

Effective-medium approximation for a percolation network: The structure factor and the Ioffe-Regel criterion

G. Polatsek

The Racah Institute, The Hebrew University, Jerusalem 91904, Israel

O. Entin-Wohlman

*School of Physics and Astronomy, Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University,
Tel Aviv 69978, Israel*

(Received 14 September 1987)

The effective-medium approximation for a percolation system is used to analyze the vibrational structure factor $S(q, \omega)$, measured in scattering experiments off self-similar samples. A sharp crossover to strong localization is found at a certain frequency ω_c , corresponding to a crossover wave vector q_c . In particular, the linewidth τ^{-1} obeys the Rayleigh law, $\tau^{-1} \simeq \omega^{d+1}$, at frequencies lower than ω_c (d is the Euclidean dimensionality), and the Ioffe-Regel strong-scattering limit, $\tau^{-1} \simeq \omega$, at high frequencies, $\omega > \omega_c$. At wave vectors less than q_c , $S(q, \omega)$ is sharply peaked at $\omega = qc$ (where c is the sound velocity) and has a small structure at ω_c . At wave vectors higher than q_c , the sharp peak is completely smeared out, while the small structure persists. The results are in qualitative agreement with experiments and with the fracton scaling model, regarding the frequency and wave-vector dependence. However, they fail to scale with ω_c alone in the low-frequency regime.

I. INTRODUCTION

The character of the vibrational spectrum of self-similar, fractal systems (e.g., percolation clusters, gels) was originally discussed by Alexander and Orbach,¹ who named it the fracton model. The main feature of the model is the crossover from low-frequency phonon excitations, to relatively-high-frequency, strongly localized fracton modes. Indications of such a behavior have been recently observed in Brillouin scattering from silica aerogels² and neutron scattering from magnetic excitations of diluted antiferromagnets.³

The fracton model is based upon scaling arguments. As such, it cannot yield detailed information of the frequency and wave-vector dependence of the structure factor, measured in these experiments. In this article we present a calculation of the structure factor within the effective-medium approximation (EMA) for a bond percolating network. Such a network appears to be homogeneous over length scales larger than the connectivity coherence length, $\xi \propto (p - p_c)^{-\nu}$, and exhibits anomalous features at length scales smaller than ξ (here p is the percolation concentration and p_c is the percolation threshold). In previous studies^{4,5} it has been found that the EMA reveals a sharp crossover from extended, phonon-like behavior to strongly localized, fracton behavior at a crossover frequency $\omega_c \propto \xi^{-2}$. The density of states changes abruptly at ω_c ,⁴ and the corresponding wave vector $q_c \propto \xi^{-1}$ marks a rapid change in the dispersion relation $\omega(q)$,⁵ interpreted as crossover to localization. These rapid changes are caused by a singularity in the solution of the EMA equations at $\omega = \omega_c$. Here we exploit the same equations to derive the structure factor, and find its features to be dominated by the same crossover frequency

and wave vector. However, we find that the EMA fails to yield scaling in terms of ω_c alone, in the frequency range below ω_c . This is in disagreement with the scaling ansatz of the fracton model,⁶ which assumes a single characteristic frequency scale for the description of the excitations of a self-similar system.

We apply the EMA to the force constants of the scalar elasticity problem⁷ of a percolating network. In this approximation, the force constants are replaced by a uniform, frequency-dependent, complex force constant, chosen in such a way that the scattering produced by one bond, for which the original force constant is maintained, is zero on the average. In Sec. II we present the basic equations resulting from this form of the EMA, and the self-consistent solution for the frequency-dependent force constant. This provides us with an expression for the EMA retarded Green's function. The Green's function is then used to calculate the structure factor.

The scattering cross section for an energy transfer ω and momentum transfer q is proportional to

$$-[1 - \exp(-\beta\omega)]^{-1/2} \text{Im}G^R(q, \omega), \quad (1)$$

where $\beta = 1/k_B T$ and $G^R(q, \omega)$ is the retarded Green's function of the vibrations. The experimental data is usually presented without the Bose factor, and the structure factor is thus given by

$$S(q, \omega) = -2 \text{Im}G^R(q, \omega). \quad (2)$$

In an ordered isotropic lattice, the Green's function, in the Debye approximation, is

$$G^R(q, \omega) = (\omega^2 - Kq^2)^{-1}, \quad (3)$$

where ω includes an infinitesimal positive imaginary part,

and K is the force constant, proportional to the square of the sound velocity (we use units in which the mass is unity). In this case, $S(q, \omega)$ is of the form of a δ function, located at $\omega = cq$, where c is the sound velocity. When weak disorder is introduced into the lattice (e.g., a low concentration of defects) the δ function broadens into a quasi-Lorentzian shape, centered around $\omega = cq$, with a finite width, τ^{-1} , whose frequency dependence obeys the Rayleigh law, $\tau^{-1} \simeq \omega^{d+1}$, where d is the Euclidean dimensionality.

In the EMA for a percolating network, the force constant K in Eq. (3) is replaced by a complex, frequency-dependent, homogeneous "force constant" $W(\omega)$, which also depends upon $p - p_c$. The real and imaginary parts of $W(\omega)$ result in an effective, frequency-dependent "sound velocity" and an effective linewidth. We present numerical results for these quantities for a simple cubic lattice in three dimensions.

We find that for q below q_c , the structure factor as a function of ω has two peaks. The first is a high and narrow one, centered around cq , where c scales as $\sqrt{p - p_c}$. The width of this peak follows the Rayleigh law. The second peak is located around ω_c and is much smaller. As q increases towards q_c , the first peak moves towards ω_c and broadens, while the second peak rises but remains at ω_c . At $q = q_c$ the two peaks merge together. For values of q higher than q_c , the structure factor exhibits a very low and broad structure. This behavior is in accordance with experimental data,^{2,3} and with the predictions of the fracton scaling model. As q_c corresponds to the inverse of the percolation coherence length ξ , the phononlike spectrum is expected to be reflected in $S(q, \omega)$ only for $q\xi < 1$. The fracton contribution is the smaller structure at ω_c . For $q\xi > 1$, the phononlike contribution disappears. In other words, wave vectors $q > q_c$ essentially probe only the localized modes. These characteristics appear as well in the effective sound velocity and line width, extracted from our expressions. Above ω_c , the dispersion relation deviates from linearity and the linewidth reaches the Ioffe-Regel strong scattering limit, $\tau^{-1} \simeq \omega$.

We discuss in Sec. III the failure of the EMA to obey scaling for frequencies less than ω_c . However, comparison of our results with experimental data can still be made because ω_c dominates over all crossover behavior. In this sense, when $p - p_c$ is finite, the breakdown of scaling within EMA is practically unimportant.

II. THE STRUCTURE FACTOR IN THE EMA

We consider a lattice of equal masses, for which the elastic potential energy is of the form

$$\frac{1}{4} \sum_{l,l'} K_{l,l'} (\mathbf{u}_l - \mathbf{u}_{l'})^2, \quad (4)$$

where \mathbf{u}_l is the displacement from equilibrium of the mass at site l , and $K_{l,l'} = K_{l',l}$ connects two nearest neighbors. The force constants $K_{l,l'}$ span a bond percolating system, obeying the probability distribution

$$P(K_{l,l'}) = p\delta(K_{l,l'} - K) + (1-p)\delta(K_{l,l'}) . \quad (5)$$

The retarded Green's function of the displacements is defined by the thermal average

$$g^R(l, l', t) = -i\Theta(t) \langle [u_l(t), u_{l'}] \rangle, \quad (6)$$

where $\Theta(t)$ is the theta function. The vector notations are omitted since for the scalar⁷ elastic energy (4) there is no coupling between different directions.

The Fourier transform of the retarded Green's function satisfies the equation

$$\left[\omega^2 - \sum_{l''} K_{l,l''} \right] g^R(l, l', \omega) + \sum_{l''} K_{l,l''} g^R(l'', l', \omega) = \delta_{l,l'}. \quad (7)$$

In the EMA one replaces all the force constants $K_{l,l'}$ by an effective uniform force constant W , except for a single bond (say, the bond 1-2). One then finds that the Green's function is given by

$$g^R(l, l', \omega) = G^R(l, l', \omega) - \sum_{i,j=1}^2 G^R(l, i, \omega) T_{ij} G^R(j, l', \omega). \quad (8)$$

Here G^R is the retarded Green's function of the homogeneous lattice in which all the force constants are replaced by W , and the 2×2 T matrix is given by

$$T = \Delta_{12} (1 + G_{12}^R \Delta_{12})^{-1}, \quad (9)$$

$$\Delta_{12} = (W - K_{12}) \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix},$$

where G_{12}^R is the 2×2 homogeneous Green's function of the sites 1 and 2. More details concerning this form of the EMA are given in Ref. 8. The effective force constant W is determined from the requirement that the T matrix vanishes when averaged with the probability distribution (5). This makes the average Green's function to be equal to the homogeneous Green's function $G^R(l, l', \omega)$ [see Eq. (8)] and leads to the EMA self-consistency equation

$$\frac{1}{d} (W - K) [1 - \omega^2 G^R(0, 0, \omega)] - W + pK = 0. \quad (10)$$

From this equation, in the $\omega = 0$ limit, one finds that the percolation threshold in the EMA is $p_c = 1/d$.

To solve for the frequency dependence of W , we note that the homogeneous Green's function is

$$G^R(l, l', \omega) = \sum_{\mathbf{q}} \exp[i\mathbf{q} \cdot (\mathbf{l} - \mathbf{l}')] G^R(\mathbf{q}, \omega), \quad (11)$$

where, for a simple cubic lattice in d dimensions

$$G^R(\mathbf{q}, \omega) = \left[\omega^2 - 2W \sum_{i=1}^d (1 - \cos q_i) \right]^{-1}. \quad (12)$$

Here q_i are the components of the wave vector in units of the inverse lattice constant.

We follow Ref. 4 and solve the EMA coupled equations (10) and (12) for frequencies of the order of $p - p_c$. Measuring W and ω^2 in units of K , we expand $G^R(0, 0, \omega)$ in powers of $\omega^2/W \propto p - p_c \ll 1$ [this is consistent with the resulting expressions, e.g., Eq. (16a) below]

$$G^R(0,0,\omega) \simeq -\psi_d \frac{1}{2W} - \left[\frac{1}{\omega^2} \right] \left[-\frac{\omega^2}{W} \right]^{d/2} \chi_d, \quad 2 < d < 4 \quad (13)$$

where ψ_d and χ_d are numerical (real) constants. In conjunction with Eq. (10), Eq. (13) leads to a complex solution,⁴

$$W(\omega) = W_1(\omega) - iW_2(\omega). \quad (14)$$

The detailed solution is carried out numerically and reveals a sharp change of behavior⁴ at $\omega = \omega_c$, where

$$\omega_c \simeq p - p_c. \quad (15)$$

At frequencies much smaller than ω_c the EMA for the vibrational spectrum has a phononlike behavior.^{4,5} At $\omega > \omega_c$, the features of the spectrum change drastically. Following the fracton scaling model, we denote the low-frequency regime ($\omega < \omega_c$) the phonon regime, and the high-frequency regime ($\omega > \omega_c$) the fracton regime. We find that the limiting behaviors of the effective force constant in the two regimes are

$$W_1 \simeq p - p_c, \quad (16a)$$

$$W_2 \simeq \omega^d / W_1^{d/2}, \quad W_2 \ll W_1, \quad \omega \ll \omega_c$$

and

$$W_1 \simeq p - p_c, \quad (16b)$$

$$W_2 \simeq \omega, \quad W_2 \gg W_1, \quad \omega \gg \omega_c.$$

Turning now to the structure factor, we use in the homogeneous Green's function, Eq. (12), the Debye approximation

$$2 \sum_{i=1}^d (1 - \cos q_i) \simeq q^2, \quad (17)$$

and so reduce Eq. (12) to the form (3). Combining Eq. (14) with Eqs. (2) and (3), the structure factor in the EMA becomes

$$S(q,\omega) = \frac{2q^2 W_2}{\omega^4 - 2\omega^2 q^2 W_1 + q^4 |W|^2}. \quad (18)$$

For fixed ω , the limiting behavior of the structure factor as a function of q , from Eq. (18), is

$$S(q) \simeq q^2, \quad q \ll q_{\max} \quad (19)$$

$$S(q) \simeq q^{-2}, \quad q \gg q_{\max}$$

where $(q_{\max})^2 = \omega^2 / |W|$.

The structure factor (18) can be rearranged to read

$$S(q,\omega) = \left[\frac{c(\omega)q}{\omega^2} \right] \left[\frac{\tau^{-1}(\omega)}{[\omega - c(\omega)q]^2 + \tau^{-2}(\omega)} - \frac{\tau^{-1}(\omega)}{[\omega + c(\omega)q]^2 + \tau^{-2}(\omega)} \right], \quad (20)$$

such that it resembles the usual quasi-Lorentzian form.

To this end we have defined

$$c(\omega) = |W(\omega)| / \text{Re} \sqrt{W(\omega)}, \quad (21)$$

$$\tau^{-1}(\omega) = \omega \text{Im} \sqrt{W(\omega)} / \text{Re} \sqrt{W(\omega)}.$$

This provides us with natural definitions for a frequency-dependent sound velocity $c(\omega)$ and a linewidth $\tau^{-1}(\omega)$, and allows us to explore their variation as a function of frequency, from the phonon to the fracton regime. Using the limiting behaviors, Eqs. (16), in Eqs. (21) we find

$$q_{\max}^2 \simeq \frac{\omega^2}{p - p_c}, \quad (22)$$

$$c \simeq (p - p_c)^{1/2},$$

$$\tau^{-1} \simeq \frac{\omega^{d+1}}{(p - p_c)^{d/2+1}},$$

for $\omega \ll \omega_c$ (phonon regime) and

$$q_{\max}^2 \simeq \omega, \quad (23)$$

$$c \simeq \omega^{1/2},$$

$$\tau^{-1} \simeq \omega,$$

for $\omega \gg \omega_c$ (fracton regime).

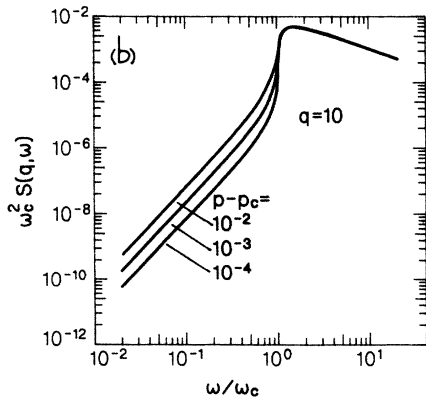
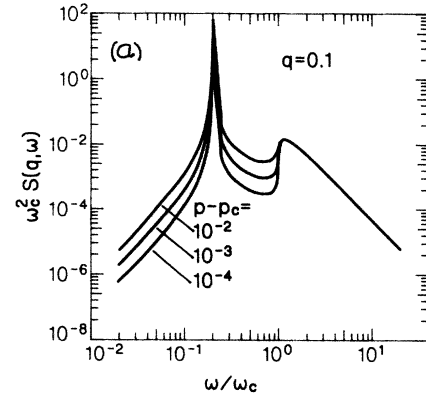


FIG. 1. The structure factor $S(q,\omega)$ as a function of ω for several values of $p - p_c$ and for fixed q . All quantities are measured in reduced units in terms of ω_c and q_c . (a) $q = 0.1$; (b) $q = 10$.

We see that in the EMA, the sound velocity in the phonon regime is independent of the frequency, and hence one has the usual linear dispersion relation. In the percolating system, c also scales with $p - p_c$. At $p = p_c$ it vanishes, and the phonons no longer exist. Note that combining Eq. (15) with the second of Eqs. (22) leads to $q_c \simeq (p - p_c)^{1/2}$, i.e., $v = \frac{1}{2}$ in the EMA.⁵ At ω_c the sound velocity crosses over to the fracton regime and becomes strongly frequency dependent, but independent of $p - p_c$, in agreement with the scaling conjecture.⁶ The linewidth follows the Rayleigh law of weak scattering, as long as the excitations are phononlike. But in the fracton regime it fulfills the Ioffe-Regel criterion⁹ for strong scattering localization, $\tau^{-1} \simeq \omega$.

Coming back to the structure factor, we now consider its frequency dependence when q is treated as a parameter. From Eqs. (16) and (18) we find

$$S(q, \omega) \simeq \frac{\omega^d}{q^2(p - p_c)^{2+d/2}}, \quad (24)$$

for ω much less than ω_c , while for ω larger than ω_c ,

$$\begin{aligned} S(q, \omega) &\simeq q^2/\omega^3, \quad \omega > q^2 \\ S(q, \omega) &\simeq 1/\omega q^2, \quad \omega < q^2. \end{aligned} \quad (25)$$

Note that our results, Eqs. (22)–(25), are restricted to the Euclidean dimensionality $2 < d < 4$, for which the expansion (13) is valid. The numerical results are presented for a three-dimensional simple cubic lattice, in the Debye approximation. We use

$$d = 3, \quad p_c = \frac{1}{3}, \quad \psi_3 \simeq 0.505, \quad \chi_3 = 1/4\pi \quad (26)$$

to obtain the roots of the polynomial in $W^{1/2}$ resulting from Eqs. (10) and (13).

Figure 1(a) depicts the structure factor (normalized by ω_c^{-2}) as a function of ω/ω_c for q less than q_c and various values of $p - p_c$, and Fig. 1(b) portrays the structure factor for q larger than q_c . When $q < q_c$, there is a high and narrow peak around $\omega \simeq cq$, and a second peak, much smaller, around ω_c . In the case $q > q_c$, there is only one peak, still around ω_c . Notice also the decay of the struc-

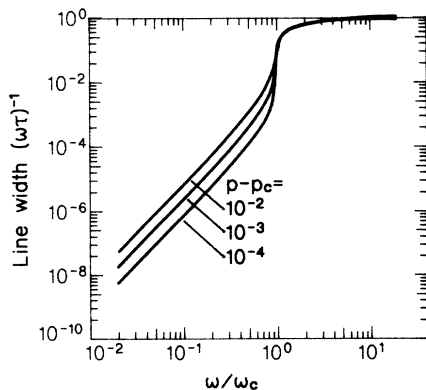


FIG. 2. The linewidth $(\omega\tau)^{-1}$ as a function of ω , in reduced units in terms of ω_c , for several values of $p - p_c$.

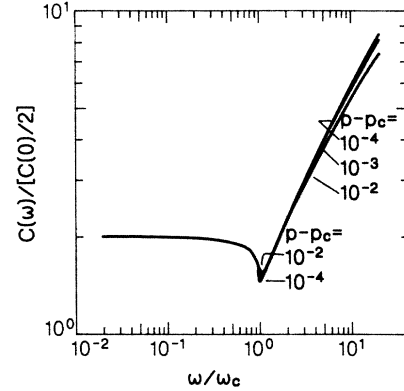


FIG. 3. The sound velocity c as a function of ω , in reduced units in terms of ω_c , for several values of $p - p_c$. Almost everywhere except at the vicinity of $\omega = \omega_c$ the lines are indistinguishable.

ture factor as ω^{-3} in Fig. 1(a) and as ω^{-1} in Fig. 1(b), in accordance with Eqs. (25). The behavior of the linewidth is depicted in Fig. 2, where we plot $(\omega\tau)^{-1}$ as a function of ω/ω_c . Below ω_c the Rayleigh law is obeyed. As p approaches p_c , the jump observed at ω_c becomes steeper, while the approach to $(\omega\tau)^{-1} = 1$ becomes slower. Finally, in Fig. 3, we exhibit the sound velocity (normalized by $[(p - p_c)/(1 - p)]^{1/2}$) as a function of ω/ω_c . As expected, it is a constant in the phonon regime, and varies as $\omega^{1/2}$ in the fracton regime. Changing p affects the plot only around ω_c , where it becomes sharper as p approaches p_c .

III. DISCUSSION

From Figs. 1 and 2 it is clear that in the EMA the structure factor and the linewidth do not scale with ω_c at frequencies below ω_c . For if it were so, all plots would have been independent of $p - p_c$. This is in disagreement with the underlying ansatz of the fracton scaling model,⁶ and also with the experimental data of Ref. 2.

This failure of scaling is most clearly seen when one rewrites the linewidth in the phonon regime in the form

$$\frac{1}{\tau\omega} \simeq \left[\frac{\omega}{\omega_c} \right]^d \frac{1}{(p - p_c)^{1-d/2}}, \quad (27)$$

using Eq. (15) and the third of Eqs. (22). The extra power of $p - p_c$ [last factor in (27)] means that the linewidth does not scale with ω_c but with a different characteristic frequency, ω_{IR} ,

$$(\omega_{\text{IR}})^d = \omega_c^d (p - p_c)^{1-d/2}, \quad (28)$$

at which $\tau\omega \simeq 1$ and crosses over into the Ioffe-Regel limit. The possibility that there exists a second characteristic frequency within the fracton scaling model has been discussed recently.⁶ But, in the case of the EMA, it is conceivable that this failure of scaling is connected with the approximation itself. This has been already pointed out in Ref. 10, in conjunction with the vibrational density of states. Indeed, in the fracton scaling model the density of states is suitably normalized.¹¹ But in the EMA the

density of states $N(\omega)$ takes the form⁴

$$\begin{aligned} N(\omega) &\simeq \omega^{d-1}/(p-p_c)^{d/2}, \quad \omega \ll \omega_c \\ N(\omega) &\simeq \text{const}, \quad \omega \gg \omega_c. \end{aligned} \quad (29)$$

If we now integrate $N(\omega)$ over the frequency, using the first expression of (29) up to ω_c and the second from ω_c up to some microscopic (Debye) frequency ω_m , we find that the result depends upon $p-p_c$. This is apparent from the complete numerical solution of the EMA equations.⁴

The absence of scaling with respect to a single characteristic frequency has implications concerning comparison with experiments. Our results for the structure factor agree qualitatively with the experimental data of Refs. 2 and 3. But, in principle, particularly for the data of Ref. 2, there is a difficulty. Since the value of the percolation concentration p of the samples can be only roughly estimated, the data is scaled² with ω_c and q_c . Moreover, most of the data is in the phonon regime, i.e., below ω_c , where in the EMA the structure factor does not scale with ω_c . In practice, p_c is not closely approached and the difference between the EMA and the experimental results cannot be markedly observed. Also, the sharp crossover of the EMA results does occur at ω_c . We also note that in three dimensions [see Eq. (28)] $\omega_{\text{IR}} \simeq \omega_c(p-p_c)^{-1/6}$, and hence, for finite values of $p-p_c$, ω_c and ω_{IR} are practically the same.

Admittedly, the EMA is a rather rough approxima-

tion. It is well known that it does not yield the correct values for p_c and critical exponents. However, it does distinguish, for example, between rigidity and scalar elasticity percolation transitions.¹² The EMA though, considers the whole system to belong to the infinite cluster. Thus, it does not allow for finite clusters, and so the form it yields for the structure factor takes into account all the atoms in the system. Presumably, the approximation becomes better as $p-p_c$ increases. However, contrary to the traditional treatments of Anderson localization,¹³ it has, at least for a percolating system, the interesting feature that it shows a sharp change of behavior in the single-particle Green's function. It therefore provides a detailed form of the structure factor which exhibits a crossover to strong localization.

Finally, we note that the magnetic excitations of diluted antiferromagnets obey a similar equation to that of the vibrations of the scalar elasticity problem. It was indeed found that the structure factor for neutron scattering off magnetic excitations has the same characteristics, experimentally³ and within¹⁴ EMA, as those presented here.

ACKNOWLEDGMENTS

Useful discussions with S. Alexander, R. Orbach, and A. Aharony are gratefully acknowledged. The work was supported by the Fund for Basic Research administered by the Israel Academy of Sciences and Humanities and by the National Science Foundation under Grant No. DMR-84-12898.

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

²E. Courtens, J. Pelous, J. Phalippou, R. Vacher, and T. Woignier, *Phys. Rev. Lett.* **58**, 128 (1987).

³Y. J. Uemura and R. J. Birgeneau, *Phys. Rev. Lett.* **57**, 1947 (1986).

⁴B. Derrida, R. Orbach, and Kin-Wah Yu, *Phys. Rev. B* **29**, 6645 (1984).

⁵O. Entin-Wohlman, S. Alexander, R. Orbach, and Kin-Wah Yu, *Phys. Rev. B* **29**, 4588 (1984).

⁶S. Alexander, *Physica* **140A**, 397 (1986); A. Aharony, S. Alexander, O. Entin-Wohlman, and R. Orbach, *Phys. Rev. Lett.* **58**, 132 (1987).

⁷S. Alexander, *J. Phys.* **45**, 1939 (1984).

⁸I. Webman, *Phys. Rev. Lett.* **47**, 1496 (1981); T. Odagaki and

M. Lax, *Phys. Rev. B* **24**, 5284 (1982).

⁹A. F. Ioffe and A. R. Regel, *Prog. Semicond.* **4**, 237 (1960).

¹⁰A. Aharony, S. Alexander, O. Entin-Wohlman, and R. Orbach, *Phys. Rev. B* **31**, 2565 (1985).

¹¹S. Alexander, C. Laermans, R. Orbach, and H. M. Rosenberg, *Phys. Rev. B* **28**, 4615 (1983); S. Alexander, *Ann. Isr. Phys. Soc.* **5**, 149 (1983).

¹²S. Feng, M. F. Thorpe, and E. J. Garboczi, *Phys. Rev. B* **31**, 276 (1985); E. J. Garboczi and M. F. Thorpe, *ibid.* **31**, 7276 (1985); **32**, 4513 (1985).

¹³S. John, H. Sompolinsky, and M. J. Stephen, *Phys. Rev. B* **27**, 5592 (1983); E. Akkermans and R. Maynard, *ibid.* **32**, 7850 (1985).

¹⁴R. Orbach and Kin-Wah Yu, *J. Appl. Phys.* **61**, 3689 (1987).