Critical Behavior of the Two-Dimensional Random Quantum Ising Ferromagnet

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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

Though *classical* phase transitions occurring at finite temperature are very well understood, our knowledge of *quantum* transitions at $T = 0$ is relatively poor, at least for systems with quenched disorder. There is, however, considerable interest in these systems since 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.

Just as the simplest model with a classical phase transition is the regular Ising model, the simplest random model with a quantum transition is arguably the Ising model in a transverse field whose Hamiltonian is given by

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

Here 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. This model should provide a reasonable description of the experimental system[6] $LiHo_xY_{1-x}F_4$ and may also be an appropriate model[7] to describe non-fermi liquid behavior in certain f-electron systems.

Naturally the random transverse field Ising model has been quite extensively studied and many *analytical* results are available[3–5,2] for the case of the one-dimensional chain. Among the surprising predictions[3] 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*[8] 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 $C_{\rm av}(r) \sim r^{-\bar{\eta}}$, where $\bar{\eta} = (3-\sqrt{5})/2 \simeq 0.38$ whereas the typical value falls off much faster, as a stretched exponential

$$C_{\rm typ}(r) \sim \exp(-\text{const. } r^\sigma), \tag{3}$$

   with $\sigma = 1/2$.

3. As the critical point is approached, ($\delta \to 0$), 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 Eq. (9), and

$$\nu_{\rm av} = 2; \qquad \nu_{\rm typ} = 1. \tag{4}$$

Unfortunately, the analytical approach is only valid in 1-d, and very little is known about the critical behavior in higher dimensions[9]. An important question is whether these striking analytical results are a special feature of 1-d, or whether they are valid more generally. 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[10,11] which considerably reduce critical slowing down. Consequently, we are able to study larger sizes and get much better statistics than in earlier work[12,13] on quantum *spin glasses*. Furthermore, cluster algorithms have an improved estimator[14] for correlation functions, which greatly reduces the statistical errors when the mean is small, so we are able to probe the distribution of correlation functions out to relatively large distances.

Our main conclusion is that the behavior of the 2-d system at the critical point is *very similar* to that of the 1-d case, see points 1 and 2 above. 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, see point 3 above.

In related work, Rieger and Kawashima[15] have studied the same model but with *continuous* imaginary time, concentrating on Griffiths-McCoy singularities in the paramagnetic phase, which are characterized by a continuously varying dynamical exponent, $z(\delta)$. Kawashima and Rieger find that $z(\delta)$ tends to infinity as the critical point is approached ($\delta \to 0$), again as in 1-d[3].

As is standard[16], 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

$$\beta_{cl}\mathcal{H}_{cl} = -\sum_{\langle i,j\rangle,\tau} K_{ij}S_i(\tau)S_j(\tau) - \sum_{i,\tau} \widetilde{K}_i S_i(\tau)S_i(\tau') \quad (5)$$

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 correlations of the $\sigma_i^z(\tau)$ in the original quantum model.

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, which is captured by having distributions for both the fields and interactions with a finite weight at the origin. We therefore take a constant distribution for the K_{ij} and a distribution for the $\widetilde{K}_i$ which falls off exponentially at *large* values. Furthermore, because of universality, the critical behavior does not depend on short distance physics and is hence independent of $\Delta\tau$, so for convenience we will take $\Delta\tau = 1$. A Hamiltonian which encapsulates these features in a way convenient for simulations is

$$\mathcal{H}_{cl} = -\sum_{\langle i,j\rangle,\tau} J_{ij}S_i(\tau)S_j(\tau) - \sum_{i,\tau} \widetilde{J}_i S_i(\tau)S_i(\tau+1), \quad (6)$$

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

$$\pi(J) = \begin{cases} 1 & \text{for } 0 < J < 1, \\ 0 & \text{otherwise,} \end{cases}$$
$$\rho(\widetilde{J}) = \begin{cases} 2\exp(-2\widetilde{J}) & \text{for } \widetilde{J} \ge 0, \\ 0 & \text{for } \widetilde{J} < 0. \end{cases} \quad (7)$$

Disorder averages are denoted by $[\cdots]_{\rm av}$ and Monte Carlo averages for a single sample are denoted by $\langle\cdots\rangle$. One controls the strength of the fluctuations, and hence tunes through the transition, by varying the classical temperature, T_{cl}. Because of universality, this should give the same critical behavior as changing the ratio of the fields to the bonds in the original quantum model, Eq. (1).

To assess the accuracy of the method, we not only performed simulations in 2-d, but also carried out simulations for the 1-d model for a similar range of sizes and compared the results with the analytic predictions discussed above. 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[11] 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.

The first task is to locate the critical point, for which we use a method suggested by D. Huse (private communication)[12,13]. One computes the Binder ratio

$$g_{\rm av} = \frac{1}{2}\left[3 - \frac{\langle M^4\rangle}{\langle M^2\rangle^2}\right]_{\rm av}, \quad (8)$$

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

$$g_{\rm av} = \widetilde{g}\left(\delta L^{1/\nu_{\rm av}}, L_\tau/L^z\right), \quad (9)$$

where $\delta = T_{cl} - T_{cl}^c$, with T_{cl}^c the value of T_{cl} at criticality. For fixed L, $g_{\rm av}$ has a peak as a function of L_τ. At the critical point, 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, a plot of $g_{\rm av}$ against $L_\tau/L_\tau^{\rm max}$ at the critical point, which has the advantage of not needing a value for z, should collapse the data. We see in Figs. 1 and 2 that this does *not* happen either in 1-d or 2-d. 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. The inset to Fig. 1 shows that this works moderately well for 1-d (though not perfectly for this range of sizes) with the expected value $\psi = 1/2$. In 2-d, the data collapse for sizes $L \ge 12$, shown in the inset to Fig. 2, 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 close similarity of the data for 1-d and 2-d, particularly the broadening of the data in the main part of the figures, suggests that z is infinite also in 2-d.

Next we consider the behavior of the equal time correlations at the critical point. Figs. 3 and 4 show data for the average and typical[8] correlations for spins separated by $r = L/2$ in 1-d and $\vec{r} = (L/2, 0)$ in 2-d. For each value of L, we took L_τ such that $g_{\rm av}$ is close to the peak[17] shown in Figs. 1 and 2. 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. Fig. 3 shows that in 1-d, the average correlation falls off with a power law while the typical value decays with an

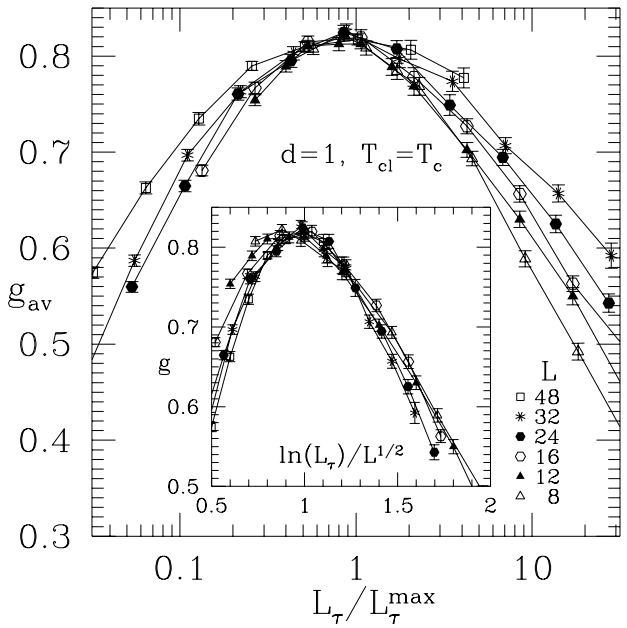

FIG. 1. A plot of the data for the average Binder ratio, $g_{\rm av}$, at the critical temperature $T_{cl} = T_c^{cl} = 0.98$ for the one-dimensional model. In the main figure the horizontal axis is $L_\tau/L_\tau^{\rm max}$ where $L_\tau^{\rm max}$ is the value of L_τ at the peak. Note that the curves do not scale but rather get broader for larger sizes, indicating activated scaling, $z = \infty$, (which is known from the analytical work[3]). The inset shows a plot appropriate for activated scaling in which the horizontal axis is $\ln L_\tau / \ln L_\tau^{\rm max}$, with $\ln L_\tau^{\rm max} \sim L^{1/2}$, which is also known from the analytical work. Scaling works quite well though there are still some small deviations for this range of sizes, even in the large L_τ limit.

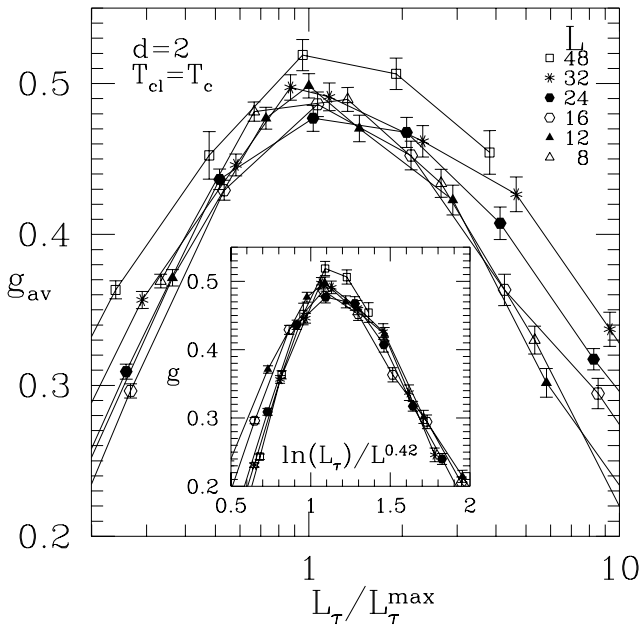

FIG. 2. As in Fig. 1 but for two dimensions, with $T_{cl} = T_c^{cl} = 2.45$. The conclusion is similar, i.e. the broadening of the curves for large L in the main plot indicates activated dynamical scaling, i.e. $z = \infty$. The data for $L = 48$ is slightly high which may indicate that the true value of T_c^{cl} is a little higher. In the inset, the data for $L \geq 12$ is seen to scale quite well with the same form $\ln L_\tau / L^\psi$ known to be exact in 1-d, but the value of $\psi = 0.42$ (shown) works better than the 1-d value of $\psi = 1/2$.

exp(−const. $L^{1/2}$) variation, as expected[3]. Note, though, that the exponent for the average, $-\tilde{\eta}$, obtained by fitting the data, gives $\tilde{\eta} = 0.53$, somewhat different from the expected[3] value of 0.38. We will discuss this discrepancy further below. The data in Fig. 4 shows that the behavior in 2-d is quite similar: the average falls off with a power law, with $\tilde{\eta}$ about 1.95, while the typical value falls off faster than a power law, (because of the downward *curvature*) consistent with a stretched exponential behavior of the form exp(−const. L^σ), with $\sigma \simeq 1/3$. The statistical errors (shown) are generally smaller than the size of the points, so the downward curvature is statistically significant. According to D.S. Fisher (private communication), the structure of the renormalization group used in Ref. 3 implies, quite generally, that $\psi = \sigma$. Our results are compatible with this.

Finally we briefly describe our data away from the critical point, keeping the same values of L and L_τ as at the critical point[17]. In 1-d, $g_{\rm av}$ scales well with the expected value $\nu_{\rm av} = 2$ and the corresponding plot in 2-d also works well, this time with $\nu_{\rm av} \simeq 1.5$. Plots of the typical correlation function (divided by the value at criticality) give an exponent close to the expected value of $\nu_{\rm typ} = 1$ in 1-d and around 0.7 in 2-d, i.e. in each case *much smaller* than the exponent for the average correlation length obtained from $g_{\rm av}$. However, attempts to determine $\nu_{\rm av}$ *directly* by scaling data for the average correlation function away from criticality were less successful. In 1-d, the fit, which works quite well, gives $\nu_{\rm av} \simeq 1.2$, much less than the expected value[3] of 2, while in 2-d we found $\nu_{\rm av} \simeq 0.75$, not significantly different from $\nu_{\rm typ}$.

This discrepancy for results from average correlation function may be due to difficulties in taking enough samples to probe the rare regions which dominate the average. It may also be why $\tilde{\eta}$ in 1-d was not found accurately. Furthermore, we do not understand the way that the critical singularities go over to Griffiths-McCoy singularities, which have a continuously variable[3,15,18] $z(\delta)$. Perhaps the latter give big corrections to scaling, thus making the size of the critical region quite small.

To conclude, we have found a strong similarity between the critical behavior of the random transverse field Ising model in one and two dimensions. 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. 3, finding a flow to the infinite disorder critical fixed point, just as in $d = 1$.

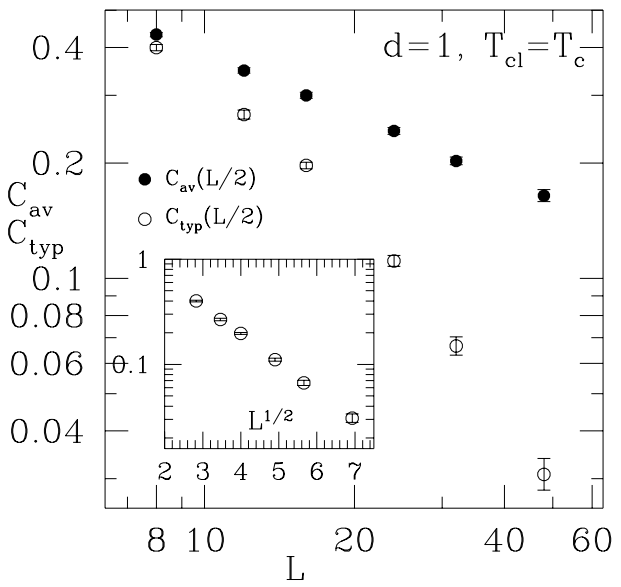

FIG. 3. The main figure shows the average and typical[8] correlations between spins $L/2$ apart at the critical point in one dimension. As expected[3], the average decays with a power law while the typical value decays faster than a power, as shown by the downward curvature in the plot. The inset shows that the typical correlation function decays as the stretched exponential, $C_{\rm typ}(L/2) \sim \exp(-\text{const. } L^{1/2})$, as expected[3].

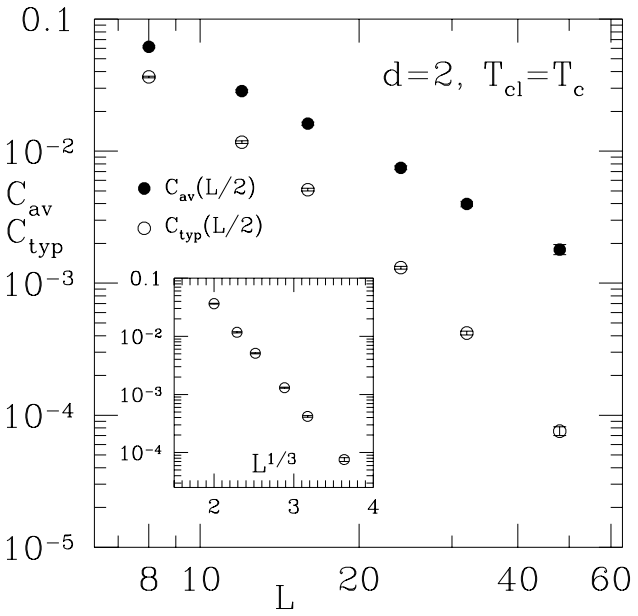

FIG. 4. A similar plot to Fig. 3 but for two dimensions. We emphasize just how similar these figures are. The most noteworthy feature is that in two dimensions, as in d=1, the typical correlation function falls off *faster* than a power law. The average falls off with a power law and a fit gives a slope of $-\tilde{\eta}$ with $\tilde{\eta} = 1.95$. The inset shows that the 2-d 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.

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