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Position-space renormalization for elastic percolation networks with bond-bending forces

Shechao Feng
Schlumberger-Doll Research, P. O. Box 307, Ridgefield, Connecticut 06877 and Physics Department, Harvard University, Cambridge, Massachusetts 02138*

Muhammad Sahimi
Department of Chemical Engineering, University of Southern California, Los Angeles, California 90089-1211

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We develop a three-parameter position-space renormalization-group method and study the percolation properties of a two-dimensional elastic network in which *both* central and rotationally invariant bond-bending forces are present. The critical exponent f, which describes the power-law behavior of the elastic moduli near the percolation threshold, is estimated for a square network and is found to be consistent with recent estimates obtained by other methods.

There has recently been considerable interest in the problem of elastic properties of random networks near the percolation threshold. Until recently this problem was mostly viewed as analogous to the problem of electrical conductivity of percolating networks. de Gennes[1] discussed the relationship between the conductance, conductivity, and bulk modulus of a percolating network which is a simple model for gelation without solvent. He set out the explicit equations governing the behavior of the last two properties and pointed out that the bulk elastic modulus of a gel, modeled by a *nonrotationally invariant isotropic force constant,* is analogous to the electrical conductivity of the system. His intuitive argument resulted in some controversy,[2] but the controversy seems to have been settled by the scaling arguments of Yu, Chaikin, and Orbach[3] which is supportive of de Gennes's argument.

Feng and Sen[4] recently considered a different model, namely, the *central force* elastic percolating network model, and provided numerical evidence that the critical properties of this model belong to a new universality class than that of percolation conductivity problem. This model, which is basically a network of springs, is rotationally invariant, but suffers from a few peculiarities, as was pointed out by Feng, Sen, Halperin, and Lobb.[5] For simple cubic lattices at all dimensions the elastic threshold is $p_c = 1$. Thus a meaningful study of this problem is limited to certain lattices, e.g., triangular and fcc lattices. Another shortcoming of this model is that the significance of the straight-bond chains in transmitting elastic forces is ambiguous, because in a nonlinear model, the straight bonds could "buckle" under compression, but not under extension. An effective medium approximation[6] has also been developed for this model which correctly predicts that $p_c = 1$ for d-dimensional simple cubic networks of randomly occupied springs and provides very reasonable estimates of p_c for many other lattices.

In this Rapid Communication we study another rotationally invariant model for the elastic moduli of percolating networks. We study a model in which *both* central and bond-bending forces are included and develop a three-parameter position-space renormalization-group[7] (PSRG) method to estimate the critical exponent f which describes the power-law behavior of the elastic moduli of the system near the elastic threshold p_c. If K and N are the bulk and shear modulus of the network, respectively, we may write (as $p \to p_c$)

$$K, N \sim (p - p_c)^f \ . \tag{1}$$

The potential energy E of the network is given by

$$E = \tfrac{1}{2}\alpha \sum_{\langle ij \rangle} [(\mathbf{u}_i - \mathbf{u}_j)\cdot \mathbf{r}_{ij}]^2 g_{ij} + \tfrac{1}{2}\beta \sum_{\langle ijk \rangle} (\delta\theta_{jik})^2 g_{ij} g_{ik} \ , \tag{2}$$

where $\mathbf{u}_i$ and $\mathbf{u}_j$ are displacements of sites i and j and $\mathbf{r}_{ij}$ a unit vector from site i to site j. g_{ij} is a random variable which takes the values 1 and 0 with probabilities p and $q = 1 - p$, for bonds that are occupied and empty, respectively. The bond-bending forces between two occupied bonds ij and ik having site i in common are given in terms of the change in angle $\delta\theta_{jik}$ at site i, which is expressed in turn as a linear function of $\mathbf{u}_i$, $\mathbf{u}_j$, and $\mathbf{u}_k$. The sums are, respectively, over all bonds, and over all pairs of bonds with a site in common. This model is essentially the same as that of Kirkwood[8] who studied vibrational properties of rodlike molecules. Keating[9] studied the elastic properties of covalent crystals with essentially the same model. The only difference here is that we have included the bending of 180° bonds. Kantor and Webman[10] have recently studied the critical properties of this model by using "the nodes and links" model of percolation networks together with scaling arguments and have proposed that $f \geq 3.6$ at $d = 2$, while Feng *et al.*[5] and Bergman[5] have employed numerical simulations and finite-size scaling technique. An experimental study of hole-punched sheets by Benguigui[5] also gave $f \simeq 3.5$ at $d = 2$. The elastic threshold of this system can be easily shown to be the same as that of the ordinary bond percolation.[5,10]

Our PSRG method is similar to that developed for percolation conductivity[11] but with a few differences which we note. We use a standard H shape RG cell that has been used extensively in the past.[7] The basic idea is to develop *three* RG transformations to relate α, β, and p to their rescaled values α', β', and p'. Since the RG cell used here is self-dual, the recursion relation,[12] $p' = p^5 + 5p^4q + 8p^3q^2 + 2p^2q^3$, for the rescaled probability of occupied bonds reproduces the exact result, $p_c = \frac{1}{2}$. For the RG cell used here the displacements $\mathbf{u}_1 = (0, \Delta)$, $\mathbf{u}_2 = (0, \Delta)$, $\mathbf{u}_5 = (0, 0)$, and $\mathbf{u}_6 = (0, 0)$ of the exterior sites of the cell are held fixed (similar to the PSRG treatment of percolation conductivity

in which the voltages of the exterior sites of the RG cell are held fixed), where Δ is a constant. (We employ a RG cell of linear dimension $b=2$.) We replace the RG cell with one bond in each direction, so that the random variable g_{ij} takes the value of unity for the occupied bonds in the rescaled network with probability p'. For each direction one has to find all configurations that transmit elastic forces across the cell which in the present case is the same as that of simple geometric connection. To do this one has to solve the equations $\partial E/\partial \mathbf{u}_3 = \partial E/\partial \mathbf{u}_4 = 0$, for the displacements $\mathbf{u}_3$ and $\mathbf{u}_4$ of the internal sites of the RG cell.

The recursion relation for α' can be approximated by

$$p' \ln\alpha' = \sum_{i=1}^{n} a_i(p) \ln h_i(\alpha,\beta) \ , \tag{3}$$

where $a_i(p)$ is the probability of the spanning configuration i, $h_i(\alpha,\beta)$ its equivalent bond stretching, and n the total number of spanning configurations; $\sum a_i(p) = p'$. This equation is written in analogy with that of Bernasconi[11] for percolation conductivity. One may also use another approximation due to Stinchcombe and Watson[11]

$$p'\alpha' = \sum_{i=1}^{n} a_i(p) h_i(\alpha,\beta) \ . \tag{4}$$

Similar equations can be written for β'. For example, for the $b=2$ cell we obtain

$$p' \ln\alpha' = p^5 \ln\alpha + 4p^4 q \ln\alpha\left(\frac{\alpha+6\beta}{2\alpha+9\beta}\right) + p^4 q \ln\alpha + (6p^3q^2 + 2p^2q^3)\ln(\alpha/2) + 2p^3q^2 \ln\left(\frac{4\alpha\beta}{2\alpha+9\beta}\right) \tag{5}$$

if we use Eq. (3). Calculation of the recursion relation for β' is somewhat more complicated. The exterior sites of the RG cell are displaced as much as $\Delta/2$ in each direction. Thus, one has to have symmetric cell configurations in which both of rescaled bonds are present. Hence we find, by solving the associated equations which are similar to those for the calculations of α', that

$$p' \ln\beta' = p^5 \ln\beta + p^4 q \ln(5\beta/9) + 2p^3q^2 \ln(\beta/3) + (4p^4q + 6p^3q^2 + 2p^2q^3)\ln(\beta/9) \ . \tag{6}$$

We now let $r=\beta/\alpha$ and $r'=\beta'/\alpha'$ to obtain a single recursion relation of the form, $r' = F(p,r,\beta)$. This relation, at the fixed point β_c, has two stable fixed points at $p = p_c = \frac{1}{2}$, namely, $r=0$ and ∞ and one stable one at $r_0 = \frac{1}{66843}$, which is the relevant fixed point. At this point the eigenvalue of the linearized RG transformation is, $\lambda_r = \partial r'/\partial r = 0.875$ (evaluated at $p_c = \frac{1}{2}$), which means that after many iterations of the RG transformation the ratio r flows stably into the point r_0. In analogy with percolation conductivity,[11] we may write

$$\frac{f}{\nu} = -\frac{\ln\lambda_\alpha}{\ln b} \ , \tag{7}$$

where $\lambda_\alpha = \partial\alpha'/\partial\alpha$. Here ν is the exponent of the correlation length of percolation which is predicted by the RG transformation to be $\nu = \ln b/\ln\lambda_p$, where $\lambda_p = \partial p'/\partial p$, evaluated at the fixed point p_c and b is the linear dimension of the RG cell. To obtain λ_α one has to iterate the recursion relations for α' and β' (or equivalently for r') many times to reach the true fixed points of α and β (i.e., to obtain recursion relations for α' and β' whose shape would not change under further rescaling). In the present problem after many iterations we obtain $\lambda_\alpha \simeq 0.1617$, which means that

$$f \simeq 3.75 \ , \tag{8}$$

where we used $\nu \simeq 1.43$, the prediction of the PSRG transformation.[12] If we use the presumably exact value $\nu = \frac{4}{3}$, we obtain $f \simeq 3.5$. Both of these estimates are consistant with the recent estimate from simulations by Feng *et al.*,[5] $f \simeq 3.3 \pm 0.5$, and by Bergman,[5] $f \simeq 3.5 \pm 0.2$, and the experimental result of Benguigui[5] mentioned above.

We remark that the small value of the relevant fixed point r_0 is not a result of our PSRG method and has physical significance. Near p_c strongly bonded regions (the so-called blobs in the language of percolation) are connected by tenuous weak regions. The strong regions can be regarded as perfectly rigid, so the elastic properties near p_c are determined by the weak regions which are quasi one dimensional and thus can be modeled as tortuous chains. If $\beta >> \alpha$ (i.e., if $r_0 >> 1$) and for any fixed chain length, it will cost less energy to accomplish a displacement of the chain ends by adjusting the length of bonds parallel to the stress, rather than bending bond angles, so that the Young modulus Y of the system scales as $Y \sim (p-p_c)^t$. However, if the value of bond-bending force constant β is much smaller than that of the stretching-force constant α, the opposite is true and the behavior of the system crosses over to $Y \sim (p-p_c)^f$, i.e., the new universality class describing our model. Therefore, a reasonable RG procedure should yield $r_0 << 1$, as is the case here.

If we use the same procedure for the percolation conductivity exponent t and use the same RG cell, we obtain, $t \simeq 1.32$. This was first obtained by Bernasconi[11] and is only 1.5% larger than the most recent estimate,[13] $t \simeq 1.3$. We find it very satisfying that the present PSRG method predicts the elastic percolation exponent f to be much larger than the conductivity exponent t, consistent with other recent results.[4-6,10] For the *central force* elastic triangular network (i.e., a triangular network of springs), Feng and Sen[4] estimated that $f \simeq 2.4 \pm 0.4$. At this point, however, we cannot rule out the possibility that the central force problem and the bond-bending one belong to the same universality class or otherwise. We are currently carrying out extensive Monte Carlo simulations to estimate f more accurately for the simple spring model. The results will be reported elsewhere.[14] The universality class of these models can also be established by using the RG flow diagrams. Work in this direction will be reported elsewhere.[15] If we use Eq. (4) together with $\nu \simeq 1.43$, we obtain $f \simeq 3.5$. This is only about 6.7% less than our estimate using Eq. (3), which indicates that our PSRG is not very sensitive to the details of either method. With the presumably exact value $\nu = \frac{4}{3}$, Eq. (4) predicts that $f \simeq 3.26$, again consistent with numerical estimates mentioned above.

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*Present address.
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