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Dynamics of percolating networks

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Abstract. The dynamic properties of the 2D percolation network are investigated, using the spectral moments method. The density of states of percolating clusters of size 10^6 or larger is calculated at the percolation threshold p_c and at different occupation probabilities varying from p_c to $p = 1$. As p increases, the phonon, fracton and high frequency regimes appear. These results can be interpreted by assuming that as p increases, the percolating cluster becomes homogeneous, giving rise to a phonon regime at low frequencies and to an accumulation of modes at the Van Hove singularities of the square lattice. The exponent of the coherence length away from the critical point is found to be identical with the mean field value. The localization of modes has been studied by computing the Green functions. Localized and extended modes are present in all the spectrum at p_c, except in the high-frequency zone where all modes are strongly localized.

Over the past few years, fractal structures have been the subject of much attention. The most widely studied systems include the percolation networks which are fractal on smaller length scales than the percolation length ξ_c. Alexander and Orbach (1982) first studied the density of states (DOS) on a fractal basis and suggested with a scaling argument that the DOS obeys a universal law above a characteristic frequency ω_c (fracton modes): $D(\omega) \simeq \omega^{\tilde{d}-1}$ ($\tilde{d}$ is the fracton dimensionality and equals $\frac{4}{3}$ for percolation fractals in all Euclidean dimensions $d \geqslant 2$). Under ω_c, the DOS follows the conventional Debye law (phonon modes) $D(\omega) \simeq \omega^{d-1}$.

Computer simulations which do not require diagonalization have been performed by several workers: Angles d'Auriac *et al* (1983); Derrida *et al* (1984) used an effective-medium approximation treatment (which did not allow them to determine critical exponents); Yakubo and Nakayama (1987, 1989) used the resonance method of Williams and Maris (1985) on large percolating clusters for the 2D and 3D square lattice; Qiming Li *et al* (1990) studied the Sturm sequence method. They all found a dimensionality close to $\frac{4}{3}$. In 1984, Aharony and Stauffer (1984) suggested that, for $d = 2$, $\tilde{d} = \frac{182}{139} = 1.309$ which is 2% lower than $\frac{4}{3}$ and this was confirmed by Keramiotis *et al* (1985). However, following Qiming Li *et al* (1990), $\frac{4}{3}$ is a good approximation, although it is probably not the exact value in all Euclidean dimensions (Normand *et al* 1988, Roman 1990). The existence of a hump or a steepness in the crossover region of the DOS in percolating clusters has been extensively discussed with contradictory results.

It has also been suggested that the fracton wavefunction has the superlocalized form

$$\Psi(r) \simeq \exp[-\tfrac{1}{2}(r/\xi(\omega))\, d_\Phi] \tag{1}$$

where $\xi(\omega)$ is the localization length and the exponent d_Φ is larger than 1. Levy and

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Souillard (1987) suggested that d_Φ equals 1.42; Aharony *et al* (1987) suggested 0.95. Recent studies, by De Vries *et al* (1989), Qiming Li *et al* (1990) and Roman *et al* (1991) observe no evidence for fracton superlocalization. Yakubo and Nakayama (1989) found d_Φ equal to 2.3, which is not consistent with any theoretical predictions.

To clarify these points, we were interested to apply our new method, the spectral moments method, which is a powerful tool for determination of linear responses (infrared, Raman scattering or inelastic neutron scattering) of harmonic systems (Benoit 1987, 1989, Benoit and Poussigue 1989). Recently, we found that the spectral moments method could provide, with some variations, the total DOS with good accuracy and the Green functions of systems. The detailed computing aspect of the method will be published elsewhere (Benoit *et al* 1991). This method allows us to work with a very large percolating cluster (up to 2×10^6). The localization of fractons is then computed with smaller lattices.

We have studied a 2D 1415×1415 square lattice at and above the percolation threshold p_c ($=0.593$), for four values of the occupation probability, to compute the DOS.

We assume now that atoms with mass m are placed at the sites of the lattice and are connected by springs. The displacements of the particles are represented by scalars; for instance, the motion is in an orthogonal direction to the plane of the lattice.

Then the set of equations of motion for site i is given by

$$m\ddot{U}_i = -\sum_j k_{ij} U_j \tag{2}$$

where $k_{ii} = -\Sigma_{j \neq i} k_{ij}$, U_j is the scalar displacement of the site j and k_{ij} are the force constants between the atoms i and j, equal to 0.125 if i and j are occupied and to 0 otherwise.

Following Aharony *et al* (1985), the DOS can be written

$$D(\omega, p) \simeq A\omega^{\tilde{d}-1} F(\omega/\omega_c) \tag{3}$$

where $F(x) = 1$ for $x \gg 1$, $F(x) = x^{d-\tilde{d}}$ for $x \ll 1$ and

$$\omega_c \approx (p - p_c)^{\nu D/\tilde{d}} \tag{4}$$

(ν is the correlation length exponent and D is the fractal (Hausdorff) dimension). For $d = 2$, $D = \frac{91}{48}$, $\nu = \frac{4}{3}$ (Stauffer 1985) and then, with $\tilde{d} = \frac{4}{3}$, $\nu D/\tilde{d} = 1.931$.

To test the accuracy of the method, we first compared the result of the moments technique for the DOS, and the exact result obtained for a regular 1415×1415 square lattice. We observed that excellent agreement is obtained; see figures 1(*e*) and 2(*e*) where the DOS is plotted versus ω and versus $u = \omega^2$, respectively.

Computations were performed from the probability $p \simeq p_c = 0.6$ to $p = 1$, with a step of 0.1, on the same lattice. The sizes of the percolating clusters and the computing times are given in table 1. The CPU times (1) are times to construct the dynamical matrix and to find the percolating cluster; the CPU times (2) are times to compute the DOS of this cluster. At $p = 1$, a unique program is used, since all the sites of the lattice form the cluster. We plot the DOS of $\log[D(\omega)]$ versus $\log \omega$ and the DOS $G(u)$ versus u, where $u = \omega^2$, in figures 1 and 2. The DOS is normalized to 1 for every figure.

In figure 1(*a*) for $p = 0.6$, the full line is the tangent of the DOS, and its slope is exactly 0.302, which is very close to 0.309. We therefore confirm the Aharony–Stauffer conjecture although 0.309 is nevertheless a good approximation of $\frac{1}{3}$. Several peaks in the DOS at $p = p_c$ (figure 2(*a*)) are localized at the following square frequencies: 0.068; 0.125; 0.170; (0.250); 0.284; (0.331); 0.370; 0.427; 0.512; (0.594); 0.637; 0.700 (where

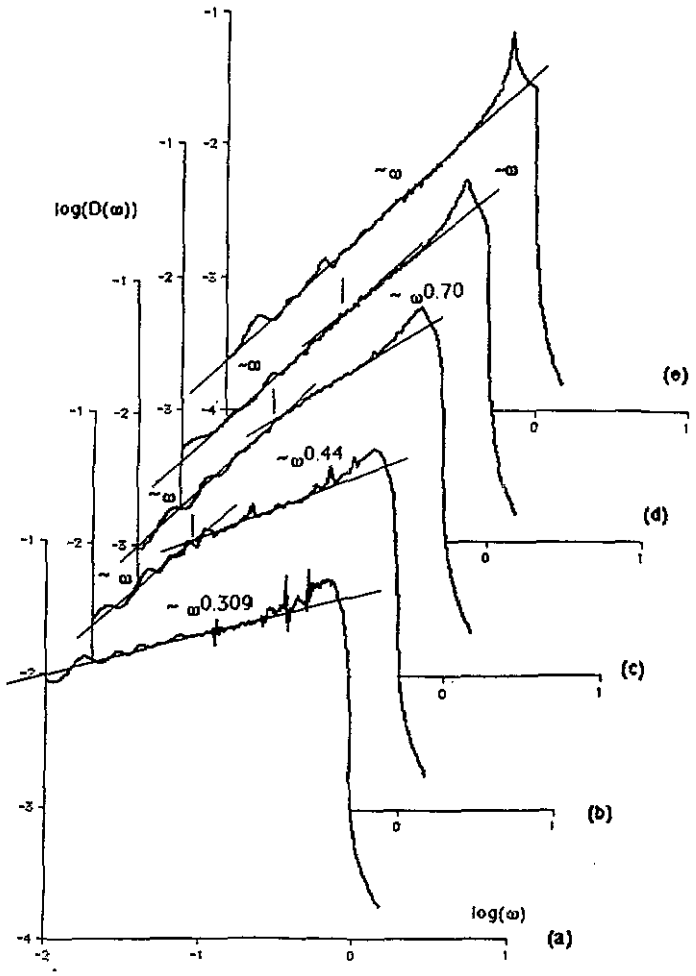

Figure 1. Density of states on a log–log scale of the percolating cluster at different occupation probabilities p, formed on a 1415 × 1415 square lattice: the straight lines are only guide for the eyes and give the slope of the DOS and ω_c. (*a*) $p = 0.6 \simeq p_c$; (*b*) $p = 0.7$; (*c*) $p = 0.8$; (*d*) $p = 0.9$; (*e*) $p = 1$.

the frequencies in parentheses correspond to peaks with low intensity). These results prove that, at the percolating threshold, regions with few sites are mainly present and behave as a homogeneous small ($n \times n$) square lattice ($2 \leqslant n \leqslant 10$). These frequencies are found when a small regular square lattice is computed, except for the two frequencies 0.284 and 0.512, which seem to be the frequencies corresponding to 0.25 and 0.5 for a small square lattice, maybe displaced because regions are connected to each other.

Above p_c (figure 1(*b*), $p = 0.7$; figure 1(*c*), $p = 0.8$; figure 1(*d*), $p = 0.9$; figure 1(*e*), $p = 1$) we observe three clear regimes; at lower frequencies than ω_c, the slope of the tangent of the DOS is about 1 so that the Debye law holds. At medium frequencies, the Aharony–Stauffer rule does not hold any longer above ω_c since, as p increases from p_c, the slope increases from 0.302 to 1. This is a new result; most percolation networks have been studied near the percolation threshold, so that the slope of the

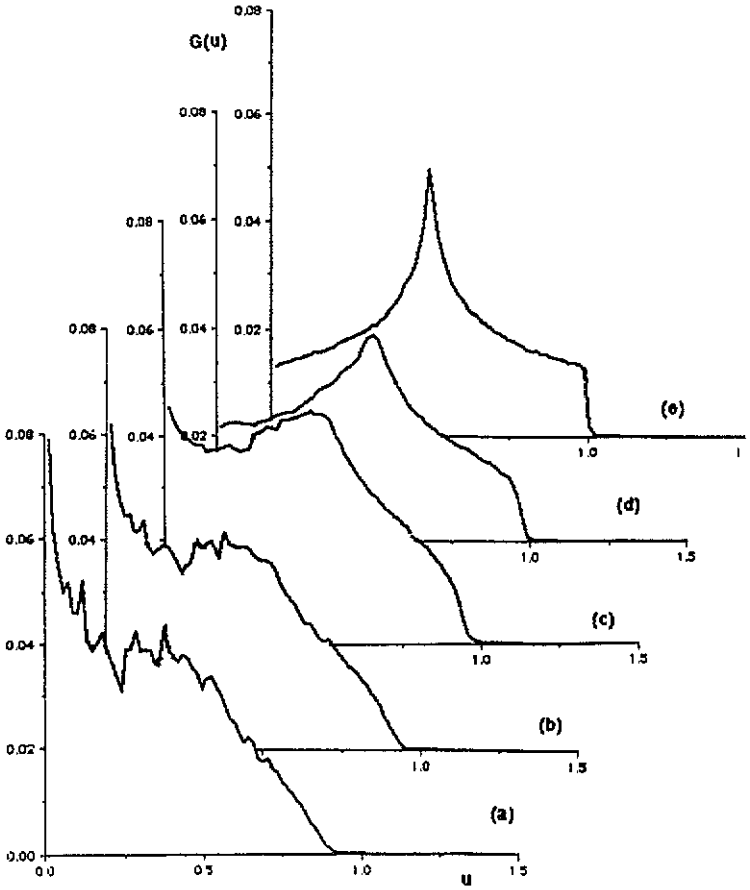

Figure 2. Plot of DOS versus $\mu = \omega^2$ at different occupation probabilities p for a 1415 × 1415 square lattice: (*a*) $p = 0.6 \simeq p_c$; (*b*) $p = 0.7$; (*c*) $p = 0.8$; (*d*) $p = 0.9$; (*e*) $p = 1$.

Table 1. p (the occupation probability of the percolation network), the sizes (the numbers of sites of the percolating cluster, formed on a 1415 × 1415 square lattice), the CPU times (1) (the times to find the percolating cluster and construct the dynamical matrix) and the CPU times (2) (the times to compute the DOS of the percolating cluster).

		CPU time	
p	Size	(1)	(2)
0.6	904 068	39 min 49 s	6 min 32 s
0.7	1 378 975	10 min 03 s	7 min 15 s
0.8	1 599 431	5 min 41 s	7 min 56 s
0.9	1 802 855	3 min 29 s	8 min 41 s
1	2 002 225	9 min 21 s	

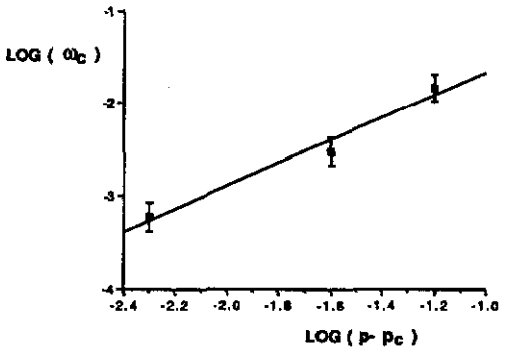

Figure 3. The characteristic frequency ω_c versus $|p - p_c|$ on a log–log scale.

tangent remains an approximation of $\frac{1}{3}$. Now, above p_c, the percolating cluster loses its fractal properties since it causes the regular square lattice to fill up and it becomes homogeneous as p grows. It is clear that equation (3) does not represent the DOS of the percolation network. Such a conclusion has already been mentioned by Yakubo *et al* (1990), when considering the magnitude of the DOS in the fracton regime. Hence, at maximum frequencies, we confirm the accumulation of 'missing modes' (Yakubo *et al* 1990) in the upper end of the fracton range at the Van Hove singularities which are the points $(\pi/a, 0)$ $(0, \pi/a)$ and $(\pi/a, \pi/a)$ of the boundary of the first Brillouin zone of the square lattice (a is the atomic distance taken to be 1 here). This is very well confirmed by figure 2 where the DOS is plotted versus u. These three regimes are called phonon modes, fracton modes and particle modes by Vacher *et al* (1990). Figure 1 tells us that the DOS does not exhibit a hump or a steepness in the crossover region.

In figure 3, we plot on a log–log scale, the frequency ω_c versus $|p - p_c|$. As expected, ω_c approaches zero when p approaches p_c. The slope of the straight line is 0.7 ± 0.2 which is in agreement with the work of Qiming Li *et al* (1990), who find a value of 1.0 ± 0.3 although the scaling theory predicts 1.913 (equation (4)). They suggested that this discrepancy is due to the difficulty in determining ω_c exactly. However, as the same result is obtained by two different numerical methods, it is necessary to analyse these results a little more. Some values of p used in this work are very far from the percolating threshold p_c and the corresponding clusters no longer have a fractal structure so that the scaling law is not, strictly speaking, true. From the work of Alexander and Orbach, the lowest frequency of the fracton modes, ω_c behaves as $\omega_c \approx (\xi_c)^{-D/d}$. In the percolation network, we have (Stauffer 1985, Feder 1988) $\xi_c \approx |p - p_c|^{-\nu}$ so that equation (4) holds close to the critical point. However, far from the critical point, percolation clusters may be described by characteristic length with a different critical exponent. If we assume that

$$\xi_c = |p - p_c|^{-\varphi} \tag{5}$$

for $p \gg p_c$, then

$$\omega_c \simeq |p - p_c|^{-\varphi D/d} \tag{6}$$

and comparison with experimental data gives $\varphi \simeq 0.5$. This is generally the classical mean field value in phase transitions. However, it is not clear to us why such a value is obtained here, although it is well known that the spatial range of magnetic correlations diverges with the same exponent as the percolation problem (Klein *et al* 1978, Stoll and Domb 1979).

In order to study the localization or extended nature of eigenstates in the fracton regime, we used the imaginary part of the Fourier transform of the time-dependent position correlation function given by (with unity masses) (Maradudin 1969)

$$H(n, n', \omega) = 2\pi\hbar[n(\omega) + 1] \sum_j e_n(j) e_{n'}(j) \frac{1}{2\omega_j} [\delta(\omega - \omega_j) - \delta(\omega + \omega_j)] \tag{7}$$

where ω_j and $e_n(j)$ are the frequency and the amplitude of mode j, and $n(\omega)$ is the Boltzmann factor. This function indicates the influence of the atom n on the atom n'; if it vanishes, there is no correlation between the atoms n and n'. The direct computation of $H(n, n', \omega)$ presents some difficulties and we worked with the following function:

$$\begin{aligned}\sigma(n, n', \omega) &= \sum_j e_n(j) e_{n'}(j) \frac{1}{2\omega_j} [\delta(\omega - \omega_j) + \delta(\omega + \omega_j)] \\ &= \sum_j e_n(j) e_{n'}(j) \delta(u - \lambda_j) = S(n, n', u)\end{aligned} \tag{8}$$

with $u = \omega^2$, $\lambda_j = \omega_j^2$ which is identically $\{1/2\pi\hbar[n(\omega) + 1]\}$ $H(n, n', \omega)$ for $\omega > 0$, symmetrical and independent of the temperature. It can be shown that, with $z = u + i\varepsilon$,

$$S(n, n', u) = (-1/\pi) \lim_{\varepsilon \to 0^+} \{\mathrm{Im}[h(n, n', z)]\}. \tag{9}$$

As the imaginary part of $h(n, n', z)$ is not a positive function everywhere, the moments method does not work directly. We thus define two positive functions the combination of which gives h, and now the moments method is applied (detailed technical aspects of the method will be published elsewhere (Benoit *et al* 1991)).

The localization of the eigenmodes is often characterized by the inverse participation ratio $P_n^{-1}(u) = \sum_{i=1}^{N} |\Phi(r_i, u)|^{2n}$, which is a measure of the effective number of sites covered by a normalized eigenstate Φ (De Vries *et al* 1989). However, first here the normalization constant of the eigenstates is unknown and secondly the presence of the Dirac function gives some difficulties. So we prefer to determine the second and the fourth spatial isotrope moments of the correlation function. For a given frequency ω (or u), the function $S(n, n', u)$ is proportional to the wave packet amplitude of the modes centred on ω (or u). We used equation (8) to calculate the second and the fourth moments of the spatial distribution of the amplitude; let us define

$$\mu_2(u) = \sum_{n'} |S(n, n', u)| (r_n - r_{n'})^2 \tag{10}$$

$$\mu_4(u) = \sum_{n'} |S(n, n', u)| (r_n - r_{n'})^4. \tag{11}$$

Then the localization ratio is

$$P(n, u) = \mu_4(u)/\mu_2(u). \tag{12}$$

Moreover $P(n, u)$ is small, and the modes are localized.

To analyse these results, we supposed that the eigenmodes vary as equation (1) with $d_\Phi = 1$. We use it as a trial function and we determine the localization ratio $L(\xi)$ for several values of ξ, using the same distances as used for the determination of (12) (figure 4). Here the atom n is the atom of 'the centre' of the percolating cluster.

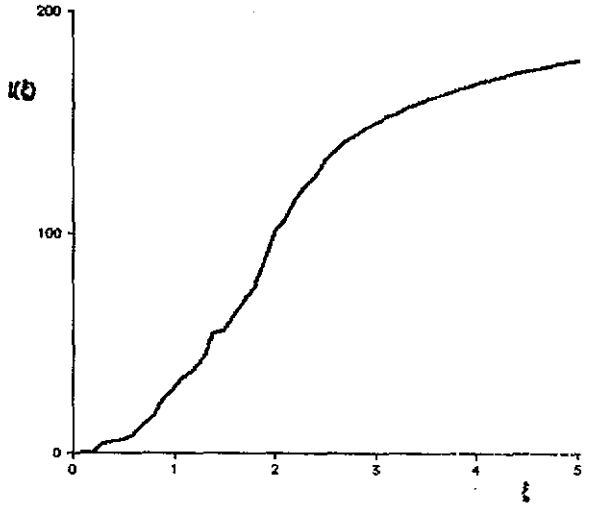

Figure 4. Localization ratio calculated assuming that the eigenmodes vary as equation (4): $L(\xi)$ versus ξ.

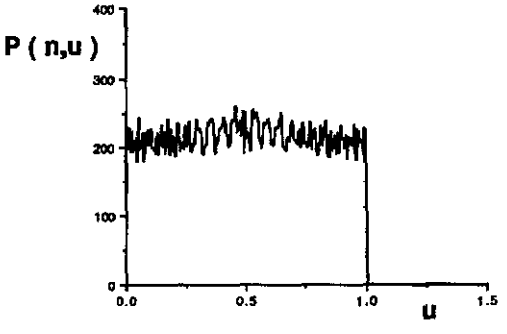

Figure 5. The localization ratio $P(n, u)$ versus u for the regular square lattice.

We have performed the calculations on a 100×100 square lattice, at different occupation probabilities; the atoms n' are randomly chosen in a circle of radius of 15 atomic distances and the average is performed over 60 atoms. We give the results in figures 5 and 6, in which we plot the ratio $P(n, u)$ versus u and in figure 7 versus $\log u$.

As expected, for the regular square lattice (figure 5), all the modes are extended. From figure 6(a) for $p = 0.9$, figure 6(b) for $p = 0.8$, figure 6(c) for $p = 0.7$ and figure 6(d) for $p = 0.6$, we observe that, as p decreases to the percolation threshold, the high-frequency modes become more and more localized, rather quickly. At $p = 0.9$, we observe that the region around $u = 0.25$ tends to be localized, a tendency confirmed at $p = 0.8$, 0.7 and 0.6; hence the mode about 0.05 is localized from $p = 0.8$ to $p = 0.6$. From figure 7(d) for $p = 0.6$, we observe a very-low-frequency region (around $u = 0.015$) where the modes tend to be localized ($\xi \simeq 2$; see figure 4).

With a new numerical method which allows us to investigate percolating clusters of greater size than previously studied clusters, we find that the DOS obeys three characteristic regimes: for medium frequencies a power-law behaviour occurs and for lower frequencies the Debye law holds, while at the maximum frequencies the

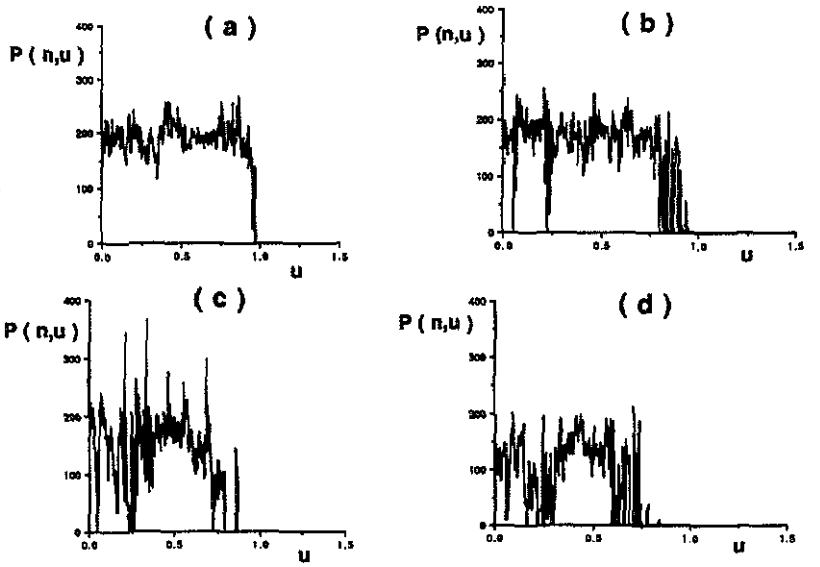

Figure 6. The localization ratio $P(n, u)$ versus u for the percolating cluster: (*a*) $p = 0.9$; (*b*) $p = 0.8$; (*c*) $p = 0.7$; (*d*) $p = 0.6$.

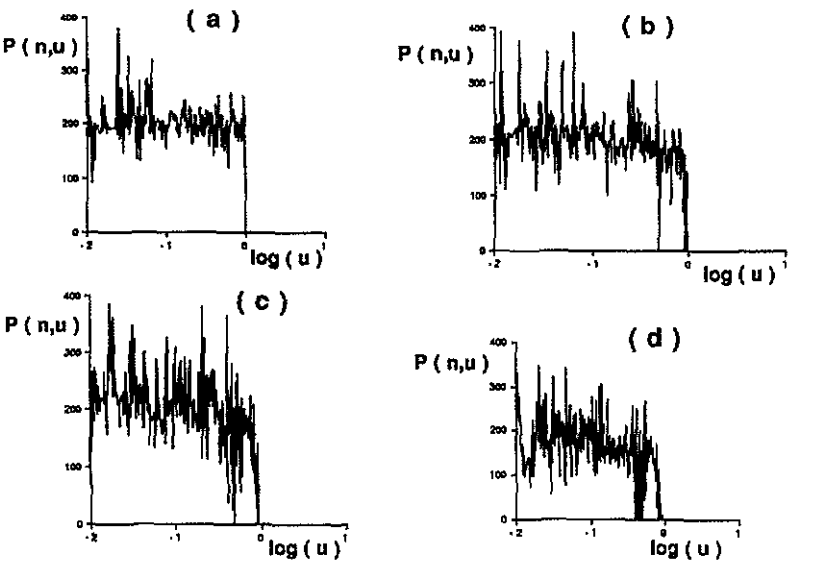

Figure 7. The localization ratio $P(n, u)$ versus $\log u$ for the percolating cluster: (*a*) $p = 0.9$; (*b*) $p = 0.8$; (*c*) $p = 0.7$; (*d*) $p = 0.6$.

Van Hove singularities appear. So, at $p > p_c$, the system appears as a whole, on length scales much greater than ξ_c, homogeneous while, on length scales much less than ξ_c, parts of it behave as homogeneous, their contribution increasing as p increases from p_c. The DOS is smoothly connected and no hump in the crossover region is exhibited. Finally, the characteristic frequency ω_c obeys a power law, giving a correlation length exponent equal to the mean field classical value. With reference to the localization or extended nature of eigenstates in fracton regime, unfortunately

our method does not allow us to calculate the exponent d_Φ exactly. We observe localization for higher frequencies and some lower frequencies but we cannot draw any conclusions about localization or superlocalization.

This work will allow us to study models which are closer to physical reality.

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