Scaling of splay and total rigidity for elastic percolation on the triangular lattice

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The randomly diluted elastic network with central force interactions is simulated on the triangular lattice using a constraint analysis of cluster displacement vectors. The exponents for the percolation of splay and total rigidity are found to be the same, $v=1.14\pm0.1$, $\gamma=1.6\pm0.3$, and $\beta=0.46\pm0.4$. The concentration of bonds that are in clusters rigid only with respect to a splay deformation is evaluated as a function of bond concentration. The area under the resulting distribution diminishes with lattice size as $\sim L^{-1.1}$, indicating that splay and total rigidity have the same threshold, $p_c \approx 0.64$.

I. INTRODUCTION

The modeling of randomly inhomogeneous elastic systems has attracted much attention, as have its predecessors in related areas, since abrupt changes in elastic, electromagnetic, rheological, etc., response, hold both theoretical and practical interest, and these changes occur at thresholds in the concentration of inhomogeneities.

In this paper we study the property of elastic connectedness in a triangular lattice composed of randomly occupied bonds which mediate a central force interaction between adjacent sites. This is easily visualized as a collection of springs each of which spans the gap between two adjacent sites of the lattice. Every gap is occupied by a spring with probability p, and is vacant with probability 1-p, so the lattice is incomplete unless p = 1. In the harmonic approximation the elastic energy for the system is

$$H = \frac{1}{2}k \sum_{\langle ij \rangle} g_{ij} [(\mathbf{u}_i - \mathbf{u}_j) \cdot \hat{\mathbf{r}}_{ij}]^2 , \qquad (1)$$

where the sum is over nearest-neighbor pairs ij, and $g_{ij}=1$ (a bond exists between sites *i* and *j*) or 0 (no bond exists) with respective probabilities *p* and 1-p. Also \mathbf{u}_i is the displacement of the *i*th site, and $\hat{\mathbf{r}}_{ij}$ is the unit vector from site *i* to site *j*. Interest in this model arose when Feng and Sen¹ studied its critical properties (for finite *k*) and found behavior different from that of the analogous conductivity problem. More recent investigations have included simulations,² effective-medium theories,³⁻⁵ renormalization-group treatments,⁶ series expansions,⁷ and mean-field theory.⁸ These approaches have yielded estimates of the critical threshold^{2,6} ($p_{cen} \approx 0.65$), the bulk modulus exponent^{1,2} ($f \approx 1.4-2.4$), the correlation length exponent^{2,6} ($\nu \approx 1.94$). Here we will consider the case $k = \infty$, so that the springs are to be considered rigid rods with no bond-angle restoring forces.

Using series expansion techniques Wang and Harris proposed⁷ an intermediate phase between those of disorder and total rigidity for the diluted central force model on a triangular lattice. This proposed splay-rigid phase

lacks stability with respect to compression and shear, but opposes an application of counter torques. Bonds in this phase have long range orientational order but no long range positional order. Wang and Harris found the threshold of splay rigidity to be $p_{SR} \equiv 0.61 \pm 0.02$. Subsequently, Tremblay, Day, and Tremblay¹⁰ (TDT) simulated the same lattice and found no evidence for such a phase. However, their method involved the use of boundary conditions (i.e., bus bars) which inhibited the formation of a splay-rigid phase.¹¹

We present the results of a simulation in which the boundary conditions are more nearly neutral, favoring neither splay rigidity nor total rigidity with respect to one another. An analysis of rigidity propagation is carried out for each realization generated. The method enabled us to calculate the critical threshold and the exponents ν , β , and γ , associated respectively with the correlation length, the probability that a bond is in the infinite cluster, and the mean square number of bonds in a cluster. Our results probably indicate the absence of the splay-rigid phase in an infinite triangular lattice or at least set an upper limit on the difference in thresholds of the two phases.

Briefly this paper is organized as follows. In Sec. II we present the method for analyzing rigidity percolation. In Sec. III we present our results and a discussion of them.

II. THE MODEL, DEFINITIONS, AND ANALYSIS OF RIGIDITY PROPAGATION

As stated above, we work in the limit $k = \infty$, i.e., the bonds are infinitely stiff but are freely hinged to other bonds at the nodes of the lattice. In this limit we may identify two kinds of elastic clusters, one possessing only splay rigidity, the other being totally rigid.

First, consider splay rigidity. For this discussion, we describe each bond b by giving its orientation θ_b and the coordinates $\mathbf{r}_b = \{x_b, y_b\}$ of a point on the bond. A splay-rigid cluster is a set of bonds $\{b_1, b_2, b_3, \ldots\}$, all of whose relative orientations, $(\theta_i - \theta_j)$, cannot be changed by any application of finite forces to the cluster. The distance between bonds $|\mathbf{r}_i - \mathbf{r}_j|$ need not be rigid under finite external forces. For instance, the simplest splay-

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rigid cluster may be found in the elementary parallelogram of the triangular lattice. The parallelogram collapses or folds up when we compress it [Fig. 1(a)], yet it resists efforts to splay out a pair of opposite sides [Fig. 1(b)]. The opposite sides thus form a splay-rigid cluster, i.e., a cluster of bonds within which all the relative bond orientations are fixed. Since the bonds in the splay-rigid cluster need not touch (see Fig. 1), one sees that this weaker form of rigidity can propagate without direct connection. Nonetheless splay rigidity obeys the cluster property,^{7,12} so that two bonds, each splay rigid with respect to a third bond, are also splay rigid with respect to each other. Using this property one can uniquely decompose any collection of bonds into its component clusters with respect to splay rigidity. Next for finite k consider the elastic response of such a cluster. Following Day et al.,⁹ and in close analogy with the definition for resistor networks,¹³ one can consider a "two terminal" experiment in which two distant bonds at positions \mathbf{r}_1 and \mathbf{r}_2 are rotated in opposite senses through an angle θ . For this situation, we can define the backbone as follows. The bond, b, is in the splay-rigid backbone if it has a neighboring bond, b', in the splay-rigid cluster, such that $\theta_{b'} - \theta_b \neq 0$. Let $n_b(\mathbf{r}_1, \mathbf{r}_2)$ denote the number of such bonds. Then the fractal dimension, d_{BB} of the splay-rigid backbone is defined through

$$n_b(\mathbf{r}_1, \mathbf{r}_2) \sim |\mathbf{r}_1 - \mathbf{r}_2|^{a_{BB}} .$$
⁽²⁾

This relation presumably holds as long as $|\mathbf{r}_1 - \mathbf{r}_2|$ is less than the correlation length for splay rigidity. As in ordinary percolation, one can have dangling ends, which do not contribute to the backbone. Such dangling ends are formed by rhombuses that lead to dead ends. Thus d_{BB} is smaller than the fractal dimension of the entire splayrigid cluster.



FIG. 1. (a) The parallelogram collapses when we compress it; it is not totally rigid. (b) The parallelogram resists efforts to splay out its opposite sides. Pairs of opposite sides are in the same splay-rigid cluster.

Next we consider total rigidity. Here the analogy with ordinary percolation is less satisfactory. The main problem is to define totally rigid clusters in such a way that the rigid backbone is contained within a single totally rigid cluster. The obvious definition of total rigidity is as follows. Two bonds are totally rigid with respect to one another, if clamping one bond prevents (for $k = \infty$) the other from having a translational or orientational displacement. This definition clearly obeys the cluster property. The definition of Ref. 10 for the totally rigid backbone seems to be a plausible one, namely, the backbone consists of bonds whose springs are compressed or stretched when the system is compressed at its boundaries. As is clear from their illustrations, in the interior of the sample there exist chain segments consisting of more than one bond which are stressed during such a compression. On the other hand, within the above definition of total rigidity, bonds in such a chain segment are certainly not totally rigid with respect to any other bonds in the backbone, since the chain segment has no resistance to a transverse stress. Thus, with these definitions all bonds in the totally rigid backbone are not in the same totally rigid cluster. As noted previously,⁷ one cannot preserve the cluster property if one defines total rigidity in terms of sites. For simulations like ours, this property is essential if we are to decompose the system into its component clusters. Accordingly, we adopt the above definition to define totally rigid cluster, ignoring possible inconsistencies with the definition of the elastic backbone given in Ref. 10.

The simulation consists of randomly populating the lattice with bonds at successively larger bond concentrations (bonds are added one at a time or in groups). At each concentration an analysis is made which classifies the current set of bonds into splay-rigid and totally rigid clusters. In this procedure it is clearly advantageous to use cluster data from a previous (lower) concentration to identify clusters. Cluster size statistics may be generated from this information. The above process is repeated for as many realizations as desired.

The method by which one identifies splay and totally rigid clusters will be described for a fixed set of N bonds (assumed for simplicity to be connected). In summary, the method is as follows. In the absence of constraints there are at most 3N displacement variables, q_i , needed to describe the two possible translations and one rotation associated with each bond. However, constraints exist among these variables since each bond is joined to at least one other, and the problem we address is how to identify and characterize these constraints. In our procedure the cluster is reconstructed by sequentially attaching bonds, starting from an arbitrary seed bond. Correspondingly, we successively include into a working set the q_i associated with each bond. After the inclusion of a bond, we use the constraints associated with its connections to others previously analyzed to eliminate dependent variables. Thus at each stage of analysis we obtain a complete set of independent variables q_i . Once we have considered all of the bonds and eliminated the linearly dependent q_i 's, we check the effect of each of the remaining q_i on the motion of pairs of bonds for the kind of joint displacements associated with splay or total rigidity. Having determined the splay and totally rigid cluster to which each bond belongs, we calculate the cluster size distribution for both types of rigidity.

Since the technique used here is different from others used in this class of problems, we give it a full description. We will assume that the set of bonds to be classified into elastic clusters has already been decomposed into sets of connected clusters. We therefore consider the analysis for a connected set of bonds. Since the longitudinal stiffness of an individual bond [k in Eq. (1)] is infinite, it is clear that, apart from a uniform translation, the displacements of all sites in a cluster can be expressed in terms of the set of angular displacements $\{\delta \theta_i\}$ of the bonds in the cluster, when the displacement of one arbitrarily chosen site is taken to be zero. We consider the limit of small displacements from equilibrium, so that all coordinates are linear functions of the $\{\delta \theta_i\}$. The equilibrium lattice spacing is taken to be unity. Thus the problem we consider is how to select from the set $\{\delta \theta_i\}$ a complete set of independent variables

$$Q_1 = \delta \theta_{i_1}, Q_2 = \delta \theta_{i_2}, \cdots$$
(3)

in terms of which any $\delta \theta_i$, or indeed the displacement of any node in the cluster can be expressed. To do this we reconstruct the cluster, starting from an arbitrarily chosen "initial," or "seed" bond, by sequentially attaching bonds, so that at any stage of the reconstruction the bonds form a connected cluster. The displacement of one site associated with the "seed" bond is taken to be zero.

In general, the reconstruction process proceeds as follows. Assume that we are at the stage in which k bonds have been chosen. (We assume that the bonds are numbered in the order in which they are chosen in the reconstruction process.) At this stage there will be m (with $m \le k$) independent variables of the type listed in Eq. (3). We assume that m > 0, but if not, the case m = 0 can be considered separately. The angular displacement of any bond can be expressed in terms of these currently independent variables as

$$\delta \theta_i = \sum_{j=1}^m A_{ij} Q_j , \quad i = 1, 2, \dots, k$$
(4)

where the coefficients A_{ij} were obtained previously in the construction. In addition, the coordinates, x_i , y_i , of the position, \mathbf{r}_i , of the *i*th node can also be expressed in terms of these variables:

$$x_i = x_i^{(0)} + \sum_{j=1}^m X_{ij} Q_j$$
, $i = 1, 2, ..., n$ (5a)

$$y_i = y_i^{(0)} + \sum_{j=1}^m Y_{ij}Q_j$$
, $i = 1, 2, ..., n$ (5b)

where the superscript (0) denotes an equilibrium value and n is the number of nodes in the cluster at this stage. Here again, the coefficients X_{ij} and Y_{ij} would have been obtained in a previous stage of the construction. We now describe the iteration procedure by which the corresponding quantities (denoted by primes) are obtained for the cluster consisting of k + 1 bonds. Accordingly, consider adding the k + 1st bond to this cluster of k bonds. There are two cases (A) and (B). In case (A) the new bond is attached to a single site in the existing cluster. In this case, adding the bond introduces no new constraint. In this case, then, the new set $\{\delta\theta\}'$ is given by $\{\delta\theta\}$ together with $\delta\theta_{k+1}$. Also Eqs. (4) and (5) can be updated in the obvious way with m' = m + 1, k' = k + 1, and n' = n + 1. In case (B) the bond connects two sites I and J which are already sites in the cluster, and therefore are sites for which Eqs. (5a) and (5b) already exist. We write equations (which do not yet take account of bond k + 1) for the positions of these sites as

$$\mathbf{r}_{I} \equiv \mathbf{r}_{I}(\{Q\}) = \mathbf{r}_{I}^{(0)} + \sum_{j=1}^{m} \mathbf{R}_{Ij} Q_{j}$$
, (6a)

$$\mathbf{r}_{J} \equiv \mathbf{r}_{J}(\{Q\}) = \mathbf{r}_{J}^{(0)} + \sum_{j=1}^{m} \mathbf{R}_{Jj} Q_{j}$$
, (6b)

where \mathbf{R}_{ij} is the vector with components X_{ij} and Y_{ij} . If $\delta \theta_{k+1}$ is the vector (perpendicular to the plane of the triangular lattice) representing the angular displacement of bond k + 1, then the constraint introduced by adding this bond gives rise to the equation

$$\delta\theta_{k+1} \times (\mathbf{r}_{J}^{(0)} - \mathbf{r}_{I}^{(0)}) + \mathbf{r}_{J}^{(0)} - \mathbf{r}_{I}^{(0)} = \mathbf{r}_{J}(\{Q\}) - \mathbf{r}_{I}(\{Q\}) .$$
(7)

The right-hand side of this equation is the relative displacement associated with the k + 1st bond calculated in terms of the independent variables associated with the system of k bonds. On the left-hand side of this equation the same quantity is expressed in terms of $\delta \theta_{k+1}$. Equation (7) is a vector equation which gives rise to two scalar equations which are each linear in the variables $\{\delta \theta_i\}$ and $\delta \theta_{k+1}$. In general, from these two equations we can always eliminate $\delta \theta_{k+1}$ in terms of the $\{Q\}$'s. However, these two formal equations may or may not be linearly independent. For instance, if the sites I and J were already rigidly connected before the k + 1st bond was added, the only constraint now present with k+1 bonds is that $\delta\theta_{k+1}$ is equal to the $\delta\theta$ representing the rotation of the rigid cluster containing sites I and J. In this example $\{Q\}' = \{Q\}$ and Eqs. (4) and (5) can be updated in an obvious way. If the two scalar equations from Eq. (7) are linearly independent, then it will be possible to solve for both $\delta \theta_{k+1}$ and for one of the Q's. Let Q_r be the variable so eliminated by the newly introduced constraint:

$$Q_r = \sum_{i=1}^{m'} B_{ri} Q_i \quad , \tag{8}$$

where the prime on the summation indicates the absence of the term for which i = r. Thus Eq. (4) yields

$$\delta \theta_{j} = \sum_{i=1}^{m'} A_{ji} Q_{i} + A_{jr} \sum_{i=1}^{m'} B_{ri} Q_{i} , \qquad (9)$$

from which one can deduce the new coefficients A'_{ji} . To do this, it is necessary to renumber the Q's if $r \neq m$.

This procedure is illustrated in Fig. 2 for the parallelogram shown in Fig. 1. In discussing this cluster we num-



FIG. 2. Here panels (a), (b), (c), and (d) show the independent angular displacements after, respectively, 1, 2, 3, and 4 bonds have been attached to form a parallelogram. In panel (d) the constraint of Eq. (7) has not yet been applied. In panel (e) a bond has been added which connects sites 2 and 3, making the overall cluster completely rigid.

ber the sites in increasing order clockwise, starting with number 1 at the lower left. Bond 1 is fixed to have one end at the origin: $\mathbf{r}_1 = (0,0)$, i.e., the displacement of this end is zero. In terms of the orientational displacement, $\delta\theta_1$ the other end is at $\mathbf{r}_4 = (1, \delta\theta_1)$ [Fig. 2(a)]. Now we add bond 2 and allow it to have orientational displacement $\delta\theta_2$ from equilibrium [Fig. (2b)]. There are no constraints so that now $\{Q\} = \delta\theta_1, \delta\theta_2$. Also at this stage

$$\mathbf{r}_1 = (0,0)$$
, (10a)

$$\mathbf{r}_4 = (1, \ \delta\theta_1) \ , \tag{10b}$$

$$\mathbf{r}_2 = \left[\frac{1}{2} - \frac{\sqrt{3}}{2}\delta\theta_2 , \frac{\sqrt{3}}{2} + \frac{1}{2}\delta\theta_2\right].$$
(10c)

Next we add bond 3 and allow it to have orientational displacement $\delta\theta_3$ [Fig. 2(c)]. There are still no constraints, so that now $\{Q\} = \delta\theta_1$, $\delta\theta_2$, $\delta\theta_3$. Now \mathbf{r}_i for i = 1, 2, 4 are as given in Eqs. (10a)–(10c), but additionally we have

$$\mathbf{r}_{3} = \left[\frac{3}{2} - \frac{\sqrt{3}}{2}\delta\theta_{2}, \frac{\sqrt{3}}{2} + \frac{1}{2}\delta\theta_{2} + \delta\theta_{3}\right].$$
(10d)

Finally, we add bond 4. This is shown in Fig. 2(d) where we note that the ends of bonds 1 and 4 are not connected. If we insist that these two ends be connected, we obtain constraint equations as in Eq. (7). Specifically, the x and y components of this equation are

$$\frac{\sqrt{3}}{2}\delta\theta_4 - \frac{1}{2} = -\frac{1}{2} + \frac{\sqrt{3}}{2}\delta\theta_2$$
(11a)

$$-\frac{1}{2}\delta\theta_{4} - \frac{\sqrt{3}}{2} = -\frac{\sqrt{3}}{2} - \frac{1}{2}\,\delta\theta_{2} - \delta\theta_{3} + \delta\theta_{1} \,. \quad (11b)$$

These equations are linearly independent in this case and their solution yields, $\delta\theta_4 = \delta\theta_2$ and $\delta\theta_3 = \delta\theta_1$, so finally for the full cluster of Fig. 1 we have simply $\{Q\} = \delta\theta_1$, $\delta\theta_2$, and the constraints are $\delta\theta_4 = \delta\theta_2$, and $\delta\theta_3 = \delta\theta_1$. If another bond were placed connecting sites 2 and 3, one would introduce for it an orientational displacement, $\delta\theta_5$ [Fig. 2(e)]. The constraint equations would then have the solutions $\delta\theta_5 = \delta\theta_2 = \delta\theta_1$. This coordinate describes an overall rigid rotation of the cluster and indicates that the whole cluster forms a single "rigid" cluster and, of course, a single "splay-rigid" cluster.

There are several advantages to this method. One obtains the exact cluster size distribution for each realization as well as an unambiguous map of the propagation of the two types of rigidity through the lattice. This map may be drawn on a terminal or printed. The method may be generalized to other lattices, higher dimensions, and different models of elastic energy. Most of the necessary operations within a computer program can be vectorized. This procedure results in a substantial saving of computational time. Since this approach identifies a minimum set of variables, it would be a useful starting point for a calculation of the bulk modulus.



FIG. 3. For each lattice size, L, the abscissa is the occupied-bond concentration p_1 , the ordinate is the fraction of realizations p_2 in which splay rigidity has percolated across the entire lattice (circles), total rigidity has percolated (squares), and splay rigidity has percolated but total rigidity has not (triangles).

III. RESULTS AND DISCUSSION

At a particular bond occupation probability, the fraction of realizations in which splay or total rigidity has traversed the sample results in a pair of cumulative distribution functions. These are plotted in Fig. 3 as are their differences for lattices of size 12 (11000), 18 (1700), 24 (500), and 36 (1000), where the number of realizations is given in parentheses. The areas under the peaks (tails put in by hand) when extrapolated to $L = \infty$ yield the value of $\Delta P = p_{\text{TR}} - p_{\text{SR}}$, the difference in the critical thresholds of splay and total rigidity. One can see that the areas decrease, as do the maxima as already found by TDT with somewhat smaller data sets than ours. A plot of $\ln \Delta P$ against $\ln L$ is shown in Fig. 4. $\Delta P \sim L^{-\lambda}$ with $\lambda = 1.1$. In view of this behavior the existence of the splay-rigid phase is unlikely. If there is a splay-rigid phase, the area under the L = 36 peak gives the upper bound $\Delta P < 0.007 \pm 0.002$ where the error estimates are somewhat subjective.

In Fig. 5 we make a log plot of the reduced bond concentration $|p_L - p_{cen}| \sim L^{-1/\nu}$ at which total rigidity has percolated across half of the realizations versus the log of the lattice size L. We expect this relationship to be linear with slope $-1/\nu$. The graph indicates $\nu = 1.14\pm 0.1$, and the best fit to this power law behavior



FIG. 4. log-log plot of the areas, ΔP , under the peaks (graphed with triangles) in Fig. 3 vs L.

occurs for $p_{cen} = 0.64 \pm 0.002$. This value of p_{cen} supercedes previous estimates. We cannot say whether or not λ and $1/\nu$ are distinct exponents.

From the above results it appears that the order parameters for splay and total rigidity are simultaneously critical. We also find that their exponents, within error, are the same. In particular, the fraction of realizations which are splay rigid but not totally rigid as a function of p has a peak of diminishing amplitude and width as one moves to larger lattices. All of the above data indicates the absence of splay rigidity on the triangular lattice as found by TDT.

For each realization of the lattice and at each bond concentration p we calculate $\langle m^k \rangle \equiv \sum_m m^k N_m / N_m$



FIG. 5. log-log plot of the occupied bond concentration p_L at which total rigidity has percolated across half of the realizations vs the lattice size L. Here $p_c \equiv p_L - p_{cen}$ and we took $p_{cen} = 0.64$.



FIG. 6. The exponent Φ_n for n = -1, 0, 1.

 $\sum_{m} mN_{m}$, the kth moment of the cluster size distribution $\overline{N_m}$. N_m is the number of clusters per bond with m bonds where $\sum_{m} m N_{m} = p N_{0}$ for bond percolation, where N_{0} is the total number of bonds in the system when p = 1. For a given lattice of size L, finite size scaling gives¹⁴ $\langle m^k \rangle \sim L^{x/\nu} f((p-p_c)L^{1/\nu})$. Near the critical point and for $L \rightarrow \infty$, f becomes a simple power law, so we obtain $\langle m^k \rangle \sim |p-p_c|^{-x}$. For L finite this implies that at the critical point $\langle m^k \rangle \sim L^{x/\nu}$. In analogy with the ordinary percolation problem¹⁴ we set $x = \beta$ $+2\gamma + n(\gamma + \beta) \equiv \Phi_n v$ and $n \equiv k - 3$. This choice of origin for n puts the intercept of Φ in the middle of the data points. The definition of x allows us to recover the usual susceptibility, infinite cluster, and gap exponents. A plot of Φ_n versus *n* for n = -1, 0, 1 should have a slope of $(\gamma + \beta)/\nu$ and an intercept of $(\beta + 2\gamma)/\nu$. From Fig. 6 we find that the slope is 1.8 ± 0.2 and the intercept is 3.2 \pm 0.16. These are combined to yield $\gamma/\nu = 1.4\pm 0.23$, and $\beta/\nu = 0.4 \pm 0.36$. If from above we take $\nu = 1.14 \pm 0.1$, then $\beta = 0.46 \pm 0.4$ and $\gamma = 1.6 \pm 0.3$. The above slope can also intercept be checked against and hyperscaling relation $dv = 2\beta + \gamma$. We obtain the $(2\beta + \gamma)/\nu = 2.2 \pm 0.76$, which is satisfied given the large error bars.

The percolation exponents for rigidity have rather large errors associated with them. At this point there is no other prediction for these quantities although the backbone exponent for total rigidity, β_{BB} , may be derived from the calculation of Day *et al.*⁹ via $\beta_{BB} = v(d - \sigma) \approx 0.07$ which is considerably smaller than $\beta \approx 0.5$ calculated here. It is possible that the difference between the two numbers be attributed to the difference in technique discussed in TDT and the response by Wang and Harris.¹¹

A field theoretic formulation of this problem would offer more insight into the simultaneous criticality of splay and total rigidity as well as further estimates of the exponents in this problem.

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