Eur. Phys. J. B **9**, 233–236 (1999)

THE EUROPEAN PHYSICAL JOURNAL B

EDP Sciences

Application of a continuous time cluster algorithm to the two-dimensional random quantum Ising ferromagnet

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Received 6 November 1998

Abstract. A cluster algorithm formulated in continuous (imaginary) time is presented for Ising models in a transverse field. It works directly with an infinite number of time-slices in the imaginary time direction, avoiding the necessity to take this limit explicitly. The algorithm is tested at the zero-temperature critical point of the pure two-dimensional (2d) transverse Ising model. Then it is applied to the 2d Ising ferromagnet with random bonds and transverse fields, for which the phase diagram is determined. Finite size scaling at the quantum critical point as well as the study of the quantum Griffiths-McCoy phase indicate that the dynamical critical exponent is infinite as in 1d.

PACS. 75.50.Lk Spin glasses and other random magnets – 05.30.-d Quantum statistical mechanics – 75.10.Nr Spin-glass and other random models

Quantum phase transitions (QPT) in random transverse Ising models at and close to their quantum critical point at zero temperature have attracted a lot of interest recently [1]. In particular in one dimension many astonishing results have been obtained with powerful analytical [2,3] and numerical [4,5]) tools. Among the most important results is that *at* the critical point time scales diverge exponentially fast, implying that the dynamical exponent is $z_{\rm crit} = \infty$. Such a behavior is reminiscent of thermally activated dynamics in classical random field systems [6], and has also been proposed for the Anderson-Mott transition of disordered electronic systems at the QPT [7].

The other important result for random transverse Ising models in any dimension is that close to the quantum critical point there is a whole region in which various susceptibilities diverge for $T \to 0$ and that all these singularities, also called Griffiths-McCoy singularities [8,9], can be parameterized by a single dynamical exponent $z(\delta)$ that varies continuously with the distance δ from the critical point [1,10]. Recently it has been argued that experimentally observed non-Fermi liquid behavior in f-electron compounds can be nicely explained within such a scenario [11]. In *one* dimension $z(\delta)$ *diverges* for $\delta \to 0$. It is not clear in how far these properties, *i.e.* $z_{\rm crit} = \infty$ and $z(\delta \to 0) = z_{\rm crit}$ also apply in higher dimensions: in 2 and 3-dimensional transverse Ising *spin glass* models a *finite* value for $z_{\rm crit}$ has been reported [12] and for finite dimensional bond *diluted* ferromagnets it has been shown [13] that $z_{\rm crit}$ is infinite only at the percolation threshold.

In this paper we therefore consider the two-dimensional random ferromagnet (without dilution) in a transverse field with the help of a new Monte-Carlo cluster algorithm that is particularly suited to handle the inherent difficulties in the study of such a random quantum system: the origin of the Griffiths-McCoy singularities are strongly coupled clusters (with strong ferromagnetic bonds and weak transverse fields) which are extremely hard to equilibrate in a conventional Monte-Carlo algorithm, therefore we had to use a cluster method. Moreover, the exponent $z(\delta)$ is a *non-universal* quantity for which reason we really have to perform the so-called Trotter-limit explained below.

A continuous time algorithm that incorporates this limit right from the beginning (in the spirit of Refs. [16, 17]) is the most efficient method we can think of. In the first part of this paper we present the method we use and apply it to the pure case in two dimensions, in the second part we present our results for the random case. In a related work [14] a short account of our results on the Griffiths-McCoy phase in the random system has been given and also a study of essentially the same model with a discrete time cluster algorithm, *not* performing the Trotter limit and therefore concentrating on the *critical* behavior, was presented.

The system we are interested in is defined by the quantum mechanical Hamiltonian

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij}\sigma_i^z\sigma_j^z + \sum_i \Gamma_i \sigma_i^x \qquad (1)$$

in which σ_i are spin-$\frac{1}{2}$ operators located on *any* d-dimensional lattice (below we consider a $L \times L$ square

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lattice with periodic boundary conditions), $\langle ij\rangle$ indicate all nearest neighbor pairs on this particular lattice, $J_{ij} \geq 0$ *ferromagnetic* interactions (either uniform $J_{ij} = J$ or random) and Γ_i transverse fields (either uniform $\Gamma_i = \Gamma$ or random – note that the sign of Γ_i can always be gauged away by a local spin rotation).

To derive our continuous time algorithm we use the Suzuki-Trotter decomposition to represent the free energy $\mathcal{F}$ of the system (1) at inverse temperature $\beta = 1/T$ as the *limit* of a (d+1)-dimensional classical Ising model [18]:

$$\mathcal{F} = -\beta^{-1} \lim_{\Delta\tau\to 0} \ln \operatorname{Tr} \exp(-\mathcal{S}_{\text{class}}), \tag{2}$$

$$\mathcal{S}_{\text{class}} = -\sum_{\tau,\langle ij\rangle} K_{ij} S_i(\tau) S_j(\tau) - \sum_{\tau,i} K'_i S_i(\tau) S_i(\tau+1).$$

Here the additional index $\tau = 1, \ldots, L_\tau$ of the now *classical* Ising spin variables $S_i(\tau) = \pm 1$ labels the L_τ d-dimensional (imaginary) time slices within which spins interact *via* $K_{ij} = \Delta\tau J_{ij}$ and among which they interact with strength $K'_i = -\frac{1}{2} \ln \tanh \Delta\tau\Gamma_i$. The number of time slices L_τ is related to $\Delta\tau$ by $\Delta\tau = \beta/L_\tau$, so that the limit $\Delta\tau \to 0$ in (2) implies $L_\tau \to \infty$.

Taking the limit $\Delta\tau \to 0$ consecutive spins with the same value along the imaginary time direction, *e.g.* $S_i(\tau)$=$S_i(\tau$+1)=$\cdots$=$S_i(\tau$+$N)$, form continuous *segments* $\overline{S}_i\{[\tau, \tau+t]\}$ of length $t = N\Delta\tau$ rather than individual lattice points. Since we are going to take this limit implicitly we will have to consider these imaginary time segments as the dynamical objects in a Monte-Carlo algorithm, and not the individual spin values at discrete imaginary times any more. These segments correspond to continuous, uninterrupted pieces of a spin's world line during which it has the same value, say +1, and its two ends, in the following called *cuts*, are those times when this spin changes to another value, say −1.

As the next step we apply the scheme of the Swendsen-Wang cluster update method [19] within the aforementioned implicit continuous time limit. Remember that in this method in order to construct the clusters to be flipped at random, neighboring spins pointing in the same direction are connected with a certain probability p: for neighbors in the space direction, for instance $S_i(\tau)$ and $S_j(\tau)$ with $\langle ij\rangle$ being nearest neighbors, it is $p_{ij} = 1 - \exp(-2K_{ij}) = 2\Delta\tau J_{ij} + \mathcal{O}(\Delta\tau^2)$ and for neighbors in imaginary time, for instance $S_i(\tau)$ and $S_i(\tau+1)$, it is $p'_i = 1 - \exp(-2K'_i) = 1 - \Delta\tau\Gamma_i + \mathcal{O}(\Delta\tau^2)$. These spin connection probabilities are now translated into probabilities for creating (cutting) and connecting segments.

The probability for connecting spins along the imaginary time direction at a particular site i over a finite time interval of length $t < \beta$ is given by the probability to set $t/\Delta\tau$ bonds, *i.e.* in the limit $\Delta\tau \to 0$

$$p_i'^{t/\Delta\tau} = (1 - \Delta\tau\Gamma_i)^{t/\Delta\tau} \to \exp(-\Gamma_i t). \tag{3}$$

This means for each site one generates new cuts in addition to the old ones from the already existing segments *via* a Poisson process with decay time $1/\Gamma_i$ along the imaginary time direction. Next one connects segments on neighboring sites i and j that have the same state and a non-vanishing time-overlap t, *e.g.* $\overline{S}_i\{[t_1, t_2]\}$ and $\overline{S}_j\{[t_3, t_4]\}$ with t now the length of the interval $[t_1, t_2] \cap [t_3, t_4]$). The probability for *not* connecting the two segments is given by

$$(1 - p_{ij})^{t/\Delta\tau} = (1 - 2\Delta\tau J_{ij})^{t/\Delta\tau} \to \exp(-2J_{ij}t) \tag{4}$$

in the limit $\Delta\tau \to 0$. Finally, one identifies clusters of connected segments and assigns each of them (and herewith all of the segments belonging to it) one value +1 or −1 with equal probability. In Figure 1 the individual steps of this cluster update procedure are illustrated. The measurement of observables is straightforward: for instance the local magnetization m_i at site i for one particular configuration of segments is simply given by the difference between the total length of all +segments and the total length of all −segments, divided by β. The expectation value for the local susceptibility is

$$\chi_i(\omega = 0) = \int_0^\beta \mathrm{d}\tau \langle \sigma_i^z(\tau)\sigma_i^z(0)\rangle_{\text{QM}} = \beta \langle m_i^2 \rangle_{\text{MC}}, \tag{5}$$

where $\langle \cdots \rangle_{\text{QM}}$ is the quantum mechanical expectation value for model (1) and $\langle \cdots \rangle_{\text{MC}}$ is an average over all configurations generated during the Monte-Carlo run.

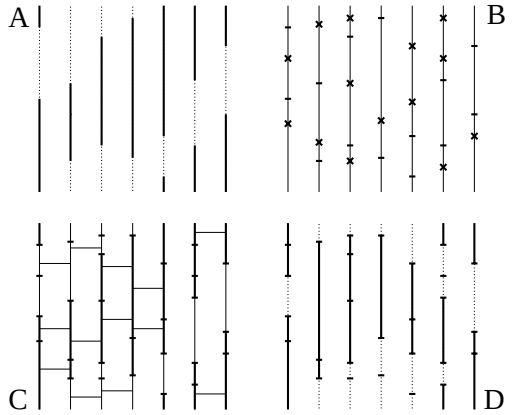

Fig. 1. Sketch of the cluster construction procedure: (a) configuration of segments before update — full (broken) lines correspond to worldline segments with spin up (down). (b) Insertion of new cuts (crosses) in addition to old ones (bars) according to a Poisson process along each worldline described by (3). (c) Connection of segments with probabilities given by (4). (d) Configuration of segments after assigning randomly a spin value to each cluster of connected segments. Before starting a new cycle (with A) the redundant cuts *within* segments are removed.

For an actual implementation of the algorithm one has to provide sufficient memory in which the information about the segments $\overline{S}_i\{[t_1, t_2]\}$ (site index i, starting point t_1, end point t_2 and state +1 or −1) is stored in linked lists. The number of segments, which of course fluctuates, is typically of the order $\mathcal{O}(\beta\Gamma_{\max}L^d)$, whereas in discrete time algorithm the number of spin values to be stored is $\beta L^d/\Delta\tau$, which diverges in the limit $\Delta\tau \to 0$.

We tested our code first for the one-dimensional pure case ($d = 1$, $J_{ij} = 1$ and $\Gamma_i = \Gamma$), for which the critical properties at $T = 0$ are identical to those of the classical

2-dimensional Ising model and are well-known exactly [20] ($\Gamma_c = 1$, $\nu = 1$, $\beta = 1/8$, $z = 1$).

As a first non-trivial application we considered the *pure* case (again $J_{ij} = 1$ and $\Gamma_i = \Gamma$) in *two* dimensions, where the quantum critical point at Γ_c is in the universality class of the classical 3-dimensional Ising model. Close to this quantum critical point quantities are expected to obey finite size scaling forms

$$\langle \mathcal{O} \rangle = L^{x_\mathcal{O}} \tilde{q}(L^{1/\nu}\delta, L^z/\beta) \tag{6}$$

with $\delta = \Gamma - \Gamma_c$ and $x_\mathcal{O}$ the finite size scaling exponent of the quantity $\mathcal{O}$. From the equivalence with the 3-dimensional classical Ising model one knows the dynamical exponent *a priori* to be $z = 1$, thus we can perform conventional one-parameter finite size scaling if one chooses the aspect ratio β/L to be constant. In Table 1 we list the results of the finite size scaling analysis of our data for system sizes up to $L = 32$ (and $\beta = 8$). Our estimates for the critical field value $\Gamma_c = 3.044(1)$ and the thermal exponent $\nu = 0.625(5)$ agree well with the series expansion result [21] and a recent DMRG study [22].

The real challenge for our algorithm (and our main motivation for implementing it) is the *random* case, which we consider now. The ferromagnetic couplings as well as the transverse field are now quenched random variables, which we define both as being uniformly distributed, *i.e.*

$$P(J_{ij}) = \begin{cases} 1, & \text{for } 0 < J_{ij} < 1 \\ 0, & \text{otherwise} \end{cases}$$

$$P'(\Gamma_i) = \begin{cases} \Gamma^{-1}, & \text{for } 0 < \Gamma_i < \Gamma \\ 0, & \text{otherwise} \end{cases} . \tag{7}$$

Observables now have to be averaged over a large number (10^3–10^4) of disorder configurations, which will be indicated by $[\dots]_{\rm av}$.

The main interest in our investigation is the determination of the dynamical exponent at and above the quantum critical point. Since both are unknown, it is hard to work with a finite size scaling form like (6). Therefore we have chosen the following procedure: first we determine the (T, Γ) phase diagram of the model (1) with (7) by calculating the averaged ratio of moments $[g]_{\rm av}$ for various system sizes L at fixed temperature $T > 0$, corresponding to a fixed system size in the imaginary time direction. Thus, at any finite temperature the system is expected to be in the universality class of the *classical* two-dimensional random bond Ising ferromagnet. For large enough system size the finite size scaling analysis to detect this classical phase transition proceeds in the conventional manner by studying the Γ-dependence of $[g]_{\rm av}$, which at Γ_c is expected to be dimensionless (*i.e.* has no system size dependence). For small temperatures (*i.e.* large system size in the imaginary time direction) the crossover region to the quantum universality class becomes larger, necessitating larger system sizes (we went up to $L = 32$) to get a reliable estimate of $\Gamma_c(T)$. By extrapolating the latter to $T = 0$, see Figure 2, we obtain for the location of the quantum critical point $\Gamma_c = \Gamma_c(T = 0) = 4.2 \pm 0.2$. Obviously the systematic error in this extrapolation is hard to estimate, the value 0.2 for our error bar is essentially a statistical error based on a quadratic approximation of the phase boundary close to Γ_c.

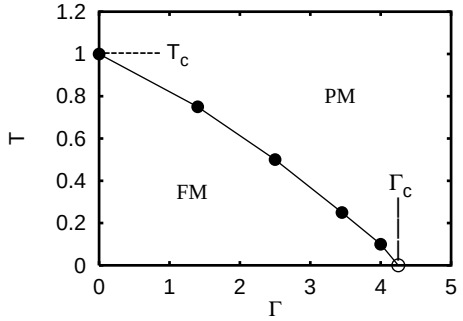

Fig. 2. The phase diagram of the two-dimensional *random* transverse Ising model. PM means paramagnetic, FM means ferromagnetic, $T_c = 1.00(1)$ is the critical temperature of the classical random Ising ferromagnet with a uniform bond distribution between 0 and 1, and $\Gamma_c = 4.2(2)$ the location of the quantum critical point we are interested in. The filled dots are obtained by analysing our Monte-Carlo data for finite temperatures as described in the text, their statistical error is smaller then the point size.

For $\Gamma = \Gamma_c$ it is $\delta = 0$ and any observable is expected to be a function of the aspect ratio β/L^z alone. On the other hand, *if* the two-dimensional case, which we consider here, is similar to the one-dimensional case where one has unconventional (or activated) scaling [2–5] one would expect $z = \infty$, which implies that $\ln \beta/L^\psi$ would be the appropriate scaling variable (with ψ a fit-parameter, playing the role of the barrier exponent in classical activated dynamics [6,7,23]). Our data scale much better according to the latter scenario with ψ close to 0.5 as in 1d (details will be published in [15]). The corresponding study of the critical behavior of the discretized model reported in [14] yields an estimate of $\psi = 0.42$.

Now we turn our attention to the Griffiths-McCoy region in the disordered phase ($\Gamma > \Gamma_c$). 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 $T = 0$ [4,5,10]

$$\Omega(\ln \chi_{\rm local}) \approx -\frac{d}{z(\Gamma)} \ln \chi_{\rm local} \tag{8}$$

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 $z(\Gamma)$ 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 Ω 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 $\beta \leq 1000$ and averaged over at least 512 samples.

Table 1. Estimates for the critical field strength and the critical exponents for the quantum phase transition of the *pure* two-dimensional transverse Ising model. The left column indicates the quantity for which the finite size scaling analysis with constant aspect ratio $\beta = L/4$ has been performed (m = magnetization, χ = uniform susceptibility and g = dimensionless ratio of moments). The values in brackets are obtained from the scaling relation $\gamma/\nu = d + z - 2\beta/\nu$ ($d = 2$ and $z = 1$ here).

	FSS form	Γ_c	ν	β/ν	γ/ν
m	$L^{-\beta/\nu}\tilde{m}(L^{1/\nu}(\Gamma - \Gamma_c))$	3.0440(2)	0.622(3)	0.5050(5)	[1.990(1)]
χ	$L^{\gamma/\nu}\tilde{\chi}(L^{1/\nu}(\Gamma - \Gamma_c))$	3.0437(1)	0.621(1)	[0.500(3)]	2.000(5)
g	$\tilde{g}(L^{1/\nu}(\Gamma - \Gamma_c))$	3.0435(2)	0.629(5)	—	—

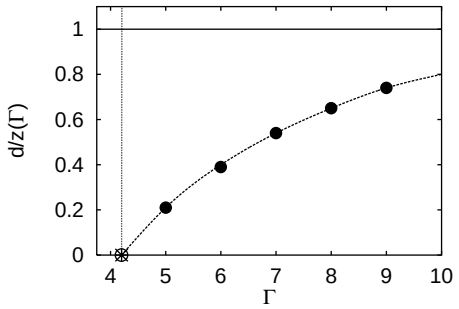

Fig. 3. The value of $d/z(\Gamma)$ obtained from analyzing the integrated probability distribution of $\ln \chi_{\rm local}$ according to (8) in the Griffiths-McCoy region. The vertical line indicates the (approximate) region of the critical point at $\Gamma_c \sim 4.2$, the open circle corresponds to $z(\Gamma_c) = \infty$ and the horizontal line at $d/z = 1$ indicates the expected limit $\lim_{\Gamma\to\infty} z(\Gamma) = d$. The broken line is just a guide to the eye, the statistical error of our estimates for d/z is smaller than the point size.

In Figure 3 we show our result for $d/z(\Gamma)$ in the Griffiths-McCoy region. For $\Gamma \to \infty$ we expect $d/z(\Gamma) \to 1$, since this is the results for *isolated* spins in random fields with non-vanishing probability weight at $\Gamma_i = 0$. The more interesting limit is $\Gamma \to \Gamma_c$. The data are well compatible with $\lim_{\Gamma\to\Gamma_c} z(\Gamma) = \infty$, implying that here, in analogy to the one-dimensional case [2,4] this limit and the *critical* dynamical exponent $z_{\rm crit}$ agree.

To summarize we have presented a new Monte-Carlo cluster algorithm in continuous imaginary time with which we studied the random transverse Ising model in two dimensions. We determined the temperature-transverse field phase diagram, estimated the location of the quantum critical point at zero temperature and performed a finite size scaling analysis at the critical point. Here we found indications for an exponential divergence of time scales ($z = \infty$) and also the dynamical exponent parameterizing the strength of the quantum Griffiths-McCoy singularities extrapolates to $z(\Gamma \to \Gamma_c) = \infty$. In this respect the phenomenology of the one-dimensional model seems to extend to higher dimension. Another aspect is the different scaling behavior of average and typical correlations in the one-dimensional case, which is present in two dimensions, too [14].

We thank F. Iglói and A. P. Young for helpful discussions. H. R.'s work was supported by the Deutsche Forschungsgemeinschaft (DFG) and is grateful to the Toho University Department of Physics for kind hospitality. N. K.'s work was supported by the grant-in-aid (No. 09740320) from the ministry of education, science, sport and culture of Japan.

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