Critical and thermodynamic properties of the randomly dilute Ising model

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The randomly bond-dilute two-dimensional nearest-neighbor Ising model on the square lattice is studied by renormalization-group methods based on the Migdal-Kadanoff approximate recursion relations. Calculations give both thermal and magnetic exponents associated with the percolative fixed point. Differential recursion relations yield a phase diagram which is in quantitative agreement with all known results. Curves for the specific heat, percolation probability, and magnetization are displayed. The critical region of the specific heat becomes unobservably narrow well above the percolation threshold p_c . This provides a possible explanation for the apparent specific-heat rounding in certain experiments.

I. INTRODUCTION

Magnetic phase transitions in randomly dilute (quenched) magnetic materials exhibit competition between percolative ("geometrically driven") and thermodynamic ("thermally driven") processes. Consider for specificity a model magnetic insulator composed of an infinite lattice of magnetic ions interacting via pairwise ferromagnetic exchange forces of finite range. Suppose that a fraction (1-p) of the exchange bonds is removed at random, leaving the remaining fraction p unchanged.¹ There is a finite fractional concentration $p = p_c$ ("critical bond concentration" or "bond percolation threshold"2) below which any given magnetic ion finds itself with probability unity a part of a *finite* magnetic cluster, uncoupled from the rest of the magnetic lattice. Because such a finite system cannot support long-range order, the lattice as a whole is nonmagnetic at all temperatures.³ For $p > p_c$ each magnetic ion may still be part of a finite cluster; however, there is a nonzero probability P(p) ("bond percolation probability") that it will be part of an infinite cluster $[P(p_c) = 0, P(1)]$ =1]. This infinite cluster can develop long-range order, so the zero-field magnetization per site M(p, T, H=0) is nonzero for temperatures T less than some critical temperature $T_c(p)$. The critical temperature $T_c(p)$ is a continuous monotonically increasing function, which for Ising models⁴ joins $T_c(p_c) = 0$ and $T_c(1) = T_c$ (pure system). It is generally (but not universally⁵) believed that critical behavior in the "dilute" region p_c is normal, i.e., characterized by critical exponents, etc., arising from the single infinite cluster and modified only by Griffiths singularities³ due

to the additional presence of arbitrarily large finite clusters.⁶ The form (universality class) of pure and dilute critical behavior may or may not differ, according to whether the pure-system specific-heat exponent α (pure) > 0 or α (pure) < 0, respectively.⁷⁻¹⁰ In the former case, the region $p \approx 1$, $T \approx T_c(p = 1)$ is characterized by crossover between pure and dilute critical behavior. At T \rightarrow 0, model properties as functions of p are related to purely percolative phenomena.^{2,11} For example. the infinite cluster orders at T=0, while finite clusters do not; hence, $M(p, T \rightarrow 0, H = 0)$ is precisely P(p) except for overall normalization. The region of the "percolation point," $p = p_c$, T = 0, exhibits its own distinct critical behavior.¹² For p $\approx p_c$, $T \approx 0$ there is crossover behavior between percolative and dilute regimes. Various forms of crossover scaling have been proposed.¹²⁻¹⁵

The purpose of this paper is to develop a method for calculating the properties of the bond-dilute Ising model for all concentrations $(0 \le p \le 1)$ and temperatures $(0 \le T < \infty)$ and in particular to study critical behavior over the full range $p_c \le p \le 1$. The method is based on a generalization of the Migdal-Kadanoff approximate recursion relations¹⁶⁻¹⁸ to inhomogeneous systems.^{19,20} In order to simplify the calculation in the dilute regime, p_c , the additional approximation is made of reducing the bond probability distribution $\mathcal{O}(K)$ to a two- δ -function form at each iterative stage of the calculation.^{19,21,22} The phase diagram, the critical and percolation exponents, and thermodynamic functions are determined in two dimensions (d=2). Crossover phenomena between percolation and critical properties are studied. In our approach the phase diagram in the p-T plane is described

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in terms of two fixed points (pure system critical and percolation) and the high- and low-tempera ture sinks. (The approximation does not yield an additional dilute critical fixed point, which is consistent⁷⁻¹⁰ with the fact that it gives $\alpha < 0$.) In the limit in which the recursion relations preserve the duality symmetry of the model¹⁷ (scale parameter $b \rightarrow 1$), not only is $T_c(p)$ exact at both ends $[p_c = \frac{1}{2}, T_c(1) = (T_c)_{Onsager}]$ but also initial slopes agree closely with exact results. The thermal and magnetic eigenvalues associated with the critical and percolation fixed points are calculated. The magnetic exponent at percolation is new and in good agreement with available data. Finally, explicit thermodynamic functions are obtained from our recursion relations using the method of Nauenberg and Nienhuis,²³ suitably generalized for the randomly dilute magnet. Specific-heat curves, displayed for a range of concentrations p both above and below percolation, are smooth for $p < p_c$, but for $p > p_c$ have cusped critical behavior near $T = T_c(p)$. What is perhaps at first unexpected is that already for $p \leq 0.8$ the critical region is so narrow that the specific heat *appears* entirely smooth to graphical accuracy. For $p \leq 0.85$ the specific heat exhibits a maximum at a temperature above $T_c(p)$, which corresponds to the development of significant short-range order. Evidence for this behavior is also cited from Monte Carlo results²⁴ and experiment.²⁵ Finally, renormalization-group calculations of the percolation probability P(p) and the magnetization are displayed.

Section II defines the model and develops the method. Section III presents our main results. In the remainder of Sec. I previous work on randomly dilute Ising systems is briefly reviewed.

Both the purely geometric (T=0) percolation problem and the quenched random dilution problem have received much attention. Series²⁶ and Monte Carlo^{24,27} methods allow numerical estimation of transition parameters such as p_c , $T_c(p)$, exponents, etc. Recently renormalization-group methods have proved very fruitful. The majority of such treatments rest on the equivalence proved by Kasteleyn and Fortuin²⁸ between the percolation problem and the $s \rightarrow 1$ limit of the s-state Ashkin-Teller-Potts (ATP) model. The ATP model can be treated via ϵ expansion^{29–31} around the critical dimensionality $d^* = 6$ or by position-space methods.³² A few authors^{29, 33, 34} have studied percolation directly by position-space methods.

Similarly, the dilution problem may be attacked via ϵ expansion^{10,35,36} about $d^* = 4$ (using the $n \rightarrow 0$ limit³⁷) or in position space.^{20,21,36,38} While ϵ expansion results are enormously useful in elucidating systematics, they require extrapolation from

 d^* down to physical dimensionalities. Also, their application has been mainly confined to exponent estimates, since it is difficult to make contact with nonuniversal properties of specific lattice models. Posi ion snace methods, while limited by recursion relations containing ad hoc approximations, do apply directly to physical dimensionalities and can be used to extract both universal and nonuniversal information. Harris and Lubensky³⁶ first showed how to use position-space recursion relations to study random systems. Kirkpatrick²⁰ applied the Migdal-Kadanoff approximate recursion relations to the dilution problem at H= 0 and calculated p_c and v_b for d=2, 3 bond-dilute Ising models. Our work extends Kirkpatrick's²⁰ to $H \neq 0$, the full $T_c(p)$, and the explicit calculation of various thermodynamic functions.³⁹ We are aware of no previous explicit renormalizationgroup calculations of thermodynamic functions belonging to the randomly dilute magnet.

II. RECURSION RELATIONS, EXPONENTS, AND THERMODYNAMIC FUNCTIONS

A. Model

Consider a nearest-neighbor $s = \frac{1}{2}$ Ising system on a square lattice and subject to randomly inhomogeneous pair couplings and local magnetic fields. The appropriate Hamiltonian (in reduced units) is

$$-\beta \mathcal{K}_{N} = \sum_{i} h_{i} \mu_{i} + \sum_{\langle i,j \rangle} K_{ij} \mu_{i} \mu_{j}, \quad \mu_{i} = \pm 1, \quad (1)$$

where N is the number of lattice sites, the subscripts i,j run over the lattice, and the second sum is over distinct nearest-neighbor pairs $\langle i,j \rangle$. The dimensionless couplings h and K are related to local magnetic fields and exchange energies by $h = g\mu_B H/k_B T$ and $K = J/k_B T$. The variables K_{ij} and h_i are independently random with probability distributions $P_1(K_{ij})$ and $P_2(h_i)$, respectively. In calculation below we shall specialize to

 $P_1(K_{ij}) = p \,\delta(K_{ij} - K) + (1 - p) \delta(K_{ij}), \quad K > 0 ,$

and

$$P_2(h_i) = \delta(h_i - h), \quad h \ge 0$$

i.e., each bond either has the value K (with probability p) or is absent (with probability 1-p), while the magnetic field is homogeneous.

It is useful to introduce the notation

$$[X]_{av} \equiv \int \prod_{\langle i,j \rangle} dK_{ij} P_1(K_{ij}) \prod_i dh_i P_2(h_i) \times X(\{K_{ij}\}, \{h_i\})$$
(3)

for the average value of any function of the set

(2)

of variables $\{K_{ij}\}, \{h_i\}$. In particular the average free energy per site of the infinite randomly dilute system is

$$\overline{f} = \lim_{N \to \infty} \frac{1}{N} \left(\ln \operatorname{Tr}_{N} e^{-\beta \mathscr{K}_{N}} \right)_{\mathrm{av}}.$$
 (4)

For the distributions (2), $\overline{f} = \overline{f}(p, K, h)$ and appropriately averaged thermodynamic quantities can be determined by differentiation. For example, the average magnetization is

$$\overline{M}(p, K, h) \equiv [\langle \mu_i \rangle]_{av} = \frac{\partial f}{\partial h} , \qquad (5)$$

the average susceptibility is

$$\overline{\chi}(p, K, h) = \frac{\partial \overline{M}(p, K, h)}{\partial h} , \qquad (6)$$

and the average specific heat per site at h = 0 is

$$\overline{c}(p, K) = k_B K^2 \frac{\partial^2 \overline{f}(p, K, h=0)}{\partial K^2} .$$
(7)

In the strong-coupling limit $K \rightarrow \infty$ (e.g., $T \rightarrow 0$ with J and H/T fixed) various thermodynamic properties of the dilute magnet are related to the functions describing percolative phenomena.^{2,11} For example, the infinite cluster orders, while each finite *n*-cluster (cluster of *n* coupled spins) has a magnetic moment of $n \tanh(nh)$. Thus,

$$\overline{M}(p, K=\infty, h) = P(p) \operatorname{sgn}(h) + \sum_{n=1}^{\infty} q_n \tanh(nh) , \qquad (8)$$

where q_n is the probability that a site chosen at random is part of an *n*-cluster. It follows that

$$|\overline{M}(p, K=\infty, 0)| = P(p); \quad \overline{\chi}(p, \infty, 0) = \sum_{n=1}^{\infty} nq_n.$$
(9)

 $\overline{\chi}(p,\infty,0)$ is, therefore, the mean size density of finite clusters at a site, which is identical to the⁴⁰ "mean cluster size" S(p) for $p < p_c$, but equal to [1-P(p)]S(p) for $p > p_c$. Near p_c , P(p) vanishes as $(p-p_c)^{\beta_p}$, while S(p) diverges as $|p-p_c|^{-\gamma_p}$. These expressions define the "percolation exponents" β_p and γ_p .

B. Recursion relations at h=0

Migdal-Kadanoff recursion relations^{16,17} were first applied to randomly inhomogeneous systems in the spin-glass context¹⁹ and thereafter used by Kirkpatrick²⁰ for the dilution problem.³⁹ The procedure consists in successive contractions by a scale factor *b* along each of the *d* Cartesian directions, resulting in a volume contraction by an overall factor b^d . Each contraction involves a bond-shifting perpendicular to the contraction and a decimation along the contraction, schematically,¹⁹

$$\overline{K}_{\perp} = \sum K_{\perp}, \quad \tanh \overline{K}_{\parallel} = \prod \tanh K_{\parallel}, \qquad (9a)$$

or, in terms of the convenient variable $\tau = \tanh K$, which is finite at both $T \rightarrow \infty$ and $T \rightarrow 0$,

$$\tanh^{-1}\overline{\tau}_{\perp} = \sum \tanh^{-1}\tau_{\perp}, \quad \overline{\tau}_{\parallel} = \prod \tau_{\parallel}.$$
(9b)

When the system is homogeneous,¹⁷ the recursion relation for the coupling along the direction of initial contraction (x) is

$$\tau'(\tau) = \tanh[b^{d-1} \tanh^{-1}(\tau^b)], \qquad (10)$$

while the coupling along the direction of final contraction (y) transforms as

$$\tau'(\tau) = [\tanh(b^{d-1} \tanh^{-1} \tau)]^b .$$
(11)

We shall refer to these as xy and yx recursion relations, respectively. They have quite different fixed-point couplings for integer b > 1. However, it is easy to interpret b as a continuous variable (the "natural" analytic continuation in b) and to take the limit $b \equiv 1 + dl$, $dl \rightarrow 0^+$ (dl is an infinitesimal). In this $b \rightarrow 1$ limit, the xy and yx recursion relations become identical and yield for $dK \equiv K'$ -K

$$\frac{dK}{dl} = (d-1)K + \frac{1}{2}(\sinh 2K) \ln \tanh K.$$
(12)

For d=2, Eq. (12) has a fixed point at $K^* = \frac{1}{2} \ln(1 + \sqrt{2})$, which agrees with Onsager's⁴¹ exact K_c . This remarkable agreement, which arises because the $b \rightarrow 1$ recursion relations preserve duality,¹⁷ does not unfortunately extend to exponents: one finds a thermal exponent $y_T = 0.754$ (exact y_T = 1) and, correspondingly, a specific-heat exponent $\alpha = 2 - d/y_T = -0.654$ [exact $\alpha = O(\ln)$]. This strongly negative α seems to be a defect of all Migdal-Kadanoff-type approximations for Ising models.

There is a close analog to (12) for percolation, which we note here for future use. The Kasteleyn-Fortuin theorem²⁸ relates the bond-percolation problem to the $s \rightarrow 1$ limit of the *s*-state ATP model. Kadanoff¹⁷ and Stephen³¹ have treated this model using the Migdal approach. From Eqs. (2.18) of Ref. (17) one obtains (with $p \equiv 1 - e^{-K}$) a recursion relation for the bond-percolation probability (*xy* asymmetric)

$$p' = 1 - (1 - p^b)^{b^{d-1}}.$$
(13)

The $b \rightarrow 1$ limit yields for $dp \equiv p' - p$ the recursion relation

$$\frac{dp}{dl} = p \ln p - (d-1)(1-p) \ln(1-p) .$$
(14)

This equation exhibits for d=2 the exact⁴² bond-

percolation fixed point $p^* \equiv p_c = 0.5$. The associated eigenvalue exponent $y_p = 2(1 - \ln 2)$ corresponds to a correlation length exponent for percolation ν_p $= y_p^{-1} = 1.629$ (series⁴³ $\nu_p = 1.34 \pm 0.02$).

For the Ising model in the presence of bond and/or field inhomogeneity the analogs of (10) and (11) determine each new local coupling $\tau'_{\alpha\beta}$ in terms of a set of original couplings $\{\tau_{ij}\}$. If each τ_{ij} is independently distributed according to a probability distribution $\mathcal{O}(\tau_{ij})$, then the probability distribution $\mathcal{O}'(\tau'_{\alpha\beta})$ for the renormalized coupling is given by³⁶

$$\mathcal{O}'(\tau_{\alpha\beta}') = \int \left(\prod_{\langle i,j \rangle} d\tau_{ij} \mathcal{O}(\tau_{ij}) \delta(\tau_{\alpha\beta}' - \tau_{\alpha\beta}'(\{\tau_{ij}\})) \right).$$
(15)

In general the same coupling τ_{ij} may contribute to several renormalized couplings, so that $\tau'_{\alpha\beta}$'s are *not* independently distributed. It is a special property of the usual ("asymmetric") interpretation^{19,20} of the Migdal-Kadanoff approximation (9) that each coupling contributes to a single $\tau'_{\alpha\beta}$, so such intercoupling correlations are absent; however, more "symmetric" interpretations (see below) can introduce such correlations. We shall make the approximation of neglecting them whenever they arise, i.e., of assuming the validity of (15) at each stage of iteration.

We specialize in what follows to the randomly bond-dilute *two*-dimensional nearest-neighbor Ising model on the square lattice. (Within the Migdal-Kadanoff framework, the generalization to d>2 is straightforward.) Although initially the couplings are either present or absent ($\tau_{ij} = 0, \tau$), corresponding to the two-peaked distribution (2), they do not remain so under iteration: the initial contraction along the x direction gives an intermediate x coupling

$$\overline{\tau}_{x} = \tanh \overline{K}_{x} = \begin{cases} \tau^{b}, & \text{with probability } p^{b} \\ 0, & \text{with probability } 1 - p^{b}. \end{cases}$$
(16)

When b of these intermediate couplings are added together in the succeding y contraction, the new coupling $K'_{\alpha\beta} = \tanh^{-1}\tau'_{\alpha\beta}$ is an integral multiple of $\tan^{-1}(\tau^{b})$,

$$K'_{\alpha\,\beta} = m \tanh^{-1}(\tau^{\,b}), \quad 0 \le m \le b , \qquad (17)$$

with corresponding probability

$$p_{m}(b) = {b \choose m} (p^{b})^{m} (1 - p^{b})^{b - m}.$$
(18)

To render calculations tractable we make the additional approximation at each iteration of forcing the full distribution (17) back to a two-peak form [cf. (2)],

$$P'(\tau'_{\alpha\beta}) = p'\delta(\tau'_{\alpha\beta} - \tau') + (1 - p')\delta(\tau'_{\alpha\beta}).$$
⁽¹⁹⁾

The parameters p' and τ' are chosen by fitting first and second moments. Thus, (xy asymmetric)

$$p'(\tau')^n = \sum_{m=0}^{b} p_m(b) [\tanh(m \tanh^{-1} \tau^b)]^n .$$
 (20)

Equation (20) with n = 1 and n = 2 determines recursion relations, $p'(p, \tau)$, $\tau'(p, \tau)$, from which fixed points, exponents, etc., can be extracted as usual. Note that Eq. (19) represents the distribution (17) *exactly* in two important limits. When p = 1 (pure system), then $p_m = 0$ for $m \neq b$; hence, p' = 1 and (20) reduces to (10) with the fixed point $K^* \equiv K_c = 0.6094$. Similarly, when¹⁹ T = 0 and $\tau = 1$ (percolation), Eq. (17) implies $\tau'_{\alpha\beta} = 0$ or 1 only; hence, (20) reduces to (13) with the fixed point $p^* \equiv p_c = 0.6180$.

Considerable ambiguity exists in the development of recursion relations within the Migdal-Kadanoff context. If we had focused on the y coupling instead of the x coupling in (16), then for b=2 we would have found in place of (20) (yx asym-



FIG. 1. Sites and bonds for Migdal-Kadanoff recursion relations. (a) The usual (asymmetric) bond-moving procedure combines the movable bond (2,5) with one of the adjacent fixed bonds, e.g., (1,4). A more symmetrical procedure is to split (2,5), asigning half to (1,4) and half to (3,6). (b) See discussion in Secs. II C and II D. Circled sites remain after x and y decimations have been performed.

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metric)

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$$b'(\tau')^{n} = 4p^{2}(1-p)^{2}\tau^{2n} + 4p^{3}(1-p)\left(\frac{2\tau^{2}}{1+\tau^{2}}\right)^{n} + p^{4}\left(\frac{2\tau}{1+\tau^{2}}\right)^{2n}$$
(21)

[cf. (11)]. Furthermore, for even *b* this usual treatment of the bond-shifting is rather asymmetrical. For b=2, for example, one moves the entire intermediate bond in one direction [see Fig. 1(a)] rather than splitting it symmetrically between the two adjacent unshifted bonds.⁴⁴ The *xy* decimation with the *symmetrical* bond-shifting gives for b=2 (*xy* symmetric),

$$p'(\tau')^{n} = p^{6}(\tanh 2z)^{n} + 2p^{4}(1-p^{2})(\tanh \frac{3}{2}z)^{n} + p^{2}(1-p^{2})(\tanh z)^{n} + 2p^{2}(1-p^{2})^{2}(\tanh \frac{1}{2}z)^{n},$$
(22)

where $\tau^2 \equiv \tanh z$. It is easy to derive a similar recursion relation for the b = 2 yx symmetric case.

Each of these four recursion relations (xy and yx), asymmetric and symmetric) has two interesting fixed points: one on the p = 1 axis corresponds to pure-system critical behavior; the other on the T=0 ($\tau=1$) axis represents percolation. The positions of these fixed points and their associated eigenvalue exponents are shown for b=2 in Table I. Note that K^* and p^* are in rather poor agreement with the exact values, ${}^{41, 42}K_c = 0.4407..., p_c = \frac{1}{2}$, and vary widely between different approximations. Eigenvalue exponents are somewhat more consistent but still only accurate to $\pm 25\%$.

One is tempted (by analogy to the pure system) to hope that taking the b + 1 limit will (a) give

improved phase-boundary parameters and (b) resolve the ambiguity between different Migdal-Kadanoff approximations. We can make no statement on (b), because we have been able to find a useful analytic continuation *only* for the *xy* asymmetric case (20). Expectation (a) turns out to be true, as we shall now show. Continuation of (10) and (11) is trivial, since *b* appears parametrically. The difficulty with (20) is that *b* is also a summation limit. We wish, therefore, to cast (17) into a form which allows the sum to be performed. Let x $= e^{-2\overline{K}} = (1 - \tau^b)/(1 + \tau^b) \leq 1$. Then

$$\tanh(m \tanh^{-1} \tau^b) = \frac{1 - x^m}{1 + x^m}$$

$$= (1 - x^m) \sum_{r=0}^{\infty} (-1)^r x^{rm}. \qquad (23)$$

The sum over m is a binomial expansion, so

$$p'\tau' = \sum_{r=0}^{\infty} (-1)^r [(1-p^b+p^bx^r)^b - (1-p^b+p^bx^{r+1})^b].$$
(24)

The corresponding expression for $p'\tau'^2$ is only slightly more complicated. Now *b* can be interpreted as a continuous variable and the analytic continuation is achieved. There is no general infinitesimal form comparable in simplicity to (12) and (14); however, there is no numerical difficulty in taking the $b \rightarrow 1$ limit. In the important special cases p = 1 (pure system) and $\tau = 1$ (percolation), Eq. (22) reduces in the $b \rightarrow 1$ limit to Eqs. (12) and (14), respectively, and yields the exact critical parameters p_c and K_c , as noted above.

Fixed-point parameters and eigenvalue expo-

Pure-sy (p*=1)	ystem fixed point Correct results	b = 2 xy asymmetric [Eq. (20)]	b=2 yx asymmetric [Eq. (21)]	b=2 xy symmetric [Eq. (22)]	b=2 yx symmetric	$b \rightarrow 1$ xy asymmetric [Eq. (24)]
<i>K</i> *	0.4407 (exact) ^a	0.6094	0.3047	0.6094	0.3047	0.4407
Ут	1 (exact) ^a	0.747	0.747	0.747	0.747	0.754
Ур		-0.264	-0.264	-0.740	-0.740	-0.128
Percol (K*)	ation fixed point $f^{1} = k_{B}T^{*}/J = 0$					
p *	1/2 (exact) ^b	0.6180	0.3820	0.3894	0.3717	0.5000
Ут		0.611	0.611	~	00	0.614
Ур	0.75 ± 0.02 (series) ^c	0.611	0.611	0.750	0.980	0.614

TABLE I. Fixed points and eigenvalue exponents for various h=0 recursion relations.

^aReference 41. ^bReference 42. ^cReference 43.

	e and a second			
Exponen	ut Quant	ity $b=2$	$b \rightarrow 1$	Exact or series
Pure syste	em			
$\nu = 1/\nu_T$	correlation l	ength 1.339	1.326	1.00 ^a
$2 - \alpha = 2/v$	r free energy	2.678	2.654	2.00 ^a
$\varphi = v_{\rm P} /v$	π "correction"	0.353	0.170	
$\beta = (2 - v_b)/(2 - v_b)$	v_{τ} magnetization	n 0.170		0.125 ^a
$\gamma = 2(v_h - 1)$	$)/v_{\tau}$ susceptibility	2.337		1.75 ^a
$\eta = 4 - 2y_h$	critical corr	elation 0.254		0.25 a
Percolatio	n			
$v_{\rm A} = 1/v_{\rm B}$	correlation l	ength 1.637	1.629	1.34 ± 0.02 b
$2 - \alpha_{s} = 2/\sqrt{2}$	mean number	3.273	3.259	2.68 ± 0.04 ^b
p	of clusters			
φ_{h}	cross-over	1	1	
$\beta_{b} = (2 - \gamma_{b})$	$/v_{P}$ percolation p	robability 0.193		0.15 ± 0.03 ^b
$\gamma_{h} = 2(\gamma_{h} - 1)$	$1)/v_{h}$ mean cluster	size 2.888		2.38 ± 0.02 b
$d_{h} = \gamma \sqrt{\nu_{h}}$	effective clus	ster 1.764		1.78 ± 0.04 ^b
	dimensional	ity		

TABLE II. Critical exponents from xy asymmetric recursion relations.

^aReference 41.

^bReference 43.

nents of the various recursion relations are summarized in Table I. The corresponding (Greek alphabet) critical exponents for the xy asymmetric recursion relations (b=2 and b-1) are given in Table II. The accuracy of the nonmagnetic exponents is limited. Section IIC discusses the magnetic exponents.

C. Recursion relations at $h \neq 0$

There is considerable arbitrariness in the Migdal-Kadanoff approach when developing recursion relations with magnetic fields: the fraction of the field at each site that is moved with the bond is arbitrary. One possibility¹⁸ is to divide the field at each site symmetrically between the four bonds at that site and then to move bonds (with attached fields) as before (Sec. IIB). This possibility is workable and gives reasonable exponents;⁴⁵ however, it has an annoying conceptual problem:⁴⁶ when interactions vanish, $K_{ii} = 0$, renormalization (of the decimation type) should leave the magnetic fields at undecimated sites unaltered. Any nonvanishing fields which move with bonds will violate this requirement. We therefore adopt the following procedure. Consider the xy asymmetric case and refer to Fig. 1(b). In the initial contraction the y bonds are moved without fields and the x decimation is performed. The renormalized field on site 13 is $\bar{h}_{13} = h_{13} + \Delta h_{13}$, with

$$\Delta h_{13} = f(K_{13,14}, K_{14,15}, h_{14}) + f(K_{12,13}, K_{11,12}, h_{12}), \quad (25)$$

where

$$f(x,y,z) = \frac{1}{4} \ln \left(\frac{(1+e^{2x+2y+2z})(e^{2y}+e^{2x+2z})}{(e^{2x}+e^{2x+2y})(e^{2x}+e^{2y+2z})} \right).$$
(26)

When in the succeeding y contraction the x bonds are moved, we allow them to carry the change in field Δh generated by the previous x decimation.⁴⁷ At this stage the new field on site 13 is $\overline{h}_{13} = \overline{h}_{13}$ $+\Delta h_8$. Finally, we decimate along the y direction and obtain the renormalized fields $h'_{\alpha^{\circ}}$

Even if one starts with the uniform initial field distribution (2), the renormalized h'_{α} will be (i) inhomogeneous and (ii) correlated among themselves and with the $K'_{\alpha\beta}$'s. As in Sec. II B we neglect all correlation. Furthermore, rather than keeping the full h distribution, we make the approximation of replacing it by a δ function in analogy to (19),

$$\mathcal{O}(h'_{\alpha}) = \delta(h'_{\alpha} - h') . \tag{27}$$

Because the order parameter in our problem is \overline{M} and h is the corresponding conjugate field see (5)], we hope that this neglect of all moments of $\mathcal{P}(h)$ higher than the first is a reasonable first approximation.⁴⁸ The averaging (19) over $\mathcal{O}(\{K_{i,i}\})$ can now be done easily. To linear order in h the magnetic-field recursion relation for b = 2 is

.

$$h' = h \{ 1 + p^{4} \tanh 4K + 4p^{3}(1-p) \tanh 3K + [6p^{2}(1-p)^{2} + 2p^{2}] \tanh 2K + [4p(1-p)^{3} + 4p(1-p)] \tanh K \}.$$
(28)

Magnetic critical exponents are obtained as usual. We find for the pure system $y_h = 1.873$ (exact⁴¹ y_h)

= 1.875) and at the percolation threshold $y_h = 1.882$ (series⁴³ $y_h = 1.89 \pm 0.02$). The corresponding magnetic exponents are shown in Table II. The Migdal-Kadanoff approximation is very satisfactory for y_h , in marked contrast to the situation for y_T .

D. Calculation of thermodynamic functions

Phase boundaries and thermodynamic data are given in Sec. III. The recursion relations (20), (21), (22), and (24) suffice to produce the former. Thermodynamic computations on the other hand are based on Eqs. (5)-(7) and require evaluation of the average free energy per site \overline{f} , which is calculated by summing the incremental integrated free energy generated at each iteration stage,^{6,23,49}

$$\overline{f} = \sum_{n=0}^{\infty} b^{-(n+1)} \times \int \left(\prod_{(i,j)} dK_{ij}^{(n)} \mathcal{O}^{(n)}(K_{ij}^{(n)}) \right) \Re(\{K_{ij}^{(n)}\}) .$$
(29)

The superscript (n) indicates the *n*th iterate and the function $\Re(\{K_{ij}\})$ is the inhomogeneous incremental free energy per site. $\Re(\{K_{ij}\})$ is the spinindependent term that occurs in the renormalization-group transformation, i.e., the relevant field belonging to the identity operator. There is some latitude in defining \Re within the Migdal-Kadanoff approach. We consider the xy asymmetric case (20) and adopt the following procedure: during the initial x contraction the y bonds $[K_{4,9}, K_{9,14}, K_{2,7},$ and $K_{7,12}$ in Fig. 1(b)] are moved, the x decimation is performed, and an incremental free energy is obtained. This increment is associated with the site to the left of the new bond. For example, summing over spin 4 in Fig. 1(b) yields a term

$$g(K_{13,14}, K_{14,15}) = \ln 2 + \frac{1}{2} \ln [\cosh(K_{13,14} + K_{14,15}) \\ \times \cosh(K_{13,14} - K_{14,15})],$$

which is associated with site 4. Now, the intermediate x bonds are moved and the y decimation is performed. This yields an additive free-energy increment at site 1 which consists of two parts which depend only on x and y bonds, respectively,

$$\Re = \Re_x + \Re_y$$
,

where

$$\mathfrak{R}_{x} = g(K_{13,14}, K_{14,15}) + g(K_{8,9}, K_{9,10})$$
(30)

and

$$\mathfrak{R}_{v} = g(K_{3,8} + K_{4,9}, K_{8,13} + K_{9,14})$$

The averaged quenched-free-energy increment is now obtained by use of (19),

$$R(p, K) \equiv \int \prod_{\langle i,j \rangle} \left[dK_{ij} \mathcal{P}(K_{ij}) \right] \mathfrak{R}(\{K_{ij}\})$$
$$= R_x(p, K) + R_y(p, K), \qquad (31)$$

and the full free energy (29) follows from summation,

$$f = \sum_{n=0}^{\infty} b^{-(n+1)d} R(p^{(n)}, K^{(n)}).$$
(32)

We calculate the average specific heat per site by carrying out the differentiation (7) numerically.

To compute thermodynamic properties in the $b \rightarrow 1$ limit, it is necessary to find R(p, K) for arbitrary integer b > 1 and then to carry out the appropriate analytic continuation. We have been able to do this only for the R_x part of (31). Therefore, in order to proceed, we are forced to make the additional simplifying approximation that the x and y contractions contribute roughly equal amounts to the incremental free energy, i.e.,

$$R(p, K) \simeq 2R_x(p, K) . \tag{33}$$

We have checked at b=2 (see Sec. III B) that the qualitative features of the specific-heat curves are unaltered by the replacement of (31) by (33). Using the approximation (33), one finds

$$R(p, K) = b \left\{ p^{b} \ln \left[1 - \left(\frac{c-1}{c+1} \right)^{b} \right] + b p \ln(1+c) + b(1-p) \ln 2 \right\}, \quad (34)$$

where $c = \cosh 2K$. In computing the $b \rightarrow 1$ limit numerically from (34), we used a linear extrpolation based on b = 1.1 and b = 1.01. The linear dependence of the specific heat on b was checked carefully for several points.

Within the assumption of Sec. II C, it is easy to find an expression for the zero-field magnetization. Based on (5),

$$\overline{M}(p, K, 0) = \frac{\partial \overline{f}}{\partial h} \bigg|_{h=0} = b^{-d} \frac{\partial \overline{f}^{(1)}}{\partial h^{(1)}} \frac{\partial h^{(1)}}{\partial h} \bigg|_{h=0}, \quad (35)$$

where $h^{(n)}$ is the average magnetic field after *n* iterations and $\overline{f}^{(n)}$ is the average free energy per site at $p^{(n)}$, $K^{(n)}$, $h^{(n)}$. Repeating this, we find that, when the initial point (p, K) flows to the zero-temperature fixed point $(p = 1, K = \infty)$, the spontaneous magnetization is given by the infinite product,⁵⁰

$$\overline{M}(p, K, 0) = \prod_{n=1}^{\infty} \left(b^{-d} \frac{\partial h^{(n)}}{\partial h^{(n-1)}} \right)_{h=0}.$$
 (36)

Note that $\partial h^{(n)}/\partial h^{(n-1)} + b^d$ as $(p, K) + (1, \infty)$, ensuring the convergence of the infinite product. The T=0 magnetization is just the percolation probability (9). Equation (36) simplifies in this case to

$$P(p) = \prod_{n=1}^{\infty} \left[1 - \frac{1}{2} (1 - p^{(n)})^2 - \frac{1}{4} (1 - p^{(n)})^4 \right], \qquad (37)$$

which we use in Sec. III C.

III. RESULTS

A. Phase boundaries

Phase boundaries and a few representative global flows are shown in Fig. 2 for the b = 2 and b \rightarrow 1 versions of the *xy* asymmetric recursion relations [Eqs. (20) and (24)]. The behavior of other recursion relations is qualitatively identical. Points of the ordered phase $T < T_c(p)$ flow to the ferromagnetic sink at p = 1, T = 0 ($\tau = 1$), while those of the disordered phase flow to the paramagnetic sink at p = 0, $T = \infty$ ($\tau = 0$). The phase-boundary points flow from the percolation fixed point to the pure-system fixed point. This implies that the critical behavior for $p > p_c$ belongs to the universality class of the pure system (i.e., exhibits puresystem exponents, etc.). This result, although presumably false, is consistent with the Harris criterion,⁷⁻¹⁰ in that the Migdal approximation yields a negative value for the pure-system specific-heat exponent α . The actual critical properties of the dilute two-dimensional Ising model are unknown. Because the pure-system specific heat diverges logarithmically, the Harris criterion is inconclusive. It is quite possible, however, that there is crossover to a distinct, nondivergent, dilute critical behavior at p < 1. The behavior shown by our Migdal-Kadanoff approximation is



FIG. 2. Phase boundaries derived from the xy asymmetric recursion relations. Scale factors b=2 ($p^*=0.618$) and $b \rightarrow 1$ ($p^*=\frac{1}{2}$) are shown. Note the large region over which T_c is a linear function of impurity concentration. Dashed curves show some representative trajectories. Arrows give direction of flow.

appropriate only for a system with α (pure) < 0; however, it may not be a gross misrepresentation for α (pure) \geq 0, provided the crossover is in some sense 'weak," a point we shall return to in Sec. III B.

The $b \rightarrow 1$ phase boundary was determined from Eq. (22) using a sequence of nonintegral b's approaching unity from above. It is probably an excellent representation of the true phase boundary. Not only are K_c (pure) and p_c given exactly (Sec. II B), but also the exact initial slope $\partial T_c(p)/\partial p |_{p=1}$ is known from a calculation of Harris,⁷ who finds 3.016. Our calculated value is 3.108, a discrepancy of only 3%. The initial slope at percolation (in terms of proper low-temperature variables) has been calculated, ⁵¹ $de^{-2K_c(\phi)}/dp |_{p=p_c=1/2} = 2 \ln 2$ = 1.386. Our calculated value is 1.33±0.01, a discrepancy of 4%.

Note finally the qualitative form of the global flows⁵²: trajectories that start near but not on the phase boundary diverge from it rapidly. Indeed, any trajectory passing through a nominal critical region, $1-p < 10^{-2}$, $t = |[T - T_c(p)]/T_c(p)| < 10^{-2}$, near the pure-system fixed point was practically indistinguishable from the phase boundary for p< 0.9. For example, if one follows the b = 2 xyasymmetric trajectory starting at p = 0.66 and $k_B[T - T_c(p)]/J = 10^{-7}$, one finds that by the time $p \simeq 0.99$, t has grown by more than four orders of magnitude. Since it is the contributions to \overline{f} [Eq. (32)] from the neighborhood of the pure-system fixed point which give rise to critical behavior,⁵³ it is clear that for p < 0.9 the region $T - T_c(p)$ of observable critical behavior in the thermodynamic functions will be exceedingly narrow. We shall see this explicitly in Sec. III B. Analysis in the linear region near the pure-system fixed point is easy: at each step of iteration t increases by a factor of b^{y_T} , while the irrelevant field, which measures distance along the phase boundary, decreases by a factor $b^{-|y_p|}$. Hence, $t \sim (1-p)^{-1/\varphi}$, where $\varphi = |y_{p}| / y_{T}$ (see Table II).

B. Specific heat

Figures 3-7 show a variety of specific-heat curves. Figures 3-5 refer to the b = 2 xy asymmetric recursion relations (17) and are based on the "correct" $R_x + R_y$ free-energy expression (31). Figure 6 refers to the b = 2 xy symmetric recursion relation (22) with the $R_x + R_y$ free energy, and emphasizes the fact that the different b = 2 recursion relations discussed in Sec. II B produce qualitatively similar curves. We emphasize the b= 2 curves despite the rather poor phase boundaries to which they correspond, because their qualitative behavior appears general and can easily



TEMPERATURE (k_BT/J)

FIG. 3. Specific-heat curves for the randomly impure Ising model on the square lattice. p is the bond concentration, i.e., a fraction 1-p of all bonds have been removed. Calculations use the b=2 xy asymmetric recursion relations (20) with the $R_x + R_y$ free energy (31). $p_c = 0.618$ in this approximation. Note the rapid disappearance of the cusp well above p_c .



FIG. 4. Specific heat at p=0.85, showing magnified inset of critical region. Data is the same as Fig. 3. Note scale of inset axes. Cusped critical behavior is present but its magnitude is very much reduced. The maximum of the specific heat occurs at a temperature well above T_c (p=0.85).



FIG. 5. Specific heat at the percolation threshold. $p_c = 0.618$ in this approximation. Data is the same as Fig. 3. A low-concentration specific heat (p = 0.2) is shown for comparison. Arrows indicate appropriate scale of vertical axis. The dashed curve (read on the right-hand scale) is a plot of 0.4185 ($K/\cosh K$)² and corresponds to the shape of the specific-heat contribution of clusters not containing closed loops (see text). Its coefficient is chosen to fit the p = 0.2 data at $k_B T/J = 4$.



FIG. 6. Specific heat in the b=2 xy symmetric Migdal-Kadanoff apprixmation (22), using the $R_x + R_y$ free energy (31). The pure-system specific heat is identical to Fig. 3, but now $p_c = 0.389$. The effect of dilution is similar to that in Fig. 3; however, a small visible cusp is still present at p=0.8.



FIG. 7. Specific heat in the $b \rightarrow 1 xy$ asymmetric Migdal-Kadanoff approximation (24) using the $2R_x$ free energy (33). T_c (pure) agrees with the Onsager value as $b \rightarrow 1$. The percolation threshold $p_c = \frac{1}{2}$ is also exact. Note, however, that the shape of the specificheat curves remains similar: the critical cusp disappears rapidly as impurity concentration is increased. The linear region for $p = p_c$ also persists (see text).

be studied in a context which is computationally simple and free of ambiguity. A calculation of specific-heat curves with the b = 2 xy asymmetric recursion relations (17) based on the "incorrect" but analytically continuable $2R_r$ free-energy expression (33) yields curves with shapes similar to those of Fig. 3. (The specific heats are approximately 20% larger and the visible cusps disappear slightly more slowly as impurity concentration is increased.) This serves to make plausible the assertion that the $R_x + R_y$ free energy may be replaced by the $2R_x$ free energy. Figure 7 displays the results obtained by using the $b \rightarrow 1$ recursion relations (24) with the (continued) $2R_r$ free energy. These curves are our best estimates for the $b \rightarrow 1$ Migdal-Kadanoff specific heat and go with the "good" b - 1 phase boundary of Fig. 2.

Focus now on Figs. 3, 6, and 7, each of which diaplays a family of specific-heat curves. Although phase-boundary data differs between approximations, the behavior of the families are similar: at p = 1 there is a bold, λ -like peak. The size of this peak decreases rapidly with increasing impurity concentration, until by p = 0.8 ($0.8 \gg p_c$) the specific-heat maximum occurs at a temperature well *above* the transition and there is hardly any detectable anomaly at $T_c(p)$. Below p = 0.8 all curves *appear* smooth to graphical accuracy. As long as $p > p_c$, there is, of course, sharp singular behavior; it occurs, however, on an unobservably small scale, as illustrated in Fig. 4. This dramatic disappearance of *observable* critical behavior occurs as a consequence of the criticalregion narrowing discussed in Sec. III A (*not* because of any pronounced decrease in the critical specific-heat amplitude).⁵⁴ This narrowing, as we have seen, is controlled by the correction exponent φ (Table II).

Is the rapid disappearance of observable critical behavior well above p_c an artifact of our approximations or is it real? We cannot answer with certainty, but there are two pieces of evidence that suggest the latter. Monte Carlo calculations of the specific heat of the d=2 site-dilute Ising model by Ching and Huber²⁴ show this effect. On the experimental side there are relatively few critical experiments with controlled random dilution. Algra et al.²⁵ have taken specific-heat data which look very similar to our curves on $Co_{1-x}Zn_x(C_2H_5NO)_6(C10_4)_2$, a site-dilute⁵⁵ s = 1/2 XY antiferromagnet. How common such behavior is and for precisely what systems it occurs are

questions that deserve investigation. Note that, if this effect is present, it is important to distinguish in the analysis of data between $T_c(p)$ and the considerably higher temperature of the rounded specific-heat maximum.

Our overall conclusion is that for the dilute system normal, sharp critical behavior, although technically present, may well be invisible not only near the percolation threshold but throughout much of the dilute region $p_c . If true, how should this be interpreted? The progressive freezing out of$ *local* $disorder (both in finite clusters and in local regions of the infinite cluster) takes place smoothly over the range <math>k_B T \approx J - 2J$. It appears that the *additional* entropy associated with the development of *long*-range order in the infinite cluster for $T \approx T_c(p)$ is quite negligible except close to p = 1.

We mention two additional and apparently general characteristics of the specific-heat curves: (i) a striking decrease with p in the specific heat on the low-temperature side of the transition very near p = 1 (0.9 < p < 1.0) and (ii) a peculiar linear region on the low-temperature side of the specific-heat maximum near and at $p = p_c$, visible particularly clearly in Fig. 5 but present also in Figs. 3, 6, and 7. We have no physical interpretation of these phenomena.⁵⁶ We comment further on point (ii): it is easy to show that any cluster of

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FIG. 8. Spontaneous magnetization of the randomly bond-dilute Ising model, calculated using the b=2 xy asymmetric recursion relations. Note that, although the critical exponent β is the same at all concentrations p, the magnetization drops off more abruptly with temperature for $p \approx p_c$ than for $p \approx 1$.

coupled Ising spins (finite or infinite) which contains no closed loops contributes to the specific heat a term proportional to $(K/\cosh K)^2$, which peaks at $T \sim 0.83 J/k_B$. Small branched chains of this type may be expected to dominate the specific heat for low p, and the shape of the specific-heat curve at p = 0.2 (Fig. 5) bears out this expectation. On the other hand, for $p_c the temperature$ $of the rounded maximum is well above <math>0.83 J/k_B$ and decreases only weakly with p. Thus, the shape of the curve at $p = p_c$ suggests a superposition of two rather distinct contributions. Whether this is connected to recent speculations about dominant cluster configurations near percolation^{13-15,57} remains obscure.

C. Magnetization and percolation probability

Figure 8 shows the spontaneous magnetization $\overline{M}(p, T)$, as calculated using the b=2 xy asymmetric recursion relations and Eqs. (36) and (37). Note via (9) that $\overline{M}(p, 0) = P(p)$. The intersection $\overline{M}(p, T) = 0$ reproduces the b=2 phase diagram of Fig. 2. Although the percolation threshold is given poorly for b=2 ($p_c=0.618$), the qualitative trends shown by the curves are all reasonable.

IV. SUMMARY

The randomly bond-dilute, two-dimensional, nearest-neighbor Ising model on the square lattice was studied by renormalization-group methods, based on the Migdal-Kadanoff approximate recursion relations. The value of the approach is that it provides a simple method for the *estimation* of the phase diagram, critical exponents, and thermodynamic functions. The approximation does not generally give correct quantitative information (except, e.g., for the phase diagram in the limit $b \rightarrow 1$), but it does seem to describe correctly some of the essential features of phase transitions in randomly dilute magnetic systems.

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