LETTER TO THE EDITOR

The bond-bending model in three dimensions

Jian Wang

Department of Chemistry, Brandeis University, Waltham, MA 02254, USA

Abstract. We discuss the bond-bending model in three dimensions. We argue that for this model loops are very important in all length scales and the rigidity percolation is non-local, exhibiting similar behaviour to the central force model.

Recently, randomly diluted elastic networks have received much attention. Two rotational invariant models, the central force model [1] (CF model), and the bond-bending model [2] (BB model), i.e. the CF model plus an angular force term between nearest-neighbouring bonds, have been studied. The computer simulation of the CF model by Feng and Sen [1], Lemieux *et al* [3], Day *et al* [4] indicate that the geometrical (percolation) exponents are different from that of the random resistor network (RRN) (e.g. $\nu_{cen} = 1.05$ compared to $\nu = 1.34$ for percolation) and the bulk modulus exponent $f_{CF} = 1.4$ is different from the conductivity exponent $t = 1.30$. This suggests that the CF model belongs to a different universality class than that of RRN. Here if either the dynamical exponents or geometrical (percolation) exponents of the two systems are different, we consider them to belong to a different universality class. The simulation by Roux and Hansen [5], however, gives $f_{CF}/\nu_{CF} = 3.0$ which is about the same as f_{BB}/ν, where f_{BB} is the bulk modulus exponent for the BB model. This makes the CF model more interesting and controversial. The study of the BB model in two dimensions, on the other hand, is much more satisfactory. All the numerical results [6–8] agree with each other and indicate that the bulk modulus exponent f_{BB} is much larger than the conductivity exponent t. Hence people believe that the BB model belongs to a different universality class than that of the RRN, in the sense that they have different dynamical exponents.

The Hamiltonian of the BB model in two dimensions can be written as

$$H = \tfrac{1}{2}k_{CF}\sum_b |\boldsymbol{u}_b \cdot \hat{\boldsymbol{R}}_b|^2 \varepsilon_b + \tfrac{1}{2}k_{BB}\sum_{\langle bb'\rangle} |\boldsymbol{u}_b \times \hat{\boldsymbol{R}}_b - \boldsymbol{u}_{b'} \times \hat{\boldsymbol{R}}_{b'}|^2 \varepsilon_b \varepsilon_{b'} \tag{1}$$

where $\boldsymbol{u}_b = \boldsymbol{u}_{s_1} - \boldsymbol{u}_{s_2}$ is the displacement associated with a bond b (connecting points s_1 and s_2), $\boldsymbol{R}_b$ is a unit vector along the direction of bond b, ε_b is an indicator variable: $\varepsilon_b = 1$ if bond b is occupied and $\varepsilon_b = 0$ otherwise, and $\langle bb'\rangle$ indicates a sum over pairs of nearest-neighbouring bonds. Here k_{CF} and k_{BB} are spring constants.

The most accurate numerical value of bulk modulus exponent f_{BB} of the BB model in two dimensions by Zabolitzky *et al* [8] gives $f_{BB} = 3.96 \pm 0.04$. This leads people [6, 9–11] to conjecture that the relation

$$f_{BB} = t + 2\nu \tag{2}$$

for the BB model is exact, where $t = 1.30$ is the conductivity exponent, $\nu = \frac{4}{3}$ is the correlation length exponent for percolation.

In three dimensions, the experimental estimate of f_{BB} gives $f_{BB} = 3.8$ [12] and $f_{BB} = 3.9 \pm 0.2$ [13] which agree very well with equation (2) if one uses $t = 1.9$ and $\nu = 0.85$ in three dimensions. Most recently, Arbabi and Sahimi [14] have carried out a computer simulation using equation (1) in three dimensions. They found that $f_{BB} = 3.78$ which also agrees with equation (2). It raises questions as how to define a BB model in three dimensions and whether equation (2) is true for the BB model, etc. The main purpose of this letter is to address those questions.

Two expressions for the BB models have appeared in the literature, one being equation (1). The other is the so-called Keating model [15] (which has been used by He and Thorpe [16]):

$$H = \tfrac{1}{2}k_{CF}\sum_b |\boldsymbol{u}_b \cdot \hat{R}_b|^2 \varepsilon_b + \tfrac{1}{2}k_{BB} \sum_{\langle bb' \rangle}' |\boldsymbol{u}_b \cdot \hat{R}_{b'} + \boldsymbol{u}_{b'} \cdot \hat{R}_b|^2 \varepsilon_b \varepsilon_{b'} \tag{3}$$

where the prime means excluding the bending of $180°$ bonds.

In fact, these two models are related. The bond-bending energy of a pair of bonds A and B (figure 1) is $\tfrac{1}{2}k_{BB}(\Delta\theta_{AB})^2$, where $\Delta\theta_{AB}$ satisfies the equation

$$|\hat{R}_{12} + \boldsymbol{u}_{12}||\hat{R}_{13} + \boldsymbol{u}_{13}| \cos(\theta + \Delta\theta_{AB}) = (\hat{R}_{12} + \boldsymbol{u}_{12}) \cdot (\hat{R}_{13} + \boldsymbol{u}_{13}) \tag{4}$$

and $\cos\theta = \hat{R}_{12} \cdot \hat{R}_{13}$. For small displacement $\boldsymbol{u}$, we can expand equation (4) to get

$$(\hat{R}_{12} \cdot \boldsymbol{u}_{12} + \hat{R}_{13} \cdot \boldsymbol{u}_{13})\hat{R}_{12} \cdot \hat{R}_{13} - \sin\theta\, \Delta\theta_{AB} = \hat{R}_{12} \cdot \boldsymbol{u}_{13} + \hat{R}_{13} \cdot \boldsymbol{u}_{12}. \tag{5}$$

From equation (5) we see that equation (3) is good only when (i) $\hat{R}_{12} \cdot \hat{R}_{13} = 0$ and (ii) there is no stretch on the bonds A and B. Note that

$$(\boldsymbol{u}_{13} \times \hat{R}_{13} - \boldsymbol{u}_{12} \times \hat{R}_{12}) \cdot \frac{\boldsymbol{R}}{|\boldsymbol{R}|} = \frac{(\boldsymbol{u}_{13} \cdot \hat{R}_{12} + \boldsymbol{u}_{12} \cdot \hat{R}_{13})}{|\boldsymbol{R}|} - (\boldsymbol{u}_{13} \cdot \hat{R}_{13} + \boldsymbol{u}_{12} \cdot \hat{R}_{12})\frac{\hat{R}_{12} \cdot \hat{R}_{13}}{|\boldsymbol{R}|} \tag{6}$$

where $\boldsymbol{R} \equiv \hat{R}_{12} \times \hat{R}_{13}$. Here we have assumed that $|\boldsymbol{R}|$ is non-zero. From equations (5) and (6), we arrive at

$$\Delta\theta_{AB} = (\boldsymbol{u}_{13} \times \hat{R}_{13} - \boldsymbol{u}_{12} \times \hat{R}_{12}) \cdot \frac{\boldsymbol{R}}{|\boldsymbol{R}|}. \tag{7}$$

Thus in two dimensions, we have

$$|\Delta\theta_{AB}|^2 = |\boldsymbol{u}_{13} \times \hat{R}_{13} - \boldsymbol{u}_{12} \times \hat{R}_{12}|^2. \tag{8}$$

Equation (8) is a very clean expression for the BB model and it can also include the bending of $180°$ bonds. This expression also enables us [17] to map it to a RRN when the CF term is irrelevant. However, equation (8) is not rotationally invariant in three dimensions. For example, we can rotate the cluster in figure 1 around bond A. From equation (1), we see that it costs energy. One can also convince oneself by calculating the number of zero frequency modes N_0 of the clusters in figures 1 and 2, for which we found $N_0 = 4$ and 3 respectively. Hence for the cluster in figure 2, one has only three translational degrees of freedom and no rotational degrees of freedom. Thus the result of Arbabi and Sahimi [14] cannot be used as a check for equation (2).

In order to keep the Hamiltonian rotationally invariant, which is a physical requirement, we may write the Hamiltonian of the BB model in three dimensions as

$$H = \tfrac{1}{2}k_{CF}\sum_b (\boldsymbol{u}_b \cdot \hat{R}_b)^2 \varepsilon_b + \tfrac{1}{2}k_{BB} \sum_{\langle bb' \rangle} (\Delta\theta_{bb'})^2 \varepsilon_b \varepsilon_{b'} \tag{9}$$
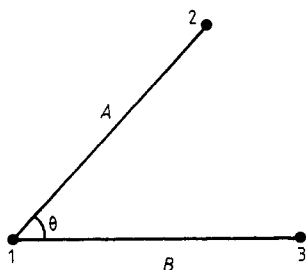
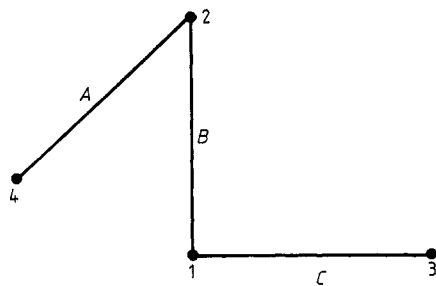**Figure 1.** The number of zero frequency modes of this cluster is 4 in three dimensions for equation (1).

Figure 2. A non-rigid cluster in three dimensions for the BB model.

where

$$\Delta\theta_{bb'} = \begin{cases} (\boldsymbol{u}_b \times \hat{R}_b - \boldsymbol{u}_{b'} \times \hat{R}_{b'}) \cdot \dfrac{\hat{R}_b \times \hat{R}_{b'}}{|\hat{R}_b \times \hat{R}_{b'}|} & \text{if } \hat{R}_b \text{ is not parallel to } \hat{R}_{b'} \\ |(\boldsymbol{u}_b + \boldsymbol{u}_{b'}) \times \hat{R}_b| & \text{if } \hat{R}_b \text{ is parallel to } \hat{R}_{b'} \end{cases} \quad (10)$$

where the last part comes from expansion of the following equation:

$$|\hat{R}_{12} + \boldsymbol{u}_{12}||\hat{R}_{13} + \boldsymbol{u}_{13}| \sin(\theta + \Delta\theta_{AB}) = |(\hat{R}_{12} + \boldsymbol{u}_{12}) \times (\hat{R}_{13} + \boldsymbol{u}_{13})|. \quad (11)$$

This is an appropriate Hamiltonian to discuss the elastic property of the three-dimensional BB model, e.g. the elastic property of a three-dimensional covalent network [18].

For the Hamiltonian defined in equation (9) the cluster in figure 2 is not rigid, because one can twist bonds A and C freely. As a result the rigidity threshold p_{rigid} should be higher than the percolation threshold p_c. A constraint counting method [19], which works surprisingly well in estimating p_{rigid} of the CF model [20], by Phillips and Thorpe predicts $p_{\text{rigid}} \sim 0.4$ for the cubic lattice for the three-dimensional BB model. This should be compared with $p_c \sim 0.25$. One should notice that the rigidity percolation of the three-dimensional BB model is very similar to that of the CF model. From equation (10), a chain having 180° bonds (a straight line) is rigid. Thus we can always renormalise a straight line to a single bond. Due to the fact that the cluster in figure 2 is non-rigid, a renormalised linear chain having more than two bonds is non-rigid. In other words, any cluster containing a singly connected bond (which is not a dangling bond; see figure 3) is non-rigid. As a consequence, a rigid cluster must at least be a biconnected cluster. In figure 4, we give an example of a biconnected cluster that is non-rigid, since plaquettes A and B can move freely without changing the angles. In order to make the cluster rigid, we need more loops in all length scales which is
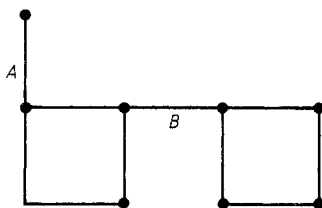

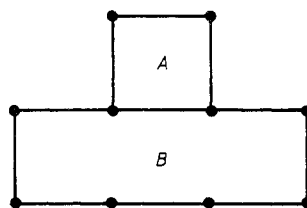**Figure 3.** A non-rigid cluster with a singly connected bond B, where A is a dangling bond.

Figure 4. A non-rigid biconnected cluster, where plaquettes A and B are not rigid connected.

reminiscent of the CF model [4]. Given a cluster one cannot tell whether it is rigid or not without looking at the whole cluster. We believe that non-locality of the rigidity percolation of the three-dimensional BB model is sufficient to change the universality class and expect that it belongs to a different universality class from that of ordinary percolation.

In order to make p_{rigid} of the BB model coincide with p_c, one needs to consider a diamond lattice with third-nearest-neighbour interaction. (Note that one needs infinitely long-range interaction to bring p_{rigid} down to p_c for a cubic lattice.) Actually, in the study of biophysics, the Hamiltonian which contains a CF term, BB term, torsion (third-nearest-neighbour interaction for the peptide plane) has been widely used (e.g. [21]) in molecular dynamics simulations, where the double helix is basically of diamond structure. This Hamiltonian would be the model to test equation (2) in three dimensions. Another possible model to look at would be the disc model proposed by Feng [22]. The advantages of working on this model are twofold. Firstly, it can be treated theoretically [23] because it contains only two-body interaction, unlike the BB model. Note that since the superelastic bulk modulus exponent S is found to be different for the disc model [22] ($S = 1.02$) and the BB model [24] ($S = 1.30$)†, it is worthwhile to study the disc model in more detail. Secondly, the BB model can be obtained by integrating out the angular part θ from the disc model, i.e.

$$\exp(-H_{BB}) = \int (D\theta) \exp(-H_{disc}) \tag{12}$$

where the integration is straightforward. Here one should extend the range of θ to infinity and let $\beta = \gamma$ in the disk model (see [22] for details of the disc model). Hopefully, equation (12) would help us to set up a field theory for the BB model.

One should also notice that a lattice-of-beams model [26] can also be formulated. In this model, each site is defined as a rigid solid with $d(d+1)/2$ degrees of freedom in a d-dimensional space, and the energy is the most general quadratic form, built with the displacements of the two ends of each bond, that satisfies the rotational invariance requirements.

In summary, we have pointed out that equation (1) is not rotationally invariant in three dimensions and the lack of rotational invariance of equation (1) invalidates the simulation result of Arbabi and Sahimi [14]. We have discussed the generalisation of equation (1) in three dimensions. We also argued that for the three-dimensional BB model, loops are very important in all length scales and the rigidity percolation is non-local, as observed for the CF model. Hence, we expect that the rigidity percolation of the three-dimensional BB model belongs to a different universality class from that of the ordinary percolation.

References

[1] Feng S and Seng P N 1984 *Phys. Rev. Lett.* **52** 216
[2] Kantor Y and Webman I 1984 *Phys. Rev. Lett.* **52** 1891

† See [25] for a discussion of the difference in S between the BB and granular disc models.

[3] Lemieux M A, Breton P and Tremblay A M S 1985 *J. Physique Lett.* **46** L1
[4] Day A R, Tremblay R R and Tremblay A M S 1986 *Phys. Rev. Lett.* **56** 2501
[5] Roux S and Hansen A 1988 *Europhys. Lett.* **6** 301
   Hansen A and Roux S 1988 Universality class of central force percolation *Preprint*
[6] Feng S C, Sen P N, Halperin B I and Lobb C J 1984 *Phys. Rev.* B **30** 5386
[7] Bergman D J 1985 *Phys. Rev.* B **31** 1696
[8] Zabolitzky J G, Bergman D J and Stauffer D 1986 *J. Stat. Phys.* **44** 211
[9] Harris A B and Lubensky T C 1986 unpublished
[10] Roux S 1986 *J. Phys. A: Math. Gen.* **19** L351
[11] Sahimi M 1986 *J. Phys. C: Solid State Phys.* **19** L79
[12] Deptuck D, Harrison J P and Zawadzki P 1985 *Phys. Rev. Lett.* **54** 913
[13] Woignier T, Phalippou J, Sempere R and Pelous J 1988 *J. Physique* **49** 289
[14] Arbabi S and Sahimi M 1988 *Phys. Rev.* B **38** 7173
[15] Keating P N 1966 *Phys. Rev.* **152** 774
[16] He H and Thorpe M F 1985 *Phys. Rev. Lett.* **54** 2107
[17] Wang J and Harris A B 1988 *Europhys. Lett.* **6** 615
   Wang J, Harris A B and Lubensky T C 1988 unpublished
[18] Phillips J C 1982 *Solid State Phys.* **37** 93
   Thorpe M F 1983 *J. Non-cryst. Solids* **57** 355
[19] Phillips J C and Thorpe M F 1985 *Solid State Commun.* **53** 699
[20] Feng S, Thorpe M F and Garboczi E 1985 *Phys. Rev.* B **31** 276
[21] Sung S and Jordan P C 1987 *Biophys. J.* **51** 661
[22] Schwartz L M, Johnson D L and Feng S 1984 *Phys. Rev. Lett.* **52** 831
   Feng S 1985 *Phys. Rev.* B **32** 510
[23] Wang J 1989 *J. Phys. A: Math. Gen.* **22** in press
[24] Bergman D J 1985 *Phys. Rev.* B **33** 1671
[25] Limat L 1988 *Phys. Rev.* B **38** 7219
[26] Roux S and Guyon E 1985 *J. Physique Lett.* **46** L999