

## Critical Behavior of the Randomly Spin Diluted 2D Ising Model: A Grand Ensemble Approach

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The critical behavior of the 2D spin diluted Ising model is investigated by a new method that combines a grand ensemble approach to disordered systems with phenomenological renormalization. We observe a continuous variation of critical exponents with the density  $\rho$  of magnetic impurities, respecting, however, weak universality in the sense that  $\eta$  and  $\gamma/\nu$  do not depend on  $\rho$  while  $\gamma$  and  $\nu$  separately do. Our results are in complete agreement with a recent Monte Carlo study.

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The present contribution is concerned with the critical behavior of the 2D spin diluted (SD) Ising model. For this model, the Harris criterion [1], according to which small amounts of disorder do (not) change the nature of the phase transition, if the corresponding pure system's specific heat exponent is positive (negative), is inconclusive, since  $\alpha_{\text{pure}} = 0$ . The critical behavior of the disordered system has been a subject of debate for many years; see [2] and references therein, and [3–10].

Currently, there appears to be widespread consensus that critical exponents of bond disordered (BD) systems in the *weak* disorder limit are the same as those of the pure system, albeit modified by logarithmic corrections [3–6]. Monte Carlo (MC) simulations of BD systems [6,7] indicated that such modifications through logarithmic corrections would persist even in the strongly disordered regime. In [9], on the other hand, a more complicated phase transition and a nondivergent specific heat are predicted. Lastly, a recent MC study of the SD system [10] produces results at variance with the findings of [3–9], in that it gives critical exponents which clearly vary with the density  $\rho$  of occupied sites.

It is this investigation, in particular, which finally convinced us to put our own transfer-matrix analysis of the SD system—both the method and its results—to public discussion, even though, or rather *because* we are aware that a deeper understanding of our approach [11] would still be welcome. In essence, we find that there is full qualitative and quantitative agreement between the MC results of Kim and Patrascioiu [10] and ours.

We study the SD system by a new method [11] which combines Morita's grand ensemble approach to disordered systems [12] with phenomenological renormalization [13]. We begin by briefly describing Morita's method of configuration averaging in systems with quenched randomness. We then state our main results, relegating details of our investigation to a separate publication [14].

Consider a system described by the Hamiltonian  $H(\sigma|\kappa)$ , where  $\kappa$  denotes the quenched disorder configuration, and  $\sigma$  the set of dynamic variables. Morita avoids configuration averaging of the free energy by

working in an enlarged phase space in which  $\kappa$ , too, is a dynamic variable, and by introducing a potential  $\phi(\kappa)$  chosen such that the new system with Hamiltonian  $H^\phi(\sigma, \kappa) = H(\sigma|\kappa) + \phi(\kappa)$  exhibits thermodynamic equilibrium properties identical to the nonequilibrium properties of the quenched system. To achieve this, the distribution  $p^\phi(\sigma, \kappa)$  generated by  $H^\phi(\sigma, \kappa)$  must be constructed such that it satisfies

$$p^\phi(\sigma, \kappa) = \frac{\exp[-\beta H^\phi(\sigma, \kappa)]}{Z^\phi} = \frac{q(\kappa)}{Z(\kappa)} \exp[-\beta H(\sigma|\kappa)] \quad (1)$$

for all  $(\sigma, \kappa)$ . Here  $Z^\phi$  and  $Z(\kappa)$  are partition functions of the grand ensemble and the quenched system at fixed  $\kappa$ , respectively;  $q(\kappa)$  is the probability distribution describing the quenched disorder. If  $\phi$  is normalized such that  $\langle \phi(\kappa) \rangle_q = 0$  [14], Eq. (1) implies

$$\ln Z^\phi = \langle \ln Z(\kappa) \rangle_q - \langle \ln q(\kappa) \rangle_q, \quad (2)$$

where  $\langle \dots \rangle_q$  denotes an average over the quenched disorder. That is,  $\ln Z^\phi$  gives the Brout free energy plus an irrelevant contribution of an entropy of mixing. Equation (2) shows that an equivalent equilibrium system exists.

In order to utilize Morita's ideas in practice, one has to find a representation for  $\phi(\kappa)$  which is adapted to the problem at hand, and one will usually have to resort to approximations [11,14–18]. For the spin diluted Ising model, one may expand  $\phi(\kappa)$  according to

$$\begin{aligned} \beta\phi(\kappa) = & \lambda_0 + \lambda_1 \sum_i k_i + \lambda_2 \sum_{(i,j)} k_i k_j + \dots \\ & + \lambda_p \sum_P \prod_{i \in P} k_i + \dots, \end{aligned} \quad (3)$$

where the occupation numbers  $k_i$  are 1 or 0, if in  $\kappa$  the site  $i$  is occupied or empty [19]. The first sum in (3) is over all lattice sites, the second over nearest neighbor pairs, and the third over all elementary plaquettes of the system. Each term serves to control one *moment* of  $p^\phi(\kappa) = \sum_\sigma p^\phi(\sigma, \kappa)$ , i.e., an expectation under  $p^\phi$  of some product of the  $k_i$ . The couplings  $\lambda_1, \lambda_2, \dots$  have to be determined as functions of temperature and field such

that the moments of  $p^\phi(\kappa)$  coincide with those of  $q(\kappa)$ , while  $\lambda_0$  is required to achieve  $\langle \phi(\kappa) \rangle_q = 0$ .

For an SD system with spin density  $\rho$ , one would have to determine the couplings of  $\phi$  so that [11,17]

$$\begin{aligned} \langle k_i \rangle_\phi &= \rho, \quad \langle k_i k_j \rangle_\phi = \rho^2, \dots \\ \left\langle \prod_{i \in P} k_i \right\rangle_\phi &= \rho^{|P|}, \dots \end{aligned} \quad (4)$$

Here  $\langle \dots \rangle_\phi$  denotes an average with respect to  $p^\phi(\kappa)$  and  $|P|$  the size of the elementary plaquette, which for the square lattice is 4. Equations (4) constitute an *infinite* set of equations for the couplings  $\lambda_1, \lambda_2, \dots$  of the *exact* potential  $\phi$ . To obtain a full solution is, in general, impossible. Interpreting (4) as a set of constraints imposed on the thermal motion of the magnetic impurities, one may, however, set up a *systematic* scheme of approximations by letting only finite subsets of this set of constraints become operative [11,17]. Implementing only  $\langle k_i \rangle_\phi = \rho$ , one would describe an annealed system, which would provide a rather poor description of quenched disorder. If, in addition, one fixes nearest neighbor correlations  $\langle k_i k_j \rangle_\phi$  at their quenched value  $\rho^2$ , the system already exhibits a percolation transition, and is therefore the first serious candidate for the description of fully frozen-in disorder. In this manner, one arrives at increasingly accurate descriptions of quenched disorder as more and more constraints are taken into account, until eventually one obtains an *exact* description of the original disordered system. The hope, of course, is that already rather simple approximations in this hierarchy might belong to the “universality class” of the quenched system.

The method was tested on the 1D system, with the following results [11,14]. In zero field,  $H = 0$ , the first nontrivial approximation involving only  $\lambda_1$  and  $\lambda_2$  already provides the exact solution. If  $H \neq 0$ , *no* finite approximation is exact. Nevertheless, the first nontrivial approximation gives thermodynamic functions usually to within 1% or less of exact results.

At all levels of approximation, one is dealing with translationally invariant equilibrium systems. Their critical behavior in  $d \geq 2$  could be obtained by standard renormalization group (RG) methods, were it not for the fact that the couplings of  $\phi$  are determined only through a set of constraints. Since it is far from obvious how these constraints should be transformed under rescaling (see, however, [17]), we decided to use phenomenological renormalization [13], which avoids this problem altogether. No explicit RG transformation in the space of couplings need be constructed. Given  $\rho$ , one just solves the system in strip geometries—with the appropriate set of constraints (4) imposed [11]. Critical temperatures  $T_c$  and the thermal correlation length exponent  $\nu_t$  are determined from standard phenomenological RG relations [13] for the correlation lengths  $\xi_M(\rho, T)$  of  $(M \times \infty)$  systems at density  $\rho$ , temperature  $T$ , and field  $H = 0$ . By varying  $\rho$ , we obtain the phase boundary  $T_c(\rho)$ , and the thermal

correlation length exponent  $\nu_t$  along the critical line. The method can also be used to study the percolation transition at  $T = 0$ ,  $\rho = \rho_c$ .

We studied four approximations, named (a)–(d). In system (a), only the first and second constraints displayed in (4) are imposed. Due to the anisotropy of the strip geometry, correlations parallel and perpendicular to the strip turn out to be different. We thus introduced system (b) where correlations parallel and perpendicular to the strip are treated as separate constraints. Systems (c) and (d) are obtained from (a) and (b) by fixing, in addition, correlations around each elementary plaquette at  $\rho^4$ . Note that results for systems (a) and (b) or (c) and (d) should approach each other as the strip width  $M$  goes to infinity. This can serve as a valuable consistency check for extrapolations of critical parameters to the infinite system values.

We now turn to the results. We computed  $T_c(\rho)$  for various  $\rho < 1$ . Values obtained for systems (a)–(d) agree very well down to  $\rho \approx 0.75$ . Below  $\rho \approx 0.75$ , the  $T_c(\rho)$  of systems (c) and (d) with the plaquette constraint turn out to be slightly larger than those of systems (a) and (b) without this constraint. As  $\rho \rightarrow 1$ , we obtain  $T_c(\rho) \rightarrow 2.2674$ , which is off the mark by less than 0.1%, and  $-T_c(\rho)^{-1} dT_c(\rho)/d\rho \rightarrow 1.579$ , which differs from the exact result 1.565 [20] by less than 1%. We have also checked the scaling form of the transition line near  $\rho_c$ ,  $\exp[-2J/k_B T_c(\rho)] \sim (\rho - \rho_c)^\varphi$ , with  $\varphi = \nu_t(\rho_c)/\nu_p$ , and we find  $\varphi = 1$  to within less than 2% for all four approximating systems [11]. Here  $\nu_p$  denotes the connectivity length exponent of the percolation transition. The percolation threshold  $\rho_c$  itself ( $\rho_c \approx 0.593$  [21]) is correctly reproduced to within 3% and 1% by systems (a) and (b) and (c) and (d), respectively; see Table I.

Figure 1 shows the correlation length exponent  $\nu$  of system (a), based on extrapolations from strip widths up to  $M = 8$  and 10 for the thermal and the percolation transitions, respectively. They clearly show a variation with the spin density  $\rho$ . For  $\rho = 0.7$  and 0.9, Table I shows that this variation *persists*, as we impose further constraints in systems (b)–(d). Note that the exponents  $\nu$  are always mutually consistent for these four approximating systems. For the percolation transition, they agree well with the exact result  $\nu_p = 4/3$  [22]. Also, the isotropic

TABLE I. Extrapolated critical parameters for percolation, and the thermal phase transition at  $\rho = 0.7$  and 0.9. Numbers in brackets give the estimated error of the last displayed digit of the preceding quantity.

	Percolation		$\rho = 0.7$		$\rho = 0.9$	
	$\rho_c$	$\nu_p$	$T_c$	$\nu_t$	$T_c$	$\nu_t$
(a)	0.609(1)	1.33(2)	1.051(1)	1.31(2)	1.902(1)	1.13(1)
(b)	0.609(1)	1.33(2)	1.050(1)	1.30(2)	1.901(1)	1.13(1)
(c)	0.587(1)	1.34(2)	1.081(1)	1.29(2)	1.901(1)	1.12(1)
(d)	0.587(1)	1.33(2)	1.080(1)	1.30(2)	1.901(1)	1.13(1)

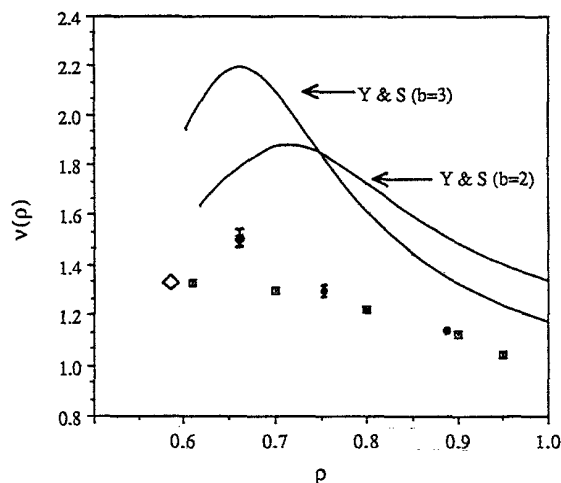


FIG. 1. Correlation length exponent  $\nu$  of system (a) for various densities  $\rho$  (open squares). The leftmost open square was determined as a connectivity length exponent  $\nu_\rho$ . The exact result  $\nu_\rho = 4/3$  is displayed as a diamond at  $\rho_c \approx 0.593$ . Results from a RSRG calculation, using the  $b = 2$  and  $b = 3$  decimation transformations of Yeomans and Stinchcombe, are given as full curves. Full circles show the Monte Carlo data of [10]; except near  $\rho_c$ , where a precise location of the phase boundary is difficult, the agreement with our model (a) results is excellent.

and anisotropic variants in the two groups of systems, (a),(b) and (c),(d), always give consistent results (as they should). While all four systems agree in "universal" characteristics of the phase transition,  $\nu_\rho$  or  $\nu_t$ , the first group can differ from the second as far as the nonuniversal parameters,  $\rho_c$  or  $T_c(\rho)$ , are concerned.

The variation of  $\nu_t$  with  $\rho$  goes against standard universality considerations, and one might well argue it to be an artifact of our simple approximations so we tried to obtain independent evidence. Turning to real-space renormalization group (RSRG) calculations [2], we noted that they, too, are able to produce similar results. The full curves in Fig. 1 are obtained from RSRG decimation transformations *à la* [23], parametrized by the spin density  $\rho$  in a manner proposed in [24]. While such an approach may still seem *ad hoc*, we find that, last but not least, recent large scale MC simulations of the SD system [10] also give a nonuniversal  $\nu_t(\rho)$  in quantitative accord with our results, as can be seen in Fig. 1.

The agreement between the results of [10] and ours goes, in fact, much deeper. We computed susceptibilities and used the finite-size scaling relation  $\chi_M(T_c) \sim M^{\gamma/\nu}$  to determine  $\gamma/\nu$ . We find  $\gamma/\nu \approx 1.75$  as in the pure system, *independently* of  $\rho$ , which implies that  $\gamma$  itself is again nonuniversal. The amplitude  $A_0$  of the critical finite-size correlation length,  $\xi_M(T_c) \approx A_0 M$ , is related to the critical exponent  $\eta$  according to  $A_0 = 1/\pi\eta$  [25]. We used this relation to determine  $\eta$ , and we find  $\eta \approx 0.25$  *independently* of  $\rho$  for the thermal transition, which is of course consistent with the  $\rho$  independence of  $\gamma/\nu$  via

the Fisher relation  $\gamma/\nu = 2 - \eta$ . We find this relation satisfied in systems (a)–(d) at *all* densities, usually to within 1% or better. The same kind of weak universality [26] is also observed in [10]; it is of the same type as that encountered in the eight-vertex model [27].

Some time ago, Derrida *et al.* [28] found analogous nonuniversal behavior of Binder's cumulant ratio in a family of self-dual bond disordered Ising models, which they ascribed to logarithmic corrections to scaling. However, as pointed out by Cardy [29], in order to disentangle logarithmic from power-law corrections to finite-size scaling, one might have to go to rather large strip widths, and our data, as yet, do *not* support the conclusion that the observed nonuniversality is only apparent and caused by logarithmic corrections; see Fig. 2 which shows the variation of the phenomenological critical exponent  $\nu_{M,M-1}$  of system (a) with system size  $M$ , and the inset which addresses this particular point. A recent MC study of the BD system [29] also yields exponents different from those of the pure system, which these authors interpret as being nonasymptotic, because they would violate the Rushbrooke relation, if one *assumes*  $\alpha = 0$  according to [3–6]. However, it turns out that the specific heat data of [30] can equally well be fitted with a *negative*  $\alpha$  [31] consistent with the Rushbrooke relation, so that these exponents may equally well be regarded as asymptotic.

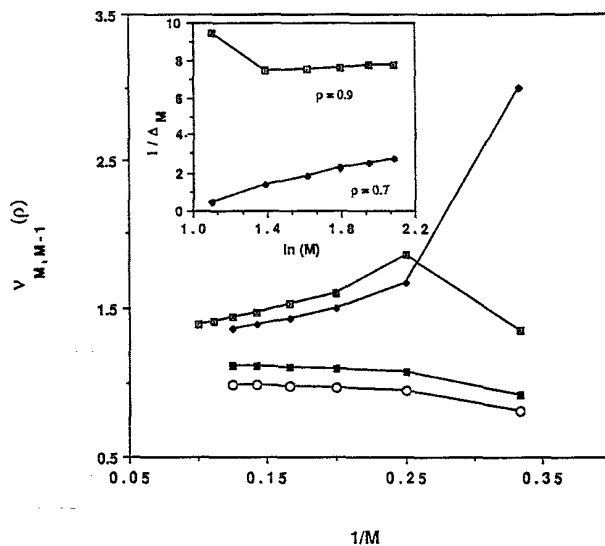


FIG. 2. Variation of the phenomenological critical exponent  $\nu_{M,M-1}$  with strip width  $M$ , for system (a); open squares: percolation; diamonds:  $\rho = 0.7$ ; full squares:  $\rho = 0.9$ ; open circles: pure system. The inset checks for the possibility of logarithmic corrections to the pure systems critical behavior. The quantity  $1/\Delta_M = [\nu_{M,M-1}(\rho) - \nu_{M,M-1}(1)]^{-1}$  is plotted vs  $\ln(M)$ . For  $\rho = 0.9$ ,  $1/\Delta_M$  is not monotonically increasing with  $M$  and levels off for large  $M$ , which is evidence against logarithmic corrections. For  $\rho = 0.7$  the data themselves are not as conclusive as for  $\rho = 0.9$ . However,  $1/\Delta_M$  appears to increase slower than linearly with  $\ln(M)$  and there is a trend for the curve to level off.

The complete set of constraints (4) imposes the condition  $\langle \prod_{i \in \omega} k_i \rangle_\phi = \rho^{|\omega|}$  for all subsets  $\omega$  of the lattice, implying that the correlation length describing the  $k_i$  correlations vanishes. Our simple approximations only fix some of these correlations. Others can, of course, be computed and are found to vary only slightly with temperature and field. We have checked that the corresponding correlation length remains small (at most a few lattice spacings) so that our systems may be regarded as "nearly" quenched. Moreover, it can be shown [11,14] that for  $H = 0$  an infinite set of couplings of the exact potential  $\phi$  vanishes, and is thus correctly taken into account already at the level of systems (a)–(d). [It implies, for instance, that in zero field system (a) already provides an exact description of the 1D quenched system.]

In summary, we have studied the critical behavior of the SD Ising model by a new method which combines a grand ensemble approach to disordered systems with phenomenological renormalization. The grand ensemble approach allows one to formulate a *systematic* scheme of approximations, which was successfully tested against exact results in 1D and (concerning exactly known properties of the phase diagram and of the percolation transition) also in 2D. Our main and surprising result in 2D is a continuous variation of critical exponents with the spin density  $\rho$  in a manner that respects weak universality. Our results are in complete qualitative and quantitative accord with those of a recent Monte Carlo study [10]. Hence, the observed variation of critical exponents is most likely *not* an artifact of our grand ensemble description of quenched disorder. Note that in the limit of weak disorder,  $\rho \rightarrow 1$ , our results would not necessarily contradict those of [3–6].

We are currently using our method to study correlated disorder and the wetting transition in the presence of surface disorder, which has recently been a subject of some controversy in the literature.

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