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Dynamic structure factor of percolation clusters at criticality

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Abstract. The dynamic structure factor of very large percolating clusters (bond and site), in two dimensions and three dimensions are calculated using the spectral moments method. Interactions are represented by the scalar model. Numerical results are presented and interpreted in terms of scaling arguments given by Alexander, Courtens and Vacher (ACV) in 1993. Concerning the $q\lambda \ll 1$ limit, our results confirm and supplement previous numerical work and are in agreement with the scaling behaviour theoretically deduced by ACV. Concerning the $q\lambda \gg 1$ limit, we have shown that the dynamic structure factor complies with the very nice asymptotic behaviour $g(q,\omega) = q^{\gamma} H(q\lambda(\omega))$ where the scaling function $H(x)$ is of power-law form $x^{-\tau'}$ in agreement with the theory. However, our results indicate a scaling behaviour with exponents that differ from those deduced by theory. The values obtained for τ' are 1.20 for the two-dimensional bond and site percolating lattices, and 1.00 for the three-dimensional percolating lattices. Comparisons with previous simulations are reported.

1. Introduction

One way of studying materials is to scatter particles from them. Two examples of this type of experiment are Raman scattering of light and scattering of thermal neutrons. These different types of scattering can be treated with the same formalism. The differential cross section $\sigma(q,\omega)$ is directly related to the Fourier transform of the thermodynamics correlation function $g(q,\omega)$, where $\hbar q$ and $\hbar\omega$ are the momentum and the energy transferred by the particle to the sample. In a perfect crystal, the displacement field can be developed by plane waves and it is easy to show that, from the Bloch theorem, determination of the correlation functions simply involves the computation of the inelastic structure factor of the unit cell. In the presence of disorder, the system must be considered as a large macromolecule and determination of the correlation functions is much more difficult. Two methods have been developed to determine these quantities. The first method consists of directly computing the differential cross section from models where the positions of particles and potential are known. Concerning percolating networks, such computations have been done, using different techniques such as direct diagonalization (Montagna *et al* 1990, Stoll *et al* 1992), resonance methods (Yakubo and Nakayama 1989) or the spectral moments method (Benoit *et al* 1992b). The spectral moments method directly provides

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the exact inelastic scattering cross section of very large systems and has been applied to determination of Raman scattering in polythiophene (Poussigue *et al* 1991) and in ordered and disordered Sierpinski gaskets (Benoit *et al* 1992a), and to inelastic neutron scattering of quasicrystals such as the Fibonacci chain (Benoit *et al* 1990) and i-AlMn (Poussigue *et al* 1994). Recently, applications of the method to the study of the propagation of sound waves and electromagnetic waves in heterogeneous systems with or without energy dissipation have been developed (Benoit *et al* 1995).

Another approach using dynamic scaling considerations, without a specific physical model, was developed by Alexander (1989) and Alexander, Courtens and Vacher (ACV) (1993) in order to interpret a variety of inelastic experiments in fractal materials such as sol–gel glasses (Boukenter *et al* 1986, Freltoft *et al* 1987), borate glasses (Fontana *et al* 1987), silica aerogel (Tsujimi *et al* 1988, Vacher *et al* 1990) and metal colloids (Duval *et al* 1987, 1992). In this work, they postulated that vibrations of random fractals should be characterized by a single unique length scale which combines the roles of a wavelength, a scattering length and a localization length. They also related the dynamic correlation function to the average strain of the fractal mass distribution. Alexander (1989) proposed a scaling form for the dynamic structure factor and introduced a new and independent exponent σ related to the average coherent strain of fractons. The first attempt to compute the dynamic structure factor and light scattering was done by Montagna *et al* (1990), using a diagonalization technique. They obtained results for site percolating (SP) networks formed on 65×65 square lattices and $29 \times 29 \times 29$ cubic lattices and claimed that the fracton excitations cannot be scaled by a single length scale. However, the single-length-scale postulate (SLSP) was confirmed by Stoll *et al* (1992), who calculated the dynamic structure factor for the bond percolating (BP) network, using a direct diagonalization technique, for 68×68 square lattices and $21 \times 21 \times 21$ cubic lattices and by Nakayama and Yakubo (1992), using a resonance technique, for SP networks formed on 500×500 square lattices.

To clarify some discrepancy between the numerical results obtained by the workers cited above, we developed a systematic study of the dynamical structure factor on very large SP and BP networks in two dimensions (500×500 square lattice) and three dimensions ($85 \times 85 \times 85$ cubic lattice) using the spectral moments method (Benoit *et al* 1992b).

Before presenting the results and discussion, we shall introduce the scaling arguments of the dynamic structure factor, as proposed by Alexander (1989) and ACV (1993), in order to interpret our numerical results.

2. Scaling theory on the dynamic structure factor

Work on the dynamics of a percolating network has been fundamentally affected by the paper of Alexander and Orbach (AO) (1982). In this paper, AO (1982) considered that scaling with the frequency ω of the fracton density of states is

$$N(\omega) \approx \omega^{\tilde{d}-1} \tag{1}$$

where the spectral dimension $\tilde{d}$ is conjectured to be equal to 4/3, in the case of scalar elasticity, independently of the fractal dimension D of the percolating network. This conjecture was confirmed by many simulations (Yakubo and Nakayama 1987, 1989, Russ *et al* 1991, Royer *et al* 1991, 1992, Rahmani *et al* 1993) (see also the review paper by Nakayama *et al* (1994)). The dispersion relation between the localization length and the frequency ω is

$$\lambda(\omega) \sim \omega^{-\tilde{d}/D}. \tag{2}$$

The following arguments are derived from the theory proposed by ACV (1993). In this work, they postulated that the vibrations of fractals should be characterized by a single unique length scale which combines the roles of a wavelength, a scattering length and a localization length. This SLSP was confirmed by simulations (Stoll *et al* 1992).

The inelastic cross section is directly related to the displacement–displacement correlation function, which is given by

$$G(q,\omega) = (n(\omega)+1)\sum_j |a_j(q)|^2 \frac{(\delta(\omega-\omega_j)-\delta(\omega+\omega_j))}{2\omega_j}$$
$$\approx \frac{kT}{\omega^2}\sum_j |a_j(q)|^2 \delta(\omega-\omega_j) \tag{3}$$

for $\omega > 0$, with $n(\omega)+1 \sim kT/\omega$ and

$$a_j(q) = \sum_{n\alpha} q_\alpha \langle \alpha n|j\rangle \exp(\mathrm{i}q\cdot r_n) \tag{4}$$

where r_n is the equilibrium position of the nth particle, ω_j and $\langle \alpha n|j\rangle$ are the frequency and the (αn) components of the eigenvector $|j\rangle$ of the jth mode, $\alpha = x, y, z$ are the Cartesian indices, kT is the thermal energy and q_α is the component α of q.

The dynamic correlation function or dynamic structure factor $g(q,\omega)$ is defined by

$$g(q,\omega) = \sum_j |a_j(q)|^2 \delta(\omega-\omega_j). \tag{5}$$

Assuming the validity of the SLSP, in the case of scalar elasticity, the function $g(q,\omega)$ has a universal scaling form and depends only on the single length scale $\lambda(\omega) \sim \omega^{-\tilde{d}/D}$:

$$g(q,\omega) = q^y H(q\lambda(\omega)) \tag{6}$$

where $q = |q|$.

ACV postulate an asymptotic behaviour of the scaling function $H(x)$ of a power-law form,

$$H(x) \sim \begin{cases} x^\tau & \text{for } x \ll 1 \\ x^{-\tau'} & \text{for } x \gg 1. \end{cases} \tag{7}$$

τ and τ' are new scaling positive exponents. It describes the modulation of the density in space by vibrations.

2.1. The $q\lambda \ll 1$ limit

The dynamic structure factor is directly connected, for a given frequency ω, to the q Fourier component of the eigenvectors of fractons with a frequency ω_j close to ω. In the $q\lambda \ll 1$ limit, we are concerned about the Fourier components of the eigenvectors which correspond to a wavelength much larger than the length scale. This limit thus corresponds to long-range motion. Within a vibrating region v_j, in the small-q limit, we can expand $\exp(\mathrm{i}q\cdot r_n)$ as

$$\exp(\mathrm{i}q\cdot r_n) = \exp[\mathrm{i}q\cdot(r_n - R^j) + \mathrm{i}q\cdot R^j]$$
$$= \exp(\mathrm{i}q\cdot R^j)[1 + \mathrm{i}q\cdot R_n^j + \cdots] \tag{8}$$

where $R_n^j = r_n - R^j$ and R^j is the 'centre' of the vibration j defined by

$$R^j = \sum_{\alpha n} |\langle \alpha n|j\rangle|^2 r_n \Big/ \sum_{\alpha n} |\langle \alpha n|j\rangle|^2. \tag{9}$$

The quantity $a_j(q)$ defined in [4] can be written as

$$a_j(q) = \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}^j)\sum_{\alpha\beta} q_\alpha D^j_{\alpha\beta} q_\beta \tag{10}$$

where

$$D^j_{\alpha\beta} = \sum_n R^j_{n\beta}\langle \alpha n|j\rangle \tag{11}$$

or in dyadic form

$$\tilde{D}^j = \sum_n \boldsymbol{R}^j_n \otimes v^j(n) \tag{12}$$

with $v^j_\alpha(n) = \langle \alpha n|j\rangle$. This quantity (12) characterizes the jth fracton. This averages out all details of the internal motion, and it is only sensitive to the average relation between the vibrational amplitudes and the position within the jth fracton. Defining an average strain tensor $\tilde{\mathbf{e}}^j(r)$, it can be shown that

$$D^j_{\alpha\beta} = \sum_n R^j_{n\beta} v^j_\alpha(\boldsymbol{R}^j) + \sum_\delta R^j_{n\beta} R^j_{n\delta} e^j_{\alpha\delta}(r) \tag{13}$$

where

$$e^j_{\alpha\beta} = \left(\frac{\partial v^j_\alpha(r)}{\partial x_\beta}\right)_0. \tag{14}$$

The first term equals zero and equation (12) can be written as the dyadic product

$$\tilde{D}^j = \sum_{n\in\nu_j} (\boldsymbol{R}^j_n \otimes \boldsymbol{R}^j_n)\cdot\tilde{\mathbf{e}}^j. \tag{15}$$

Since the $\boldsymbol{R}^j$ in the vibrating region ν_j are all of the order of λ, we obtain a scaling relation relating the magnitude of $\tilde{D}$ and $\tilde{e}$:

$$D^j \sim \lambda^{D+2} e^j. \tag{16}$$

Alexander (1989) assumes the scaling form

$$\langle \tilde{e}^2\rangle \sim \langle v^2\rangle \lambda^{-2\sigma} \tag{17}$$

where σ is a new scaling index describing modulation of the density in the embedding space by the vibration. The mean-squared amplitude is given by

$$\langle v^2\rangle \sim \lambda^{-D}. \tag{18}$$

By equation (5), one obtains

$$g(q,\omega) \sim N(\omega)\sum_j |a_j(q)|^2. \tag{19}$$

From equations (10), (16) and (17) and using the relations (1) and (2), one obtains that

$$g(q,\omega) \sim q^\gamma \omega^{-\alpha} \tag{20}$$

where $\gamma = 4$ and

$$\alpha = 1 - (2\sigma - 4)\tilde{d}/D. \tag{21}$$

To preserve the scaling form (equations (6) and (7)), one deduces that

$$y = 2\sigma - D/\tilde{d} \tag{22}$$

and

$$\tau = \frac{D}{\tilde{d}}\alpha. \tag{23}$$

2.2. The $q\lambda \gg 1$ limit

In this limit, we are concerned about the Fourier components of the eigenvectors which correspond to a wavelength much smaller than the length scale. The phase factor $\exp(i\boldsymbol{q}\cdot\boldsymbol{r}_n)$ is therefore uniform over small regions of size $l_q \sim q^{-1} \ll \lambda$.

The vibrating region ν will contain $(\lambda/l_q)^D \sim (q\lambda)^D$ blobs of this size. Each blob will contain $(qa)^{-D}$ particles. With $\boldsymbol{R}^{jb}$, the centre of the mass of particles in the blob b in the fracton region ν_j (small by construction), one obtains

$$\begin{aligned}\exp(i\boldsymbol{q}\cdot\boldsymbol{r}_n) &= \exp[i\boldsymbol{q}\cdot(\boldsymbol{r}_n - \boldsymbol{R}^{jb}) + i\boldsymbol{q}\cdot\boldsymbol{R}^{jb}] \\ &= \exp(i\boldsymbol{q}\cdot\boldsymbol{R}^{jb})[1 + i\boldsymbol{q}\cdot\boldsymbol{R}_n^{jb} + \cdots]\end{aligned} \tag{24}$$

where $\boldsymbol{R}_n^{jb} = \boldsymbol{r}_n - \boldsymbol{R}^{jb}$. Therefore the quantity

$$a_j(q) \approx \sum_b \exp(i\boldsymbol{q}\cdot\boldsymbol{R}^{jb}) \sum_{\substack{\alpha \\ n\in b}} q_\alpha \left[1 + i\sum_\beta q_\beta R_{n\beta}^{jb}\right]\langle\alpha n|j\rangle. \tag{25}$$

Let us define U_α^{jb}, the average displacement on the blob of volume V_b, by

$$U_\alpha^{jb} = \frac{1}{V_b}\sum_{n\in b}\langle\alpha n|j\rangle \sim q^D \sum_{n\in b}\langle\alpha n|j\rangle. \tag{26}$$

So one obtains

$$a_j(q) \approx \sum_{b\alpha} q_\alpha q^{-D} U_\alpha^{jb} \exp(i\boldsymbol{q}\cdot\boldsymbol{R}^{jb}) + i\sum_b \exp(i\boldsymbol{q}\cdot\boldsymbol{R}^{jb}) \sum_{n\in b} q_\alpha q_\beta R_{n\beta}^{jb}\langle\alpha n|j\rangle. \tag{27}$$

Phase factors $\exp[i\boldsymbol{q}\cdot(\boldsymbol{R}^{jb} - \boldsymbol{R}^{jb'})]$ clearly appear in evaluating $g(q,\omega)$ (equation (3)). For larger q and very disordered systems, one has to conclude that there is no coherence between the scattering of different blobs.

Thus, $g(q,\omega)$ is composed of two contributions:

$$g(q,\omega) = g_1(q,\omega) + g_2(q,\omega) \tag{28}$$

where the first term results from the separate motion of blobs and is given by

$$g_1(q,\omega) = \sum_j (q\lambda)^D [q^{-D}\boldsymbol{q}\cdot\boldsymbol{U}^{jb}]^2 \delta(\omega - \omega_j) \tag{29}$$

and the second is related to the internal strain of the blob due to the jth fracton and is given by

$$g_2(q,\omega) = \sum_j (q\lambda)^D \left[\sum_{\substack{\alpha\beta \\ n\in b}} q_\alpha q_\beta R_{n\beta}^{jb}\langle\alpha n|j\rangle\right]^2 \delta(\omega - \omega_j). \tag{30}$$

Assuming that

$$|\boldsymbol{U}^{jb}| \sim q^x \lambda^{-D} \tag{31}$$

ACV, from equation (26), deduced that $g_1(q,\omega)$ complies with the power law

$$g_1(q,\omega) \sim q^{\delta_1}\omega^{\beta_1} \tag{32}$$

where

$$\beta_1 = \tilde{d} - 1 \tag{33}$$

and

$$\delta_1 = 2\sigma - D \tag{34}$$

where, to preserve the scaling form (equations (6) and (7)), one deduces that

$$x = 2(\sigma - 1) \tag{35}$$

and

$$\tau_1' = D - D/\tilde{d}. \tag{36}$$

Following the same method as developed for $g(q, \omega)$, in the $q\lambda \ll 1$ limit, one obtains for the $g_2(q, \omega)$

$$g_2(q, \omega) \sim N(\omega)(q\lambda)^D q^4 (\tilde{D}^{jb})^2 \tag{37}$$

where the elements of $\tilde{D}^{jb}$ are given by

$$D^{jb}_{\alpha\beta} = \sum_{\substack{n \in b \\ \delta}} R^{jb}_{n\beta} R^{jb}_{n\delta} e^{jb}_{\alpha\delta}. \tag{38}$$

Integration over the blob, in the continuous limit, gives

$$|\tilde{D}| \sim q^{-(D+2)} |\tilde{e}| \tag{39}$$

with

$$\langle |\tilde{e}|^2 \rangle \sim \lambda^{-2\sigma - D}. \tag{40}$$

One can deduce that

$$g_2(q, \omega) \sim q^{\delta_2} \omega^{\beta_2} \tag{41}$$

where

$$\delta_2 = -D \tag{42}$$

and

$$\beta_2 = 2\sigma \tilde{d}/D + \tilde{d} - 1 \tag{43}$$

and, from equation (7),

$$\tau_2' = 2\sigma + D - D/\tilde{d}. \tag{44}$$

From Stoll *et al* (1992), one expects that overall motions of small blobs control the limit $q\lambda \gg 1$, i.e. τ_1'. The internal strain of blobs would dominate for $q\lambda \sim 1$.

3. Numerical results

In this study, we compute the dynamic structure factor (equation (5)) of the site and bond two-dimensional (2D) square and three-dimensional (3D) cubic percolating networks. In all the systems below, we assume that atoms of mass $m = 1$ are placed on the lattice sites. Interactions are represented by the scalar potential. The spring constant is taken to be $K_{ij} = 0$ if either sites i or sites j are unoccupied and $K_{ij} = 1$ otherwise. Each system consists of a single very large cluster: the infinite cluster.

For harmonic solids, the moments method was first used by Montroll (1942) to calculate the density of one-phonon states. In the dynamics of condensed matter, the exact evaluation of the response was developed by Benoit (1987, 1989) and applied to different systems (Benoit *et al* 1990, 1992a,b, Poussigue *et al* 1991, 1994, Royer *et al* 1991, 1992, Rahmani *et al* 1993, 1994).

In this work, using the spectral moments method, we developed calculations of $g(q, \omega)$ for percolating systems formed on 500×500 square and $85 \times 85 \times 85$ cubic lattices for values of site and bond occupation probability p near p_c (0.5 in two dimensions and 0.249

in three dimensions for BP and 0.593 in two dimensions and 0.312 in three dimensions for SP).

The fractal dimension D of these systems is $D = 1.89$ and $D = 2.5$ in two dimensions and three dimensions, respectively. Several tests were performed on three clusters formed on cubic and square lattices of different sizes. We report here the results of clusters of 178 205 sites (2D BP), 108 326 sites (2D SP), 226 940 sites (3D BP) and 106 993 sites (3D SP). All exponents are the average of 25 values of q and ω in the studies of ω dependence and q dependence of $g(q, \omega)$, respectively. For all clusters the computations were done for 100 different wavevectors $\pi/100 \leqslant q \leqslant \pi$. We also note that the computations were done for 200 different frequencies $\omega_{max}/200 \leqslant \omega \leqslant \omega_{max} = \sqrt{4d}$, with d the space dimension.

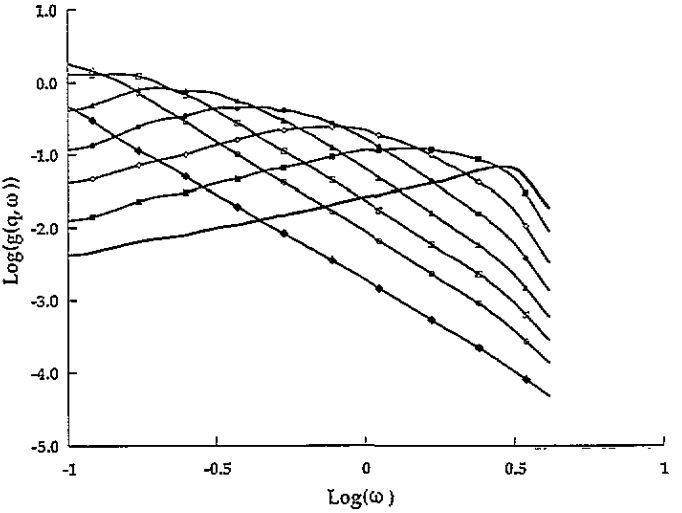

Figure 1. The dynamic structure factor $g(q, \omega)$ versus ω on a log–log scale, for the 2D BP cluster for eight values of q: —♦—, $q = 0.079$; —○—, $q = 0.198$; —□—, $q = 0.314$; —▲—, $q = 0.498$; —●—, $q = 0.789$; —◇—, $q = 1.251$; —■—, $q = 1.982$; ——, $q = 3.142$.

In figures 1 and 2, we report, on a log–log scale, the frequency dependence of the dynamic structure factor $g(q, \omega)$ for the $d = 2$ and $d = 3$ BP clusters for some values of the wavevector. The abscissa indicates the frequency ω. In order to show that the data collapse well, we report in figures 3 and 4 on a log–log scale, the $q\lambda(\omega)$ dependence of the function $H(q\lambda(\omega)) = q^{-\gamma} g(q, \omega)$ for the $d = 2$ and $d = 3$ SP clusters. The abscissa indicates the quantity $q\lambda(\omega)$. Curves are obtained by averaging over 50 values of the wavevector q. We define ω_0 as the frequency at which $g(q, \omega)$ has a maximum value for each fixed wavenumber q. As $q\lambda(\omega_0) = 1$, for $\omega \gg \omega_0$ ($\omega \ll \omega_0$) this corresponds to the $q\lambda \ll 1$ ($q\lambda \gg 1$) limit. In figures 5–8, the wavevector dependence of the function $g(q, \omega)/q^2$ for the $d = 2$ and $d = 3$ BP and SP clusters for some values of the frequency are reported, on a log–log scale. The abscissa indicates the wavevector q. We define q_0 as the wavevector at which the function $g(q, \omega)/q^2$ has a maximum value for each fixed frequency ω. As $q_0\lambda(\omega) = 1$, for $q \gg q_0$ ($q \ll q_0$) this corresponds to the $q\lambda \gg 1$ ($q\lambda \ll 1$) limit.

The length scale versus the frequency for the 2D and 3D clusters are plotted, on a log–log scale, in figures 9 and 10, respectively.

Let us consider the results concerning the 2D BP cluster. From figure 9, we observe that the scaling length complies with the power law $\lambda(\omega) \sim \omega^{-0.73 \pm 0.02}$. From equation (2),

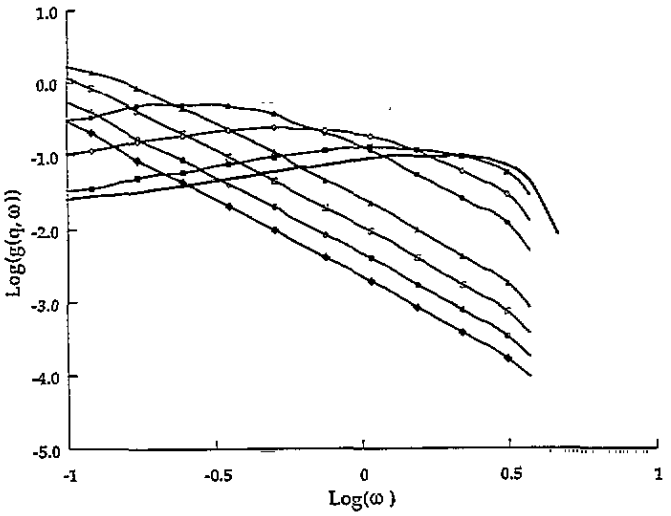

Figure 2. The dynamic structure factor $g(q,\omega)$ versus ω, on a log–log scale, for the 3D BP cluster for eight values of q: —♦—, $q = 0.079$; —○—, $q = 0.125$; —□—, $q = 0.198$; —▲—, $q = 0.314$; —●—, $q = 0.498$; —◇—, $q = 1.251$; —■—, $q = 1.982$; ——, $q = 2.736$.

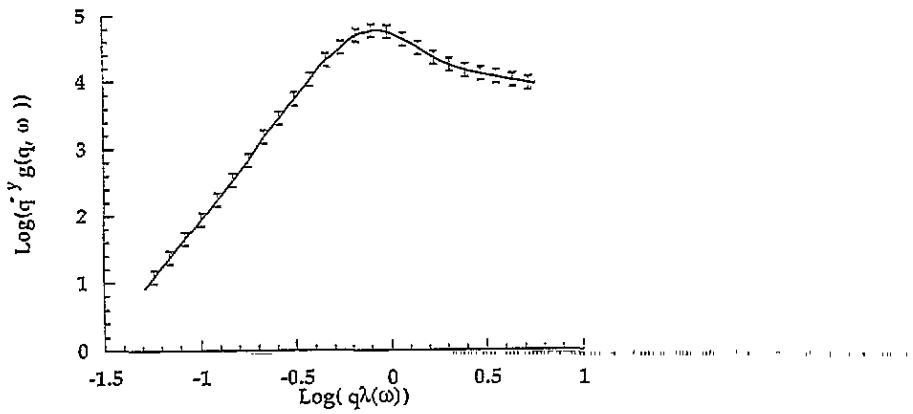

Figure 3. The function $q^{-\gamma}g(q,\omega)$ versus $q\lambda(\omega)$, on a log–log scale, for the 2D SP cluster.

$\lambda(\omega) \sim \omega^{-\tilde{d}/D}$. According to the AO conjecture $\tilde{d} = 4/3$, with $D = 1.89$, one obtains $\tilde{d}/D = 0.705$. The agreement is very good.

Considering the asymptotic behaviour of the dynamic structure factor in the $q\lambda \ll 1$ limit, the results show (figures 1 and 5) that the function $g(q,\omega) \sim q^{\gamma}\omega^{-\alpha}$ with $\gamma = 4.00 \pm 0.05$ and $\alpha = 2.31 \pm 0.03$ (table 1). These values are obtained by averaging over 25 different wavenumbers ($\pi/100 < q < \pi/4$) for α and 25 different frequencies ($5\omega_{max}/8 \leqslant \omega \leqslant 3\omega_{max}/4$) for γ. The behaviour of $g(q,\omega)$ and the value of γ are in complete agreement with the theory (equations (20), (21) and (22)). One obtains from equation (23) $\tau = 3.28$ with $\tilde{d} = 4/3$. Using equation (22), one finds that $\sigma = 1.07$ with the AO conjecture (table 1). These results are in agreement with the intuitive notion that $\sigma \geqslant 1$ (ACV 1993).

In the $q\lambda \gg 1$ limit, the theory predicts the dynamic structure factor

$$g(q,\omega) \sim Aq^{\delta_1}\omega^{\beta_1} + Bq^{\delta_2}\omega^{\beta_2} \tag{45}$$

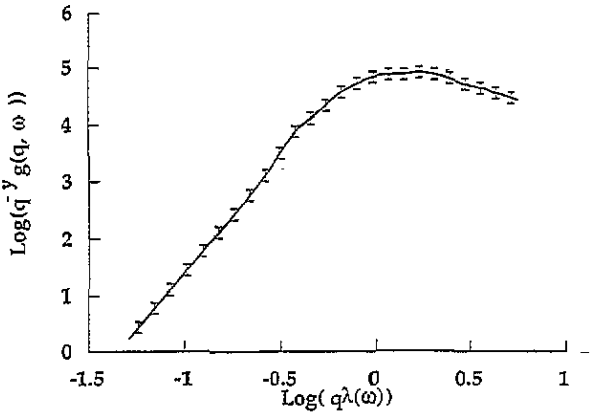

Figure 4. The function $q^{-y}g(q,\omega)$ versus $q\lambda(\omega)$, on a log–log scale, for the 3D SP cluster.

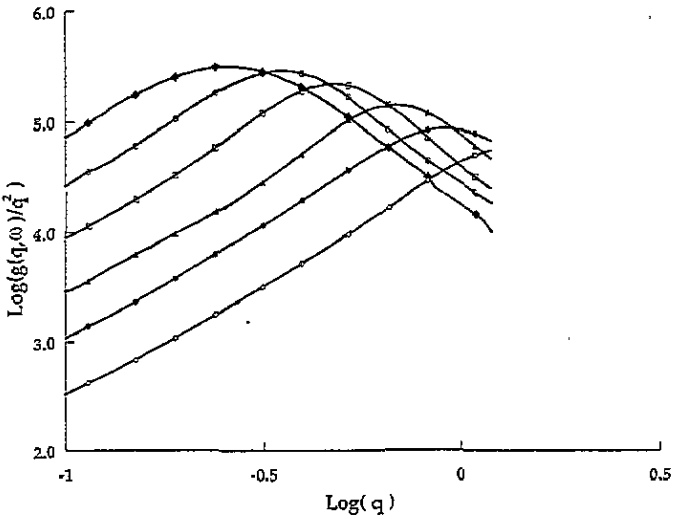

Figure 5. The dynamic structure factor $g(q,\omega)$ versus q, on a log–log scale, for the 2D BP cluster for six values of ω: —♦—, $\omega = 0.226$; —○—, $\omega = 0.353$; —□—, $\omega = 0.552$; —▲—, $\omega = 0.862$; —●—, $\omega = 1.346$; —◇—, $\omega = 2.101$.

where δ_1, β_1, δ_2 and β_2 are given by equations (33) and (34) and equations (42) and (43) as functions of σ, $\tilde{d}$ and D. From the value of σ obtained in the $q\lambda \ll 1$ limit, one obtains $\delta_1 = 0.25$, $\beta_1 = 0.33$, $\delta_2 = -1.89$ and $\beta_2 = 1.84$ (table 2). The computation (figures 1 and 5) shows that $g(q,\omega) \sim q^{\delta}\omega^{\beta}$ with the presence of two regimes. For $q\lambda \sim 1$ the values of the exponents are dependent on the values of q and ω. However, for sufficiently larger q (or smallest ω), this limit is found to have very nice asymptotic behaviours $g(q,\omega) \sim q^{\delta}\omega^{\beta}$ with $\delta = -0.55$ and $\beta = 0.88$, which are quite different from the expected values. These values are obtained by averaging over 25 different wavenumbers ($\pi/4 < q < \pi$) for β and 25 different frequencies ($\omega_{max}/200 \leqslant \omega \leqslant \omega_{max}/8$) for δ.

However, as mentioned by ACV, it is possible to assume the presence of an additional factor $(q\lambda)^{z}$ in equation (31) or in equation (40). Then, equation (28) is now written with

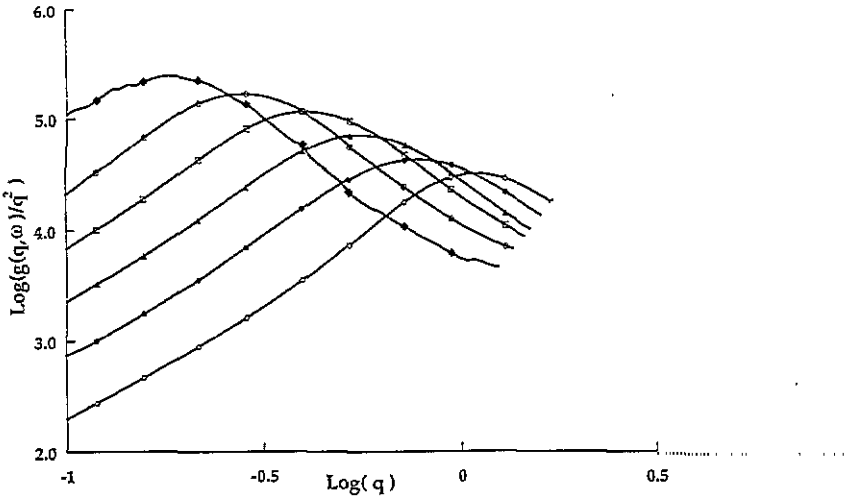

Figure 6. The dynamic structure factor $g(q, \omega)$ versus q, on a log–log scale, for the 2D SP cluster for six values of ω: —♦—, $\omega = 0.226$; —○—, $\omega = 0.353$; —□—, $\omega = 0.552$; —▲—, $\omega = 0.862$; —○—, $\omega = 1.346$; —◇—, $\omega = 2.101$.

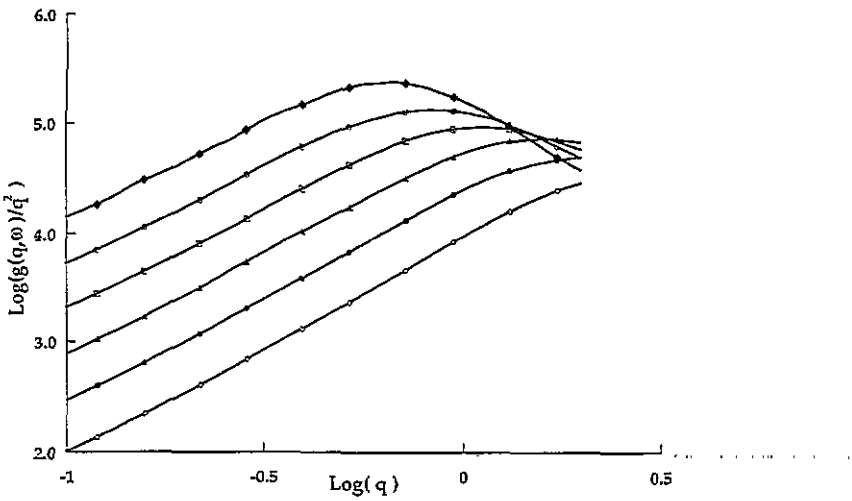

Figure 7. The dynamic structure factor $g(q, \omega)$ versus q on a log–log scale, for the 3D BP cluster for six values of ω: —♦—, $\omega = 0.353$; —○—, $\omega = 0.552$; —□—, $\omega = 0.862$; —▲—, $\omega = 1.346$; —●—, $\omega = 2.101$; —◇—, $\omega = 3.281$.

equations (32) and (41) as

$$g(q, \omega) \sim Aq^{\delta_1 + z_1} \omega^{\beta_1 - z_1 \tilde{d}/D} + Bq^{\delta_2 + z_2} \omega^{\beta_2 - z_2 \tilde{d}/D}. \tag{46}$$

By comparison with the computed values of δ and β, for the first term, resulting from the separate motion of the blobs, we find that $z_1 = -0.80$ from the q dependence and $z_1 = -0.78$ from the frequency dependence of the dynamic structure factor. Now, if we assume that the second contribution resulting from the internal strain of the blob is dominant, one obtains $z_2 = 1.34$ from the q dependence and $z_2 = 1.36$ from the frequency

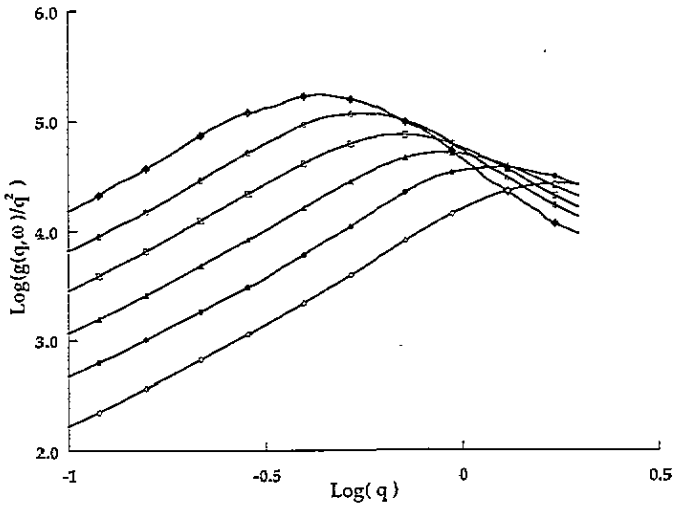

Figure 8. The dynamic structure factor $g(q, \omega)$ versus q, on a log–log scale, for the 3D SP cluster for six values of ω: —♦—, $\omega = 0.226$; —○—, $\omega = 0.353$; —□—, $\omega = 0.552$; —▲—, $\omega = 0.862$; —●—, $\omega = 1.346$; —◇—, $\omega = 2.101$.

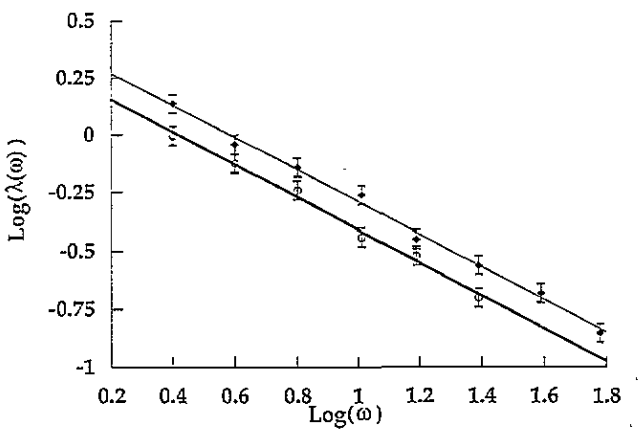

Figure 9. The values of the wavelength $\lambda(\omega)$ plotted as a function of frequency ω on a log–log scale, for the 2D percolating clusters: ♦, 2D SP; ○, 2D BP.

dependence.

The same analyses have been performed on the three other clusters. The results are summarized in tables 1 and 2. We have also reported the results obtained by Stoll *et al* (1992) and Nakayama and Yakubo (1992).

4. Discussion and conclusion

First, we note the excellent agreement with the theory, for the four clusters, concerning the scaling law of the length scale $\lambda(\omega)$ (figures 9 and 10 and tables 1 and 2). This behaviour was verified by Stoll *et al* (1992) for the localization length on 2D and 3D BP clusters. In our computation, $\lambda(\omega)$ corresponds to a wavelength, defined as the inverse of the value of q for which the Fourier components of the eigenvectors of fractons with a frequency ω are

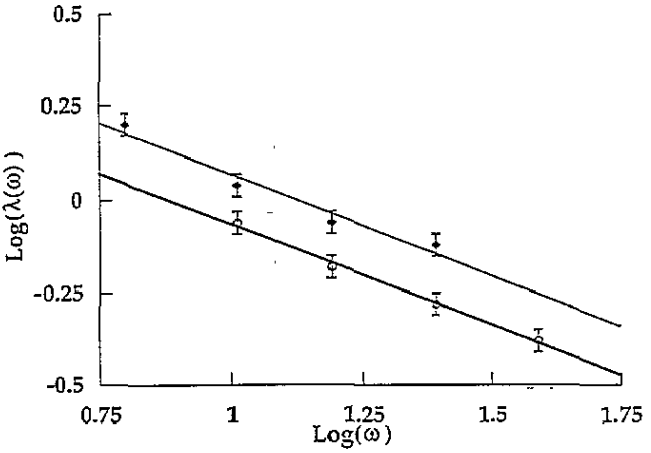

Figure 10. The values of the wavelength $\lambda(\omega)$ plotted as a function of frequency ω on a log–log scale, for the 3D percolating clusters: ○, 3D SP; ♦, 3D BP.

Table 1. Values of the exponents γ, α, $\tilde{d}$, σ and τ for the four percolating clusters in the $q\lambda \ll 1$ limit. $(\tilde{d}/D)_{num}$ are deduced from figures 9 and 10. $(\tilde{d}/D)_{theo}$ are calculated from the fixed values of $D = 1.89$ and $\tilde{d} = 1.33 \pm 0.02$.

	γ	α	$\tilde{d}$	$(\tilde{d}/D)_{num}$	$(\tilde{d}/D)_{theo}$	σ	τ
2D BP	4.00 ± 0.05	2.31 ± 0.03	1.33 ± 0.02	0.73 ± 0.02	0.70 ± 0.01	1.07 ± 0.04 1.05[a]	3.28 ± 0.10 3.32[a]
2D SP	3.98 ± 0.05	2.34 ± 0.03	1.33 ± 0.02	0.70 ± 0.02	0.70 ± 0.01	1.05 ± 0.04 1.11[b]	3.33 ± 0.10 3.32[b]
3D BP	4.00 ± 0.05	2.03 ± 0.03	1.33 ± 0.02	0.55 ± 0.02	0.53 ± 0.01	1.03 ± 0.05 1.1[a]	3.82 ± 0.11 3.65[a]
3D SP	4.00 ± 0.05	1.98 ± 0.03	1.33 ± 0.02	0.53 ± 0.02	0.53 ± 0.01	1.08 ± 0.05	3.72 ± 0.11

[a] From Stoll *et al* (1992).
[b] From Nakayama and Yakubo (1992).

maximum. These results are in agreement with the SLSP of ACV.

As can be shown in table 1, in the $q\lambda \ll 1$ limit, where q^{-1} is much larger than the fracton size, for the four models we note that, in agreement with the theory, $g(q, \omega) \sim q^{4.00 \pm 0.05}$. From the β-value or from the scaling form of the 2D and 3D SP systems (figures 3 and 4), one obtains $\tau \simeq 3.30$ for the 2D systems and $\tau \simeq 3.77$ for the 3D systems, in agreement with the values of Stoll *et al* ($\tau(2D) \simeq 3.32$ and $\tau(3D) \simeq 3.65$) obtained for 2D and 3D BP networks, and of Nakayama and Yakubo ($\tau(2D) \simeq 3.20$) for the 2D SP cluster.

We note that in the four systems the values obtained for σ are in accordance with the conclusion of ACV that $\sigma > 1$.

The only precise work concerning the $q\lambda \gg 1$ limit is that of Nakayama and Yakubo (1992) on the 2D SP cluster. They found that $\beta = 1.7$, in accordance with the theoretical behaviour of the $g_2(q, \omega)$ contribution (equation (43)) but in complete disagreement with our present results. We find, for the four models, that the values computed for the exponents are

Table 2. Values of the exponents δ, β, δ_1, β_1, z_1, δ_2, β_2 and z_2 for the four percolating clusters for fixed values of $\tilde{d} = 1.33 \pm 0.02$ in the $q\lambda \gg 1$ limit.

	δ	β	$\tilde{d}$	δ_1	β_1	$z_1 = \delta - \delta_1$	$z_1 = (\beta_1 - \beta)D/\tilde{d}$	δ_2	β_2	$z_2 = \delta - \delta_2$	$z_2 = (\beta_2 - \beta)D/\tilde{d}$
2D BP	-0.55 ± 0.10	0.88 ± 0.05	1.33 ± 0.02	0.25 ± 0.01	0.33 ± 0.02	-0.80 ± 0.10	-0.78 ± 0.10	-1.89	1.84 ± 0.10	1.34 ± 0.20	1.36 ± 0.10
2D SP	-0.57 ± 0.10 -1.60[a]	0.80 ± 0.05 1.7[a]	1.33 ± 0.02	0.21 ± 0.01	0.33 ± 0.02	-0.78 ± 0.11	-0.67 ± 0.10	-1.89	1.81 ± 0.10	1.32 ± 0.20	1.43 ± 0.10
3D BP	-0.65 ± 0.10	0.65 ± 0.05	1.33 ± 0.02	-0.44 ± 0.02	0.33 ± 0.02	-0.21 ± 0.14	-0.60 ± 0.08	-2.50	1.43 ± 0.1	1.85 ± 0.25	1.46 ± 0.10
3D SP	-0.53 ± 0.10	0.57 ± 0.05	1.33 ± 0.02	-0.34 ± 0.02	0.33 ± 0.02	-0.19 ± 0.14	-0.45 ± 0.08	-2.50	1.48 ± 0.1	1.97 ± 0.25	1.70 ± 0.10

[a] From Nakayama and Yakubo (1992).

between the theoretical values obtained for both contributions $\delta_1 > \delta > \delta_2$ and $\beta_1 < \beta < \beta_2$. However, introduction of exponent z leads to results that are in accordance with the theory; it is especially precise for 2D percolating networks where values obtained from the frequency dependence are in complete agreement with the values of z obtained from the wavevector dependence (table 2). This result holds for both contributions. The agreement is not so good for 3D percolating networks, but the values obtained from the frequency and wavevector dependence are in accordance if errors in the computed values are taken into account. These results show that it is not possible to neglect coherence between the scattering of different blobs, even in the $q\lambda \gg 1$ limit. This coherence arises from relations which exist, through the dynamics matrix, between the structure and components of the eigenvectors of the fractons. It is thus not possible to assume that the motion of the centre of the blobs are completely uncorrelated, since the phase factor and the components of the eigenvectors are not completely independent.

In conclusion, in this work, we computed the dynamic structure factor of four percolating networks. Concerning the $q\lambda \ll 1$ limit, our results confirm and supplement the previous numerical work and are in agreement with the scaling behaviour theoretically deduced by ACV.

Concerning the $q\lambda \gg 1$ limit, our results indicate a scaling behaviour with exponents that differ from those obtained from theory assuming the simple scaling law (31) and (40). However, we have shown that the dynamic structure factor also complies with the very nice asymptotic behaviour $g(q,\omega) = q^y H(q\lambda(\omega))$, where the scaling function $H(x)$ is of power-law form $x^{-\tau'}$, if we introduce an additional contribution $(q\lambda)^z$ in equations (31) and (40). The values obtained for τ' are about 1.20 for the 2D bond and SP lattices, respectively and 1.00 for the 3D lattices (table 3). These values do not correspond to the theoretical values given by equations (36) and (44) but are again consistent with the SLSP conjecture. Let us note that analysis of the data obtained by Stoll *et al* (1992) gives, for the slope of the scaling function, a value of about 1.30 ± 0.2 for the 2D BP lattice and 1.1 ± 0.1 for the 3D lattices. In the 2D lattice, the slope of the scaling function is dependent on the value of the wavevector for the region $q\lambda \sim 1$; close to this value, one obtains a slope of around 1.7, which could explain the disagreement with the results of Nakayama and Yakubo (1992). Computations with different types of interacting potential and different types of self-similar structure are now under way. The first results show that the SLSP conjecture, tested until now only with the percolating networks, is certainly more universal.

Table 3. Values of the exponents τ' from the values of δ and β for the four percolating clusters for fixed values of $\tilde{d} = 1.33 \pm 0.02$ in the $q\lambda \gg 1$ limit. τ'_1 (theo) and τ'_2 (theo) are given by equations (36) and (44), respectively.

	δ	β	$\tilde{d}$	$\tau'(\beta)$	$\tau'(\delta)$	τ'_1 (theo)	τ'_2 (theo)
2D BP	-0.55 ± 0.10	0.88 ± 0.05	1.33 ± 0.02	1.25 ± 0.10	1.27 ± 0.2 1.30 ± 0.20[a]	0.47 ± 0.01	2.61 ± 0.10
2D SP	-0.57 ± 0.10	0.80 ± 0.05	1.33 ± 0.02	1.14 ± 0.10	1.25 ± 0.2	0.47 ± 0.01	2.57 ± 0.10
3D BP	-0.65 ± 0.10	0.65 ± 0.1	1.33 ± 0.02	1.22 ± 0.2	0.85 ± 0.25 1.10 ± 0.10[a]	0.62 ± 0.01	2.68 ± 0.15
3D SP	-0.53 ± 0.10	0.57 ± 0.1	1.33 ± 0.02	1.07 ± 0.20	0.80 ± 0.3	0.62 ± 0.01	2.78 ± 0.20

[a] From Stoll *et al* (1992).

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References

Alexander S 1989 *Phys. Rev.* B **40** 7953
Alexander S, Courtens E and Vacher R 1993 *Physica* A **195** 286
Alexander S and Orbach R 1982 *J. Physique Lett.* **43** L625
Benoit C 1987 *J. Phys. C: Solid State Phys.* **20** 765
——1989 *J. Phys.: Condens. Matter* **1** 335
Benoit C, Poussigue G and Assaf A 1992a *J. Phys.: Condens. Matter* **4** 3153
Benoit C, Poussigue G and Azougarh A 1990 *J. Phys.: Condens. Matter* **2** 2519
Benoit C, Poussigue G, Rousseau V, Lakhliai Z and Chenouni D 1995 *Modelling Simul. Mater. Sci. Eng.* **3** 161
Benoit C, Royer E and Poussigue G 1992b *J. Phys.: Condens. Matter* **4** 3125
Boukenter A, Champagnan B, Duval E, Dumas J, Quinson J F and Serugetti J 1986 *Phys. Rev. Lett.* **57** 2391
Duval E, Boukenter A, Achibat T, Champagnon B, Serugetti J and Dumas J 1992 *Phil. Mag.* B **65** 181
Duval E, Mariotto G, Montagna M, Pilla O, Villiani G and Barland M 1987 *Europhys. Lett.* **3** 333
Fontana A, Rocca F and Fontana M P 1987 *Phys. Rev. Lett.* **58** 503
Freltoft T, Kjems J and Richter D 1987 *Phys. Rev. Lett.* **59** 1212
Montagna M, Pilla O, Villiani G, Mazzacurati V, Roucco G and Signorelli G 1990 *Phys. Rev. Lett.* **65** 1136
Montroll E W 1942 *J. Chem. Phys.* **10** 218
Nakayama T and Yakubo K 1992 *J. Phys. Soc. Japan* **61** 2601
Nakayama T, Yakubo K and Orbach R 1994 *Rev. Mod. Phys.* **66** 381
Poussigue G, Benoit C, de Boissieu M and Currat R 1994 *J. Phys.: Condens. Matter* **6** 659
Poussigue G, Benoit C, Sauvajol J L, Lere-Porte J P and Chorro C 1991 *J. Phys.: Condens. Matter* **3** 8803
Rahmani A, Benoit C and Poussigue G 1993 *J. Phys.: Condens. Matter* **5** 7941
——1994 *J. Phys.: Condens. Matter* **6** 1483
Royer E, Benoit C and Poussigue G 1991 *High Performance Computing* ed M Durand and F El Dabaghi (Amsterdam: Elsevier) p 513
——1992 *J. Phys.: Condens. Matter* **4** 561
Russ S, Roman H E and Bunde A 1991 *J. Phys.: Condens. Matter* **3** 4797
Stoll E, Kolb M and Courtens E 1992 *Phys. Rev. Lett.* **68** 2472
Tsujimi Y, Courtens E, Pelous J and Vacher R 1988 *Phys. Rev. Lett.* **60** 2757
Vacher R, Courtens E, Coddens G, Heidemann A, Tsujimi Y, Pelous J and Foret M 1990 *Phys. Rev. Lett.* **65** 1008
Yakubo K and Nakayama T 1987 *Phys. Rev.* B **36** 8933
——1989 *Phys. Rev.* B **40** 517