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Abstract

It is proposed that the randomly diluted elastic network of Hooke's-law central-force springs in two dimensions may have a hitherto unrecognized splay-rigid phase in which the bulk and shear moduli vanish but the Frank elastic constant, K , is nonzero. Exponents for the associated splay-rigidity percolation and torsional resistance are estimated by series-expansion techniques. These exponents are related to that for K through the node-link picture.

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Physics

Bond Orientational Order in the Randomly Diluted Elastic Network

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It is proposed that the randomly diluted elastic network of Hooke's-law central-force springs in two dimensions may have a hitherto unrecognized splay-rigid phase in which the bulk and shear moduli vanish but the Frank elastic constant, K , is nonzero. Exponents for the associated splay-rigidity percolation and torsional resistance are estimated by series-expansion techniques. These exponents are related to that for K through the node-link picture.

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This Letter is concerned with the properties of the randomly diluted elastic network of central-force springs, for which the elastic potential energy, V , is $V = \sum V_b$, where the sum is over nearest-neighbor bonds on a triangular lattice and

$$V_b = \frac{1}{2} k \epsilon_b [(\mathbf{u}_1 - \mathbf{u}_2) \cdot \hat{\mathbf{R}}_{12}]^2.$$

Here k is the force constant of the springs, $\mathbf{u}_1$ and $\mathbf{u}_2$ are the displacements of the sites at the ends of the spring b from their respective equilibrium positions $\mathbf{R}_1$ and $\mathbf{R}_2$, $\hat{\mathbf{R}}_{12}$ is a unit vector in the direction $\mathbf{R}_1 - \mathbf{R}_2$, and, for each bond, ϵ_b is a random variable assuming the values 1, with probability p , and 0, with probability $1 - p$, corresponding respectively to the bond b being present or absent from the lattice. This model has received considerable attention recently,¹⁻⁴ but a comprehensive analytic treatment of it has yet to appear. The present work is a precursor to a mean-field theory in that we here, for the first time, identify order-parameter fields which can describe the crossover that must occur at the threshold from a type of percolation to a type of rigidity susceptibility. The analogy with the resistor network has been recognized, but not yet formulated concretely. By exploring this analogy in detail, we have been led to identify bond-angle coordinates as the above-mentioned order-parameter fields. Our result that there is a bond-angle rigid phase intervening between the disordered phase and the "rigid" (i.e., solid) phase, although novel to this problem, is similar to that obtained for two-dimensional melting⁵ and thus puts this problem into a more general context than heretofore.

To describe our result, it is useful to recall the nature of the crossover from percolation to conductivity in the analogous diluted resistor network,^{6,7} for which the "Hamiltonian," H , is

$$H = \sum_b \frac{1}{2} \sigma \epsilon_b (V_{b1} - V_{b2})^2,$$

where $V_{b1} - V_{b2}$ is the voltage difference across the bond b . For this model, the susceptibility $\chi(x, x')$ is taken to be

$$\chi_\lambda(x, x') = [\text{Tr}\{e^{-H} \psi_\lambda(x) \psi_{-\lambda}(x')\} / \text{Tr} e^{-H}]_{\text{ran}},$$

where $\psi_\lambda(x) = e^{-i\lambda V(x)}$, $[\]_{\text{ran}}$ indicates an average over the random bond variables ϵ_b , Tr indicates integration over all V variables from $-\infty$ to $+\infty$, and similarly for the displacements in the elastic model. One can write

$$\chi_\lambda(x, x') = [\exp(-\frac{1}{2} \lambda^2 R_{x,x'})]_{\text{ran}}, \quad (1)$$

where $R_{x,x'}$ is the resistance between sites x and x' . We now consider the interpretation of $\chi_\lambda(x, x')$ for large σ . First of all, note that $R_{x,x'} = \infty$ if sites x and x' are not in the same cluster, so that

$$\chi_\lambda(x, x') = [\nu_{x,x'} \exp(-\frac{1}{2} \lambda^2 R_{x,x'})]_{\text{ran}},$$

where $\nu_{x,x'}$ is the pair-connectedness function of bond percolation: $\nu_{x,x'} = 1$ if sites x and x' are connected (in the same cluster) and is zero otherwise.

In configurations where $\nu_{x,x'} = 1$, $R_{x,x'} = r_{x,x'}/\sigma$, where $r_{x,x'}$ is the resistance when $\sigma = 1$. Thus for large σ ,

$$\begin{aligned} \chi_\lambda(x, x') &= \left[\nu_{x,x'} \left(1 - \frac{\lambda^2}{2\sigma} r_{x,x'} \cdots \right) \right] \\ &= \chi^{(p)}(x, x') \left[1 - \frac{\lambda^2}{2\sigma} r_{x,x'}^{\text{av}} \cdots \right] \end{aligned} \quad (2a)$$

$$\sim \chi^{(p)}(x, x') \left[1 - \frac{\lambda^2}{2\sigma} |x - x'|^\phi \right], \quad (2b)$$

where $\chi^{(p)}(x, x')$ is the susceptibility for percolation and $r_{x,x'}^{\text{av}}$ is the configurationally averaged dimensionless resistance between sites x and x' subject to these sites being in the same cluster. One can say that $\chi_\lambda(x, x')$ defines a percolation problem in the limit $\sigma \rightarrow \infty$. This so-defined percolation problem is, of course, identical to the traditional percolation problem. In this formulation^{6,7} the critical exponents describing the diluted resistor network can be expressed in terms of the exponents for percolation and the crossover exponent ϕ of Eq. (2b).

It is useful to consider the new percolation problem defined by the analogous operation $k \rightarrow \infty$ for the di-

luted elastic network. In so doing we require that any "elastic-connectedness" function $\nu_{x,x}^{\text{el}}$, we may introduce should obey the cluster property, namely, if in any random configuration $\nu_{x,y}^{\text{el}} = 1$ and $\nu_{y,z}^{\text{el}} = 1$, then $\nu_{x,z}^{\text{el}} = 1$. If $\nu_{x,y}^{\text{el}}$ is defined for pairs of sites x, y , then this property does not always hold, as the configuration in Fig. 1 shows. Here sites x and y are rigidly connected, as are sites y and z . However, sites x and z are not rigidly connected. Thus we are led to formulate rigidity in terms of bonds. For a pair of bonds, $b_1 = (x_1, x_2)$ and $b_2 = (x_3, x_4)$ a natural set of generalized displacements, $Q_i(b_1, b_2)$ for $i = 1, \dots, 8$ are for $i = 1, 2$, a uniform translation of all four points in either the x or y directions; for $i = 3$, a uniform rotation of all four points about their center of mass; for $i = 4$, a relative compression in which bonds b_1 and b_2 are moved relative to one another as rigid units along the line joining their centers; for $i = 5, 6$, individual compression of either bond b_1 or bond b_2 ; for $i = 7$, a splay distortion in which b_1 is rotated about its center through an angle θ and b_2 is rotated about its center through an angle $-\theta$; and for $i = 8$, a bend, in which the two bonds are rotated about their centers by the same angle, θ . These generalized displacements (in Fig. 2 the modes Q_7 and Q_4 are illustrated) form a complete set for the four sites in question but are not necessarily orthogonal to one another. We define rigidity in terms of these generalized displacements as follows: In a given configuration two bonds b_1 and b_2 are rigid with respect to a set of generalized displacements $\{Q_i\}$ if, for all Q_i ,

$$\langle Q_i | G | Q_i \rangle < \infty, \quad (3)$$

where G is the elastic Green's function, i.e., the inverse of the potential-energy matrix, V , for the random configuration in question. [Although V^{-1} is singular, G can be defined as $G = \lim_{\eta \rightarrow 0} (V + i\eta I)^{-1}$, where I is the identity matrix.] Alternatively, Eq. (3) may be expressed as

$$\langle Q_i | \phi_0 \rangle = 0, \quad \text{for all } |\phi_0\rangle,$$

where $|\phi_0\rangle$ is a zero-energy eigenfunction of V . Equation (3) states that the response to a generalized force conjugate to Q_i is finite, i.e., the restoring force for the displacement Q_i is nonzero. If $\{Q_i\}$ is taken to be the set of splay distortions $Q_7(b_1, b_2)$, then one can show that this definition of rigidity does satisfy the cluster

FIG. 1. A cluster in which sites x and y are rigidly connected as are y and z , but for which x and z are not rigidly connected.

property introduced above, and we coin the term splay rigidity to describe this type of partial rigidity. It is also easy to show that rigidity with respect to the set of relative bond compressions, $Q_4(b_1, b_2)$, does not satisfy the cluster property. For example, in Fig. 2 bonds A and B are both splay rigid and relative-compression rigid as are bonds B and C . However, bonds A and C , although splay rigid, are not relative-compression rigid. It is possible to define what we may call "total rigidity" as follows. In the following a nontrivial displacement $Q_n(b, b')$ of the bonds b, b' is one such that $Q_n(b, b')$ is orthogonal to the uniform translations $Q_1(b, b'), Q_2(b, b')$ and to the rotation $Q_3(b, b')$. Bonds b and b' are totally rigid if, for any such nontrivial displacement, $Q_n(b, b')$, one has $\langle Q_n(b, b') | G | Q_n(b, b') \rangle < \infty$. This condition indicates that there is a nonzero restoring force associated with any nontrivial displacement. This total rigidity is what has previously been called "rigidity." Note that even total rigidity only obeys the cluster property if it is referred to bonds rather than to sites.

The analog of $\chi_\lambda(x, x')$ is here

$$\chi_\lambda^{\text{el}}(b, b') = [\text{Tr} \{ \psi_\lambda(b) \psi_{-\lambda}(b') e^{-V} \} / \text{Tr} e^{-V}]_{\text{ran}},$$

where $\psi_\lambda(b) = \exp\{i\lambda [\hat{k} \times \hat{R}_{12} \cdot (\mathbf{u}_1 - \mathbf{u}_2)]\}$, where $\hat{k}$ is a unit vector perpendicular to the plane of the lattice. To motivate this definition, note that $\psi_\lambda(b) \times \psi_{-\lambda}(b') \sim \exp[iF_7 Q_7(b, b')]$, where $F_7 \sim \lambda$ is the generalized force conjugate to the splay distortion, $Q_7(b, b')$. The analog of Eq. (1) is

$$\chi_\lambda^{\text{el}}(b, b') = \left[\exp \left(- \frac{\lambda^2}{2k} n_{b, b'} \right) \right]_{\text{ran}}, \quad (4)$$

where $n_{b, b'}$ is the dimensionless torsional resistance

FIG. 2. (a), (b) A plaquette for which opposite sides are rigid both with respect to splay [in (a)] and with respect to compression [in (b)]. In these diagrams the arrows show the generalized force conjugate (a) to splay (Q_7) and (b) to relative compression (Q_4). (c) A cluster in which bonds A and B are rigidly connected with respect both to splay and compression, as are B and C . Note that A and C are rigid only with respect to splay. Over large distances compression rigidity propagates one dimensionally, whereas splay propagates in various directions, e.g., bonds A and D are splay rigid.

between bonds b and b' , defined by the ratio of the appropriate angle of response, θ , to applied torque, Γ . We use Eq. (4) to define elastic connectedness: $\nu_{b,b'}^{\text{splay}} \equiv \lim_{k \rightarrow \infty} \exp[(-\lambda^2/2k)n_{b,b'}]$, so that $\nu_{b,b'}^{\text{splay}} = 1$ if the two bonds are splay rigid with respect to one another and is zero otherwise. For large k , the analog of Eq. (2) is

$$\chi_{\lambda}^{\text{el}}(b, b') = [\nu_{b,b'}^{\text{splay}}]_{\text{ran}} [1 - (\lambda^2/2k)n_{b,b'}^{\text{av}}] \\ \sim \chi^{\text{splay}}(b, b') [- (\lambda^2/2k) |r_b - r_{b'}|^{\phi_{\text{el}}/\nu_{\text{SR}}}],$$

where $\chi^{\text{splay}}(b, b')$ is the splay-rigidity-percolation susceptibility, $n_{b,b'}^{\text{av}}$ is the configurationally averaged dimensionless torsional resistance between bonds subject to their being in the same splay-rigid cluster, ϕ_{el} is the elastic crossover exponent which describes the way $n_{b,b'}^{\text{av}}$ scales with distance between bonds, $|r_b - r_{b'}|$, and ν_{SR} is the correlation-length exponent for splay rigidity.

We now consider the location of the threshold for splay rigidity to percolate. For a diluted network, the mean cluster size for ordinary percolation diverges at p_c and the mean size of totally rigid clusters has been shown¹ to diverge at a larger value of p , which we denote $p_{\text{TR}} > p_c$. The important question is now: At what value of p (denoted p_{SR}) will the mean size of splay-rigid clusters diverge? Since (viz. see Fig. 2) splay rigidity propagates through some structures which are not totally rigid as well as through all that are, it is clear that $p_{\text{SR}} \leq p_{\text{TR}}$. Moreover, to make such a large splay-rigid cluster totally rigid requires the addition of a *finite fraction* of cross linkages. Thus we intuit the *inequalities*

$$p_c < p_{\text{SR}} < p_{\text{TR}}, \quad (5)$$

so that at $p = p_{\text{SR}}$ a transition into a splay-rigid phase occurs, and then at $p = p_{\text{TR}}$ a transition into a totally rigid phase occurs.

These inequalities are borne out by several calculations. For instance, let us define $\chi^{\text{splay}} = \sum_b \chi_{bb'}^{\text{splay}} \equiv [n_b^2]_{\text{ran}}$ and $\chi^{\text{rigid}} = [n_b^{\text{rigid}}]_{\text{ran}}$, where n_b^{splay} (n_b^{rigid}) is the number of bonds in a cluster which is splay rigid (totally rigid). We evaluate these "susceptibilities" in the tree approximation within which the dual lattice of triangles is treated as a Cayley tree of coordination number 3. This approximation is equivalent to a form of mean-field theory and yields $\chi^{\text{rigid}} = 3p + 12p^3/(1 - 2p^2)$ and $\chi^{\text{splay}} = 3p + 12p^3/(1 - p - p^2)$, so that

$$\chi^{\text{splay}} = (3, 0, 12, 12, 24, 36, 60, 96, 156, 264, 420, 564), \\ \chi_2 = (3, 0, 48, 36, 216, 324, 828, 1512, 3084, 6012, 11232, 18696), \\ \chi\xi^2 = (0, 0, 6, 24, 72, 180, 402, 852, 1704, 3342, 6312, 11538), \\ \chi_{\text{el}} = (0, 0, 6, 10, 28, 54, 110, 208, 390, 760, 1353.5, 2075.4).$$

$p_{\text{TR}} = 1/\sqrt{2} \sim 0.71$, which is greater than $p_{\text{SR}} = (-1 + \sqrt{5})/2 \sim 0.62$. One might argue that fluctuations caused by circuitous connections or other nonlocal effects could invalidate this result. At least for one special model of percolation on a lattice of rhombi we have been able to show unambiguously⁸ that a splay-rigid phase does occur, i.e., $p_{\text{SR}} < p_{\text{TR}}$.

In this splay-rigid phase one defines the Frank elastic constant, K , by $E = \frac{1}{2} K \int [\nabla (\partial_y u_x - \partial_x u_y)]^2 dx dy$, where $u(x, y)$ is the displacement field and E is the energy associated with nonuniform twisting. If opposite sides (of length L) of a square are rotated through angles θ and $-\theta$, respectively, then $E \sim 2K\theta^2$. In the node-link picture⁹ the energy is that of $(L/\xi)^2$ links, each of length equal to the correlation length, ξ , at whose ends bonds suffer a relative angular displacement $Q_7(b, b') \sim a\theta\xi/L$, where a is the lattice constant. Thus in the node-link picture

$$E \sim (L/\xi)^2 (a\theta\xi/L)^2 k\xi^{-\phi_{\text{el}}/\nu_{\text{SR}}},$$

so that $K \sim \xi^{-\phi_{\text{el}}/\nu_{\text{SR}}} \sim (p - p_{\text{SR}})^{\phi_{\text{el}}}$. The shear and bulk elastic moduli are, of course, zero in the splay-rigid phase, as in a hexatic liquid.⁵ They become nonzero at the higher threshold at $p = p_{\text{TR}}$. In d spatial dimensions the node-link picture in terms of a single Frank elastic constant yields $K \sim |p_{\text{SR}} - p|^f$, with $f = (d - 2)\nu_{\text{el}} + \phi_{\text{el}}$. This result should not be applied in high spatial dimension where f attains its mean-field value, probably obtained if we set $d = 6$, $\nu_{\text{el}} = \frac{1}{2}$, and $\phi_{\text{el}} = 1$. This relation, although analogous to that for the resistor network,^{6,7} is not to be identified with previous relations [e.g., Eq. (13) of Ref. 2] which do not make reference to K .

To obtain numerical estimates of the critical exponents describing the splay-rigidity threshold, we have developed series expansions in powers of p up to order p^{12} for the following quantities:

$$\chi^{\text{splay}} \sim (p_{\text{SR}} - p)^{-\gamma_{\text{SR}}}, \quad (6a)$$

$$\chi_2 = [n_b^3]_{\text{ran}} \sim (p_{\text{SR}} - p)^{-2\gamma_{\text{SR}} - \beta_{\text{SR}}}, \quad (6b)$$

$$\chi\xi^2 = \sum_b \chi^{\text{splay}}(b, b') |r_b - r_{b'}|^2 \\ \sim (p_{\text{SR}} - p)^{-\gamma_{\text{SR}} - 2\nu_{\text{SR}}}, \quad (6c)$$

$$\chi_{\text{el}} \equiv \sum_b n_{b,b'}^{\text{av}} \chi_{b,b'}^{\text{splay}} \sim (p_{\text{SR}} - p)^{-\gamma_{\text{SR}} - \phi_{\text{el}}}. \quad (6d)$$

For percolation, Eq. (6b) follows from the fact that n_b scales as $|p_c - p|^{-\beta - \gamma}$, and we assume the same result here. We obtained

In each case the k th number in the string is the coefficient of p^k in the series expansion for the quantity in question. We analyzed these series using Padé and differential Padé approximants¹⁰ and obtained the values $p_{SR} = 0.61 \pm 0.02$, $\gamma_{SR} = 0.95 \pm 0.1$, $\beta_{SR} = 0.45 \pm 0.02$, $\nu_{SR} = 0.60 \pm 0.15$, and $\phi_{el} = 0.95 \pm 0.15$, where the uncertainties are somewhat subjective. Although our value of p_{SR} does satisfy Eq. (5) with⁴ $p_{TR} = 0.65 \pm 0.005$, we regard the heuristic argument for Eq. (5) as its ultimate justification. These exponents can just barely satisfy the scaling relation $2\beta + \gamma = d\nu$, if we set $\gamma_{SR} = \phi_{el} = 1$, $\beta_{SR} = \frac{1}{4}$, and $\nu_{SR} = \frac{3}{4}$. These results will be presented in more detail shortly.

This formulation has recently enabled us to develop the first mean-field theory¹¹ in terms of variables related to $\psi_\lambda(b)$, from which the splay-rigidity ordering occurs in agreement with Eq. (5) and which also describes the total-rigidity transition. These results as well as numerical simulations¹² concerning this new splay-rigidity threshold will be presented elsewhere.

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