The Random Transverse Field Ising Ferromagnet: the Simplest Disordered Model with a Quantum Phase Transition

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Abstract

After an introduction to quantum phase transitions, we study the quantum phase transition in the two-dimensional random Ising model in a transverse field by Monte Carlo simulations. We find results similar to those known analytically in one-dimension: the dynamical exponent is infinite and, at the critical point, the typical correlation function decays with a stretched exponential dependence on distance. Away from the critical point, there may be different exponents for the divergence of the average and typical correlation lengths, again as in one-dimension, but the evidence for this is less strong.

I. INTRODUCTION TO QUANTUM PHASE TRANSITIONS

Most studies of critical phenomena investigate *classical* phase transitions, i.e. those which occur at finite temperature, where one passes through the system by changing the temperature itself. By now, classical transitions are very well understood. *Quantum* transitions, by contrast, occur at $T = 0$, and one tunes through the transition by changing some parameter in the Hamiltonian. Our understanding of quantum transition is relatively poor, at least for systems with quenched disorder. There is, however, considerable interest in these systems since, as we shall see, they (i) exhibit new universality classes, and (ii) display "Griffiths-McCoy"[1,2] singularities even away from the critical point, due to rare regions with stronger than average interactions.

We start by discussing two examples of quantum phase transitions. The quantum phase transition that has been studied *for the longest time* is the metal-insulator transition in a disordered metal[3]. For sufficiently strong disorder, the metal is an insulator at zero temperature because all states are localized, while for weak disorder there are extended states so the system can conduct even at zero temperature. Theoretically,[3] there has been a lot progress, both analytically and numerically, on a model with no electron-electron interactions. Among the results are reasonably precise estimates for exponents at the metal-insulator transition in three-dimensions, and the prediction that all electron states are localized by even an infinitesimal amount of disorder in two dimensions. However, almost nothing is known theoretically about the metal insulator transition if one includes interactions.[4] In particular, since the Coulomb interaction is long range, it may well change the universality class. Experimentally,[5] there has never been a consensus as to the values of the exponents, with different groups claiming quite different values. Difficulties in determining exponents include the need to extrapolate the data to zero temperature, and uncertainties as to the size of the critical region. Furthermore, there have been recent strong claims for a metal-insulator transition in *two-dimensions*.[6] If confirmed this would

indicate that not only can Coulomb interactions change the critical behavior at transitions *between phases*, but also the *nature of the allowed phases* themselves.

Recently, the quantum phase transitions which have *been studied in the greatest detail* are those between quantum Hall "plateau" states[7] in two-dimensional layers of electrons in semiconducting heterostructures in a magnetic field. Developments in fabrication of semiconductors have permitted great control over, for example, the amount of disorder, which has opened the door to precise experiments. Some experiments[8] have indicated a diverging correlation length exponent ν of about 7/3, in agreement with numerical calculations,[9] which, again, neglect electron interactions. However, the the role of interactions is unclear and, furthermore, some recent experiments[10] have cast the whole idea that the "transitions" between plateaus are quantum phase transitions by claiming that the width of the transition region does not extrapolate to zero in the limit of zero temperature.

The above two examples indicate that our knowledge of quantum phase transitions with disorder is very poor compared with, for example, our understanding of classical phase transitions at a finite temperature. Even with disorder, the latter are rather well understood. Theoretically, one of the great successes in classical phase transitions has been the perturbative renormalization group (ϵ-expansion). The main reason for our poor understanding of quantum phase transitions with disorder is that this technique does not seem to apply. Rather the renormalization group trajectories generally flow to strong coupling in the presence of disorder[11]. Hence numerical simulations seem to be the most promising way of getting quantitative information about quantum phase transitions with disorder. Because the problem is very difficult, in this paper we will confine our attention to one system, the simplest random system with a quantum phase transition, the Ising model in a transverse field.

II. THE MODEL

Since quantum phase transitions with disorder are poorly understood, it is desirable to study the simplest (random) model with a quantum phase transition, with the hope that one might be able to find an exact solution in some cases. Furthermore, such a model may be especially suitable for numerical simulations.

For classical transitions, the simplest model is the Ising model. Much has been learned from Onsager's exact solution in two dimensions and from Monte Carlo simulations (as well as other techniques) in three dimensions. Furthermore, we now know that the critical behavior of the Ising model applies to all systems in the Ising universality class, even though the *microscopic* Hamiltonians may be very different. Hence the results are of rather wide generality.

We argue that the corresponding simple model for quantum transitions is the spin-1/2 Ising model in a transverse field. The Hamiltonian is given by

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij}\sigma_i^z\sigma_j^z - \sum_i h_i\sigma_i^x \ , \tag{1}$$

where the $\{\sigma_i^\alpha\}$ are Pauli spin matrices, and the nearest neighbor interactions J_{ij} and

transverse fields h_i are both independent random variables. In this talk we shall confine our attention to this system.

There is at least one experimental system[12] which seems to correspond to this model, $LiHo_xY_{1-x}F_4$. The magnetic ion is Ho^{3+}, which has its electronic levels split by crystal fields such that the lowest level is a doublet within which only a single component (z) of angular momentum has non-zero matrix elements. Thus, confining our attention to the lowest level, the system is an Ising model. Furthermore, a field transverse to the z-direction splits the doublet in the same way as the transverse field splits the $\sigma^z = \pm 1$ states in the transverse Ising model, and a sufficiently large field can be applied to depress T_c to zero. The interactions are long range dipole-dipole and, depending on the concentration x, the system can either be a spin glass or a random ferromagnet. Unfortunately, even for the ferromagnetic samples, the frustrating effects of the dipole-dipole interactions seems to be rather large, and very slow, glassy relaxation has been observed[13] which has so far obscured the physics that we will discuss here.

In addition, recently it has been proposed[14] that the non Fermi liquid behavior observed in a number of f-electron compounds[15] may be due to Griffiths-McCoy singularities (to be discussed below), and, furthermore, it is suggested that an appropriate model to describe these singularities is the random Ising model in a transverse field that we study here.

As discussed in more detail in the next section, analytical results have been obtained[16] in one dimension and surprising results obtained. The goal of our own work, to be discussed in the subsequent sections, is to investigate the model in two dimensions by Monte Carlo simulations, to see if the surprising results found in 1-d also apply in higher dimensions.

III. ANALYTICAL RESULTS

An important feature of the random transverse Ising model is that exact *analytical* results are available[16–18,2] for the case of the *one-dimensional chain*. These results turn out to be very different from what one finds for classical transitions. Among the surprising predictions[16] for the critical behavior in 1-d are:

1. The dynamic critical exponent, z, is infinite. Instead of a characteristic time scale ξ_τ varying as a power of a characteristic length scale ξ according to $\xi_\tau \sim \xi^z$, one has instead an exponential relation

$$\xi_\tau \sim \exp(\text{const. } \xi^\psi), \tag{2}$$

   where $\psi = 1/2$. This is called *activated* dynamical scaling.

2. Distributions of the equal-time σ^z-σ^z correlations, are very broad. As a result *average* and *typical*[19] correlations behave rather differently, since the average is dominated by a few rare (and hence *atypical*) points. At the critical point, for example, the average correlation function falls off with a power of the distance r as

$$C_{\text{av}}(r) \sim r^{-\lambda}, \tag{3}$$

where $\lambda = (3 - \sqrt{5})/2 \simeq 0.38$, whereas the typical value falls off much faster, as a stretched exponential

$$C_{\rm typ}(r) \sim \exp(-\text{const. } r^{\sigma}), \tag{4}$$

with $\sigma = 1/2$.

3. As one approaches the critical point ($\delta \to 0$) the average and typical correlation *lengths* both diverge but with *different* exponents, i.e. $\xi_{\rm av} \sim \delta^{-\nu_{\rm av}}$; $\xi_{\rm typ} \sim \delta^{-\nu_{\rm typ}}$, where δ, the deviation from criticality, is defined precisely below, and

$$\nu_{\rm av} = 2; \qquad \nu_{\rm typ} = 1. \tag{5}$$

A special feature of one-dimension is that the model can be mapped on to free fermions[20] and so precise numerical studies can be carried out by diagonalization for rather large sizes[21] Figs. 1 and 2 show results[21] obtained by this approach for the correlations at the critical point. The pronounced difference between the average and typical correlation functions is clearly seen, with the typical correlation function falling off much faster than the usual power law.

In addition to novel critical behavior, the one-dimensional random transverse field Ising model also has striking singularities in the paramagnetic phase. These are of the type first discussed by Griffiths[1] for a random classical system, but are much more pronounced in the quantum case. They come from local regions in which the interactions happen to be stronger than average and/or the transverse fields are weaker than average, so that these regions can be viewed as "locally in the ferromagnetic phase", even though the whole sample is paramagnetic. Spins in such regions effectively act as one large spin, as a result of which their dynamics is very slow. A simple phenomenological picture[22], leads to the prediction that the average, on-site, time-dependent correlation function, varies as a power of (imaginary) time, with an exponent, $z(\delta)$, varying continuously with δ, the deviation from the critical point. This general picture has been confirmed by numerics[21,23,24] both in one-dimension and higher dimensions. If $z(\delta)$ is sufficiently large (in practice greater than the space dimension, d) the average local susceptibility will diverge. A surprising feature of one-dimension[16,21] is that $z(\delta) \to \infty$ as $\delta \to 0$, so there will *always* be a region of the paramagnetic phase where the susceptibility diverges. The divergence of the susceptibility in a finite region of the paramagnetic phase was first found many years ago by McCoy[2], and hence Griffiths singularities in quantum systems are often called Griffiths-McCoy singularities.

Here we concentrate on the critical behavior. However, related work of Rieger and Kawashima[25] has focused on Griffiths-McCoy singularities in the paramagnetic phase.

IV. CLUSTER MONTE CARLO

An important question is whether these striking analytical results are a special feature of 1-d, or whether they are valid more generally. Unfortunately, the analytical approach of Fisher[16] (and also the numerical method using free fermions[21]) is only valid in 1-d,

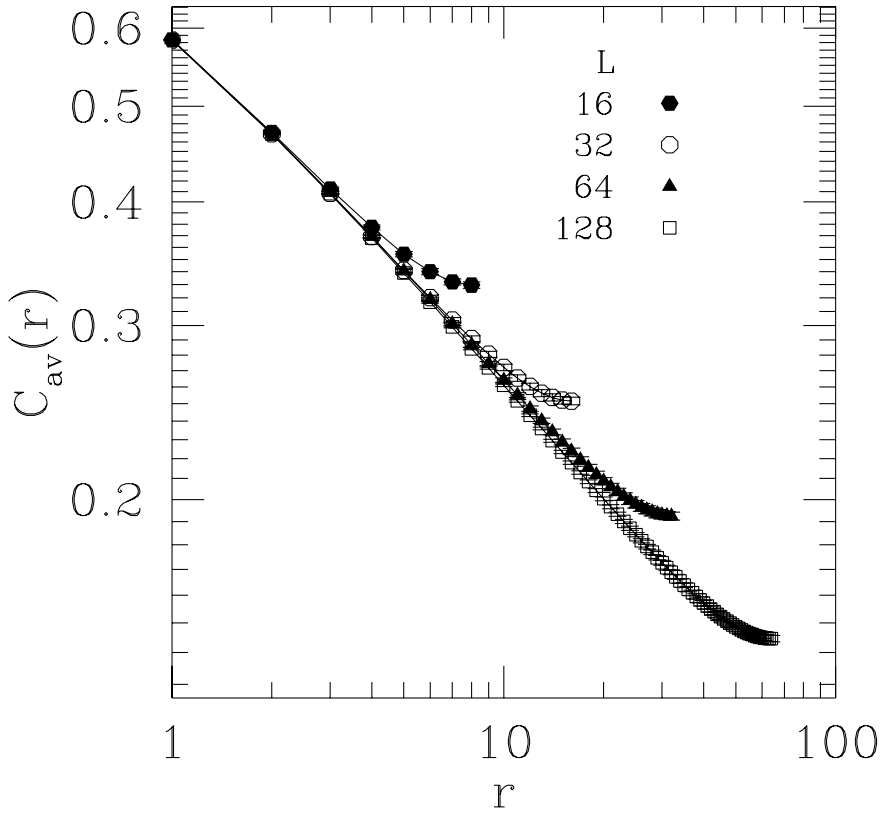

FIG. 1. Data for average correlation function at the critical point in 1-d obtained by the free fermion method[21]. The behavior for large sizes clearly shows power law behavior. A fit[21] gives a power close to the expected value[16] of $-(3-\sqrt{5})/2 \approx -0.38$.

and very little is known about the critical behavior in higher dimensions[26]. Here, we make a first step in investigating this question by performing large-scale Monte Carlo simulations of the random transverse field Ising *ferromagnet* in two dimensions. Because the ferromagnet has no frustration we are able to use highly efficient cluster algorithms[27,28] which considerably reduce critical slowing down. In these algorithms one flips not a single spin but a cluster, chosen in such a way that the typical cluster size turns out to be the size over which spins are correlated. Consequently, we are able to study larger sizes and get much better statistics than in earlier work[24] on quantum *spin glasses*. We use the Wolff[28] algorithm because it is slightly simpler to implement and is also somewhat faster than the Swendsen-Wang[27] algorithm. In the Wolff algorithm, for a given configuration, one just grows a single cluster centered on a randomly chosen site, whereas in the original Swendsen-Wang approach one assigns all sites to clusters.

An additional benefit of the cluster algorithms is that there are "improved estimators"[29] for calculating correlation functions which have much smaller error bars than the conventional method when the mean is very small. If one wants to compute the

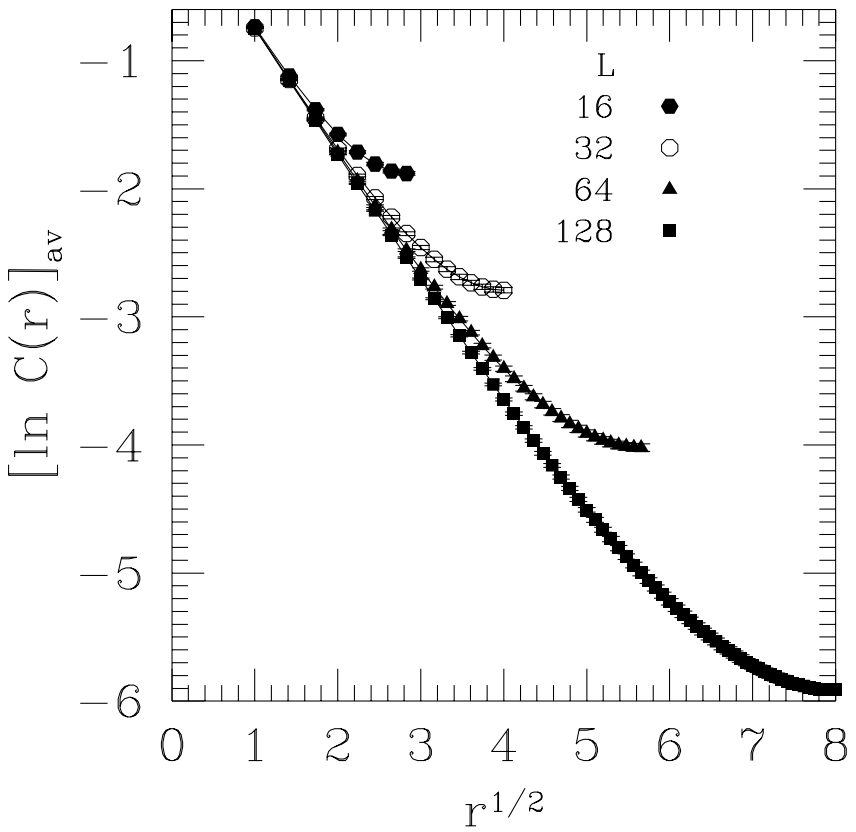

FIG. 2. Data for the average of the log of the correlation function at the critical point in 1-d obtained by the free fermion method[21]. This is a reasonable definition for the log of the typical correlation function. The data clearly fits well the predicted[16] stretched exponential behavior, $[\ln C(r)]_{\rm av} \sim -{\rm const.}r^{1/2}$.

correlation function between spins at sites i and j say, then, conventionally, one generates many configurations and each configuration gives a factor of 1 to the sum if the spins are parallel and -1 if they are anti-parallel. Hence, the variance is close to one if the mean is small. By contrast, in the Swendsen-Wang method, from a spin configuration one constructs clusters and the configuration contributes a factor 1 if sites i and j are in the same cluster and 0 (not -1) if they are in different clusters[29]. Hence the variance is equal to the mean and so the error bars are much reduced compared with the conventional scheme if the mean is small. Roughly speaking, if the mean is ϵ say, then the conventional method requires $1/\epsilon^2$ statistically independent configurations for the error to be comparable to the mean, whereas the improved estimator only requires $1/\epsilon$ configurations. There is also an improved estimator for the Wolff algorithm[29].

The main conclusion from our studies is that the behavior of the 2-d system at the critical point is *very similar* to that of the 1-d case. There are some difficulties in interpreting our data away from the critical point but, nonetheless, here too there is some

evidence for behavior similar to that in 1-d. A preliminary account of these results has appeared elsewhere[30]. In their related work, Rieger and Kawashima[25] studied essentially the same model, concentrating, as mentioned above, on Griffiths-McCoy singularities in the paramagnetic phase. They find that the continuously varying dynamical exponent, $z(\delta)$, tends to infinity as the critical point is approached ($\delta \to 0$), again as in 1-d[16].

V. IMAGINARY TIME FORMALISM

As is standard[31], we represent the d-dimensional quantum Hamiltonian in Eq. (1) by an effective classical "Hamiltonian" in (d+1)-dimensions, where the extra dimension, imaginary time, is of size $\beta \equiv 1/T$ and is divided up into L_τ intervals each of width $\Delta\tau = \beta/L_\tau$. The effective classical Hamiltonian is given by

$$\beta_{cl}\mathcal{H}_{cl} = -\sum_{\langle i,j\rangle,\tau} K_{ij}S_i(\tau)S_j(\tau) - \sum_{i,\tau} \widetilde{K}_i S_i(\tau)S_i(\tau') \tag{6}$$

where, $\tau' = \tau + \Delta\tau$, $S_i(\tau) = \pm 1$, $K_{ij} = \Delta\tau J_{ij}$, $\exp(-2\widetilde{K}_i) = \tanh(\Delta\tau h_i)$, and $\beta_{cl} \equiv 1/T_{cl}$ where T_{cl} is an effective "classical" temperature (not equal to the real temperature which is the inverse of the size in the time direction). Note that the disorder is quenched and so the interactions are independent of τ. Correlations of the classical Ising spins, $S_i(\tau)$, correspond to imaginary time $\sigma_i^z(\tau)$ correlations in the original quantum model. These are the correlations that we are interested in here.

In order to capture the random quantum critical behavior in the intermediate size systems that we can simulate, we wish the disorder to be effectively quite strong. In particular, we would like some of the fields to be *much* stronger than the bonds in their vicinity and vice-versa. This is captured by having distributions for both the fields and interactions with a finite weight at the origin. This is satisfied by a constant distribution for the K_{ij} and a distribution for the $\widetilde{K}_i$ which falls off exponentially at *large* values. Furthermore, the critical behavior does not depend on short distance physics and is hence independent of $\Delta\tau$, so for convenience we will take $\Delta\tau = 1$. It is also possible to study the continuous imaginary time[32] version of the model; this was done in the related work of Rieger and Kawashima[25]. A Hamiltonian which encapsulates these features in a way convenient for simulations is

$$\mathcal{H}_{cl} = -\sum_{\langle i,j\rangle,\tau} J_{ij}S_i(\tau)S_j(\tau) - \sum_{i,\tau} \widetilde{J}_i S_i(\tau)S_i(\tau+1), \tag{7}$$

where τ runs over integer values, $1 \le \tau \le L_\tau$, and the distributions of the interactions are given by

$$\pi(J) = \begin{cases} 1 & \text{for } 0 < J < 1, \\ 0 & \text{otherwise,} \end{cases}$$
$$\rho(\widetilde{J}) = \begin{cases} 2\exp(-2\widetilde{J}) & \text{for } \widetilde{J} \ge 0, \\ 0 & \text{for } \widetilde{J} < 0. \end{cases} \tag{8}$$

Disorder averages are denoted by $[\cdots]_{\rm av}$ and Monte Carlo averages for a single sample are denoted by $\langle\cdots\rangle$. Note that $[J]_{\rm av} = [\widetilde{J}]_{\rm av} = 1/2$, so the *average* interactions are isotropic.

However, the perfect correlation of the disorder in the τ direction leads, as we will see, to very anisotropic behavior. One controls the strength of the fluctuations, and hence tunes through the transition, by varying the classical temperature, T_{cl}.

The size of the system in the space direction denoted by L, so there are $N = L^d L_\tau$ sites in the sample. We studied sizes up to $L = 48$ and $L_\tau = 2048$ using the Wolff[28] cluster algorithm. We found that no more than 100 sweeps were required for equilibration, even for the largest lattices. At least 1000 samples were averaged over.

VI. RESULTS

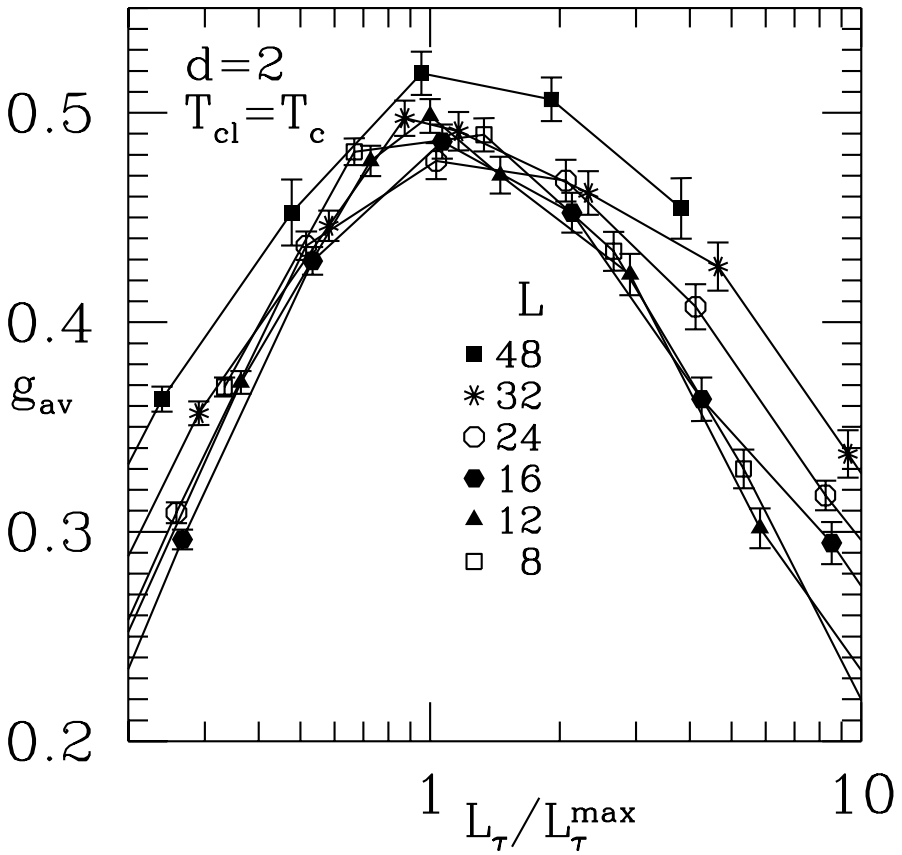

FIG. 3. Data for the Binder ratio, g_{av}, in two dimensions, at the critical point $T_{cl} = T_c^{cl} = 2.45$. This plot would collapse the data if conventional dynamical scaling, with a finite z, were appropriate, see Eq. (11). By contrast, the curves clearly *broaden* for larger L. The data for $L = 48$ is slightly high which may indicate that the true value of T_c is a little higher.

The first task is to locate the critical point, for which we use a method suggested by D. Huse (private communication). One computes the Binder ratio

$$g_{\rm av} = \frac{1}{2}\left[3 - \frac{\langle M^4 \rangle}{\langle M^2 \rangle^2}\right]_{\rm av}, \tag{9}$$

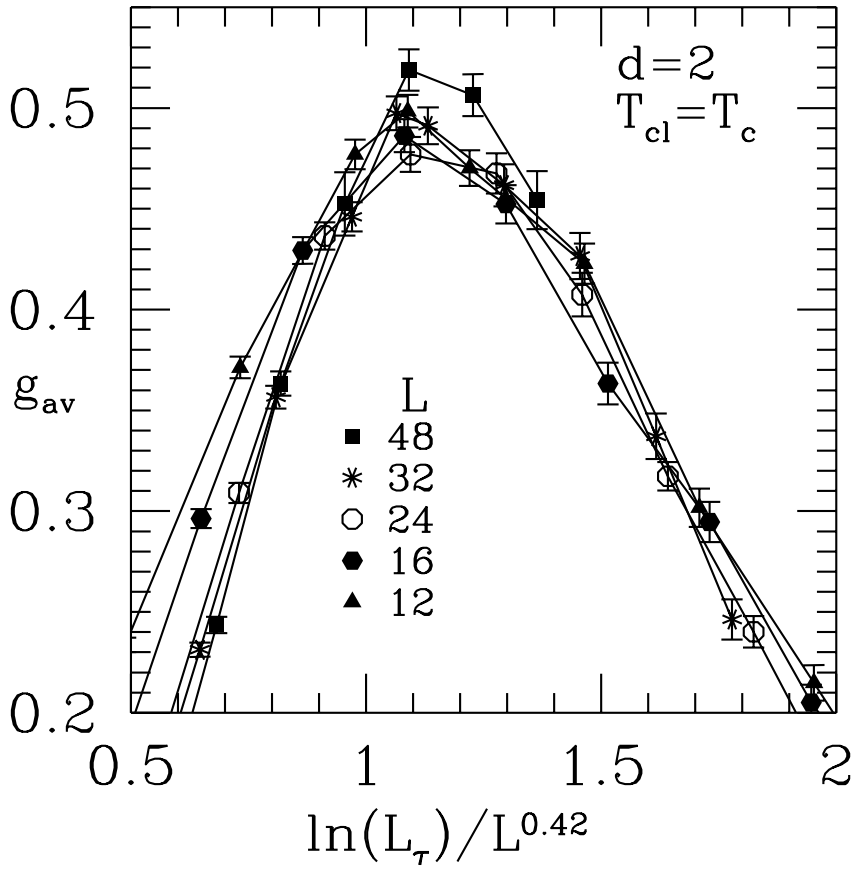

FIG. 4. A scaling plot for the Binder ratio assuming activated dynamical scaling, see Eq. (12), for the data for $L \geq 12$. The scaling is seen to be quite good with the value of $\psi = 0.42$. This works better than the 1-d value of $\psi = 1/2$.

where $M = \sum_{i,\tau} S_i(\tau)$, which (assuming, for now, that z is finite) has the finite-size scaling form

$$g_{\rm av} = \widetilde{g}\left(\delta L^{1/\nu_{\rm av}}, \frac{L_\tau}{L^z}\right). \tag{10}$$

At the critical point, $\delta = 0$, this becomes

$$g_{\rm av} = \widetilde{\widetilde{g}}\left(\frac{L_\tau}{L_\tau^{max}}\right) \quad (\delta = 0), \tag{11}$$

with $L_\tau^{max} \sim L^z$. For fixed L, $g_{\rm av}$ has a peak as a function of L_τ. At the critical point[33], T_c^{cl}, the peak height is independent of L and the values of L_τ at the maximum, $L_\tau^{\rm max}$, vary as L^z. Furthermore, from Eq. (11), a plot of $g_{\rm av}$ against $L_\tau/L_\tau^{\rm max}$ at the critical point, should collapse the data. This plot has the advantage of not needing a value for z.

We see in Fig. 3 that this does *not* happen in 2-d, and neither does it happen in 1-d[30]. Rather the curves clearly become broader for larger sizes. This is easy to understand since we know that for 1-d z is infinite and it is the *log* of the characteristic time which scales with a power of the length scale. This suggests that the scaling variable should be $\ln L_\tau / \ln L_\tau^{\rm max}$ with $\ln L_\tau^{\rm max} \sim L^\psi$, say, or, in other words, at criticality,

$$g_{\rm av} = \widetilde{\widetilde{g}}\left(\frac{\ln L_\tau}{\ln L_\tau^{max}}\right) \quad (\delta = 0). \tag{12}$$

In 2-d, the data collapse for sizes $L \geq 12$, shown in Fig. 4, is quite good for $\psi = 0.42$, and not quite so good with the 1-d value, $\psi = 1/2$, though we would not claim that $\psi = 1/2$ is ruled out. The small L_τ region in Fig. 4 corresponds to high temperature, and hence is likely not to be in the scaling region. Consequently, the observed lack of scaling in this region is not surprising. The broadening of the data in Fig. 3, and the reasonably good fit in Fig. 4 suggests that z is infinite in 2-d as well as in 1-d[16].

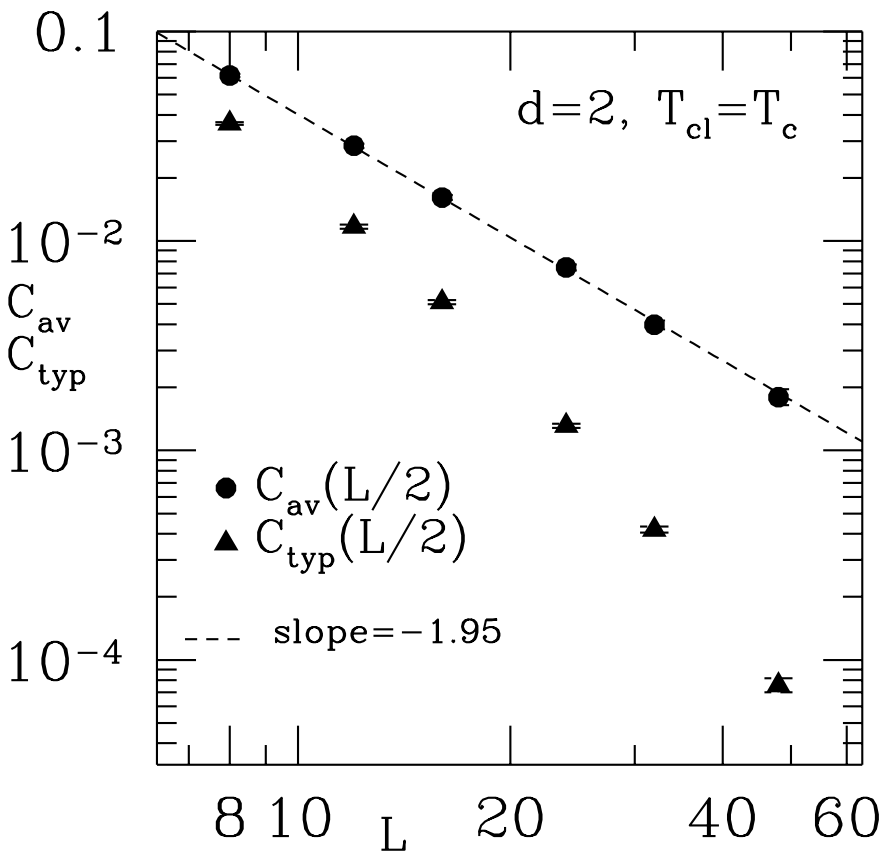

FIG. 5. A plot of the average and typical correlation functions at the critical point in two dimensions. The average falls off with a power law and a fit gives a slope of $-\lambda$ with $\lambda = 1.95$. The curvature in the data for the typical value shows that it falls off *faster* than a power law.

Next we consider the behavior of the equal time correlations at the critical point using the improved estimator[29]. Fig. 5 shows data for the average and typical[19] correlations for spins separated by $\vec{r} = (L/2, 0)$. For each value of L, we took L_τ such that $g_{\rm av}$ is close to the peak[34], see Fig. 3. According to finite size scaling, the dependence on L for a finite system should be the same as the dependence on r in a bulk system. The data in Fig. 5 shows that the average falls off with a power law, with λ about 1.95, while the typical value falls off faster than a power law, (because of the downward *curvature*). The statistical errors (shown) are generally smaller than the size of the points, so the downward

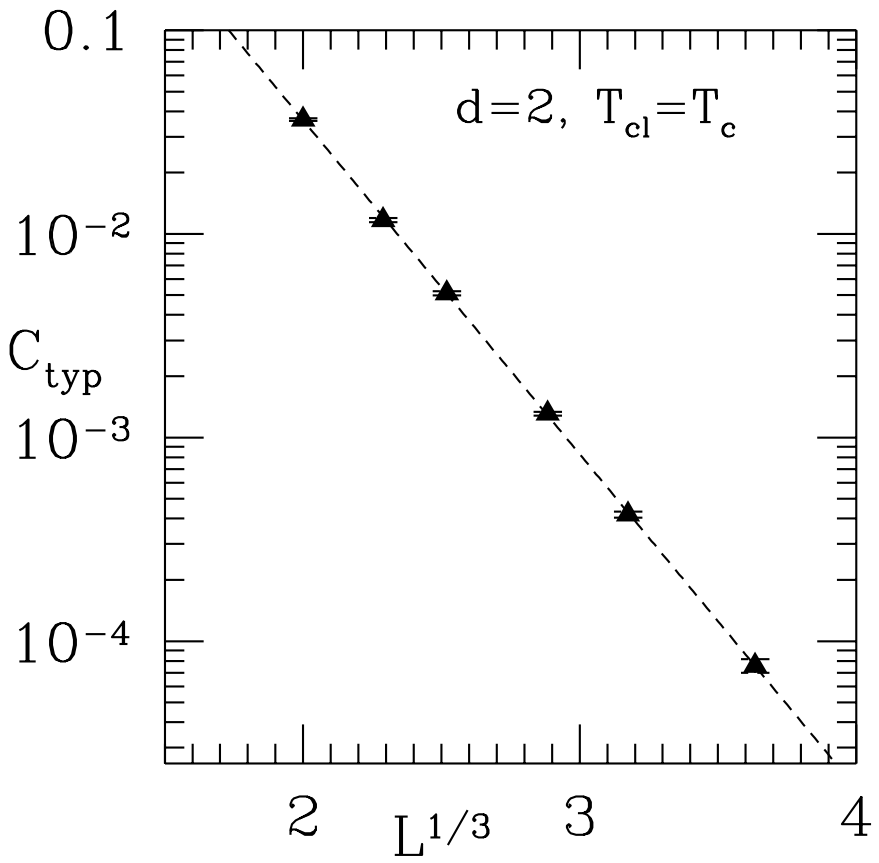

FIG. 6. A plot of the typical correlation function at the critical point in two dimensions. The data is consistent with a stretched exponential form, $\exp(-\text{const. } L^{\sigma})$, but with $\sigma = 1/3$ rather than the value of 1/2 found in 1-d.

curvature is statistically significant. Fig. 6 shows that the data for the typical correlation function is consistent with a stretched exponential behavior of the form $\exp(-\text{const. } L^{\sigma})$, with $\sigma \simeq 1/3$. The value of σ seems to be different from the 1-d result of 1/2 (the data is curved on the appropriate plot) but we are not able to determine it with great precision. D.S. Fisher (private communication) has argued that if the fixed point structure of the renormalization group persists to higher dimension, then one has $\sigma = \psi$, though both could be different from the 1-d value of 1/2. We do not feel that our data are inconsistent with this.

Finally we briefly describe our data away from the critical point, keeping keep the same values of L and L_τ as at the critical point. A plot of $g_{\rm av}$ scales well with the this time with $\nu_{\rm av} \simeq 1.5$. In addition, a plot of the typical correlation function (divided by the value at criticality) gives an exponent, ν_{typ}, close to around 0.7, i.e. about half the value of ν_{av} just as in one dimension[16]. However, attempts to determine $\nu_{\rm av}$ *directly* by scaling data for the average correlation function away from criticality were less successful; $\nu_{\rm av} \simeq 0.75$, not significantly different from $\nu_{\rm typ}$ and much less than the value of ν_{av} found from the Binder ratio.

This discrepancy for results from average correlation function was also found in similar

Monte Carlo simulations in one dimension[30] and may be due to difficulties in taking enough samples to probe the rare regions which dominate the average. Another concern with the data away from the critical point is that we do not understand the way that the critical singularities go over to Griffiths-McCoy singularities, which have a continuously variable[16,25,21] $z(\delta)$. Perhaps the latter give big corrections to scaling, thus possibly making the size of the critical region quite small.

VII. CONCLUSIONS

To conclude, we have found a strong similarity between the critical behavior of the random transverse field Ising model in one and two dimensions. The evidence that $z = \infty$ and that the typical correlations at the critical point decay with a stretched exponential function of distance are quite strong, but the evidence for different exponents for the average and typical correlations in two dimensions is weaker because of discrepancies involving the data for the average correlation function. It is natural to speculate that the behavior found in one dimension may go over qualitatively to *all* finite dimensions, though we have no direct evidence. It would certainly be interesting to check if similar behavior also occurs in three dimensions. It also would be interesting to try to obtain these results analytically by extending the methods used in one dimension[16].

After this work was completed, we heard that S.-C. Mau, O. Motrunich and D. A. Huse (private communication) have implemented numerically for $d > 1$ the renormalization group approach used in Ref. 16, finding a flow to the infinite disorder critical fixed point, just as in $d = 1$. This is consistent with our finding the the main features of the behavior in one dimension go over into two dimensions.

ACKNOWLEDGMENTS

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