RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 31, NUMBER 4 15 FEBRUARY 1985

Scaling approach to phonon-fracton crossover

A. Aharony
School of Physics and Astronomy, Tel Aviv University, Tel Aviv 69978, Israel

S. Alexander,* O. Entin-Wohlman,† and R. Orbach
Department of Physics, University of California, Los Angeles, California 90024

(Received 31 October 1984)

A scaling approach is formulated for the vibrational modes, from phonon to fracton, of a fractal network. The ratio of fracton-to-phonon density of vibrational states at crossover is found to be noncritical, i.e., independent of the crossover length scale. A steplike increase in the density of states at crossover is justified by an appeal to the normalization requirement on a fractal network. Applications are made to different fractal models. Recent effective-medium-approximation results are shown to violate scaling.

The crossover between the long wavelength (low frequency) phonon (ph) and the short length scale (high frequency) fracton (fr) vibrational excitations was first discussed by Alexander and Orbach.[1] Assuming a scaling form for the dispersion relations between the frequency ω and the characteristic length scale of the mode, $\lambda_\omega \equiv \lambda$, one can write[1,2]

$$\omega(\lambda^{-1}) = \lambda^{-a} f(\xi\lambda^{-1}) \ , \tag{1}$$

where[1]

$$\omega_{\rm fr}(\lambda^{-1}) \propto \lambda^{-[1+(\theta/2)]}, \ \ \lambda/\xi \to 0 \ , \tag{2a}$$

and

$$\omega_{\rm ph}(\lambda^{-1}) \propto \xi^{-\theta/2}\lambda^{-1}, \ \ \lambda/\xi \to \infty \ . \tag{2b}$$

Here θ is a characteristic dynamical index related to the scaling properties of the elastic consants, the conductivity, or the diffusion constant.[3] Thus, $a = 1 + (\theta/2)$. Let ξ represent the characteristic length at which the vibrational eigenstates change their character from phonon to fracton ($\lambda > \xi$, phonon; $\lambda < \xi$, fracton). Then, as shown in Ref. 1, crossover frequency, $\omega_{\rm co}$, can be defined ($\omega < \omega_{\rm co}$, phonon; $\omega > \omega_{\rm co}$, fracton) which must scale as

$$\omega_{\rm co} \propto \xi^{-[1+(\theta/2)]} \ . \tag{3}$$

From Eq. (2b), the velocity of sound obeys

$$c_s \propto \xi^{-\theta/2} \ . \tag{4}$$

It is evident from Eq. (2) that the phonon frequency, towards $\omega = 0$ (large λ), is always higher than the extrapolated fraction value one would obtain from Eq. (2a) for the same λ (because $\theta > 0$). The two dispersion curves [Eqs. (2a) and (2b)] must then cross at higher ω. It seems natural to associate the crossover frequency ($\omega_{\rm co}$) with the dispersion curve crossing, and to assume the following: (a) $\omega(\lambda^{-1})$ is monotonic increasing in λ^{-1}, and (b) $\omega(\lambda^{-1})$ has a positive second derivative. This procedure was used by Alexander[4] and Alexander, Laermans, Orbach, and Rosenberg.[5] This shape now appears to contradict results of the calculation for a percolation model within the effective medium approximation (EMA)[6] which exhibited an inflection point in the dispersion curve in the crossover region. More important, the above assumptions[4,5] [(a) and (b)] lead to a density of states which decreases when one crosses from the phonon to the fracton regime. This appears to contradict the relevant experimental results[5] (for example, for epoxy resins[7]), and also the EMA calculations of Derrida, Orbach, and Yu.[8]

Both experimental and EMA calculations appear to exhibit a large increase in the density of states in the crossover region. Tua, Putterman, and Orbach[9] have suggested some remedies for this inconsistency.

In this Rapid Communication we use a scaling approach to the density of states in an attempt to clarify the nature of the crossover region. Our results are summarized in Fig. 1. The density of states crosses over from the phonon behavior $N_{\rm ph}$ [Eq. (6b)] to the fracton behavior $N_{\rm fr}$ [Eq. (6a)] near $\omega_{\rm co}$ [Eq. (3)]. The apparent step in N is given by Eq. (10). The power-law relation between ΔN and $\omega_{\rm co}$ should be observed experimentally.

Consider the scaling behavior of the density of vibrational states. We write

$$N(\omega) = A\omega^{p-1} f(\omega/\omega_{\rm co}) \ . \tag{5}$$

We find it convenient to use a vibrational-mode normalization per unit mass (i.e., per atom). In the fracton regime,

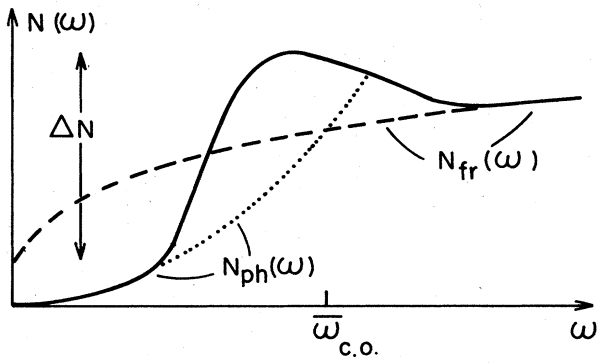

FIG. 1. Crossover of the density of vibrational states (solid line). The dotted (dashed) lines represent the continuation of the phonon (fracton) asymptotic behavior into the crossover regime.

one knows that[1,4,5] (broken line in Fig. 1)

$$N_{\rm fr}(\omega) = A\omega^{p-1}, \quad \omega/\omega_{\rm co} >> 1 \ , \tag{6a}$$

where an explicit expression for p will depend on the particular fractal model chosen, and will be discussed below. The prefactor in Eq. (5), A, does not depend on $\omega_{\rm co}$. In the phonon regime, one must have $N_{\rm ph}(\omega) \propto \omega^{d-1}$. The only way in which one can satisfy these requirements and Eq. (5) simultaneously is if one has in the phonon regime (dotted line in Fig. 1)

$$N_{\rm ph}(\omega) \propto \omega_{\rm co}^{p-d}\omega^{d-1}, \quad \omega/\omega_{\rm co} << 1 \ . \tag{6b}$$

This immediately leads to $f(x) \to 1$, $x \to \infty$; $f(x) \to x^{d-p}$, $x \to 0$, implying that the ratio

$$N_{\rm fr}(\omega_{\rm co})/N_{\rm ph}(\omega_{\rm co}) = C \ , \tag{7}$$

where C is noncritical (independent of $\omega_{\rm co}$). Because p in Eq. (6) will be restricted to $1 \leq p \leq d$ (see below), one also notes that

$$N_{\rm ph}(\omega) < N_{\rm fr}(\omega), \quad \omega << \omega_{\rm co} \ ,$$

because by construction $d-p \geq 0$. Furthermore, we have taken the vibrational spectrum to be normalized per atom, so that the integral of $N_{\rm fr}(\omega)$ [Eq. (6a)] from 0 to the upper cutoff $\omega_{\rm fD}$ (see Ref. 5) is unity. This crossing over to phonon excitations for ω less than $\omega_{\rm co}$ must mean that one always misses some states in the low-frequency region (as long as $\omega_{\rm co}$ is finite). The number of missing modes depends on the point where the curves of Eqs. (6a) and (6b) cross. This frequency, $\bar{\omega}_{\rm co}$, is expected to be proportional to $\omega_{\rm co}$, i.e., to scale as Eq. (3). Then,

$$\int_0^{\bar{\omega}_{\rm co}} [N_{\rm fr}(\omega) - N_{\rm ph}(\omega)]\, d\omega \propto \bar{\omega}_{\rm co}^{p} \propto \omega_{\rm co}^{p} \ . \tag{8}$$

This means that $N(\omega)$ has to be larger than the extrapolated low-frequency value of $N_{\rm fr}(\omega)$ somewhere in the crossover regime to assure overall normalization for the number of vibrational modes as shown by the full line in Fig. 1. This has implications for the shape of the scaling function $f(x)$ in Eq. (5). In particular, $f(x)$ has to approach its asymptotic limits as

$$f(x) \to 1, \quad x \to \infty \ , \tag{9a}$$

for large argument upon comparison of Eqs. (5) and (6a). However, from Eq. (8), $f(x)$ must be greater than 1 for at least some range of x to preserve normalization. For small argument, comparing Eqs. (5) and (6b), leads to

$$f(x) \propto x^{d-p} << 1, \quad x \to 0 \ . \tag{9b}$$

Scaling considerations are obviously insufficient for a precise determination of the shape of the scaling function $f(x)$ when $x \sim 1$. Equation (8) and our observation that $f(x)$ must exceed 1 for at least some range of x could therefore lead to a sharp feature at crossover which could be interpreted visually as a "step" of size Δf in $f(x)$ (see Fig. 1). The result would be a step in $N(\omega)$ with

$$\Delta N(\omega) = A\omega_{\rm co}^{p-1}\Delta f \ , \tag{10}$$

from the assumed scaling form [Eq. (5)]. This would in no manner contradict our previous result [Eq. (7)]. The ratio of the extrapolated density of states [Eq. (6)] at any frequency proportional to $\omega_{\rm co}$ is constant [Eq. (7)] when $N(\omega)$ is a scaling function. Nevertheless, a step in $N(\omega)$ will scale like Eq. (10). Both results are manifestations of the scaling form of Eq. (5). This steplike increase in $N(\omega)$ at $\omega_{\rm co}$ appears to be called for from EMA calculations (but see below) and upon comparison with experiments.

The scaling prefactor exponent p can be related to the frequency scaling index for fractal models.[1] This is discussed in detail in Refs. 4 and 5. In essence there are two model options.

(a) Infinite cluster only. One is dealing with a single cluster which is fractal at short distances and d dimensional (Euclidean) on large length scales. One then has

$$p = \bar{\bar{d}} = \frac{2\bar{d}}{2+\theta} \ , \tag{11}$$

where $\bar{\bar{d}}$ is the fracton dimension[1] and $\bar{d}$ the fractal (Hausdorff) dimension of the fractal network. This is the model discussed by Tua *et al.*[9] In this model, the mass density is critical

$$\rho \propto \xi^{\bar{d}-d} \propto \omega_{\rm co}^{\bar{\bar{d}}[(d/\bar{d})-1]} \ . \tag{12}$$

(b) Finite and infinite clusters. The alternative[3-5] is to assume that one has a Stauffer[10] distribution of finite clusters. As shown in Refs. 4 and 5, one has

$$p = 2d/(2+\theta) \tag{13}$$

so that the mass density ρ becomes independent of ξ.

In both cases (a) and (b), the required inequality $1 \leq p \leq d$ is satisfied for percolation. Models with $p < 1$ are, however, possible and appear in some situations.[11]

If one compares our results exhibited in Eq. (6) with the EMA calculations of Derrida *et al.*[8] it becomes obvious that the EMA density of states does not have a scaling form. The phonon and fracton EMA densities of states scale as

$$N_{\rm ph}^{\rm EMA}(\omega) \propto \omega_{\rm co}^{-d/2}\omega^{d-1} \ ,$$
$$N_{\rm fr}^{\rm EMA}(\omega) = \text{const} \ , \tag{14}$$

respectively. Thus, upon comparison with the scaling form of Eq. (6), respectively,

$$p_{\rm ph}^{\rm EMA} = d/2 \ ,$$
$$p_{\rm fr}^{\rm EMA} = 1 \ . \tag{15}$$

We believe this inconsistency reflects the breakdown of hyperscaling[9] within the EMA, at least for $d > 2$, representing another aspect in which EMA has mean-field features.

Another manifestation of the fact that $N^{\rm EMA}(\omega)$ does not have a scaling form is the magnitude of the step in $N^{\rm EMA}(\omega)$ at crossover exhibited in Ref. 8. It increases as $\omega_{\rm co} \to 0$ violating both Eqs. (7) and (10) of this paper.

We have shown that the ratio $N_{\rm fr}(\omega)/N_{\rm ph}(\omega)$ is noncritical at $\omega = \omega_{\rm co}$, and that normalization conditions could reasonably lead one to expect a steplike increase in $N(\omega)$ at crossover. This behavior is required by the observed temperature dependence of the specific heat T^3 as measured in nearly all amorphous materials. This was recognized in Ref. 5, and used to advantage in Ref. 9 in an attempt to construct a phenomenological density-of-states curve for phonons and fractons. The effective medium approximation results of Ref. 8 also exhibit this increase, but its predicted critical behavior has been shown above to be incorrect.

There must be an experimental manifestation of this effect for measurements other than specific heat if the application is to be as general as claimed in Ref. 5. Very recent neutron diffraction experiments by Rosenberg[12] have shown an upward departure of $N(\omega)$ from ω^2 when plotted on a log-log graph, the extracted crossover frequency changing in the direction predicted by Eq. (10) when the length scale was changed (amount of hardener) in epoxy resin. Optical-absorption experiments[13] may also have shown the increase in $N(\omega)$ at frequencies expected to be equal to ω_{co} in the relevant material.

We recognize that all these pieces of "evidence" are somewhat circumstantial at this stage, but at least none of them conflicts with our interpretation. We suggest that direct investigation of the vibrational density of states in the energy regime expected to contain the crossover energy (or length scales of order the crossover length) in amorphous or polymeric materials[14] is in order, and would provide important insight into their geometrical structures.

This research was supported by the National Science Foundation under Grant No. DMR 81-15542 by the U.S.–Israel Binational Science Foundation (BSF), Jerusalem, and by the Israel Academy of Sciences and Humanities.

---

*Permanent address: The Racah Institute, The Hebrew University, Jerusalem, Israel.

†Permanent address: School of Physics and Astronomy, Tel Aviv University, Tel Aviv 69978, Israel.

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

[2]A somewhat similar scaling form was suggested by R. Rammal and G. Toulouse [J. Phys. (Paris) Lett. **44**, L13 (1983)], but the normalization of the density of states was not accounted for.

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

[4]S. Alexander, Ann. Isr. Phys. Soc. **5**, 144 (1983).

[5]S. Alexander, C. Laermans, R. Orbach, and H. M. Rosenberg, Phys. Rev. B **28**, 4615 (1983).

[6]O. Entin-Wohlman, S. Alexander, R. Orbach, and K.-W. Yu. Phys. Rev. B **29**, 4588 (1984).

[7]S. Kelham and H. M. Rosenberg, J. Phys. C **14**, 1737 (1981).

[8]B. Derrida, R. Orbach, and K.-W. Yu, Phys. Rev. B **29**, 6645 (1984).

[9]P. Tua, S. Putterman, and R. Orbach, Phys. Lett. **98A**, 357 (1983).

[10]D. Stauffer, Phys. Rep. **54**, 1 (1979).

[11]I. Webman and G. Grest, Phys. Rev. (to be published).

[12]H. M. Rosenberg (unpublished).

[13]U. Strom, J. R. Hendrickson, R. J. Wagner, and P. C. Taylor, Solid State Commun. **15**, 1871 (1974).

[14]D. N. Batchelder and M. N. Wybourne, Phys. Rev. Lett. **53**, 580 (1984).