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Density of states on fractals : « fractons »

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Résumé. — Nous calculons la densité d'états sur un fractal en tenant compte des propriétés d'échelles pour le volume et la connectivité. Nous utilisons la méthode de Green développée par ailleurs, qui utilise une relation au problème de diffusion. Nous avons trouvé que, pour compter les modes correctement, on doit avoir un espace réciproque avec une nouvelle dimensionnalité de fracton

$$\bar{\bar{d}} = 2\,\bar{d}/(2 + \bar{\delta})\,.$$

Ici, $\bar{d}$ est la dimension effective, et $\bar{\delta}$ est l'exposant que caractérise la variation de la constante de diffusion avec la distance. Par exemple, nous trouvons pour les amas de percolation, $\bar{\bar{d}} = 4/3$, quelle que soit la dimensionnalité Euclidienne d à la précision numérique disponible. Nous discutons le « crossover » vers un comportement normal aux basses fréquences pour des fractals finis, et pour la percolation au-dessus du seuil de percolation p_c. Nous examinons aussi la pertinence de nos prédictions en les confrontant à des résultats expérimentaux sur les protéines.

Abstract. — The density of states on a fractal is calculated taking into account the scaling properties of both the volume and the connectivity. We use a Green's function method developed elsewhere which utilizes a relationship to the diffusion problem. It is found that proper mode counting requires a reciprocal space with new intrinsic fracton dimensionality $\bar{\bar{d}} = 2\,\bar{d}/(2 + \bar{\delta})$. Here, $\bar{d}$ is the effective dimensionality, and $\bar{\delta}$ the exponent giving the dependence of the diffusion constant on distance. For example, we find for percolation clusters $\bar{\bar{d}} = 4/3$ within the numerical accuracy available, independent of the Euclidean dimensionality d. Crossover to normal behaviour at low frequencies is discussed for finite fractals and for percolation above the percolation threshold p_c. Relevance to experimental results on proteins is also discussed.

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The purpose of this note is to calculate the density of states on fractals. We do this using a Green's function technique [1], which avoids the use of boundary conditions and wave vector counting. We show that the usual relationship between the density of states and the Euclidean dimensionality (d) does not apply. The density of states cannot be described in terms of an anomalous dimensionality ($\bar{d}$) alone but requires an additional index describing the internal structure. We determine a fracton dimensionality ($\bar{\bar{d}}$) of the relevant reciprocal space which assures proper mode counting for a fractal in terms of the index governing diffusion ($\bar{\delta}$) and the anomalous or fractal dimension ($\bar{d}$). The density of states for free particles and for lattice vibrations is determined. We apply these results to polymer chains, the triangular Sierpinski gasket, and to percolation networks.

We were directly motivated by the recent work of Stapleton *et al.* [2] who found an anomalous temperature dependence for the ESR spin-lattice relaxation time of iron in several proteins. They interpreted their measurements in terms of an anomalous vibrational density of states arising from a suggested fractal structure for the proteins. However, they included only the anomalous dimensionality $\bar{d}$ in their analysis.

The density of states on fractals should also be of interest in other situations. Examples would be the role of geometrical disorder in amorphous systems, and the specific heat of fractal-like systems in the intermediate temperature range (see below).

1. **Method of calculation.** — We consider problems defined on a fractal so that both the available volume and the connectivity are determined by the fractal geometry. An explicit way of realizing a fractal model is to consider solutions of the relevant equations on a network of wires connected in a suitable geometry [3]. We take the network to be homogeneous. Our results will apply for times or frequencies such that the associated distances are much larger than the size of the individual bonds making up the network, but much smaller than the total size of the network. Formally, we are assuming that one can define some local geometry on the fractal in which the Laplacian has its usual form (i.e. is equivalent to a local q^2 expansion). This is defined by the wires for a network model. While this may not be possible for all conceivable fractals, we believe it is certainly possible for most cases in which one would be interested. One finds that the formal relationship between problems initially described by Laplacians (or by equivalent finite difference equations [4]) is maintained.

The structure of the diffusion equation is such that it can be mapped onto a master equation, which in turn has the same form as the free particle Schrödinger equation and the equation of motion for mechanical vibrations (see Sec. 3 of Ref. [3], and Ref. [5]). This will enable us to map the eigenvalue density of states for the quantum vibrational problem onto the eigenvalue density of states of the diffusion problem. The latter can be obtained from the single site Green's function for the diffusion problem [1] :

$$N(\varepsilon) = -\frac{1}{\pi}\,\mathrm{Im}\,\langle \tilde{P}_0(-\varepsilon + i0^+)\rangle \tag{1}$$

where $\tilde{P}_0(\varepsilon)$ is the Laplace transform of $P_0(t)$, the autocorrelation function, with ε the spectral parameter. In physical terms, if a particle is initially at the origin at time $t = 0$, the probability of finding it there at time t is given by $P_0(t)$. We now calculate this quantity directly.

On a fractal one expects, in general, anomalous diffusion [6]. We write,

$$\langle r^2(t)\rangle \propto t^{2/(2+\bar{\delta})}, \tag{2}$$

where $\bar{\delta}$ is an index which depends on the geometry (i.e. it is the diffusion constant scaling exponent). In general, one expects $\bar{\delta} \neq 0$. The total volume available on the fractal, within the diffusion distance, is

$$V(t) \propto \langle r^2(t)\rangle^{\bar{d}/2}, \tag{3}$$

where $\bar{d}$ is the anomalous or fractal dimensionality. Thus,

$$\langle P_0(t) \rangle \propto [V(t)]^{-1} \propto t^{-\bar{d}/(2+\bar{\delta})} . \tag{4}$$

We have thus assumed that the diffusion length is given by a power law (Eq. (2)) and that it is the only relevant length scale in the problem. Using equation (1), one is immediately led to the eigenvalue density of states for the diffusion problem :

$$N(\varepsilon) \propto \varepsilon^x , \tag{5}$$

where

$$x = [\bar{d}/(2 + \bar{\delta})] - 1 . \tag{6}$$

As shown explicitly in reference [1], the spectral parameter ε can be related to the energy eigenvalues of the vibrational problem by replacing ε by ω^2 and multiplying by ω :

$$N(\omega) \propto \omega^p , \tag{7}$$

where

$$p = 2x + 1 = [2\bar{d}/(2 + \bar{\delta})] - 1 . \tag{8}$$

We refer to the quantized vibrational states on a fractal as fractons.

For positive $\bar{\delta}$, x and p are always smaller than the anomalous dimension result ($x = (\bar{d}/2) - 1$, $p = \bar{d} - 1$, as suggested in Ref. [2]). The reason for the difference is that the scale dependence of the elastic constants is also anomalous (i.e. it depends on $\bar{\delta}$). It is not sufficient to consider only the mass scaling described by $\bar{d}$.

Our results, equations (5)-(8), can be described by a « mode counting » reciprocal space of effective dimensionality

$$\bar{\bar{d}} = 2\bar{d}/(2 + \bar{\delta}) . \tag{9}$$

We shall call this the fracton dimensionality. For a standard Laplacian ($\Delta \to q^2$) expansion, this is the relevant dimensionality. It determines the relevant Hilbert space for Laplacian equations on the fractal. We emphasize that the fracton dimensionality ($\bar{\bar{d}}$) is an intrinsic property of the fractal geometry. It differs from the mass scaling exponent, or the fractal dimensionality ($\bar{d}$), and from the diffusion constant scaling exponent ($\bar{\delta}$), in being independent of the manner in which the fractal is embedded in an external space (of Euclidean dimension d). The d dependence of $\bar{d}$ and $\bar{\delta}$ cancels out in equation (9).

We note that this seems to be the natural extension of a gradient expansion to fractals. The obvious alternative of expanding in undistorted real space gradients leads to a singular expansion ($\varepsilon \sim q^{2+\bar{\delta}}$) and a reciprocal space of dimensionality $\bar{d}$ (using Eq. (2)).

2. **Some examples.** — It is useful to consider some examples.

a) Consider a one dimensional chain whose configuration is described by a random walk or self-avoiding walk. One has

$$N^\nu \propto r , \tag{10}$$

where N is the length (number of units) of the chain. Thus,

$$\bar{d} = \nu^{-1} . \tag{11}$$

For diffusion *along* the chain,

$$N^2(t) \propto t ,$$

and from equations (10) and (11),

$$\langle r^2(t) \rangle \propto \langle N^{2\nu}(t) \rangle \propto t^{\nu}, \tag{12}$$

so that

$$\bar{\delta} = 2(\bar{d} - 1), \tag{13}$$

leading to (Eqs. (6), (8), and (9)),

$$x = 1/2, \quad p = 0, \quad \text{and} \quad \bar{\bar{d}} = 1. \tag{14}$$

The fracton dimension ($\bar{\bar{d}}$) for this problem is identically one, and is independent of ν.

b) Consider a triangular ($d = 2$) Sierpinski gasket. One has [3, 7]

$$\bar{\delta} = [(\ln 5)/(\ln 2)] - 2 \approx 0.322, \tag{15a}$$

$$\bar{d} = (\ln 3)/(\ln 2) \approx 1.585, \tag{15b}$$

but the fracton dimension is (Eq. (9)),

$$\bar{\bar{d}} = 2(\ln 3)/(\ln 5) \approx 1.365. \tag{16}$$

Thus, the gasket is somehow more one dimensional than suggested by $\bar{d}$. For the eigenvalue density of states, one has the spectral parameter exponent (Eq. (6)),

$$x = [(\ln 3)/(\ln 5)] - 1 \approx -0.317, \tag{17a}$$

and the fracton ω exponent (Eq. (8)),

$$p = [2(\ln 3)/(\ln 5)] - 1 \approx 1.365. \tag{17b}$$

c) Consider a critical percolation network. Taking the infinite cluster at the critical percolation concentration p_c, one has from straight forward scaling considerations [8],

$$\bar{d} = d - (\beta/\nu), \tag{18}$$

where d is the Euclidean dimensionality of the external space, and [3, 6]

$$\bar{\delta} = (t - \beta)/\nu, \tag{19}$$

where t is the conductivity exponent. Thus,

$$\bar{\bar{d}} = 2(d\nu - \beta)/(t - \beta + 2\nu). \tag{20}$$

Table I. — *The fracton dimensionality $\bar{\bar{d}}$ defined in equation* (9) *and the eigenvalue density of states indices x* (*Eq.* (6)) *and p* (*Eq.* (8)) *as a function of the Euclidean dimensionality of the percolation problem* (d). *The fractal dimensionality $\bar{d}$* (*Eq.* (18)) *and $\bar{\delta}$* (*Eq.* (19)) *were computed from the numerical values in reference*[8].

d	$\bar{\bar{d}}$	x	p	$\bar{d}$	$\bar{\delta}$
2	1.36	− 0.32	0.36	1.9	0.80
3	1.42	− 0.29	0.42	2.5	1.55
4	1.39	− 0.30	0.39	3.3	2.71
5	1.44	− 0.28	0.44	3.8	3.3
∞	4/3	− 1/3	1/3	4	4

We give results for $\bar{\bar{d}}$ in table I as a function of the Euclidean dimensionality (d) for Stauffer's values [8] of the indices t, β, and ν for the percolation problem. One notes the very weak dependence of the fracton dimensionality ($\bar{\bar{d}}$) on the Euclidean dimensionality (d) of the percolation problem. This is in sharp contrast to the behaviour of $\bar{d}$ and $\bar{\delta}$. The table certainly suggests the conjecture that, for percolation on the infinite cluster,

$$\bar{\bar{d}} = 4/3\,, \tag{21}$$

independent of d (see note added in proof).

3. **Crossover and finite size effects.** — The Laplace transform of equation (2) yields a relation between length scale and the Laplace transform spectral parameter ε. We are able to find a characteristic diffusion length scale appropriate to the spectral parameter ε, λ_ε, which varies as [3]

$$\lambda_\varepsilon \propto \varepsilon^{-1/(2+\bar{\delta})}\,. \tag{22a}$$

Mapping onto the vibrational problem as before,

$$\lambda_\omega \propto \omega^{-2/(2+\bar{\delta})}\,. \tag{22b}$$

Fractal behaviour is found for length scales less than the size (L) of a fractal object. For larger length scales, the solutions are, in essence, uniform over the fractal and the density of states is determined by the boundary conditions. Crossover to fractal behaviour occurs when $\lambda_\varepsilon \lesssim L$, or for energies

$$\varepsilon_{\text{c.o.}} \approx \omega^2_{\text{c.o.}} \gtrsim L^{-(2+\bar{\delta})}\,, \tag{23}$$

where the subscript c.o. means crossover. For $\varepsilon > \varepsilon_{\text{c.o.}}$ (or $\omega > \omega_{\text{c.o.}}$), the eigenvalue density of states is then given by equation (5) (or Eq. (7)). For a percolation network above p_c, one predicts normal d-dimensional low frequency vibrational density of states ($p = d - 1$) crossing over to fracton behaviour for vibrational frequencies above (Eq. (23))

$$\omega_{\text{c.o.}}(p) \propto \xi_p^{-(2+\bar{\delta})/2} \tag{24}$$

where ξ_p is the percolation correlation length.

4. **Discussion.** — We conclude with some remarks concerning the relevance of our results to experiment. We have analysed the eigenvalue density of states for diffusion on a fractal geometry, and mapped our results onto the vibrational eigenvalue density of states for systems with the same geometrical structure. For the vibration problem, this assumes that both the elastic constants and the inertial mass are appropriate to a free fractal. It is important to emphasize that this is not necessarily a proper physical description. It is, in fact, hard to think of a situation where the vibration spectrum of a polymer would be adequately described by our free fracton model. For gels, the mass density is always dominated by the solvent, and therefore scales with the Euclidean dimensionality of the external space (d). Any fractal anomalies would only reflect the scaling properties of the elastic constants. It is conceivable that something similar occurs for proteins where one would also expect an essentially uniform density. This might be relevant to the interpretation of the results of Stapleton *et al.* [2] and to other measurements in which the vibrational density of states of proteins is important [9].

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Note added in proof. — Professor T. C. Lubensky has noted (private communication) that some intriguing consequences follow if one takes seriously the results of the table for the percolation problem. He notes that if one assumes that $\bar{\bar{d}} = 4/3$, independent of d, one can use equation (20) to generate an expression for the exponent t in terms of ν and β :

$$t = (1/2)\left[\nu(3\,d - 4) - \beta\right].$$

Two consequences are worth noting.

1) Using the values of β and ν following from the den Nijs conjecture at $d=2$ (M. P. M. den Nijs, *Physica* (Utrecht) **A 95** (1979) 449) : $\beta = 5/36$ and $\nu = 4/3$, one finds $t = 91/72 = 1.264$. This differs from $t \cong 1.1$ presented by S. Kirkpatrick (*La matière mal condensée*, Ed. by R. Balian, R. Maynard and G. Toulouse (North-Holland publishing company, Amsterdam) 1979, p. 321), and is not in accord with the relation $t = \nu$ (A. K. Sarychev and A. P. Vinogradoff, *J. Phys.* **C 14** (1981) L-487). A very recent finite size scaling (simulations on finite size strips) of B. Derrida and J. Vannimenus (submitted for publication, 1982) finds $t \cong 1.28$, in close accord with the above consequence ($t = 1.264$) of setting $\bar{\bar{d}} = 4/3$.

2) The links and node model led A. S. Skal and B. I. Shklovskii [*Fiz. Tekh. Poluprov.* **8** (1974) 1582 (*Sov. Phys. : Semicond.* **8** (1975) 1029)] to define $t = (d - 2)\,\nu + \zeta$. Setting $\bar{\bar{d}} = 4/3$, solving for t, and using appropriate scaling relationships, leads to the expression, valid for all d,

$$\zeta = (1/2)\,(\beta + \gamma).$$

G. S. Grest and M. J. Stephen (*Phys. Rev. Lett.* **38** (1977) 567) and C. Dasgupta, A. B. Harris and T. C. Lubensky (*Phys. Rev.* **B 17** (1978) 1375) show that $\zeta_{\text{pert}} = 1 + 0(\varepsilon^2)$ where $\varepsilon = 6 - d$. If we use perturbation theory results for β and γ (R. G. Priest and T. C. Lubensky, *Phys. Rev.* **B 13** (1976) 4159; **B 14** (1976) 5125; D. J. Amit, *J. Phys.* **A 9** (1976) 1441) :

$$\beta = 1 - (1/7)\,\varepsilon - (61/7^3\,3^2\,2^2)\,\varepsilon^2 + \cdots$$

$$\gamma = 1 + (1/7)\,\varepsilon + (565/7^3\,3^2\,2^2)\,\varepsilon^2 + \cdots$$

we find

$$\zeta_{\text{pert}} = 1 + \varepsilon^2/49$$

as required to $0(\varepsilon^2)$. For $d = 2$, $t_{\text{pert}} = \zeta = 1.33$, obviously outside the range of « safe » convergence ($\varepsilon = 4$), but remarkably close to the conjecture ($\bar{\bar{d}} = 4/3$) value of $t = 1.264$.

Finally, from another perspective, R. Rammal and Angles d'Aurioc (submitted for publication, 1982) have found values for $\bar{d}$ and $\bar{\delta}$ for the Sierpinski sponge in d dimensions. They find

$$\bar{d} = [\ln(d + 1)]/\ln 2\,, \qquad \bar{\delta} = \{\,[\ln(d + 3)]/\ln 2\,\} - 2$$

so that

$$\bar{\bar{d}} = 2[\ln(d + 1)]/\ln(d + 3)\,.$$

These results agree with ours for the case we considered, $d = 2$. In addition, the asymptotic $d \to \infty$ limit for $\bar{\bar{d}}$ is 2, quite different from the $d \to \infty$ limit for the percolation problem, 4/3. The ratio, $\bar{\bar{d}}/\bar{d} = (\ln 4)/[\ln(d + 3)]$ is always less than unity for $d \geqslant 2$, exhibiting the same trend as we have exhibited for $d = 2$.

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