Chapter 7

Percolation and the Potts Model

7.1   Introduction

To introduce bond dilution correctly and use bond dilution to map the percolation model onto the thermal, we need more powerful tools. These tools are provided by the Kasteleyn-Fortuin mapping [Kasteleyn and Fortuin 1969], which relates the percolation model to a particular limit of the Potts model [Stauffer 1979].

7.2   Random Bond Percolation and the Potts Model

The Potts model is a generalization of the Ising model. As in the Ising model we have a lattice with a spin at each vertex. In the Potts model however, the spins can be in one of s states rather than the two states of the Ising model. The Hamiltonian $-\beta H$ is

$$-\beta H = J \sum_{ij} \left(\delta_{\sigma_i \sigma_j} - 1 \right) + h_p \sum_i \left(\delta_{\sigma_i 1} - 1 \right). \tag{7.1}$$

The σ_i specify the direction of the Potts spin, $\delta_{\sigma_i \sigma_j}$ is the Kronecker delta and is one if the two spins at i and j are in the same state and zero otherwise. The term $\delta_{\sigma_i 1}$ is zero unless the Potts spin at site i is in the state we have designated as $\sigma_i = 1$ and h_p is the Potts applied field. The values of J and h_p are always taken to be greater than or equal to zero.

The partition function z is

$$z = \sum_{\{\sigma\}} \exp(-\beta H), \tag{7.2}$$

where the sum is over the configurations of the Potts spins or Potts states. The free energy per spin $f(J, h_p, s)$ is

$$f(J, h_p, s) = -\frac{k_B T}{N} \ln(z), \tag{7.3}$$

where N is the number of spins on the lattice and we have made the s dependence explicit.

The Kasteleyn-Fortuin mapping states that the derivative of $f(J, h_p, s)$ with respect to s evaluated at $s = 1$ is the mean number of finite clusters per site (generating function) in the random bond percolation model. To obtain this result we first rewrite z as

$$z = \sum_{\{\sigma\}} \left\{ \prod_{i \neq j} \left[e^{-J}(1 - \delta_{\sigma_i \sigma_j}) + \delta_{\sigma_i \sigma_j}) \right] \right\} \left\{ \prod_{i} \left[e^{-h_p}(1 - \delta_{\sigma_i 1}) + \delta_{\sigma_i 1} \right] \right\}. \tag{7.4}$$

We regroup terms and write

$$z = \sum_{\{\sigma\}} \left\{ \prod_{i \neq j} \left[(1 - e^{-J}) \delta_{\sigma_i \sigma_j} + e^{-J} \right] \right\} \left\{ \prod_{i} \left[(1 - e^{-h_p}) \delta_{\sigma_i 1} + e^{-h_p} \right] \right\}. \tag{7.5}$$

If $s = 1$ we have from Eq. (7.4) that $z = 1$. Consequently

$$\left. \frac{df(J, h_p, s)}{ds} \right|_{s=1} = -\frac{k_B T}{N} \left. \frac{dz}{ds} \right|_{s=1}. \tag{7.6}$$

To investigate the derivative of the partition function with respect to s we start with the simpler case of $h_p = 0$. From Eq. (7.5) the partition function becomes

$$z = \sum_{\{\sigma\}} \left\{ \prod_{i \neq j} \left[(1 - e^{-J}) \delta_{\sigma_i \sigma_j} + e^{-J} \right] \right\}. \tag{7.7}$$

We expand this product and look at the term that results from all factors coming from the e^{-J} term , which we call z_1

$$z_1 = \sum_{\{\sigma\}} e^{-J N_b}, \tag{7.8}$$

where N_b is the number of possible bonds in the lattice. That is, N_b equals the number of places where a bond could be. The sum over $\{\sigma\}$ in Eq. (7.8) results in a factor of s^N, where N is the number of lattice sites or spins. The reason for this factor is that there are no delta functions to restrict the sum. From these considerations it follows that

$$\left. \frac{dz_1}{ds} \right|_{s=1} = N e^{-J N_b}. \tag{7.9}$$

We can interpret Eq. (7.9) as follows. Because $J \geq 0$, the quantity e^{-J} can be thought of as the probability $1 - p$ that a bond is **not** occupied or filled. Then the term e^{-JN_b} is the probability that there are no filled bonds on the lattice. Although we have defined a bond percolation problem, we count the clusters by counting sites, so if there are no bonds each site is an isolated one site cluster and N is the number of clusters when all bonds are unoccupied.

What happens if $h_p \neq 0$? The factor

$$z_{h_p} = \prod_i \left[(1 - e^{-h_p}) \delta_{\sigma_i 1} + e^{-h_p} \right] \tag{7.10}$$

can be expanded to give a sum of terms. Each term connects a subset n of the N Potts spins to the ghost, and each spin connected to the ghost is no longer free to contribute a factor of s in the sum over $\{\sigma\}$ because it is fixed by the $\delta_{\sigma_i 1}$ term to be in the state $\sigma_i = 1$. Because $h_p \geq 0$, the factor $1 - e^{-h_p}$ can be interpreted as the probability that a spin is attached to the ghost. If we multiply the two factors z_1 and z_{h_p}, differentiate with respect to s and set $s = 1$, we obtain

$$\left. \frac{d(z_1 z_{h_p})}{ds} \right|_{s=1} = e^{-JN_b} \sum_{n=0}^{N} (N - n) \frac{N!}{n!(N-n)!} e^{-h_p(N-n)} (1 - e^{-h_p})^n. \tag{7.11}$$

Equation (7.11) is the mean number of clusters with no bonds present; the sum is over all configurations of the ghost bonds.

Consider the case in which we take from the product in Eq. (7.7) only those terms with one factor of $(1 - e^{-J})$. We label this contribution z_2. We have

$$z_2 = N_b e^{-J(N_b - 1)} (1 - e^{-J}) \sum_{\{\sigma\}} \delta_{\sigma_a \sigma_b}. \tag{7.12}$$

The sum over $\{\sigma\}$ gives a factor s^{N-1}; which is a factor s^{N-2} for the one site clusters times a factor s for the single two site cluster created by the $\delta_{\sigma_a \sigma_b}$ linking the Potts states of the pair of spins at $\{a, b\}$. With the previous interpretation of e^{-J}, the factor $e^{-J(N_b - 1)} (1 - e^{-J})$ is the probability that only one bond is present and N_b is the number of places that one bond can be placed.

As before, we can include the ghost field by multiplying z_2 by z_{h_p} in Eq. (7.10), taking the derivative of the product with respect to s as in Eq. (7.11) and setting $s = 1$.

$$\left. \frac{d(z_2 z_{h_p})}{ds} \right|_{s=1} = e^{-J(N_b - 1)} (1 - e^{-J}) \sum_{n=0}^{N} \sum_{m=\alpha}^{\min\{2,n\}} (N - n - 1 + \delta_{m2}) \frac{(N-2)!(1 + \delta_{m1})}{(n-m)!(N-n+m)!}. \tag{7.13}$$

The upper bound on the second sum $\min\{2, n\}$ means that the sum over m goes from α to the minimum of the two values, 2 or n. The lower bound on the second sum is $\alpha = 0$ if $n \leq N - 2$. Or $\alpha = 1$ if $n = N - 1$ and $\alpha = 2$ if $n = N$.

We could continue this process but at this stage the point should be clear. Namely, the derivative of $f(J, h_p, s)$ with respect to s evaluated at $s = 1$ is the mean number of clusters per site in the random bond percolation model.

7.3 Correlated Site-Random Bond Percolation and the Dilute Potts Model

We can generalize the mapping discussed in Sec. 7.2 to the other percolation models discussed in Chapter 6. To do so we use the dilute s state Potts model. Before introducing this model we need to express the Ising Hamiltonian Eq. (1.4) in terms of lattice gas variables. This rewriting reflects the association of a down spin with an occupied site and an up spin with an empty site.

We introduce the occupation number n_i, which is 1 if a site is occupied and 0 if it is not. The n_i are related to the Ising spin variable s_i, which can take on the values ± 1, by

$$n_i = \frac{1 - s_i}{2}. \tag{7.14}$$

The Ising Hamiltonian

$$-\beta H_I = K \sum_{ij} s_i s_j + h \sum_i s_i \tag{7.15}$$

can be rewritten using Eq. (7.14) as

$$-\beta H_I = (cK + h)N - \beta H_{\mathrm{LG}}, \tag{7.16}$$

where the coordination number $c = N_b/N$. and

$$-\beta H_{\mathrm{LG}} = K_{\mathrm{LG}} \sum_{ij} n_i n_j - \frac{K_{\mathrm{LG}}}{2} \sum_{ij} (n_i + n_j) - 2h \sum_i n_i. \tag{7.17}$$

The term $K_{\mathrm{LG}} = 4K$ and the lattice gas Hamiltonian is often written in the form

$$-\beta H_{\mathrm{LG}} = K_{\mathrm{LG}} \sum_{ij} n_i n_j - \Delta \sum_i n_i, \tag{7.18}$$

where the chemical potential Δ is

$$\Delta = cK_{\mathrm{LG}} + 2h. \tag{7.19}$$

We now define the dilute Potts model [Murata 1979, Coniglio and Klein 1980] by the Hamiltonian

$$-\beta H_{\mathrm{DP}} = J\sum_{ij}(\delta_{\sigma_i\sigma_j} - 1)n_in_j + h_p\sum_i(\delta_{\sigma_i 1} - 1)n_i + H_{\mathrm{LG}}. \tag{7.20}$$

This model has occupied sites ($n_i = 1$) and empty sites ($n_i = 0$). Each occupied site has a Potts spin which can, as with the random pure Potts model, take one of s states. The partition function is

$$z_{\mathrm{DP}} = \sum_{\{\sigma\}}\sum_{\{n\}}e^{-\beta H_{\mathrm{DP}}}, \tag{7.21}$$

and the free energy per site is given by

$$f_{\mathrm{DP}}(J, K_{\mathrm{LG}}, h, h_p, s) = -\frac{k_BT}{N}\ln(z_{\mathrm{DP}}), \tag{7.22}$$

where we have again made the s dependence explicit.

The distribution of the occupied sites is governed by H_{LG}. All of the percolation models we discussed in Chapter 6 can be obtained by using the Kasteleyn-Fortuin mapping and taking the appropriate limits of the coupling constants J and K_{LG}. A straightforward adaptation of the technique used to obtain random bond percolation from the pure Potts model results in the relation

$$\left.\frac{df_{\mathrm{DP}}(J, K_{\mathrm{LG}}, h, h_p, s)}{ds}\right|_{s=1} = G(J, K_{\mathrm{LG}}, h, h_p), \tag{7.23}$$

where $G(J, K_{\mathrm{LG}}, h, h_p)$ is the mean number of clusters per site in a percolation model where the occupied sites are distributed according to the lattice gas Boltzmann factor and the bonds between occupied sites at i and j with a probability

$$p_{b(ij)} = 1 - e^{-J}. \tag{7.24}$$

If we set $K_{\mathrm{LG}} = 0$, the sites are distributed at random and the Kasteleyn-Fortuin mapping produces the mean number of clusters per site for the random site-random bond percolation model. If $K_{\mathrm{LG}} = 0$ and $J = \infty$, it follows from Eq. (7.24) that a bond is present between two occupied sites with probability one. We would then have random site percolation. To obtain the random bond model we can either set $K_{\mathrm{LG}} = \infty$ and let $h \to 0_-$ or let K_{LG} be any nonzero value and set $h = -\infty$ so that all sights are filled with probability one.

7.4 Mapping of Thermal to Percolation Models: The Critical Point

For the purpose of mapping the correlated site-random bond percolation model onto the critical point of the Ising model we require the full dilute state Potts model. We will first

consider the simpler case of $h = h_p = 0$. The dilute Potts Hamiltonian from Eqs. (7.15) and (7.20) is

$$-\beta H_{\mathrm{DP}} = \sum_{ij} \left\{ J[\delta_{\sigma_i \sigma_j} - 1]n_i n_j + K_{\mathrm{LG}} n_i n_j - \frac{K_{\mathrm{LG}}}{2}[n_i + n_j] \right\}. \qquad (7.25)$$

We now chose

$$J = \frac{K_{\mathrm{LG}}}{2}, \qquad (7.26)$$

so that

$$p_b = 1 - e^{-K_{\mathrm{LG}}/2}. \qquad (7.27)$$

The Potts Hamiltonian for a pair of sites i and j with J given in Eq. (7.26) is

$$-\beta H_{\mathrm{DP}(ij)} = \frac{K_{\mathrm{LG}}}{2}[\delta_{\sigma_i \sigma_j} - 1]n_i n_j + K_{\mathrm{LG}} n_i n_j - \frac{K_{\mathrm{LG}}}{2}[n_i + n_j]. \qquad (7.28)$$

This Hamiltonian is equivalent to an $s + 1$ state pure Potts model with the $s + 1$ states being $b_{i0} \equiv n_i = 0$; that is the state is "empty," and $b_{i\alpha}, \alpha = 1 \cdots s$ correspond to $n_i = 1$ and σ_i at the site i taking on the possible states $1 \cdots s$. To see that this is a proper Potts model we check Eq. (7.26) to see if the $s + 1$ states of the Potts variable b_i have the right interaction.

Consider the state $n_i = n_j = 0$. From Eq. (7.26), $-\beta H_{\mathrm{DP}(ij)} = 0$. The state $n_i = n_j = 1$ and $\sigma_i = \sigma_j$ also has $H_{\mathrm{DP}(ij)} = 0$, which corresponds to the variables $b_i = b_j$ in the $s + 1$ pure Potts model. If $n_i = 1$ and $n_j = 0$ or $n_i = n_j = 1$ and $\sigma_i \neq \sigma_j$, then $-\beta H_{\mathrm{DP(ij)}} = -K_{\mathrm{LG}}/2$. This corresponds to $b_i \neq b_j$. These results can be summarized as follows: If $J = K_{\mathrm{LG}}/2$, then $H_{\mathrm{DP}}(s) = H_P(s + 1)$ and

$$-\beta H_P(s + 1) = \frac{\beta K_{\mathrm{LG}}}{2} \sum_{ij} [\delta_{b_i b_j} - 1]. \qquad (7.29)$$

We still need to show that the percolation model is isomorphic to the thermal model. We will not quite do that. Instead, we argue that at the thermal critical point the percolation model also has a transition and that all the percolation exponents are the same as the Ising model. This latter result can be shown in several ways. A renormalization group argument has been used and is outlined in Coniglio and Klein [1980] and in more detail in Monette's thesis [1990]. We will investigate the relation between the pair connectedness function and the pair correlation function for $T > T_c$ and below the percolation threshold (finite cluster region).

The pair connectedness function plays the same role in percolation that the pair correlation function plays in thermal models [Essam 1982, Klein and Stell 1985]. For

example, the integral of the pair connectedness function $g_p(r)$ is related to the mean size of the finite clusters. That is,

$$\int_0^\infty g_p(r)d\vec{r} \propto \chi_p. \tag{7.30}$$

In the same way the pair correlation function $g(r)$ is related to the susceptibility.

$$\int_0^\infty g(r)d\vec{r} \propto \chi_T. \tag{7.31}$$

The pair connectedness function is defined as the probability that occupied sites at a and b belong to the same cluster. It is simple to see that for the dilute s state Potts model

$$g_p(r) = \frac{d}{ds}\left[\frac{\sum_{\{\sigma\}}\sum_{\{n\}}[1-\delta_{\sigma_a\gamma}][1-\delta_{\sigma_b\gamma}]n_a n_b e^{-\beta H_{\mathrm{DP}}}}{z_{\mathrm{DP}}}\right]_{s=1}, \tag{7.32}$$

where γ is a fixed but arbitrary Potts state and z_{DP} is given in Eq. (7.21). The way to see this is to note that if the Potts spins at a and b are in different clusters, there is no additional restriction on the sum over their configurations other than they cannot be in the state γ, which is imposed by the factors $(1-\delta_{\sigma_a\gamma})(1-\delta_{\sigma_b\gamma})$. Such terms produce a factor $(s-1)^2$ and hence vanish in the limit $s \to 1$. However, if there is a connection between the spins at a and b so that they are in the same cluster, then the sum over the Potts states produces only a factor of $(s-1)$ which is eliminated by differentiation with respect to s. This factor of $(s-1)$ makes it unnecessary to differentiate the denominator in Eq. (7.32) so that it becomes equal to z_{LG} in the limit $s \to 1$.

These considerations imply that the right-hand side of Eq. (7.32) is the sum of configurations, weighted by the dilute Potts Boltzmann factor, that have a diagram connecting the spins at a and b. From our mapping Eq. (7.32) can also be written as

$$g_p(r) = \frac{d}{ds}\left[\frac{\sum_{\{\sigma\}}\sum_{\{n\}}[1-\delta_{\sigma_a\gamma}][1-\delta_{\sigma_b\gamma}]e^{-\beta H_P(s+1)}}{z_P(s+1)}\right]_{s=1}. \tag{7.33}$$

We are interested in the asymptotic form of $g_p(r)$ which is known [Essam 1972] to scale in the same way as the pair correlation function. Namely,

$$\lim_{r\to\infty} g_p(r) \sim \frac{e^{-r/\xi_p}}{r^{d-2+\eta_p}}. \tag{7.34}$$

Consequently, we can write

$$\tilde{g}_p(r) = \frac{d}{ds}\left[\sum_{\{\sigma\}}\sum_{\{n\}}\frac{\delta_{\sigma_a\gamma}\delta_{\sigma_b\gamma}e^{-\beta H_P(s+1)}}{z_P(s+1)}\right]_{s=1}, \tag{7.35}$$

and obtain the same scaling form as Eq. (7.34). This results holds because the terms we have neglected in Eq. (7.33) are independent of r.

Now consider the function

$$g(r) = \frac{\sum_{\{b\}} \delta_{b_a \gamma} \delta_{b_b \gamma} e^{-\beta H_P(s+1)}}{z_P(s+1)}. \tag{7.36}$$

Equation (7.36) is the correlation function of the Ising model in the limit $s \to 1$. We know that this function is also composed of only connected graphs (see Chapter 2). Moreover, they are the same graphs as in Eq. (7.35) weighted by the same Boltzmann factor. Hence the scaling law should be the same up to a constant. This result implies $T = T_c, \nu = \nu_p$, and $\eta = \eta_p$. From two exponent scaling we conclude that all the exponents are equal.

This mapping is however not an isomorphism. The critical exponents of the percolation and thermal quantities are the same, but it is known numerically that the amplitudes are different [Kertesz et al. 1983]. We can not only make the mapping into an isomorphism, but make the mapping work at any value of the magnetic field (not just $h = 0$) by the simple technique of symmetrizing the percolation model [Hu 1984]. If we add to the dilute Potts Hamiltonian in Eq. (7.25) a term of the form

$$J[\delta_{\sigma_i \sigma_j} - 1](1 - n_i)(1 - n_j) + \tilde{h}_p[\delta \sigma_i 1 - 1](1 - n_i), \tag{7.37}$$

then there are clusters between empty as well as full sites. In Ising language there are up spin as well as down spin clusters.

We could also add a term to the Hamiltonian in Eq. (7.15) of the form

$$K_{\text{LG}}[1 - n_i][1 - n_j], \tag{7.38}$$

which changes the relation between K_{LG} and the Ising coupling constant K to $K_{\text{LG}} = 2K$. The relation between the bond probability p_b and the lattice gas coupling constant also changes to $p_b = 1 - e^{-K_{\text{LG}}}$ rather than the relation in Eq. (7.27).

The meaning behind the mathematics is that the percolation clusters are a physical realization of the fluctuations. At the critical point the clusters associated with the divergent connectedness length are the fluctuations associated with the divergent susceptibility in the thermal model. We can use a similar mapping to generate a percolation model for the spinodal.

7.5 Mapping of Thermal to Percolation Models: The Spinodal

To map the spinodal onto the percolation model [Klein 1980] it is more convenient to use the Landau-Ginsburg free energy. We can use this form of the free energy because the

spinodal is intrinsically a mean-field construct. We begin by writing down the Landau-Ginsburg free energy for the dilute s state Potts model derived by Coniglio and Lubensky [1980]. A derivation of this form of the dilute Potts free energy f_p can be found in the thesis of L. Monette [1990].

$$f_p = -\frac{r_1}{2}(s-1)\psi_p^2 - (s-1)h_p\psi_p + \frac{1}{3}w_1 s(s-1)(s-2)\psi_p^3 + \frac{1}{2}w_2 s(s-1)\phi\psi_p^2 + f(\phi). \quad (7.39)$$

The parameters r_1 and w_2 are given by

$$r_1 = c\Big(1 - c\frac{J}{2}\Big), \quad (7.40)$$

and

$$w_2 = \frac{c^3}{2}JK^{1/2}. \quad (7.41)$$

Note that we have used the Ising coupling constant K. The parameter w_1 is of no interest in this discussion except that it does not vanish at the spinodal. The term $f(\phi)$ is the standard Landau-Ginsburg free energy.

We use the Hubbard-Stratonovich transformation [Amit 1984] to express the parameters in $f(\phi)$, Eq. (1.9), in terms of the Ising coupling constant. In particular, the value of ϕ at the spinodal is [Monette 1990]

$$\phi_s = \pm\frac{\sqrt{(cK-1)c}}{c^2 K}. \quad (7.42)$$

We have obtained ϕ_s as in Chapter 5 and used the relation between the Landau-Ginsburg parameters and the Ising or lattice gas parameters obtained from the Hubbard-Stratonovich transformation.

The order parameter ϕ is proportional to the magnetization m. To obtain the proportionality constant we note that as $T \to 0$ or $K \to \infty$, the value of the magnetization at the spinodal must approach ± 1. Remember that h is the applied field divided by $k_B T$ and consequently either no spin will flip if $2cK > h$ or they all do if $2cK \le h$. Note that $2c$ is the number of bonds out of a vertex. The spinodal value of ϕ in Eq. (7.42) does not approach 1 as $K \to \infty$ but instead ϕ_s approaches zero. Therefore the relation between ϕ and m must be

$$m = cK^{1/2}\phi_s, \quad (7.43)$$

which approaches 1 as $K \to \infty$.

To obtain the percolation generating function we again use the Kastaleyn-Fortuin mapping. We differentiate f_p in Eq. (7.39) with respect to s and obtain

$$G(J, K, h) = \frac{1}{2}(-r_1 + w_2\phi)\psi_p^2 - h_p\psi_p + \frac{1}{3}w_1\psi_p^3. \quad (7.44)$$

The percolation transition occurs when the coefficient of the ψ_p^2 term vanishes. If we use Eqs. (7.40) and (7.41), Eq. (7.44) implies that

$$c\left(1 - c\frac{J}{2}\right) = c^3 2JK^{1/2}\phi_s, \tag{7.45}$$

where we have set $\phi = \phi_s$ because we are interested in the value of the bond probability that makes the percolation transition coincide with the spinodal. We use Eq. (7.43) and reduce Eq. (7.45) to

$$cJ = \frac{2}{1 + m_s}, \tag{7.46}$$

where m_s is the value of the magnetization at the spinodal. We can rewrite Eq. (7.46) in a more familiar form by multiplying the numerator and denominator of the right-hand side of Eq. (7.46) by $1 - m_s$ and using Eqs. (7.42) and (7.43) to express m_s^2 as a function of K. We have

$$J = 2(1 - m_s)K. \tag{7.47}$$

We have assumed that the up spins are metastable and the down spins are the stable phase. If we want to express J in terms of the density of the up spins ρ, we have

$$1 - m_s = 2(1 - \rho_s), \tag{7.48}$$

or

$$J = 4(1 - \rho_s)K = K_{\mathrm{LG}}(1 - \rho_s). \tag{7.49}$$

This value of J implies the bond probability

$$p_b = 1 - e^{K_{\mathrm{LG}}(1 - \rho_s)}, \tag{7.50}$$

which reduces to the value in Eq. (7.27) at the critical point.

Suggestions for Further Reading

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