Critical Behavior and Griffiths-McCoy Singularities in 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. At the critical point, the dynamical exponent is infinite and the typical correlation function decays with a stretched exponential dependence on distance. Away from the critical point there are Griffiths-McCoy singularities, characterized by a single, continuously varying exponent, z', which diverges at the critical point, as in one-dimension. Consequently, the zero temperature susceptibility diverges for a *range* of parameters about the transition.

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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 Ising model, the simplest random model with a quantum transition is arguably the Ising model in a transverse field whose Hamiltonian is given by

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

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] $\mathrm{LiHo}_x\mathrm{Y}_{1-x}\mathrm{F}_4$ 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 surprising *analytical* results are available[3–5] for the case of dimension $d = 1$. For example, 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[3] $\xi_\tau \sim \exp(\text{const. } \xi^\psi)$, where $\psi = 1/2$. This is called *activated* dynamical scaling. In addition, distributions of the equal-time σ_i^z–σ_{i+r}^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 $C_{\rm av}(r) \sim r^{-\tilde\eta}$, where[3] $\tilde\eta = (3 - \sqrt{5})/2 \simeq 0.38$ whereas the typical value falls off much faster, as a stretched exponential $C_{\rm typ}(r) \sim \exp(-\text{const. } r^\sigma)$, with $\sigma = 1/2$. As the critical point is approached, the average and typical correlation *lengths* both diverge but with *different* exponents[3], i.e. $\xi_{\rm av} \sim \delta^{-\nu_{\rm av}}$; $\xi_{\rm typ} \sim \delta^{-\nu_{\rm typ}}$, where δ is the deviation from criticality, and $\nu_{\rm av} = 2, \nu_{\rm typ} = 1$. Finally, there are strong Griffiths-McCoy singularities at low temperature even away from the critical point, coming from rare regions which are "locally in the wrong phase". These are characterized by a single continuously varying exponent[9], $z'(\delta)$, which *diverges* as $\delta \to 0$.

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 is only valid in 1-d, and very little is known in higher dimensions. Senthil and Sachdev[10] have studied the model in Eq. (1) with site dilution and shown that activated dynamical scaling occurs along that part of the zero temperature phase boundary which is precisely *at* the percolation concentration. However, it is not clear if this result also holds for the rest of the phase boundary, and, to our knowledge, there are no results at all for other, more general, models. Here, we investigate the behavior of the random transverse field Ising ferromagnet in *two* dimensions by performing large-scale Monte Carlo simulations. Because the ferromagnet has no frustration we are able to use highly efficient cluster algorithms which considerably reduce critical slowing down. Our main conclusion is that the behavior of the 2-d system *is* very similar to that of 1-d.

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 the following "box" distribution

$$\pi(J_{ij}) = \begin{cases} 1, & \text{for } 0 < J_{ij} < 1 \\ 0, & \text{otherwise} \end{cases}$$
$$\rho(h_i) = \begin{cases} h^{-1}, & \text{for } 0 < h_i < h \\ 0, & \text{otherwise} \end{cases} . \quad (2)$$

As is standard[11], we represent the d-dimensional quantum Hamiltonian in Eq. (1) by an effective classical action in (d+1)-dimensions, where the extra dimension, imaginary time, is of size $\beta \equiv 1/T$, and is divided up into $L_\tau \equiv \beta/\Delta\tau$ intervals each of width $\Delta\tau$ in the limit $\Delta\tau \to 0$. The partition function can then be written as $Z = \lim_{\Delta\tau\to 0} \mathrm{Tr}\exp(-S)$, where the effective classical action is given by

$$S = -\sum_{\langle i,j\rangle,\tau} K_{ij} S_i(\tau) S_j(\tau) - \sum_{i,\tau} \widetilde{K}_i S_i(\tau) S_i(\tau') \quad (3)$$

where, $\tau' = \tau + \Delta\tau$, $S_i(\tau) = \pm 1$,

$$K_{ij} = \Delta\tau J_{ij}, \quad \text{and} \quad \exp(-2\widetilde{K}_i) = \tanh(\Delta\tau h_i). \quad (4)$$

To study large systems sizes with small statistical errors, we use cluster algorithms which simultaneously flip many spins. For our results on Griffiths-McCoy singularities we have developed[12] a variant of the loop algorithm[13] in which the required limit $\Delta\tau \to 0$ is explicitly taken. We shall call this the *continuous imaginary time* algorithm. It represents the original quantum Hamiltonian exactly (apart from statistical errors). We tune through the transition by varying h.

In our simulations which determine for critical exponents, we use a different approach, and exploit universality according to which the universal quantities should be independent of $\Delta\tau$ and so, for convenience, we set $\Delta\tau = 1$. We then have a three-dimensional Ising model, with disorder perfectly correlated in one direction, which we simulate using the Wolff[14] cluster algorithm. We shall call this the *discrete imaginary time* algorithm. It does *not* represent the quantum Hamiltonian exactly but is expected to be in the same universality class. Furthermore, for this algorithm we find it convenient to parameterize the strength of fluctuations by an effective classical temperature $T_{cl} \equiv 1/\beta_{cl}$, (not equal to the real temperature which is the inverse of the size in the time direction) and write $Z = \mathrm{Tr}\exp(-\beta_{cl}\mathcal{H}_{cl})$ where

$$\mathcal{H}_{cl} = -\sum_{\langle i,j\rangle,\tau} J_{ij} S_i(\tau) S_j(\tau) - \sum_{i,\tau} \widetilde{J}_i S_i(\tau) S_i(\tau+1). \quad (5)$$

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

$$\pi(J_{ij}) = \begin{cases} 1 & \text{for } 0 < J_{ij} < 1, \\ 0 & \text{otherwise,} \end{cases}$$
$$\rho(\widetilde{J}_i) = \begin{cases} 2\exp(-2\widetilde{J}_i) & \text{for } \widetilde{J}_i \ge 0, \\ 0 & \text{for } \widetilde{J}_i < 0, \end{cases} \quad (6)$$

which, from Eq. (4), is similar to Eq. (2). We tune through the transition by varying the classical temperature, T_{cl}.

The lattice is of size L in the space directions, and we denote disorder averages by $[\cdots]_{\rm av}$ and Monte Carlo averages by $\langle\cdots\rangle$. For both algorithms we employ periodic boundary conditions in all directions.

First of all we discuss our results for the location of the critical line using the continuous imaginary time algorithm. We do this by computing the Binder ratio

$$g_{\rm av} = \frac{1}{2}\left[3 - \frac{\langle M^4\rangle}{\langle M^2\rangle^2}\right]_{\rm av}, \quad (7)$$

where $M = \sum_i \int_0^\beta S_i(\tau)\, d\tau$, At any finite temperature the system is expected to be in the universality class of the classical two-dimensional classical random bond Ising ferromagnet. For small temperatures the size of the classical critical region shrinks and we need to study larger sizes (we went up to $L = 32$) to get a reliable estimate of $h_c(T)$. By extrapolating the latter to $T = 0$, see Fig. 1, we obtain for the location of the quantum critical point $h_c = h_c(T=0) = 4.2 \pm 0.2$.

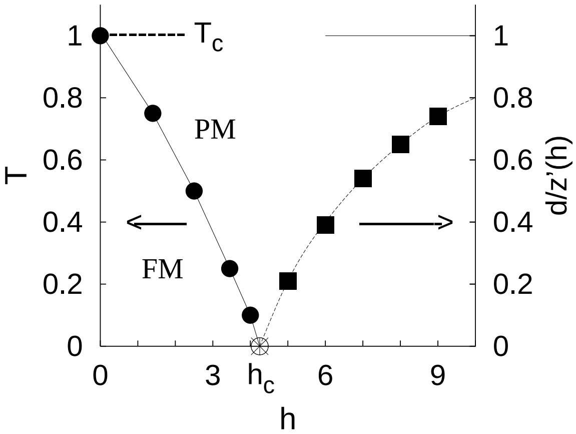

FIG. 1. Results obtained with the continuous imaginary time algorithm. The left hand axis indicates the phase diagram of the $d = 2$ random transverse Ising model: PM means paramagnetic, FM means ferromagnetic, $T_c = 1.00(1)$ is the critical temperature of the classical random Ising ferromagnet ($h_i = 0$) with the box bond distribution in Eq. (2), and $h_c = 4.2(2)$ the location of the quantum critical point we are interested in. The right hand scale indicates the values of $d/z'(h)$ obtained from analyzing the integrated probability distribution of $\ln\chi_{\rm local}$ according to (8) in the Griffiths-McCoy region, $h > h_c$. The open circle corresponds to $z'(h_c) = \infty$ and the horizontal line at $d/z' = 1$ indicates the expected limit $\lim_{h\to\infty} z'(h) = d$. The broken line is just a guide to the eye.

Now we turn our attention to the Griffiths-McCoy region in the disordered phase ($h > h_c$). Due to the presence of strongly coupled regions in the system the probability distribution of excitation energies (essentially inverse tunneling times for these ferromagnetically ordered clusters) becomes extremely broad. As a consequence we expect the probability distribution of local susceptibilities to have an algebraic tail at $T = 0$[15–18]:

$$\Omega(\ln \chi_{\rm local}) \approx -\frac{d}{z'(h)} \ln \chi_{\rm local}, \qquad (8)$$

where $\Omega(\ln \chi_{\rm local})$ is the probability for the logarithm of the local susceptibility χ_i at site i to be larger than $\ln \chi_{\rm local}$. The dynamical exponent[9] $z'(h)$ varies continuously with the distance from the critical point and parameterizes the strengths of the Griffiths-McCoy singularities also present in other observables. At finite temperatures the distribution of $\chi_{\rm local}$ is chopped off at β, and close to the critical point one expects finite size corrections as long as L or β are smaller than the spatial correlation length or imaginary correlation time, respectively. We used $\beta \le 1000$ and averaged over at least 512 samples.

In Fig. 1 we show our results for $d/z'(h)$ in the Griffiths-McCoy region. For $h \to \infty$ we expect $d/z'(h) \to 1$, since this is the result for *isolated* spins in random fields with non-vanishing probability weight at $h_i = 0$. The more interesting limit is $h \to h_c$. The data are well compatible with $\lim_{h\to h_c} z'(h) = \infty$, as in one-dimension[3,15]. The average susceptibility $[\chi]_{\rm av}$ diverges like[18] $[\chi]_{\rm av} \sim T^{d/z'(h)-1}$ for $T \to 0$. Hence, if $\lim_{h\to h_c} z'(h)$ is universal, *i.e.* does not depend on the details of the disorder, as is the case in 1-d, $[\chi]_{\rm av}$ diverges quite generally in a *range* about the quantum critical point for systems with Ising symmetry.

Next we describe our results for critical exponents using the discrete imaginary time algorithm, for which we studied sizes up to $L = 48$ and $L_\tau = 2048$. We found that no more than 100 sweeps were required for equilibration, even for the largest lattices. At least 1000 samples were averaged over.

We locate the $T = 0$ critical point by a method already used for the quantum spin glass[19]. We compute the Binder ratio, Eq. (7) , which (assuming, for now, that z is finite) has the finite-size scaling form

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

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 Fig. 2 that this does *not* happen. 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. A corresponding scaling plot is shown in the inset to Fig. 2. The data collapse for sizes $L \ge 12$, 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. We have also performed analogous calculations for one-dimension[20] with very similar results. The close similarity of the data for 1-d and 2-d, and the broadening of the data in the main part of Fig. 2, suggests that z is infinite in 2-d, as well as in 1-d.

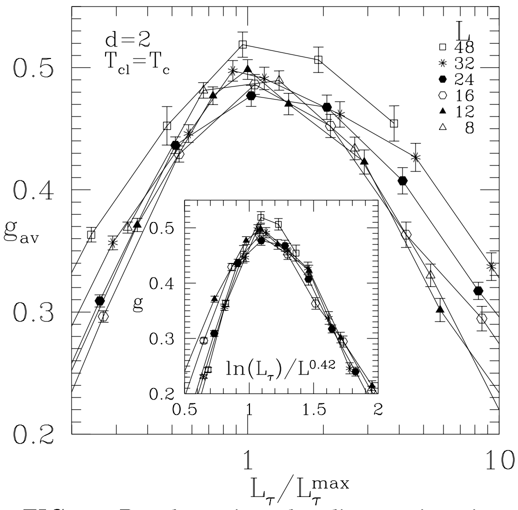

FIG. 2. Results using the discrete imaginary time algorithm at the quantum critical point, $T_{cl} = T_c^{cl} = 2.45$. In the main figure the horizontal axis is $L_\tau/L_\tau^{\rm max}$ where $L_\tau^{\rm max}$ is the value of L_τ at the peak. Note that the curves do not scale but rather get broader for larger sizes, indicating activated scaling, $z = \infty$, 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 $L \ge 12$ 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 $\psi = 1/2$.

Next we consider the equal time correlations at the critical point. Fig. 3 shows data for the average and typical[8] 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[21] shown in Fig. 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.

The data in Fig. 3 shows that the average correlation function 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 $\exp(-{\rm const.}\ L^\sigma)$, 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. This behavior is of the form expected in one dimension[3], except that there $\sigma = 1/2$, a result which is reproduced by our 1-d simulations[20]. Moreover, in one dimension $\psi = \sigma$, and this relation also holds in higher dimensions[22] provided that the fixed point is similar, *i.e.* has infinitely strong disorder. Our data is compatible

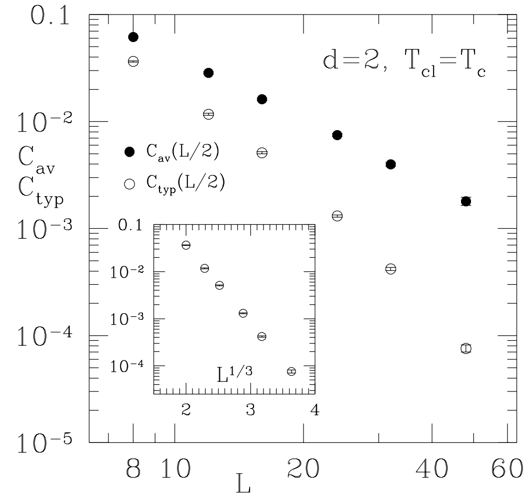

FIG. 3. The main figure shows the average and typical[8] correlations between spins $L/2$ apart at the critical point. The average falls off with a power law, and a fit gives a slope of $-\tilde{\eta}$ with $\tilde{\eta} = 1.95$. However, the curvature of the data for the typical correlation function shows that this falls off *faster* than a power law. The inset shows that 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[3] in 1-d.

with this result though neither σ nor ψ are determiend with precision. Additional results, including the whole distribution of correlation functions, will be presented in a separate publication.

To conclude, we have found a strong similarity between the critical behavior of the random transverse field Ising model in one and two dimensions. In particular, both z and $\lim_{h\to h_c} z'(h)$ are infinite. Previous simulations on quantum spin glasses[18] (for which the mean of the distribution of the J_{ij} is zero) in two dimensions, found these quantities to be apparently finite. However, it is plausible that the asymptotic result should be infinite also for quantum spin glasses, and that the finite result found is an artifact of the smaller sizes used there. (Those studies also used a non-random transverse field.)

Two of us (NK and HR) have implemented numerically for $d = 2$ a natural generalization of the renormalization group procedure used in Ref. 3 for $d = 1$. After this work was completed, we heard that S.-C. Mau, O. Motrunich and D. A. Huse (private communication) used a similar approach and observed a flow to the infinite disorder critical fixed point, just as in $d = 1$.

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