

Random bond Ising chain in a transverse magnetic field: A finite-size scaling analysis.

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(May 27, 1994)

Abstract

We investigate the zero-temperature quantum phase transition of the random bond Ising chain in a transverse magnetic field. Its critical properties are identical to those of the McCoy-Wu model, which is a classical Ising model in two dimensions with layered disorder. The latter is studied via Monte Carlo simulations and transfer matrix calculations and the critical exponents are determined with a finite-size scaling analysis. The magnetization and susceptibility obey conventional rather than activated scaling. We observe that the order parameter- and correlation function-probability distribution show a nontrivial scaling near the critical point which implies a hierarchy of critical exponents associated with the critical behavior of the generalized correlation lengths.

75.10Hk, 75.50Lk

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Quite recently there has been a growing interest in the zero-temperature quantum critical behavior of *disordered* spin systems. Thermal fluctuations are absent here and the phase transition is driven by the interplay between randomness and quantum fluctuations. In order to tune the system to criticality one can either vary the strength of the disorder, as for instance in spin- $\frac{1}{2}$ XXZ-chains [1], or one can control the strength of the quantum fluctuations directly by an external transverse magnetic field in spin models with a strong Ising anisotropy. The latter case is particularly interesting since experimentalists became able to investigate the effect of a transverse field on the glass transition in the Ising spin glass $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$ at low temperatures [2]. On the theoretical side much progress has been made since then: the infinite range model has been solved analytically [3–5], a Migdal-Kadanoff renormalization group calculation has been made [6], the critical exponents in 2 and 3 dimensions have been determined via Monte Carlo simulations [7,8] and new results for the one-dimensional case have been derived via a renormalization-group analysis [9].

In the latter papers focusing on the critical behavior in finite dimensions of these quantum models it has been pointed out that their universal properties are identical to those of classical Ising models with layered disorder [10]. Especially the Ising spin chain in a transverse field can be mapped onto the McCoy-Wu model [11–13], for which various exact results have been derived. The critical exponents of the order-parameter β and the correlation length ν as well as the dynamical exponent z has been found recently via a renormalization-group (RNG) analysis by D. Fisher [9].

The aim of the present paper is to perform a numerical investigation of the finite-size scaling behavior of the Ising spin chain in a transverse magnetic field. Such an analysis has not been performed yet for this model and bears some new features concerning the finite-size scaling of anisotropic systems [14]. It can also be seen as a test-ground for numerical methods applied to systems, for which — in contrast to this model — no quantitative theoretical prediction are at hand (e.g. for the cases considered in [7,8]). And finally it provides a check to what extent analytical predictions, like those made in [9] and which are valid asymptotically for an infinite system with rather unusual properties, can be detected

in systems of finite size.

The model under consideration is described by the quantum Hamiltonian

$$H_Q = - \sum_i J_i \sigma_i^z \sigma_{i+1}^z - \Gamma \sum_i \sigma_i^x, \quad (1)$$

where σ are spin- $\frac{1}{2}$ Pauli matrices, Γ is the transverse field strength and the exchanges J_i are quenched random variables obeying a distribution $P(J)$. At zero temperature the system (1) has a ferromagnetic phase transition to long-range magnetic order at a critical value Γ_c , which depends on the bond distribution $P(J)$. We are interested in the critical properties of this transition. However, as shown in [9,11,13], the magnetization behaves already non-analytically at higher values of Γ_c giving rise to e.g. a divergence of the longitudinal susceptibility at higher values of Γ .

The ground state energy of this one-dimensional quantum model (1) is equal to the free energy of the two-dimensional classical Ising model [15]

$$H = - \sum_{i,j} \tilde{J}_i S_{i,j} S_{i+1,j} - K \sum_{i,j} S_{i,j} S_{i,j+1} \quad (2)$$

at a certain finite temperature T . Here $S_{i,j} = \pm 1$ are classical Ising spins, the site index i runs along the x (space) direction and the index j along the τ (imaginary time) direction of a two-dimensional square lattice. Following [7,8] we can rescale the bond strengths \tilde{J}_i and coupling constant K without changing the universal properties. For numerical convenience we set $K = 1$ and take a binary distribution

$$P(\tilde{J}) = \frac{1}{2} \delta(\tilde{J} - j_1) + \frac{1}{2} \delta(\tilde{J} - j_2), \quad (3)$$

where we put $j_1 = 1$. The layered random bond Ising model (2) with the bond distribution (3) has a ferromagnetic phase-transition at a critical temperature T_c defined by [11]

$$\log \coth(1/T_c) + \log \coth(j_2/T_c) = 4/T_c \quad (4)$$

and the universal properties (like exponents etc.) are identical to those of the quantum chain (1) at Γ_c and zero temperature. Therefore we study model (2) at $T_c(j_2)$ by Monte-Carlo

simulations of rectangular lattices of size $L \times L_\tau$. The largest size in the τ -direction was $L_\tau = 160$ whereas that in the space direction x , which corresponds to the length of the quantum chain (1), was $L = 16$. Hence the disorder average over the distribution (3) could be done exactly by generating all, non-equivalent bond-configurations (whose number is approximately $2^L/L$). To have more confidence on the data from the Monte-Carlo simulation we have compared our results to those obtained from transfer matrix calculations. The advantage of the latter method is that the results are exact, but the drawback is that one is limited to small system sizes $L \leq 10$. In all cases we found no significant deviations between the results of the two methods.

The correlation length of the quantum chain (1) diverges as $\xi \sim (\Gamma - \Gamma_c)^{-\nu}$ when approaching the ferromagnetic transition. The characteristic relaxation time of the quantum dynamics is expected to diverge as $\tau \sim \xi^z$, with z being the dynamical exponent. These two diverging scales can naturally be found in the classical model (2): due to the extreme anisotropy one expects the correlation length in the space (or x) direction to diverge like $\xi \sim (T - T_c)^{-\nu}$ and the correlation length in the imaginary time (or τ) direction like $\xi_\tau \sim (T - T_c)^{-z\nu}$. Following a nice argument by L. Mikheev [16] one might imagine the system close to T_c as being composed of roughly rectangular, ferromagnetic/paramagnetic domains, which are located (in the space direction) at segments of the chain where strong/weak bonds are dominating. The correlation length ξ_τ in the time direction is then given by the average distance of domain walls in semi-infinite strips of width ξ being ferromagnetically ordered, thus $\xi_\tau \propto \exp(a\xi)$ (see e.g. [17]). This supports very much an activated dynamics scenario with $z = \infty$, as found in the RNG analysis [9]. However, we begin the analysis by assuming a finite z and will see how far we get.

At the critical point (i.e. $T = T_c$) various thermodynamic quantities are expected [14] to depend only on the scaling variable L/L_τ , the aspect ratio or the shape of the system. For instance we would have for the averaged spontaneous magnetization

$$M = [\langle m \rangle]_{\text{av}} \approx L^{-\beta/\nu} \widetilde{m}(L_\tau/L^z), \quad (5)$$

where $m = (L_\tau L)^{-1} |\sum_{i,j} S_{i,j}|$ is the magnetization per site, $\langle \dots \rangle$ means the thermal average and $[\dots]_{\text{av}}$ means the disorder average. In figure 1 we show a scaling plot according to (5) obtained by Monte-Carlo simulations for different shapes and sizes (note that the disorder average is done exactly) at $j_2 = 0.1$ and $T = T_c = 1.32038$. It yields $\beta/\nu = 0.17 \pm 0.01$ and $z = 1.65 \pm 0.05$. We also looked at $j_2 = 0.05$ for which $T_c = 1.14710$, and obtain $z = 1.70 \pm 0.05$ and $\beta/\nu = 0.18 \pm 0.01$. The RNG prediction is $\nu = 2$ (for the averaged correlation length) $\beta = (3 - \sqrt{5}) \approx 0.38$ [9], which yields a ratio $\beta/\nu \approx 0.19$ that agrees roughly with our estimate.

The exponent z decreases as j_2 increases approaching $z = 1$ for $j_2 = 1$ and indicating the crossover to the pure case. This is the reason why we used small values for j_2 to ensure that what we see is the critical behavior of the disordered model. On the other hand we tried to avoid too small values of j_2 in the Monte-Carlo simulations, since then the critical temperature decreases too much and equilibration becomes more difficult.

The insert of figure 1 shows the scaling behavior of the susceptibility at $j_2 = 0.1$,

$$\chi(L, L_\tau) = L_\tau L [\langle m^2 \rangle]_{\text{av}} \approx L^{\gamma'/\nu} \tilde{\chi}(L_\tau/L^z), \quad (6)$$

for which we find $\gamma'/\nu = 2.3 \pm 0.1$ (we used the value $z = 1.65$ that was obtained from the scaling of the magnetization). Note that γ' is not the critical exponent that describes the divergence of the susceptibility in an infinite system by approaching the temperature T_c from above, since this quantity is expected to diverge already at a temperature higher than T_c [9,11]. The prediction for an anisotropic system obeying hyperscaling [14] is $\gamma'/\nu + 2\beta/\nu = d + z$. Inserting $d = 1$ and the values for β/ν and z given above this relation is fulfilled very well. For the magnetization and the susceptibility conventional scaling seems to work well for these system sizes.

The averaged cumulant $g_{\text{av}} = 0.5 \cdot [3 - \langle m^4 \rangle / \langle m^2 \rangle^2]_{\text{av}}$ is expected to scale like

$$g_{\text{av}}(L, L_\tau) = \tilde{g}(L_\tau/L^z) \quad (7)$$

and a scaling plot is shown in figure 2 with $z = 1.55 \pm 0.05$ for $j_2 = 0.1$, which is slightly lower than the estimate from the spontaneous magnetization. Furthermore the data collapse

is not as good as in figure 1. Even worse is the scaling behavior of the cumulant $\bar{g} = 0.5 \cdot (3 - [\langle m \rangle^4]_{\text{av}} / [\langle m \rangle^2]_{\text{av}}^2)$. A systematic shift in the maximum to smaller values for increasing system sizes L indicates that this quantity is not dimensionless as expected naively. The natural scaling assumption $[\langle m \rangle^k]_{\text{av}} \approx L^{-k\beta/\nu} \tilde{m}_k(L_\tau/L^z)$ does not seem to be correct here. As a consequence, the order parameter probability distribution $P(\mathcal{M}) = [\delta(\langle m \rangle - \mathcal{M})]_{\text{av}}$ does not scale in a trivial way like $P(\mathcal{M}) \approx L^{\beta/\nu} \tilde{P}(\mathcal{M}L^{\beta/\nu}, L_\tau/L^z)$ — as it does e.g. in conventional spin glasses [18] — which we checked explicitly by looking at the magnetization histograms for systems with constant aspect ratios $L_\tau \approx L^z$.

To have an independent check of this scenario we have compared the above results with those obtained from the transfer matrix calculation. We have used the method recently introduced in [19] for the exact calculation of the free energy derivatives. The method has been extended to a finite rectangular lattice with periodic boundary condition in both directions. By expressing the cumulants of the magnetization as derivatives of the free energy, we have computed g_{av} and \bar{g} for systems sizes up to 8×256 . Since there are no numerical derivatives involved and the average over disorder is performed by summing over all possible configurations, the calculation yields the exact values. In all cases we did not find significant difference between these results and those of the Monte-Carlo simulations.

We have also calculated the averaged spin-correlation function at T_c , which is defined as

$$C(r, t) = [\langle S_{i,j} S_{i+r, j+t} \rangle]_{\text{av}} . \quad (8)$$

For the averaged correlations in the time direction $C(0, t)$ one expects [14] for $L_\tau \propto L^z$ a behavior

$$C(0, t) \propto t^{-\eta_\perp} + (L_\tau - t)t^{-\eta_\perp} , \quad (9)$$

where the second term on the r.h.s. takes into account the periodic boundary conditions. In the insert of figure 3 we have depicted $C(0, t)$ for various system sizes L with L_τ chosen at the maximum of $g_{\text{av}}(L_\tau)$, so that $L_\tau \propto L^z$. From the fit we conclude that $\eta_\perp = 0.23 \pm 0.01$.

Concerning the spatial correlation function $C(r, 0)$ Shankar and Murthy report a result (see equations 3.39 and 3.43 in [13]), which is

$$C(r, 0) \propto \exp(-a\sqrt{r}) + \exp(-a\sqrt{L-r}), \quad (10)$$

where the second term on the r.h.s. takes again into account the periodic boundary conditions. This form yields a nice least square fit to our numerical data, as shown in figure 3. Note that comparing (9) and (10) one observes that “space” and “time” seem to scale like $r \sim (\log t)^2$, as predicted in [9].

D. Fisher argues [9] that the result (10) holds for the *typical* correlations (i.e. those corresponding to the maximum of their probability distribution), whereas the average should decay algebraically, since the latter should be dominated by rare, strongly correlated regions of the spin chain. We tried to fit $C(r, 0)$ to an algebraic decay similar to (9) with a different exponent η_{\parallel} , which gave much worse results. However, stipulating

$$C(r, 0) \approx r^{-\eta_{\parallel}} \tilde{c}(r/L, L_{\tau}/L^z), \quad (11)$$

the relation $C(L/2, 0) \approx L^{-\eta_{\parallel}} \tilde{c}(L_{\tau}/L^z)$ should hold, which gives indeed an acceptable data-collapse for $\eta_{\parallel} = 0.40 \pm 0.02$ (using our estimate $z = 1.70$). The latter result agrees well with the result $\eta_{\parallel} \approx 0.38$ obtained in [9]. Furthermore it is consistent with the scaling relation $\eta_{\perp}/\eta_{\parallel} = z$ (within the errorbars) and $\eta_{\parallel} = d + z - \gamma'/\nu = 2\beta/\nu$. We would like to stress that our data are compatible with both equations (10) and (11), which, however, are based on assumptions excluding each other.

Next we study the probability distribution of correlation functions in the spatial direction through the analysis of the associated generalized correlation lengths [20,21]. The analysis is carried out using the transfer matrix approach, for more details see [21,22]. We focus on the spatial correlation function for which we can use the general results for products of random matrices. In this case the latter consists of a succession of transfer-matrices from row i to row $i + 1$ in the spatial direction, each of which is made by L_{τ} spins. Since the generalized correlation lengths to be defined below are related to the first two Lyapunov exponents of an infinite product of transfer matrices we have to choose L very large ($\sim 10^6$). An advantage of this approach is that one is left with only one scaling variable at the critical point since L_{τ}/L^z is zero.

In general each moment of the probability distribution of the correlation function defines a characteristic length scale which we denote by ξ_q where q is the order of the moment [20,21]:

$$\xi_q^{-1} = - \lim_{r \rightarrow \infty} \frac{1}{rq} \ln [G_i(r)^q]_{\text{av}} \quad (12)$$

where $G_i(r)$ is the connected correlation function between the row i and the row $i + r$. For example ξ_1 is the characteristic length scale of the average correlation function, while ξ_0 is that of the typical correlation function. We shall then call ξ_0 the typical correlation length and ξ_1 the average correlation length. It can be shown that if $q > q'$ then $\xi_q \geq \xi_{q'}$ [22]. Taking into account this hierarchy, the usual finite-size scaling hypothesis [14] for the spatial generalized correlation lengths would be

$$\xi_q^{-1} = L_\tau^{-1/z_q} \tilde{\zeta}_q((T - T_c) L_\tau^{1/z_q \nu_q}) \quad (13)$$

where the z_q can be called “generalized dynamical exponents”. From the relation $\xi_q \geq \xi_{q'}$ for $q > q'$ it follows that $z_q \geq z_{q'}$ and $\nu_q \geq \nu_{q'}$. In the scaling form (13) it is assumed that the ξ_q diverges all at the same temperature T_c , which in general need not to be the case, see for instance [20]. As consequence, especially for large q (13) should be modified allowing for a q -dependent T_c . However, we stick to the scaling form (13) with T_c given by the ferromagnetic phase transition temperature.

We have calculated (for technical details see [21,22]) the z_q by computing the exponents ξ_q at the critical point T_c for different j_2 for systems of sizes up to $L_\tau = 8$. The length of the product was 10^6 . The exponent z_q increases as j_2 decreases. We get (with at least 10 percent accuracy)

j_2	z_0	z_1	z_2	
0.10	1.74	2.04	2.63	
0.05	2.12	3.23	5.26	

(14)

In all cases we found a good scaling at the critical temperature T_c given by (4). Our statistics is not accurate enough to investigate higher correlation lengths. The dynamical exponents

increase systematically with decreasing j_2 and it cannot be ruled out that $z_q \rightarrow \infty$ for $j_2 \rightarrow 0$. Since the other exponents (as ν_q , see below, or β see above) are less susceptible to a variation in j_2 we have to leave it open here, whether this behavior indicates a cross-over or an actual non-universality of z_q with respect to j_2 .

The exponent ν_q are obtained from the data collapse using (13). In this case we computed the generalized correlation lengths for temperatures $T > T_c$ and for system sizes up to $L_\tau = 7$. Again the length of the product was 10^6 . With this statistics we were able to estimate only the first two exponents. The data for $j_2 = 0.1, 0.05$ and 0.01 leads to $\nu_0 \simeq 0.7$ and $\nu_1 \simeq 1$, in agreement with the analytical result of [13] but disagrees with the RNG result $\nu_1 = 2$ [9]. In figure 4 we show a scaling plot for ξ_0 .

We briefly discuss the time-correlation length for which we consider a semi-infinte strip in the time-direction ($L_\tau \rightarrow \infty$). While for the spatial correlations we have an infinite product of random matrices, in the case of time-correlations the transfer matrix is always the same since the randomness is only in the spatial direction. In this situation for each realization of disorder the correlation length is given by the inverse of difference between the first two eigenvalues of the transfer matrix and yields, if averaged, the inverse of the typical correlation length, ξ_0^{-1} (note that this is equivalent to averaging the logarithm of the correlation function). For the typical time-correlation length we stipulate again the usual finite-size scaling form [14]

$$\xi_{\tau,0}^{-1} = L^{-\tilde{z}_0} \tilde{\zeta}_{\tau,0}((T - T_c) L^{1/\tilde{\nu}_0}). \quad (15)$$

For $j_2 = 0.1$ we found, for example, $\tilde{z}_0 \approx 1.3$ and $\tilde{\nu}_0 \approx 1$. Note that $\tilde{z}_0 \neq z_0$ and $\tilde{\nu} \neq \nu$.

To summarize we performed a detailed finite-size scaling analysis of the zero-temperature phase transition occurring in a random bond Ising chain by tuning the transverse magnetic field to some critical value. For this model many analytical results are known and our analysis shows a good agreement with the results of Shankar and Murthy [13] and concurs also with the RNG prediction of the existence of different length scales with different critical exponents ν [9]. However, we do not find the same values as those reported in the latter.

One possible explanation of this fact might be the following: D. Fisher [9] estimated the *average* correlations by only taking into account the very rare events, which, in our notation (12) for the generalized correlation length ξ_q corresponds to the limit $q \rightarrow \infty$. Consequently his result $\nu = 2$ should be an upper bound of our ν_q . What is denoted by *typical* correlations in [9] seems to us more related to our averaged correlation functions.

Our finite-size analysis leads to finite values for the dynamical exponent z , which might be due to the small system sizes we were confined to. However, for $j_2 \rightarrow 0$ we find $z \rightarrow \infty$ in agreement with a RNG-picture [9]. Furthermore we find that the order-parameter probability distribution scales non-trivially at the critical temperatures. We made this observation also in connection with the cumulants of the probability distribution of correlation functions and we found a hierarchy of critical exponents for the generalized correlation lengths. Despite these facts the numerical value β/ν for the finite-size scaling of the averaged spontaneous magnetization concurs with the prediction made in [9].

All these phenomena merit further investigation (a more detailed discussion on these results will be given elsewhere [23]), especially with respect to the Griffiths singularities occurring already at temperatures above T_c [9,13]. Finally we would like to mention that there is also a large overlap of the scenario we have encountered here with what might occur in two- and three-dimensional Ising spin glass in a transverse field [7,8].

ACKNOWLEDGMENTS

AC is grateful to G. Parisi, E. Marinari and A. Vulpiani for an interesting discussion and thanks the Institut für Theoretische Physik of the University of Köln for hospitality where part of this work was done. HR would like to thank L. Mikheev and A. P. Young for many extremely valuable discussions. He acknowledges the allocation of about 10^5 processor hours on the transputer cluster Parsytec-GCel1024 from the Center of Parallel Computing (ZPR) in Köln. This work was performed within the SFB 341 Köln-Aachen-Jülich.

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FIGURES

FIG. 1. Scaling plot of the magnetization $M(L, L_\tau)$ for $j_2 = 0.1$ at T_c . It yields $z = 1.65 \pm 0.05$ and $\beta/\nu = 0.17 \pm 0.01$. The insert shows the scaling plot of the susceptibility $\chi(L, L_\tau)$ with $\gamma'/\nu = 2.3 \pm 0.1$ and z as for M .

FIG. 2. Scaling plot of the averaged cumulant $g_{\text{av}}(L, L_\tau)$ for $j_2 = 0.1$ at $T = T_c$ with $z = 1.55 \pm 0.05$.

FIG. 3. **Insert:** Correlation function in the (imaginary) time direction $C(0, t)$ for $j_2 = 0.05$ at $T = T_c$. The system sizes are 4×16 , 6×32 , 8×64 , 12×100 and 16×160 , i.e. their aspect ratio is close to the maximum of the cumulant g_{av} and therefore roughly constant. The full curve is a least square fit to $C(0, t) \propto t^{-\eta_\perp} + (160 - t)^{-\eta_\perp}$ and yields $\eta_\perp = 0.23 \pm 0.01$. **Left part:** Correlation function in the space direction $C(r, 0)$ for $j_2 = 0.05$ at $T = T_c$. The system size is 16×160 , close to the maximum of g_{av} . The full line is a least square fit to $C(r, 0) \propto \exp(-a r^{1/2}) + \exp(-a (L - r)^{1/2})$ with $a = 0.62$.

FIG. 4. Scaling plot for the typical correlation length in the spatial direction $\xi_0^{-1} L_\tau^{1/z_0}$ versus $(T - T_c) L_\tau^{1/z_0 \nu_0}$. The upper data-set is for $j_2 = 0.05$, where $z_0 = 2.12$ and $\nu_0 = 0.7$ has been used, the lower data-set is for $j_2 = 0.1$, where $z_0 = 1.74$ and $\nu_0 = 0.7$.







