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DYNAMIC STRUCTURE FACTOR OF FRACTALS

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The dynamic structure factor $S(q, \omega)$ of the vibrational modes of a deterministic fractal is analyzed as a function of both frequency (ω) and momentum (q) transfer. It is found that $S(q, \omega)$ is peaked at $q_{max} \approx \omega^{1/(2+\theta)}$, where θ is the anomalous diffusion exponent, and is a scaling function of $q^{(2+\theta)}/\omega$. The results are obtained by a novel recursion method for the calculation of the vibration Green's function of a deterministic fractal. They confirm predictions based upon the fracton scaling model.

1. Introduction

The dynamics of disordered systems is a subject of considerable interest. In particular, much work has been devoted to studies of geometrically disordered systems (e.g. percolation clusters) by scaling considerations [1,2], by numerical simulations [3] and by scattering experiments [4,5]. These structures appear to be homogeneous at length scales longer than the connectivity length ξ, and exhibit fractal characteristics at shorter length scales. The dynamic excitations of the latter regime are termed fractons [1,2]. Fracton modes are localized; their localization length decreases rapidly with increasing frequency [2] and is smaller than ξ. By scaling considerations it was argued [1] that the fracton density of states $N(\omega)$ varies as $\omega^{\tilde{d}-1}$, where ω is the frequency and $\tilde{d}$ is the fracton dimensionality [1]. The excitations pertaining to the homogeneous regime are phonons, with sound velocity that depends upon ξ. Thus, within the scaling picture, the low-frequency portion of the spectrum consists of extended phonons and the higher-frequency part of localized fractons. The crossover frequency ω_x tends to zero as ξ increases (e.g. as the percolation threshold is approached), $\omega_x \approx \xi^{-(2+\theta)}$, where θ is the exponent characterizing the diffusion on a fractal [6]. The crossover from fractons to phonons has recently been established by light scattering experiments [4]. Fracton modes were also invoked to interpret Raman scattering data of silica aerogels [7].

An excitation spectrum is commonly probed by inelastic neutron or light scattering, which measures the dynamic structure factor $S(q, \omega)$ as a function of frequency and momentum transfer of the scattered particles. This method has recently been applied to silica aerogels [4] and also to diluted antiferromagnets [5], in which the short-length-scale spin modes are expected to have fracton features [2].

The detailed form of the dynamic structure factor of tenuous systems is yet unknown. Some general remarks can be made using scaling arguments [8] and an explicit analysis was carried out within the effective medium approximation [9]. Here we present an exact calculation of the dynamic structure factor of a fractal object [10].

The concept of fractal geometry, first introduced by Mandelbrot [11], has turned out to be a most useful tool in studies of tenuous materials. For example, silica aerogels at short length scales are characterized by their fractal dimensions [4]. The same is true for a percolating system close enough to the percolation threshold [12]. It is therefore of interest to investi-

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gate the dynamic properties of a fractal structure. In section 2 we compute $S(q, \omega)$ for a modified version of the Sierpinski gasket [11] (see fig. 1). We present there a novel recursion method for calculating the vibration Green's function of a deterministic fractal. We find that $S(q, \omega)$ has a well-defined maximum as a function of q or ω and exhibits single-variable scaling. The analysis of the peak position as a function of frequency confirms the fracton model prediction [1,2,8]. Section 3 includes some conclusions.

2. The structure factor

The determination of $S(q, \omega)$ necessitates the knowledge of the full Green's function of the vibrating structure. We present here a new algorithm for a successive construction of the Green's function, and use it to derive a recursion relation for $S(q, \omega)$. The algorithm is extremely efficient and can be exploited in computations of other properties related to vibration dynamics, e.g. the heat diffusion.

The model considered (see fig. 1) is a version of the two-dimensional Sierpinski gasket [11], on which we solve the scalar elasticity equations

$$-m\omega_+^2 u_i = \sum_{nn} t(u_{nn,i} - u_i), \quad \omega_+ = \omega + i\eta, \qquad (1)$$

where u_i is the displacement of the ith mass from its equilibrium position, nn denotes nearest-neighbours and t is the spring constant. The distance between two vertices of different triangles is set to zero in order to make the structure geometrically self-similar. This structure is more amenable to efficient calculations than the usual Sierpinski gasket. Though it is not self-similar, the low-frequency spectrum rapidly converges (as a function of iteration order) to that of the common Sierpinski gasket [11]. It simulates a structure with holes on all length scales – a feature exhibited by some of the systems [4] studied in scattering experiments.

The solution to eq. (1) may be written in terms of the retarded Green's function, whose i,j- matrix element is denoted $G_{ij}(\omega_+)$. Here i and j are site indices. The structure factor is then given by

$$S(q, \omega) = -\frac{1}{\pi} \operatorname{Im} \sum_{ij} \exp[i\boldsymbol{q}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)] G_{ij}(\omega_+), \qquad (2)$$

in which ω is the real part of ω_+ and $\boldsymbol{R}_i$ denotes the coordinate of the ith site.

We now outline the derivation of the recursion relation for the Green's function matrix elements which are used in eq. (2) to obtain the recursion formulae

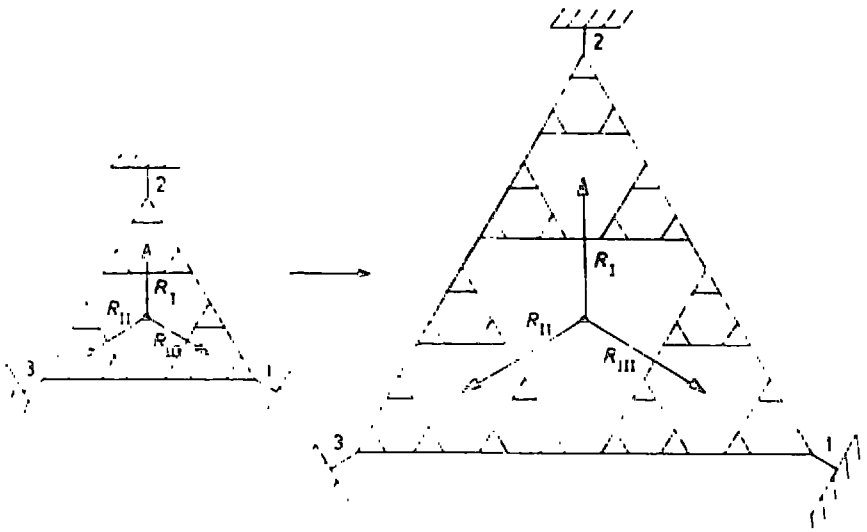

Fig. 1. Two stages in the construction of the gasket.

of $S(q, \omega)$. Suppose we know the full Green's function of the $(n-1)$th stage, $G^{(n-1)}$. The Green's function of the nth stage, $G^{(n)}$, can be written, in matrix notation, as

$$\mathbf{G}^{(n)}=[\mathbf{g}^{-1}+\mathbf{\Gamma}]^{-1}, \tag{3}$$

where

$$\mathbf{g}=\begin{pmatrix} \mathbf{G}^{(n-1)} & 0 & 0 \\ 0 & \mathbf{G}^{(n-1)} & 0 \\ 0 & 0 & \mathbf{G}^{(n-1)} \end{pmatrix} \tag{4}$$

and $\mathbf{\Gamma}$ is a coupling matrix, connecting the three $(n-1)$th gaskets to form the nth stage gasket. Note that $\mathbf{G}^{(n)}$ is an N matrix, where N is the number of sites ($N=3^n$) in the nth stage gasket. Referring to fig. 1, one notes that there are only six nonzero matrix elements in $\mathbf{\Gamma}$, the ones connecting together the three $(n-1)$th stage gaskets. Expanding eq. (3), it is easily seen that each term of the expansion includes those matrix elements of $\mathbf{\Gamma}$, and the diagonal (α) and nondiagonal (β) matrix elements of $\mathbf{G}^{(n-1)}$ with respect to the external sites of the $(n-1)$th stage. (For example, G_{11} and G_{12} in fig. 1.) It therefore follows that

$$\mathbf{G}^{(n)}=\mathbf{g}-\mathbf{g}\mathbf{T}\mathbf{g}, \qquad \mathbf{T}=\mathbf{\Gamma}[\mathbf{I}+\mathbf{g}\mathbf{\Gamma}]^{-1}, \tag{5}$$

and to obtain $\mathbf{T}$ explicitly, one has to invert a 6 by 6 matrix. The elements of the symmetric matrix $\mathbf{T}$ are given in terms of α and β, which in turn, are calculated recursively. The evaluation of $S(q, \omega)$ involves the site coordinates. To incorporate those into the recursive procedure, we have adopted an hierarchical scheme in which the coordinates of each site are defined with respect to the center of the smallest gasket to which it belongs, the latter being measured with respect to the second smallest gasket, and so on.

The results are presented for a gasket of 3^{10} sites and wavevectors q at an angle $\pi/4$ relative to one of the edges (this direction is incommensurate with the gasket symmetry axes). $S(q, \omega)$ has a well-defined maximum as a function of q or ω (see fig. 2). The analysis of the peak position, q_{max}, as a function of frequency yields

$$q_{max} \approx \omega^{2/(2+\theta)}, \tag{6}$$

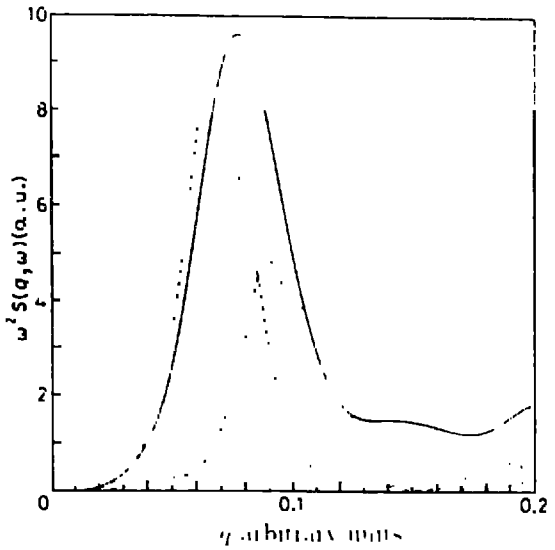

Fig. 2. Typical curves of $\omega^2 S(q, \omega)$ versus q for three closeby frequencies belonging to different subsets.

which confirms the fracton model prediction [1,2]. Here $2+\theta=\ln(5)/\ln(2)$. Indeed, eq. (6) agrees with the scaling assumption [1,2] for the mass m and the coupling constant t, in conjunction with the basic relation $\omega^2=t/m$. Thus, excitations of frequency ω correspond to modes of spatial variation q_{max}^{-1}. The spectrum of the gasket includes a small number of nondegenerate eigenvalues characteristic to its specific construction procedure [13]. These were neglected in the analysis of the overall shape and scaling properties and we concentrated on eigenstates characteristic to the fractal nature of the structure. Most of these eigenvalues are highly degenerate. They separate into subsets of frequencies [13], within each the frequencies relate by $\omega_i^2=2^{2+\theta}\omega_{i-1}^2$ (or $q_{max,i}=2q_{max,i-1}$), where i enumerates members of the same subset. The degeneracy of the ω_i^2 eigenvalue is approximately proportional to 3^i.

The fracton model assumes the existence of a single, frequency-dependent, length that sets up the scale for the dynamics [1,2]. This implies scaling of the structure factor with a single length. We now construct this scaling.

In terms of the (normalized) eigenmodes ϕ_n and eigenfrequencies ω_n, the structure factor takes the form

$$S(q,\omega)=\sum_{\alpha} o_{\alpha}(q)\, o_{\alpha}^{*}(q)\, \delta(\omega^{2}-\omega_{\alpha}^{2})$$

where $o_{\alpha}(q)$ is the spatial Fourier transform of $o_{\alpha}(\boldsymbol{R})$. As $S(q,\omega)$ satisfies the sum rule $\int d\omega\, \omega S(q,\omega)=1$, the assumption of single-length scaling implies

$$S(q,\omega)=\omega^{2}F(\omega/q^{(2+\theta)/2}), \tag{7}$$

where F is a scaling function. To test this form, we have calculated $S(q,\omega)$ for successive eigenfrequencies belonging to the same subset. For numerical reasons, the δ function was eliminated, by adding an arbitrarily small imaginary term $i\eta$ to ω^2, calculating $S(q,\omega)$, and then multiplying the result by η. For $|\omega^2-\omega_{\alpha}^2|<\eta$, the result is independent of η. Effectively, this procedure is equivalent to the calculation of $\sum' o_{\alpha}^{*}(q)\, o_{\alpha}(q)$, where the sum runs over all degenerate states of eigenfrequency ω_{α}. The corresponding curves as a function of q, fall one onto the other when the q axis is rescaled by a factor of 2 for each successive frequency (see fig. 3). Hence, though the shape of $S(q,\omega)$ of two frequencies belonging to different subsets is not the same, the structu factor of frequencies of the same subset obey the scaling form (7), which again confirms the fracton model predictions [8].

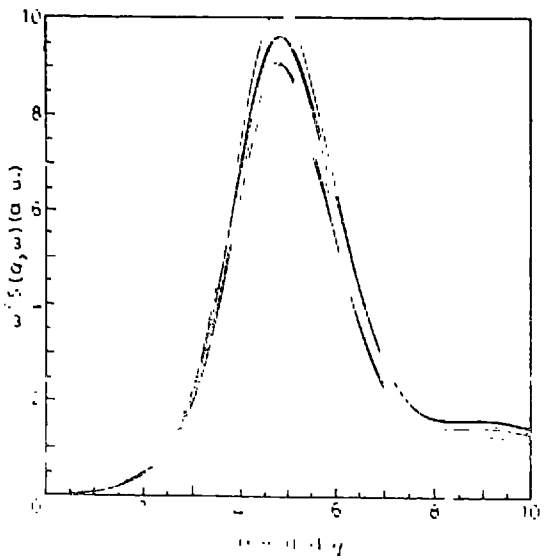

Fig. 3. Rescaled curves of $\omega^{-2}S(q,\omega)$ for eigenvalues belonging to a given subset.

A technical point should be noted. The structure factor and hence the scaling function F are expected to obey scaling in the $\eta\to 0$ limit. The deviation from exact scaling observed in fig. 3 is due to numerical iterative approach towards that limit: one chooses a value for η, calculates the approximate eigenvalue, reduces η, then recalculates the eigenvalue until the desired accuracy is achieved. The nonsystematic deviations from scaling can be removed by further iterations. The scaling of the structure factor is, however, clearly demonstrated by fig. 3.

3. Summary

We have shown that the excitation spectrum pertaining to the equation of motion (1) obeys single length scaling for a fractal structure. This holds not only for the peak position of the structure factor, but for its shape as well.

This computation cannot describe the phonon–fracton crossover, as it is valid only in the fracton regime. To consider the entire frequency range, the effective medium approximation (EMA) was exploited [9]. The spirit of this model is to replace a random system by an effective homogeneous (and periodic) medium, which one can solve for the dynamics. The parameters of the effective medium depend, in a self-consistent way, upon the parameters of the random system. The line shape of the structure factor, within EMA, can be written in terms of an effective sound velocity and linewidth, τ^{-1}, both functions of frequency [9]. One can then analyze their limiting behaviours, in the phonon ($\omega<\omega_{\times}$) and in the fracton ($\omega>\omega_{\times}$) regimes. By interpolating between these two limits and using the EMA line shape, Courtens et al. [4] were able to fit beautifully their Brillouin scattering data.

Within EMA, the sound velocity, up to $\omega_{\times}$, was found [9] to be independent of ω. Above $\omega_{\times}$ it increased with ω. The scattering width τ^{-1} followed the Rayleigh law in the phonon regime, $\tau^{-1}\propto\omega^{d+1}$, and became proportional to the frequency in the fracton regime, thus confirming the Ioffe-Regel limit for

fractons, derived from scaling arguments [8]. However, within EMA, the linewidth did not scale with ω_c. It is conceivable that this failure of scaling is connected with the approximations involved in the effective medium approach. The calculation presented here indicates that in the fracton regime the dynamics does obey single variable scaling.

We finally speculate upon the spatial extension of the eigenfunctions corresponding to a given frequency. The 3^l degeneracy of the ω_l^2 mode suggests that there is a representation in which each eigenfunction extends over 3^{n-l} sites. This implies that the spatial extension is approximately $2^{n-l} > 1/q_{max}$, in a complete agreement with the width of the computed structure factor. The spatial extension of the wavefunctions is most effectively probed by the heat diffusivity; it would be of interest to explore this quantity.

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References

[1] S. Alexander and R. Orbach, J. Phys. (Paris) 43 (1982) L625.

[2] S. Alexander, Ann. Israel Phys. Soc. 5 (1983) 144.
R. Orbach, Science 231 (1986) 814.
O. Entin-Wohlman, in: The T.D. Holstein Symposium: Condensed Matter Physics, R. Orbach ed. (Springer, Berlin, 1986), p. 160.

[3] K. Yakubo and T. Nakayama, Phys. Rev. B 36 (1987) 8933.

[4] E. Courtens, J. Pelous, J. Phalippou, R. Vacher and T. Woignier, Phys. Rev. Lett. 58 (1987) 128;
R. Vacher, T. Woignier, J. Pelous and E. Courte, Phys. Rev. B 37 (1988) 6500;
E. Courtens, R. Vacher, J. Pelous and T. Woignier, Europhys. Lett. 6 (1988) 245;
Y. Tsujimi, E. Courtens, J. Pelous and R. Vacher, Phys. Rev. Lett. 60 (1988) 2757.

[5] Y.J. Uemura and R.J. Birgeneau, Phys. Rev. B 36 (1987) 7024.

[6] Y. Gefen, A. Aharony and S. Alexander, Phys. Rev. Lett. 50 (1983) 77.

[7] A. Boukenter, B. Champagnon, E. Duval, J. Quinson and J. Serughetti, Phys. Rev. Lett. 57 (1986) 2391;
A. Boukenter, E. Duval and J. Serughetti, Phys. Rev. Lett. 59 (1987) 604.

[8] A. Aharony, S. Alexander, O. Entin-Wohlman and R. Orbach, Phys. Rev. Lett. 58 (1987) 132;
A. Aharony, O. Entin-Wohlman and R. Orbach, in: Time Dependent Effects in Disordered Materials, T. Riste and R. Pynn, eds. (Plenum, New York, 1988), p. 233.

[9] G. Polatsek and O. Entin-Wohlman, Phys. Rev. B 37 (1988) 7726.
G. Polatsek, O. Entin-Wohlman and R. Orbach, Phys. Rev. (1989) in press.

[10] U. Sivan, R. Blumenfeld, Y. Meir and O. Entin-Wohlman, Europhys. Lett. 7 (1988) 249.

[11] B.B. Mandelbrot, The Fractal Geometry of Nature (Freeman, San Fransisco, 1982).

[12] A. Aharony, in: Scaling Phenomena in Disordered Systems, R. Pynn and A. Skjeltorp, eds. (Plenum, New York, 1985), p. 335.

[13] E. Domany, S. Alexander, D. Bensimon and L.P. Kadanoff, Phys. Rev. B 28 (1983) 3110.