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1990 J. Phys. A: Math. Gen. 23 2211

(http://iopscience.iop.org/0305-4470/23/11/042)

J. Phys. A: Math. Gen. **23** (1990) 2211-2216. Printed in the UK

COMMENT

On three-dimensional elastic percolation networks with bond-bending forces

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Received 14 June 1989, in final form 30 January 1990

Abstract. This is a comment on a recent paper by Jian Wang regarding the elastic energy of three-dimensional percolation networks with bond-bending forces. We give the details of the elastic energy that was used in our recent simulation of such systems and show that, contrary to Wang's claim, for a simple cubic network used in our study, our elastic energy is equivalent to that given by him, and is rotationally invariant. From the elastic energy of the system we also derive a rotationally invariant continuum representation of the system. The relation between this model and several other models that have previously been developed for studying elastic properties of disordered media is also clarified.

Elastic percolation models with various microscopic force laws have recently received considerable attention [1]. The central force (CF) [2] and the bond-bending (BB) models [3] are the two elastic percolation models which have been extensively studied in two dimensions [4-6], while the study of these two models in three dimensions has been very limited. In general, the elastic Hamiltonian of such systems is given by

$$H=\frac{\alpha}{2}\sum_{\langle ij\rangle} g_{ij}[(\boldsymbol{u}_i-\boldsymbol{u}_j)\boldsymbol{R}_{ij}]^2+\frac{\beta}{2}\sum_{\langle jik\rangle} g_{ij}g_{ik}(\delta\theta_{jik})^2 \tag{1}$$

where $\boldsymbol{u}_i$ is the displacement of site i, and $\boldsymbol{R}_{ij}$ a unit vector from i to j. Here, g_{ij} is a random variable which takes a non-zero value or 0 with probabilities p and $1-p$, respectively, and essentially represents the elastic constant of the bond ij, and α and β denote the CF and the BB force constants, respectively. The angular (or BB) force between occupied bonds ij and ik are given in terms of the change in the angle $\delta\theta_{jik}$ at site i.

Near the percolation threshold p_c the elastic moduli Y of the network obey the scaling law, $Y\sim(p-p_c)^f$, where f is a critical exponent. The most accurate numerical simulation of the BB model in two dimensions has yielded [5] $f\simeq 3.96\pm 0.04$, which totally supports the scaling relation [7, 8]

$$f=t+2\nu \tag{2}$$

between f and the critical exponent t which describes the conductivity σ of the network near p_c, $\sigma\sim(p-p_c)^t$, where ν is the exponent of correlation length ξ_p of percolation, $\xi_p\sim(p-p_c)^{-\nu}$; for two-dimensional systems one has $t\simeq 1.3$ and $\nu=4/3$. While earlier numerical simulations [9] had indicated that $f\simeq 1.45$ for the CF model in two dimensions, more recent and extensive simulations [10, 11] have strongly suggested

0305-4470/90/112211+06$03.50

that $f \simeq 3.9$ for the CF model in two dimensions, so that, as far as Y is concerned, the CF and BB models may belong to the same universality class in two dimensions. The situation for three-dimensional systems is not yet clear. Our recent large scale Monte Carlo simulations of the BB model in three dimensions [12] yielded $f \simeq 3.78$, which completely supports equation (2), where $t(d=3) \simeq 2$ and $\nu(d=3) \simeq 0.88$. However, in a recent letter Wang [13] discussed the BB model in three dimensions and presented a rotationally invariant expression for $\delta\theta_{jik}$, on which basis he claimed that the model which we used in our computer simulations [12] in three dimensions does not actually represent a true BB model, because our expression for $\delta\theta_{jik}$ was claimed to be non-rotationally invariant.

The purpose of this comment is to give the details of the elastic Hamiltonian that we used in our simulations [12] and show that, for a simple cubic network, it is equivalent to that given by Wang [13]. We then use our discrete elastic Hamiltonian and derive a rotationally invariant continuum representation for our system. The relation between this BB model and several other models of disordered elastic solids is then clarified.

In order to calculate the nodal displacements $\boldsymbol{u}_i$, one has to take into account the contributions to $\boldsymbol{u}_i$ of all bonds and all pairs of bonds in which i is a node of at least one of the bonds. One then determines the elastic energy H and minimises it with respect to $\boldsymbol{u}_i$ for every node i. Thus, one has to write down the equation of motion (EOM), $\partial H/\partial \boldsymbol{u}_i = 0$ for every i. Minimisation of the first sum on the right side of equation (1) with respect to $\boldsymbol{u}_i$ is straightforward and needs no explanation. However, the precise form of the second sum on the right side of equation (1) (the contribution of the BB forces) involves a pair of bonds and does require some explanation. In our simulations [12], for the BB term of equation (1), we considered two types of contributions, one coming from a pair of bonds in which i is the centre of the pair of bonds, and the other coming from a pair of bonds in which i is the end node of one of the bonds. This means that, for any i, the set of all bonds that have to be considered in the EOM is that shown in figure (1). For $p \simeq 1$, there are some clusters which can be deformed without any cost to the elastic energy. This is caused by the symmetry of the network. However, as $p \to p_c$, this symmetry is destroyed, and the deformation of *any* cluster of bonds, and the change in the angle between any pair of bonds costs some elastic energy. Therefore, the percolation threshold of our model coincides with that of ordinary percolation, $p_c \simeq 0.25$ for a simple cubic network (see also below). We now show that our elastic Hamiltonian is identical to that proposed by Wang [13] in the special limit of a simple cubic network.

Wang [13] has presented an expression for $\delta\theta_{jik}$ which, in our notation, is given by

$$\delta\theta_{jik} = \begin{cases} (\boldsymbol{u}_{ij} \times \boldsymbol{R}_{ij} - \boldsymbol{u}_{ik} \times \boldsymbol{R}_{ik})(\boldsymbol{R}_{ij} \times \boldsymbol{R}_{ik})/|\boldsymbol{R}_{ij} \times \boldsymbol{R}_{ik}| & \boldsymbol{R}_{ij} \text{ not } \| \text{ to } \boldsymbol{R}_{ik} \quad (3a) \\ |(\boldsymbol{u}_{ij} + \boldsymbol{u}_{ik}) \times \boldsymbol{R}_{ij}| & \boldsymbol{R}_{ij} \| \text{ to } \boldsymbol{R}_{ik} \quad (3b) \end{cases}$$

where $\boldsymbol{u}_{ij} = \boldsymbol{u}_i - \boldsymbol{u}_j$, whereas we had used [12]

$$(\delta\theta_{jik})^2 = |(\boldsymbol{u}_{ij} \times \boldsymbol{R}_{ij} - \boldsymbol{u}_{ik} \times \boldsymbol{R}_{ik})|^2 \quad (4)$$

for the case when $\boldsymbol{R}_{ij}$ is not parallel to $\boldsymbol{R}_{ik}$; when $\boldsymbol{R}_{ij}$ is parallel to $\boldsymbol{R}_{ik}$, our equation is identical to Wang's. In a simple cubic network, any two bonds are either perpendicular to each other, or are parallel with one another. Clearly, for the perpendicular bonds, $|\boldsymbol{R}_{ij} \times \boldsymbol{R}_{ik}| = 1$. Now consider the EOM, $\partial H/\partial u_x = 0$, in the x direction. Let $\boldsymbol{u}_i = (u_x, u_y, u_z)$ be the displacement vector for site i of the lattice. The location of i is identified by the indices l, m and n. We only consider the contribution of BB forces

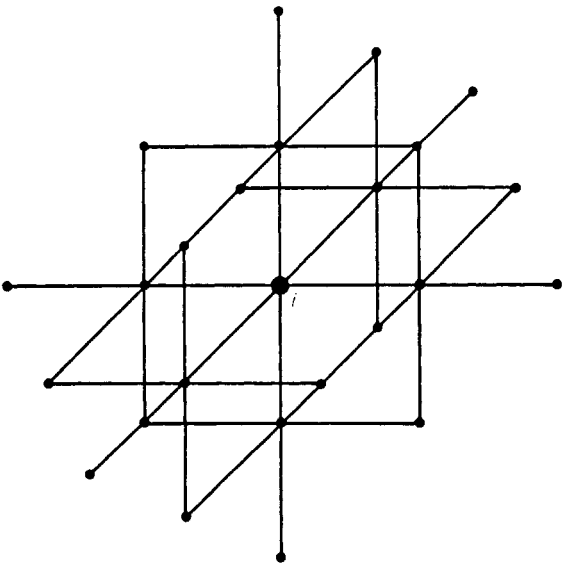

Figure 1. The set of all bonds that contribute to the determination of the displacement $\boldsymbol{u}_i$ of node i.

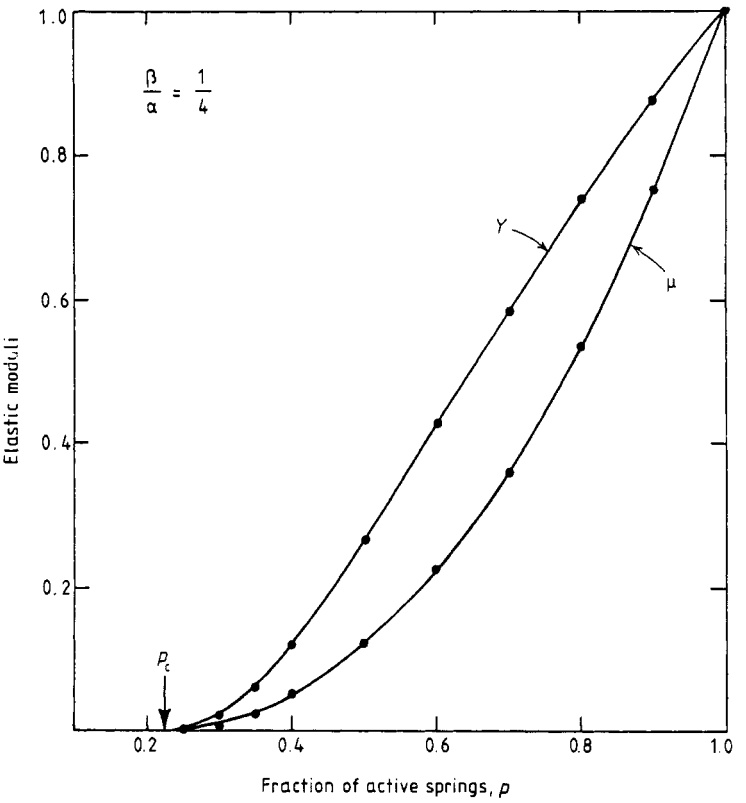

Figure 2. Young's modulus Y and shear modulus μ of a simple cubic network with $L = 20$ against the fraction p of active springs.

in the cluster of figure (2), i.e., $\partial(\delta\theta_{jik})^2/\partial u_x$, since the contribution of CF is straightforward and unambiguous. If we expand Wang's expression, equation (3*a*), to determine the contribution of BB forces to the EOM, we obtain, for a simple cubic lattice

$$\begin{aligned}\partial(\delta\theta_{jik})^2/\partial u_x = \beta(&u_y^{l+1,m+1,n} - u_y^{l-1,m-1,n} - u_y^{l-1,m+1,n} - u_y^{l+1,m-1,n} + u_z^{l+1,m,n+1} \\ &+ u_z^{l-1,m,n-1} - u_z^{l-1,m,n+1} - u_z^{l+1,m,n-1} + 4u_x^{l,m+1,n} + 4u_x^{l,m-1,n} \\ &+ 4u_x^{l,m,n+1} + 4u_x^{l,m,n-1} - 16u_x^{l,m,n}).\end{aligned} \tag{5}$$

On the other hand, for a pair of bonds in which i is the central node we used [12], $\delta\theta_{jik} = |(\boldsymbol{u}_{ij} \times \boldsymbol{R}_{ij} - \boldsymbol{u}_{ik} \times \boldsymbol{R}_{ik})|$, whereas for the pair of bonds in which i is the end node, we used $\delta\theta_{ijk} = |(\boldsymbol{u}_{ji} \times \boldsymbol{R}_{ji} - \boldsymbol{u}_{jk} \times \boldsymbol{R}_{jk})|$, keeping in mind that for this pair of bonds j is the central node. These configurations together make a contribution to the EOM which is identical to equation (5), i.e., Wang's expression. When the angle between the two bonds is 180°, we used a similar treatment. If i is the central node of the pair of bonds, $\delta\theta_{jik} = |(\boldsymbol{u}_{ij} \times \boldsymbol{R}_{ij} - \boldsymbol{u}_{ik} \times \boldsymbol{R}_{ik})| = |(\boldsymbol{u}_{ij} + \boldsymbol{u}_{ik}) \times \boldsymbol{R}_{ij}|$ (since $\boldsymbol{R}_{ij} = -\boldsymbol{R}_{ik}$), which is equivalent to equation (3*b*). Likewise, if i is the end node of one of the bonds, then, $\delta\theta_{jik} = |(\boldsymbol{u}_{ji} \times \boldsymbol{R}_{ji} - \boldsymbol{u}_{jk} \times \boldsymbol{R}_{jk})| = |(\boldsymbol{u}_{ji} + \boldsymbol{u}_{jk}) \times \boldsymbol{R}_{ji}|$ (since $\boldsymbol{R}_{ji} = -\boldsymbol{R}_{jk}$), which is again equivalent to equation (3*b*), considering that j is the central node of the pair of the bonds. We agree with Wang [13] that equations (3*a*) and (3*b*) are the most general expressions for the change in the angle between a pair of bonds in a three-dimensional network (because for all two-dimensional networks, the vectors $(\boldsymbol{u}_{ij} \times \boldsymbol{R}_{ij} - \boldsymbol{u}_{ik} \times \boldsymbol{R}_{ik})$ and $\boldsymbol{R}_{ij} \times \boldsymbol{R}_{ik}$ are always parallel regardless of the type of the network, whereas the same is not generally true for three-dimensional networks). However, for the BB model in a *simple cubic network* his equations are equivalent to those we used in our work [12].

We now derive a rotationally invariant continuum representation of the BB model that we used in our simulations [12]. We first consider a closely related system, the so-called Keating model [14], the Hamiltonian of which is given by

$$H = \frac{\alpha}{2} \sum_{\langle ij \rangle} g_{ij}[(\boldsymbol{u}_i - \boldsymbol{u}_j)\boldsymbol{R}_{ij}]^2 + \frac{\beta}{2} \sum_{\langle jik \rangle} g_{ij}g_{ik}(\boldsymbol{u}_{ij} \cdot \boldsymbol{R}_{ik} + \boldsymbol{u}_{ik} \cdot \boldsymbol{R}_{ij})^2. \tag{6}$$

For every cluster of bonds in a simple cubic network equations (1) and (6) are identical, except that the bending of 180° (collinear) bonds is not allowed in equation (6). He and Thorpe [15] employed this model to study the percolation and elastic properties of glasses, although f was not estimated. Gazis *et al* [16] utilised a variation of the model (see below) in their study of surface elastic waves in various crystals, while Mindlin [17] used a somewhat similar model to study disordered systems comprised of unconsolidated spherical grains under hydrostatic pressure. Consider now the EOM in the x direction equation for the Keating model, which is given by (assuming $g_{ij} = g_{ik} = 1$);

$$\begin{aligned}\alpha(&u_x^{l+1,m,n} + u_x^{l-1,m,n} - 2u_x^{l,m,n}) + \beta(u_y^{l+1,m+1,n} + u_y^{l-1,m-1,n} - u_y^{l-1,m+1,n} \\ &- u_y^{l+1,m-1,n} + u_z^{l+1,m,n+1} + u_z^{l-1,m,n-1} \\ &- u_z^{l-1,m,n-1} - u_z^{l+1,m,n-1} + 4u_x^{l,m+1,n} \\ &+ 4u_x^{l,m-1,n} + 4u_x^{l,m,n+1} + 4u_x^{l,m,n-1} - 16u_x^{l,m,n}) = 0.\end{aligned} \tag{7}$$

Equation (7) is valid for every node (except, possibly, for the boundary nodes) of a simple cubic lattice. This is precisely the equation that we used in our simulations [12], except that we also included the bending of collinear bonds. It is also identical to Wang's expression, for a simple cubic lattice, equation (3*a*) (compare equations

(5) and (7)). A similar equation was used by Gazis *et al* [16], except that in their model there is also a CF between every site and its second-nearest-neighbour nodes. All terms of equation (7) can be expressed in terms of difference operators. Thus, using Taylor's series, such difference operators can be expressed in terms of the partial derivatives of the continuous function $\boldsymbol{u}_i(x, y, z)$. Then, if we assume that the wavelengths of deformations are much longer than the lattice constant a, all but the second derivatives of $\boldsymbol{u}_i$ can be neglected. In the continuum limit, one obtains

$$(C_{11}-C_{12}-2C_{44})\sum_j \frac{\partial^2 u_j}{\partial x_j^2}\boldsymbol{e}_j + C_{44}[2\nabla(\nabla\cdot\boldsymbol{u})-\nabla\times(\nabla\times u)]+C_{12}\nabla(\nabla\cdot\boldsymbol{u})=\boldsymbol{0} \tag{8}$$

where $u_j = u_x$, u_y, u_z, $x_j = x$, y, z and $\boldsymbol{e}_j$ are the corresponding unit vectors in the x, y and z directions. Here $C_{11}=\alpha/a$, $C_{12}=0$ and $C_{44}=4\beta/a$ are the usual elastic (Lamé) constants of the lattice (in this case C_{11} is simply Young's modulus since $C_{12}=0$). If the CF between a neighbour and its second-nearest neighbour is not neglected, then $C_{11}=(\alpha+4\gamma)/a$, $C_{12}=2\gamma/a$ and $C_{44}=2(\gamma+2\beta)/a$, where γ is the stretching force constant between a site and its second-nearest neighbours. In this case, one has to include in equation (7) the appropriate terms representing the CF between node i and its second-nearest neighbours. As already mentioned, the only difference between the Keating and BB models is that, in the former model the bending of collinear bonds is not allowed. However, the bending of such bonds can be represented as a CF between a site and its second-nearest neighbour. Therefore, equation (8) is equally applicable to the BB model, except that, for the simple cubic network, the coefficient C_{12} would no longer be zero (although its value would be quite small). Clearly, equation (8) is rotationally invariant.

We should point out that equation (8) is very similar to that used by Schwartz *et al* [18] in their study of vibrational modes in granular media (see equation (5) of [18]). The main difference between equation (8) and theirs is that, similar to Mindlin [17], they also included the *torques* that arise as a result of the rotation of two contacting particles with respect to each other. Moreover, they did not include a CF between two contacting particles. Feng [19] has laready shown that the exponent f for this model in two dimensions is the same as that of the BB model, so that the inclusion of the torques does not change the scaling behaviour of the BB model.

Equation (8) is applicable to any percolation network in which the size L of the system is much larger than the correlation length ξ_p of percolation. Obviously, for such a system the elastic constants C_{11}, C_{12} and C_{44} would be dependent on p. If, however, $L \ll \xi_p$, the sample spanning percolation cluster is a fractal object, then we expect equation (8) to break down. This is similar to scalar transport (e.g., diffusion and hydrodynamic dispersion) in percolation networks, in which for $L \ll \xi_p$, one has anomalous transport that cannot be described by the usual continuum diffusion or convective diffusion equations (see Sahimi and Imdakm [20] and references therein).

We have also carried out Monte Carlo simulations on a cubic network with $L=20$ and have determined the elastic moduli of the network. In figure (2), we present Young's modulus Y and the shear modulus μ as a function of the fraction of active springs p. It is clear that, contrary to Wang's claim [13], all elastic moduli of the network vanish at the threshold of ordinary percolation.

We would like to thank Jian Wang for a useful correspondence. Partial support of this work by the National Science Foundation Grant No CBT 8615160, and the San Diego SuperComputer Centre is gratefully acknowledged.

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