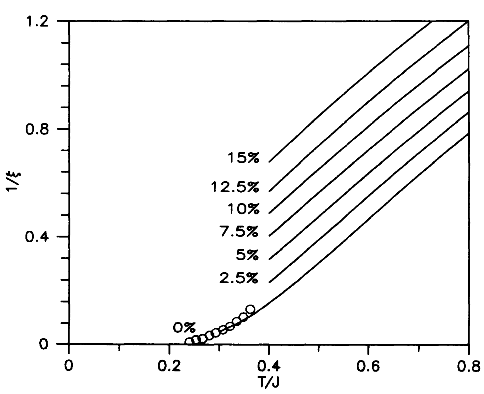

FIG. 2. $\xi^{-1}(T,x)$ for t/J=1 and (o) the experimental data of Ref. [15] for the undoped La_2CuO_4 (we set a=1); our calculation falls within not shown experimental error bars.

Once it is established that the spin dynamics of doped antiferromagnets is described by Eq. (6), we can now address the experimental result of Imai, Slichter, and collaborators [5] that at high temperatures the spin-lattice relaxation rate, $1/T_1$, is nearly doping and temperature independent in the doping range 0%–15%. From Eq. (6) one obtains $1/T_1 \sim \int d\mathbf{q} \lim_{\omega\to 0} \chi''(\mathbf{q},\omega)/\omega \sim \chi_Q/\xi^2$. Indeed, we find that χ_Q/ξ^2 and therefore $1/T_1$ is nearly doping and temperature independent in a broad doping range. Earlier, it has been shown [3] that near the critical point, temperature, and parameter independence of $1/T_1$ follows from the Josephson hyperscaling law; our results show that such arguments are applicable even for substantial doping.

Now we turn to the Gaussian component of the spin-echo decay rate, $1/T_{2G}$, which is given by (after Pennington and Slichter [16])

$$\frac{1}{T_{2G}^2} = \frac{0.69}{8}\sum_{r\neq 0} a_r^2, \quad a_r = -\int \frac{d^2\mathbf{q}}{(2\pi)^2} e^{i\mathbf{q}\cdot\mathbf{r}} F_q^2 \frac{\chi(\mathbf{q})}{g^2\mu_B^2}, \tag{8}$$

where $\chi(\mathbf{q})$ is the static susceptibility and F_q hyperfine form factor. We evaluate this quantity by generating series directly for T/T_{2G} and then using Padé approximants. We take $J = 1500$ K (in the region of experimental comparisons calculated $1/T_{2G}$ is not sensitive to the choice of J) and the values of hyperfine couplings determined for $YBa_2Cu_3O_{6.63}$ in Ref. [17]. The motivation for doing so is that a number of experiments [18] indicate that the hyperfine couplings do not change substantially from La_2CuO_4 to $YBa_2Cu_3O_{6+x}$. Our results for $1/T_{2G}$ are plotted in Fig. 3 along with the experimental data of Imai, Slichter, and collaborators [6] for the insulator. The results are in excellent agreement with the experiments; note that no adjustable parameters are used. We also find good agreement at high temperatures ($T > J/2$) with the 4×4 cluster calculation for $x=0$ [19].

Recently, linear in temperature T_{2G} above 200 K has been reported by Takigawa [8], which is consistent with the QC prediction in the range of comparisons. The slope of the linear high temperature part of the data [8] is larger in $YBa_2Cu_3O_{6.63}$ than in La_2CuO_4; in our study, we indeed find that the slope increases with increasing doping and t/J ratio (Fig. 3, inset).

To summarize, in our high temperature series expansion study we find that spin fluctuations in the t-J model exhibit quantum critical scaling behavior. Particularly,

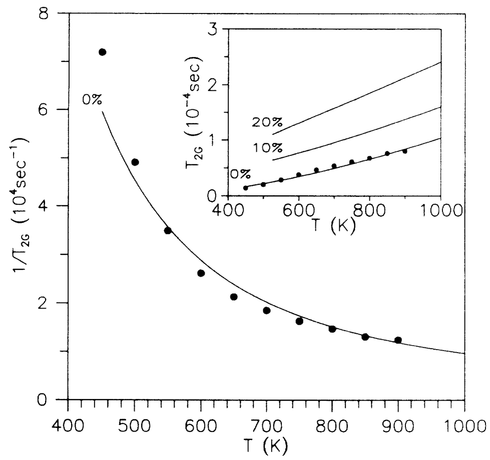

FIG. 3. The spin-echo decay rate $1/T_{2G}(T)$ in the Heisenberg model (i.e., for x=0) calculated without adjustable parameters and (●) the experimental data of Ref. [6] for La_2CuO_4. Inset: $T_{2G}(x,T)$ for t/J=1.

for a broad range of t/J ratio, doping, and temperatures (1) the numerical data for both $S(\mathbf{q})$ and $\chi(\mathbf{q})$ collapse to the universal scaling function computable in the $O(N)$ QNLσ model, (2) the characteristic energy scale for spin fluctuations, $\bar{\omega}$, is proportional to temperature, and (3) $1/\xi$ is nearly linear in temperature. The disagreement of the slope of $1/\xi$ with the prediction based on fully renormalized $T = 0$ value of c is likely to be caused by the lattice corrections above $T = 0.6J$. One may speculate that the absence of such corrections to the scaling functions of Eqs. (2) and (6) is related to the fact that in the QNLσ model they are much less dependent on the cutoff and N (for a relevant discussion see Ref. [20]). Our results are consistent with the conclusion of Refs. [2,3] that in the Shraiman-Siggia model [21] the presence of fermions does not alter the universality class of the $z=1$ critical point separating phases with Néel and short range order. While the t-J model might not be quantitatively applicable for the doped cuprates, we believe that a broad region of the quantum critical behavior is a general feature of moderately doped antiferromagnets.

In the second part of our study, we calculated the spin-echo decay rate, $1/T_{2G}$, recently measured in a number of the high T_c compounds. Our results for $x=0$ (i.e., in the Heisenberg model), obtained with no adjustable parameters are in excellent agreement with the experiments in La_2CuO_4 [5,6] and show that the hyperfine couplings do not vary substantially from $YBa_2Cu_3O_{6.63}$ to La_2CuO_4. We also find qualitative agreement with the experimental data on $1/T_{2G}$ in $YBa_2Cu_3O_{6.63}$ [8] and show that for moderate doping, $1/T_1$ is nearly doping and temperature independent, in agreement with both the experimental data in $La_{2-x}Sr_xCuO_4$ [5] and earlier analysis based on the QNLσ model [3].

Our results provide additional support to the conjecture of Ref. [4] that the high temperature quantum critical behavior [1–3] is a common feature shared by many of the cuprate superconductors. More detailed study of this and related subjects will be presented in a subsequent publication [10].

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