Critical Behaviour of the Randomly Spin–Diluted 2-d Ising Model — A Grand Ensemble Approach

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Abstract

The critical behaviour of the randomly spin-diluted Ising model in two space dimensions is investigated by a new method which combines a grand ensemble approach to disordered systems proposed by Morita with the phenomenological renormalization group scheme of Nightingale. Accurate approximations for the phase diagram and for the connectivity length exponent of the percolation transition are obtained. Our results suggest that the thermal phase transition of the disordered system might be different from that of the pure system: 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 qualitative and quantitative agreement with a recent Monte–Carlo study.

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The present contribution is concerned with the critical behaviour of the randomly spin-diluted (SD) Ising model in two space dimensions. For this model, the Harris criterion [1] according to which small amounts of disorder do (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 behaviour of the disordered system has been a subject of debate for many years; see e.g. [2] and references therein, and [3-10].

Currently, there appears to be widespread consensus — based upon a field–theoretic reformulation of the system with weak bond–disorder (BD) in the critical regime — that, in this limit, critical exponents of the disordered system are the same as those of the pure system, albeit modified by logarithmic corrections [3-6]. Numerical simulations of BD systems [7,8] indicate that such modifications through logarithmic corrections would persist even in the strongly disordered regime. This consensus is, on the other hand, being questioned in [9], where a more complicated phase transition, and a non–divergent specific heat are predicted. Lastly, a very recent large–scale Monte–Carlo study of the SD Ising system [10] produces results which are 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 certainly still be welcome. In essence, we find that there is full qualitative and quantitative agreement between the Monte–Carlo 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. Within this approach, a hierarchy of approximating equilibrium systems is constructed, whose critical behaviour in turn is obtained by phenomenological renormalization. We then state the main results, relegating a detailed description of the method to a separate publication.

Consider a disordered system described by the Hamiltonian \( H(\sigma|\kappa) \), where \( \kappa \) denotes the quenched disorder configuration, and \( \sigma \) the set of dynamic variables of the system. Morita’s approach 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 non-equilibrium properties of the original quenched system. To achieve this, the distribution \( p^\phi(\sigma, \kappa) \) generated by \( H^\phi(\sigma, \kappa) \) must be constructed such that it satisfies

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

for all \((\sigma, \kappa)\), or equivalently \( -\beta \phi(\kappa) = \ln[q(\kappa)/Z(\kappa)] + \ln Z^\phi \). Here \( Z^\phi \) and \( Z(\kappa) \) are partition functions of the grand ensemble and the quenched system with fixed impurity configuration \( \kappa \), respectively; \( q(\kappa) \) is the probability distribution describing the quenched disorder. If \( \phi \) is normalized such that its configuration average vanishes \[14\], Eq. (1) implies

\[
\ln Z^\phi = < \ln Z(\kappa) >_q - < \ln q(\kappa) >_q , \tag{2}
\]

where \( < .. >_q \) 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.

Eqs. (1) and (2) are not very useful for practical calculations. In order to utilize Morita’s ideas, 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 \[11,15–17\]. For the spin–diluted Ising model, one may expand \( \phi(\kappa) \) according to

\[
\beta \phi(\kappa) = \lambda_0 + \lambda_1 \sum_i k_i + \lambda_2 \sum_{(i,j)} k_i k_j + \ldots + \lambda_P \sum_P \prod_{i \in P} k_i + \ldots \tag{3}
\]

where the \( k_i \) are occupation numbers taking the value 1 or 0 if in \( \kappa \) the site \( i \) is occupied or empty \[18\]. The first sum in (3) is over all lattice sites, the second over nearest neighbour pairs, and the third over all elementary plaquettes of the system. Each term serves to control one moment of the probability distribution \( p^\phi(\kappa) = \sum_\sigma p^\phi(\sigma, \kappa) \) - i.e. an expectation under \( p^\phi \) of some product of occupation numbers. The couplings \( \lambda_1, \lambda_2, \ldots \) have to be determined as functions of temperature and field such that the moments of \( p^\phi(\kappa) \) coincide with those of \( q(\kappa) \). The constant \( \lambda_0 \) is required to achieve \( < \phi(\kappa) >_q = 0 \).

For a randomly spin-diluted system with density \( \rho \) of magnetic impurities, one would have to determine the couplings of \( \phi \) so that

\[
< k_i >_\phi = \rho , \quad < k_i k_j >_\phi = \rho^2 , \ldots , < \prod_{i \in P} k_i >_\phi = \rho^{|P|} , \tag{4}
\]
and so on [11,16]. Here $< . >_\phi$ denotes an average with respect to $p^\phi(\kappa)$ and $|P|$ the size of the elementary plaquette, which for the square lattice is 4. Eqs. (4) constitute an infinite set of equations for the couplings $\lambda_1, \lambda_2, \ldots$ of the 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 [11,16]. Implementing only $< k_i >_\phi = \rho$, one would describe an annealed system at density $\rho$ of magnetic impurities. Such a system would condense and order at low temperatures and would thus provide a rather poor description of the quenched system. If, in addition, one fixes nearest neighbour correlations $< k_i k_j >_\phi$ of particle locations at their quenched value $\rho^2$, the condensation phenomenon no longer occurs and the system exhibits, e.g., a percolation transition. Such a system is already a serious candidate for the description of fully frozen-in disorder. In this manner, one arrives at increasingly accurate descriptions of the quenched system as more and more constraints are taken into account, until eventually one would obtain 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.

Except for the one dimensional system [11], this program cannot be carried through to the end, and for $d \geq 2$ we know of no exact solution of even the simplest approximating systems. At all levels of approximation, though, one has to do with translationally invariant equilibrium systems. Their critical behaviour could, for instance, be obtained by standard RG methods, were it not for the fact that the couplings of $\phi$ are only determined through a set of constraints. Since it is far from obvious how these constraints should be transformed under rescaling (see, however, [16]), 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].

If $\xi_M(\rho, T)$ denotes the correlation length of an $(M \times \infty)$-system at density $\rho$, temperature $T$, and field $H = 0$, an approximation to the critical point $T_c$ is given by the fixed point of the phenomenological RG relation $\xi_M(\rho, T)/M = \xi_{M'}(\rho, T')/M'$. An approximation to the correlation length exponent $\nu$ may be obtained by linearizing this relation about its fixed point [13]. Note that $\rho$ is a parameter of this procedure. By varying $\rho$, we can obtain the phase boundary $T_c(\rho)$, and the thermal correlation length expo-
component $\nu_t$ along the critical line. Analogous relations can be used to study the percolation transition at $T = 0, \rho = \rho_c$.

We have studied four approximating systems, named (a) - (d). In system (a), only the first and second constraint displayed in (4) are imposed on the system. Due to the anisotropy of the strip geometry, correlations parallel and perpendicular to the strip turn out to be different. We have 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 the results obtained from systems (a) and (b) or (c) and (d) should approach each other as the strip widths $M$ and $M'$ go to infinity. This can serve as a valuable consistency check for extrapolations of critical parameters obtained from fixed points of the phenomenological RG relations to the infinite system values.

We now turn to the results. We have computed critical temperatures $T_c(\rho)$ for various densities $\rho < 1$. The values obtained for systems (a) - (d) agree very well down to $\rho \approx 0.75$. Below $\rho \approx 0.75$, critical temperatures of the approximating systems with the plaquette–constraint imposed turn out to be slightly larger than those of systems (a) and (b) without this constraint. Extrapolating a parabolic interpolation of the $T_c(\rho)$ values for $\rho = 0.9, \rho = 0.95, \rho = 0.975$ to $\rho = 1$, we obtain $T_c(\rho) \to 2.2674$, as $\rho \to 1$, which is off the mark by less than 0.1%, and $T_c(\rho)^{-1} dT_c(\rho)/d\rho \to 1.579$, as $\rho \to 1$, which differs from the exact result 1.535 [19] by less than 3%. We have also checked the scaling form of the transition line near the percolation transition at $\rho_c$, $\exp[-2J/k_B T_c(\rho)] \sim (\rho - \rho_c)^\varphi$, 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 ($\rho_c \approx 0.593$ [20]) is correctly reproduced to within 3% and 1% by systems (a),(b) and (c),(d) respectively; see table I.

Fig. 1 shows our results for the correlation length exponent $\nu$ of system (a), based on extrapolations from strip widths up to $M = 8$ and $M = 10$ for the thermal and the percolation transitions, respectively. They clearly show a variation with the density $\rho$ of magnetic impurities. For $\rho = 0.7$ and $\rho = 0.9$, table I shows that this variation persists, as we impose further constraints in approximating systems (b)–(d). Note that the correlation length exponents are always mutually consistent for these four approximating systems. For the percolation transition, they agree well with the expected exact result $\nu_p = 4/3$ of den Nijs [26]. Also, the isotropic and anisotropic vari-
ants 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, \( \nu_p \) or \( \nu_t \), the first group can differ from the second as far as non-universal parameters of the phase transitions, i.e. \( \rho_c \) or \( T_c(\rho) \), are concerned.

Table 1: Extrapolated critical parameters for the percolation transition, and the thermal phase transition at densities \( \rho = 0.7 \) and \( \rho = 0.9 \) of magnetic impurities. 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) |

The variation of critical exponents with the density \( \rho \) is at variance with what would be expected from universality arguments, and one might well argue it to be an artefact of our simple approximations. So independent evidence is clearly welcome. Therefore, we turned to standard real-space renormalization group (RSRG) calculations for this system [2], and noted that they, too, are able to produce similar results: Some time ago, Tsalilis and Levy [21] used the RSRG to compute phase diagrams of bond diluted models, and they propose, inter alia, a set of RSRG transformations parametrized by the density \( \rho \) of bonds. Applying this idea to the SD problem, and using techniques of [22], we obtain the full curves shown in Fig. 1. While such an approach may still seem ad hoc, we find that, last but not least, very recent large scale Monte–Carlo simulations of the SD system [10] also give a non–universal \( \nu_t(\rho) \) in quantitative accord with our results, as can be seen in Fig. 1.

The agreement between the results of Kim and Patrascioiu [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 \( \gamma/\nu \simeq 1.75 \) as in the pure system, and independently of \( \rho \), which implies that \( \gamma \) itself is again non–universal. The amplitude \( A_0 \) of the critical finite–size correlation length, \( \xi_M(T_c) \simeq A_0 M \), is known to be related to the critical exponent \( \eta \)
according to \( A_0 = 1/\pi\eta \) \[23\]. We have 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 by all our extrapolated values for all our approximating systems, usually to within 1% or better. The same kind of weak universality \[24\] is also observed in \[10\], and it is of the same type as that encountered in Baxter’s 8–vertex model \[25\].

At this point let us mention that some time ago Derrida et al. \[27\] found analogous non-universal behaviour of Binder’s cumulant ratio in a family of self–dual bond disordered Ising models, which they ascribed to logarithmic corrections to finite–size scaling. However, as pointed out by Cardy \[28\], 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 non–universality is only apparent and caused by logarithmic corrections to finite–size scaling; 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 insert which addresses this particular point.

The complete set of constraints (4) imposes the condition \(< \prod_{i \in \omega} k_i >_\phi = \rho^{|\omega|}\) for all subsets \( \omega \) of the lattice, implying that occupancy of lattice sites is uncorrelated, or in other words that the correlation length describing the \( k_i \)-correlation functions 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 lengths remain small (at most a few lattice spacings) so that the approximating systems may be regarded as virtually quenched. Moreover, it can be shown \[11\] that in zero external field an infinite set of couplings of the exact potential \( \phi \) vanishes, and is thus correctly taken into account already at the level of our simple approximating systems (It implies, for instance, that in zero field our system (a) already provides an exact description of the quenched system in 1-d).

In summary, we have studied the critical behaviour of the spin–diluted Ising model by a new method which combines a grand ensemble approach to disordered systems with phenomenological renormalization. Where a comparison with exact results (concerning the phase diagram but also universal aspects of the percolation transition) is possible, our data compare favourably with earlier RG analyses of the system (see e.g. \[2\] and Refs. therein). We know of no a-priori reason why the present method should be intrinsically better in describing the percolation transition, where we get a
value of \( \nu_p \) consistent with the exact result of den Nijs, than in describing the thermal phase transition at \( \rho_c < \rho \leq 1 \), where our results indicate a continuous variation of critical exponents with \( \rho \) — in a manner that respects weak universality. Indeed, a recent Monte–Carlo study [10] produces results completely in accord with ours, both qualitatively and quantitatively. Hence, the observed variation of critical exponents is most likely not an artefact of our grand ensemble description of quenched disorder.

A deeper understanding of our method would certainly still be welcome. Let us mention in closing that it is easily adapted to the study of correlated disorder. Preliminary results for a 1-d system, where comparison with an exact solution is possible [29] do look encouraging. We are currently also using our method to study 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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**Figure captions**

**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 of the percolation transition. The exact result $\nu_p = 4/3$ 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 the percolation transition, where a precise location of the phase boundary is difficult, the agreement with our model (a) results is excellent.

**Fig. 2:** Variation of the phenomenological critical exponent $\nu_{M,M-1}$ with strip width $M$, for approximating system (a); open squares: percolation; diamonds: $\rho = 0.7$, full squares: $\rho = 0.9$, open circles: pure system. The insert checks for the possibility of logarithmic corrections to the pure systems critical behaviour: 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.