

**A RENORMALIZATION-GROUP ATTEMPT TO OBTAIN THE EXACT
TRANSITION LINE OF THE SQUARE-LATTICE BOND-DILUTE
ISING MODEL**

by

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ABSTRACT

Two different renormalization-group approaches are used to determine approximate solutions for the paramagnetic-ferromagnetic transition line of the square-lattice bond-dilute first-neighbour-interaction Ising model. The first one (in two different versions, named RG1 and RG2) consists in substituting a single bond for an H-shaped cluster. In the second one (RG3, RG4, RG5 and RG6) we take advantage of the self-duality of the square-lattice and define a duality renormalization operation. All six renormalization groups are defined as operations on the p - t space, where p is the independent occupancy probability, and $t = th (J/K_B T)$. Both approaches yield very good results, including the exact values $t_c = \sqrt{2} - 1$ and $p_c = 1/2$ (for all six RG's) and $dt_c/dp \Big|_{p=1} = 8 - 6\sqrt{2}$ (for RG5 and RG6), as well as the correct asymptotical behaviour in the neighbourhood of $t = 1$ (that is, $T=0$). The transition lines obtained through RG5 and RG6 are very likely to be extremely close (better than 0,5% in the most unfavourable case) to the exact solution; moreover, one of the two might be the exact one.

The Hamiltonian of the square-lattice bond-dilute spin-1/2 first-neighbour-interaction ferromagnetic Ising model can be written as:

$$H = \sum_{i,j} J_{ij} \sigma_i \sigma_j$$

where $\sigma_i, \sigma_j = \pm 1$, and J_{ij} is a random variable with probability distribution $P(J_{ij}) = (1-p) \delta(J_{ij}) + p \delta(J_{ij}-J)$, $J > 0$. The sum is taken over all pairs of nearest-neighbouring atoms of a plane square lattice. There have been in recent years several attempts ⁽¹⁻⁶⁾ to obtain exact or approximate information concerning the paramagnetic-ferromagnetic transition line of this model. So far, the only available exact results (see Table I) are the critical temperature for $p=1$ ⁽⁷⁾, the critical probability for $T=0$ ⁽⁸⁾, the asymptotical behaviour in the neighbourhood of $T=0$ ⁽³⁾, including upper and lower bounds on T_c , and finally the derivative $dT_c/dp|_{p=1}$ ⁽¹⁾.

We present here two different approaches for the above problem. The first one is a standard application of expansion-type real-space renormalization group; the cluster we have used is the H-cluster, introduced by Reynolds et al. ⁽⁹⁾, which proves to be very efficient, since it is self-dual.

We use throughout the paper the variable $t = \beta J$ (where $\beta = 1/k_B T$), which is very convenient in the treatment of such problems^(5,10), and will be referred to as the thermal transmittivity of the bond.

The overall transmittivity distribution of an H-cluster whose elementary bonds have distribution

$$P(t) = P(t; p, t_0) = (1-p) \delta(t) + p \delta(t-t_0) \quad (1)$$

is given by (see also Reference (5)):

$$\begin{aligned} P_H(t) = P_H(t; p, t_0) = & \left[(1-p)^5 + 5p(1-p)^4 + 8p^2(1-p)^3 + 2p^3(1-p)^2 \right] \delta(t) + \\ & + \left[2p^2(1-p)^3 + 6p^3(1-p)^2 \right] \delta(t-t_0^2) + 2p^3(1-p)^2 \delta(t-t_0^3) + \\ & + p^4(1-p) \delta \left(t - \frac{2t_0^2}{1+t_0^4} \right) + 4p^4(1-p) \delta \left(t - \frac{t_0^2 + t_0^3}{1+t_0^3} \right) + \\ & + p^5 \delta \left(t - \frac{2t_0^2 + 2t_0^3}{1+2t_0^3+t_0^4} \right) \end{aligned}$$

We now define a renormalization operation (RG1) on the parameter t_0 by holding p fixed and calculating t_0' so that

$$\langle t \rangle_{P'} = \langle t \rangle_{P_H}, \quad (2)$$

where $P'(t) = P(t; p, t_0')$. We seek the fixed points of the function $t_0'(t_0)$. For each p satisfying $1/2 \leq p \leq 1$ we have a non-trivial fixed point $t_0(p)$; the line of such points in the $p-t_0$ space is expected to be an approximation to the transition line we are looking for.

Let us add that although we cannot prove it, we strongly believe (6,11) that this method leads to the exact solution in the limit of increasingly large clusters. For results, see Table I:

We can also get an estimate for the critical exponent ν_t (defined by $\xi_t \sim |T - T_c|^{-\nu_t}$, where ξ_t is the usual correlation length), by taking $p=1$. We have:

$$\nu_t \approx \ln b / \ln \lambda_t,$$

where b is the expansion factor of the RG (in the present case $b=2$) and $\lambda_t = dT'/dT |_{T=T_c} = dt'_0/dt_0 |_{t_0 = t_c}$. This gives us $\nu_t \approx 1.149$, to be compared with the exact value $\nu_t = 1$. In a completely analogous way, we can make $t_0 = 1$ and renormalize p thus obtaining a function $p'(p)$ (see also Reference (9)), whose derivative λ_p in the fixed point $p=1/2$ leads us to an estimate of the critical exponent ν_p (defined by $\xi_p \sim |p-p_c|^{-\nu_p}$, where ξ_p is the mean cluster size:

$$\nu_p \approx \ln b / \ln \lambda_p = 1.428 ,$$

to be compared with the value $\nu_p = \ln 3 / (2 \ln(3/2)) \approx 1.3547^{(12)}$.

An alternative renormalization group (RG2) can be defined by requiring that equations (2) and

$$\langle t^2 \rangle_{p'} = \langle t^2 \rangle_{p_H} \tag{3}$$

be simultaneously satisfied. $P'(t)$ now denotes $P(t; p', t_0')$.

We thus get p' and t_0' as functions of p and t_0 . Equating p' to p and t_0' to t_0 leads to the non-trivial fixed points $(1/2, 1)$ and $(1, \sqrt{2} - 1)$. A flow line extends from the first to the second of these points, as suggested by Harris ⁽¹⁾. The slope of this line at both fixed points is obtained through diagonalization and search for eigenvectors of the Jacobian matrix of the joint functions $p'(p, t_0)$ and $t_0'(p, t_0)$. This line is a better approximation to the exact transition line than that obtained by RG1 (see Table I).

We now proceed to the exposition of the second approach (RG3, RG4, RG5 and RG6). Given a transmittivity t , we define its dual transmittivity as $t_D = (1-t) / (1+t)$. The word "dual"⁽¹³⁾ stems from the fact that, given a cluster (or two-terminal graph⁽⁶⁾) with bond transmittivities $\{t_i\}$, its dual cluster will have transmittivities $\left\{ \frac{1 - t_i}{1 + t_i} \right\}$.

For instance, let us consider a series arrangement of two bonds with transmittivities t_1 and t_2 : the overall transmittivity will be given by ⁽⁵⁾ :

$$t_s = t_1 t_2 \tag{4}$$

On the other hand, the overall transmittivity of a parallel arrangement of two bonds is given by

$$t_p = \frac{t_1 + t_2}{1 + t_1 t_2} . \tag{5}$$

We immediately verify that equation (5) may be written as follows:

$$\frac{1 - t_p}{1 + t_p} = \frac{1 - t_1}{1 + t_1} \cdot \frac{1 - t_2}{1 + t_2} , \tag{5'}$$

which clearly has the same functional form as (4), thus exhibiting the duality between t and $\frac{1-t}{1+t}$.

Now if t is a random variable with probability distribution P , let P_D be its dual distribution, that is, the probability distribution of the dual random variable t_D . P_D is given by

$$P_D(t) = \frac{2}{(1+t)^2} P\left(\frac{1-t}{1+t}\right). \quad (6)$$

In our particular case, $P(t)$ is given by equation (1), so that $P_D(t)$ is given by

$$P_D(t) = P_D(t;p,t_0) = (1-p) \delta(t-1) + p \delta\left(t - \frac{1-t_0}{1+t_0}\right) \quad (7)$$

We verify that P and P_D satisfy

$$\frac{2}{1+t_0} \langle t \rangle_P + \langle t \rangle_{P_D} = 1,$$

and

$$\left(\frac{2}{1+t_0}\right)^2 \kappa_2(P) = \kappa_2(P_D) \quad (8)$$

where $\kappa_2(P) \equiv \langle t^2 \rangle_P - [\langle t \rangle_P]^2$ is the second-order cumulant associated to P .

We next define a renormalization group (RG3) by holding p fixed and imposing the following condition:

$$\langle t \rangle_P = \langle t \rangle_{P_D}, \quad (9)$$

where $P'_D(t) = P_D(t;p,t'_0)$. This is justified by the self-duality of the lattice. We get a line of fixed points joining the points $(1/2,1)$ and $(1, \sqrt{2} - 1)$, in complete analogy with RG1. For results see Table I. We notice that this approach does not allow us to calculate the critical exponents ν_t and ν_p , since both the expansion factor b and the derivatives λ_p and λ_t have absolute value equal to unity, thus leading to an indeterminacy in the calculation of the critical exponents.

Another way to define a renormalization group (RG4) , analogous to RG2, is to require that equations (9) and

$$\kappa_2(P) = \kappa_2(P'_D) \quad (10)$$

be simultaneously satisfied, where $P'_D(t) = P_D(t;p',t'_0)$. The flow line joining the non-trivial fixed points $(1/2,1)$ and $(1,\sqrt{2}-1)$ gives us once more an approximation for the transition line we are seeking.

Comparing the results of RG3 and RG4 with the available exact results (Table I), we notice that the exact solution is in a sense intermediate between those obtained by RG3 and RG4. This led us to substitute a new condition for Eq. (10). This condition is based on the following heuristical argument : for RG3, we have $P_D = P'_D$ on the fixed points $t'_0 = t_0$, so that Eq. (8) gives us

$$\left(\frac{2}{1 + t_0} \right)^2 \kappa_2(P) = \kappa_2(P'_D) \quad (11)$$

Equation (11) could be taken as an accessory condition for RG3, since it imposes no further restrictions than those automatically, created by Eq. (9) and the fact that $t_0' = t_0$. We were thus led to consider an intermediate condition between those Eqs. (10) and (11), namely

$$\frac{2}{1 + t_0'} \kappa_2 (P) = \kappa_2 (P_D') \quad (12)$$

or

$$\frac{2}{1 + t_0} \kappa_2 (P) = \kappa_2 (P_D') \quad (13)$$

We define a renormalization group (RG5) by simultaneously requiring that Eqs. (9) and (12) be satisfied, and another one (RG6) through use of (9) and (13). Again, we get a flow line joining the fixed points $(1/2, 1)$ and $(1, \sqrt{2} - 1)$, which is intermediate between those of RG3 and RG4. As we see in Table I, the results obtained by means of RG5 and RG6 agree with all available exact results. In Table II we present a few points that lie in the transition lines obtained by RG5 and RG6. Figure 1 shows these lines in both p - T and p - t spaces.

We now proceed to a summary analysis of our results. As we can notice in Table I, all six RG's presented lead to results that agree fairly well among them, which allows us to suppose that these results are close to the exact solution as well. In fact, it would not be surprising if one of the two solutions obtained by means of RG5 and RG6, (which differ among them by less than 0,2% for the variable t in the most unfavourable situation) was found to be the exact one, since they agree perfectly with all available exact results. At any rate, comparing the solutions of RG3, RG4, RG5 and RG6, we may evaluate the error (inferior to 0.5% in mid-range) of the solutions of RG5 and RG6.

The derivative $dt_o/dp \Big|_{p = 1/2}$ deserves a special commentary. Bergstresser⁽³⁾ found rigorous upper and lower bounds for $t_c(p)$ (Eq. (45) of his paper); those bounds are depicted in Fig. 1. It is a straightforward matter to verify that all solutions from RG1 to RG6 fall within these bounds; as a matter of fact, this would be the case (at least in a neighbourhood of $p = 1/2$) whenever $-4 \leq dt_o/dp \Big|_{p = 1/2} \leq -2$. Incidentally, we remark that Fisch⁽⁴⁾, through use of Bergstresser's results, presents the value $dt_o/dp \Big|_{p = 1/2} = -2$ as being the exact one; however, it is not clear to us that he has not overlooked second-order corrections in Bergstresser's Eqs. (42) and (43). Also, our second derivative $d^2T/dp^2 \Big|_{p = 1}$ disagrees with the value suggested by Harris⁽¹⁾.

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REFERENCES

1. Harris A B - J. Phys. C: Solid State Phys. 7, 1671-92 (1974)
2. Plischke M and Zobin D - J. Phys. C: Solid State Phys. 10, 295-312 (1977)
3. Bergstresser T K - J. Phys. C: Solid State Phys. 10, 3831-49 (1977)
4. Fisch R - J. Statistical Phys. 18, 111-4 (1978)
5. Yeomans J M and Stinchcombe R B - J. Phys. C: Solid State Phys. 12, 347-60 (1979)
6. Tsallis C - to be published.
7. See for example Huang K, "Statistical Mechanics", Chapter 17, John Wiley and Sons (1963)
8. See for example Shante V K S and Kirkpatrick S - Adv. Phys. 20, 325-55 (1971)
9. Reynolds P J, Klein W and Stanley H E - J. Phys. C: Solid State Phys. 10, L167-72 (1977)
10. Nelson D R and Fisher M E - Ann. Phys. 91, 226-74 (1975)
11. Magalhães A C N, Tsallis C and Schwachheim G - to be published
12. Reynolds P J, Stanley H E and Klein W - J. Phys. A: Math. Gen. 11, L199-207 (1978); also Klein W, Stanley H E, Reynolds P J and Coniglio A (preprint).
13. For an analysis of duality within this context, see Syozi I - "Transformation of Ising Models" - Vol. 1, 270-329, Collection "Phase Transitions and Critical Phenomena" edited by Domb C and Green M S (Academic Press, 1972)

CAPTION FOR FIGURES AND TABLES

Fig. 1: Full lines - Transition line obtained by means of RG5 or RG6 (they are undistinguishable within the present scale) in a) p-t space, and b) p-T space. Broken lines - Rigorous upper and lower bounds⁽³⁾ for a) the critical transmittivity t_o , and b) the critical temperature T_c .

Table I

Summary of the results obtained by means of RG1 to RG6, as well as the exact available ones.

Table II

Critical transmittivities (t_o) and temperatures (T_c) obtained by means of RG5 and RG6 for various values of p.

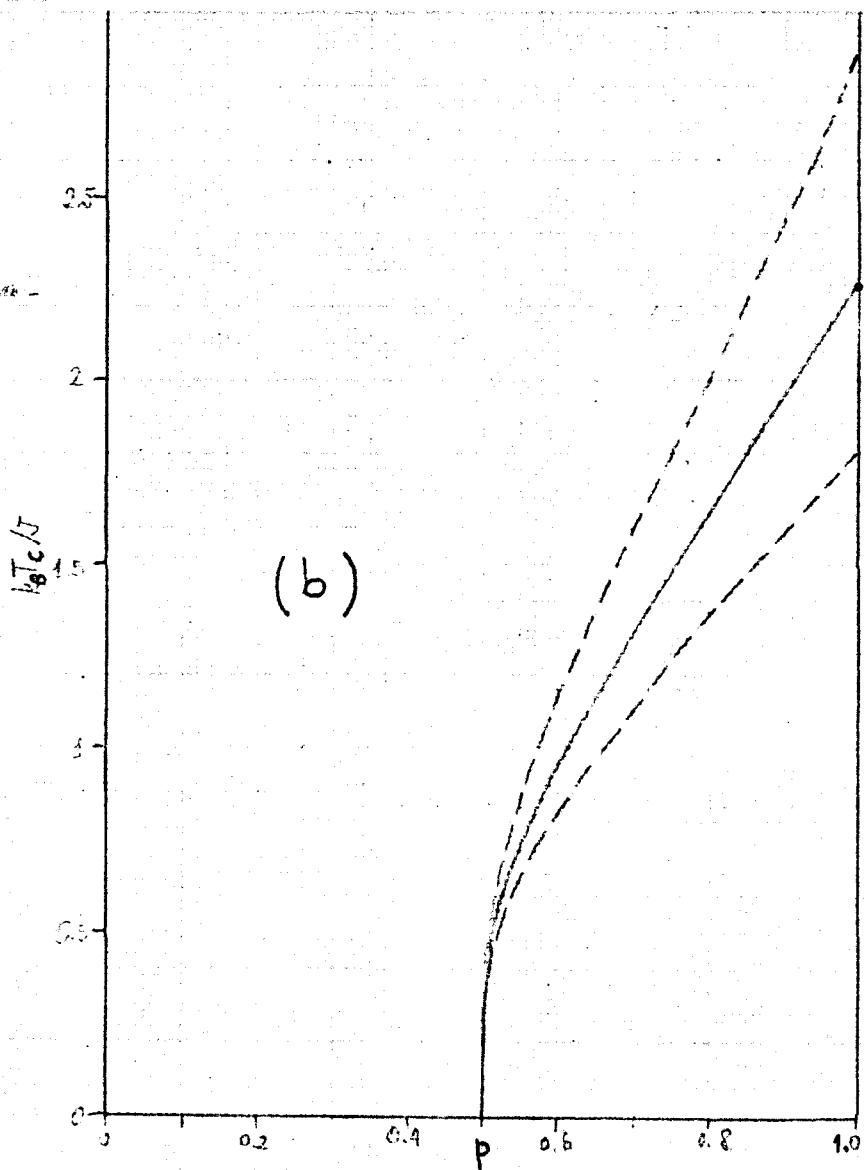
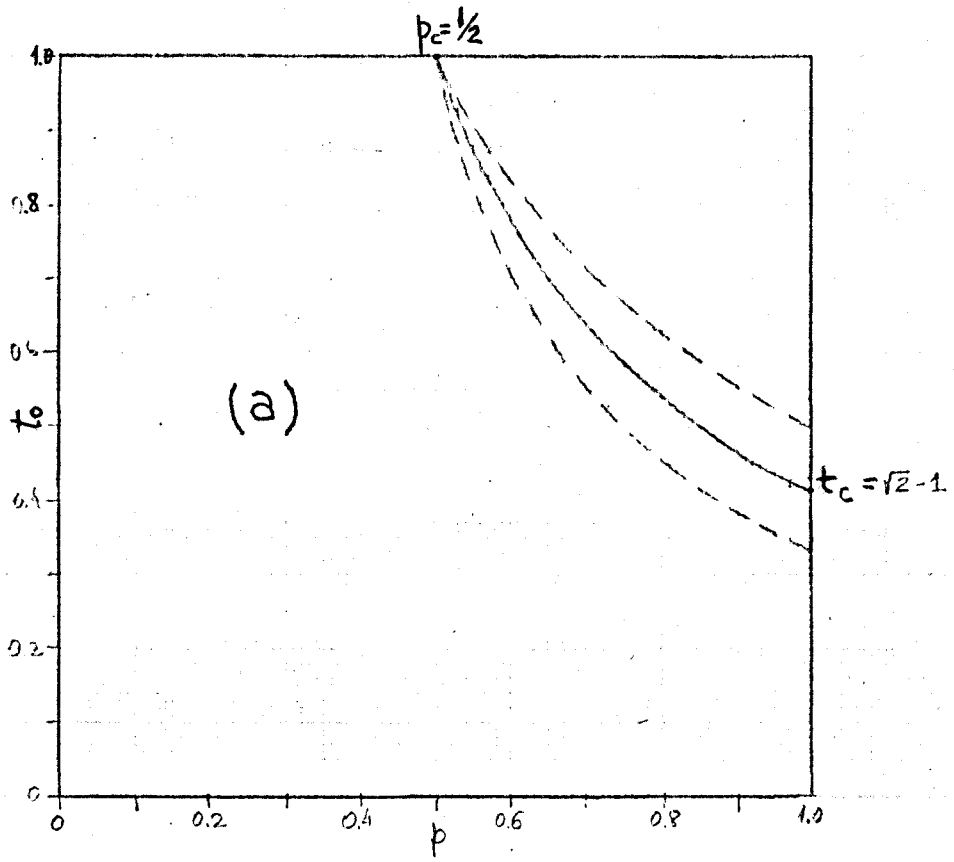


Fig. 1

TABLE I

RG	Eqs.	t_c	$-\frac{dt_o}{dp} \Big _{p=1}$	$\frac{1}{T_c} \frac{dT_c}{dp} \Big _{p=1}$	$\frac{d^2 t_o}{dp^2} \Big _{p=1}$	$-\frac{1}{T_c} \frac{d^2 T_c}{dp^2} \Big _{p=1}$	p_c	$-\frac{dt_o}{dp} \Big _{p=1/2} = 2 \frac{de^{-2\beta J}}{dp} \Big _{p=1/2}$
1	(2)	$\sqrt{2} - 1$	$\frac{65-31\sqrt{2}}{42} \approx 0.5038$	1.3800	1.30	0.45	1/2	2
2	(2), (3)	$\sqrt{2} - 1$	$\frac{3994+12509\sqrt{2}}{44183} \approx 0.4908$	1.3444	1.19	0.30	1/2	2.687
3	(9)	$\sqrt{2} - 1$	1/2	1.3696	1.18	0.16	1/2	$8/3 \approx 2.667$
4	(9), (10)	$\sqrt{2} - 1$	$\sqrt{2}/3 \approx 0.4714$	1.2912	1.17	0.48	1/2	3
5	(9), (12)	$\sqrt{2} - 1$	$6\sqrt{2} - 8 \approx 0.4853$	1.3293	1.14	0.23	1/2	$14/5 = 2.8$
6	(9), (13)	$\sqrt{2} - 1$	$6\sqrt{2} - 8$	1.3293	1.10	0.12	1/2	2.857
exact	—	$\sqrt{2} - 1$ ⁽⁷⁾	$6\sqrt{2} - 8$	1.3293 ⁽¹⁾	—	—	1/2 ⁽⁸⁾	$\epsilon [2, 4]$ ⁽³⁾

TABLE II

p	t_o (RG5)	KT_c/J (RG5)	t_o (RG6)	KT_c/J (RG6)
0.5	1	0	1	0
0.55	0.876844	0.734243	0.875351	0.737722
0.6	0.780307	0.955881	0.778727	0.959575
0.65	0.702744	1.145867	0.701490	1.149124
0.7	0.639135	1.321510	0.638262	1.324090
0.75	0.586063	1.488875	0.585511	1.490740
0.8	0.541129	1.650844	0.540814	1.652059
0.85	0.502604	1.809024	0.502447	1.809712
0.9	0.469212	1.964407	0.469151	1.964709
0.95	0.439994	2.117642	0.439981	2.117714
1	0.414214	2.269185	0.414214	2.269185