Percolation on Elastic Networks: New Exponent and Threshold

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Bond percolation on elastic networks involving nearest-neighbor forces is studied by numerical simulations. With purely central forces, the bulk and shear moduli go to zero, with an exponent f, and at a threshold p_{cen}, which are significantly higher than the exponent t and threshold p_c of the corresponding purely isotropic force or the equivalent electrical conduction problem. An interesting crossover is observed when both central and isotropic forces are included.

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de Gennes[1] pointed out that the elastic modulus of a gel, modeled by an *isotropic force* constant, is analogous to the electrical conductivity of an electrical network. In this paper we show strong evidence that the *central-force* elastic percolation problem belongs to a *new* universality class.

de Gennes' results are based on a lattice percolation model for gelation without solvent.[1-3] In this model, each lattice site represents one polyfunctional unit. Two reacted neighboring units are linked by a bond. When the fraction p of the reacted bonds exceeds a critical value p_c, a gel is formed, corresponding to the formation of an infinite cluster in the percolation problem.[4]

The elastic forces between the reacted nodes give rise to a random network of elastic bonds. We describe the elastic forces by the Born model.[5] In this model, the potential energy of the lattice is given by

$$V=\tfrac{1}{2}(\alpha-\beta)\textstyle\sum_{ij}[(\vec{U}_i-\vec{U}_j)\cdot\hat{r}_{ij}]^2 g_{ij} + \tfrac{1}{2}\beta\textstyle\sum_{ij}(\vec{U}_i-\vec{U}_j)^2 g_{ij}\,. \quad (1)$$

Here $\vec{U}_i$ and $\vec{U}_j$ are displacements of node i and node j; $g_{ij}=1$ for the bonds that are occupied with a probability p, and $g_{ij}=0$ for the bonds that are empty with a probability $1-p$; and, $\hat{r}_{ij}$ is the unit vector from node i to node j. Despite its difficulty with rotational invariance[6] when β is nonzero, Born model (1) is a useful practical model which is qualitatively correct in many instances.[7,8] The purely *isotropic* Born model, i.e., $\beta=\alpha$ in (1), reduces to a scalar problem, and, hence, to the usual universality class of the conductivity problem, as noted by de Gennes.[1]

A far more interesting problem arises when such a reduction to the scalar model is *not* possible. The simplest example of this is offered by the model in which the nearest-neighbor forces are central, i.e., when $\beta=0$ in Eq. (1). Thus, forces are involved only when a bond stretches or contracts, just like an ordinary spring. The purely central-force Born model *is* rotationally invariant. The often used simple hypercubic lattices have no shear rigidity for any p and no bulk rigidity for any $p<1$ with nearest-neighbor central forces. Therefore, we study three-dimensional (3D) face-centered cubic (fcc) and 2D triangular lattices.

We determine numerically the bulk modulus K in 3D. For the 2D triangular lattice there are only two independent moduli, K and the shear modulus N; and we compute both. For the case of purely central forces, $\beta=0$, we find as p approaches p_{cen} from above that

$$K, N \sim (p-p_{cen})^f, \quad \beta=0. \quad (2)$$

For the purely isotropic case, $\alpha=\beta$, one finds that[1]

$$K, N \sim (p-p_c)^t, \quad \alpha=\beta, \quad (3)$$

where, for the 2D triangular lattice,

$$p_{cen}=0.58, \quad f=2.4\pm0.4; \qquad p_c=0.3473 \quad t=1.2\pm0.3, \quad (4)$$

and for the 3D fcc lattice,

$$p_{cen}=0.42, \quad f=4.4\pm0.6; \qquad p_c=0.119, \quad t=1.6\pm0.3. \quad (5)$$

The values of t were estimated by us on the same network with $\alpha=\beta$, as a check of our program, and agree well, within the error bars, with the commonly accepted best estimates: $t=1.3$ in 2D and $t=1.8$ in 3D for the conductivity exponents,[9-17] and with the latest estimates[14,15] of t, which are somewhat higher. In estimating t, we used the known values of p_c, as is customary.[9-17]

Because of the difference in the exponents f and t we propose that the central-force elastic percolation problem belongs to a *different* universality class from that of the conduction problem. This, in our opinion, reflects the differ-

ence in symmetry properties of the Hamiltonian when $\beta=0$, which is intrinsically of vector nature, as opposed to that when $\alpha=\beta$, which is essentially of scalar nature [x, y, z equations decouple, see Eq. (6) below]. This difference can be likened to the difference between the Heisenberg model and the Ising model in the magnetic context.

Admittedly, the central-force nearest-neighbor model is oversimplified, but it suffices to show the existence of a new universality class. Furthermore, a crossover behavior near $p_{\rm cen}$ will be seen when central forces dominate.

A practical, and qualitatively correct, way to include the bond-bending forces is to use the Born model, Eq. (1).[5-8] The crossover behavior can be easily illustrated in this case. In Fig. 1, we show K versus p from the results of simulations, when $\beta/\alpha=0.1$. We see that when $\alpha \gg \beta$, there is strong crossover behavior from isotropic-force-like behavior near $p \approx p_c$ to central-force-like behavior near $p \approx p_{\rm cen}$. For $p < p_{\rm cen}$, the noncentral forces provide the rigidity to the lattice, and near p_c, which is much smaller than $p_{\rm cen}$, the isotropic forces should dominate. Thus, near p_c, one expects the exponent to be t. Numerical estimate of the exponent for the case $\beta/\alpha = 0.1$ yields the value $t = 1.2 \pm 0.3$, supporting our intuitive expectation.

Next consider the explicit differences between

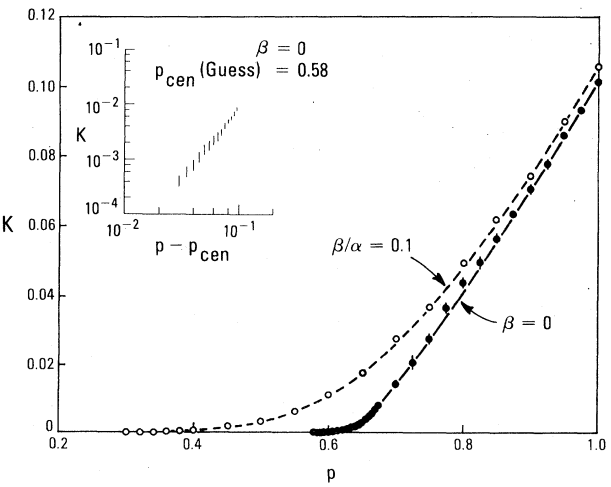

FIG. 1. Bulk moduli vs p for the cases when the force is purely central ($\beta=0$), and when the noncentral force is small ($\beta/\alpha=0.1$), for the 2D triangular lattice of 946 modes. A strong crossover is observed near $p_{\rm cen}$ in the latter case. Inset shows one $\log K$ vs $\log(p-p_{\rm cen})$ plot.

the electrical conduction and the purely central-force model. For the purely isotropic Born force-constant model, $\alpha=\beta$ in Eq. (1), the μth component of force on the atom i is given by

$$F_{i\mu} = \beta \sum_i (U_i - U_j)_\mu g_{ij} . \qquad (6)$$

For the interior nodes, $F_{i\mu}=0$ for each component $\mu=1$, 2, and 3. Equation (6) is identical to Kirchhoff's equations on an electric network, when $U_{i\mu}$ and $U_{j\mu}$ are interpreted as the voltages and β the conductance, and $F_{i\mu}$ the externally injected current into node i. Thus, the equation for each Cartesian component maps onto a scalar Kirchoff's equation. In the case of central forces only, $\beta=0$, the μth component of force on the atom i is given by

$$F_{i\mu} = \alpha \sum_i [(\vec{U}_i - \vec{U}_j)\cdot \hat{r}_{ij}](\hat{r}_{ij})_\mu g_{ij} . \qquad (7)$$

For interior atoms, $F_{i\mu}=0$, but the different Cartesian components $U_{i\mu}$ ($\mu=1$, 2, 3) in Eq. (7) do not decouple, and hence do *not* map onto the scalar electrical problem. Strictly speaking, the fact that Eqs. (6) and (7) do not map onto each other does not prove that the central-force elastic problem and the electrical network problem belong to different universality classes.

That the threshold $p_{\rm cen}$ can be different from p_c is perhaps not so surprising. For example, one can envision an infinite cluster in which there exists a node which has only two nonstraight bonds connected to it. Because with purely central forces, the bonds can pivot freely without costing any energy, this structure is not able to transmit any elastic forces, i.e., $K, N=0$, although the structure is definitely connected.

Above $p_{\rm cen}$, there is a part of the infinite cluster which participates in transmitting the elastic forces. This structure is analogous to the backbond of the usual percolation cluster,[13] i.e., the part of the connected network that participates in carrying current. Clearly, with central forces only, the bonds that do not stretch or compress are equivalent to dead ends. In Fig. 2, we have identified by the solid lines those occupied bonds that are either stretched or compressed. The dotted lines show the occupied bonds that are neither stretched nor compressed. The cluster formed by the solid lines gives the central-force "backbone." For clarity, we show only a part of the network which was subjected to a hydrostatic pressure.

To continue with these illustrations, consider a simple cubic lattice with central forces only. It is well known that the shear modulus is identi-

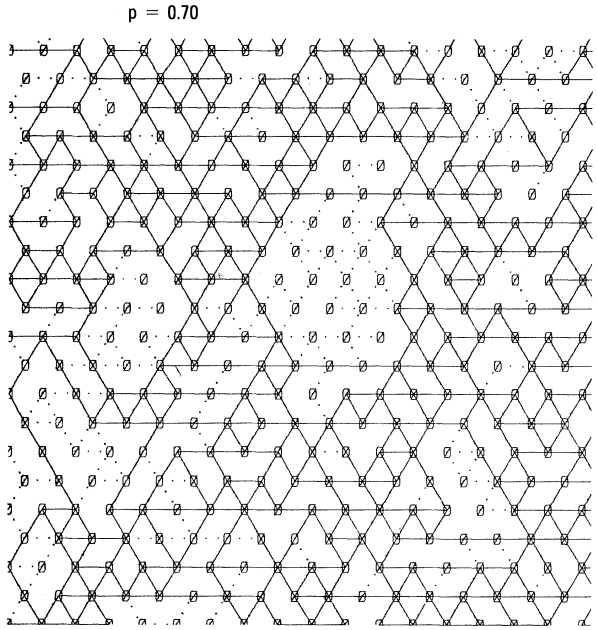

FIG. 2. Simulation of displacements of a 2D triangular lattice subjected to a hydrostatic pressure. The occupied bonds that stretched or shrank are shown by the solid lines and other occupied bonds by dotted lines. The rigid elastic backbone is given by the connected network of solid bonds. For clarity only a small portion of the network is shown.

cally zero in this case. One can also show that the bulk modulus goes to zero when an infinitesimally small fraction of bonds are missing, i.e., $p_{cen}=1$ in this case.

It is curious that the effective medium theory for the continuum case[18,19] also gives a p_{cen} which is different from p_c for inclusions of the same shape.

The details of the numerical simulations are as follows: In 3D we used a cubic sample of an fcc lattice with 666 nodes, and in 2D rectangular samples of triangular lattice with 946 nodes (~30 ×30) and 1661 nodes (~40×40). In both models (6) and (7), we assign a set of random numbers n_{ij}, between 0 to 1, on each bond of the lattice in each realization. Then we remove the bonds for which $n_{ij}>p$ where p is decreased successively from unity. The boundary nodes are given fixed vector displacements corresponding to a macroscopic strain.[20] The interior nodes are then allowed to relax until zero force condition on the interior nodes is achieved. The forces on the surface nodes are then used to obtain the stress. Since the strain is given, we can easily compute the elastic moduli. The entire procedure is repeated for a number of realizations. Each realization, i.e., an entire sequence of p for one set of n_{ij}, required from 2 to 4 CPU hours on a VAX computer.

The exponents are then estimated from the slope of a log-log plot of K, N, etc., versus ϵ, $\epsilon=p-p_{cen}$ for the central force (see inset in Fig. 1 for an example), and $\epsilon=p-p_c$, for the isotropic case. The values of ϵ are chosen to be small enough ($\epsilon_{max}\sim 0.09$) to lie in the critical region, but large enough ($\epsilon_{min}\sim 0.03$ for 30×30) such that the coherence length $\xi_{cen}\sim\epsilon^{-\nu_{cen}}$ is smaller than L, the macroscopic size of the sample. As a first guess, we assume arbitrarily that the rigid-structure percolation incurring near p_{cen} is short range in nature, and thus ν_{cen} is taken as ν of the connectivity problem.[12] We have typically used ten realizations for calculating the K,N versus p relation, and the error bars in Eqs. (4) and (5) reflect fluctuations among various realizations. Choosing ϵ as we did seems to have circumvented the finite-size effects, for we find in 2D $f=2.3\pm0.4$ for 40×40 and $f=2.5\pm0.4$ for 30×30 lattices.

We use the known values of p_c to estimate t, as is customarily done.[9,10,12-17] We believe that the agreement between t for the model (3) calculated from our program and other known values[12-17] of t shows that neither the statistical nor the finite-size errors of our program are devastatingly great. The difference between f and t is outside the range of numerical error.

In the central-force model we do not know the precise values p_{cen}, and this compounds the error in estimating f. Since the value of f is so large, p_{cen} cannot be obtained very accurately from identifying the values of p where the moduli have become zero. We vary p_{cen} slightly until $\log K$ or $\log N$ versus $\log\epsilon$ best fits a straight line. The exact values of t are still being argued,[12-17] and there is certainly a need to improve our estimate of f.

It is this large difference between f and t, *much* beyond possible numerical errors, that makes us believe in the difference in the universality classes between the central-force elastic problem and the conduction problem.

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