Effective-medium theory of percolation on central-force elastic networks

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(Received 15 August 1984)

We show that effective-medium theory gives an excellent description of regular lattices when nearest-neighbor central-force springs are present with probability p. Effective-medium theory shows that all the elastic constants go to zero at $p_{\rm cen}=dp_c$ where d is the dimension and p_c is the effective-medium estimate of the ordinary percolation threshold.

I. INTRODUCTION

There has been considerable interest in the elastic properties of random systems recently.[1–4] While much of this attention has focused on the critical properties of the random elastic network as it breaks up, it is of considerable interest to describe the overall behavior. We focus our attention in this paper on the central-force elastic percolation model.[1] We show that the simplest effective-medium theories give excellent agreement with numerical simulations for most values of p, the bond occupation probability, except for a very small range of values of p near $p_{\rm cen}$, on both the triangular network and on the fcc lattice.

Although it is unlikely that the present model will apply directly to any real physical system, it is an important one as it is the simplest member of a general class of models. These models are made up of units that can be connected but still transmit no elastic restoring forces. In the present case, the units are bonds and a pair of two and just two connected bonds form a "free hinge" as there are no angular forces. The whole network has finite elasticity for high values of p because the high connectivity "locks" all the free hinges. As bonds are removed from the pure system, local *floppy* regions are created which eventually prevent the rigid regions (i.e., the parts of the network that have finite elasticity) from percolating and the system loses its elasticity. Thus the breakup of the system is determined by *rigidity percolation* and not ordinary *connectivity percolation.*

The most important physical manifestation of this phenomenon is in the *covalent random networks*[5] where the local movement is not a free hinge but the dihedral angle associated with three connected bonds. The energy required to change the dihedral angle is small compared to that needed to change the bond lengths and bond angles, so it is reasonable to neglect it as a first approximation. This leads to a division of covalent random networks into low coordinated *polymeric glasses* and high coordinated *amorphous solids.*[5]

The other class of models for the elastic percolation phenomenon[2–4] involve specifying a sufficient number of microscopic forces so that all connected parts of the lattice are rigid by themselves and the elastic percolation transition occurs at the ordinary percolation threshold p_c, albeit with different exponents.[2–4]

The system under consideration is made up of Hooke springs connecting nearest-neighbor sites i,j to give a potential,

$$V=\frac{\alpha}{2}\sum_{\langle ij\rangle}[(\vec{u}_i-\vec{u}_j)\cdot\hat{r}_{ij}]^2p_{ij}\ , \tag{1}$$

where the angular brackets denote a sum over nearest-neighbor pairs which are connected by springs with spring constant α and p_{ij} is a random variable that is associated with each bond and is 0,1 with probability $1-p,p$. The $\vec{u}_i$ are the displacements from equilibrium and $\hat{r}_{ij}$ is a unit vector connecting nearest-neighbor pairs in equilibrium.

In the next section, we show how a constraints counting argument can be used to give an estimate of $p_{\rm cen}$ where the elastic constants of the system vanish. In Secs. III and IV we develop effective-medium theories for the elastic constants for $p>p_{\rm cen}$ from two different viewpoints, both of which lead to the same result. The first one is a direct generalization of the method developed in the study of electrical conduction near percolation threshold, and the second one applies the coherent-potential approximation to the present problem.

II. CONSTRAINTS METHOD

The simplest way to estimate where the transition takes place is to use a constraints argument.[5] When p is small, the system consists of disconnected pieces and hence has many *zero-frequency modes* whose number is given by the number of degrees of freedom (Nd) minus the number of constraints ($\frac{1}{2}zNp$). Thus, the effective-medium estimate of the fraction f of zero-frequency modes is given by

$$f=(Nd-\tfrac{1}{2}zNp)/Nd=1-\frac{zp}{2d} \tag{2}$$

so that f goes to zero at $p_{\rm cen}=2d/z$.

Next consider comparison of this result with numerical simulations. We have computed f numerically for a 168 atom triangular network (see inset in Fig. 1) and a 108

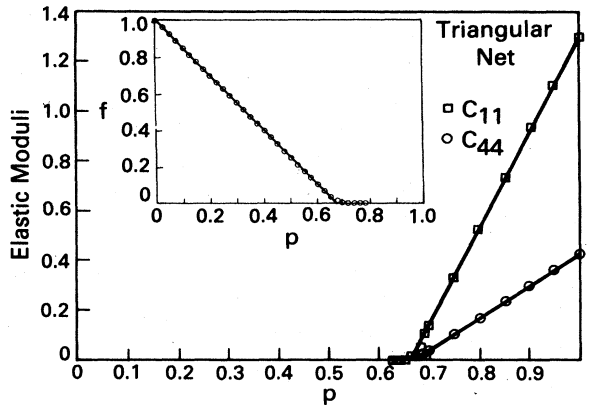

FIG. 1. Elastic constants C_{11} and C_{44} averaged over three configurations for a 440 atom triangular network. For the pure system ($p=1$), $C_{44}=C_{11}/3=\alpha\sqrt{3}/4$. The inset shows the fraction of zero-frequency modes f for a 168 atom triangular network averaged over three configurations. The straight lines are from the effective-medium theories described in the text.

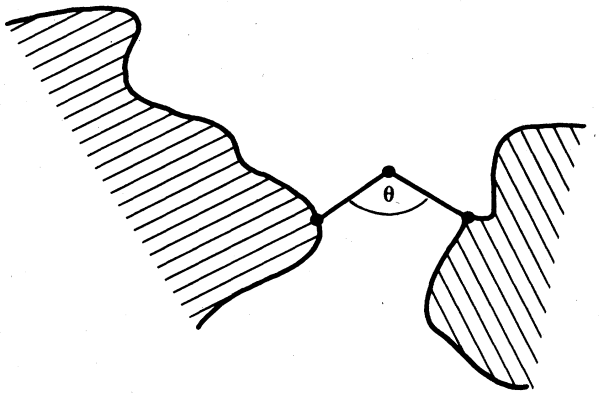

FIG. 3. Showing a two coordinated bridge connecting two regions. This bridge is ineffective in transmitting any elastic restoring force and can be trimmed.

atom fcc lattice (see inset in Fig. 2). Both lattices had periodic boundary conditions and f was obtained by directly diagonalizing the dynamical matrix formed from (1) and counting the number of modes with eigenvalues of zero. It can be seen that Eq. (2) describes the results well except near $p_{\rm cen}$ where the very small deviations from (2) are due to a combination of finite size and critical effects.

A similar constraint counting argument for 1, rather than d, degrees of freedom per site, which is the case for the electrical conduction problem, leads to the effective-medium estimate for the ordinary percolation (i.e., the connectivity problem)[6] of $p_c=2/z$, and hence

$$p_{\rm cen}=p_c d \ . \tag{3}$$

The transition described here takes place well before ordinary percolation occurs because many connections in the network produce no elastic restoring force.[1] A simple example is shown in Fig. 3. Configurations like this correspond to one example of the *floppy regions.*[5]

III. STATIC METHOD

For $p>p_{\rm cen}$, it is of interest to develop a mean-field theory for the elastic constants. We have done this in two ways, both of which lead to the *same result.* The one that is simpler conceptually is to adapt an argument used by

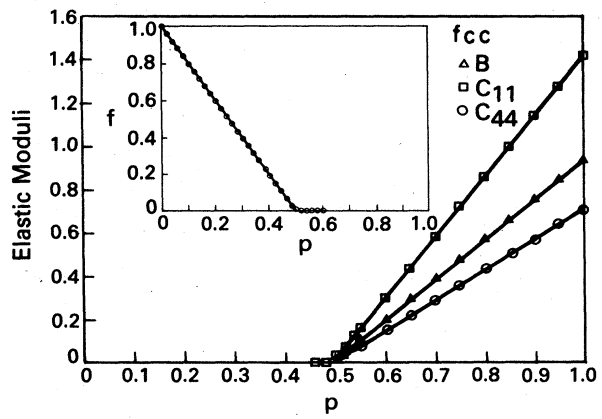

FIG. 2. Elastic constants C_{11}, C_{44}, and $B=(C_{11}+2C_{12})/3$ averaged over three configurations for a 500 atom fcc lattice. For the pure system ($p=1$), $C_{11}=2C_{12}=2C_{44}=\alpha\sqrt{2}/b$, where b is the nearest-neighbor separation. The inset shows the fraction of zero-frequency modes f for a 108 atom fcc lattice averaged over three configurations. The straight lines are from the effective-medium theories described in the text.

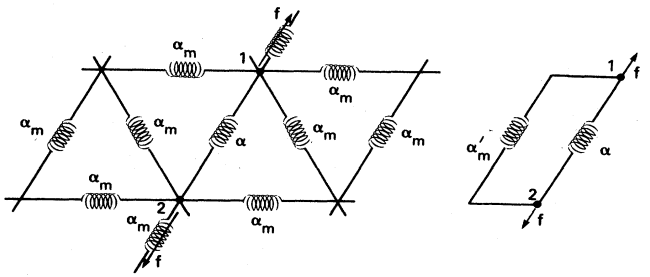

FIG. 4. Showing the notation for constructing the effective-medium theory. On the left-hand side a single bond between sites 1 and 2 is modified by having a spring constant α rather than α_m. The strain existing before the modification can be reestablished by applying a force f across the bond as shown. On the right-hand side, we show an equivalent circuit for the bond joining 1 and 2 as described in the text. The springs α'_m and α are connected in parallel.

Kirkpatrick[6] for the electrical resistor network. Suppose a uniform stress (uniaxial, hydrostatic, etc.), is applied to a lattice where all the springs are α_m and that the atoms labeled 1,2 in Fig. 4 have a relative displacement, along $\hat{r}_{12}$ of δu_m. Now substitute a single "wrong bond" α as shown in Fig. 4 and imagine an *extra external force* f applied to 1 and 2 as shown to restore 1 and 2 to their positions *before* α was substituted for α_m. It is then easily seen that f should be

$$f=\delta u_m(\alpha_m-\alpha) . \tag{4}$$

From the superposition principle, the relative displacement δu between 1 and 2 induced by f when the system is unstressed is the same as the *extra displacement* between 1 and 2 when there is an applied uniform strain δu_m but no f. Then δu is the "fluctuation" in relative displacement of 1,2 due to the introduction of the wrong bond α. The relation between f and δu can be obtained in the following way. If the force f is applied to 1,2 when *all* the springs are α_m, there will be an effective spring constant $\alpha_{\rm eff}=\alpha_m/a^*$ where $0<a^*<1$ takes account of all the connections between 1,2 including the direct one in this uniform system. We will calculate a^* later, but for now treat it as a known constant. If the α_m spring between 1 and 2 is *removed,* then the new effective constant α'_m between 1 and 2 is

$$\alpha'_m=\alpha_m/a^*-\alpha_m \tag{5}$$

as shown in Fig. 4. If α is added in parallel to α'_m and the force f applied, then the relative displacement δu of 1 and 2 is given by

$$f=\delta u(\alpha'_m+\alpha) \tag{6}$$

or

$$\delta u=\delta u_m(\alpha_m-\alpha)/(\alpha_m/\alpha^*-\alpha_m+\alpha) . \tag{7}$$

The effective-medium result is obtained by choosing α_m so that the average value $\langle \delta u \rangle$ of δu is zero to give

$$\left\langle \frac{\alpha_m-\alpha}{\alpha_m/\alpha^*-\alpha_m+\alpha} \right\rangle =0 . \tag{8}$$

For a distribution $P(\alpha)$ of spring constants α this leads to

$$\int \frac{P(\alpha)}{1-a^*(1-\alpha/\alpha_m)} d\alpha=1 . \tag{9}$$

For the present case of interest $P(\alpha')=p\delta(\alpha-\alpha')+(1-p)\delta(\alpha')$ gives

$$\frac{\alpha_m}{\alpha}=\frac{p-a^*}{1-a^*} \tag{10}$$

which goes to zero when $p_{\rm cen}=a^*$.

The quantity a^* is obtained for the perfect lattice as follows. The force $\vec{F}_i$ on the atom i is given by

$$\vec{F}_i=-\frac{\partial V}{\partial \vec{u}_i}=-\sum_j \overleftrightarrow{D}_{ij}\cdot\vec{u}_j , \tag{11}$$

where

$$\overleftrightarrow{D}_{ij}=\begin{cases} -\alpha_m \hat{r}_{ij}\hat{r}_{ij}, & j\neq i \\ \alpha_m \sum\limits_{j'\neq i} \hat{r}_{ij'}\hat{r}_{ij'}, & j=i \end{cases} . \tag{12}$$

These equations can be inverted by Fourier transformation to give

$$\vec{u}_k=-\overleftrightarrow{D}^{-1}(\vec{k})\cdot\vec{F}_k , \tag{13}$$

where $\overleftrightarrow{D}(\vec{k})$ is the $d\times d$ dynamical matrix for a Bravais lattice, and $\vec{F}_k$ and $\vec{u}_k$ are the Fourier transforms of the $\vec{F}_i$ and $\vec{u}_i$, respectively:

$$\begin{aligned}\overleftrightarrow{D}(\vec{k})&=\sum_{i,j}\overleftrightarrow{D}_{ij}\exp[i\vec{k}(\vec{r}_j-\vec{r}_i)] \\ &=\alpha_m\sum_{\hat{\delta}}[1-\exp(ia\vec{k}\cdot\hat{\delta})]\hat{\delta}\hat{\delta} ,\end{aligned} \tag{14}$$

where $\hat{\delta}$ is a unit vector in the direction of one of the z nearest neighbors and a is the nearest-neighbor separation. Putting $\vec{F}_j=f\hat{r}_{12}(\delta_{j1}-\delta_{j2})$, the negative of the externally applied force as shown in Fig. 4, we find that

$$\begin{aligned}\vec{u}_2-\vec{u}_1=\frac{f}{N}\sum_{\vec{k}}&[2-\exp(ia\vec{k}\cdot\hat{r}_{12}) \\ &-\exp(-ia\vec{k}\cdot\hat{r}_{12})]\overleftrightarrow{D}^{-1}(\vec{k})\cdot\hat{r}_{12} ,\end{aligned} \tag{15}$$

which defines

$$\begin{aligned}a^*=\frac{\alpha_m}{N}\sum_{\vec{k}}&[2-\exp(ia\vec{k}\cdot\hat{r}_{12}) \\ &-\exp(-ia\vec{k}\cdot\hat{r}_{12})]\hat{r}_{12}\cdot\overleftrightarrow{D}^{-1}(\vec{k})\cdot\hat{r}_{12} .\end{aligned} \tag{16}$$

As all bonds are equivalent, we can replace $\hat{r}_{12}$ by any of the nearest-neighbor bonds $\hat{\delta}$, sum over all nearest-neighbor bonds and divide by z to give

$$\begin{aligned}a^*&=\frac{2\alpha_m}{Nz}\sum_{\vec{k}\delta}\mathrm{Tr}\{[1-\exp(ia\vec{k}\cdot\hat{\delta})](\hat{\delta}\hat{\delta})\cdot\overleftrightarrow{D}^{-1}(\vec{k})\} \\ &=\frac{2}{Nz}\sum_{\vec{k}}\mathrm{Tr}(1)=\frac{2d}{z}=p_{\rm cen} .\end{aligned} \tag{17}$$

Thus, the result (11) can be written[7,8] as

$$\frac{\alpha_m}{\alpha}=\frac{p-p_{\rm cen}}{1-p_{\rm cen}} . \tag{18}$$

Since all the elastic constants C_{ij} of the network are linear functions of α_m only, we conclude that they all go to zero linearly at $p_{\rm cen}$, and that any ratio of two elastic constants is independent of p. In particular, the ratio of the bulk modulus to the shear modulus of the triangular network is *always* 2.

Next consider comparison of this result with the numerical simulations. The straight lines from Eq. (18) are plotted in Figs. 1 and 2 for the triangular and the fcc lattices and show excellent agreement with simulations except for a very small critical region near $p_{\rm cen}$. Such close agreement between simulations and effective-medium theories is rare although it does occur for the conductivity problem[6] in $2d$. The deviations are larger in $3d$ for the conductivity problem[6] than in the results for springs in Figs. 1 and 2. Indeed $2d/z$ appears to be a *superior* estimate for $p_{\rm cen}$ than $2/z$ is for p_c. This is particularly apparent in comparing the results for the fcc lattice in this paper and those in Ref. 6. In general, we would expect effective-medium theories to do better in higher dimensions.

The numerical simulations were done by removing bonds at random in a lattice with periodic boundary conditions, imposing an appropriate external small strain ϵ (which redefines the vectors that define the large periodic cell) and relaxing as fully as possible by moving atoms towards positions where there is no force on them. The elastic constants were obtained by computing the potential energy of the system via Eq. (1) and using $V=\frac{1}{2}C\epsilon^2$. This procedure has some advantages over that used previously[1] in that all atoms are treated equivalently and there are no "surface atoms." Typical strains used were $\epsilon=10^{-5}$.

There are some subtle and important differences in the numerical simulations done in this work and those done previously.[1] In Fig. 3, the two bonds can be removed as they do not produce a restoring force. (Dangling bonds are also removed as in the conductivity problem.[6]) However, when $\theta=180°$ in Fig. 3, there are two ways to proceed. In Ref. 1, it was assumed that there was a restoring force as given by the potential (1), whereas in the present work we assume there is none and remove such configurations. This has the effect of increasing $P_{\rm cen}$ from ≈ 0.58 nearer to $\frac{2}{3}$. We remove such configurations because "buckling" can occur in compression rendering the connection in Fig. 3 ineffective even if $\theta=180°$. This model can be visualized as replacing all 180° bonds by $180°-\Delta$, evaluating the elastic properties for a small strain $\epsilon \ll \Delta$, and letting $\Delta \to 0$. Both models (i.e., Ref. 1 and the present one) are equally valid and of course the effective-medium theories do not distinguish between them. In the numerical simulations to calculate f, as described previously, it was found that f was slightly larger for the $\Delta=0$ case than for the small Δ case. However, this was only appreciable around $p_{\rm cen}$ and too small an effect to show on the scale of the insets in Figs. 1 and 2.

IV. COHERENT-POTENTIAL APPROXIMATION

We now consider a multiple-scattering approach in which all repeated scatterings from the same bond are summed to give a coherent-potential approximation (CPA).[9] We find that same result (18) is obtained from this method. Writing the Hamiltonian for the system as

$$H=H_0+V\ , \tag{19}$$

where

$$H_0=\sum_i \frac{\vec{p}_i^{\,2}}{2M}+\frac{\alpha_m}{2}\sum_{\langle ij\rangle}[(\vec{u}_i-\vec{u}_j)\cdot\hat{r}_{ij}]^2 \tag{20}$$

and

$$V=\frac{\alpha-\alpha_m}{2}[(\vec{u}_1-\vec{u}_2)\cdot\hat{r}_{12}]^2 \tag{21}$$

represents a single "defect" bond in an effective medium α_m as shown in the left-hand side of Fig. 4. It is convenient to define Green's functions for the system described by H_0 as

$$\overleftrightarrow{P}_{ij}=\sum_n \left[\frac{\langle 0\,|\,\vec{u}_i\,|\,n\rangle\langle n\,|\,\vec{u}_j\,|\,0\rangle}{\omega-\omega_n+\omega_0} - \frac{\langle 0\,|\,\vec{u}_j\,|\,n\rangle\langle n\,|\,\vec{u}_i\,|\,0\rangle}{\omega+\omega_n-\omega_0}\right], \tag{22}$$

where $\overleftrightarrow{P}_{ij}$ is a $d\times d$ matrix. A similar quantity $\overleftrightarrow{G}_{ij}$ is defined for the system described by H. We rewrite (21) in matrix form with

$$\overleftrightarrow{V}_{ij}=(\alpha-\alpha_m)\hat{r}_{12}\hat{r}_{12}m_{ij}\ , \tag{23}$$

where $m_{ij}=(\delta_{1i}\delta_{1j}+\delta_{2i}\delta_{2j}-\delta_{1i}\delta_{2j}-\delta_{2i}\delta_{1j})$ arises from the translational invariance of each bond. It is easy to show that the Dyson equation is satisfied, i.e.,

$$\overleftrightarrow{G}=\overleftrightarrow{P}+\overleftrightarrow{P}\cdot\overleftrightarrow{V}\cdot\overleftrightarrow{G}\ , \tag{24}$$

where $\overleftrightarrow{P}$, $\overleftrightarrow{G}$, and $\overleftrightarrow{V}$ are considered as matrices in both site indices (i,j) and in a d-dimensional vector space. Remembering that we are considering a single defect bond, Eq. (24) can be rewritten as

$$\overleftrightarrow{G}=\overleftrightarrow{P}+\overleftrightarrow{P}\cdot\overleftrightarrow{T}\cdot\overleftrightarrow{P}\ , \tag{25}$$

where

$$\overleftrightarrow{T}_{ij}=\frac{\alpha-\alpha_m}{1-2(\alpha-\alpha_m)\hat{r}_{12}(\overleftrightarrow{P}_{11}-\overleftrightarrow{P}_{12})\cdot\hat{r}_{12}}\hat{r}_{12}\hat{r}_{12}m_{ij} \tag{26}$$

has the same *form* as $\overleftrightarrow{V}_{ij}$ but with a renormalized coefficient. Setting $\langle\overleftrightarrow{T}\rangle=0$, we find

$$\left\langle\frac{\alpha-\alpha_m}{1-2(\alpha-\alpha_m)\hat{r}_{12}\cdot(\overleftrightarrow{P}_{11}-\overleftrightarrow{P}_{12})\cdot\hat{r}_{12}}\right\rangle=0 \tag{27}$$

which is analogous to (8) except that it applies at all frequencies ω and the effective force constants $\alpha_m(\omega)$ are functions of the frequency. Note that *all elements* of the T matrix are set equal to zero by (27) as all the T matrices have the form of a scalar multiplying m_{ij}. The method of Sec. III can also be easily generalized to finite frequencies.

The pure system Green's functions $\overleftrightarrow{P}_{ij}$ obey the equation of motion (noting that $\overleftrightarrow{P}_{11}=\overleftrightarrow{P}_{22}$ and $\overleftrightarrow{P}_{12}=\overleftrightarrow{P}_{21}$)

$$M\omega^2 P_{11}=1+\frac{z\alpha_m}{d}\hat{r}_{12}\cdot(\overleftrightarrow{P}_{11}-\overleftrightarrow{P}_{12})\cdot\hat{r}_{12}\ , \tag{28}$$

where P_{11} is the magnitude of the isotropic site diagonal Green's function. As $\omega^2\to 0$, Eq. (27) reduces to the previous result (8) with again $a^*=2d/z$.

V. CONCLUSIONS

There is a slight difference between these two versions of effective-medium theory for $p > p_{cen}$. In the first, the elastic constants C_{ij} are calculated, and the various masses are irrelevant. In the second, the sound velocities are calculated in the long-wavelength limit. This leads to the elastic constants if it is assumed that the effective mass is independent of p. In reality, the effective mass will depend on p, but this dependence is expected to be much weaker than the dependence on p of the elastic constants near p_{cen}, analogous to the conductivity case. An account for such effects is obviously beyond the capabilities of effective-medium theories.

To summarize, we have shown that simple effective-medium theories give a remarkably good overall description of the dilute elastic systems with Hooke springs. The detailed behavior around p_{cen} is a subject still under study.

ACKNOWLEDGMENTS

We thank P. Sen for many useful conversations on this problem, and also R. J. Elliott, B. Halperin, B. Nickel, and L. Schwartz for clarification on particular points. Two of us (S.F. and M.F.T.) would like to thank Schlumberger-Doll Research Center for their hospitality during part of this work. The support of the Office of Naval Research and the National Science Foundation is gratefully acknowledged by M.F.T. and E.G.

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