

ENERGETIC AND ENTROPIC ELASTICITY OF THE SIERPIŃSKI GASKET

Yacov KANTOR

School of Physics and Astronomy, Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University,
Tel Aviv 69978, Israel

Two complementary (energetic and entropic) models of the problem of elasticity on the Sierpiński gasket are compared and discussed. Both models are known to exhibit a power-law scaling of the elastic constants. These results are compared with the properties of random systems, and it is shown that the Sierpiński gasket is significantly more stable than a "typical" random system. In the energetic elasticity model the elastic constants decay very slowly with increasing length scale while in the entropic elasticity model the excluded-volume effects are able to stabilize the shape of the gasket, i.e. its relative shape fluctuations decay with increasing system size.

1. Introduction

In recent years there has been a renewed interest in the elastic properties of inhomogeneous materials. In many such systems one can identify a correlation ξ , above which the material can be treated as homogeneous. The linear elastic response of *homogeneous* solids is characterized by the elastic stiffness tensor C_{ijkl} . This tensor is simply related to the volume and shape dependence of the free energy F of the solid [1]: $C_{ijkl} = (1/V) \partial^2 F / \partial \epsilon_{ij} \partial \epsilon_{kl}$, where V is the volume of the system, while ϵ_{ij} is the applied strain. At finite temperature T , both the energy U and the entropy S contribute to the shape dependence of $F = U - TS$. For the purpose of the theoretical research one can *roughly* divide the inhomogeneous systems into two groups: (a) Materials whose elementary grains are very large will belong to the *energetic elasticity* group. The weakly compacted sandstone is a typical member of such a group. Under applied external distortion the entropy of these materials remains unchanged, and the change in the free energy F can be attributed to the increase in the energy U . (b) Materials consisting of very small "building blocks", e.g. polymeric systems such as rubbers and gels [2], belong to the *entropic elasticity* group. The distortion of a polymeric network reduces the available phase space thus de-

creasing the entropy of the system and increasing its free energy [3].

The "borderline" between the two groups is not sharp, and depends on such properties as grain size, geometry and temperature. One may quantify the difference between the types of the systems by comparing their relative fluctuations [4].

Frequently, at length scales $L < \xi$ the geometrical properties of the systems can be characterized by a fractal dimension d_f [5] which relates the mass N of the object to its linear size L : $N \sim L^{d_f}$. In the fractal regime one may expect a power-law dependence on length of the various physical properties such as resistance or force constants. These power laws can be used to infer the properties on length scales $L > \xi$ by assuming a smooth crossover from the fractal regime to a homogeneous regime. In some cases, such as colloidal aggregates [6,7] there is no crossover to the homogeneous regime, and the fractal behavior is limited by the finite size of the aggregate. In these systems one directly measures the length-scale dependence of the elastic properties [7]. The theoretical analysis of the vibrations in the fractal regime led to the discovery [8] of modes denoted "fractons", with a peculiar power-law scaling of the density of states. More recently, these states have been observed experimentally [9].

In this paper, I compare several approaches [10–12] to the elasticity of a particular regular fractal – the Sierpiński gasket [5]. I show that certain properties of that object differ from what one could call “a typical random fractal”. Nevertheless, the system permits one to quantify several important concepts of the elastic behavior of inhomogeneous systems.

2. The Sierpiński gasket – basic properties

The Sierpiński gasket is a deterministic fractal defined by the following iterative procedure [5]. A triangle is subdivided into four triangles by lines connecting the mid-points of its edges, followed by removal of the central triangle and inflation of the entire system by a factor of 2. The procedure is repeatedly applied to each of the remaining triangles. The fractal dimension of the gasket is $d_f = \ln 3 / \ln 2 \approx 1.585$.

A considerable number of investigations [13, 14] dealt with the properties of various models defined on the Sierpiński gasket, hoping that it will provide a qualitative insight into the general behavior of random fractals, as well as supply some quantitative estimates for critical exponents. Gefen et al. [13] investigated the scaling of the conductivity of a resistor network having the topology of the Sierpiński gasket: equal resistors have been placed along the edges of the present triangles of the gasket, and it has been shown that the resistance of a two-dimensional gasket increases by a factor 5/3 after each iteration, leading to the power-law dependence of the two-point conductance $\Sigma \sim L^{-\zeta_r}$, with $\zeta_r = \ln(5/3) / \ln 2 \approx 0.737$. (For a d -dimensional gasket $\zeta_r = \ln[(d+3)/(d+1)] / \ln 2$.) Since the fractal dimension of the Sierpiński gasket is close to the fractal dimension of the backbone of the percolating cluster, it has been suggested [13], that the value of ζ_r obtained for the gasket could approximate the conductivity exponent of a random system. Later, an appreciable discrepancy in the numerical values has been found. However, the gasket remained one of the simplest, but,

nevertheless, nontrivial models for testing the properties of the random systems.

3. Energetic elasticity models

The behavior of elasticity and conduction in a continuum are governed by similar differential equations. Thus, it was frequently assumed that the critical behavior of both properties is identical. Bergman has suggested [15] to use the Sierpiński gasket to look for possible differences between the problems. In its simplest form, one replaces the resistors described in the previous section by springs [10], i.e. uses central forces between the neighboring nodes of the network, and measures the changes in the elastic response of the system under the rescaling. Different elastic moduli can be measured by applying a variety of displacements to the external corners of the gasket. It has been found [10] that all possible force constants k (which are the analogues of the conductance Σ in the electric case) halve after each iteration, leading to the scaling relation $k \sim L^{-\zeta_e}$, with $\zeta_e = 1$. (This result remains unchanged if one considers a d -dimensional gasket.)

The behavior of the central force model is governed by a single force constant, which describes the properties of the elementary spring. A more general case was considered by introducing a three-terminal element at each node of the gasket [10], as well as by considering three-body bending forces on the gasket [11]. Both models have the same effect of adding an energetic cost to the change of the angle between the bonds. However, these modifications did not change the behavior of the effective elastic moduli of the gasket, and ζ_e remained 1.

The immediate conclusion from the above results is that the critical behavior of elasticity differs from the behavior of conductivity. The subsequent investigations of the energetic elasticity of percolating systems revealed significant differences between the predictions of the Sierpiński gasket model and the behavior of random systems: in the presence of central forces the rigidity threshold was found to be significantly larger than the percolation threshold [16].

i.e. the geometric continuity was insufficient to support stress. In the presence of bending forces ζ_c is significantly larger than ζ_r , and its value is primarily determined by the bending forces [17]. The differences in the behavior can be attributed to the fact that the Sierpiński gasket consists of the “most stable structures” – triangles, while the elastic response of a percolating system is primarily determined by the long tortuous paths [17].

So far we considered a purely energetic model. What happens to the system at finite temperature T ? The fluctuations δ of the gasket size can be related to the force constant k via [18]

$$k\delta^2 \approx k_B T. \quad (1)$$

Therefore the relative fluctuations of the Sierpiński gasket decay with increasing length scale:

$$\delta/L \approx (\sqrt{k_B T/k})/L \sim L^{\zeta_c/2-1} = L^{-1/2}.$$

By contrast, for percolation clusters, where $\zeta_c \approx 3$, the relative fluctuations increase with increasing length scale. Thus, for most tenuous structures large fluctuations will (on sufficiently large length-scales) eventually break the validity of the energetic approach which essentially assumed small fluctuations [4].

4. Elasticity of polymeric networks

Linear and branched polymers are examples of entropy-dominated tenuous structures. They do not have a “ground-state shape”, and can be defined only by the *connectivity*, while their relative shape fluctuations are of order unity. The radius of gyration (rms size) R_g of such a system can be usually related to its *internal* linear size L (in the case of a linear polymer L is the number of monomers, while in the case of a polymeric surface L is the linear size of a stretched surface) by a power law: $R_g \sim L^\nu$. In such a situation one cannot use the regular elastic stiffness tensor. However, the scaling $k \sim L^{-2\nu}$ of a typical force constant k can be easily determined: since the typical fluctuation δ satisfies eq. (1), and δ is of order R_g ,

the force constant [19] $k \approx k_B T/R^2 \sim L^{-2\nu}$. Thus, the elasticity exponent $\zeta_c = 2\nu$ for polymeric structures.

The success of the scaling theory in polymer physics rests on detailed investigation of linear polymers [2]. The treatment of more complicated objects usually relies on approximate theories. It is believed that on sufficiently long length-scale a tenuous network without self-avoidance (i.e. without the excluded-volume, or steric, interactions) can be correctly described by a network of harmonic springs which have a vanishing equilibrium length (“Gaussian network”). It can be shown [20,21] that the squared radius of gyration R_{g0}^2 of such a polymeric network is proportional to the mean resistance of a resistor network, which has the same topology as the polymeric network. Therefore, in the absence of the self-avoidance in polymer having the connectivity of a Sierpiński gasket we should expect $R_{g0} \sim L^{\nu_0}$, with $\nu_0 = \zeta_r/2 \approx 0.368$. (For the gasket we define L as the length of a stretched fractal, i.e. it is proportional to 2^n , where n is the number of iterations of the gasket.)

Excluded-volume interactions cause an expansion of the system (compared with the case without self-avoidance) and an increase in ν . From a dimensional analysis one finds that the self-avoidance becomes irrelevant when the structure is embedded in space dimension [20] $d > d_c \equiv 4d_r/\zeta_r$. For a structure with the connectivity of a two-dimensional Sierpiński gasket the upper critical dimension $d_c \approx 8.6$. For $d < d_c$ we can approximate the free energy F by a Flory-type expression [22]:

$$\frac{F}{k_B T} = \left(\frac{R_g}{R_{g0}}\right)^2 + \nu \left(\frac{N}{R_g^d}\right)^2 R_g^d, \quad (2)$$

where we omit the dimensionless prefactors of order unity. The first term on the right of (2) is the elastic (entropic) free energy of a network (R_{g0} is the radius of gyration of the same network without self-avoidance). The second term is an estimate of the repulsive interaction energy (the squared density of the monomers $(N/R_g^d)^2$ is a mean-field-type estimate of the number of pairs of monomers coming into close

contact with each other in a unit volume). By minimizing (2), we find $R_g \sim L^\nu$, with $\nu_F = (\bar{z}_r + 2d_f) / (d + 2)$.

For a polymer with the connectivity of the Sierpiński gasket in $d=2$, $\nu_F=0.977$. Notice, that for $d < d_k \equiv \bar{z}_r + 2d_f - 2$, we have $\nu_F > 1$. In general, the definition of the internal size L is somewhat arbitrary (the value of ν depends on that definition) and ν can exceed unity. However, with the particular definition of L for the Sierpiński gasket, such result would mean that the system is overstretched, and the Flory approximation fails. For the gasket the approximation breaks down at space dimension $d_k \approx 1.907$. We should keep in mind that the expression for d_k has been obtained within an approximate treatment, and it is quite possible that even at $d=2$ the system is already completely stretched.

5. Monte Carlo simulation of the entropic model

During and Kantor [12] considered a two-dimensional model system which is described by the Hamiltonian

$$\frac{H}{k_B T} = \sum_{i,j \text{ nn}} V_{\text{att}}(|\mathbf{r}_i - \mathbf{r}_j|) + \sum_{i,j} V_{\text{rep}}(|\mathbf{r}_i - \mathbf{r}_j|), \quad (3)$$

where \mathbf{r}_i is the position of the i th atom. The attractive potential V_{att} acts only between pairs $\langle i, j \rangle$ of atoms, which are nearest neighbors on a regular Sierpiński gasket, thus ensuring the *connectivity* (but *not the shape*) of the gasket. $V_{\text{att}}(r) = 0$, for $r < b$, and ∞ otherwise. (This type of "tethering potential" has been previously used to investigate self-avoiding surfaces [23].) The excluded-volume interaction was implemented by a hard-core repulsive potential V_{rep} , which acts between *any pair* $\{i, j\}$ of atoms. The physical properties of the system are determined by the entropy, and the force constants are strictly proportional to T .

The configuration space of the structure has been sampled using the Monte Carlo (MC) method [24] which consisted of randomly picking an atom and attempting to displace it in a randomly chosen direc-

tion. To verify the standard assumption that without the excluded volume the system should approach the behavior of a Gaussian network, an equilibration was performed for a modified version of the model in which V_{rep} was restricted to act only between the nearest neighbors of the network, and an excellent agreement with the theoretical prediction has been found.

In the MC simulation R_g was measured for a sequence of gasket sizes L . For small L the effective value of ν was somewhat smaller than unity, but it increased with increasing L and tended towards $\nu = 1.002 \pm 0.005$, leaving the Flory estimate outside the error bars. Since $\nu \leq 1$, the result suggests that $\nu = 1$ *exactly*. This conclusion also follows naturally from a simple inspection of fig. 1: we notice that on short length scales the structure is quite featureless. However, on larger length scales the "regular" shape of the gasket becomes apparent. This behavior, resembling homogeneous structure, indicates that $\nu = 1$.

The "shape stability" permits introduction of regular elastic compliance tensor $S_{\mu\nu}$, and its MC measurement from the strain fluctuations [25]:

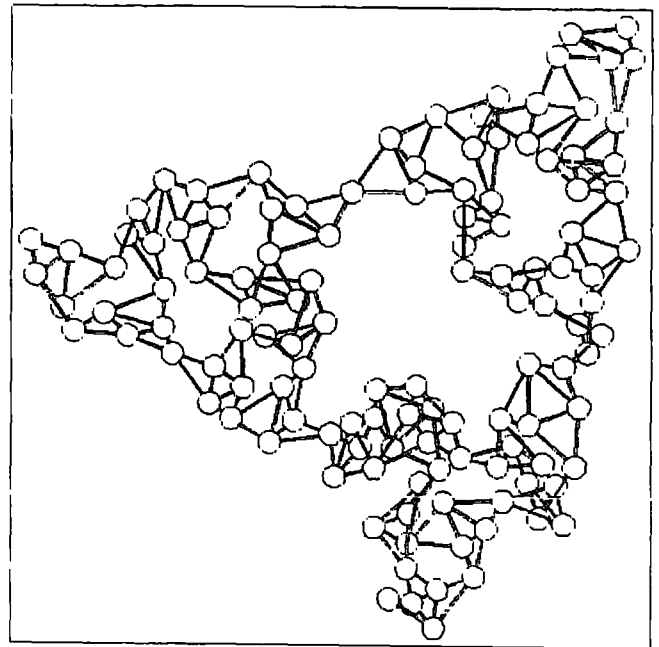


Fig. 1. A typical equilibrium configuration of a polymer which has the connectivity of the Sierpiński gasket.

$S_{ijkl} = (A/k_B T) \langle \epsilon_{ij} \epsilon_{kl} \rangle$, where A is the area of the system, while ϵ_{ij} is the thermally induced strain. All non-vanishing elements of S_{ijkl} had the same L -dependence, and were consistent with the (expected) isotropic symmetry, thus reducing the results to two independent constants with the same scaling properties. From the L -dependence of the elastic moduli one obtains an estimate of the entropic elasticity exponent $\zeta_c = 0.90 \pm 0.15$, which is close to the value 1 expected in the energetic elasticity models of the gasket [10,11] with central forces (with or without bending forces), and somewhat exceeds the value 0.737 which would follow from a scalar elasticity model [11]. The result is, obviously, inconsistent with $\zeta_c = 2\nu = 2$, which would be expected in a polymeric system.

The most surprising part of the results described in this section is the fact, that the excluded-volume effects are able to stabilize the shape of the fractal. Once we accept such stability, the scaling of the elastic constants becomes quite natural: One could assume that beyond a certain length scale, the fluctuations are small and the entire system can be approximately described by a simply *energetic* Hamiltonian. Since we have shown that the relative fluctuations of the energetic elasticity model on a Sierpiński gasket do not grow, such an effective description will remain valid also on even larger length-scales.

6. Discussion

In this work several elasticity models on Sierpiński gasket have been compared. It has been shown, that the gasket is significantly more stable than "a typical random fractal". The indications of the exceptional behavior came from the fact that the relative fluctuations of energetic models do not grow, and that the excluded volume in the entropic model stabilizes the structure. Both behaviors are related to an exceptionally high connectivity and to the fact that the fractal consists of stable structures – triangles. Only further investigation of additional models will show in a more quantitative way, which properties of fractals cause such an exceptional behavior.

From the theoretical point of view the results indicate that some additional parameter (besides the fractal and spectral dimensions) might enter the theory of fractal polymers. The results also imply that one should not use the Sierpiński gasket as a prototype for explaining the properties of gels [26], unless one has experimental evidence for the presence of such connectivity in a gel. The exceptional geometry of the Sierpiński gasket, however, does not mean that such "highly triangulated" structures are rare, since in certain random aggregation processes such stable structures may be preferably created.

Acknowledgement

This research was supported by the US–Israel Binational Science Foundation through Grant No. 87-00010, and by the Bat Sheva de Rothschild Foundation.

References

- [1] J.H. Weiner, *Statistical Mechanics of Elasticity* (Wiley, New York, 1983).
- [2] P.G. de Gennes, *Scaling Concepts in Polymer Physics* (Cornell Univ. Press, Ithaca, 1979).
- [3] S.F. Edwards, *J. Phys. A* 1 (1968) 15.
- [4] Y. Kantor and T.A. Witten, *J. Phys. (Paris)* 45 (1984) L 675.
- [5] B. B. Mandelbrot, *Fractals: Form, Chance and Dimension* (Freeman, San Francisco, 1987); *The Fractal Geometry of Nature* (Freeman, San Francisco, 1982).
- [6] A.I. Medalia and F.A. Hechman, *J. Colloid Interface Sci.* 36 (1971) 173.
J. Eisenlauer and E. Killman, *J. Colloid Interface Sci.* 74 (1980) 108;
K. Kusaka, N. Wada and A. Tasaki, *Japan. J. Appl. Phys. S* (1969) 599;
S.R. Forest and T.A. Witten, *J. Phys. A* 12 (1979) L 309.
- [7] L. Ye, D.A. Wenz, P. Sheng, S. Bhattacharya, J.S. Huang and M.J. Higgins, *Exxon preprint* (1989).
- [8] S. Alexander and R. Orbach, *J. Phys. (Paris)* 43 (1982) L 625.
R. Rammal and G. Toulouse, *J. Phys. (Paris)* 44 (1983) L 13.

- [9] J. Fricke. *Sci. Am.* 256 (1988) 92.
E. Courtens, J. Pelous, J. Phalippou, R. Vacher and T. Woignier. *Phys. Rev. Lett.* 58 (1987) 128.
E. Courtens, R. Vacher, J. Pelous and T. Woignier. *Europhys Lett* 6 (1988) 245.
T. Freltoft, J. Kjems and D. Richter. *Phys. Rev. Lett.* 59 (1987) 1212.
- [10] D.J. Bergman and Y. Kantor. *Phys. Rev. Lett.* 53 (1984) 511.
- [11] S. Alexander. *J. Phys. (Paris)* 45 (1984) 1939.
- [12] E. Duering and Y. Kantor. Tel Aviv University preprint (1989).
- [13] Y. Gefen, A. Aharony, B.B. Mandelbrot and S. Kirkpatrick. *Phys. Rev. Lett.* 47 (1981) 1771.
- [14] Y. Gefen, B.B. Mandelbrot and A. Aharony. *Phys. Rev. Lett.* 45 (1980) 855.
M. Stephen. *Phys. Lett. A* 32 (1981) 67.
R. Rammal and G. Toulouse. *Phys. Rev. Lett.* 49 (1982) 1194.
S. Alexander. *Phys. Rev. B* 27 (1983) 1541.
S. Alexander and E. Halevi. *J. Phys. (Paris)* 44 (1983) 805.
E. Domany, S. Alexander, D. Bensimon and L.P. Kadanoff. *Phys. Rev. B* 28 (1983) 3110.
R. Rammal. *Phys. Rev. B* 28 (1983) 4871.
S. Alexander. *Phys. Rev. B* 29 (1984) 5504.
- [15] D.J. Bergman. *Santa Barbara Workshop on Disordered Systems* (1983).
- [16] S. Feng and P.N. Sen. *Phys. Rev. Lett.* 52 (1984) 216.
- [17] Y. Kantor and I. Webman. *Phys. Rev. Lett.* 52 (1984) 1891.
- [18] L. Landau and I. Lifshitz. *Statistical Physics* (Pergamon Press, London, 1958) ch. 12.
- [19] P.G. de Gennes. *Polymers* 9 (1976) 587.
- [20] M.E. Cates. *Phys. Rev. Lett.* 53 (1984) 926; *J. Phys. (Paris)* 46 (1985) 1059.
- [21] Y. Kantor. in: *Proceedings of the 5th Jerusalem Winter School on Statistical Mechanics of Membranes and Surfaces*, D.R. Nelson, T. Piran and S. Weinberg, eds. (World Scientific, Singapore), to be published.
- [22] P. Flory. *Principles of Polymer Chemistry* (Cornell Univ. Press, Ithaca, 1971).
- [23] Y. Kantor, M. Kardar and D.R. Nelson. *Phys. Rev. Lett.* 57 (1986) 791.
- [24] A. Baumgärtner. in: *Application of the Monte Carlo Method in Statistical Physics*, K. Binder, ed. (Springer, Berlin, 1984), p. 145.
- [25] M. Parinello and A. Rahman. *Phys. Rev. Lett.* 45 (1980) 1196.
- [26] J. Bastide and F. Boue. in: *Statphys 16*, ed. H.E. Stanley (North-Holland, Amsterdam, 1986), p. 251.