Extended Fractons and Localized Phonons on Percolation Clusters

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We investigate the localization behavior of vibrational modes of infinite percolation clusters above the critical concentration in two and three dimensions using the method of level statistics. We find that all eigenstates are localized in \( d = 2 \), including the low frequency phonon states. In \( d = 3 \) we obtain evidence for a localization-delocalization transition. But contrary to the common view this transition occurs for frequencies above the phonon fracton crossover giving rise to a new regime of extended fracton states.

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Percolation represents one of the standard models for disordered systems. Its applications range from transport in composites and in amorphous and porous media to the properties of branched polymers and gels, for recent reviews see e.g. [1,2]. One intriguing aspect is the vibrational dynamics of percolation networks. Since the pioneering discovery of localized lattice vibrations (‘fractons’) by Alexander and Orbach [3,4], much work has been devoted to the study of their properties [5–14] and the investigation of various applications [15–18] and in particu-lar its implication on the localization behavior has been discussed in a controversial way. Analogies with random walks seem to indicate that the crossover characterizes a transition between localized fractons and extended phonons. This view has been mostly accepted for three-dimensional systems (1,2,13,18,19, see also [15]), but not yet been proven. Analogies with the Anderson model [21], in contrast, suggest the absence of a localization-delocalization transition for two-dimensional systems. But since these analogies are not exact, even the value of the critical dimension has not been established for vibrations [12].

It is the purpose of this Letter to clarify the localization properties of the vibrational excitations. We employ the method of level statistics which has been used successfully to determine the localization-delocalization transition (LDT) in the Anderson model [22–24]. We find that the localization properties of the vibrations are not related to the fracton-phonon crossover (FPC) at \( \omega_c \). Our results suggest that (i) in \( d = 2 \) all states are localized and (ii) the LDT in \( d = 3 \) occurs at a critical frequency \( \omega_c \) well above \( \omega_c \). Accordingly the vibrational modes in \( d = 3 \) are extended phonons below \( \omega_c \) and localized fractons above \( \omega_c \), while the regime between \( \omega_c \) and \( \omega_c \) is characterized by extended excitations with a fracton-type dispersion (‘extended fractons’).

We consider the incipient infinite site percolation cluster on a square lattice and a simple cubic lattice, both above the critical concentrations \( p_c \approx 0.59275 \) and \( 0.3116 \), respectively. On length scales below the correlation length \( \xi \sim |p - p_c|^{-\nu} \), the cluster is self-similar and characterized by the fractal dimension \( d_f \). Above \( \xi \), the cluster appears homogeneous. The correlation exponent \( \nu \), the fractal dimension \( d_f \), and the spectral dimension \( d_s \) depend on the space dimension \( d \): \( \nu \approx 4/3, d_f \approx 91/48 \) and \( d_s \approx 1.3173 \) in \( d = 2 \); \( \nu \approx 0.875, d_f \approx 2.524 \), and \( d_s \approx 1.328 \) in \( d = 3 \).

We assume that equal masses \( M \) are placed on each occupied site and nearest neighbor cluster sites \( n \) and \( n + \delta \) are coupled by equal (scalar) force constants \( k_{n,n+\delta} \). In this case, different components of displacements decouple and we obtain the same equation of motion for lattice vibrations for all components \( u_n(t) \),

\[
M \frac{d^2}{dt^2} u_n(t) = \sum_{\delta} k_{n,n+\delta} [u_{n+\delta}(t) - u_n(t)],
\]

where the sum runs over all nearest neighbor sites \( n + \delta \) of site \( n \). The standard ansatz \( u_n(t) = u_{n,\omega} \exp(-i\omega t) \) leads to the corresponding time independent vibration equation. Setting \( M = k_{n,n+\delta} = 1 \) (which determines the unit of the frequency) we obtain

\[
-\omega^2 u_{n,\omega} = \sum_{\delta} (u_{n+\delta,\omega} - u_{n,\omega}),
\]

which represents an eigenvalue equation that can only be solved numerically.

For obtaining an analytical estimate of the way the characteristic length in the vibration problem depends on the frequency \( \omega \) and on the correlation length \( \xi \), one can employ the analogy between the corresponding diffusion equation and the vibration equation, Eq. (1).
In the diffusion problem, the characteristic length is the root-mean-square displacement $R(t) = \langle r^2(t) \rangle^{1/2}$ of a diffusing particle (random walker). At criticality, $R(t)$ scales as $R(t) \sim t^{1/d_w}$ with the random walk dimension $d_w = 2d_f/d_s$. Above $p_c$, the finite correlation length $\xi$ gives rise to a finite ‘correlation’ time $\tau_\xi \sim \xi^{d_w}$. Below $\tau_\xi$, the random walker discovers the fractal part of the infinite cluster and $R(t) \sim t^{1/d_w}$, while above $\tau_\xi$, on length scales where the cluster is homogeneous, diffusion is normal and $R(t) \sim t^{1/2}$. Since the (discretized) diffusion equation reduces to the vibration equation, Eq. (2), when the first time derivative is substituted by a second time derivative, we can obtain a corresponding characteristic length $\Lambda(\omega)$ for the vibration problem by substituting $t^{-1}$ in $R(t)$ by $(1/t)^2 = \omega^2$. This yields

$$\Lambda(\omega) \sim \begin{cases} \omega^{-2/d_w}, & \text{for } \omega \gg \omega_\xi \sim \xi^{-1/2} \sim \xi^{-d_w/2}, \\ \omega^{-1}, & \text{for } \omega \ll \omega_\xi. \end{cases} \quad (3)$$

The expression for the crossover frequency $\omega_\xi$ that separates the fracton from the phonon regime can be written as

$$\omega_\xi = \omega_0 (p - p_c)^{d_w\nu/2}, \quad (4)$$

where the proportionality factor $\omega_0$ depends on the details of the underlying lattice.

The scaling for the vibrational DOS $g(\omega)$ can be derived in an analogous way. By construction, the crossover frequency $\omega_\xi$ separating the fracton regime with $g(\omega) \sim \omega^{d-1}$ from the phonon regime with $g(\omega) \sim \omega^{d-1}$ is expected to be identical with $\omega_\xi$ from Eq. (4). We have determined $\omega_0$ from the DOS for percolation clusters on the square lattice and the simple cubic lattice for several concentrations above $p_c$. The crossover from the fracton to the phonon regime is smooth (see also [14]). We find $\omega_0 \approx 15$ in $d = 2$ and $\omega_0 \approx 6$ in $d = 3$ for the parameter in Eq. (4). Both numbers are in good agreement with earlier (less extensive) numerical calculations of the DOS [13].

In order to see the difference of the characteristic length $\Lambda$ described by Eq. (3), we have numerically solved Eq. (2) using the Lanczos algorithm. Figure 1 shows the wavelength $\lambda(\omega)$ that we calculated by Fourier transform of the eigenstates at several frequencies and concentrations in $d = 2$ and in $d = 3$. The data nicely confirm that the wavelength $\lambda$ is the characteristic length $\Lambda$ discussed above. At the FPC, the wavelength crosses over from fracton behavior for high frequencies to phonon behavior for low frequencies according to Eq. (3). The values of the crossover frequency $\omega_\xi$ are well described by Eq. (4). In addition, the prefactor $\omega_0$ is exactly the same as for the crossover frequencies that were previously determined for the vibrational DOS $g(\omega)$, since the crossover occurs exactly at $\omega = \omega_\xi$ in Fig. 1. Thus, the characteristic length $\Lambda$ can be identified with the wavelength of the modes.

Next we address the localization behavior of the vibrational excitations. We want to know if there is an intimate relationship between the FPC and the localization behavior, such that, for example, phonons are extended and fractons are localized, as one might infer from the analogies with random walks discussed above. This analogy suggests a LDT both in the phonon regime ($\omega < \omega_\xi$) and $-2/d_w$ in the fracton regime ($\omega > \omega_\xi$) according to Eq. (4). In $d = 3$, we used the effective value $d_w = 3.4$ that governs diffusion on length scales of the order of the correlation length considered here. The asymptotic value $d_w = 3.8$ applies only to considerably larger length scales. The figure shows that $\omega_\xi$ is the FPC frequency for the wavelength.

In the following we address the questions: (i) Are the phonon states in $d = 2$ (for $\omega < \omega_\xi$) extended or localized states? (ii) Does the localization-delocalization transition (LDT) for vibrations in $d = 3$ occur at the same frequency as $\omega_\xi$? For answering these questions, we have applied the method of level statistics, which proved to be a powerful tool for the electronic case recently [22, 24].
In conducting disordered electronic systems, the energy spacing distribution \( P(s) \) of consecutive eigenvalues (levels) \( E_i \) shows the universal random matrix theory result \([25,26]\), which is well approximated by the appropriate Wigner surmise, \( P(s) = (\pi/2)s \exp(-\pi s^2/4) \). Here, \( s = |E_{i+1} - E_i|/\Delta \) where \( \Delta \) is the mean level spacing in the energy interval considered. For localized states the uncorrelated eigenvalues are described by the Poisson distribution, \( P(s) = \exp(-s) \). In contrast to \( P(s = 0) = 1 \) for localized states, the probability that two eigenvalues are close in energy decreases to zero for extended states, because of the level repulsion due to the overlap of the corresponding eigenstates. For finite systems, the shape of \( P(s) \) is in between the two limiting cases and approaches one of them with increasing system size. \( P(s) \) is system size independent only directly at the transition. Hence, the knowledge of the nearest neighbor spacing distribution \( P(s) \) for several system sizes tells whether the eigenstates are localized or extended in the limit of infinite system size.

**FIG. 2.** Second moments \( I_0(\omega) \) of the level spacing distribution \( P(s) \) for vibrational modes of 3d percolation clusters with site concentration \( p = 0.37 \). The symbols denote different system sizes \( L \) (radius of the clusters in topological space), \( L = 50 \) (\( \Box \)), \( L = 62 \) (\( \bigcirc \)), \( L = 75 \) (\( \triangle \)), \( L = 90 \) (\( \nabla \)), \( L = 110 \) (\( \ominus \)), and \( L = 150 \) (+), corresponding to cubic systems with linear sizes ranging from 30 to 107. The correlation length was determined to be \( \xi \approx 3.3 \). The LDT occurs for \( \omega_c = 0.24 \).

Since it is tedious to compare the \( P(s) \) distributions for several system sizes and other model parameters, we calculate the size dependence of the quantity \( I_0 = \langle s^2 \rangle /2 \), which is related to the second moment of the level spacing distribution \( \langle s^2 \rangle = \int_0^\infty s^2 P(s) ds \). If the eigenstates are localized, \( I_0 \) increases monotonously with increasing system size approaching the Poisson limit \( I_0^{\text{loc}} = 1 \) for infinite system size. If the modes are extended, \( I_0 \) decreases monotonously until it reaches the random matrix theory limit \( I_0^{\text{ext}} = 0.637 \). At the transition \( I_0^{\text{crit}} \) is scale invariant, but its precise value depends on the boundary conditions. Other moments of the distribution give similar results.

We apply the method of level statistics to vibrations of incipient infinite percolation clusters at several concentrations ranging from \( p = 0.61 \) to \( p = 0.8 \) in \( d = 2 \), and from \( p = 0.32 \) to \( p = 0.5 \) in \( d = 3 \). Up to six different cluster sizes are compared for each concentration. The clusters were generated by the Leath method and the eigenvalues were computed with a Lanczos algorithm. For the vibrational modes, the level spacing is \( s = |\omega_{i+1}^2 - \omega_i^2|/\Delta \) since the eigenvalue \( \omega^2 \) in Eq. (2) corresponds to the energy eigenvalue \( E \) for electrons. Representative results are shown in Fig. 2 and in the inset of Fig. 2.

In Fig. 2 the LDT can clearly be observed for vibrations of clusters in \( d = 3 \) at \( p = 0.37 \). For low frequencies, \( \omega < \omega_c \), \( I_0(\omega, L) \) decreases with increasing system size \( L \), indicating extended modes, while it increases for \( \omega > \omega_c \), as expected for localized modes. Directly at the critical frequency \( \omega_c \approx 0.24 \), \( I_0(\omega, L) \) is independent of \( L \). This value of the LDT frequency \( \omega_c \) is well above the corresponding FPC frequency \( \omega_p \approx 0.053 \) that we obtained from Eq. (1) with \( \omega_0 \approx 6 \). Consequently, we discover a novel intermediate regime of extended fracton modes for \( \omega_p < \omega < \omega_c \).

Using plots similar to Fig. 2 we determined the LDT frequency \( \omega_c(p) \) for nine concentrations \( p \). All values of \( \omega_c(p) \) are well above the respective FPC at \( \omega_p(p) \). Our results for \( d = 3 \) are summarized in Fig. 3 which shows the phase diagram. The critical frequencies \( \omega_c(p) \) can be fitted by \( \omega_c(p) \approx 27(p - p_c)^{2\nu/\nu} \) (dashed line in Fig. 3), suggesting that \( \omega_c(p) \) scales as \( \omega_p(p) \), but with a different prefactor (\( \omega_0 \approx 27 \) instead of \( \omega_0 \approx 6 \)).

**FIG. 3.** Phase diagram of vibrational modes of percolation clusters in \( d = 3 \). The FPC at \( \omega_p(p) \) is marked by the continuous black line. The black discs indicate the LDT at \( \omega_c(p) \). Finite size effects do only occur in the shaded region at very low frequencies. While the vibrational modes are (extended) phonons for low frequencies \( \omega < \omega_c(p) \) and localized fractons for \( \omega > \omega_c(p) \), a new intermediate regime of extended fractons is located between the two curves.
Next we consider $d = 2$. The results of the level statistics for vibrational modes on incipient infinite percolation clusters at $p = 0.75$ are shown in the inset of Fig. 4. We find no indication of a LDT. For $\omega > 0.15$, the modes turn out to be localized since $I_0(\omega)$ increases with increasing system size. This limit is well below the FPC frequency $\omega_c \approx 0.43$ that we obtained from Eq. (4) with $\omega_0 \approx 15$. Hence, we can conclude that the vibrational modes remain localized even for frequencies well below the FPC frequency $\omega_c$. For very small frequencies $\omega$, the level statistics does not provide a conclusive picture due to the restricted system sizes. Our results for the localization behavior in $d = 2$ are summarized in the main part of Fig. 4.

![Phase diagram of vibrational modes of percolation clusters in $d = 2$](image)

**FIG. 4.** Phase diagram of vibrational modes of percolation clusters in $d = 2$. The black line separates localized fractons with $\lambda(\omega) \sim \omega^{-2/4}$ from localized phonons with $\lambda(\omega) \sim \omega^{-1}$. In the shaded region, the method is not specific since finite size effects occur. The inset shows $I_0(\omega)$ for site concentration $p = 0.75$. The symbols correspond to different system sizes, $L = 70$ ($\bigcirc$), $L = 100$ ($\bigcirc$), $L = 150$ ($\triangle$), $L = 220$ ($\triangledown$), $L = 350$ ($\bullet$), and $L = 500$ ($+$), corresponding to quadratic systems with linear sizes ranging from 95 to 680. There is no indication of extended states.

In conclusion, we have applied level statistics to investigate the localization behavior of vibrational excitations on the infinite percolation cluster in $d = 2$ and $d = 3$. We have found that above $p_c$, two length scales have to be distinguished. (i) The wavelength $\lambda$ is strongly related to the density of states $g(\omega)$ and its scaling can be derived from the analogy to diffusion. At $\omega_c$, both $\lambda(\omega)$ and $g(\omega)$ cross over from fractal to normal behavior. (ii) The localization length is supposed to diverge at the localization-delocalization transition, which occurs in $d = 3$ at a critical frequency $\omega_c$, that is considerably larger than the fracton-phonon crossover frequency $\omega_c$. As a consequence, a novel regime of extended fractons exists in the phase diagram of vibrations in $d = 3$. These extended states might be observable in real experiments. In $d = 2$ there is no localization-delocalization transition, so also the phonon modes are localized. Thus, the vibrational modes in percolation systems show features characteristic of both classical diffusive and electronic systems. For a complete understanding of the problem both analogies are useful and necessary.

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