Dynamic scaling in diluted systems: Deactivation through thermal dilution

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Activated scaling is confirmed to hold in transverse field-induced phase transitions of randomly diluted Ising systems. Quantum Monte Carlo calculations have been made not just at the percolation threshold (p_c) but also well below and above it. We follow the evolution of the activated scaling at zero temperature in the phase transition from ferromagnetic to quantum Griffiths phase ($p>p_c$) at the phase boundary ($p=p_c$) and for transitions inside the nonferromagnetic quantum Griffiths phase ($p<p_c$). A novel deactivation phenomenon inside the nonferromagnetic Griffiths-McCoy phase ($p<p_c$) is observed using a thermal (in contrast to random) dilution of the system.

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The presence of quenched disorder in quantum phase transitions at zero temperature is a topic of current interest. Two of the most important special properties of the disordered quantum phase transitions are the appearance of *activated dynamic scaling* and the existence of *Griffiths-McCoy singularities* [1,2] even away from the critical point.

Activated dynamic scaling was first analytically proved to hold in the disordered one-dimensional Ising model in a transverse field [3], and there are many other results for this model in the literature [4–8]. The disordered Ising model in a transverse field considered as a quantum spin glass provides a reasonable description of the system $LiHo_xY_{1-x}F_4$ [9] and also, considering the existence of long-range correlated disorder in it, may be an appropriate model to describe non-Fermi-liquid behavior in certain *f*-electron systems [10–12]. Activated dynamic scaling implies the existence of an infinite dynamic critical exponent ($z=\infty$). It means that instead of the typical power-law relationship between the characteristic time scale and the characteristic length scale, $\xi_\tau \sim \xi^z$, a new exponential relation appears, $\xi_\tau \sim \exp(\text{const} \times \xi^\psi)$ with $\psi=\frac{1}{2}$ for the one-dimensional Ising model [3]. There are almost no analytical results for higher dimensions. The activated dynamic scaling seems to disappear for two-dimensional [13] and three-dimensional Ising glass systems [14], but it has been proved to hold in the disordered two-dimensional Ising model in a transverse field by means of quantum Monte Carlo simulations [15,16] and renormalization-group analysis [17]. The only analytical prediction of activated scaling in dimensions higher than 1 has been made for the dilution probability transition at the percolation threshold (p_c) of a diluted Ising system in a transverse field [18], where percolation critical exponents have been found.

The phase boundary of this model at $T=0$ was studied a long time ago [19–21] and is expected to have a multicritical point and a straight vertical phase boundary separating the ferromagnetic phase from the quantum Griffiths phase at the percolation threshold. The existence of this boundary and the activated scaling predicted by Senthil *et al.* has been recently checked by means of quantum Monte Carlo simulations, comparing the dilution probability transitions at constant transverse fields for p values below and above the one corresponding to the multicritical point [22].

However, there is no study of the existence of activated scaling for transitions tuned by the transverse field in diluted Ising systems. These systems present a great advantage: fixing the probability of occupied places (p) and varying the transverse field (Γ) at $T=0$, it is possible to follow the evolution of the activated scaling at zero temperature in the phase transition from ferromagnetic to quantum Griffiths phase ($p>p_c$) at the phase boundary ($p=p_c$) and for transitions inside the nonferromagnetic quantum Griffiths phase ($p<p_c$). In this paper, we will use the diluted Ising model in a transverse field to directly determine the existence and evolution of activated scaling in the three different zones of the phase diagram. We will show how the activated scaling exists not just at the percolation threshold but well above it and how it reaches a maximum near the phase boundary ($p=p_c$) keeping mostly constant for values $p<p_c$. We start from the two-dimensional ($d=2$) diluted Ising model in a transverse field with the Hamiltonian given by

$$\mathcal{H}=-\sum_{\langle i,j\rangle} \varepsilon_i\varepsilon_j\sigma_i^z\sigma_j^z-\Gamma\sum_i \varepsilon_i\sigma_i^x, \tag{1}$$

where $\varepsilon_i\in\{0,1\}$ are quenched random variables producing the dilution. $\varepsilon_i=1$ with probability p and $\varepsilon_i=0$ with probability $1-p$. In order to perform the Monte Carlo calculations, we use the Suzuki-Trotter decomposition [23] and we map the phase transition at $T=0$ of the two-dimensional quantum system in a three-dimensional classical system with action

$$\mathcal{S}=-K_{\text{hor}}\sum_{\tau,\langle i,j\rangle} \varepsilon_i\varepsilon_j s_i(\tau)s_j(\tau)-K_{\text{ver}}\sum_{\tau,i} \varepsilon_i s_i(\tau)s_i(\tau+1) \tag{2}$$

with $K_{\text{hor}}=\Delta\tau$, $K_{\text{ver}}=-(1/2)\ln[\tanh(\Delta\tau\Gamma)]$, and $\Delta\tau\to 0$. This limit may be taken into account exactly considering a continuous time algorithm [16], however making use of the universality between the model with $\Delta\tau\to 0$ and the model with $\Delta\tau\neq 0$, we may simulate the usual discrete Ising model, but with anisotropic interactions. In order to avoid problems

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arising from the critical slowing down at the critical point, we use the Wolff single cluster algorithm [24]. It is important to notice that once a spin is diluted, the whole imaginary time axis (Trotter axis) is also diluted, which means that the random disorder in a quantum system is equivalent to the long-range correlated disorder in classical systems [25] giving rise to a different universality class. In order to obtain the $T=0$ phase boundary, we fix the occupied site probability (p) and we consider different values of the transverse field (Γ) at intervals of $\Delta\Gamma=0.02$. We really do not fix the probability but rather the concentration, which means that we do not use a grand-canonical distribution of the vacancies but rather a canonical distribution, however both kinds of constraints are supposed to belong to the same universality class [26].

The critical magnetic field for each probability is determined by a method previously used for Ising spin glasses [13,14]. First it is necessary to compute the Binder cumulant average from a certain number of realizations of the disorder (in our case, we consider 500 different realizations). This is done for a fixed value of (Γ,p) and for a fixed value of the size (we consider the values $L=8,12,16,24$). Then we study the evolution of such a cumulant for different sizes of the Trotter axis (we consider up to $L_\tau=600$). Due to the dynamic scaling form of the Binder cumulant, it has a peak as a function of L_τ. At the critical point $[\Gamma_c(p)]$, the peak height is independent of L and the values of L_τ at the maximum, $(L_\tau)_m$, vary as L^z for conventional dynamic scaling and as $(L_\tau)_m \sim \exp(\text{const}\times L^{\psi})$ for activated scaling. Of course, all the nonuniversal quantities, such as, for example, the critical values of the transverse field, will depend on the model and in particular on $\Delta\tau$. In the present work, we choose $\Delta\tau=\frac{1}{5}$.

The results for the phase boundary at $T=0$ are shown in Fig. 1 together with the phase boundary obtained for the classical system by means of conventional scaling. The points where the existence of activated scaling is going to be checked are $p=1$ (pure case), $p=0.8,0.7$ ($p>p_c$), $p=0.6 \simeq p_c \simeq 0.59$ [27], and $p=0.55,0.5$ ($p<p_c$). The results for $(L_\tau)_m$ vs L are presented in Fig. 2. Note how the scaling is not activated for the pure case ($p=1$) where the dynamical exponent is found to be $z\approx 1$, but it starts to activate as the dilution is increased. To ensure that for diluted cases the scaling is activated, Fig. 3 presents a plot of $\ln(L_\tau)_m$ vs L. The straight line behavior for the values $p\neq 1$ clearly indicates that the scaling is activated. The evolution of the values $\psi(p)$ is presented in the inset. Note how it grows monotonically until $p\simeq p_c$ and then it keeps approximately constant inside the ($p<p_c$) zone.

So, basically, the results presented indicate that the scaling is activated not just near the percolation threshold but well above it, and that it keeps nearly constant when the transition considered occurs inside the nonferromagnetic Griffiths-McCoy quantum zone ($p<p_c$), at least for the values of p considered, which are near p_c (it may also be a maximum). It would be interesting to investigate whether ψ keeps growing, or is indeed a constant for $p<p_c$. Note that

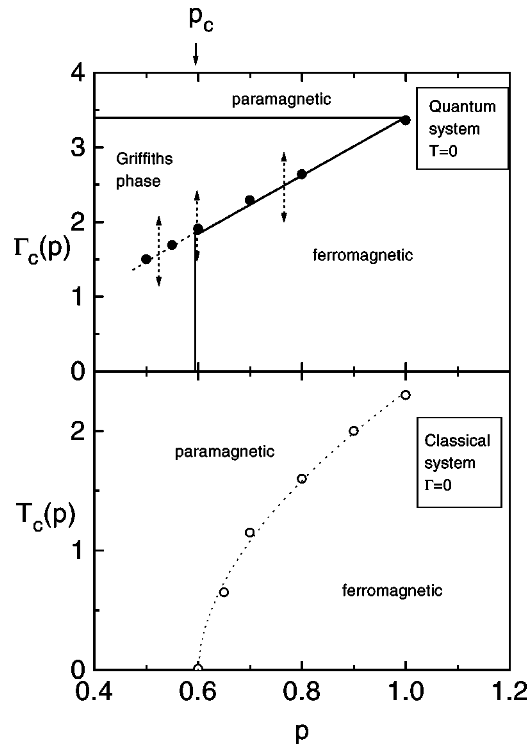

FIG. 1. Phase diagram calculated for the classical model, T_c vs p (white points), and for the quantum model at $T=0$, Γ_c vs p (black points). The dashed line in the classical model indicates a power-law fitting behavior of $T_c(p)$ with $p_c=0.6$. Dotted line indicates the phase boundary in the nonferromagnetic Griffiths region ($p<p_c$). The three arrows indicate the transitions to be investigated above the percolation threshold, at the percolation threshold, and below the percolation threshold.

we have been using, up to now, a *purely random* procedure to produce the diluted samples.

The existence of the Griffiths-McCoy zone is due to rare regions that are locally in the wrong phase. Basically, there are some strongly coupled regions or clusters in the ferromagnetic phase even for spin concentrations smaller than the percolation threshold of the system. These zones are found studying the tail of local susceptibilities [7,28–33]. The quantum transitions allow the existence of these clusters in the wrong phase but they are very difficult to detect in classical systems. As we have shown, the phase transitions (tuned by the transverse field) due to these rare regions also present activated scaling.

However, there might be a possible way to deactivate the scaling inside the Griffiths zone for values of $p<p_c$. Using the Suzuki-Trotter formalism, the existence of the wrong phase comes from clusters that are infinite in the imaginary time direction, but they still are *finite* in the perpendicular slices. That is the reason why it is possible to "feel" the effect of the dilution by the existence of an activated scaling. However, if the dilution is not introduced randomly, but incorporates an *infinite correlation length* between spins and vacancies, some of the clusters formed in the slices may be considered to have *infinite size*. The wrong phase arising in these clusters is equivalent to the pure system ordered phase and is not affected by disorder. In this case, the system in the

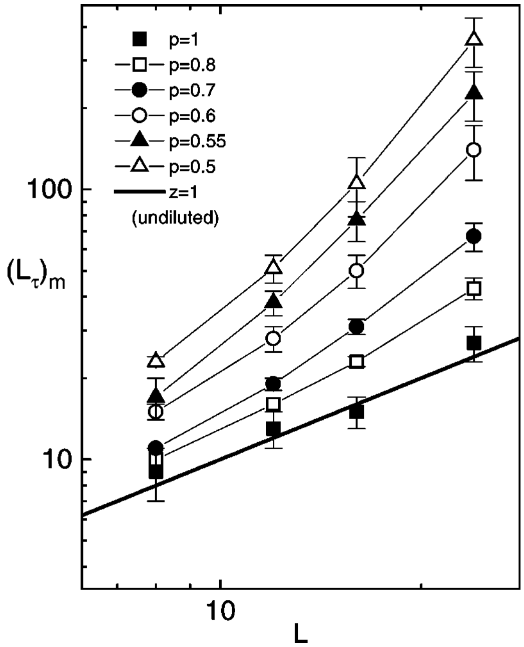

FIG. 2. $(L_\tau)_m$ vs L for different values of the spin concentration. Thin straight lines are just a guide for the eye. Thick line represents the behavior expected for the pure system $(z=1)$.

Griffiths zone is expected to show deactivated scaling. Of course, this will happen only if the phase transition is due to the existence of strongly coupled regions (i.e., if the system has an occupation probability $p<p_c$), but if the magnetic

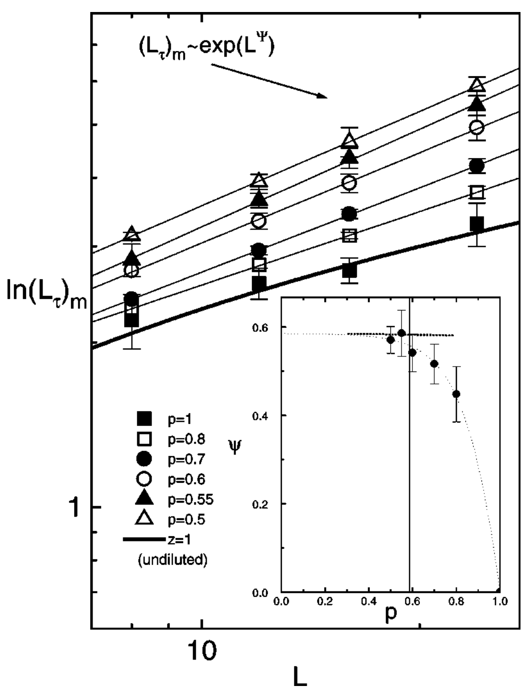

FIG. 3. $\ln(L_\tau)_m$ vs L for different values of the spin concentration. Thin lines are the linear fittings and the thick line is the behavior expected for the pure system $(z=1)$. Inset shows the behavior of the exponent $\psi(p)$. Dotted line is a sigmoidal fitting with $\psi=1$ for $p=1$.

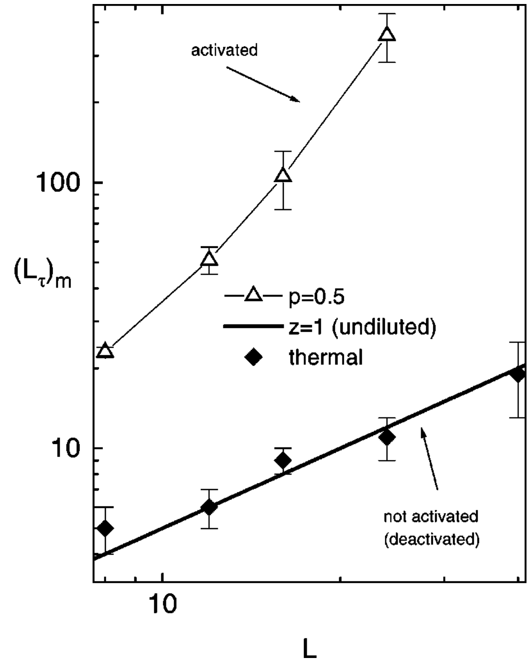

FIG. 4. $(L_\tau)_m$ vs L for a randomly diluted system with spin concentration $p=0.5$ and a thermally diluted system. The thin line is a guide for the eye, and the thick line represents the behavior expected for the pure case $(z=1)$ excepting proportional factors. Note how the scaling has been deactivated for the thermal case.

response is due to the whole system (i.e., $p>p_c$), the introduction of long-range correlated disorder will affect changing the universality class of the system (as in thermal classic transitions [25]) and enhancing the activation of the scaling [12].

A way to produce this kind of dilution is by using the *thermal* dilution instead of a random dilution [34]. With this kind of dilution, the system belongs to the universality class of *long-range correlated disordered systems* with an exponent $a=2-\eta$ [35], where η is equal to 0.25 for the classical $(d=2)$ Ising model (the way to produce thermal dilution is described in [34]). Basically the procedure is as follows. The pure system is first thermalized to criticality and then one kind of spin is turned into a vacancy. The main property of thermally diluted samples is that the spins and the vacancies are distributed in clusters of all sizes and are not randomly distributed in small clusters. This resulting distribution of spins and vacancies produces a *deactivation* of the dynamic scaling in the $p<p_c$ region due to the fact that the larger diameter clusters, made up of Trotter spin tubes, are less sensitive to the surrounding vacancies. The samples produced by thermal dilution at criticality will have a spin concentration near $p=0.5$, so we can compare them only with samples diluted randomly with probability $p=0.5$. Both kinds of dilution will be at the nonferromagnetic Griffiths phase since in both cases $p_c(a)>0.5$ [36].

The analysis performed has been exactly the same as before, but now going up to $L=40$. By the Binder cumulant we have been able to determine the critical transverse magnetic field $[\Gamma_c(\text{thermal})\simeq 3.13]$ and the relation between $(L_\tau)_m$ and L. Figure 4 compares the behavior of the thermal dilution with the behavior of the random dilution with $p=0.5$. The thick line represents the pure behavior (except for the proportional factors). Clearly, the scaling has been deactivated, as expected, and $z\simeq 1$ as corresponds to the behavior of the pure system. This phenomenon could never happen for a system with $p>p_c$.

In conclusion, quantum Monte Carlo calculations in diluted Ising models in a transverse field at $T=0$ show that dynamic scaling holds above the percolation threshold ($p>p_c$), at the percolation threshold ($p=p_c$), and below the percolation threshold ($p<p_c$). The evolution of the activated scaling has been characterized, showing how it grows monotonously towards the value corresponding to the percolation threshold and how it appears to remain nearly constant in the ($p<p_c$) zone for values of p near p_c. A new way to deactivate the scaling in the nonferromagnetic quantum Griffiths zone ($p<p_c$) by thermal dilution has been proposed. The expected deactivation works due to the fact that phase transitions come from strongly coupled regions, and not from the whole sample. The deactivation has been clearly confirmed by means of quantum Monte Carlo simulations.

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