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Vibrational properties of percolating clusters: Localization and density of states

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The vibrational integrated density of states (DOS) of two-dimensional percolating clusters is calculated using a novel numerical technique. It is confirmed that the density of states is characterized by an $\omega^{1/3}$ power-law behavior in the fracton regime, while a transition to a Debye-type spectrum occurs at lower frequencies. The dependence of the crossover frequency ω_c and the coefficient A_D of the Debye term in the DOS on the concentration p of the percolating cluster are numerically determined. By use of finite-size scaling methods, the localized nature of all the vibrational modes is established. We find that the fracton states as well as the phonon states are exponentially localized. There is no evidence for fracton superlocalization. However, there is a power-law dependence of the localization length versus frequency in the fracton regime, which crosses over to an exponential dependence in the low-frequency regime.

Over the past few years, there has been a growing interest in the vibrational properties[1-3] of systems of atoms which have fractal geometry. A model system that is known to display fractal behavior over a range of length (frequency) scales is percolating clusters.[4,5] The structure of percolating clusters above the percolation threshold is fractal on a scale smaller than ξ, the percolation correlation length, and becomes homogeneous on larger length scales. Alexander and Orbach[1] first suggested that the density of states (DOS) of the vibrational modes of percolating clusters obeys a universal law $N(\omega)\sim\omega^{\tilde{d}-1}$ above a characteristic frequency ω_c. It has been conjectured[1] that the fracton dimensionality $\tilde{d}$ equals $\frac{4}{3}$ for percolation fractals in all dimensions. While $\tilde{d}$ is probably not exactly $\frac{4}{3}$ in all dimensions,[6,7] it is nevertheless an extremely good approximation. Vibrational excitations in this regime are called "fractons." At very low frequencies ($\omega<\omega_c$), the DOS follows the ordinary Debye law $N(\omega)\sim\omega^{d-1}$, where d is the space dimensionality. The crossover behavior of the DOS has been seen in computer simulations of two-dimensional percolating[8,9] clusters as well as in experiments.[10] However, no detailed study of the crossover frequency ω_c between the phonon and fracton regime for different concentrations exists to compare with the scaling predictions. We also find, in agreement with the two previous numerical studies of the density-of-states,[8,9] no evidence for a discontinuity around ω_c which was first suggested by the effective-medium theory of Derrida, Orbach, and Yu.[11]

Somewhat surprisingly, very little is known about the localization or extended nature of eigenstates in the fracton regime. Rammal and Toulouse[3] suggested that fractons are localized, since $\tilde{d}\simeq\frac{4}{3}$ which is less than 2. It has been argued[12] that the vibrational excitations in disordered systems, such as percolating clusters or a system of atoms with random masses and the nearest-neighbor force constant, follow those of the electronic excitations in disordered systems. In particular, for $d=2$ it is expected[12] that the vibrational excitations are always localized and the localization length λ_c behaves as $\lambda_c\sim\exp[1/\omega^2]$. Recently, Levy and Souillard[13] suggested that the fracton wave function has the following superlocalized form

$$\psi(r)\sim\exp\{-[r/\lambda_c(\omega)]^{d_\phi}\}\,, \tag{1}$$

where $\lambda_c(\omega)$ is the frequency-dependent localization length and the exponent d_ϕ is larger than 1 (thus the name superlocalized wave function). For the percolating cluster, Levy and Souillard[13] suggested that $d_\phi=D/\tilde{d}$, where D is the fractal dimension. For $d=2$, since $D=\frac{91}{48}\simeq1.896$, this gives $d_\phi=1.42$. Aharony, Entin-Wohlman, and Orbach[14] have suggested that $d_\phi=(2-\tilde{d})D/\tilde{d}$, which gives a value of less than 1, $d_\phi=0.95$ for $d=2$. Therefore, an open question remains whether superlocalization is correct and if so, what is the exact value of the exponent d_ϕ? To clarify this point, Yakubo and Nakayawa[15] performed detailed numerical calculations using the equation-of-motion method in two-dimensional percolating clusters. However, this result $d_\phi=2.3\pm0.1$ is much higher than all the previous estimates of d_ϕ. Therefore, it is clear that a more detailed study is needed for percolating clusters to clarify the nature of the fracton state.

In this paper, we present a numerical study of the vibrational modes of two-dimensional (2D) percolating networks with concentrations $p\geq p_c$. Through detailed studies of the integrated density-of-states (IDOS), it is confirmed that there are two distinct frequency regimes (phonon and fracton regions) in the DOS separated by ω_c. The dependence of ω_c and A_D on p is determined. Using finite-size scaling techniques, the localization character of the vibrational modes is established and the frequency dependence of the localization length is also obtained. Finally, within the finite-size scaling technique we find no indication of superlocalization for the fracton wave functions.

Consider a lattice characterized by site disorder that is composed of N particles of equal mass that are connected

by linear springs. The displacements u_n of the mass points are given by

$$-z_n u_n + \sum_m K_{nm} u_m = m_n \omega^2 u_n , \quad (2)$$

where the sum is over the nearest neighbors of site n and $z_n = \sum_m K_{nm}$. For site percolation, a given lattice site is occupied by a particle of mass $m_n = 1$, with probability p and is unoccupied with probability $1-p$. The force constant is taken to be $K_{nm} = 0$, if either site n or m is unoccupied and $K_{nm} = 1$, otherwise. Since only sites in the same cluster are connected, each cluster vibrates independently. In the model, the displacement u_n is a scalar. Equation (2) is completely analogous to the tight-binding Hamiltonian of the electronic problem where a considerable amount of analytic and numerical work has been carried out over the last fifteen years. The most straightforward approach to obtain the eigenvalues ω and the corresponding eigenvectors is simply to diagonalize the dynamical matrix. However, only relatively small clusters ($N < 3000$) can easily be diagonalized directly due to limitations on computer memory. To study the low-frequency regime in greater detail and to observe the crossover frequency ω_c, one needs a much larger system ($N > 10^4$). Here we investigate the crossover regime at the vicinity of ω_c for N in the range 10^4 to 10^5 using three different techniques.

For calculating the IDOS, the first technique we employed was the Sturm sequence method. The method consists of an application of Gaussian elimination on the consecutive columns or rows of the matrix $(E\hat{1} - H)$, where $E = \omega^2$ and $H_{nm} = K_{nm} - z_n \delta_{nm}$. The Gaussian elimination of the elements of the matrix is applied until the matrix is reduced to a triangular form. The IDOS is then calculated by counting the fractonal number of positive elements in the diagonal of the reduced triangular matrix. For details of the calculation, see Refs. 16 and 17. The advantage of using this method is both economy in storage and speed. The computing time rises as $M^{3(d-1)} \times N$, which allows us to consider very long strips with length N of considerable width M. It also does not require matrix inversion. In our calculations, we have used systems as large as 160×1280 and 320×640 for the 2D case.

In Fig. 1 we plot the DOS of the 2D percolating cluster for different concentrations of p as a function of frequency ω. For high energies, the DOS behaves as $\omega^{1/3}$ consistent with the Alexander-Orbach conjecture of $N(\omega) \sim \omega^{1/3}$ for the fracton regime. For each concentration p there exists a frequency ω_c below which the DOS changes to a regular Debye regime where $N(\omega) \sim \omega$ for a 2D system. The DOS is clearly described by two regimes (fracton and phonon) separated by a crossover frequency ω_c. In Fig. 2, the crossover frequency ω_c is plotted versus the concentration p. As p approaches p_c, the crossover frequency ω_c approaches zero as expected. To a good approximation, $\omega_c \sim A_f |p - p_c|^{(1.0 \pm 0.3)}$, where $A_f = 1.04$. This is in qualitative agreement with the predictions of the scaling theory which gives $\omega_c \sim |p - p_c|^{\nu[1+(\theta/2)]}$, where ν is the correlation length exponent and θ is the anomalous diffusion exponent. For very short times t, the diffusion is anomalously slow and the diffusion length $R \sim t^{1/2+\theta}$. For

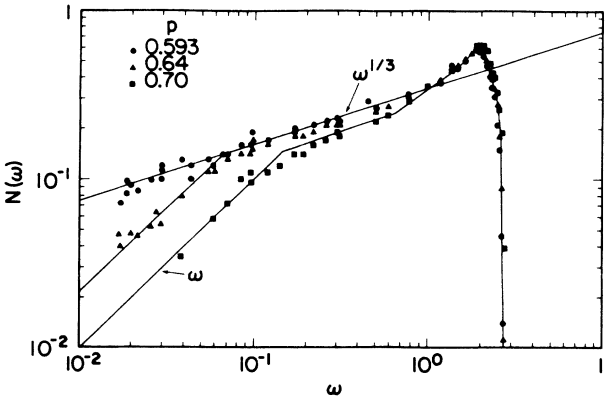

FIG. 1. The DOS $N(\omega)$ for 2D site-percolating clusters at three different percolation concentrations, $p_c = 0.593$. Solid lines are only a visual guide.

a 2D percolating cluster,[6] $\nu = 4/3$ and $\theta = 0.87$, thus $\nu[1+(\theta/2)] = 1.91$ which is larger than the value of (1.0 ± 0.3) found in our numerical studies. The discrepancy is probably due, as can be seen from Fig. 1, to the fact that ω_c is very difficult to determine.

In Fig. 2, we plot also the coefficient A_D of the Debye term in the DOS, where $N(\omega) = A_D \omega$. The coefficient A_D is inversely proportional to the sound velocity and $|p - p_c|$. It has been argued[18] that $A_D \sim |p - p_c|^{\beta - t}$, where β is the exponent of the infinite cluster and t is the conductivity exponent. For a 2D percolating cluster,[6,19] $\beta = \frac{5}{36}$ and $t \simeq 1.3$, and therefore $A_D \sim |p - p_c|^{-1.16}$. Our numerical results give $A_D \sim |p - p_c|^{-1.10 \pm 0.05}$, in excellent agreement with the analytical arguments. Thus, we conclude that the coefficient A_D of the Debye DOS can be numerically calculated very accurately, while the crossover frequency ω_c, which is not as well defined, is very difficult to determine. Our numerical results of the DOS do not show any drastic change in the crossover region. It has been suggested[15] that the absence of the hump in the

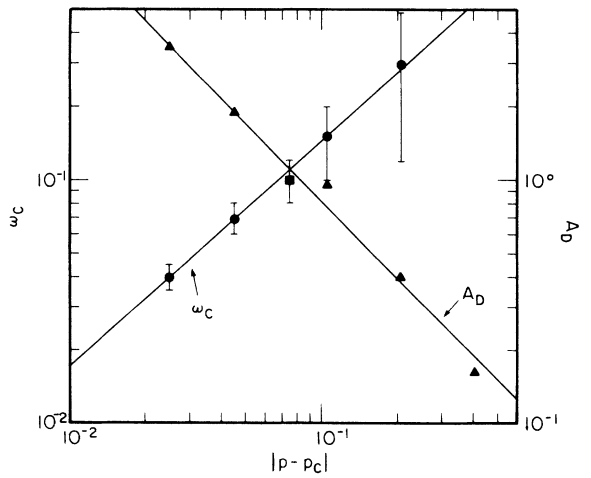

FIG. 2. The crossover frequency ω_c and the coefficient A_D of the Debye term of the DOS vs $|p - p_c|$ on a log-log scale.

vicinity of the crossover region implies the appearance of excess DOS in the phonon regime. We systematically analyzed our results to look for such an excess and did not find it. In fact, $A_D/|p-p_c|^{\beta-t}$ is independent of p and equal to its Debye value for the perfect lattice.

Now, let us turn to the nature of the eigenstates on a percolating cluster. Here we use the wire or strip method which has already been developed[20-22] and used with great success for the electronic motion in simple disordered lattice models. Note that this method has never been used for the phonon problem. However, because of the formulation of the phonon problem as given in Eq. (2), it can be made analogous to the electronic problem. In the strip method, one considers coupled 1D systems. Each 1D system is described by an equation of motion of the form in Eq. (2). The corresponding sites of the nearest-neighbor 1D system are coupled by an interchain matrix element K_{nm} which is equal to one if both sites are present, but is equal to ϵ if one site is missing and equal to ϵ^2 if both sites are missing. In the present work, M chains are coupled into a 2D array with interchain coupling K_{nm}. The additional term K_{nm} is necessary to ensure that the lattice is connected. For M regularly placed chains of length N, one determines the largest localization length λ_M as $N\rightarrow\infty$. In particular, by studying λ_M/M vs M, one obtains a reasonable estimate of the mobility-edge trajectory. At exactly the mobility edge, we found[20] for a large number of electronic problems $\lambda_M/M\simeq 0.6$, while for extended and localized states we found that λ_M/M vs M increases or decreases, respectively. The localization length for the 2D percolating system can be obtained by either plotting M/λ_M vs M from which the slope gives $1/\lambda_c$ or by scaling all the numerical data of λ_M/M to follow a simple scaling function of the form $\lambda_M/M=f(\lambda_c/M)$, where f is a universal function of its argument. For our studies here, we used M from 2 through 128 and $\epsilon=10^{-4}$ with N up to 50000. We found that our results are independent of ϵ provided that $\epsilon<10^{-3}$. Using both of these techniques, we have calculated λ_c as a function of frequency or energy for two concentrations p. As shown in Fig. 3 for $p=p_c=0.593$, $\lambda_c(\omega)\sim\omega^{-0.75}$ for all frequencies.[13,21] This agrees reasonably well with the predictions of the scaling analysis $\lambda_c(\omega)\sim\omega^{-\tilde{d}/D}=\omega^{-0.70}$. For $p=0.70$, we have $\lambda_c(\omega)\sim\omega^{-0.75}$ for $\omega>\omega_c=0.1$ (in the fracton regime), while for lower frequencies (in the phonon regimes) we obtain exceptionally large values for the localization length. We used M up to 128 and $N=6000$ to determine λ_c for these low frequencies. Our numerical results suggest that as we lower the frequency ω past ω_c, a drop in the $\lambda_c(\omega)$ is observed. Then at even lower frequencies a faster increase is seen. This nonmonotonic dependence of $\lambda_c(\omega)$ vs ω is a very interesting behavior that we do not completely understand. It might be related to the change in the DOS from a $\omega^{1/3}$ to ω dependence, since in the phonon regime the DOS decreases more rapidly than in the fracton regime. This change may be reflected in $\lambda_c(\omega)$, at least around ω_c. It is also possible that this is due to the fact that our largest width M is 128. From the equivalence of electron localization with phonon localization[12] for a system with random masses and constant force constants, one would expect an exponential behavior for $\lambda_c(\omega)\sim\exp(1/\omega^2)$. Our data for λ_c is qualitatively consistent with this dependence. However, it is very interesting that for high frequencies $\omega>\omega_c$, the localization length follows a simple power law. Experimentally, this crossover from exponential to power-law behavior of the frequency dependence of the localization length has not been observed.

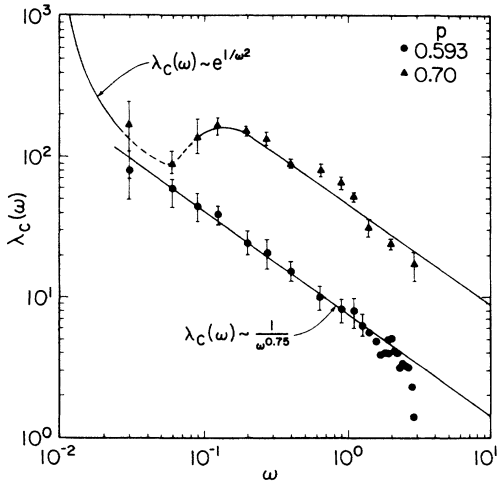

FIG. 3. The localization length $\lambda_c(\omega)$ versus frequency ω for two different percolation concentrations, $p=p_c=0.593$ and $p=0.70$. For $p=0.70$ there is a nonmonotonic behavior for $\lambda_c(\omega)$.

Finally, we have very systematically searched for the superlocalization behavior of the fracton wave functions suggested by Levy and Souillard[13] and Aharony *et al.*[14] Contrary to the findings of Yakubo and Nakayama,[15] where the wave function was found to decay faster than exponential with $d_\phi=2.3\pm 0.1$, we found no indication for superlocalization in our studies with the transfer method. The entire transfer method is based on finding in Green's function by using recursion relations and assuming that the length dependence in Green's function scaled as $G\sim e^{N/\lambda_c}$. As the length N of the strip increases, if λ_c eventually approaches a constant value, this means that for at least large lengths, the Green's function and therefore the wave functions behave as a simple exponential and not as in the form given by Eq. (1). It is possible, however, that for short distances the wave function might behave as in Eq. (1) with $d_\phi>1$. However, this cannot be checked by the transfer method, which is based on letting $N\rightarrow\infty$. This interpretation is consistent with the results of Ref. 15 in which the eigenvalues and eigenvectors in the fracton regime are obtained by diagonalizing a large matrix, but only the short length dependence of the wave functions was used to look for superlocalization. We have also looked systematically for superlocalization[13] at the classical percolation[19,20] threshold for a 3D quantum-percolation model. It has been argued[13] that in the case of a 3D quantum percolation, all states at p_c are superlocalized, since the first extended states appear at the quantum-percolation threshold p_q. While it is clear that all states at $p_c<p_q$ are clearly localized, the issue is whether they are superlocalized. For a 3D tight-binding

model on the simple cubic lattice with random sites $p_c = 0.311$, while $p_q = 0.42$.[20] In this case, we find no indication of superlocalization. While we cannot rule out the fact that the wave function might be superlocalized at short lengths, we see no evidence in either the phonon or quantum electronic case that $d_\phi \neq 1$ for very large lengths.

In conclusion, we showed agreement with previous work that the DOS is characterized by an $\omega^{1/3}$ power behavior in the fracton regime, while a transition to a Debye-type spectrum occurs at lower frequencies. There is no excess Debye DOS at the crossover frequency ω_c. In the phonon regime, we have that $N(\omega) = A_D \omega$, in agreement with the scaling predictions. We also found that ω_c scales as $|p - p_c|^{1.0}$ in qualitative agreement with the scaling predictions, but with a lower exponent. Using the very accurate finite-size scaling methods, we numerically established that all the vibrational modes are exponentially localized. We found that in the fracton regime, the localization length has a power-law dependence on frequency in agreement with the scaling predictions. In the phonon regime, the localization length depends exponentially on frequency. Finally, our studies showed no evidence of fracton superlocalization.[23]

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