## John Carroll University

From the SelectedWorks of Anthony Roy Day

June 9, 1986

## Rigid backbone: A new geometry for percolation

Anthony Roy Day, *John Carroll University* R. R. Tremblay A.-M. S. Tremblay



Available at: https://works.bepress.com/anthony\_day/11/

## **Rigid Backbone:** A New Geometry for Percolation

A. R. Day, R. R. Tremblay, and A.-M. S. Tremblay

Département de Physique et Centre de Recherche en Physique du Solide, Université de Sherbrooke, Sherbrooke, Québec J1K 2R1, Canada (Received 26 December 1985)

It is shown that the diluted two-dimensional central-force problem belongs to a new class of percolation problems. Geometric properties such as the fractal dimension of the backbone, the correlation-length exponent, and the connectivity are completely different from those of previously studied percolation problems. Explicit calculations of the backbone and the construction of an algorithm which identifies the infinite rigid cluster clearly demonstrate the absence of singly connected bonds, the overwhelming importance of loops, and the long-range nature of the rigidity.

PACS numbers: 64.60.Cn, 05.70.Jk, 62.20.-x, 63.70.+h

The percolation model<sup>1</sup> has, for a number of years, been a source of insight into many diverse physical phenomena.<sup>2</sup> Recently, it has been employed to understand elastic properties of tenuous media such as gels,<sup>3,4</sup> sinters,<sup>5</sup> or even certain glasses.<sup>6,7</sup> It was originally suggested by de Gennes<sup>3</sup> in the polymer context that the critical properties of the elastic moduli at the percolation threshold would be the same as those of the conductivity. It has become evident, however, that this is not generally true,<sup>8-10</sup> one of the reasons lying in the different tensorial character of the problem.

Recent work has concentrated on two models of elasticity percolation, the bond-bending model<sup>9,11</sup> and the central-force model.<sup>8,12</sup> It has become clear that they have different critical elastic behavior but the full nature of this difference and its underlying causes have not yet been generally appreciated. In this Letter we address this issue: We present the first analysis of the geometry of the percolating rigid clusters for the two-dimensional central-force model. While the backbone geometry of the bond-bending universality class is the same as that of ordinary percolation,<sup>9</sup> we show here that for the central-force model, the geometry is both quantitatively and qualitatively different. We compute the backbone fractal dimension<sup>13, 14</sup> to exhibit a quantitative difference and present graphic and algorithmic evidence which show qualitative differences such as the absence of singly connected bonds, the importance of loops, and the essentially long-range nature of elastic connectivity.

The best-understood model for elasticity percolation is the so-called bond-bending model.<sup>9,11</sup> That model is the simplest realization of a general class of models<sup>15</sup> where geometric connection implies elastic connection. For these models the threshold,  $p_c$ , and the percolation critical exponents  $\beta_p$ ,  $\nu_p$ ,  $\gamma_p$ , and  $\alpha_p$  are identical to those of the equivalent geometric problem. "Dynamic" exponents, however, depend on the problem: Namely, the exponent f which governs the elastic moduli is different from the exponent t which governs the conductivity. Nevertheless, the basic physics which controls these exponents can be readily understood in both cases from the "nodes-linksblobs" picture<sup>14</sup> of percolation clusters. In fact, it is fair to say that in the vast majority of percolation problems encountered to date, even continuum percolation,<sup>16</sup> the basic geometric features of the percolation clusters, such as the scaling of the number of singly connected bonds, are identical and the differences arise only at the level of the "dynamics."

For the class of models of interest here, however, geometric connection (the existence of a bond) does not imply complete elastic connection because the number of constraints associated with the existence of a bond is smaller than the number of degrees of freedom associated with the sites it connects. The percolation threshold is higher<sup>8</sup> than that of the corresponding standard percolation problem. Thorpe<sup>6</sup> has suggested the name "rigidity percolation" for this class of models, distinguishing it from the "elasticity percolation" universality class mentioned above. In this paper, we study the simplest rigidity-percolation model, namely the two-dimensional central-force model.<sup>8</sup> Extensions to other models that are of more physical significance are discussed in the conclusion.

*Model.*—The central-force Hamiltonian depends on the Euclidean distances between sites and hence is in general a nonlinear function of the coordinates. We study here the linear-response limit of this Hamiltonian on a random triangular net of unit masses and springs,

$$H = \frac{1}{2} \sum_{ij} k_{ij} [(\mathbf{u}_i - \mathbf{u}_j) \cdot \hat{\mathbf{r}}_{ij}]^2, \qquad (1)$$

where  $k_{ij}$  equals k = 1 with probability p and vanishes with probability 1 - p,  $\mathbf{u}_i$  is the displacement at site *i*, and  $\hat{\mathbf{r}}_{ij}$  is a unit lattice vector between sites *i* and *j*. This model was first studied numerically by Feng and Sen<sup>8</sup> using a relaxation technique. They found a critical probability  $p_{cen} = 0.58$  and an exponent f = 2.4 $\pm 0.4$ . Later, extensive simulations using an exact transfer-matrix technique on long strips<sup>12</sup> and finitesize scaling have found  $p_{cen} = 0.65 \pm 0.005$ ,  $\nu_{cen} = 1.05$  $\pm 0.15$ , and  $f = 1.4 \pm 0.2$ . The values for  $p_{cen}$  and for the correlation length exponent  $\nu_{cen}$  have been independently confirmed.<sup>17</sup> The value of  $f/\nu_{cen}$  is also confirmed in the present work. Note that the value of  $v_{cen}$  is significantly different from the usual percolation result  $v = \frac{4}{3}$  suggesting, but not proving, some differences at the geometric level.

Simulations for the backbone.-We perform simulations on rectangular sections of triangular nets, containing  $L \times L$  unit triangles.<sup>18</sup> We work at  $p = p_{cen}$  and apply a macroscopic strain to the boundaries, minimizing the energy with a conjugate gradient technique. For example, the elastic constant  $C_{11}$  is obtained from the total elastic energy resulting from a displacement of rigid bus bars at the top and bottom boundaries with sites on the fixed vertical boundaries constrained to move vertically. We are interested in the strain in each bond. For that purpose, unacceptable numerical errors accumulate unless calculations are performed with 64-bit (quadruple precision) accuracy. 32-bit accuracy also gives acceptable results if the conjugate gradient is iterated beyond its theoretical limit for exact matrix inversion.<sup>19</sup> This accumulation of errors is probably related to the loop structure of the rigid backbone, which we discuss below, and may explain why the original relaxation method of Feng and Sen<sup>8</sup> was inaccurate. Sizes L = 10 to 28 are considered. Calculation times per sample range from 8 s for L = 10 to 300 s for L = 28 on an IBM 4381 computer.

*Rigid backbone.*—Results for the bond-strain distribution of the L = 12 samples are displayed as a histogram in Fig. 1. The distribution has two peaks, one centered approximately around the applied strain per bond and the other one at zero strain. The bonds in the first peak are identified as being on the rigid backbone. Except for a few bonds near the boundaries, the bonds belonging to the rigid backbone are the same when boundary conditions are changed to compute

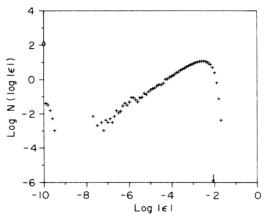


FIG. 1. Histogram for logarithm of the number of bonds N having a strain  $\epsilon$  within equally spaced logrithmic intervals of 0.1. The data point (lozenge) at  $\epsilon = 10^{-10}$  is the number of bonds with a strain  $\epsilon \le 10^{-10}$ . The data are for L = 12 and  $p = p_{cen} = 0.65$ . The arrow indicates what the strain in each bond would be at p = 1.

other elastic moduli. We find also that the distribution of local strains is independent of the bond orientation in contrast to the situation at p=1 where the bonds orthogonal to the applied strain stay unstretched: This statistical isotropy near the percolation threshold is completely analogous to the situation encountered in ordinary percolation.  $N_B$ , the number of strained bonds, is evaluated for a few hundred sample realizations of size L = 10 to L = 28. The fractal dimension of the backbone  $\overline{d}_{BB} = 1.94^{+0.06}_{-0.1}$  is obtained directly from the plot in Fig. 2 of  $\log_{10} N_B$  versus  $\log_{10} L$ . This result should be contrasted to the usual percolation result<sup>20</sup>  $\overline{d}_{BB} = 1.62 \pm 0.02$  which indicates that the rigid backbone is much more compact than the usual one.  $\overline{d}_{BB}$  for the rigid backbone is in fact close to the upper bound  $\overline{d}_{BB} = 2$ . Figure 2 also shows a log-log plot of the average elastic modulus  $C_{11}$  vs L. The slope gives  $f/v_{cen} = 1.35 \pm 0.1$  which is consistent with the result of Lemieux, Breton, and Tremblay,<sup>12</sup>  $f/v_{cen} = 1.35$  $\pm 0.25.$ 

Figure 3 displays a typical realization of the rigid backbone. We have explicitly checked that the unstrained bonds (dotted lines) can be removed without affecting the rigidity of the structure. At first sight, the presence of many single-thickness strands may seem surprising but they are a feature of the linearized Hamiltonian Eq. (1). The response in the linear problem is the same under tension and compression: Clearly, single-thickness strands have an elastic modulus under tension and so in the linear problem these strands are part of the rigid backbone. Note that these are not singly connected bonds: They always occur in "parallel" with other bonds to form the rigid backbone (sometimes the boundaries play the role of the parallel bonds). In the nonlinear problem, these strands are unstable under compression, while in the linear model, they are unstable to forces other than those applied at the boundaries (e.g., gravity).

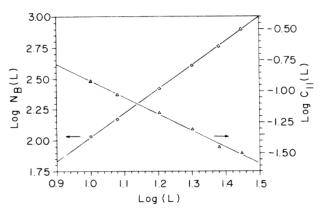


FIG. 2. Plotted against  $\log L$ , on the left-hand logarithmic vertical scale, the number of bonds on the backbone  $N_B$  (lozenges), and on the right-hand logarithmic scale, the elastic modulus  $C_{11}$  (triangles).

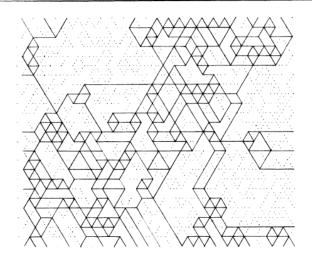


FIG. 3. Typical realization of the backbone for the linearized central-force problem on the random triangular net at  $p = p_{cen} = 0.65$ . Dots between sites indicate occupied but unstressed bonds.

The most important feature of the rigid backbone is that there are no singly connected bonds which carry all the stress in contrast with the bonds that carry all the current in the random resistor network. The backbone consists of loops and, as we show below, loops appear on all length scales.

Infinite rigid cluster.—The following algorithm sheds light on the structure of the rigid spanning cluster (including dangling ends).<sup>21</sup> By a rigid cluster, we mean a set of sites which, under any conceivable applied force, are completely rigidly connected by bonds, i.e., which satisfy the Maxwell condition<sup>22</sup>  $f - c - 3 \le 0$ , where fis the number of degrees of freedom, i.e., twice the number of connected sites, and c the number of constraints (which in general differs from the number of bonds).

We first generate a set of occupied bonds which is then scanned for rigidity by the following iterative procedure. We start with the basic rigid unit, a bond, and look for adjacent bonds forming the simplest rigid cluster, a triangle. At first, the rigid cluster grows locally by forming triangles, that is by annexing pairs of bonds<sup>23</sup> that form a closed loop from the rigid cluster back to the rigid cluster. Possible realizations are shown in Figs. 4(a) and 4(b). When the rigid cluster can no longer grow in this manner, it becomes a single generalized rigid part and other adjacent but not yet rigidly connected clusters start to grow independently by the same rule.<sup>24</sup> When that process is complete, it is repeated with the generalized rigid parts as basic units; i.e., triangles made up of the generalized rigid parts are found as in Fig. 4(c). The rigidity property of a cluster is a property of the whole cluster and is very different from the connectivity property of ordinary percolation. To illustrate what we mean, consider cut-

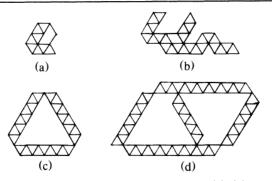


FIG. 4. Some examples of rigid clusters. (a), (b) Clusters that would be found at the first level of iteration. (c) "Generalized triangle" found at the second level of iteration. (d) More complicated loop structure that is missed by the triangle rule.

ting any one bond in Fig. 4(c): The cluster is reduced to four rigid clusters. In ordinary percolation cutting one bond can at most divide a cluster into two parts. These observations are consistent with a growth of the backbone above threshold which is more rapid (smaller value of  $\beta/\nu = d - \overline{d}_{BB}$ ) in the rigidity problem than in ordinary percolation.

It is quite possible *a priori* that elasticity percolation is controlled by the clusters found at the first level of iteration and that loop structures like those of Fig. 4(c)are irrelevant. To test if this is the case, we used the scaling technique of Kirkpatrick<sup>13</sup> to calculate the critical probability for rigidity percolation using only the clusters found at the first level. We found  $p_c$ =  $0.745 \pm 0.01$ . We then used the same scaling technique to find the critical probability for rigidity percolation using the clusters found by iterating the triangle rule on all length scales. We found  $p_c = 0.70$  $\pm 0.01$ , clearly indicating the importance of loops. This  $p_c$  is still larger<sup>25</sup> than  $p_{cen}$  for two reasons. The first is that our algorithm only includes the simplest loop structures and misses higher-order loops such as that of Fig. 4(d). The second reason is that singlethickness strands of bonds do not satisfy the Maxwell condition. As is clear from Fig. 3, these are an important part of the backbone. Despite the latter difference between the rigid backbone and the infinite rigid cluster as defined here, we expect that both have the same qualitative loop structure.

In conclusion, we have shown that rigidity percolation in the central-force model introduces a qualitatively new type of percolation problem. In this problem, "connectivity" is not local but long range and loops on all length scales are the most important feature of the percolating clusters in the sense that they provide the rigid structure. The fact that triangles on all length scales (or more generally loops) provide the rigidity clearly demonstrates that the central-force model does not renormalize into the bond-bending model as has been suggested earlier by other groups. These new types of percolation clusters are clearly an interesting theoretical problem but this problem would be of limited physical applicability if it only occurred in the two-dimensional central-force model. However, the long-range nature and the loop structure (or higher-dimensional generalization thereof) of the clusters is most likely a general feature of all elasticity percolation problems where the bonds introduce less than d constraints per bond in d dimensions. Phillips and Thorpe<sup>7</sup> have suggested that chalcogenide glasses of the type  $Ge_xS_{1-x}$  are a physical realization of such a rigidity percolation problem because of the weakness of the energy associated with the dihedral angle.

We are indebted to Professor M. F. Thorpe for numerous useful suggestions and encouragment and to J. P. Dussault for mathematical advice. One of us (A.-M.S.T.) also benefitted from discussions with J. C. Angles-d'Auriac, J. P. Clerc, L. Puech, and R. Rammal. One of us (R.R.T.) thanks the Natural Sciences and Engineering Research Council (NSERC) for a Science 1967 predoctoral fellowship. The work of another of us (A.-M.S.T.) is supported by the program "Attaché de recherche" and by an individual operating grant from NSERC. Funds from the "Fonds FCAR" Québec are gratefully acknowledged. Computing time was provided by Université de Shebrooke. NSERC and the Atmospheric Environment Service provided access to the Cray computer in Dorval.

<sup>1</sup>Percolation Structures and Processes, edited by G. Deutscher, R. Zallen, and Joan Adler, Annals of the Israel Physical Society Vol. 5 (Hilger, Bristol, 1983).

<sup>2</sup>R. Zallen, in Ref. 1, p. 3.

<sup>3</sup>P. G. de Gennes, J. Phys. (Paris), Lett. **37**, L1 (1976).

<sup>4</sup>S. Alexander, J. Phys. (Paris) **45**, 1939 (1984).

<sup>5</sup>D. Deptuck, J. P. Harrison, and P. Zawadski, Phys. Rev. Lett. **54**, 913 (1985).

<sup>6</sup>M. F. Thorpe, J. Non-Cryst. Solids **57**, 355 (1983).

<sup>7</sup>J. C. Phillips and M. F. Thorpe, Solid State Commun. 53,

699 (1985); H. He and M. F. Thorpe, Phys. Rev. Lett. 54, 2107 (1985).

<sup>8</sup>S. Feng and P. N. Sen, Phys. Rev. Lett. **52**, 216 (1984).

<sup>9</sup>Y. Kantor and I. Webman, Phys. Rev. Lett. **52**, 1891 (1984).

<sup>10</sup>D. J. Bergman and Y. Kantor, Phys. Rev. Lett. **53**, 571 (1984).

<sup>11</sup>S. Feng, P. N. Sen, B. I. Halperin, and C. J. Lobb, Phys. Rev. B **30**, 5386 (1984).

 $^{12}$ M. A. Lemieux, P. Breton, and A.-M. S. Tremblay, J. Phys. (Paris), Lett. **46**, L1 (1985).

<sup>13</sup>S. Kirkpatrick, in *Ill-Condensed Matter*, edited by R. Balian, R. Maynard, and G. Toulouse, Les Houches Summer School Proceedings Vol. 31 (North-Holland, Amsterdam, 1979).

<sup>14</sup>R. Pike and H. E. Stanley, J. Phys. A **14**, L-169 (1981); A. Coniglio, Phys. Rev. Lett. **46**, 250 (1981).

<sup>15</sup>L. M. Schwartz, S. Feng, M. F. Thorpe, and P. N. Sen, Phys. Rev. B **32**, 4607 (1985).

<sup>16</sup>W. T. Elam, A. R. Kerstein, and J. J. Rehr, Phys. Rev. Lett. **52**, 1516 (1984).

<sup>17</sup>M. Sahimi and J. D. Goddard, Phys. Rev. B **32**, 1869 (1985).

<sup>18</sup>The case p = 1 can be used to check that this corresponds to having a single external length scale in the problem.

<sup>19</sup>F. G. Ciarlet, Introduction à l'Analyse Numérique et à l'Optimisation (Masson, Paris, 1982), p. 200.

<sup>20</sup>L. Puech and R. Rammal, J. Phys. C **16**, L1197 (1983); H. J. Herrmann and H. E. Stanley, Phys. Rev. Lett. **53**, 1121 (1984).

<sup>21</sup>The backbone cannot easily be defined within an algorithm which counts the number of constraints.

<sup>22</sup>M. F. Thorpe, in *Physics of Disordered Materials*, edited by D. Adler, H. Fritzsche, and S. R. Ovshinsky (Plenum, New York, 1985).

<sup>23</sup>Single bonds connecting back to the cluster are obviously included.

<sup>24</sup>Note that in this scheme, the bus bars are considered as generalized rigid parts.

<sup>25</sup>We expect that the thresholds of the various models should be found in the following order of increasing p (with  $0.649 \le p \le 0.70$ ): linear model, nonlinear model under extension, nonlinear model under compression, constraintcounting algorithm (equivalent to no zero-frequency modes). Some of these thresholds may also be equal.