Scattering of Fractons, the Ioffe-Regel Criterion, and the $\frac{4}{3}$ Conjecture

Amnon Aharony[(a)]
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

and

S. Alexander, Ora Entin-Wohlman,[(a)] and R. Orbach
Department of Physics, University of California, Los Angeles, Los Angeles, California 90024
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The relaxation time for scattering of vibrational modes by structural irregularities in d-dimensional random systems is shown to cross over from $1/\tau \sim \omega^{d+1}\omega_c^{-d}$ for phonons ($\omega < \omega_c$, the crossover frequency between phonon and fracton vibrational excitations) to $1/\tau \sim \omega^{5-3\tilde{d}}$ for fractons ($\tilde{d}$ is the fracton dimensionality). The Ioffe-Regel criterion for localization, $\omega\tau \sim 1$, and a scaling *Ansatz*, then lead to the Alexander-Orbach value, $\tilde{d} = \frac{4}{3}$, and $1/\tau \sim \omega$ for all $\omega > \omega_c$.

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Many random systems (e.g., percolation clusters, polymers, rubbers, gels) behave like homogeneous materials for length scales L large compared with some "correlation length" ξ, and exhibit *fractal geometry* for $L < \xi$. Much recent interest has concentrated on the *dynamics* on such systems,[1-7] which is known to be *anomalous* for $L < \xi$. Particularly, the elastic properties are described by *phonons* for long wavelengths, $\lambda \gg \xi$, and by localized vibrational states, called *fractons*,[3] for $\lambda \ll \xi$. The dispersion relation crosses over from $\lambda_{\rm ph} = c/\omega \sim \xi^{-\theta/2}/\omega$ for the wavelength of phonons with frequency ω (c is the velocity of sound), to $\lambda_{\rm fr} \sim \omega^{-2/(2+\theta)}$ for the characteristic "localization length" of fractons. The exponent θ characterizes the spatial decay of the classical diffusion coefficient,[1] and the scaling properties of the conductivity or the elastic constants (for scalar coupling).[8] The length $\lambda_{\rm fr}$ is believed to be the only length scale describing fracton states.[3,6,7]

The above crossover occurs at a frequency $\omega_c \sim \xi^{-(2+\theta)/2}$, at which the density of vibrational states on a single cluster also crosses over from $N_{\rm ph}(\omega) \sim \omega^{d-1} \times \omega_c^{\tilde{d}-d}$ to[9] $N_{\rm fr}(\omega) \sim \omega^{\tilde{d}-1}$, with the "fracton dimensionality" $\tilde{d} = 2D/(2+\theta)$, where D is the fractal dimensionality (mass$\sim L^D$ for $L < \xi$). Similar crossover phenomena are expected for spin waves in isotropic magnets and in other linear problems.[5]

Alexander and Orbach[3] noted that $\tilde{d}$ was approximately $\frac{4}{3}$ for percolating networks in all dimensions $d, d \geq 2$, and suggested that $\tilde{d} = \frac{4}{3}$ may be an exact relation. Although this *Alexander-Orbach conjecture* appears to break down[10] very weakly in $d = 6 - \varepsilon$, $\tilde{d} = \frac{4}{3} \times [1 - (\varepsilon/126) + O(\varepsilon^2)]$, it remains controversial at $d = 2$.[11,12] For other systems, e.g., lattice animals, the conjecture is known to break down slightly.[13] Published attempts to derive $\tilde{d}$ from the *geometry* of "growth" sites remain inconclusive.[14,15]

In the present Letter we consider some aspects of *quantum diffusion* in the fracton regime. We study the scattering of vibrational modes by *structural inhomogeneities* (e.g., local fluctuations in the atomic mass distribution or in the elastic constants). In the phonon regime, this is dominated by *Rayleigh scattering*[16,17] *which yields a relaxation time* $\tau(\omega)$ given by

$$1/\tau \sim \omega^2 N_{\rm ph}(\omega) \sim \omega^{d+1}\omega_c^{-d}. \qquad (1)$$

In this equation, ω_c is the same crossover frequency into the fracton regime, as defined above. In the following, we shall identify another crossover frequency, $\omega_{\rm IR}$, above which we expect the Ioffe-Regel[18,19] behavior,

$$\omega\tau(\omega) \sim 1. \qquad (2)$$

Assuming scaling, and that the modes in the fracton regime are characterized by the frequency ω and the unique length $\lambda_{\rm fr}(\omega)$, Eq. (1) implies the scaling form

$$1/\tau = \omega f(\omega/\omega_{\rm IR}). \qquad (3)$$

This identifies $\omega_{\rm IR}$ with the crossover frequency to the fracton regime, ω_c.[3] The assumption that the fracton states have an Ioffe-Regel-Mott character then implies that $f(x) \to$ const for $x \gg 1$, and that Eq. (2) holds for all $\omega \gg \omega_c$.

Under these conditions, $\lambda_{\rm ph}(\omega) = c/\omega$ and the scattering length, $c\tau$, coincide at $\omega_{\rm IR} = \omega_c$. They are also equal to the Thouless[20] localization length Λ_T at this frequency $\{\Lambda_T \approx [N(\omega)D(\omega)]^{-1/(d-2)}\}$, defined from the quantum diffusion constant $D(\omega) \approx c^2\tau$ at $\omega_{\rm IR}$.[21]

This is clearly a crossover condition. At higher frequencies, the scattering becomes strong, and the weak scattering description by Rayleigh scattering, Eq. (1), and by a diffusion constant, $D(\omega)$, becomes inadequate. Nevertheless, one would expect the single length scale (Ioffe-Regel-Mott) character of the eigenfunctions to hold also at higher frequencies.[22] The fracton model[3,5,6] achieves this by giving the short-length-scale multiple scattering correlations a geometric fractal description.

So far, we have described the results of scaling with the assumption of a single crossover frequency; that is, $\omega_c = \omega_{\rm IR}$. As we show below, a consistent *direct* calculation of τ in the fracton regime yields,

$$1/\tau \propto \omega^{5-3\tilde{d}}. \tag{4}$$

This result is consistent with scaling and with the Ioffe-Regal criterion [Eq. (2)] *only if the Alexander-Orbach conjecture holds,* i.e., if there exists a quantum fracton dimensionality $\tilde{d}_q = \frac{4}{3}$. If $\tilde{d} = \tilde{d}_q = \frac{4}{3}$, then our result can be summarized in Fig. 1. The width $(1/\tau)$ of the imaginary part of the response function should obey Eq. (1) for $\omega < \omega_c$, and Eq. (2) for $\omega > \omega_c$. This prediction seems to be qualitatively consistent with recent neutron scattering results[23] on the dilute isotropic antiferromagnet $\mathrm{Mn_{0.5}Zn_{0.5}F_2}$.

The breakdown of the phonon behavior at the Ioffe-Regel point is also confirmed by an analysis of the thermal conductivity of a number of glasses and other amorphous materials,[24] extracting the phonon mean free path using the kinetic heat conduction formula. These authors state, "The data ... therefore do not support the suggestion that bulk glasses are fractal. In our opinion, the dynamics of bulk glasses are better described in terms of phonon localization due to strong scattering from static density fluctuations." But we have just seen that strong scattering leads to the Ioffe-Regel condition, and that, together with scaling, this leads directly to a fracton interpretation with $\tilde{d} = \frac{4}{3}$. The fact that the material may not exhibit a fractal static structure is irrelevant. The overall mass distribution may not be fractal (as it is not for a percolating network), but the atomic network which contributes to the elasticity may be. That is, the dynamics are controlled by $\tilde{d}$, while the total mass distribution may appear Euclidean $(D = d)$.

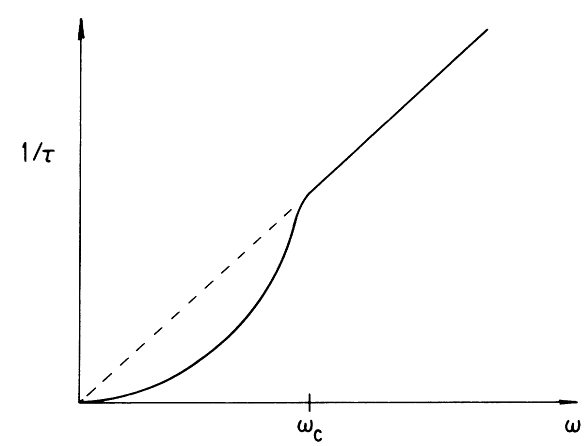

FIG. 1. Schematic plot of $1/\tau$, crossing over from Rayleigh scattering [Eq. (1) in the text] for $\omega < \omega_c$ to Ioffe-Regel behavior [Eq. (2) in the text] for $\omega > \omega_c$.

The more remarkable conclusion of our calculation is that the Ioffe-Regel condition leads directly to $\tilde{d} = \frac{4}{3}$. This should be true, therefore, for all the materials analyzed by Graebner and co-workers.[24]

Values of $\tilde{d} \neq \frac{4}{3}$ always imply an additional "Ioffe-Regel" frequency for fractons, $\omega_{\rm IR}^{\rm fr}$. By writing

$$1/\tau = \omega(\omega/\omega_{\rm IR}^{\rm fr})^{4-\tilde{3}}, \tag{4$'$}$$

it is seen that $\tilde{d} \neq \frac{4}{3}$, Eq. (4′) contradicts the uncertainty principle ($1/\tau$ greater than ω) either at low frequencies ($\tilde{d} > \frac{4}{3}$, $\omega < \omega_{\rm IR}^{\rm fr}$), or at high frequencies ($\tilde{d} < \frac{4}{3}$, $\omega > \omega_{\rm IR}^{\rm fr}$). In these regions, the scattering becomes strong even on the fractal, and (in complete analogy to the breakdown of the Rayleigh law above $\omega_{\rm IR}$) the scattering description becomes meaningless. All the observed[7,10–15] values for $\tilde{d}$ obey $\tilde{d} \leq \frac{4}{3}$. For systems with $\tilde{d} < \frac{4}{3}$, we expect a new crossover in the quantum-scattering–dominated regime (short length scale) to $\tilde{d} = \frac{4}{3}$. This crossover probably arises because of the rearrangement of the energy spectrum as a result of the strong scattering.

The way to derive Eq. (1) consists of a *d*-dimensional generalization of the Born approximation used originally by Rayleigh.[17] Alternatively, we take as an assumption the use of the golden rule of time-dependent perturbation theory, from which,

$$1/\tau(\omega) \sim |V|^2 N(\omega), \tag{5}$$

where $N(\omega)$ is the density of states and V represents a matrix element for the transition out of the initial state into a state with the same frequency ω. For a distribution of coupling constants, the perturbation Hamiltonian is $\frac{1}{2}\sum_{\langle ij\rangle}\Delta K_{ij}(\phi_i - \phi_j)^2$, where ϕ_i is the displacement of atom *i*. With use of the normal mode expansion, the amplitude of each normal mode scales as $\omega^{-1/2}$. Usually $\phi_i - \phi_j$ scales like the strain $\nabla\phi_i$ and is proportional to $\phi/\lambda_{\rm ph} \propto \omega^{1/2}$. Thus, $|V|^2 \propto \omega^2\langle|\Delta K|^2\rangle$ where the fluctuations in K have to be evaluated on a length scale on which they are statistically independent. Because there are (fractal) connectivity correlations up to scale ξ, $\langle|\Delta K^2|\rangle$ will in general be proportional to a power of ξ. With the normalization we have chosen for the density of states[9] $[N(\omega) = \omega^{d-1}\omega_c^{\tilde{d}-d}]$, one finds $\langle|\Delta K^2|\rangle \propto \xi^D \propto \omega_c^{-d}$ which generates Eq. (1) (for $\omega_{\rm IR} \simeq \omega_c$).

Our derivation of Eq. (4) starts from noting that the equations of motion for the vibrational modes on the fractal network are exactly the same as Kirchhoff's equations for a resistor network.[3,5,25–27] If one maps the region between two sites on the fractal onto an effective quasi one-dimensional "link," then the effective length of such a "link" is proportional to the *resistance* between the two end points.[27,28] This can be generalized to the envelope of a fraction wave function with a spatial decay proportional to $\exp[-R(x)]$. Here, $R(x) \sim x^{\tilde{\zeta}}$ is the resistance between points at a Euclidean distance x from each other. The exponent $\tilde{\zeta}$ is given by[1,4] $\tilde{\zeta} = 2 + \theta - D$

$=(2-\tilde{d})D/\tilde{d}$.[29]

We now coarse grain our fractal into units of linear size $\lambda_{\rm fr}$, and evaluate the matrix element $V \sim (\phi_i - \phi_j)^2$ for one such unit. Because the relevant basic length scale is $R(\lambda_{\rm fr})$, we expect the local strain, which behaved as $\phi/\lambda_{\rm ph}$ in the phonon regime, to scale as $\phi/R(\lambda_{\rm fr}) \sim [\omega^{1/2}R(\lambda_{\rm fr})]^{-1} \sim \omega^{(3/2)-\tilde{d}}$. An alternative derivation is based on the analogy between the strain $(\nabla\phi)$ and the current between the terminals of the resistor network. For a fixed stress (or voltage difference), the strain scales as the conductance, i.e., as $1/R \sim \omega^{2-\tilde{d}}$. Finally then, $\phi_i - \phi_j \sim \omega^{(3/2)-\tilde{d}}$, or[30] $|V|^2 \sim \omega^{6-4\tilde{d}}$. Together with $N_{\rm fr}(\omega) \sim \omega^{\tilde{d}-1}$, this proves Eq. (4).[8]

The philosophy of this calculation is to try to describe strong scattering in real (d-dimensional) space by (relatively) weak scattering on a fractal geometry. Our calculation shows that this can be combined consistently with the Ioffe-Regel criterion only when $\tilde{d} = \frac{4}{3}$. We emphasize that the "weak scattering" result on a fractal [Eq. (4)] is very different from what one would get from Rayleigh scattering [Eq. (1)] in $\tilde{d}$ dimensions ($1/\tau \sim \omega^{\tilde{d}+1}$): The two results only agree when $\tilde{d}=1$.

As already noted, Eq. (4) reproduces the Ioffe-Regel criterion [Eq. (2)] consistently only for $\tilde{d} = \frac{4}{3}$. When $\tilde{d} \neq \frac{4}{3}$, one can no longer continue to identify the phonon Ioffe-Regel frequency $\omega_{\rm IR}$ with ω_c. Equation (1) must be changed to

$$1/\tau = \omega(\omega/\omega_{\rm IR})^d. \qquad (1')$$

The phonon and fracton lifetimes are equal at ω_c. Equating Eqs. (1′) and (4′), one finds

$$\omega_c^{d-4+3\tilde{d}} = (\omega_{\rm IR})^d/(\omega_{\rm IR}^{\rm fr})^{4-3\tilde{d}} \qquad (6)$$

for the relationship between the crossover frequency ω_c and the phonon Ioffe-Regel frequency $\omega_{\rm IR}$. In the more common case, $\tilde{d} < \frac{4}{3}$, one then requires $\omega_c < \omega_{\rm IR} < \omega_{\rm IR}^{\rm fr}$. One crosses over from Eq. (1′) to Eq. (4′) at ω_c, but now $\omega_c\tau(\omega_c) > 1$. Equation (2) is reached only at the higher frequency $\omega_{\rm IR}^{\rm fr}$. Above this frequency, we would predict a "quantum" strong scattering regime on the fractal in which $\tilde{d}$ is renormalized to $\tilde{d}_q = \frac{4}{3}$.

This discussion assumes that the phonon Ioffe-Regel frequency, $\omega_{\rm IR}$, is sufficiently low compared to the Debye frequency (equivalently, that $\lambda_{\rm IR}$ is large on an atomic scale). This is apparently always the case for phonons in amorphous materials (see Ref. 24 for recent results). We note that in theoretical discussions (e.g., Ref. 21) it is common to choose $\lambda_{\rm IR}$ as the elementary length scale. The strong-scattering regime then disappears from the theory.

In conclusion, we have demonstrated that the Alexander-Orbach conjecture $\tilde{d} = \frac{4}{3}$ has a very strong connection with the very general Ioffe-Regel criterion for localization of the fractons, and demonstrated difficulties arising from other values of $\tilde{d}$. While this is not a rigorous proof, it certainly suggests that a scaling description of the strong scattering regime in disordered materials requires the Alexander-Orbach percolation value $\tilde{d} = \frac{4}{3}$. We believe this makes it plausible that the high-frequency modes in disordered materials will display this type of behavior irrespective of their detailed microscopic structure.

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[a]Permanent address: School of Physics and Astronomy, Tel Aviv University, 69978 Tel Aviv, Israel.

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[21]We note the obvious implication that the Anderson localization edge, ω_l, is lower than the Ioffe-Regel frequency, $\omega_{\rm IR}$. Because the two are always comparable in $d=3$, this requires some comment. The crossover frequency, ω_c, is equal to $\omega_{\rm IR}$ for $\tilde{d}=\frac{4}{3}$. We define ω_c as the transition to the strong scattering regime [as in our original qualitative arguments (Ref. 3)]. For $\omega > \omega_c$, the real part of the self-energy becomes large, and the density of states must change. The two-phonon creation (and annihilation) terms in the harmonic Hamiltonian also become important. All treatments of the Anderson localization of phonons treat localization as a weak scattering phenomenon (e.g., the density of states is found to be unchanged). This can be seen in the two most detailed recent theoretical treatments by S. John, H. Sompolinsky, and M. J. Stephen, Phys. Rev. B **27**, 5592 (1983), and by E. Akkermans and R. Maynard, Phys. Rev. B **32**, 7850 (1985). The latter paper explicitly assumes conservation of phonon number, and this weak scattering assumption at ω_l is quite generally accepted. By definition, it is violated at ω_c. Because ω_c is defined as a crossover frequency, the numerical factors are somewhat arbitrary. Using the results of S. John [Phys. Rev. Lett. **53**, 2169 (1984)], and our Eq. (2), we obtain $\omega_l/\omega_c \simeq (1/2\pi)^{1/2}$.

[22]Clearly the localization length has to be the longest length scale. The possibility that it again becomes longer than the wave length and the scattering length above ω_c, so that they regain a separate identity, seems very unlikely (assuming the scattering does not get weak).

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[29]An interesting implication of this argument is that it identifies the index d_ϕ introduced to describe the decay of fraction wave functions with $\tilde{\zeta}$. This considerably simplifies the discussion of relaxation and decay phenomena in the papers by S. Alexander, O. Entin-Wohlman, and R. Orbach: J. Phys. (Paris), Lett. **46**, L549, L555 (1985); Phys. Rev. B **32**, 6447, 8007 (1985); Phys. Rev. B **33**, 3935 (1986).

[30]The fractal correlations *on the fractal* are explicitly accounted for by the scaling indices. There is therefore no problem in assigning them to the inner cutoff $[\langle|\Delta K^2|\rangle = \text{const}]$.