Phonon-Fracton Crossover on Fractal Lattices

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The spectral properties of a d-dimensional bond-percolating network have been examined by real-space rescaling methods. Both the triangular and face-centered-cubic lattices have been studied with the d-dimensional Sierpinski gasket used to model the backbone. The vibrational density of states has been calculated as a function of $p-p_c$ and we find that two excitation regimes exist which are characterized by two separate dimensionalities. There is a low-frequency phonon regime and a higher-frequency fracton regime. The specific heat exhibits a smooth crossover from phonon to fracton behavior as a function of $p-p_c$.

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Recently there has developed a growing interest in the dynamical properties of structures which have a fractal geometry.[1] Alexander and Orbach[2] were the first to point out that three dimensionalities are required to describe excitations on fractals: the embedding (Euclidean) dimension d; the Hausdorff (fractal) dimension D; and the fracton (spectral) dimension $\tilde{d}$. The fractal dimension D describes how the mass of the geometrical object depends on length scale, whereas the spectral dimension $\tilde{d}$ characterizes the low-frequency behavior of the density of states. It is well known[3] that percolating networks near the critical threshold p_c have a self-similar (fractal) geometry on small length scales and a homogeneous (Euclidean) structure on larger scales. The length scale which separates these two regions is the percolation correlation length ξ_p which diverges as p_c is approached from above. Orbach and co-workers[4–6] have recently used scaling arguments and effective-medium-approximation calculations to predict that there is a sharp increase in the density of vibrational states at a crossover frequency ω_c which corresponds to excitations with wavelengths of the order of ξ_p. They have conjectured[4,5,7] that glasses and perhaps all amorphous materials may exhibit similar behavior which can be understood in terms of a crossover from phonons to fractons.

In order to elucidate this question concerning the sharp rise in the vibrational density of states (DOS) at a well-defined frequency, we have calculated exactly the DOS for a system of masses and springs on a percolating network in both $d=2$ and $d=3$. We have used a model for the backbone of the infinite cluster which has a self-similar geometry on length scales from the nearest-neighbor lattice spacing up to the correlation length ξ_p and which has a Euclidean geometry at length scales above ξ_p. Our results indicate that a crossover from Euclidean (Debye) to fracton behavior occurs in the DOS as p_c is approached from above, but the change is rather smooth with no apparent sharp increase in the DOS at a crossover frequency.[8]

Figure 1 illustrates how we construct our fractal lattice in $d=2$. We begin with a uniform triangular lattice which consists of both upward- and downward-pointing equilateral triangles. The lattice spacing on this lattice is denoted as L. At each subsequent stage of construction we inscribe downward-pointing triangles inside each of the upward-pointing triangles and the new lattice spacing is denoted as a. At any level n of construction the Euclidean lattice spacing L is related to a in the simple way $L=2^n a$. The lattice generated in this manner has holes of all sizes from the lattice spacing a up to the Euclidean length L. We identify this length L with the percolation correlation length and since this latter length diverges as p approaches p_c with a characteristic exponent ν, we can relate p to the level n of iteration with $p=p_c+(1-p_c)(L/a)^{-1/\nu}$. Hence $n=0$ corresponds to a uniform lattice ($p=1$) whereas $n\rightarrow\infty$ describes the self-similar geometry of the infinite cluster at p_c. A similar method of construction can be used in $d=3$ if we describe a face-centered-cubic lattice in terms of tetrahedra stacked along the cube diagonal with each upward-pointing triangle in Fig. 1 representing the base of a tetrahedron. In both cases we have not included any finite clusters nor dangling bonds.

We now consider the excitation spectrum of these systems when each site represents a mass and each bond represents a spring of length a. All masses and springs are identical and the Hamiltonian is assumed to

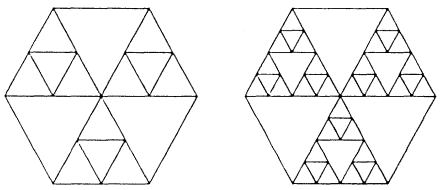

FIG. 1. Fractal lattice in $d=2$ for $n=1$ and $n=2$.

have the Born form for which the equations of motion are separable and hence reduce to a scalar problem. This model has the advantage that the spectral properties can be calculated exactly by use of real-space rescaling techniques[9-11] combined with functional integral methods.[12,13] In the limit $L/a=1$ $(n=0)$ we have a regular Euclidean lattice and the eigenstates have the Bloch form with the low-frequency DOS scaling as

$$N(\omega^2) \sim (\omega^2)^{(d-2)/2}. \quad (1)$$

In the opposite limit $L/a=\infty$ $(n=\infty)$ we have a d-dimensional Sierpinski gasket. The excitation spectrum in this case has been studied previously by several groups[12,14,15] and the low-frequency DOS behaves as above with d replaced by the spectral dimension $\tilde{d}$. For both $d=2$ and $d=3$ the spectral dimension is given by $\tilde{d}=2\ln(d+1)/\ln(d+3)$, whereas the fractal dimension is $D=\ln(d+1)/\ln(2)$.

Figure 2 shows our results for the DOS in $d=3$ for $n=0$, 1, 2, and 9. As we increase n, or equivalently approach p_c, the continuous spectrum gradually breaks up into a collection of narrower bands separated by gaps with localized modes in the gaps and at the band edges. Qualitatively similar results are found in two dimensions.[16] An alternate way of describing these lattices is to regard the fractal region on length scales from a to L as a unit cell in the Euclidean structure. For small values of n we can easily calculate the eigenvalues as a function of wave vector Q and we plot these curves for $n=1$ and $n=2$ in Fig. 3. We have only plotted the dispersion curve along $\Gamma\kappa$ of the first Brillouin zone and in this case the zone boundary is located at $2\pi/L$. Notice that as the fractal region grows many of the modes become independent of Q. These modes are localized within the unit cell and are highly degenerate. In fact, for large values of n, the mode at $\omega^2=4$ exhausts $\frac{1}{2}$ of the total DOS. The low-frequency part of the spectrum consists of a Euclidean band whose weight in the total DOS and width decrease as we approach p_c. The maximum frequency of this lowest band corresponds to a mode with wavelength equal to the correlation length and we identify this as a crossover frequency ω_c. We find that ω_c scales as $(p-p_c)^{\nu D/\tilde{d}}$ and that the weight of this band scales as $(p-p_c)^{\nu D}$. As n increases the number of bands and gaps also increases but the weight of the band modes decreases and the DOS is dominated by the modes with no dispersion (localized within the unit cell). However, the crossover is rather smooth and there is no sharp structure in the DOS at ω_c. Our calculations indicate that the higher-frequency part of the DOS is composed of both extended and localized states and that the extended states do not simply accumulate at ω_c. These results are also supported by the recent numerical calculations of Grest and Webman[17] who have calculated the vibrational properties of percolation clusters for a simple-cubic lattice. They find a smooth crossover between a phonon and fracton regime in the DOS as well as evidence for both extended and localized states at high frequencies.

Dangling ends and finite clusters could be added to the present model. The dangling bonds could then be eliminated to yield a distribution of effective masses for the backbone which may remove the large degeneracy of some of the gap modes. Finite clusters would contribute additional gap modes but we do not expect

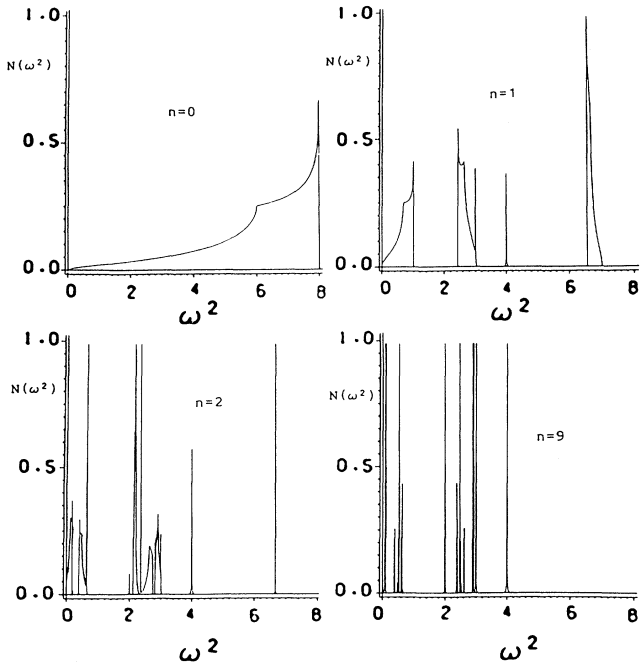

FIG. 2. Density of states $N(\omega^2)$ plotted as a function of ω^2 for $n=0$, 1, 2, and 9 in three dimensions.

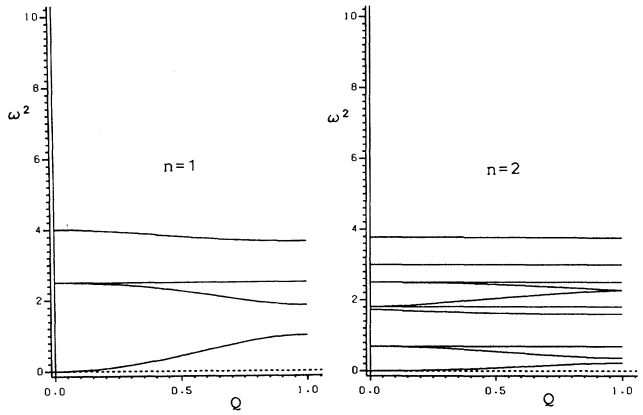

FIG. 3. Dispersion curves ω^2 vs Q in $d=3$ for $n=1,2$.

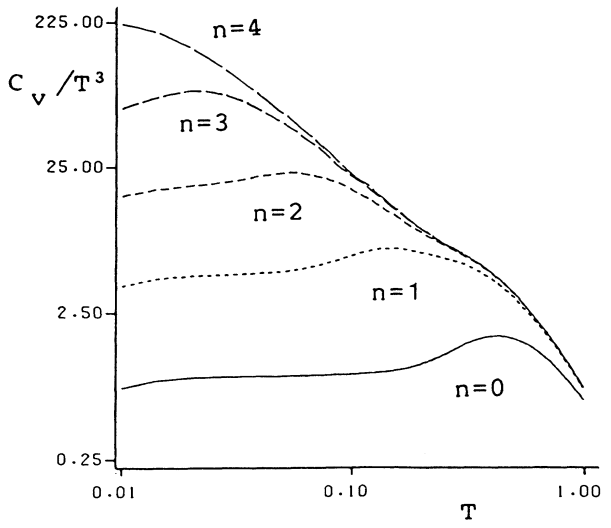

FIG. 4. C_V/T^3 plotted as a function of T on a log-log scale in $d=3$ for $n=0$–4.

these additional modes to accumulate at a well-defined crossover frequency.

We have also calculated the specific heat C_V, and Fig. 4 shows our results for $d=3$ where we have plotted C_V/T^3 vs T on a log-log scale. There is a Debye region at low T which gradually shrinks as n increases. In both $d=2$ and $d=3$ the curves can be described by a scaling form

$$C_V/T^d \sim (\xi_p^{-D/\tilde{d}})^{\tilde{d}-d} f(T\xi_p^{D/\tilde{d}}). \quad (2)$$

The prefactor arises because of the reduction in bandwidth of the lowest band and corresponds to the anomalous behavior of the sound velocity at p_c which scales as $\xi_p^{(1-D/\tilde{d})}$. The peak in the curves at low temperature is due to the deviation of the Euclidean band from a Debye spectrum and not due to fractons.[8] The position of this peak scales as $\xi_p^{-D/\tilde{d}}$.

The fractal lattices used here are similar to the recently discovered quasicrystals[18–20] which are crystals with quasiperiodic translational order. Our lattices are neither random nor translationally invariant but they do have orientational order in that all triangles and tetrahedra have the same orientation in space. The real quasicrystals also exhibit self-similar properties not unlike our fractal lattices and we would expect the thermodynamic properties of these materials to exhibit non-Euclidean behavior at low temperatures.

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