

# Floppy modes and the free energy: Rigidity and connectivity percolation on Bethe lattices

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We show that the negative of the number of *floppy modes* behaves as a *free energy* for both connectivity and rigidity percolation, and we illustrate this result using Bethe lattices. The rigidity transition on Bethe lattices is found to be first order at a bond concentration close to that predicted by Maxwell constraint counting. We calculate the probability of a bond being on the infinite cluster and also on the overconstrained part of the infinite cluster, and show how a *specific heat* can be defined as the second derivative of the free energy. We demonstrate that the Bethe lattice solution is equivalent to that of the random bond model, where points are joined randomly (with equal probability at all length scales) to have a given coordination, and then subsequently bonds are randomly removed. [S1063-651X(99)07202-5]

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## I. INTRODUCTION

Connectivity percolation on Bethe lattices or infinite statistically homogeneous Cayley trees was thoroughly analyzed by Fisher and Essam [1] and provides a useful model for percolation. Rigidity on Cayley trees was first studied by Moukarzel, Duxbury, and Leath [2], henceforth referred to as MDL. This model has  $g$  degrees of freedom per site, with  $g=1$  corresponding to connectivity percolation being a special case, and so may be regarded as an extension of the work of Fisher and Essam [1]. In this paper, we develop a free energy for the rigidity percolation problem, and as an example of its use, we show how to locate the bulk rigidity transition on the Bethe lattice. We use the term *Bethe lattice*, rather than *Cayley tree*, to emphasize the bulk behavior of lattices containing no loops away from the boundary [1,3].

We have previously suggested that a free energy can be defined as the negative of the number of floppy modes [4]. In this paper we prove this assertion for the case of random-bond dilution in a general lattice with  $g$  degrees of freedom per site and with  $z$  nearest neighbors, connected by  $b=1$  bars. For  $g=1$ , this gives *connectivity* percolation. For  $g=d$  it models a central force network with pointlike nodes in  $d$  dimensions [5,6]. However, if the nodes of the lattice are bodies with rotational degrees of freedom,  $g=d(d+1)/2$  in a  $d$ -dimensional space. Note that when bodies exist on each node of a lattice, it makes sense to consider models where more than one bar (or spring) connects each pair of bodies. These models were introduced, discussed, and extensively analyzed in Ref. [2]. Here we concentrate on the simplest cases of pointlike nodes with one bar between each pair of nodes.

We prove that this free energy has the correct convexity property and hence a *specific heat* can be defined from the second derivative. This definition of the free energy reduces to the known result for connectivity percolation when  $g=1$ , where it becomes the negative of the total number of isolated clusters [7]. This latter result can either be found

directly [7] or as the  $s \rightarrow 1$  limit of the  $s$  state Potts model [8]. For rigidity, this free energy allows us to locate the bulk transition on the Cayley tree, and we refer to this as the Bethe lattice solution [3]. We confirm that for  $b=1$  and  $g \geq 2$  the rigidity transition is always first order on the Bethe lattice, whereas of course it is second order for connectivity percolation where  $g=1$ . On the triangular lattice, rigidity percolation is second order [9–11], in contrast to the first order transition on the Bethe lattice. The nature of the rigidity transition is a subtle question, depending on the network, and this has not always been taken into account [12]. For connectivity percolation, the transition is always second order [1,13].

MDL developed a general solution, using a transfer-matrix technique, for a network of rigid bodies, each with  $g$  degrees of freedom generically connected by  $b$  bars, as sketched in Fig. 1. Initially each rigid body has  $z$  neighbors, and the rigidity of the network is studied as the bonds are randomly removed. For  $b \leq g$ , this type of network is always floppy, unless the tree is attached to a rigid surface (busbar), in which case rigidity may or may not propagate away from the busbar, depending on the degree of dilution.

We amplify the work of MDL by using the free energy and the associated Maxwell construction [14], to remove boundary constraints in the analysis of bond-diluted Cayley

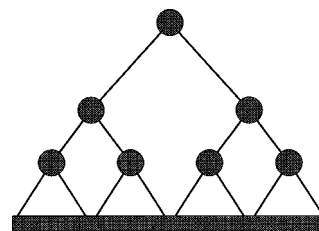


FIG. 1. Showing one branch of a tree (with coordination  $z=3$ ) with a single bar ( $b=1$ ) connecting each pair of sites. The bonds are present with probability  $p$ . Each site, shown as a shaded circle, has  $g$  degrees of freedom. Only the first few levels from the rigid busbar are shown.

trees, and hence obtain the bulk or Bethe lattice solution. This constraint equation leads to a *higher* rigidity threshold than that found in MDL. In analogy with thermally driven thermodynamic transitions, we interpret the threshold found in MDL as a *spinodal* point and use  $p_s$  when referring to it in this paper. We use  $p_c$  to refer to the *bulk* threshold.

The layout of this paper is as follows. In the next section (Sec. II) we develop results applicable to general bond-diluted lattices; namely the proof that the negative of the number of floppy modes acts as a free energy for studying bond-diluted connectivity and rigidity percolation, and we derive the associated Maxwell construction [14] or consistency condition. We review the main equations from MDL for the Cayley tree, and evaluate the probability  $P_\infty$  of being in the infinite rigid cluster and also the probability  $P_{ov}$  of being in the overconstrained part of the infinite cluster, both defined in the bulk far from the busbar.

In Sec. III, we discuss the *random-bond model* [15], where  $z$  bonds join each site with other sites, regardless of distance, and then these bonds are randomly diluted. This model is solved using the integer algorithm, the pebble game [9,10,16], for the connectivity case  $g=1$ ,  $z=3$  and the rigidity case  $g=2$ ,  $z=6$ . We demonstrate that in the thermodynamic limit, the random-bond model is equivalent to a Bethe lattice.

In Sec. IV, we show that for  $g=1$ , the familiar connectivity case is recovered. This analysis is examined for a general  $z$ , specializing to  $z=3$  to illustrate the detailed behavior for connectivity percolation.

In Sec. V, we give detailed results for a Bethe lattice with  $g=2$  and  $z=6$  as an example of a first-order rigidity transition. We apply the consistency condition to locate the first order transition in the bulk, and show that the results are equivalent to the random-bond model. We also give results for the probability  $P_\infty$  of being on the infinite cluster and the probability  $P_{ov}$  of being on its overconstrained part. We show that the results for the number of floppy modes are equivalent to the  $g=2$  random-bond model. We present a table summarizing important results for a range of values of  $g$  and  $z$ .

Throughout this paper we focus our attention on bond dilution where the number of bars  $b=1$ . Results for  $b \geq 2$  and/or for site dilution can probably be obtained in a similar manner.

## II. FORMALISM

### A. General

In this subsection we develop a free energy for both connectivity and rigidity problems on general lattices, and show that this leads to a consistency constraint on the number of floppy modes that is useful in locating first-order transitions. These results are applied to Cayley trees in the next sections.

A constraint counting method (also called *Maxwell counting*) has been very useful as a conceptual tool in understanding rigidity, and in particular the rigidity of glasses [4,17–19]. The Maxwell counting approach centers on the number of floppy modes, where we define  $f(p)$  as the average number of floppy modes per degree of freedom. We consider generic networks where each site has  $g$  degrees of freedom with central forces that connect to  $z$  neighbors. Bonds are

randomly present with probability  $p$ . An exact relation on any bond-diluted lattice is

$$f(p) = \frac{F}{gN} = 1 - \frac{z}{2g} [p - r(p)], \quad (1)$$

where  $F$  is the total number of floppy modes. There are  $N$  sites in the network and  $r(p)$  is the probability that a bond is redundant, i.e., its removal does not change the number of floppy modes in the system. Equation (1) demonstrates that we can count either floppy modes or redundant bonds, and although early work has emphasized counting floppy modes [4,18], they are equivalent. In Maxwell counting,  $r(p)$  is assumed to be zero for  $p < p_m$  and the rigidity threshold is taken to occur at  $f(p_m) = 0$ , which leads to the *Maxwell estimate* of the rigidity threshold,

$$p_m = 2g/z. \quad (2)$$

Within this approximation it is evident that

$$\begin{aligned} f(p) &= 0 & \text{for } p \geq p_m, \\ f(p) &= 1 - p/p_m & \text{for } p \leq p_m, \end{aligned} \quad (3)$$

so that  $f(p)$  changes slope at  $p_m$ . We emphasize that Maxwell counting is not correct, but does provide a useful initial approximation. In reality,  $f \neq 0$  for  $p \geq p_m$  and is nonzero right up to  $p=1$  as there is always a small probability of having a floppy inclusion if  $p \neq 1$ . This is a *Lifshitz* type of argument [20].

We note that  $f(0) = 1$  and  $f(1) = 0$ , and hence from Eq. (1) we have  $r(0) = 0$  and

$$r(1) = 1 - \frac{2g}{z}. \quad (4)$$

Equivalently, the following relation must be satisfied:

$$\int_0^1 f^{(1)} dp = -1. \quad (5)$$

These consistency conditions remove boundary constraints from the calculation and hence enable prediction of *bulk* critical behavior. This is a key new element of the Cayley tree theory, which was lacking in MDL, and which we now refer to as the bulk or Bethe lattice solution. In particular it allows us to locate the bulk critical point  $p_c$  when the transition is first order. In MDL, the point at which the finite real solution to the mean-field equations ceased to exist was identified as the critical point. Here we label that point as  $p_s$  and reinterpret it as the spinodal point in analogy with thermally driven first-order transitions.

We now show that the number of floppy modes acts as a free energy in both connectivity and rigidity problems. To demonstrate this, we recall the relation developed by Jacobs and Thorpe [10],

$$f^{(1)}(p) = -\frac{z}{2g} \left( 1 - \frac{N_0}{N_B} \right) = -\frac{z}{2g} \frac{N_I}{N_B}, \quad (6)$$

where  $f$  is the number of floppy modes per degree of freedom,  $N_0$  is the number of overconstrained bonds on the lattice,  $N_I$  is the number of isostatic bonds on the lattice,

$$N_B = \frac{pzN}{2} = N_0 + N_I \quad (7)$$

is the total number of bonds present on the lattice, and the first derivative  $f^{(1)} = \partial f / \partial p$ . The relation (6) is obtained by removing a single bond, chosen at random, and ascertaining the probability that this bond is in an overconstrained region (in which case the number of floppy modes is unchanged) or else the number of floppy modes is reduced by 1. That is (for one removed bond),  $\Delta F = (1 - N_0/N_B)$ , and if we now remove  $\Delta N_B$  bonds, we have

$$\frac{\partial F}{\partial N_B} = - \left( 1 - \frac{N_0}{N_B} \right) \quad (8)$$

and the result (6) follows. By comparing Eqs. (1) and (6), we see that the number of overconstrained bonds is given by the rate of change of the number of redundant bonds,

$$\frac{\partial r(p)}{\partial p} = \frac{N_0}{N_B}. \quad (9)$$

We can use a similar argument to derive the important result

$$f^{(2)}(p) = \frac{z}{2g} r^{(2)}(p) \geq 0, \quad (10)$$

where the second derivative  $f^{(2)} = \partial^2 f / \partial^2 p$ . We demonstrate this as follows. If we remove one bond, chosen at random, then the change in the number of overconstrained bonds is given by

$$\Delta N_0 = - \frac{N_0}{N_B} (1 + \lambda), \quad (11)$$

where  $\lambda \geq 0$ , because when an overconstrained bond is removed, the number of overconstrained bonds is reduced by at least one, and sometimes by more. If we remove  $\Delta N_B$  bonds, we therefore have

$$\frac{\partial N_0}{\partial N_B} = \frac{N_0}{N_B} (1 + \lambda). \quad (12)$$

Using this, we find

$$\frac{\partial}{\partial N_B} \frac{N_0}{N_B} = \frac{1}{N_B} \left( \frac{\partial N_0}{\partial N_B} - \frac{N_0}{N_B} \right) = \frac{\lambda}{N_B} \frac{N_0}{N_B} \quad (13)$$

and hence using Eqs. (9) and (10),

$$f^{(2)}(p) = \frac{\lambda z}{2pg} \frac{N_0}{N_B} \geq 0 \quad (14)$$

establishing that  $-f(p)$  is a convex function of the fraction of bonds present,  $p$ . Note that we must ensemble-average the results (12) and (14) so that  $\lambda$  is to be interpreted as an ensemble-averaged quantity.

Therefore, we can use  $-f(p)$  as a free energy, and if there is any ambiguity the system will always be in the lowest free energy (maximum floppy modes) state. The quantity  $-f(p)$  is convex as required of a free energy, and we will refer to  $f(p)$  interchangeably as the fraction of floppy modes or as the free energy. Note that the proof above is given for arbitrary  $g$  and  $z$ , but is restricted to  $b=1$  and bond dilution. Because  $f^{(2)}(p)$  is the second derivative of a free energy and is positive definite, we can regard it as a specific heat and it is calculated explicitly in subsequent sections [21].

## B. Cayley trees

Following MDL, we consider trees which have coordination number  $z$  with  $g$  degrees of freedom per site, which form a Cayley tree network attached to a rigid boundary which we call a busbar. This is shown in Fig. 1. The busbar is not necessary for connectivity when  $g=1$ , but is of vital importance for rigidity when  $g \geq 2$ . We define  $T_0^n$  to be the probability that a bond on a *branch*,  $n$  levels away from the busbar, is part of the infinite rigid cluster. In general, if the sites of the tree have  $g$  degrees of freedom, rigidity is transmitted to the next level of the tree provided at least  $g$  of the bonds to the lower level are occupied *and* provided that the sites at the ends of these bonds are rigid. This gives the recurrence relation

$$T_0^{n+1} = \sum_{k=g}^{z-1} \binom{z-1}{k} (pT_0^n)^k (1-pT_0^n)^{z-1-k}, \quad (15)$$

where  $T_0^n$  is the probability that a bond  $n$  levels from the busbar is rigid. If we take the thermodynamic limit (very large  $n$ ), Eq. (15) iterates to a steady-state solution, which we call  $T_0$  and is given by

$$T_0 = \sum_{k=g}^{z-1} \binom{z-1}{k} (pT_0)^k (1-pT_0)^{z-1-k}. \quad (16)$$

From this equation, we can find the probability of having a single degree of freedom with respect to the (distant) boundary

$$T_1 = \binom{z-1}{g-1} (pT_0)^{g-1} (1-pT_0)^{z-g}, \quad g \neq 1 \quad (17)$$

and more generally for  $l$  degrees of freedom with respect to the boundary

$$T_l = \binom{z-1}{g-l} (pT_0)^{g-l} (1-pT_0)^{z-g+l-1}, \quad 1 \leq l \leq g-1. \quad (18)$$

Summing over all possibilities, we have the useful sum rule

$$\sum_{l=0}^g T_l = 1. \quad (19)$$

Equation (16) is the self-consistent equation for the rigidity order parameter on bond-diluted Cayley trees. MDL also considered a more general class of problem in which another degree of freedom  $b \geq 2$  [the number of constraints (or bars)

between each pair of sites] is allowed. They also considered the case of site dilution, which is trivially related to bond dilution on a Cayley tree for  $b=1$  only.

For trees with  $b=1$ , the probability that a bond is overconstrained is  $pT_0^2$ , i.e., a bond is overconstrained if it is present *and* both of the sites at its ends are already rigidly connected to the busbar. Such bonds are the *overconstrained* bonds of the infinite cluster, as no other bonds are overconstrained far from the busbar, which is the bulk solution that we are seeking. Thus from Eq. (6) we have

$$f^{(1)}(p) = -\frac{z}{2g} \left( 1 - \frac{pT_0^2}{p} \right) = -\frac{z}{2g} (1 - T_0^2). \quad (20)$$

Differentiating a second time gives

$$f^{(2)}(p) = \frac{z}{g} T_0 \frac{\partial T_0}{\partial p}. \quad (21)$$

Since  $T_0 \geq 0$ , we must have solutions where

$$\frac{\partial T_0}{\partial p} \geq 0 \quad (22)$$

to be acceptable.

In a similar way the probability that a bond is connected to the infinite rigid cluster via the busbar at one end, but has one degree of freedom at the other, is  $2pT_0T_1$ . Such bonds are the *isostatic* bonds associated with the infinite cluster [9–11]. Thus the total probability that a bond that is present belongs to the infinite cluster  $P_\infty$  is

$$P_\infty = T_0^2 + 2T_0T_1. \quad (23)$$

The probability that a bond that is present belongs to the overconstrained part of the backbone is given by

$$P_{ov} = T_0^2. \quad (24)$$

Since the number of redundant bonds  $r(p)$  is zero for  $p \leq p_c$ , and after finding  $r^{(1)}(p) = T_0^2$  from Eq. (20) using Eq. (1), we must have

$$r(p) = \int_{p_c}^p T_0^2 dp. \quad (25)$$

In particular, combining Eq. (25), with the consistency condition (4), we have

$$r(1) = \int_{p_c}^1 T_0^2 dp = 1 - \frac{2g}{z}. \quad (26)$$

This is the key new component of the theory developed here. As in MDL, we solve the tree equations for the order parameter  $T_0$  but now we use Eq. (26) to identify the rigidity threshold  $p_c$ . Once we have  $p_c$ , the number of floppy modes at any  $p$  is given by [from Eq. (1) using Eq. (25)]

$$f(p) = 1 - \frac{z}{2g} \left[ p - \int_{p_c}^p T_0^2 dp \right]. \quad (27)$$

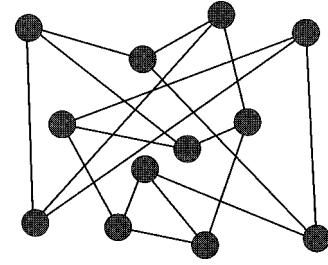


FIG. 2. A sketch of the random-bond model with a single bar  $b=1$  along the  $z=3$  bonds from each site. The bonds are present with probability  $p$ . Each site, shown as a shaded circle, has  $g$  degrees of freedom. Only  $N=12$  sites are shown in this sketch. In simulations using the pebble game, we use  $N=262\,144$ .

The condition (4) may be regarded as a *Maxwell condition*, in analogy with that commonly used to locate the first-order transition in thermodynamic systems [14].

### III. RANDOM-BOND MODEL

The *random-bond model* consists of  $N$  sites thrown down randomly, with each site joined at random to  $z$  other sites (without regard to distance) to form a  $z$ -coordinated network. Small rings appear with probability  $O(1/N)$ . It is convenient to show this network in a plane as in Fig. 2, where  $z=3$ . The dimension of this model is only defined through the number of degrees of freedom  $g$  associated with each site. In the Bethe lattice and in the random-bond model, there are no loops in the thermodynamic limit  $N \rightarrow \infty$  and so in a diagrammatic expansion all terms agree and the models are equivalent. For finite Cayley trees, there are loops involving the busbar, as can be seen in Fig. 1. Likewise, there are loops in the random-bond model, as can be seen in Fig. 2. So the equivalence is only in the bulk thermodynamic limit. We find this is a useful alternative viewpoint on the Bethe lattice limit.

We have numerically examined connectivity percolation having  $g=1$ ,  $z=3$ , and the  $g=2$ ,  $z=6$  rigidity percolation case using the random-bond model. These simulation results are compared with the corresponding exact Bethe lattice calculations in the next two sections. The pebble game [9,10,16] was used to find the number of floppy modes and the derivatives  $f^{(1)}(p)$  and  $f^{(2)}(p)$  for the  $g=2$ ,  $z=6$  case. For connectivity percolation with  $g=1$ , a similar pebble game algorithm can be constructed where only one pebble is assigned to a site [22]. In fact, as long as a site represents a rigid body having  $g$  degrees of freedom and not a point, the pebble game can be straightforwardly generalized by assigning  $g$  pebbles to each site [23].

For the connectivity percolation case, however, we actually used the  $g=2$  pebble game (two pebbles per site) by invoking an interesting mapping that makes  $g=2$  rigidity percolation equivalent to connectivity percolation. This mapping is valid for any generic network and is not limited to the random-bond model. The mapping consists of adding a single *ghost* site to the  $N$  site network. The ghost site has  $g=2$  as do all other sites in the network. Additional  $N$  bonds are placed between each of the  $N$  sites in the network and the ghost site. With this additional ghost site and its associated bonds, the network consists of edge sharing triangles. That

is, any three sites in the network that are connected are mutually rigid because they form edge sharing triangles with the ghost site common to all triangles.

The ghost site and its associated bonds allow connectivity to be a sufficient condition for a set of sites to be mutually rigid. Since rigid clusters are those that are connected, a one-to-one mapping between clusters in a  $g=2$  network to a  $g=1$  network is established. However, the number of floppy modes of the  $g=2$  network (with the ghost site) will be two more than the number of rigid clusters. These floppy modes can be viewed as two translational motions for the ghost site and one rotational motion of each rigid cluster about the ghost site. By accounting for these two extra modes, an exact mapping is established.

#### IV. CONNECTIVITY PERCOLATION

The analysis in Sec. II holds for any value of  $g$ . For  $g=1$  we recover and extend the familiar results of connectivity percolation [1,13] for random-bond dilution on a tree with coordination  $z$ . In this section we use a general  $z$  as much as possible, but then focus on  $z=3$  to simplify the algebra when necessary. For  $g=1$ , Eq. (16) reduces to

$$T_0 = [1 - (1-p)T_0]^{z-1}. \quad (28)$$

Expanding near  $p_c$ , it is easy to show that the order parameter  $T_0$  vanishes as

$$T_0 \sim \frac{2(p-p_c)}{p_c(1-p_c)} \quad \text{with} \quad p_c = \frac{1}{z-1}. \quad (29)$$

The number of redundant bonds  $r(p)$  can be found from Eq. (25) by using Eq. (28) to first calculate  $\partial T_0/\partial p$  and then doing the integration to give

$$r(p) = T_0 \left[ \left( \frac{z-2}{z} \right) (1+p-pT_0) - (1-p) \right], \quad (30)$$

where  $T_0$  is obtained by solving the polynomial (28). Notice that the *fraction* of bonds in overconstrained regions on the infinite cluster is given from Eqs. (23) and (24) and using  $T_1 = 1 - T_0$ ,

$$\frac{P_{ov}}{P_\infty} = \frac{T_0^2}{T_0^2 + 2T_0T_1} = \frac{T_0}{2-T_0}. \quad (31)$$

When  $p=1$ , we have  $T_0=1$ , so that the ratio (31) becomes unity, meaning that the entire tree is overconstrained (no dangling ends). Near  $p=p_c$ , and using Eq. (29), the fraction of overconstrained bonds in the infinite cluster goes to zero linearly as

$$\frac{P_{ov}}{P_\infty} \sim \frac{p-p_c}{p_c(1-p_c)}, \quad (32)$$

so that as the connectivity percolation transition is approached, the infinite cluster becomes completely isostatic. For  $z=3$  we can solve the quadratic equation (28) to get

$$T_0 = 0 \quad \text{for} \quad p \leq p_c, \quad (33)$$

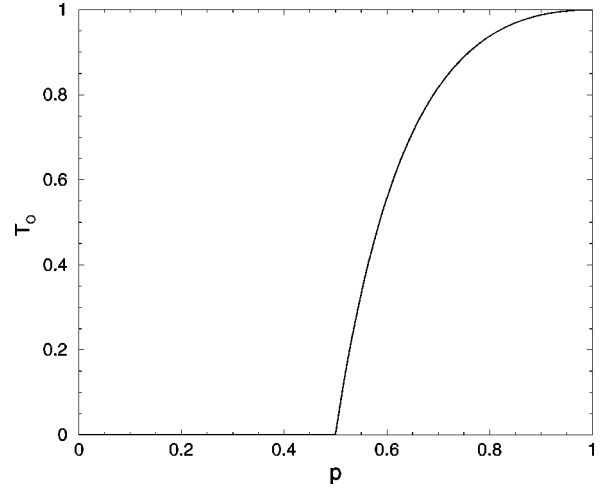


FIG. 3. The result for bond diluted connectivity percolation on a Bethe lattice for  $T_0$  is shown for coordination number  $z=3$  and with  $g=1$  degrees of freedom per site. The probability that a bond is present is  $p$ , and percolation occurs at  $p_c=0.5$ .

$$T_0 = \frac{(2p-1)}{p^2} \quad \text{for} \quad p \geq p_c,$$

where  $p_c=1/2$ , and is shown in Fig. 3.

We can use Eq. (30) to check that we get the same value of  $p_c$  by noting that we correctly reproduce  $r(1) = 1/3$  [see Eq. (4)]. Therefore the transition is indeed second order. Having found  $p_c$ , we find  $f(p)$  and  $r(p)$  from Eqs. (25) and (27),

$$f(p) = 1 - \frac{3p}{2} \quad \text{for} \quad p \leq p_c, \quad (34)$$

$$f(p) = \left( \frac{1-p}{p} \right)^3 \frac{(3p-1)}{2} \quad \text{for} \quad p \geq p_c$$

and

$$r(p) = 0 \quad \text{for} \quad p \leq p_c, \quad (35)$$

$$r(p) = \frac{1}{3} \left( \frac{2p-1}{p} \right)^3 \quad \text{for} \quad p \geq p_c$$

and by differentiating Eq. (34),

$$f^{(1)}(p) = -\frac{3}{2} \quad \text{for} \quad p \leq p_c, \quad (36)$$

$$f^{(1)}(p) = -\frac{3}{2} \frac{(1-p)^2(p^2+2p-1)}{p^4} \quad \text{for} \quad p \geq p_c$$

and differentiating again

$$f^{(2)}(p) = 0 \quad \text{for} \quad p \leq p_c, \quad (37)$$

$$f^{(2)}(p) = \frac{6(2p-1)(1-p)}{p^5} \quad \text{for} \quad p \geq p_c.$$

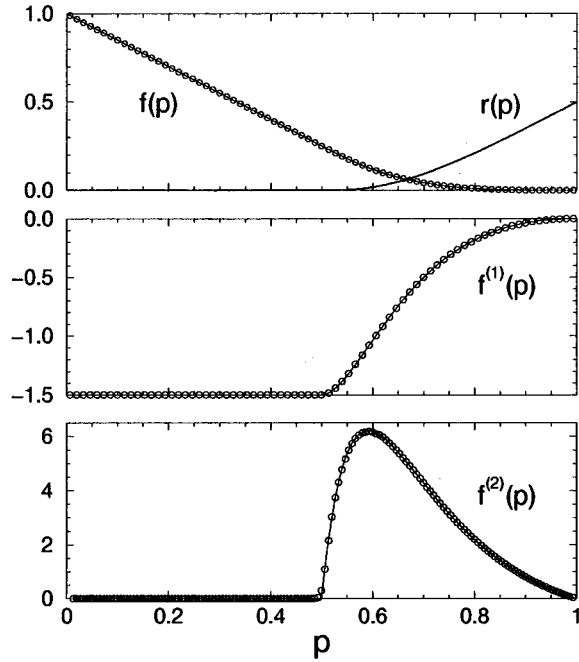


FIG. 4. Results for bond diluted connectivity percolation on a Bethe lattice for the number of floppy modes  $f(p)$  and the first two derivatives. The number of redundant bonds  $r(p)$  is also shown. The second derivative  $f^{(2)}(p)$  acts as a specific heat for this problem. Results are for coordination number  $z=3$  and with  $g=1$  degrees of freedom per site. The probability that a bond is present is  $p$ , and percolation occurs at  $p_c=0.5$ . The open circles are from computer simulations of the random bond model using the pebble game as described in Sec. III, using  $N=262\,144$  sites and averaging over 2000 realizations. The Maxwell estimate [Eqs. (2) and (3)] for the number of floppy modes is a straight line that follows the  $f(p)$  at small  $p$ .

These results (34)–(37) are shown in Fig. 4. We note that this second derivative, which is like a specific heat, is strongly peaked around  $p=1-1/\sqrt{6}=0.59$ , although it does go to zero at  $p_c=0.50$ . Note also that  $f$ ,  $f^{(1)}$ , and  $f^{(2)}$  are all continuous at  $p_c$ , with  $f^{(3)}$  being the first derivative to show a discontinuity [4].

The number of overconstrained bonds in the infinite cluster is  $P_{ov}$  and is given from Eq. (24) by

$$P_{ov} = \left( \frac{2p-1}{p^2} \right)^2 \quad \text{for } p \geq p_c \quad (38)$$

and the fraction of bonds in the infinite cluster  $P_\infty$  is given by Eq. (23),

$$P_\infty = 1 - \left( \frac{1-p}{p} \right)^4 \quad \text{for } p \geq p_c, \quad (39)$$

which has been derived by Essam and Fisher [1] [see their Eq. (35b)], although it should be noted that they have an extra factor of  $p$  as they normalized to all bonds, not just those *present*. These results are shown in Fig. 5. The reader might be concerned that some overconstrained bonds are *not* associated with the infinite cluster. This is not so on a Cayley tree in the asymptotic limit, where only the infinite cluster reaches back to the busbar. All other clusters are isolated and contain no overconstrained bonds, except finite rigid clusters

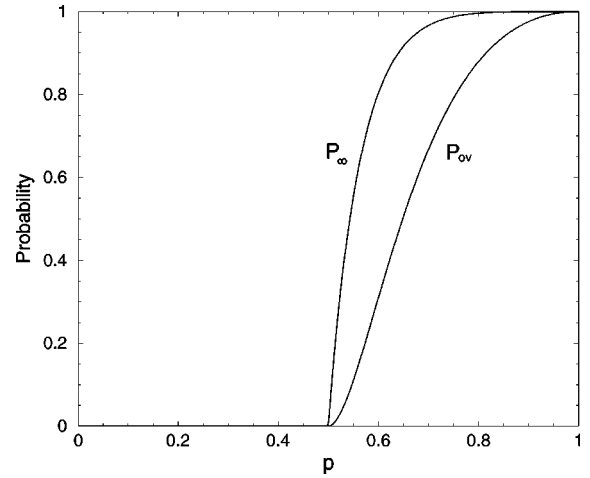


FIG. 5. Results for bond diluted connectivity percolation on a Bethe lattice for the probability of being on the infinite cluster  $P_\infty$  and the probability of being on the overconstrained part of the infinite cluster  $P_{ov}$ . Results are for coordination number  $z=3$  and with  $g=1$  degrees of freedom per site. The probability that a bond is present is  $p$ , and percolation occurs at  $p_c=0.5$ .

attached to the busbar which are considered to be surface effects and hence are ignored in the bulk or Bethe lattice solution.

In the connectivity case  $f^{(1)}(p)$  and the order parameters  $T_0$ ,  $P_{ov}$ , and  $P_\infty$  are continuous at the transition, and so connectivity percolation is of a conventional second-order type, as indeed it is on real lattices like the triangular network [13].

## V. RIGIDITY PERCOLATION

In the rigidity case we must numerically solve Eq. (16) for  $T_0$  and hence find the other quantities of interest. We first solve the self-consistent Eq. (16), by simple iteration, to find  $T_0$ , which is shown in Fig. 6 for  $g=2$  and  $z=6$ . The analog of the Maxwell construction (4) is then used to find  $p_c$ . This

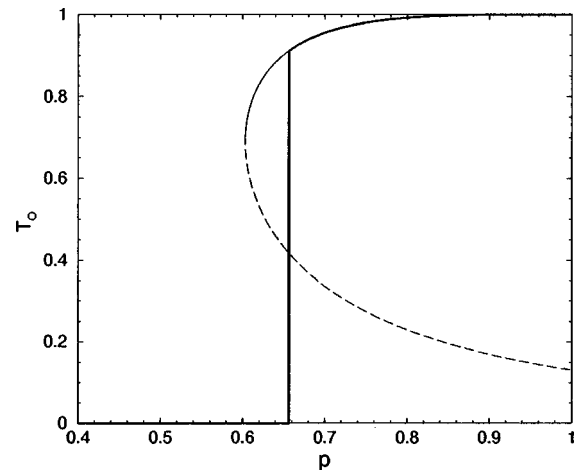


FIG. 6. Results for bond diluted rigidity percolation on a Bethe lattice for  $T_0$  are shown for coordination number  $z=6$  with  $g=2$  degrees of freedom per site. The probability that a bond is present is  $p$  and percolation occurs at  $p_c=0.656$  shown by the vertical line. The thin line extends out to the spinodal point at  $p_s=0.603$  and the dashed line shows the unstable solution.

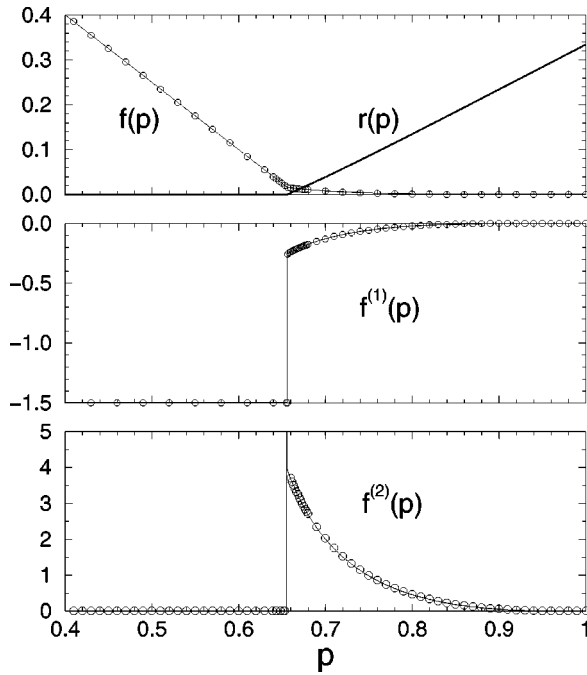


FIG. 7. Results for bond diluted rigidity percolation on a Bethe lattice for the number of floppy modes  $f(p)$  and the first two derivatives. The number of redundant bonds  $r(p)$  is also shown. The second derivative  $f^{(2)}(p)$  acts as a specific heat for this problem. Results are for coordination number  $z=6$  and with  $g=2$  degrees of freedom per site. The probability that a bond is present is  $p$  and percolation occurs at  $p_c=0.656$ . The open circles are from computer simulations of the random-bond model using the pebble game described in Sec. III, using  $N=262\,144$  sites and averaging over 2000 realizations. The Maxwell estimate [Eqs. (2) and (3)] for the number of floppy modes is a straight line that follows the  $f(p)$  at small  $p$ .

is shown as the jump in Fig. 6 at  $p_c=0.656$ . The other possible solutions are ruled out by application of Eq. (4) and hence we have a first-order jump from a rigid to a floppy state. The point at  $p_s=0.603$  can be interpreted as a spinodal point [24]. The dashed line is unstable as can be seen from Eq. (22). Having found  $T_0$  and  $p_c$ , we can find  $f(p)$ ,  $f^{(1)}(p)$ ,  $f^{(2)}(p)$ , and  $r(p)$  as shown in Fig. 7. It can be seen that there are no redundant bonds for  $p \leq p_c$  and hence  $f^{(1)}$  and  $f^{(2)}$  are flat in this region, as also happens for connectivity percolation as shown in Sec. IV. In Fig. 7, we also show the results from the random-bond model, discussed in Sec. III, and find that the results are exactly the same as expected. Note that with the random-bond model, the first-order transition occurs naturally and no Maxwell construction is needed, as the pebble game always finds the bulk equilibrium solution.

In Fig. 8, we show results for  $P_\infty$  and  $P_{ov}$  from Eqs. (23) and (24), respectively. It can be seen that most of the infinite cluster is overconstrained, even at the first-order transition.

In the connectivity case as shown in Figs. 3 and 5, the order parameter ( $T_0$ ,  $P_\infty$ , or  $P_{ov}$ ) is continuous at  $p_c$ , whereas in the rigidity case as shown in Figs. 6 and 8 the order parameter has a large first-order jump at  $p_c$ . The quantity  $f^{(1)}(p)$ , which acts like an energy, also has a large first-order jump. One could argue that in the rigidity case, a metastable rigid state exists for any  $p_c > p > p_s$ . Note that for

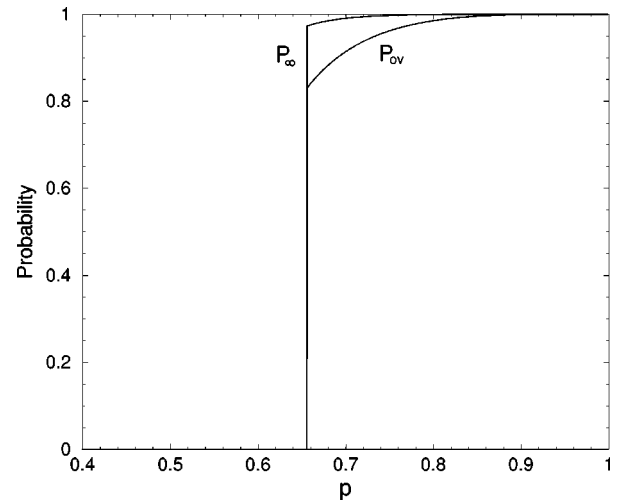


FIG. 8. Results for bond-diluted rigidity percolation on a Bethe lattice for the probability of being on the infinite cluster  $P_\infty$  and the probability of being on the overconstrained part of the infinite cluster  $P_{ov}$ . Results are for coordination number  $z=6$  with  $g=2$  degrees of freedom per site. The probability that a bond is present is  $p$ , and percolation occurs at  $p_c=0.656$ .

connectivity percolation, the boundary conditions are irrelevant, and no difference is found with or without a rigid busbar. This is not so for rigidity percolation, where there are three real solutions [25] for all  $p_s < p < 1$ , with an *unstable* solution at finite  $T_0$  existing in this regime as shown by the dashed line in Fig. 6. In order for the stable finite  $T_0$  solution to be found, the boundary rigidity must lie *above* the unstable fixed point. Any boundary rigidity below this value iterates to the  $T_0=0$  solution. This curious effect of the boundary condition in rigidity percolation, even on the bulk Bethe lattice solution, needs further study.

It is useful to compare the results for  $p_c$  with that predicted by Maxwell counting. Maxwell counting would predict  $p_m=2g/z=2/3$  in *both cases* studied here. In the connectivity case this is markedly different than the exact result  $p_c=1/2$  because there are many floppy modes at  $p_c$  in that case, as can be seen from Fig. 4. In contrast, in the rigidity case, the Maxwell estimate is close to the Bethe lattice result  $p_c=0.655$  and there are rather few floppy modes at  $p_c$  as shown in Fig. 7. It is remarkable that Maxwell counting does so well in locating the position of *both* first-order and second-order [6,18] rigidity transitions.

Results of calculations for a range of values of  $g$  and  $z$  for bond diluted Bethe lattices are summarized in Table I. In all rigidity cases (i.e.,  $g > 1$ ) there is a large jump in the order parameter  $T_0$ ,  $P_\infty$ , or  $P_{ov}$  at the critical point  $p_c$ , although the jump does decrease with increasing  $z$  for a given  $g$ . On real lattices, there will also be a *Lifshitz tail* [20] in the number of redundant bonds  $r(p)$  (see Figs. 4 and 7) extending into the regime  $p < p_c$  all the way to  $p=0$ . Notice that the Bethe lattice result does correctly reproduce the Lifshitz tail in  $f(p)$  in the region  $p_c \leq p \leq 1$ .

It is seen from Fig. 7 that the random-bond model is numerically equivalent to the Bethe lattice results, as expected from our previous discussion. The pebble game is an exact algorithm for a particular network and gives the exact number of floppy modes (and the associated derivatives). There

TABLE I. This table gives a summary of results for bond-diluted Bethe lattices with  $g$  degrees of freedom per site which are joined by  $b=1$  bars to  $z$  neighbors. The Maxwell estimate for the transition  $p_m$  is given as well as the spinodal point  $p_s$  and the critical point  $p_c$ . The number of floppy modes at the spinodal point is  $f(p_s)$  and at the critical point is  $f(p_c)$ . The jumps in the order parameters are given for  $T_0$ , the probability  $P_\infty$  that a bond is present and is part of the infinite cluster, and the probability  $P_{ov}$  that a bond is present and is overconstrained.

$g$	$z$	$p_m$	$p_s$	$p_c$	$f(p_s)$	$f(p_c)$	$T_0(p_c^+)$	$P_\infty(p_c^+)$	$P_{ov}(p_c^+)$
1	$z$	$\frac{2}{z}$		$\frac{1}{z-1}$		$\frac{z-2}{2(z-1)}$	0	0	0
2	6	0.667	0.603	0.656	0.096	0.016	0.911	0.972	0.830
2	8	0.500	0.447	0.482	0.106	0.035	0.860	0.940	0.740
2	10	0.400	0.354	0.381	0.115	0.048	0.833	0.918	0.694
2	15	0.267	0.232	0.248	0.129	0.071	0.793	0.882	0.629
3	8	0.750	0.646	0.748	0.138	0.003	0.984	0.992	0.968
3	10	0.600	0.521	0.596	0.131	0.007	0.964	0.987	0.929
3	15	0.400	0.348	0.393	0.129	0.016	0.935	0.968	0.874

is therefore no *hysteresis* in the results of the pebble game on the random-bond model, and in these large samples the system flips from the rigid state to the floppy state around  $p_c = 0.656$  as a single bond is removed in a given sample. This is a very unusual situation as most numerical techniques, like Monté Carlo, encounter hysteresis near a first-order transition [26].

## VI. CONCLUSIONS

In this paper we have shown that the free energy is negative of the number of floppy modes. This generalizes a previous result [7] which gives the free energy as the total number of clusters in connectivity percolation, where there is a single floppy mode associated with each isolated cluster. In connectivity percolation, the free energy can also be found as the limit  $s \rightarrow 1$  of the  $s$  state Potts model [8]. No equivalent approach has been possible for rigidity.

We have used the free energy and the associated Maxwell

type construction, or self-consistency condition, to show that the rigidity transition is always first order on Bethe lattices. It is necessary to use this construction in order to remove boundary constraints. In previous work [2,25], a boundary-dependent transition was found at the spinodal point  $p_s$ . As is expected from experience with thermodynamic transitions, metastability and boundary effects can be important [24] in the regime  $p_s < p < p_c$ , and this needs further investigation.

While rigidity concepts have been extensively applied to experiments in chalcogenide glasses [18,19], first-order jumps in experimental quantities have never been observed (although see recent Raman results in chalcogenide glasses [27]).

## ACKNOWLEDGMENTS

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