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Transfer-matrix scaling for diluted Ising systems

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A transfer-matrix scaling technique is developed for randomly diluted systems and applied to the site-diluted Ising model on a square lattice. For each connected configuration between adjacent columns, the contribution of the respective transfer matrix to the decay of correlations is considered only as far as the ratio of the two largest eigenvalues, allowing an economical incorporation of configurational averages. Predictions for the phase boundary at and near the percolation and pure Ising limits, and for the correlation exponent η at those limits, agree with exactly known results to within 1% error with largest strip widths of only $L=5$. The exponent η remains near the pure value ($\frac{1}{4}$) for all intermediate concentrations until it turns over to the percolation value at the threshold.

The transfer matrix (TM) provides exact solutions for a number of low-dimensional pure systems; when applied to finite-width strips and combined with finite-size scaling, it has also proved to be extremely powerful and accurate for nonsolvable pure cases.[1] Applications of "strip-scaling" techniques to random systems have, however, been few, despite the enormous interest in such problems as the spin glass, random field and dilute magnets, ceramic superconductors, etc. This is because the form so far utilized[2-4] deals with particular realizations of the random system which need not be representative unless appropriate averaging (or self-averaging) is employed, resulting in very large scale computing on extremely long strips and/or many realizations.

Here we provide a strip-scaling approach for random systems, in which the disorder averaging is carried out as one proceeds along the strip. This does not have the deficiencies noted above.

We apply the method to the two-dimensional site-diluted Ising model.[5] This is one of the best studied of all random systems, and includes well-understood special limits (the pure Ising case, and percolation) and so is particularly suitable for testing the new technique. At the same time the system raises interesting questions, such as the discrepancy between different field-theoretic predictions[6-9] for the bulk and correlation function critical behavior. We provide decisive results on this controversy, by direct evaluation of the correlation exponent η, and also give an accurate phase diagram.

In the TM scaling formulation, the central quantity to be considered is the correlation length ξ. For a pure system, this is given by

$$\xi^{-1}=-\ln(\lambda_2/\lambda_1)\ , \tag{1}$$

where λ_1,λ_2 are the two largest eigenvalues of the TM.[10] Equation (1) is obtained by iteratively applying the (same) TM, keeping only leading terms in the long-distance limit.

For a random system, the decay of thermal correlations is still given through the iterative product of (nonidentical) TM's from one column to the next; however, the randomness makes configurational averaging necessary. In previous work[2-4] this was done by generating strips of length $N\gg 1$ and carrying out the actual TM products, so the end result would presumably reflect the properties of a representative sample. A correlation length was extracted from the largest even- and odd-sector eigenvalues of the iterated TM, $\lambda_{\rm even}$ and $\lambda_{\rm odd}$, via[2-4]

$$(\xi^{-1})_{\rm ave}=-(1/N)\ln(\lambda_{\rm odd}/\lambda_{\rm even})\ . \tag{2}$$

While (2) has not the same rigor as (1) for pure systems, it is nevertheless a sensible choice to make, to obtain a quenched average of the decay of correlations, since it at least partly exploits the self-averaging by the system. The difficulty of judging when the strip is sufficiently long remains and, for diluted systems, how to avoid the effects of disconnections.

In our approach the starting point is the TM formulation of the percolation problem.[11] In this case, which is the zero-temperature limit of diluted magnets, the (geometric) correlation length is given by the largest eigenvalue of a TM, whose elements are related to the probability that two adjacent site columns (each with occupied and vacant sites) are linked to each other and to the origin. Care is thus taken of the correlations between frozen spins; as the temperature is raised from zero, each of the possible links represented by the nonzero elements of the geometric TM is weakened by thermal fluctuations. We take these into account still within the framework of a single matrix, so the exact column-by-column character of the average of disorder configurations will be preserved. It is necessary to modify each nonzero element of the original matrix by incorporating properties of the spin TM between the corresponding site column states. As the physical property under investigation is

the rate of decay of correlations, analogy with the leading contribution towards this in pure systems suggests taking the ratio of the two largest eigenvalues of the spin TM, and multiplying the corresponding geometric TM element by it. If i and j are two site column states connected to each other and to the origin, with respective probabilities P_i and P_j, and the spin TM T^{ij} between these columns has λ_1^{ij} and λ_2^{ij} as its largest eigenvalues, the matrix element of the "thermal-geometric" TM of our formulation is then

$$\mathcal{T}_{ij}=\sqrt{P_iP_j}(\lambda_2^{ij}/\lambda_1^{ij}) . \tag{3}$$

The averaged correlation length is given by $(\xi^{-1})_{\text{ave}}=-\ln\Lambda_1$, where Λ_1 is the largest eigenvalue of $\mathcal{T}$.

The following comments are in order.

(a) As the temperature $T\to 0$, the two largest eigenvalues of all thermal TM's become degenerate, and (3) shows that $\mathcal{T}$ reduces correctly to the geometric TM of Ref. 11.

(b) As the concentration p of magnetic sites approaches 1, the only remaining nonzero element of $\mathcal{T}$ is along the diagonal, connecting two fully occupied columns; denoting by λ_1^{pure} and λ_2^{pure} the largest eigenvalues of the corresponding thermal TM, $\Lambda_1=\lambda_2^{\text{pure}}/\lambda_1^{\text{pure}}$ for $p=1$, and the pure system limit is correctly obtained.

(c) As befits quenched problems, disorder and thermal aspects are not being averaged together. We represent the effect of thermal fluctuations on each given geometric configuration by the ratio of the respective largest thermal eigenvalues, and the disorder average is performed at a later step, in obtaining the largest eigenvalue of $\mathcal{T}$. Thus we make the analog of the configurational average of the factor $e^{-1/\xi}$ in the correlation function (related to its decay between two adjacent columns) and it is indeed the correlation function which is self-averaging.

(d) The procedure outlined contains the approximation that the complex contribution given by each thermal TM is truncated and replaced by that of its two largest eigenvalues. As the thermal TM's corresponding to distinct disorder configurations do not commute with each other, the influence of higher-ranking eigenvalues does not vanish identically; however, it is expected to die out asymptotically, thus minimizing the truncation effects mentioned above. We cannot rigorously prove this statement, and must thus refer to the quality of the results in order to check its validity as a working assumption. Note that from (a) above, this approximation is asymptotically correct in the low-temperature regime. For other disordered systems this must be true as well, provided that one can start from a suitable TM description of the ground-state correlations.

We have studied strips on a square lattice with periodic boundary conditions. We first present results for the critical curve.

Along the critical line $T_c=T_c(p)$, the correlation length ξ diverges in the infinite system limit. In phenomenological scaling between strip widths L and L', this is where $\xi_L/L=\xi_{L'}/L'$.[1] With one variable, this condition would give a fixed point. Here, where two variables T, p occur, we fix p and find the associated critical temperature $T_c(p)$ for each L/L'. The results for $L/L'=3/2$, 4/3, 5/4 are shown in Fig. 1 (with T given in units of the exchange constant), and are qualitatively similar to those provided by simple analytic scaling approaches[5] and by recent Monte Carlo simulations.[12]

At the pure Ising critical temperature $T_c(1)$ and the percolation critical concentration p_c (where T_c goes to zero) our results are $T_c(1)=2.367\,640\,4$, $2.320\,811\,7$, $2.293\,823\,9$; $p_c=0.582\,141\,9$, $0.590\,956\,7$, $0.588\,696\,0$, respectively, for $L/L'=3/2$, 4/3, 5/4. These are to be compared with the exact $T_c(1)=2.269\,185\,3\ldots$ (known from duality) and the best estimate[13] $p_c=0.592\,745\pm 0.000\,002$. The above results coincide with those obtained by Nightingale[14] and Derrida and De Seze[11] respectively in their separate treatments of these two special limits by strip scaling. This coincidence is guaranteed within our generalized procedure for the random system.

Another quantity for which exact analytic results are known[15] for comparison is the reduced slope $[1/T_c(1)][dT_c(p)/dp]_{p=1}$ of the critical curve at the pure limit. This is not provided in the pure Ising or percolation special cases, so it is a more severe test of our approach. Results from $L/(L-1)$ scalings up to $L=7$ are given in Table 1, together with an extrapolated value whose error, about 1%, is a measure of the divergence of different extrapolations. The exact result[15] is safely within the error bars.

Near the percolation threshold, the crossover exponent

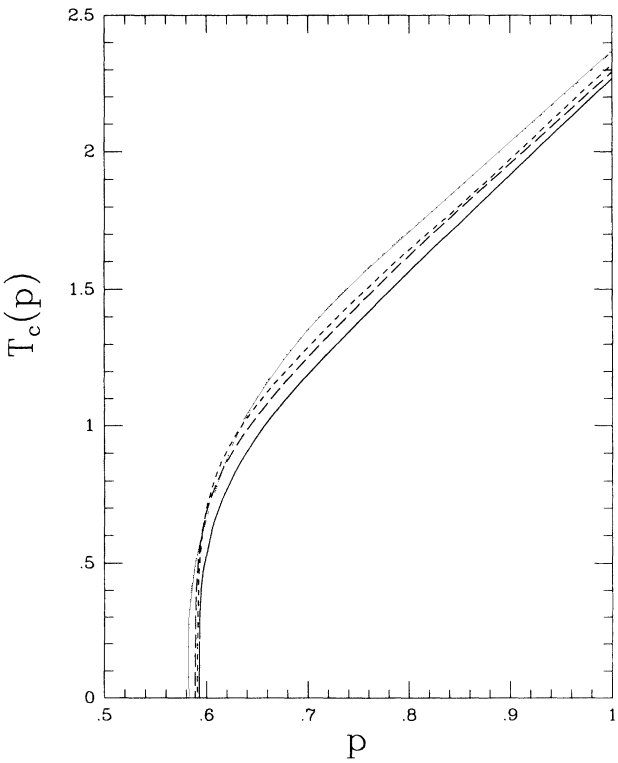

FIG. 1. Approximate phase diagrams from phenomenological renormalization between strips of width L and $L-1$: dots, $L=3$; short dashes, $L=4$; long dashes, $L=5$. Solid line: interpolated curve (see text).

TABLE I. Reduced slope of critical curve at the pure system limit ($p=1$).

L/L'	$\frac{1}{T_c(1)}\left[\frac{dT_c(p)}{dp}\right]_{p=1}$
3/2	1.4461
4/3	1.4765
5/4	1.5032
6/5	1.5165
7/6	1.5223
Extrapolated	1.57±0.015
Exact[a]	1.565

[a]Reference 15.

ϕ gives the power-law dependence of $e^{-2/T_c(p)}$ on $(p-p_c)$. As ϕ is known exactly to be 1,[16] this can provide another test of our results.

Figure 2 gives a plot of $\ln(p-p_c)$ vs $1/T_c$ for p near p_c for $L/L'=5/4$. The data fall very close to a straight line of slope -2 as shown, and the limiting slope gives $2/\phi=1.99\pm0.01$, in very good agreement with the exact result.

As can be seen from Fig. 2, the range of T_c for which $e^{-2/T_c(p)}\simeq C(p-p_c)$ goes up to T_c somewhat greater than 0.5, and Fig. 1 shows that this exponential regime is joined by a relatively narrow crossover region to one where $T_c(p)$ is linear in $(p-p_c)$ with essentially the $p=1$ limiting slope. An interpolation employing the exact values of $T_c(1)$, p_c, and the limiting slope, and an extrapolate from successive $L/(L-1)$ scalings for the constant C ($C\sim4$), provides a very accurate "interpolated" critical curve, shown as the solid line in Fig. 1. This will be useful below.

We now turn to the exponent η. Accurate values of η can be obtained from the correlation length calculated at the critical point, on a strip of width L, via[17] $\eta_L=L/[\pi\xi_L(T_c)]$. Figure 3 gives the corresponding results for η for strips with $L=2,3,4,5$ using the "interpolated" critical curve. The black square at $p=p_c$ is the exact percolation value $\eta=5/24$,[18] and that at $p=1$ is the exact pure value $\eta=1/4$. It is apparent that the values of η at $p=p_c$, $p=1$ approach the exact ones as L increases. The numerical results are $\eta(p=p_c)=0.216\,35$, $0.213\,06$, $0.212\,56$, $0.211\,47$ and $\eta(p=1)=0.277\,30$, $0.264\,51$, $0.257\,84$, $0.254\,71$ for $L=2,3,4,5$, respectively. Again, these two special cases have been treated previously,[11,14] and our results for these limits coincide with those already obtained.

The results for η at intermediate p are new. In Fig. 3 they converge with increasing L to a value not much different from the pure value $\eta=1/4$ for all p, except $p\sim p_c$, where the percolation value is approached.

This conclusion is to be compared with current field theory results for random Ising models in two dimensions.[6-9] The theories (with some exceptions, e.g., Ref. 7) agree in predicting that the specific heat singularity is

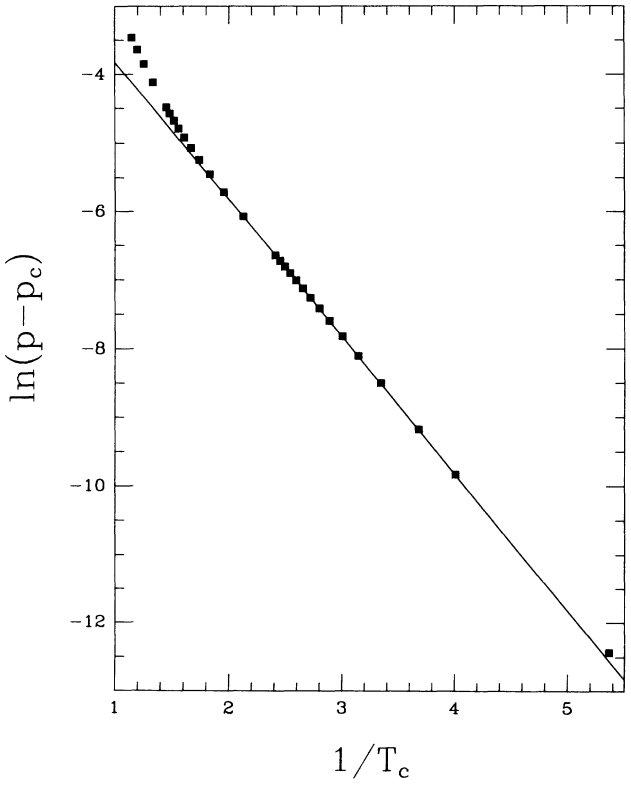

FIG. 2. Exponential behavior at low temperatures; data from 5/4 scaling. The solid line has slope -2 and is a guide to the eye.

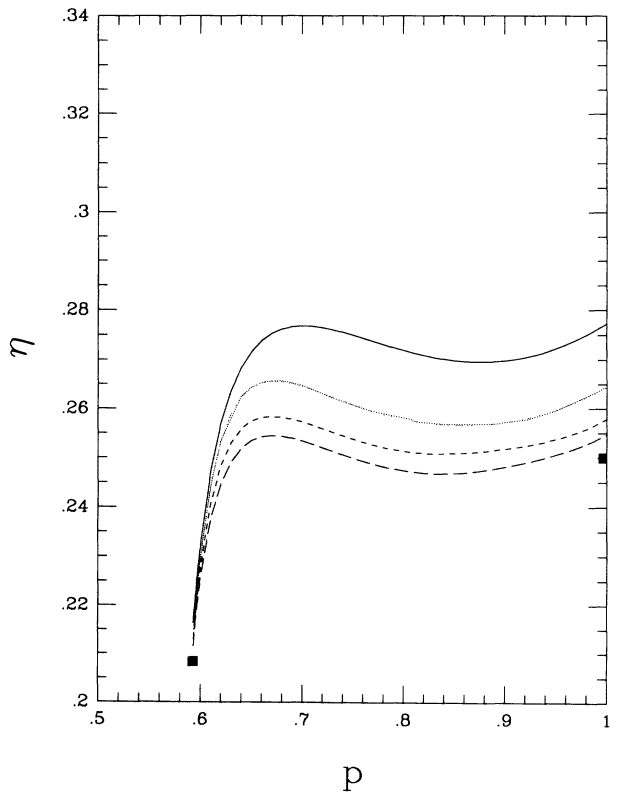

FIG. 3. Correlation exponent η from correlation-length amplitudes, along interpolated critical curve, for strip widths $L=2,3,4,5$ (top to bottom). Black squares at (0.592 75, 5/24) and (1, 1/4).

of $\ln\ln(T-T_c)$ type rather than the $\ln(T-T_c)$ of the pure case. But one group of theories[7,9] predicts that the asymptotic pair correlation is as in the pure case ($\langle\sigma_0\sigma_r\rangle \sim r^{-\eta}$, $\eta=1/4$), while the other[6] concludes that the correlation has the form $\langle\sigma_0\sigma_r\rangle \sim e^{-A(\ln r)^2}$. Our results clearly support the first class of predictions.

Recent very large Monte Carlo simulations on the random-bond Ising model at a particular (self-dual) concentration[8] also provide indirect evidence in favor of the first class of results. A direct evaluation of η, again pointing to the pure result, has also been obtained[4(b)] for the same random bond Ising model by strip scaling on long realizations of the random system.

We conclude that the new transfer matrix scaling method gives a reliable and accurate treatment of the site-diluted Ising model. The results for η at intermediate concentrations give clear evidence in favor of one of the competing classes of field-theoretic treatments.[6-9] We are at present generalizing the method for treating the random-field Ising ferromagnet and the random-bond Ising model.

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