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Vibrational properties of random percolating networks

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Abstract. The vibrational density of states (DOS) of very large percolating clusters (bond and site), is calculated in three dimensions using the spectral moments method. It is confirmed that for site (bond) percolation, the slope of the DOS in the fracton regime is strongly dependent on the occupation probability p and the particle interactions. For the bond percolation, the DOS presents a more complex behaviour in the low-frequency region than the Debye law observed in the site percolation. Interactions are represented by the Born Hamiltonian with first and second nearest neighbours. Several models are studied: for each model, it is possible to define critical exponents. A comparison with experimental results on silica aerogels is reported.

1. Introduction

In the last few years, there has been a growing interest in the dynamical properties of fractal structures: theoretical analysis (Alexander and Orbach 1982, Alexander 1983, 1986, 1989), computer simulation (Angles d'Auriac *et al* 1983, Derrida *et al* 1984, Yakubo and Yakayama 1987, 1989, Qiming Li *et al* 1990, Roman 1990, Roman *et al* 1991 and Royer *et al* 1992a, b), and experiments (Courtens *et al* 1987, 1988, Vacher *et al* 1988, 1990, and Reichenauer *et al* 1989). These investigations provide a scaling of the vibrational density of states with a power $(\tilde{d} - 1)$ of the frequency above a phonon to fracton crossover frequency ω_c ; \tilde{d} is the *spectral* dimension and characterizes the connectivity of a system. The crossover frequency is supposed to separate phonons at lower frequencies from localized vibrations (fractons) at high frequencies (Alexander and Orbach 1982).

Fractons were first introduced by studying percolation systems with scalar (isotropic) elastic forces model, where the *fracton* dimensionality $\tilde{d} = 4/3$, was conjectured to hold in d dimensions for $d \geq 2$ (Alexander and Orbach 1982). Yakubo and Yakayama (1987, 1989) using a resonance technique verified this conjecture for $d = 2$ and $d = 3$. However, the case $d = 2$ seems to be particular with $\tilde{d} \simeq 0.31$ (Aharony *et al* 1985 and Royer *et al* 1992a, b). In this model, the potential is the Born Hamiltonian (Born and Huang 1956, Feng and Sen 1984). It was shown that this potential fails to take into account the vector nature of the most realistic elastic systems, and that percolating networks can have very different critical exponents from those of a scalar model, notably the elastic modulus exponent (Feng *et al* 1984, Bergman 1985). In this paper, we consider the following potential

$$v = \frac{1}{2} \sum_{\substack{i,j \\ (NN)}} k_{ij} \{ \alpha (\mathbf{u}_i - \mathbf{u}_j)_{\parallel}^2 + \delta (\mathbf{u}_i - \mathbf{u}_j)_{\perp}^2 \} + \frac{1}{2} \sum_{\substack{i,j \\ (NNN)}} k_{ij} \{ \gamma (\mathbf{u}_i - \mathbf{u}_j)^2 \} \quad (1)$$

where NN denotes that the summation is performed over the first nearest-neighbouring pairs (i, j) and NNN over the next-nearest-neighbouring pairs (i, j) , $(\mathbf{u}_i - \mathbf{u}_j)_{\parallel}$ is the relative

displacement in the direction of the bond (i, j) and $(\mathbf{u}_i - \mathbf{u}_j)_\perp$ is the relative displacement in the perpendicular direction. For random site (bond) percolation, k_{ij} is a random variable which takes the value 1 if the sites i and j are both (bond (i, j)) occupied, and 0 otherwise. α , δ and γ are the elastic interaction strength parameters.

When $\gamma = 0$, by changing the parameters α and δ , two extreme cases can be noted (Feng and Sen 1984): for $\alpha = \delta$, the purely isotropic model introduced above, which was associated by de Gennes to conductivity problem (de Gennes 1976); for the central force model, i.e. $\delta = 0$, the Hamiltonian (1) represents a random network of springs and the problem is intrinsically of vector nature (Feng and Sen 1984).

Feng and Sen (1984) showed by numerical study of bulk and shear moduli of 3D face-centred cubic (FCC) and 2D triangular lattices, that the central force elastic percolation problem belongs to a different universality class from conduction problems. In the case of simple hypercubic percolating networks, both numerical study (Feng *et al* 1984, Bergman 1985) and effective medium approximation (EMA) (Feng *et al* 1985) predicted that the elastic threshold $p_c = 1$ for the central model.

To extend the study with vector elastic forces to such lattices, Kantor and Webman (1984) and Feng (Feng and Sahimi 1985, Feng 1985a) considered the bond-bending force model, which has been used extensively to describe elastic and vibrational properties of molecular (Kirkwood 1939) and solid state systems (Keating 1966, de Leeuw *et al* 1985 and Wooten and Weaire 1987) and those of disordered tenuous structures (Feng *et al* 1984, Webman and Grest 1985). These studies showed that a crossover length scale l_c exists, such that for a quasi-one-dimensional chain, when the correlation length $\xi < l_c$ ($\xi \sim |p - p_c|^{-\nu}$, where the critical exponent ν is a positive constant), the fracton properties of the system are governed by the bond-stretching motion, which scales in the same way as the scalar model ($\tilde{d} = 4/3$); whereas when $\xi > l_c$, the bond-bending motion (which has a different scaling behaviour) becomes dominant, and there is a crossover from effective spectral dimension $\tilde{D} = 0.8$ to $\tilde{d} = 4/3$ as the wavelength decreases from the $\lambda > l_c$ regime to the $\lambda < l_c$ one (Feng 1985a). The calculation of the Young's modulus Y and the conductivity Σ showed an elastic modulus exponent f : $Y \sim |p - p_c|^f$, greater than the conductivity exponent t : $\Sigma \sim |p - p_c|^t$.

By experimental probes, Vacher *et al* (1990) identified three crossovers and two distinct regions in the fracton regime of the DOS of silica aerogels. These contributions were associated to bend- and stretch-dominated elasticities. Further, the values of the spectral dimensions appear to be non-universal.

2. Models and DOS calculations

In this work, using a numerical technique, we direct our interest to elastic properties of the site and bond 3D cubic percolating networks. In all the systems below, we assume that atoms of mass $m = 1$ are placed at the sites of the lattice and the parameter $\alpha = 0.125$. Each system consists of a single, very large cluster: the infinite cluster.

We use the spectral moments method, which could provide the exact response function of very large harmonic systems, whatever the structure, the type of the forces and the dimension (Benoit 1987, 1989, Benoit and Poussigue 1989). The method consists of determining the moments of the response function directly from the dynamical matrix $3N \times 3N$, where N is the system size: for instance the dielectric susceptibility of the system if we are studying infrared absorption, Raman scattering or the differential cross section if we are studying inelastic scattering of light or neutrons. The method has been used for the study of the

dynamics of quasi-crystals (Benoit *et al* 1990), polythiophene (Poussiguet and Benoit 1990, Poussiguet *et al* 1991) and the Sierpinski gasket (Benoit *et al* 1992a). More recently, we have shown that, with some variations, this method could provide the total DOS with good accuracy and the displacement correlation functions of the system (Benoit *et al* 1992b). Thanks to its simple computing aspects, the spectral moments method has allowed us to work with very large clusters (up to 10^6 atoms) in d dimensions ($2 \leq d \leq 6$) (Royer *et al* 1991, 1992a, b).

We have developed calculations of DOS, on a 105^3 cubic lattice for different values of site (bond) occupation probability $p > p_c$. Two models are studied, the purely nearest-neighbour interactions model ($\gamma = 0$), hereafter referred to as the first model, and the second one with next-nearest-neighbour interactions ($\gamma \neq 0$).

2.1. First model ($\gamma = 0$)

To test the accuracy of our algorithm, we have computed the DOS of the 105^3 simple cubic lattice ($p = 1$; $N = 1\,157\,625$), where interactions are represented by the scalar potential ($\alpha = \delta$). We have plotted in figure 1 the DOS $G(u)$ versus square frequency $u = \omega^2$. We note the excellent agreement between our results (circles) and the exact result obtained for an infinite simple cubic lattice (solid line). We have plotted in figure 3(e), the DOS $g(\omega)$ versus ω on a log-log scale. As one can expect, the results show in the low-frequency region a Debye law.

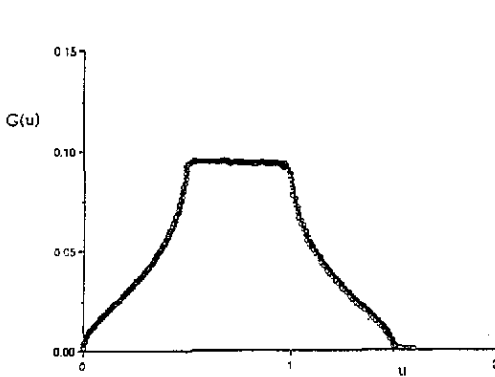


Figure 1. The DOS $G(u)$ versus u for a 105^3 simple cubic lattice (open circles). The solid line (—) indicates the exact solution for the infinite system.

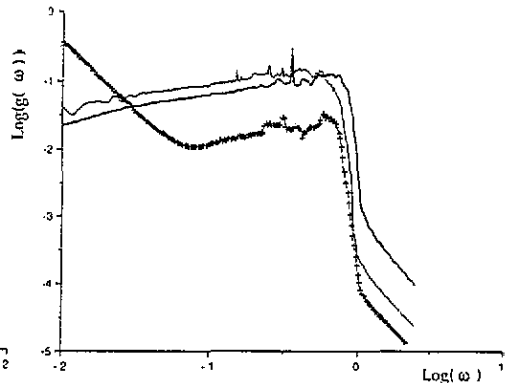


Figure 2. The DOS on a log-log scale for 3D site percolating network size 105^3 at $p = 0.33$ ($p_c = 0.3112$) for three values of δ/α ($\gamma = 0$): $\delta/\alpha = 0.0$ crosses; $\delta/\alpha = 0.5$ —; $\delta/\alpha = 1.0$ - - -. The percolating cluster size is 205 312 sites.

Let us begin by the site percolation. In figure 2, we have plotted the DOS $g(\omega)$ versus ω for three values of the ratio δ/α at $p = 0.33$ near to the percolation threshold $p_c = 0.3112$: for $\delta = 0$ (the purely central force model), the system has a finite fraction of zero frequency modes which decreases as p increases. The rigidity of the system vanishes at p close to p_c . As δ/α increases the rigidity of the system increases, and high-frequency modes appear to the detriment of lower-frequency one. When $\alpha = \delta$ (scalar model), the system is macroscopically rigid. In this later case, we have computed the DOS for several values of the occupation probability p (figure 3).

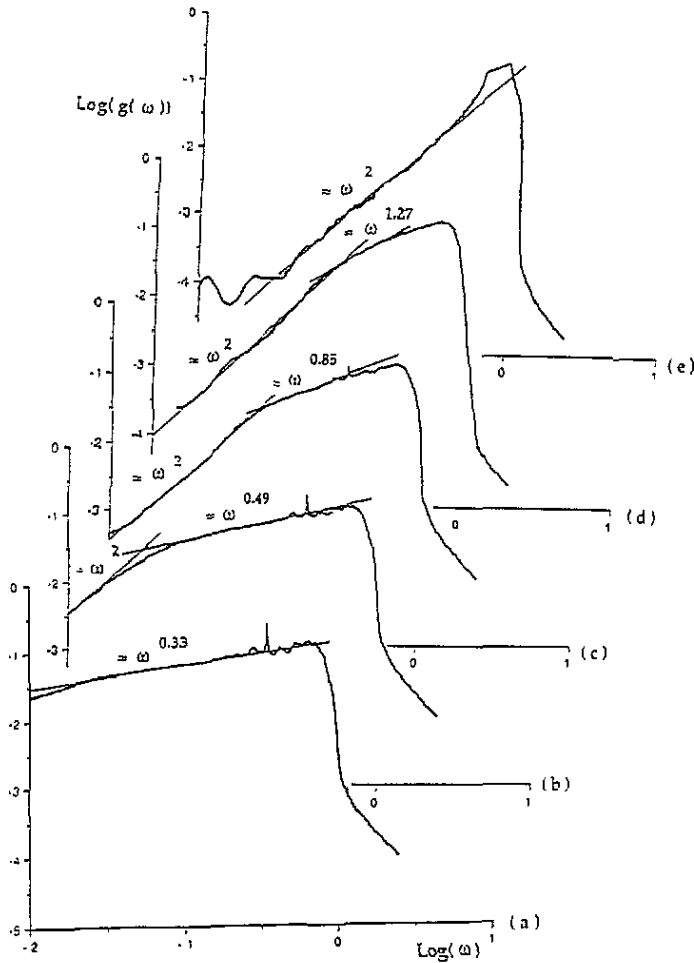


Figure 3. The scalar model DOS $g(\omega)$ on a log-log scale for 3D site percolating cluster at different values of p ($p_c = 0.3112$), formed on a 105^3 cubic lattice: the straight lines give the slope of the DOS and ω_c . (a) $p = 0.33$, (b) $p = 0.4$, (c) $p = 0.5$, (d) $p = 0.6$ and (e) $p = 1$. The percolating cluster sizes are respectively 205 312, 413 627, 566 305, 691 997 and 1 157 625 sites.

Our results show, as expected, that near p_c the DOS of the 3D site percolating cluster has a fracton behaviour, with the conjectured fracton dimension $\bar{d} = 4/3$, figure 3(a) ($p = 0.33$; $N = 205\,312$). Above p_c (figure 3(b): $p = 0.4$ ($N = 413\,627$); in (c): $p = 0.5$ ($N = 566\,305$); (d): $p = 0.6$ ($N = 691\,997$)), a crossover frequency ω_c is observed, given by the intersection of the straight lines, such that for $\omega < \omega_c$, the DOS $g(\omega)$ is Debye-like, with, as argued in Feng (1985a):

$$g(\omega) \simeq Ad\omega^2 \quad (2)$$

where

$$Ad = [C_t(p)]^{-3} \quad (3a)$$

and

$$C_t(p) \sim |p - p_c|^{(t-\beta)/2} \tag{3b}$$

is the sound speed of the system; the exponent β describes how the strength P of the infinite network goes to zero at the percolation threshold,

$$P \sim (p - p_c)^\beta \tag{3c}$$

while for $\omega > \omega_c$, the DOS is fracton-like, with

$$g(\omega) \simeq \omega^{\bar{d}(p)-1} \tag{4}$$

where $\bar{d}(p)$, deduced from the effective slope of the log-log plot of the DOS fracton region, can be understood as an effective spectral dimension of the system. For $p_c < p < 1$, we note that $\bar{d}(p)$ depends on $p(\frac{4}{3} < \bar{d}(p) < 3)$, for p relatively larger than p_c , as it has been noted in the case of 2D site percolating clusters (Royer *et al* 1992a).

With

$$\omega_c \simeq C_t(p)/\xi \tag{5}$$

one obtains

$$\bar{d} = 2D/(2 + (t - \beta)/\nu) \tag{6}$$

where $D = d - \beta/\nu$ is the fractal dimension of the system.

No steepness or hump of the DOS exists in the crossover region in the vicinity of ω_c . When $p = 1$ (figure 3(e)), at lower frequencies, two peaks appear at 0.011 and 0.023 which correspond to the first (0.0106) and the second (0.0212) minimal frequencies of a cubic lattice of size 105^3 (Landau and Lifshitz 1967), followed by a Debye law ($g(\omega) \sim \omega^2$) in agreement with previous investigations (Yakubo and Yakayama 1987, 1989). At higher frequencies, the peak at $\omega = \sqrt{0.125}$ which appears in all the spectra, is related to vibrations of a single site connected by a single bond to a relatively rigid block (Grest and Webman 1984). Other peaks related to the local structure element of the cluster can be identified in figure 4(a), (b) and (c) where we have plotted the DOS $G(u)$ versus $u = \omega^2$.

In figure 5(a), the crossover frequency ω_c is plotted versus the occupation probability p . As p approaches p_c , ω_c approaches zero with the scaling $\omega_c \sim |p - p_c|^{1.52 \pm 0.03}$. This is in agreement with the predictions of the scaling theory,

$$\omega_c \sim |p - p_c|^{\nu D/\bar{d}}. \tag{7}$$

For a 3D site-percolating cluster $\nu = 0.83$ (Stauffer 1979) and $D = 2.5$, with $\bar{d} = \frac{4}{3}$, $\nu D/\bar{d} = 1.56$ which is in the order of the value of our study. In 2D, Royer *et al* (1992a) showed a discrepancy between their calculation of $\nu D/\bar{d}$ and theoretical probes; we think that 2D is a singular case as we will see below. Another feature of our calculations is concerning the conductivity exponent t . In figure 5(b), we have plotted the coefficient Ad of the Debye term in DOS, $g(\omega) \simeq Ad\omega^2$, the slope is -2.42 ± 0.02 . Using equations (3a) and (3b), Ad obeys the scaling law,

$$Ad \sim |p - p_c|^{-3(t-\beta)/2} \tag{8}$$

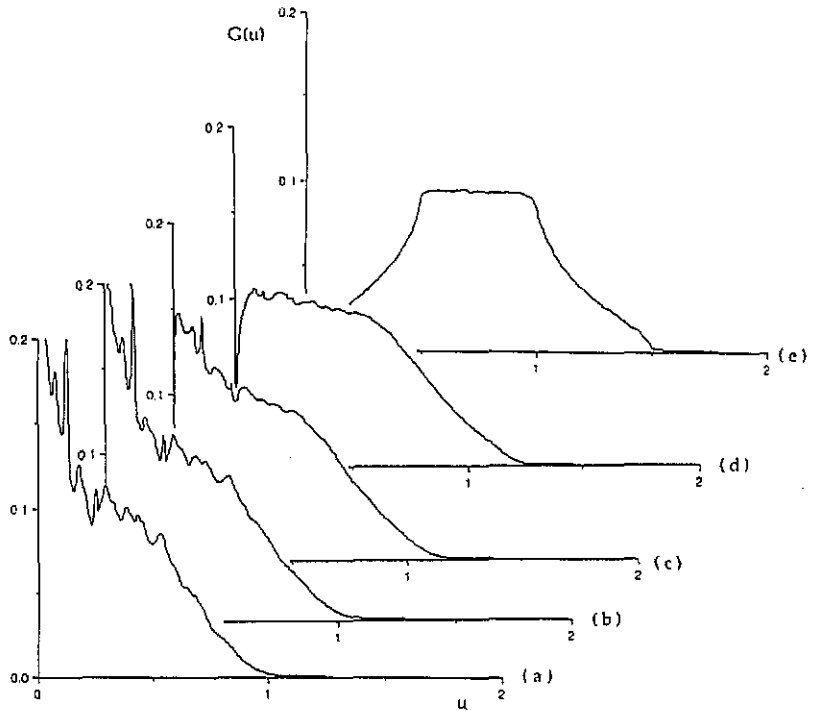


Figure 4. Plot of the scalar model DOS $G(u)$ versus $u = \omega^2$ at different values of p for a 105^3 cubic lattice: (a) $p = 0.33$, (b) $p = 0.4$, (c) $p = 0.5$, (d) $p = 0.6$ and (e) $p = 1$.

with $\beta = 0.4$ (Gaunt and Sykes 1983) and $t = 2.0$ (Kantor and Webman 1984). For 3D site percolating cluster, the exponent $-3(t - \beta)/2 = -2.4$ which is close to our estimated value.

The case of bond percolation is more complex. In figure 6, we have plotted for several values of $p > p_c$, where $p_c = 0.2489$, the DOS $g(\omega)$ versus ω on a log-log scale for a 3D bond-percolating network of size 105^3 : (a) $p = 0.265$ ($N = 498\,757$); (b) $p = 0.3$ ($N = 803\,796$); (c) $p = 0.4$ ($N = 1\,067\,201$); (d) $p = 0.5$ ($N = 1\,133\,152$) and (e) $p = 1$ ($N = 1\,157\,625$). In figure 6(a) at low frequencies, the fracton regime is governed by an effective spectral dimension $\bar{d} = 0.35 \pm 0.02$. As p approaches 1 (figure 6(b), (c) and (d)), like in the site percolation, three different regions are observed: one can recognize the phonons (i.e. $g(\omega) \sim \omega^2$), only when p is sufficiently larger than p_c . Intermediate regions correspond to fracton modes. The same results are noted in 2D bond-percolating clusters as illustrated in figure 7, where clusters are formed on a 1100^2 square lattice: (a) $p = 0.52$ ($N = 954\,528$); (b) $p = 0.6$ ($N = 1\,147\,654$); (c) $p = 0.8$ ($N = 1\,207\,768$) and (d) $p = 1$ ($N = 1\,210\,000$). At $p = 0.52$ (figure 7(a)) near $p_c = 0.5$, the effective spectral dimension is $\bar{d} = 0.37 \pm 0.02$. The discrepancy between our estimated values and the conjecturing value of $\bar{d} = \frac{4}{3}$ of site percolating cluster is due to the difference between the mean connectivity in these systems and will be discussed later.

As discussed by Alexander (1984), the Born-Huang scalar potential is not explicitly invariant under rigid rotation ($\delta \neq 0$). Assuming this invariance, the equilibrium condition dictates that the non-central force constant must vanish ($\delta = 0$). In other words, the corrected Born model requires purely nearest-neighbour interactions to be central only (Keating 1966).

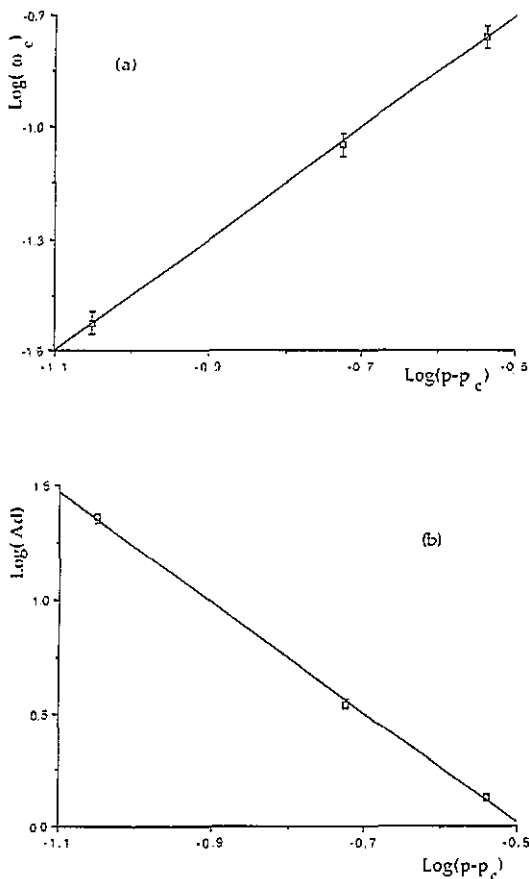


Figure 5. (a) The crossover frequency ω_c ; (b) the coefficient Ad of the Debye term of the scalar model DOS, versus $|p - p_c|$ on a log-log scale.

By introducing the next-nearest-neighbour interactions, Kaplan (1961) showed in the case of 3D cubic lattices, that the equilibrium condition does not restrict the choice of the force constants.

2.2. Next-nearest-neighbour model ($\gamma \neq 0$)

A qualitatively correct way to include bond-bending forces is to extend the interactions to next-nearest-neighbours in the Born Hamiltonian (equation 1 with $\gamma \neq 0$). This model is rotationally invariant, and has an elastic rigidity threshold equal to the geometrical connectivity threshold.

Two cases are studied here: the first central and the next non-central nearest-neighbour potential ($\delta = 0$ and $\gamma \neq 0$); and the non-central first and second nearest-neighbour potential ($\alpha = \delta \neq 0$) and $\gamma \neq 0$). We will present the results obtained for the case of the site percolation problem. The same behaviour is noted in bond percolation.

In figure 8, we have represented on a log-log scale the DOS $g(\omega)$ versus ω in the case of the first central and second nearest-neighbour model of the 3D site percolating network (10^5) at $p = 0.33$, where the percolating cluster size is 205 312 sites. One can show

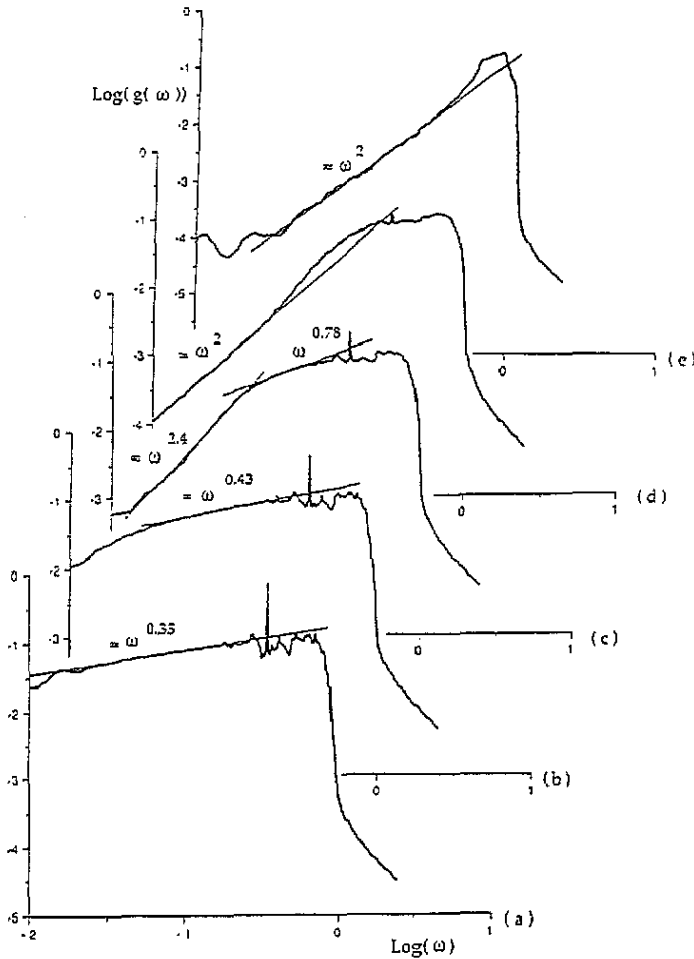


Figure 6. The scalar model DOS $g(\omega)$ on a log-log scale for a 3D bond percolating cluster at different values of p ($p_c = 0.2489$), formed on a 10^3 cubic lattice: The straight lines give the slope of the DOS. (a) $p = 0.265$, (b) $p = 0.3$, (c) $p = 0.4$, (d) $p = 0.5$ and (e) $p = 1$. The percolating cluster sizes are respectively 498 757, 803 796, 1 067 201, 1 133 152 and 1 157 625 sites.

that the more important the ratio γ/α the more rigid the system is, as expected, and zero frequency modes are reduced. For $\gamma \ll \alpha$, the system is fairly soft and the DOS of lower frequencies is important ($\gamma/\alpha = 0.01$). In this case, we note the presence of two different regions. As γ/α increases, the high frequency region decreases, while two new fracton contributions appear in the low-frequency region. The slopes are dependent on γ/α . It is difficult to hold the effective spectral dimensions, but one can observe (for example with $\gamma/\alpha = 0.7$) a characteristic behaviour: particle modes at high frequency and a fracton region, for approximately $\log \omega > -1.5$, exhibits two different contributions with a crossover near $\log \omega \simeq -1.12$; at very low frequencies (for $\log \omega < -1.5$), a phonon regime is expected, (not taken into account by our model). It is, qualitatively, in agreement with previous works (Webman and Grest 1985, Feng 1985a), in the case of the bond-bending model, where the fracton regime appears to be a combination of two contributions associated with bond-stretching motions and bond-bending ones. The latter is less pronounced in our model than in the bond-bending one.

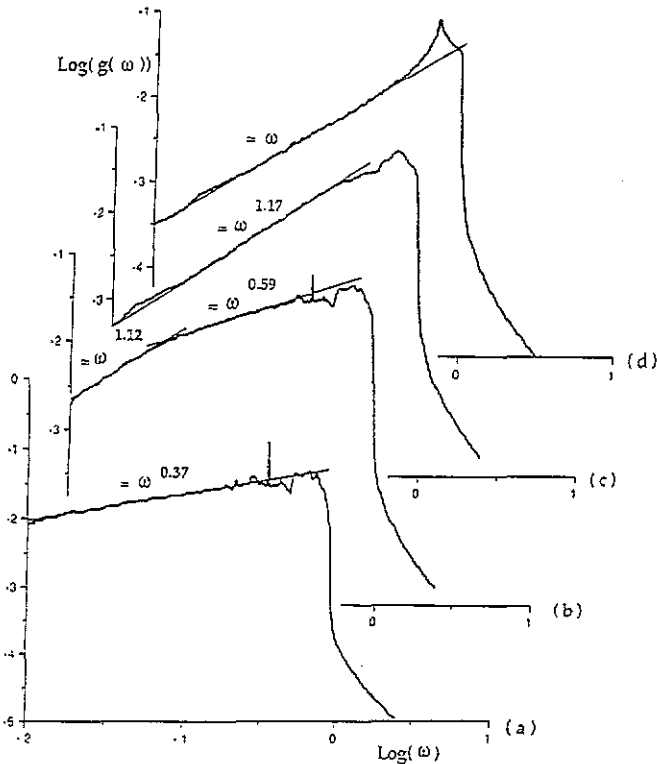


Figure 7. The scalar model DOS $g(\omega)$ on a log-log scale for a 2D bond percolating cluster at three values of p ($p_c = 0.5$), formed on a 1100^2 square lattice: (a) $p = 0.52$, (b) $p = 0.6$, (c) $p = 0.8$ and (d) $p = 1$. The percolating cluster sizes are respectively 954 528, 1 147 654, 1 207 678 and 1 210 000 sites.

Finally, we plot in figure 9 the DOS $g(\omega)$ obtained by the first and second nearest-neighbour model of the 3D site percolating network at $p = 0.4$ ($N = 413\,627$) for three values of the ratio γ/α , versus ω on a log-log scale. This value of p is chosen due to our aim of studying the ω_c evolution. The main feature of this model is that, as in the scalar model, the three regimes are conserved: phonons at low frequencies, particle modes at high frequencies and fractons in the intermediate region. As the ratio increases, we observe, on one hand an increasing of the crossover frequency ω_c , and on the other hand that the upper fracton region shows a deviation of the slope from the scalar one ($\gamma/\alpha = 0$). In order to illustrate the variation of ω_c with γ/α , we have plotted in figure 10(a) on a log-log scale $\omega_c(\gamma/\alpha)$ versus γ/α , the slope is 0.13 ± 0.03 . In figure 10(b) we have plotted the coefficient Ad of the Debye term versus γ/α , and the slope is -0.41 ± 0.02 . By analogy with the bond-bending model we can assume that the sound speed $C_f(p)$ of our system obeys a relation (3b),

$$C_f(p) \sim |p - p_c|^{(f-\beta)/2}$$

where f is the elastic modulus exponent of our present model. At the lower fracton region, the effective spectral dimension is virtually insensitive to the γ/α variation. Thus, in this region one can reproduce the same relations as (2, 3a and 3b), so that the coefficient Ad is

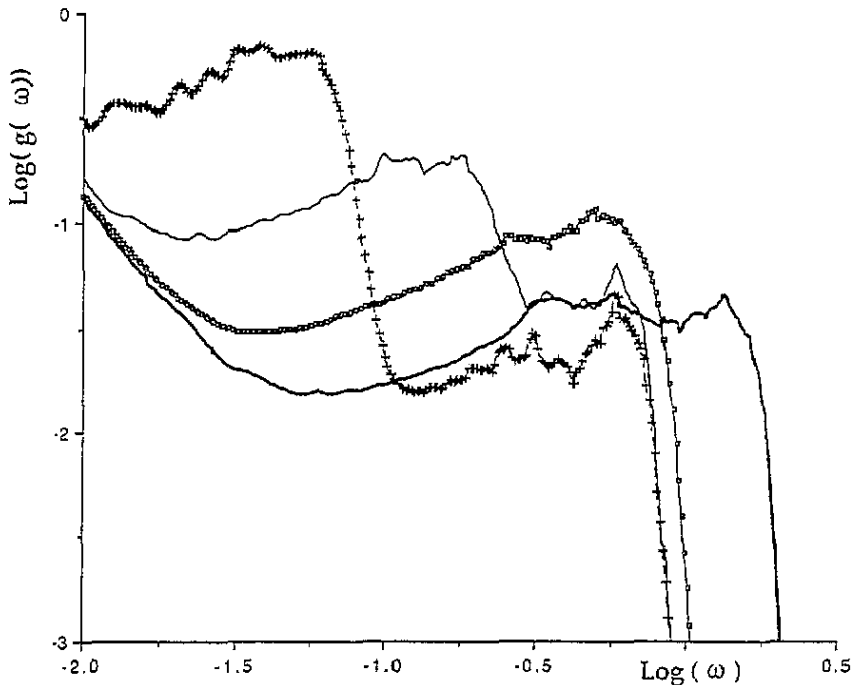


Figure 8. The DOS on a log-log scale for a 3D site percolating network size 10^5 at $p = 0.33$, for four values of γ/α ; $\delta = 0$ (first central and second non-central neighbouring model): $\gamma/\alpha = 0.01$ crosses; $\gamma/\alpha = 0.10$ —; $\gamma/\alpha = 0.70$ open squares; $\gamma/\alpha = 5.00$ —. The percolating cluster size is 205 312 sites.

given by (8),

$$Ad \sim |p - p_c|^{-3(f-\beta)/2} \quad (9)$$

with $\omega_c \sim (\gamma/\alpha)^{0.13 \pm 0.03}$ and $Ad \sim (\gamma/\alpha)^{-0.41 \pm 0.02}$, one can show that the exponent f is given by,

$$f = \frac{2}{3} \left(\frac{0.41 \nu D}{0.13 \bar{d}} + \frac{3\beta}{2} \right) \quad (10)$$

if we suppose that $\bar{d} = \frac{4}{3}$ in (10) then $f = 3.7 \pm 1.0$ which is in the range of the elastic modulus of the bond-bending and granular models (Feng 1985a, b).

3. Discussion and conclusion

In this paper we have studied the dynamical properties of very large 2D and 3D site- and bond-percolating clusters, with different types of interacting potentials. These results complete the results concerning the 2D site percolating networks published in Royer *et al* 1991, 1992a, b. The discussion will take into account the results of these preceding papers.

First, we confirm that for the site- and bond-percolating clusters the effective spectral dimension for the 2D system does not verify the Alexander and Orbach conjecture ($\bar{d} = \frac{4}{3}$).

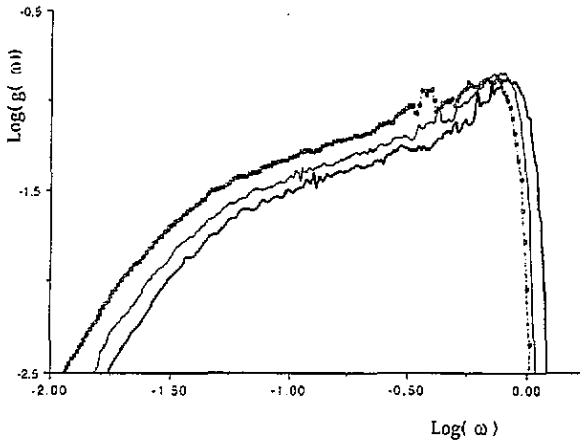


Figure 9. The DOS on a log-log scale for a 3D site percolating network size 10^5 at $p = 0.4$, for three values of $\gamma/\alpha = \gamma/\delta$ (first and second non-central neighbouring model): $\gamma/\alpha = 0.10$ open squares; $\gamma/\alpha = 0.50$ —; $\gamma/\alpha = 5.00$ ——. The percolating cluster size is 413 627 sites.

Further, this exponent is dependent on the choice of probability law in the case of the 2D percolating network. Indeed, for p near p_c , the spectral dimension is 1.302 for the site percolating network (Royer *et al* 1992a), whereas \bar{d} takes the value 1.37 ± 0.02 for the bond one. These values are different from the $\frac{4}{3}$. However, for the 3D networks, we note that \bar{d} , for both types of system, converges to the conjectured value, although the bond case presents a larger effective spectral dimension value ($\bar{d} = 0.35$).

As d increases from 3 to 6 we have found that for site percolating clusters (Royer *et al* 1991, 1992b) \bar{d} is always close to $\frac{4}{3}$ and that the total DOSS are identical, at the percolating threshold, whatever the Euclidean dimension ($d \geq 3$). This effect means that the moments of the DOS are identical for these systems; but the moments of order n are given by the trace of the dynamical matrix at power n :

$$\mu_n = \text{Tr}(D^n).$$

The similarity of the trace of the matrix at the power n , regardless of the Euclidean dimension is strongly related to the connectivity of the system and to the probability of finding a given number of neighbours for a site of the system. In fact, it is strongly connected to the probability of finding a particle on a given site at time t , this particle being on this site at time $t = 0$ (Rammal and Toulouse 1983). At low frequency, i.e. for long time t , the high Euclidean dimension systems will present the same behaviour, due to the large possibilities to travel through the lattice, while in 2D systems it should be more or less problematic, depending on the type (site or bond) of the percolating cluster.

The second point concerns the behaviour of the DOS as p increases from p_c to 1. Let us recall that we do not use on our models any boundary condition. In fact, a periodic model of cubic percolating clusters would present a low-frequency Debye regime under a crossover frequency ω_c . In real physical percolating cluster systems, even near p_c , we will have three regimes: phonon, fracton, and particle. We note however that with the site percolating cluster a phonon regime appears rapidly indicating that the system quickly becomes rigid. Such an effect is absent in the bond percolation (figure 6), where the phonon

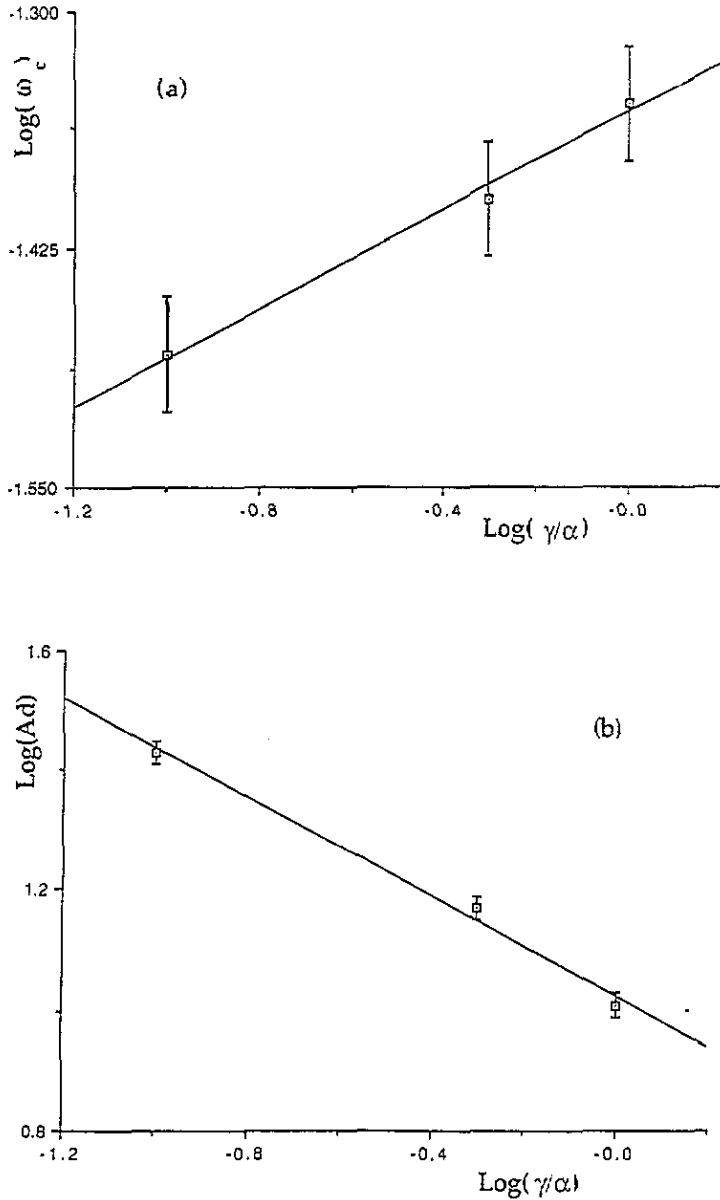


Figure 10. (a) The crossover frequency ω_c ; (b) The coefficient Ad of the Debye term of the first and second non-central neighbouring model dos versus the ratio $\gamma/\alpha = \gamma/\delta$ on a log-log scale, at $p = 0.4$ for a 3D site percolating network of size 105^3 .

regime appears only for p close to 1. These results are very interesting as they show that, for the site percolating networks, a phonon regime is present even for $p = 0.4$, where the system seems to be fractal. In figure 11, we have reported the log-log plot of N versus R_g (the radius of gyration). We note that the fractal dimensionality does not change dramatically when p goes from 0.33 to 0.4 ($D = 2.5$ and $D = 2.6$ respectively), and experimentally the

0.4 percolating network will appear as a good fractal system. However the slope of the DOS jumps from 0.33 to 0.49. The conclusion is that we must be very careful when deducing a spectral dimension from experiments.

The third point concerns the comparison of our calculation with the DOS obtained for silica aerogel (Vacher *et al* 1990). The authors have found four contributions to DOS: the phonon mode region at very low frequency, followed by two distinct regions in the fracton mode regime, and particle modes at high frequency. The authors interpreted their results on the existence of two different scaling behaviours. Based on the work of Feng (1985a), they supposed that a crossover frequency ω'_c exists in the fracton regime, such that, when the frequency $\omega > \omega'_c$, the fracton properties of the system are governed by the bond-stretching motion, which scales the same way as in the scalar model with $\bar{d}_s = 1.9$ –2.2. Whereas, when $\omega < \omega'_c$, the bond-bending motions are dominant with an effective spectral dimension $\bar{d}_b = 0.9$ –1.3. This can be seen in figure 8 where four frequency regimes can be found: a Debye regime (present in the real system), a fracton regime with two kinds of behaviour (for $\gamma/\alpha = 0.7$ for example) and a particle regime. However we note that we have also found two fracton regimes for the bond percolating network with $p = 0.3$ which is close to p_c (0.2488).

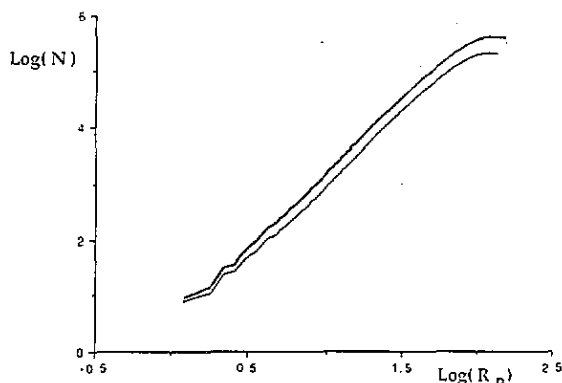


Figure 11. Results for the number of particles N in a site percolating cluster (10^5) at $p = 0.33$ (solid line) and at $p = 0.4$ (bold line) as a function of the radius of gyration R_n , on a log-log scale.

So it seems as a general conclusion of this paper that it is difficult to interpret the experimental data obtained with only a simple model. The DOSs are strongly dependent on the structure, and interacting potential. Therefore, it is necessary to build a model based on the physical reality, i.e. a model using a credible structure and interacting atomic potentials.

References

- Aharony A, Gefen Y, Kapitulnik A and Murat M 1985 *Phys. Rev. B* **31** 4727–7422
 Alexander S 1983 *Phys. Rev. B* **27** 1541
 Alexander S 1984 *J. Physique B* **45** 1939
 Alexander S 1986 *Physica A* **140** 397
 Alexander S 1989 *Phys. Rev. B* **40** 7953
 Alexander S and Orbach R 1982 *J. Phys. (Paris) Lett.* **43** L625
 Angles d'Auriac J C, Benoit A and Rammal R 1983 *J. Phys. A: Math. Gen.* **16** 4039
 Benoit C 1987 *J. Phys. C: Solid State Phys.* **20** 765
 Benoit C 1989 *J. Phys.: Condens. Matter* **1** 335
 Benoit C and Poussiguet G 1989 *High Performance Computing* ed J L Delaye and E Gelenbe (Amsterdam: North Holland) p 347

- Benoit C, Poussigues G and Assaf A 1992a *J. Phys.: Condens. Matter* **4** 3153
- Benoit C, Poussigues G and Azougarh A 1990 *J. Phys.: Condens. Matter* **2** 2519
- Benoit C, Royer E and Poussigues G 1992b *J. Phys.: Condens. Matter* **4** 3125
- Bergman D J 1985 *Phys. Rev. B* **31** 1696
- Born M and Huang K 1956 *Dynamical Theory of Crystal Lattices* (Oxford: Clarendon)
- Courtens E, Pelous J, Phalippou J, Vacher R and Woignier T 1987 *Phys. Rev. Lett.* **58** 128
- Courtens E, Vacher R, Pelous J and Woignier T 1988 *Europhys. Lett.* **6** 245
- de Gennes P G 1976 *J. Phys. (Paris)* **37** L1
- de Leeuw S W, He H and Thorpe M F 1985 *Solid State Commun.* **56** 343
- Derrida B, Orbach R and Kin-Wah Yu 1984 *Phys. Rev. B* **29** 6645
- Feng S 1985a *Phys. Rev. B* **32** 5793
- Feng S 1985b *Phys. Rev. B* **32** 510
- Feng S and Sahimi M 1985 *Phys. Rev. B* **31** 1671
- Feng S and Sen P N 1984 *Phys. Rev. Lett.* **52** 216
- Feng S, Sen P N, Halperin B I and Lobb C J 1984 *Phys. Rev. B* **30** 5386
- Feng S, Thorpe M F and Garboczi E 1985 *Phys. Rev. B* **31** 276
- Grest G S and Webman I 1984 *J. Physique Lett.* **45** L1155
- Gaunt D S and Sykes M F 1983 *J. Phys. A: Math. Gen.* **16** 783
- Kantor Y and Webman I 1984 *Phys. Rev. Lett.* **52** 1891
- Kaplan H 1961 *Phys. Rev.* **125** 1905
- Keating P N 1966 *Phys. Rev. B* **152** 774
- Kirkwood J G 1939 *J. Chem. Phys.* **7** 506
- Landau L and Lifshitz E 1967 *Theorie de l'Elasticité VII* (Moscow: Mir) p 144
- Poussigues G and Benoit C 1990 *Phonons '89 (Heidelberg)* (Singapore: World Scientific) p 165
- Poussigues G, Benoit C, Sauvajol J-L, Lere-Porte J-P and Chorro C 1991 *J. Phys.: Condens. Matter* **3** 8803
- Qiming Li, Soukoulis C M and Grest G S 1990 *Phys. Rev. B* **41** 1713
- Rammal R and Toulouse G 1983 *J. Phys. (Paris) Lett.* **44** L-13
- Reichenauer G, Fricke J and Buchenau U 1989 *Europhys. Lett.* **8** C4
- Roman H E 1990 *J. Stat. Phys.* **58** 375
- Roman H E, Russ S and Bunde A 1991 *Phys. Rev. Lett.* **66** 1643
- Royer E 1992b *Thesis* (Montpellier University, France)
- Royer E, Benoit C and Poussigues G 1991 *High Performance Computing II* ed M Durand and F El Dabaghi (London: Elsevier) (Amsterdam: North-Holland) p 513
- Royer E, Benoit C and Poussigues G 1992a *J. Phys.: Condens. Matter* **4** 561
- Stauffer D 1979 *Phys. Rev.* **54** 1
- Vacher R, Courtens E, Coddens C, Heidemann A, Tsujimi Y, Pelous J and Foret M 1990 *Phys. Rev. B* **65** 1008
- Vacher R, Woignier T, Pelous J and Courtens E 1988 *Phys. Rev. B* **37** 6500
- Webman I and Grest G S 1985 *Phys. Rev. B* **31** 1689
- Wooten F and Weaire D 1987 *Solid State Phys.* **40** 1
- Yakubo K and Yakayama T 1987 *Phys. Rev. B* **36** 8933
- Yakubo K and Yakayama T 1989 *Phys. Rev. B* **40** 517