Percolation with first- and second-neighbor bonds: Renormalization-group calculation of critical exponents

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We propose a real-space renormalization-group approach for the bond-percolation problem in a square lattice with first- and second-neighbor bonds. We treat the respective probabilities as independent variables. Two types of cells are constructed. In one of them we consider the lattice as two interpenetrating sublattices, first-neighbor bonds playing the role of intersublattice links. This allows the calculation of both critical exponents ν and γ , without resorting to any external field. Values found for the critical indices are in good agreement with data available in the literature. The phase diagram in parameter space is also obtained in each case.

I. INTRODUCTION

The percolation problem¹ has been extensively studied in recent years. In analogy with thermal phase transitions we can define critical exponents,² and a number of techniques initially devised for thermal problems is used to calculate these exponents.³⁻⁵ Specifically, real-space renormalization group has been successfully applied to this problem by several authors.⁴⁻⁸

In this paper we apply the real-space renormalization-group (RG) techniques to the bondpercolation problem in a square lattice, taking into account both nearest- and next-nearest-neighbor bonds, with probabilities p and q of being active, respectively. We treat p and q as independent variables (that is, no *a priori* relation between them is assumed). This will allow us to find the phase diagram for the system. To our knowledge, a phase diagram has not been found or proposed in any other treatment of this problem.

Two types of cells are considered. Both display the symmetry and the connectivity of the original lattice, which is important in order to achieve accurate results with relatively small cells.^{5, 8, 9}

In one type of cell, we make use of the fact that the original lattice may be decomposed into two square interpenetrating sublattices, each one formed by second-neighbor bonds, coupled by the firstneighbor bonds [see Fig. 3(a)]. Thus, for a given sublattice, the first-neighbor bonds act like an external field and this allows the calculation of both exponents ν and γ , without resorting to any "applied" field (in the percolation problem, the "applied" field is simulated by a "ghost" site connected to every lattice site by "ghost" bonds^{5, 8, 10}).

Up to now, the only approach treating p and q as independent variables⁴ evaluates solely the

correlation-length exponent, using a decimation procedure.

II. SIMPLE-CELL APPROXIMATION

We recall briefly the pure first-neighbor-bond case treated in Ref. 8. One chooses a $b \times b$ cell. The cell has the same symmetry as the original lattice and each bond has a probability p of being active. The renormalization transformation casts it into a primitive cell in the renormalized lattice, each renormalized bond now having probability p' of being active. Both the original and the renormalized cells have the property of generating the entire lattice by suitable primitive translations. (Figure 1 shows the case b = 2.)

A recursion relation is defined when some prescription relates the two probabilities p and p'. In this case, a natural one⁵⁻⁸ is to count for p' all paths that traverse—that is, "percolate" through—the original cell in a given direction, for example, vertically. We then get, for a given b,

$$p'_{a} = R_{b}(p) \quad . \tag{1}$$



FIG. 1. (a) A $b \times b$ cell in a square lattice with only nearest-neighbor bonds; here b = 2. (b) A renormalized cell.

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Clearly the same recursion relation would be obtained if we had considered the horizontal direction. For b = 2 the above definition leads to^{5,7,8}

$$R_{2}(p) = p^{5} + 5p^{4}(1-p) + 8p^{3}(1-p)^{2} + 2p^{2}(1-p)^{3}$$
$$= 2p^{5} - 5p^{4} + 2p^{3} + 2p^{2}$$

for we have two paths with two active bonds [135 and 246 in Fig. 1(a)], eight paths with three active bonds and so on. In what concerns the "vertical percolation," that is, entering the cell through sites 1 or 2 and leaving it through 5 or 6, it is irrelevant whether bonds 12, 47, and 28 are active or not, so the counting of paths in Fig. 1(a) takes into account only the five remaining bonds.

From the fixed point $p^* = R_b(p^*)$, the correlationlength exponent⁵ follows: $\nu = \ln b / \ln \lambda_1$, where $\lambda_1 = (dp'/dp)_{p^*}$. Also, p^* represents the renormalization-group approximation⁵ to the critical concentration p_c for the given lattice. The cells of the type shown in Fig. 1 give the exact result $p_c = \frac{1}{2}$ for any value of b. This can be seen from duality arguments and is demonstrated elsewhere.^{7,8}

The counting of percolating paths becomes difficult as b increases, so we make use of a computer program which generates the exact recursion relation once the cell and the prescription for p' are given. With this program we have generated all the recursion relations of this paper. For the pure p case,⁸ the values of the exponent v for cells with b from 2 up to 5 approach quite rapidly the accepted value¹¹ 1.34 ± 0.02 , indicating that errors decrease as b increases.

Now, we connect also second-neighbor sites, the respective bonds having probability q of being active, and construct a $b \times b$ cell such that for q = 0 it reduces to the one considered previously. The case b = 2 is shown in Fig. 2. Again, we count for p' all paths traversing the cell in the vertical direction, that is, such that one reaches the nearest-neighbor cell in the original lattice. In Fig. 2(a) this corresponds to counting paths beginning at points 1 or 2 and reaching points 5 or 6. For q' we count paths traversing the cell along the diagonal direction, that is, such that the next-nearest neighbor cell is reached. In Fig. 2(a) this corresponds to counting all paths beginning at point 1 and reaching the point labeled 9. Paths passing through points outside the cell, such as 12749, are not counted. Again there is a verticalhorizontal symmetry and in addition, a northwestnortheast symmetry in the definition of q'. With these prescriptions we obtain, for a given b

$$p' = \tilde{R}_b(p,q) \quad , \tag{2a}$$

$$q' = \tilde{Q}_b(p,q) = qQ_b(p,q) \quad , \tag{2b}$$

where

$$\tilde{R}_b(p,0) = R_b(p) \quad , \tag{2c}$$



FIG. 2. Cell in the original lattice (a) is transformed into the one shown in (b). Full circles denote sites belonging to the cell, whereas sites belonging to neighboring cells are shown as empty circles. (c) Typical plot of the RG flow lines in the approximation of Sec. II. The heavier line ABseparates "percolating" (outside) and "nonpercolating" (inside) regions.

the latter being defined by relation (1). We have factored out q in Eq. (2b); from our definition and from our cell this is always possible.

The renormalization-group flow in parameter space is shown in Fig. 2(c). We comment on the main features of this diagram. The interesting fixed point is $B(p^* = \frac{1}{2}, q^* = 0)$, as expected. Due to the factorized form of Eq. (2b), the matrix for the linearized transformation in the vicinity of this fixed point is triangular $(\partial q'/\partial p = 0 \text{ if } q = 0)$. Hence, the relevant eigenvalue of the transformation $\lambda_1 = (\partial p' / \partial p)_B$ leads, in view of relation (2c), to the same exponent as in the pure p case, in accordance with universality. The second eigenvalue, $\lambda_2 = (\partial q' / \partial q)_B$, is smaller than 1.

The curve AB separates the parameter space into two regions: the external (internal) part comprises points such that we do (do not) percolate through the lattice. Curve AB is then a phase boundary for the problem. It is interesting to follow the flow line along this boundary, for it shows the secondneighbor "interaction" becoming irrelevant, approaching $q^* = 0$ as successive renormalizations are performed.

A line of fixed points at p = 1 is also found. Its origin can be traced back to the fact that $Q_b(p,q)$ [for instance in Fig. 2(a)] is the probability of reaching site labeled 4, and this is clearly 1 when p = 1, whatever the value of q; hence, $\tilde{Q}_b(1,q) = q$. It should be pointed out, however, here and in Secs. III and IV, that the physically interesting region of the parameter space is the vicinity of the phase boundary AB.

Except for the trivial fixed point $p^* = q^* = 0$, no additional fixed point is found.

We would expect the phase boundary to cross the q axis at $q_c = \frac{1}{2}$, for the lattice formed only by secondneighbor bonds is also a square lattice. Our calculations give $q_c = 0.442$ for b = 2 and $q_c = 0.445$ for b = 3, approaching, although slowly, the value $\frac{1}{2}$.

The intercept of the curve *AB* with the line p = q gives $p_c = q_c = 0.275$ for b = 2 and $p_c = q_c = 0.264$ for b = 3, which is to be compared with 0.252(+0.003, -0.007), found by Magalhães *et al.*,⁷ whose treatment assumes the *a priori* relation p = q.

III. DECOMPOSITION INTO TWO SUBLATTICES

The cells and renormalization-group transformations considered in Sec. II have the advantage of being a relatively simple and natural extension of the pure first-neighbor-bond problem, reducing to it when q = 0 and giving reasonable numerical results. However, at p = 0, the cells do not respect the "twosublattice symmetry" of the original lattice, that is, its decomposition into two disconnected sublattices for p = 0 is not preserved under the renormalizationgroup transformation. This gives rise to a not quite correct behavior of the flow lines on the q axis. In other words, at p = 0, we would expect to have the same behavior along the q axis in the vicinity of q_c as we have in the neighborhood of p_c on the p axis. From the point of view of the renormalization group this amounts to requiring that the intersection of curve AB with the q axis be a fixed point. In a cell of the type shown in Fig. 2(a) this does not happen, for in this renormalization transformation, q generates contributions for p' even if initially p = 0 [for example, path 145 in Fig. 2(a)]. It might be argued that the existence or not of a fixed point at A and the behavior of the flow lines near it are not (directly) physically observable, being only auxiliary quantities, the important thing being the phase boundary itself. We shall see below, however, that the appearance of a fixed point at A depends on the use of the twosublattice symmetry and this has the effect of changing the curvature of the phase boundary [see Figs. 3(c) and 3(d)].

Having in mind the idea of displaying explicitly the two-sublattice symmetry, we introduce a cell of the type shown in Fig. 3(a) which, under renormalization, becomes the one shown in Fig. 3(b). Two prescriptions defining renormalized p' and q' as functions of p and q are discussed in Secs. III A and III B below.



FIG. 3. Cell in the original lattice (a) and transformed in the renormalized lattice (b). Full circumferences denote sites belonging to the cell, whereas sites belonging to neighboring cells are shown as half-circumferences. Firstneighbor bonds are dashed and second-neighbor bonds are represented by full lines. α and β refer to the sublattices. (c) and (d): qualitative plots of the RG flow lines in the approximations of Secs. III A (c) and III B (d). The heavy line *AB* separates "percolating" and "nonpercolating" regions.

A. First RG transformation

Refer to Fig. 3(a). For p' we count all paths starting at sites α_1 or α_2 which end at sites β_1 or β_2 , that is, paths in which there is a change of sublattice. This is consistent with the idea that p bonds are now thought of as intersublattice links. For q' we count all paths going from site α_1 or α_2 to site α_5 or α_6 , but only through sites in the given sublattice α . Here again, the symmetry of the cell makes several definitions equivalent, such as starting at α_1 or α_3 and going to α_7 or α_8 for q' and from α_1 or α_3 to β_1 or β_3 for p'. With these definitions we get

$$p' = P_b(p,q) = pF_b(p,q)$$
, (3a)

$$q' = R_b(q) \quad . \tag{3b}$$

Note that Eq. (3b) involves only second-neighbor probabilities and the functional dependence of q' on q is the same as that obtained in Eq. (1). This comes from the fact that, within a given sublattice, q plays the same role as p in the pure first-neighbor-bond problem. Note also that there must be at least one factor p in each contribution to p'; hence, the form of Eq. (3a). The renormalization flow is shown in Fig. 3(c). Point $A(p^*=0,q^*=\frac{1}{2})$ is now a fixed point; the same is true of $B(p^*=\frac{1}{2},q^*=0)$. The line of fixed points has disappeared but there remains a fixed point at $C(p=1,q=\frac{1}{2})$, whose existence comes from the particular form of Eq. (3b).

At *A* the Jacobian matrix is diagonal, for both $\partial q'/\partial p$ and $\partial p'/\partial q$ are zero, but now $\lambda_1 = \partial q'/\partial q$ and $\lambda_2 = \partial p'/\partial p$ are both larger than 1. From Eq. (3b) it follows that the exponent $\nu = \ln b/\ln \lambda_1$ coincides with those referred to in Sec. II, in accordance with universality. On the other hand, λ_2 is a "magnetic"-like eigenvalue, in the sense that nearest-neighbor bonds are the analogs of a "onespin operator" in a thermal problem, for each sublattice. In the Appendix it is shown that the "susceptibility" exponent² γ is given by $\gamma = \ln \lambda_2 / \ln \lambda_1$.

We have performed calculations for b = 2, 3, 4 for $F_b(0,q)$.

In order to estimate the value to which our results should converge as $b \to \infty$, we extrapolate^{6,12} $\ln \lambda_2$ against $\ln b$, obtaining the value 1.9 for the fractional dimension¹² $d_f = 2 - \eta = \ln \lambda_2 / \ln b$. With the scaling relation $\gamma = \nu d_f$ and the previously extrapolated value⁸ of ν , we obtain the limiting value $\gamma \cong 2.5$, in good agreement with data available in the literature, namely, 2.435 (Ref. 6), 2.375 (Ref. 2), and 2.279 (from the data of Ref. 8).

At the fixed point *B* there is only one relevant eigenvalue, namely $\partial p'/\partial p$ (the Jacobian matrix is triangular at *B*). From this, we get $\nu = 1.042$ for b = 2and $\nu = 1.099$ for b = 3. These values show a poorer convergence than those previously calculated for this exponent. The reason is that in this case our renormalization transformations and cells do not reduce to those considered in the pure *p* case when q = 0.

The phase boundary AB, shown in Fig. 3(c), has now changed with respect to that in Fig. 2(c). This can be understood if we consider the situation p = 0and q slightly less than $\frac{1}{2}$. We then expect each sublattice to develop large clusters of active bonds. Thus, an infinitesimal amount of intersublattice bonds will connect these large clusters and an infinite cluster will be formed, that is, the system percolates. This means that the phase boundary must be tangent to the q axis at A. Clearly, the same argument does not apply at B: if, in a large cluster of first-neighbor bonds, one adds some second-neighbor bonds, most of them will be "wasted," for they will connect sites already connected by p bonds. Note, however, that with the recursion relations (3) the curvature of the boundary at B has the same sign as that at point B in Sec. II [Fig. 2(c)], implying the existence of an inflection point.

We shall see that with the recursion relations defined in Sec. III B, no change of curvature along the boundary is observed [see Fig. 3(d)].

B. Second RG transformation

We now introduce contributions from p to the renormalized probability q'; for p' we keep the same definition leading to Eq. (3a). As at least two firstneighbor bonds are needed to contribute to q' [for instance, to go from α_1 or α_2 to α_5 or α_6 in Fig. 3(a)], we can write the new recursion relations as

$$p' = pF_b(p,q) \quad , \tag{4a}$$

$$q' = p^2 G_b(p,q) + R_b(q)$$
, (4b)

where $R_b(q)$ is the same as in Eq. (3b).

Before defining $G_b(p,q)$ we note that the form of Eqs. (4) implies both the existence of a fixed point at $A(p^*=0,q^*=\frac{1}{2})$ and the same values of ν and γ obtained at this fixed point in Sec. III A, regardless of the functional dependence of G_b on p and q. This is because A has coordinate $p^*=0$, $(\partial q'/\partial p)_A$ is still zero, and $(\partial q'/\partial q)_A$ has the same value as before.

We now complete the definition of q'. At first sight, it might seem reasonable to take all nearestneighbor bonds into account. However, if this is done, the symmetry between sublattices α and β will be lost, in the sense that calculating q' with paths going from α_1 or α_2 to α_5 or α_6 gives a different result than using paths from β_1 or β_2 to β_5 or β_6 . In order to keep this symmetry, we do not take into account pbonds connecting sites in the cell to sites in a nearest-neighbor cell. This corresponds in Fig. 3(a) to exclude bonds such as $\beta_1\alpha_6$, $\beta_2\alpha_5$, and $\beta_2\alpha_6$.

to exclude bonds such as $\beta_1 \alpha_6$, $\beta_2 \alpha_5$, and $\beta_2 \alpha_6$. With this prescription, $B(p^* = \frac{1}{2}, q^* = 0)$ is a fixed point and the Jacobian matrix is still triangular at B. The eigenvalue $\lambda_1 = (\partial p'/\partial p)_B$ is, of course, the same as in Fig. 3(a), but the second eigenvalue is slightly larger than 1 and increases as b goes from 2 to 3 [see the flow line along the boundary AB of Fig. 3(d)]. This implies the existence of another fixed point on this boundary, which we call D in Fig. 3(d). Both the fixed point C and the straight flow line ACof Fig. 3(c) are no longer present.

For b = 2, D is located at $(p^* = 0.486, q^* = 0.010)$; there is only one relevant eigenvalue at this fixed point, namely, $\lambda_1 = 1.958$, from which we get $\nu = 1.031$. These values are to be compared with $(p^* = 0.3894; q^* = 0.1516)$ and $\nu = 0.861$ obtained by Young and Stinchcombe.⁴ Larger cells are needed to improve this value of ν .

IV. CONCLUSIONS

The phase boundary AB of Fig. 3(d) is very similar to the one obtained by van Leeuwen¹³ for the Ising model with first- and second-neighbor interactions. There, the enlargement of the parameter space by the introduction of second-neighbor couplings shifts the original fixed point along the phase boundary. In the present case, however, due to our definition of the renormalization transformations, both points D and B occur. Had we taken all p bonds into account, it would have been possible to get contributions to q' made out of only p bonds, and B would no longer be a fixed point. But then symmetry between α and β sublattices would be broken, as stated above.

As already remarked at the end of Sec. III A, there is no change in curvature along the phase boundary in Fig. 3(d). This means that now, near point *B*, the condition for percolation is less restrictive. This, in turn, comes from the introduction of a *p* dependence in Eq. (4b), which clearly makes possible the percolation with smaller values of *q*, for a given *p*. On physical grounds, we expect that the diagram in Fig. 3(d) be our best representation of what actually occurs in the true infinite lattice.

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APPENDIX

Let $u = \frac{1}{2} - q$, so $u_c = K_c p_c^{1/\phi}$ is the equation of the critical line (or phase boundary) near the critical point (p, u) = (0, 0), where ϕ is the "crossover" ex-

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ponent. Clearly, as the effect of the linearized renormalization transformation in the neighborhood of the critical point is to transform the pair (p,u) into $(\lambda_2 p, \lambda_1 u)$, one has $\phi = \ln \lambda_2 / \ln \lambda_1$. If the average cluster size diverges as $S(0,u) \sim u^{-\gamma}$, then it is easily shown¹⁴ that $S(p,u) \sim (u - K_c p^{1/\phi})^{-\gamma}$, hence, $S(p,0) \sim p^{-\gamma/\phi}$. As $S(p,u) = \sum_s s^2 \langle n_s \rangle$, where $\langle n_s \rangle$ is the average number of clusters of size s per site, we can define the quantities $\langle n_s \rangle_0$ and $\langle n_s \rangle_p$ through $S(0,u_0) = \sum_s s^2 \langle n_s \rangle_0$ and $S(p \to 0, u_0) = \sum_s s^2 \langle n_s \rangle_p$, where u_0 is a fixed small value.

We are interested in studying the effect of introducing a small amount of p bonds on the behavior of the average cluster size: then we can take $p \leq 1/N$, where $N \rightarrow \infty$ is the total number of sites. The presence of a p bond will make finite clusters couple, that is, it will lower by one unit the number of clusters of two given sizes and will raise the number of clusters with greater size. If we assume that the coupled clusters were most probably of a size close to the average (this is a reasonable assumption as long as we are dealing with large numbers, so the spread in the probability distributions shrinks down as $1/\sqrt{N}$), one has

$$\langle n_s \rangle_p \simeq \begin{cases} \langle n_s \rangle_0 - 1/N = \langle n_s \rangle_0 - Ap, \quad S \sim S_0 \\ \langle n_s \rangle_0, \quad \text{otherwise} \end{cases},$$

where $S_0 = S(0, u_0)$ and A is a constant. Then,

$$S(p \to 0, u_0) \cong \sum_{s} s^2 \langle n_s \rangle_0 - BS_0^2 p \quad (B = \text{const})$$

or

$$[S(p \to 0, u_0) - S(0, u_0)]/p \cong -B[S(0, u_0)]^2$$

from which one has $S(p, 0) \sim 1/p$ or $\gamma/\phi = 1$.

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