(b) Calculate the critical exponent ν and compare its value with the exact result. Explain why b is given by $b^2 = 3$. Give a qualitative argument for why the renormalization group argument might work better for small cells on a triangular lattice than on a square lattice. ■

It is possible to improve our renormalization group results for p_c and ν by enumerating the spanning clusters for larger b. However, because the 2^N possible configurations for a $N = b^2$ cell increase rapidly with b, exact enumeration is not practical for $b > 7$, and we must use Monte Carlo methods if we wish to proceed further. Two Monte Carlo approaches are discussed in Project 12.13. The combination of Monte Carlo and renormalization group methods provides a powerful tool for obtaining information on phase transitions and other properties of materials.

As summarized in Table 12.1, the various critical exponents for percolation in two dimensions are known exactly. For example, the exponent ν, corresponding to the divergence of the connectedness length, is $\nu = 4/3$. It is interesting that the theory for this result is based on algebraic reasoning (too abstract to be summarized here), even though percolation is a geometrical phenomena. The most accurate estimate of p_c for the square lattice is $p_c = 0.59274621(13)$. We note that although there has been much work on percolation, only numerical estimates for p_c are known for most lattices.

12.6 ■ PROJECTS

Most of the following projects require larger systems and more computer resources than the problems that we have considered so far, but most are not much more difficult conceptually. More ideas for projects can be obtained from the references.

Project 12.12 Cell-to-cell renormalization group method

In Section 12.5 we discussed the cell-to-site renormalization group transformation for a system of cells of linear dimension b. An alternative transformation is to go from cells of linear dimension b_1 to cells of linear dimension b_2. For this cell-to-cell transformation, the rescaling length b_1/b_2 can be made close to unity. Many errors in a cell-to-cell renormalization group transformation cancel, resulting in a transformation that is more accurate in the limit in which the change in length scale is infinitesimal. We can use the fact that the connectedness lengths of the two systems are related by $\xi(p_2) = (b_1/b_2)^{-1}\xi(p_1)$ to derive the relation

$$\nu = \frac{\ln b_1/b_2}{\ln \lambda_1/\lambda_2}, \tag{12.28}$$

where $\lambda_i = dR(p^*, b_i)/dp$ is evaluated at the solution to the fixed point equation, $R(b_2, p^*) = R(b_1, p^*)$. Note that (12.28) reduces to (12.26) for $b_2 = 1$. Use the results you found in Problem 12.10d for one of the spanning criteria to estimate ν from a $b_1 = 3$ to $b_2 = 2$ transformation. ■

Project 12.13 Estimates for two-dimensional percolation

One way to estimate $R_L(p)$, the total probability of all the spanning clusters on a lattice of linear dimension L, can be understood by writing $R_L(p)$ in the form

$$R_L(p) = \sum_{n=1}^{N} S(n) P_N(n, p), \tag{12.29}$$

where

$$P_N(n, p) = \binom{N}{n} p^n q^{(N-n)}, \tag{12.30}$$

and $N = L^2$. The binomial coefficient $\binom{N}{n} = N!/[(N-n)!\,n!]$ represents the number of possible configurations of n occupied sites and $N - n$ empty sites; $P_N(n, p)$ is the probability that n sites out of N are occupied with probability p. The quantity $S(n)$ is the probability that a random configuration of n occupied sites spans the lattice. A comparison of (12.18) and (12.29) shows that for $L = 2$ and the vertical spanning criterion, we have $S(1) = 0$, $S(2) = 2/6$, $S(3) = 1$, and $S(4) = 1$. What are the values of $S(n)$ for $L = 3$?

We can estimate the probability $S(n)$ by Monte Carlo methods. One way to sample $S(n)$ is to add a particle at random to an unoccupied site and check if a spanning cluster exists. If a spanning cluster does not exist, add another particle at random to a previously unoccupied site. If a spanning cluster exists after s particles are added, then let $S(n) = S(n) + 1$ for all $n \geq s$ and generate a new configuration. After a reasonable number of configurations, the results for $S(n)$ can be normalized. Of course, this procedure can be made more efficient by checking for a spanning cluster only after the total number of particles added is near $s \sim p_c N$.

(a) Write a Monte Carlo program to sample $S(n)$. Store the location of the unoccupied sites in a separate array. To check your program, first sample $S(n)$ for $L = 2$ and $L = 3$ and compare your results to the exact results for $S(n)$. Consider larger values of L and determine $S(n)$ for $L = 4$, 5, 8, 16, and 32. Because the number of sites in the lattice can become very large, the direct evaluation of the binomial coefficients using factorials is not possible. One way to proceed is to approximate the probability of a configuration of n occupied sites by a Gaussian:

$$P_N(n, p) \approx \binom{N}{n} p^n q^{(N-n)} \approx (2\pi Npq)^{-\frac{1}{2}} e^{-(n-pN)^2/2Npq}. \tag{12.31}$$

(b) As pointed out by Newman and Ziff, the Gaussian approximation for $P_N(n, p)$ is not sufficiently accurate for high precision studies. Instead, they used the following method. The binomial distribution is a maximum for a given N and p when $n = n_{\max} = pN$. Set this value to 1 for the moment. Then compute $P_N(n)$ iteratively for all other n using

$$P_N(n, p) = \begin{cases} P_N(N, n-1, p)\dfrac{N-n+1}{n}\dfrac{p}{1-p} & (n > n_{\max}) \\ P_N(N, n+1, p)\dfrac{n+1}{N-n}\dfrac{1-p}{p} & (n < n_{\max}). \end{cases} \tag{12.32}$$

Then calculate the normalization coefficient $C = \sum_n P_N(n, p)$ and divide all the $P_N(n, p)$ by C to normalize the probability distribution.