

Transport phenomena in disordered elastic solids

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ABSTRACT

Classical waves propagating in disordered media have their paths distorted and are dispersed by scattering from heterogeneities. If the strength of the disorder is sufficiently great, the waves no longer propagate: all the energy is converted into random fluctuations of the medium and is localized within a finite region of space characterized by the localization length ℓ . In 1D, any degree of random heterogeneity is sufficient to cause localization. In higher dimensions, a certain critical value of disorder is required. This effect, although purely elastic, is much like heat conduction since it involves the conversion of propagating energy into localized random fluctuations. A model of the localization of classical waves can be developed by replacing the continuum with a dynamical system of coupled springs and masses. Scattering from a heterogeneity (i.e., a lattice defect) results in an exponentially damped mode centered about the defect. Localization itself is the cumulative result of this tendency of disorder to convert propagating energy into localized vibrational modes; the localization length can be estimated as the reciprocal of the largest Lyapunov exponent of the dynamical system associated with the disordered lattice.

Key words: localization – disordered media – transport phenomena

1 WAVE PROPAGATION IN RANDOM MEDIA

Broadly speaking, the effects of multiple scattering on a wave propagating in a disordered medium are:

- The path length is increased.
- The pulse is dispersed.
- The pulse is attenuated as energy is shifted from the direct arrival into the multiple scattering coda.

These ideas are well understood in seismology and can be proved via perturbation theory for a weakly disordered medium. A review of the mathematical literature can be found in Asch *et al.* (1991). However, a new phenomenon enters the picture if the degree of disorder of the medium is sufficiently great. Waves whose wavelength is large compared to the correlation length of the disorder no longer propagate at all: the energy becomes trapped in a finite region of the model, characterized by a *localization* length ℓ , and is converted into random fluctuations. Now in most cases in seismology, the localization length (i.e., the length associated with complete trapping of the energy) is much longer than the length scale of the observation. But the physical mechanism causing localization, this conversion of

propagating energy into localized fluctuations, is readily observed as coda Q. In a sense, an analogy exists with anisotropy, where distinctions are sometimes made between effective and true anisotropy. Anisotropy results from ordering at some length scale. This could be microscopic ordering of molecules in a crystal, mesoscopic ordering of cracks, or macroscopic ordering of sedimentary layers. The mechanism of anisotropy is essentially the same in each case, only the length scale is different. Isotropy results from disorder. At the microscopic level, glasses or other amorphous solids are isotropic by virtue of their disorder. When anisotropic crystals are randomly arranged into a rock, the result is macroscopically isotropic. The fundamental issue is the relevant length scale of order or disorder.

Similarly, while we tend to think of intrinsic attenuation as somehow resulting in the production of heat, with apparent attenuation being simply the complex rearrangement of propagating energy, heat is in essence the macroscopic manifestation of disordered motion. It hardly seems to matter at what length scale this disordered motion takes place. To say that multiple scattering attenuation is only apparent attenuation is like saying that a layered medium is only apparently anisotropic, whereas the anisotropy is precisely a man-

ifestation of the layering. In fact lattice waves (called phonons in quantum mechanics) are the principle mechanism by which heat is conducted in solids, at least in insulators and semiconductors where electron conduction is not important. For perfect crystals, whose only departure from order is the boundary, the mean free path of phonon-disorder collisions is essentially the size of the sample, which makes for extremely efficient heat conduction; whereas, highly disordered substances such as glass make good thermal insulators because of the localization of the lattice vibrations.

In order to try to get to the physical essence of scattering attenuation in macroscopically disordered media it is useful to focus on the mechanism by which propagating energy is converted into localized vibrations. The concept of localization arose during the first systematic investigations of the dynamical properties of lattices with defects by I.M. Lifshitz. In the third of a series of papers published in Russia during the Second World War, Lifshitz showed that localized vibrational modes could occur in which the frequency was outside the band of frequencies allowed for the normal modes of the perfect lattice (Lifshitz, 1944). Due to the circumstances under which Lifshitz' work was published, it remained unknown in the west for a number of years. The current phase of theoretical work on localization began with the pioneering paper by Philip Anderson (1958). Anderson's model was of lattices—regular or irregular—of electron spins (or other entities) each of whose energy was a random variable. Then, provided the interparticle potential decayed sufficiently fast as a function of distance (faster than r^{-3}), and the disorder was stronger than some critical value, Anderson was able to show rigorously that the electron wave function was localized in space asymptotically with time.

As will be seen, with a slight change of variables, Anderson's model of electron spin diffusion is mathematically identical to the problem of the vibrational properties of a classical mechanical lattice with a random distribution of masses. The interparticle potential energy corresponds to the spring constants on the lattice. Of course, one cannot expect the physics of the two problems to be the same, but it will be possible to apply certain rigorous results from quantum mechanical localization to the propagation of classical waves in disordered media. The connection between these two problems has only recently begun to be exploited in geophysics. In a series of papers, Ping Sheng, Zhao-Qing Zhang, Benjamin White, George Papanicolaou, and others ((Sheng *et al.*, 1986b), (Sheng *et al.*, 1986a), (White *et al.*, 1989), and (White *et al.*, 1990)) applied localization theory to give a complete statistical characterization of the multiple scattering coda in randomly layered 1D elastic solids. One of their goals was to use

the multiple scattering coda to be able to make inferences about the earth's subsurface. They treated the problem of plane waves propagating in 1D media whose random layering is small (i.e., whose correlation length is small) compared to the wavelength of the probing beam. In this problem the localization length is the "skin depth" associated with multiple scattering. In other words, since the envelope of such a plane wave decays exponentially with distance $e^{-z/\ell(f)}$, $\ell(f)$ is the frequency dependent localization length. Since this means that

$$\ell^{-1} = \lim_{L \rightarrow \infty} \left(-\frac{1}{L} \ln |T| \right)$$

where T is the transmission coefficient and L is the propagation distance, a plausible approximation to the localization length for finite L is then

$$\ell(f) \approx \frac{-L}{\ln |T|}.$$

Given the exponential nature of the decay, it is natural to think of the multiple scattering as a relaxation mechanism. Hence there is a Q , $\pi f \ell / v(f)$, where v is the phase velocity. Then from Kramers-Krönig, the velocity dispersion is

$$\frac{1}{v(f)} - \frac{1}{v(\infty)} = \mathcal{H} \left(\frac{1}{2\pi f \ell} \right)$$

where \mathcal{H} is the Hilbert transform, v_i are the layer velocities, $v(\infty) \equiv v_\infty = \langle v_i^{-1} \rangle^{-1}$ is the infinite frequency (ray theoretic) effective velocity, and the angled brackets denote averaging. (The zero frequency effective velocity is $v_0 = \langle v_i^{-2} \rangle^{-1/2}$.)

Many other useful results follow from knowing the localization length as a function of frequency; for example, when the medium is stationary, it gives a complete characterization of the backscattered power spectrum—with no dependence on the detailed form of the medium. In Sheng *et al.* (1986a) and Sheng *et al.* (1986b), it is argued that $\ell(f)$ is given approximately by $\ell(f) = c_1 + c_2/f^2$. With such a simple functional form, it is not difficult to find the analytic Hilbert transform in a table of integrals. The following dispersion formula results:

$$v(f) = v_\infty \left(1 - \frac{v_\infty \sqrt{c_2/c_1}}{2\pi c_1 f^2 + c_2} \right).$$

In White *et al.* (1990), examples of the calculation of the coefficients c_1 and c_2 from sonic well-log data are given. One example is shown in Figure 1. For this example the localization length at 20 Hz is about 25 km.

Questions remain as to the accuracy with which the two parameters c_1 and c_2 can be estimated from in-situ measurements and to the validity of the two-parameter approximation for $\ell(f)$. For example, it is pointed out in Scales (1993) that the long-wavelength estimates of

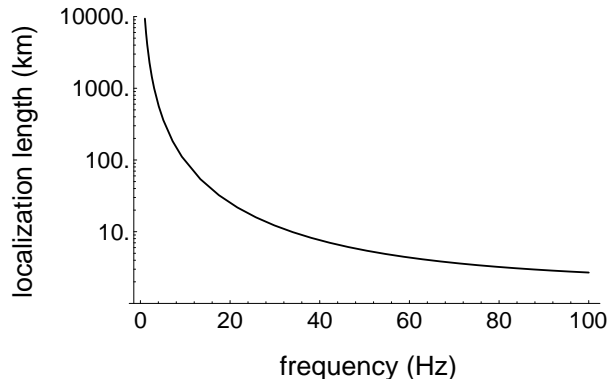


Figure 1. Localization length as a function of frequency computed from a P-wave sonic log by White *et al.* (1990).

velocity obtained via localization theory by White *et al.* (1990) are significantly at variance with the Backus effective velocity v_0 . No attempt will be made to address this issue here; the goal is to construct a physical model of localization that is simple enough to be amenable to direct analysis, while providing a foundation for further work on the practical application of this theory to wave propagation in realistic earth models. The path that will be taken involves replacing the usual continuum description of solids with a coupled dynamical system. There are a number of ways of visualizing this transition. On the one hand, one can take a microscopic view of the solid and imagine solving $F = ma$ for an arrangement of molecules on a lattice. At sufficiently low energies, a harmonic approximation to the interparticle potential energy is valid, hence Hooke's law. (Of course, no one would argue for the use of truly atomic scale lattices to study elastic wave propagation. For iron, for example, with a binding energy of around .4 eV and a lattice spacing of about 2.8 Å, maximum lattice frequencies are on the order of $10^{13} Hz$. On the other hand, Askar (1985) shows that using this value of the binding energy in a Morse potential gives a value of Young's modulus (spring constant divided by the lattice spacing) very close to the experimentally determined value.) At the other extreme, the lattice equations are equivalent to a finite difference approximation to the wave equation on the continuum. In any case, let us regard the masses as homogeneous units of some sort, layers perhaps, and the Hooke's law spring constants as the coefficients of linear forces connecting the units.

From a physical point of view the lattice theoretic approach has the advantage that the problem can be completely characterized in terms of the eigenmodes of the lattice, which are straightforward to compute. The localization itself is seen to arise from the effects of individual lattice defects, which give rise to eigenmodes whose envelopes decay exponentially away from

their maximum values centered on the defects. From a mathematical point of view, a dynamical systems approach allows one to reduce the analysis of localization to the study of the asymptotic properties of products of (small) random matrices. We will see, for example, that the localization length ℓ can be identified with the reciprocal of the largest Lyapunov exponent of this product of random matrices. Further, since a product of random matrices has a spectrum of Lyapunov exponents, in principle one can study the fine details of the decay of energy, and even quantify the effects of finite N fluctuations on the estimates of localization.

2 LATTICE DYNAMICAL SYSTEMS

It is not necessary to look at wave propagation in a complicated random earth model to see localization. In fact localization appears in discrete dynamical systems of only a few degrees of freedom. And these systems do not even have to be random. The term *disordered* is used nowadays to refer generically to these complex systems, with true randomness being a special case. For example, Gellermann *et al.* (1994) study the onset of localization for classical waves propagating in layered dielectrics whose layering is governed by a Fibonacci recursion. The idea is that the Fibonacci medium, although complex, is deterministic and can therefore be studied analytically. Figure 2 shows the result of a calculation of the transmission coefficient of a scalar wave propagating in a Fibonacci dielectric. This 1D layered medium is made up of alternating units of type A and B arranged according to the recursion:

$$S(0) = A; S(1) = B; S(n+1) = \{S(n), S(n-1)\}$$

where the curly braces denote concatenation. Thus, for example, the fifth order Fibonacci sequence would be: $BABABBAB$. The number of elements of the n -th order sequence is equal to the n -th Fibonacci number. From the figure it is clear that with increasing order (i.e., complexity), the transmission coefficient goes to zero at various frequencies. The obvious scale invariance of the transmission response is predicted by a renormalization group analysis.

2.1 Equations of motion for a 1D Newtonian lattice

Our laboratory for studying localization will be the disordered 1D chain. There are N point masses m_ℓ connected by $N - 1$ Hooke's law springs of stiffness k_ℓ . The end masses are fixed, as shown in Figure 3 and the longitudinal displacement of the ℓ -th mass x_ℓ is measured relative to its equilibrium position. The masses

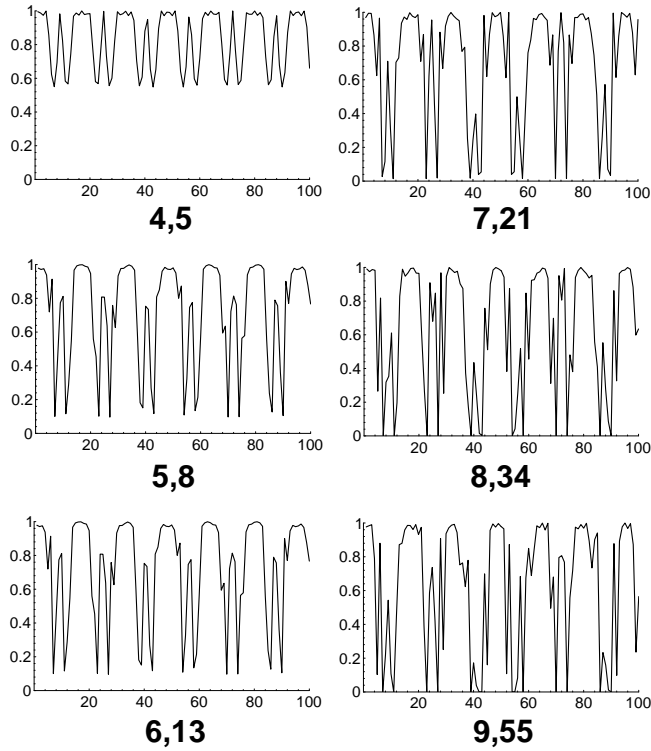


Figure 2. Acoustic transmission coefficient as a function of frequency (arbitrary units) for Fibonacci sequences of two materials whose slowness differs by 50%. The number on the left of each pair is the order of the Fibonacci sequence; the number on the right is the number of layers in the sequence. After Gellermann *et al.* (1994).

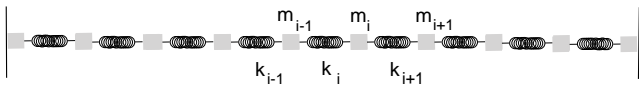


Figure 3. A simple mechanical system exhibiting localization of energy. Masses m_i are connected via springs of stiffness k_i . The end masses are fixed. Longitudinal displacement of the i -th mass x_i is measured relative to its equilibrium position.

and spring constants need not be thought of in molecular terms, although this is one possibility. They represent homogeneous units of some sort. The perfectly ordered version of this model has a long and illustrious history beginning with two of the Bernoullis (who apparently formulated the complete solution to the problem as a sum of normal modes) and continuing to this day. A vast survey of the theory of general harmonic lattices is given in Maradudin *et al.* (1971).

The kinetic energy of the system is

$$T = \frac{1}{2} \sum_{\ell=0}^N m_{\ell} \dot{x}_{\ell}^2 \quad (1)$$

and the potential energy is (assuming only nearest neighbor interactions)

$$V = \frac{1}{2} \sum_{\ell=0}^N k_{\ell+1} (x_{\ell+1} - x_{\ell})^2. \quad (2)$$

The equations of motion are

$$m_{\ell} \ddot{x}_{\ell} - k_{\ell+1} (x_{\ell+1} - x_{\ell}) - k_{\ell} (x_{\ell-1} - x_{\ell}) = 0. \quad (3)$$

This form illustrates the fact that the force on any given mass is due to the compression or extension of the two springs to which it is connected, which in turn depends only on the change of the spring's length relative to its relaxed length.

Assuming a sinusoidal time dependence, the equation for the spatial part of the motion is

$$-m_{\ell} \omega^2 z_{\ell} = k_{\ell+1} z_{\ell+1} - (k_{\ell+1} + k_{\ell}) z_{\ell} + k_{\ell} z_{\ell-1} \quad (4)$$

where $x_{\ell} \equiv z_{\ell} e^{i\omega t}$. In vector notation this can be written

$$(T + \omega^2 M) \mathbf{z} = 0 \quad (5)$$

where M is the mass matrix $M = \text{diag}(m_{\ell})$ and T is the tridiagonal matrix of spring constants: $T(\ell, \ell) = -(k_{\ell+1} + k_{\ell})$, $T(\ell, \ell + 1) = k_{\ell+1}$, and $T(\ell + 1, \ell) = k_{\ell}$.

2.2 Free oscillations of the 1D lattice

The free oscillations of the lattice are fundamental in understanding both the dynamical properties of the medium such as transport of energy, and the thermodynamic properties. Since the free energy for the solid is a sum of the energies of each mode, the actual distribution of eigenfrequencies has a direct impact on the macroscopic thermodynamic properties.

Let us begin the discussion by examining the well known properties of the ordered monoatomic 1D lattice: $m_{\ell} = m$, $k_{\ell} = k$ for all ℓ . Then the equation for the free oscillations reduces to

$$(T - \omega^2 I) \mathbf{z} = 0. \quad (6)$$

Since the spring constants are all equal to k , then T reduces to k times

$$\begin{bmatrix} -2 & 1 & 0 & 0 & \dots \\ 1 & -2 & 1 & 0 & \dots \\ 0 & 1 & -2 & 1 & \dots \\ \vdots & & & \ddots & \\ 0 & \dots & 0 & 1 & -2 \end{bmatrix}. \quad (7)$$

The eigenvalues of this matrix are known to be (for example cf. (Smith, 1978))

$$\omega_{\ell}^2 = -2 + 2 \cos\left(\frac{\ell\pi}{N}\right) \quad (8)$$

while the eigenvectors are

$$\mathbf{z}_{\ell} = \{\sin(\ell\pi/N), \sin(2\ell\pi/N), \dots, \sin((N-1)\ell\pi/N)\}. \quad (9)$$

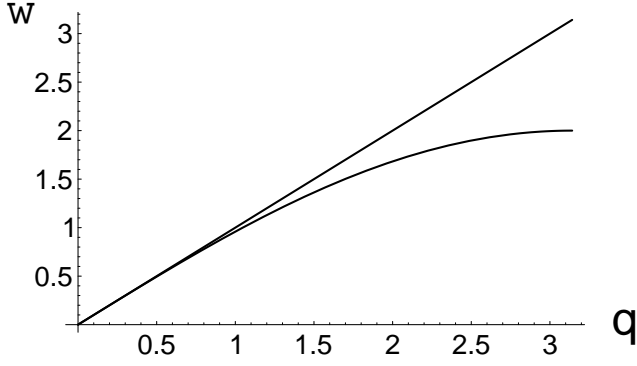


Figure 4. The continuum dispersion relation is linear with a slope given by the wavespeed. For a homogeneous lattice $\omega = 2\sqrt{k/m} \sin(qa/2)$. This figure shows a comparison of the two using units in which $c = a = 1$. In general, the maximum wavenumber for the lattice is q/a and therefore the maximum frequency is $2\sqrt{k/m}$. This plot shows half of the first Brillouin. There are corresponding negative wavenumber solutions at each frequency. Thus for each frequency there are plane waves propagating in both directions on the lattice.

Since the tridiagonal matrix is essentially a discrete second difference operator, it makes sense that the eigenvectors would just be sines or cosines—specifically sines if the endpoints of the lattice are fixed. This is true for all frequencies in the analogous continuum problem for a string. But in the discrete case the structure of the eigenvectors depends in an important way on the inherently dispersive properties of lattices. To see this, consider a plane wave solution of Equation 4; i.e., a solution of the form $e^{iq\ell a}$, where ℓ is the index and a is the lattice spacing and q is the wavenumber (to avoid confusion with the spring constant k).

$$-\frac{m}{k}\omega^2 e^{iq\ell a} = e^{iq(\ell+1)a} - 2e^{iq\ell a} + e^{iq(\ell-1)a}. \quad (10)$$

Which implies that

$$\frac{m}{k}\omega^2 = 2(1 - \cos qa) = 4\sin^2\left(\frac{qa}{2}\right). \quad (11)$$

So the dispersion relation on the lattice is

$$\omega = 2\sqrt{\frac{k}{m}} \sin \frac{qa}{2}. \quad (12)$$

Figure 4 shows a plot of $2\sin(q/2)/q$, corresponding to the departure from dispersion-free behavior for a lattice on which $c = a = 1$.

Next, in Figure 5, some of the 50 eigenvectors associated with a 50 point homogeneous lattice $k_\ell = m_\ell = 1$ are shown. The first 25 or so eigenvectors are purely sinusoidal, beyond which point they become modulated sinusoids.

Another way of looking at the free oscillations of the lattice is to recast the eigenvalue problem Equation 4 as a recursion relation:

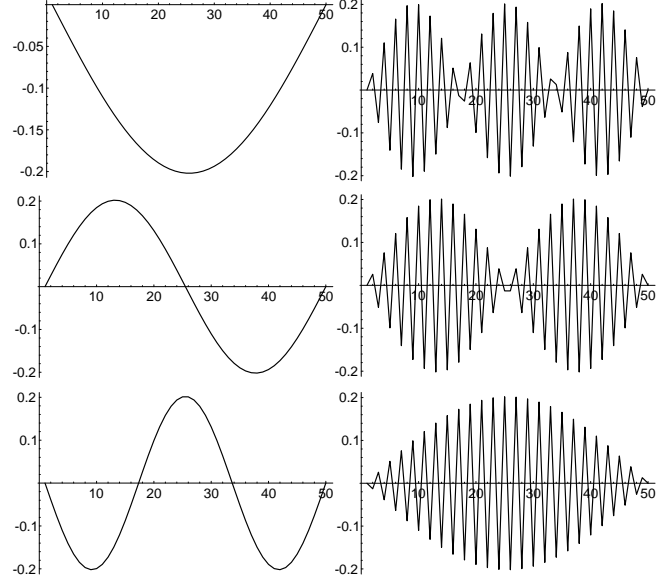


Figure 5. A sampling of the free oscillations of the 50 point homogeneous lattice. As the wavelength of the mode gets shorter, the granularity of the lattice becomes more important and the modes begin to depart from purely sinusoidal behavior. On the left are the lowest frequency three modes, on the right the highest frequency three modes.

$$z_{\ell+1} = \left(2 - \frac{m\omega^2}{k}\right)z_\ell - z_{\ell-1} \quad (13)$$

can be re-written

$$\begin{pmatrix} z_\ell \\ z_{\ell+1} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 2 - \frac{m\omega^2}{k} \end{pmatrix} \begin{pmatrix} z_{\ell-1} \\ z_\ell \end{pmatrix}. \quad (14)$$

Defining the matrix

$$B = \begin{pmatrix} 0 & 1 \\ -1 & 2a \end{pmatrix} \quad (15)$$

where $a = 1 - \frac{m}{2k}\omega^2$, it follows by induction that

$$\begin{pmatrix} z_\ell \\ z_{\ell+1} \end{pmatrix} = B^\ell \begin{pmatrix} z_0 \\ z_1 \end{pmatrix}. \quad (16)$$

The eigenvalues of B are $\lambda_{1,2} = a \pm \sqrt{a^2 - 1}$. If $|a| > 1$ ($\omega^2 > 4k/m$) then the z_ℓ solutions are exponentially growing or decaying and cannot satisfy the zero displacement boundary conditions. If $|a| < 1$ ($\omega^2 < 4k/m$), then the solutions are oscillatory and can be made to satisfy the boundary conditions.

Taking $z_0 = 0$, then

$$\begin{pmatrix} z_{N-1} \\ z_N \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 2a \end{pmatrix}^N \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (17)$$

Obviously this equation cannot produce an eigenvector for arbitrary values of a . For example, if we are trying to compute normal modes whose displacement vanishes at both ends of the lattice, then only using a associated with an eigenvalue will result in z_N being zero.

2.3 The Diatomic Lattice

These ideas are readily extended to lattices which are regular arrangements of any number of species. For example, suppose that we have alternating heavy and light “atoms” on the chain. The equations of motion are

$$m_1 \ddot{x}_{2\ell} = k(x_{2\ell+1} - 2x_{2\ell} + x_{2\ell-1}) \quad (18)$$

$$m_2 \ddot{x}_{2\ell+1} = k(x_{2\ell+2} - 2x_{2\ell+1} + x_{2\ell}). \quad (19)$$

Proceeding as before, we insert plane waves of the form $x_{2\ell} = Ae^{qa2\ell - \omega t}$ and $x_{2\ell+1} = Be^{qa(2\ell+1) - \omega t}$ into the equations of motion—being careful to keep even and odd sites separate. In this case the maximum value of the wavenumber q is $\pi/2a$ since the lattice spacing is now $2a$ rather than a . We have

$$m_1 A \omega^2 = 2kA - 2kB \cos(qa) \quad (20)$$

$$m_2 B \omega^2 = 2kB - 2kA \cos(qa). \quad (21)$$

This is a linear system for A and B . Introducing the reduced mass $1/m = 1/m_1 + 1/m_2$, the determinant of this system gives the following expression for ω

$$\omega^4 - \frac{2k}{m} \omega^2 + \frac{4k^2}{m_1 m_2} \sin^2(qa) \quad (22)$$

the roots of which are

$$\omega_{\pm}^2 = \frac{k}{m} \left[1 \pm \sqrt{1 - \frac{4m}{m_1 m_2} \sin^2(qa)} \right]. \quad (23)$$

In general, the number of branches of the dispersion curve depends on the number of types of elements on the lattice. The lower frequency branch ω_-^2 is called the *acoustic* branch and has fundamentally different behavior than the higher frequency or *optical* branch. This can be seen by looking at the long wavelength limit of the dispersion relations and group velocities. As qa goes to zero the dispersion relation and group velocity of the acoustical branch looks just like the monoatomic case, but with the equivalent mass m . On the other hand, the long wavelength limit of ω_+ is independent of q , so the group velocity goes to zero; this indicates non-propagating oscillations as q goes to zero.

The term optical refers to the fact that for typical diatomic lattices, the frequencies involved are in the infrared, and under electromagnetic stimulation, it is this mode that is excited. A detailed treatment of this mode therefore requires that we take into account the presence of electromagnetic charge by inserting a force term of the form QE , where Q is the charge and E is the applied field.

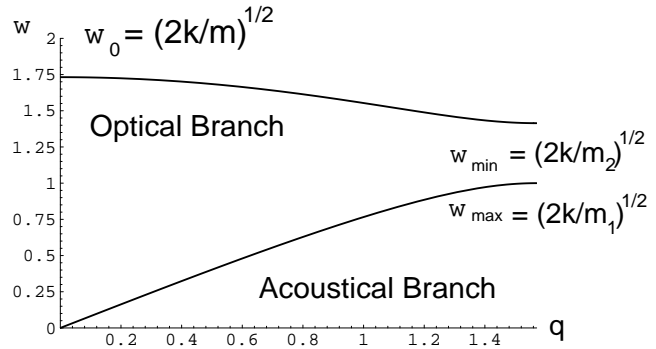


Figure 6. The optical (top) and acoustical (bottom) branches of the dispersion curve for a diatomic lattice with alternating masses $m_1 = 2$ and $m_2 = 1$, $k = 1$, and a lattice spacing $a = 1$.

3 LOCALIZED STATES

3.1 Point Defects

For the homogeneous lattice all the eigenmodes are nonzero everywhere except at the nodal points. In that sense they have global extent. Suppose we disturb the regularity of the lattice by perturbing either a spring constant or a mass. Rayleigh’s principle ((Rayleigh, 1945), Volume II, Sec. 88) says that if a single mass is reduced (or a spring constant increased) then all the frequencies are unchanged or increased, but not by more than the distance to the nearest unperturbed frequency. Similarly, if a single mass is increased (or a spring constant decreased) then all the frequencies are unchanged or decreased, but not by more than the distance to the nearest unperturbed frequency.

In spite of this apparent symmetry between the effects of increasing versus decreasing masses (or decreasing versus increasing spring constants), there is a profound difference in practice. Because the low frequency limit is zero (at least for the monoatomic chain), decreasing a spring constant, and hence one or more frequencies, cannot result in new frequencies outside the band of frequencies allowed by the dispersion relation for the homogeneous or perfect lattice. On the other hand, increasing a spring constant can result in perturbing an eigenfrequency beyond the maximum allowed by the homogeneous dispersion relation ($2\sqrt{k/m}$ for the monoatomic chain). If this happens the resulting eigenmode must be exponentially damped. One way to see that this is so is to observe that for complex wavenumbers the sine in the dispersion relation becomes a sinh, which can match any frequency whatsoever. The result also follows from the discussion following Equation 16.

This effect is illustrated in Figure 7 which shows the two highest frequency eigenmodes for systems with, respectively, one and two perturbed spring constants. In the first case, a single frequency is pushed into the

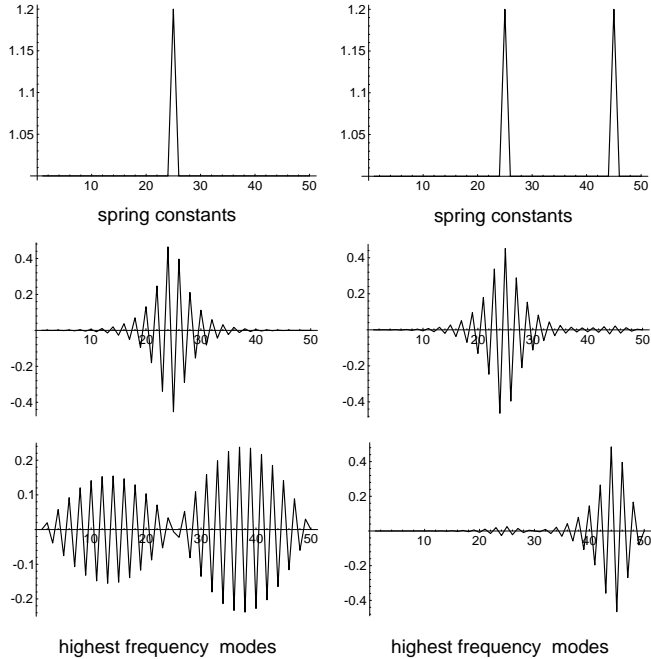


Figure 7. Perturb a single site by increasing its spring constant (or decreasing its mass). Rayleigh’s principle says that this will result in increasing (or leaving unchanged) the frequencies. Increasing a single spring constant sufficiently results in a single eigenvalue being pushed out of the band of frequencies allowed by the homogeneous dispersion relation. This must therefore be associated with a localized mode. Perturbing two lattice sites in this case pushes two frequencies outside the allowed band, resulting in two localized modes.

forbidden band beyond $2\sqrt{k/m}$, resulting in a single localized eigenmode. Increasing two spring constants sufficiently results in two eigenfrequencies in the forbidden (or *impurity*) band and therefore two localized eigenmodes. (It is possible, by making a sufficiently large change in a single spring constant, to generate more than one localized mode centered on the impurity.) As a single spring constant is perturbed by ϵ , then the envelope of the highest frequency mode switches from convex to concave (i.e., becomes exponentially damped) at precisely that value of ϵ which pushes the first perturbed eigenfrequency into the impurity band.

The corresponding experiment, that of decreasing a single spring constant, does not result in a localized mode because the minimum frequency for the monoatomic chain is zero. For the diatomic chain, however, we should expect to see localized modes associated with decreasing a spring constant since the optical branch of the dispersion curve has a nonzero minimum frequency; pushing a frequency off the bottom of the optical branch would necessarily result in an exponentially damped eigenmode, just as pushing a frequency off the top of the acoustical branch does.

3.1.1 Reflection and Transmission Coefficients

As an aside, it is straightforward to derive the reflection and transmission coefficients for the 1D chain with point defects. There are three special cases, a mass defect, a spring constant defect, and combination of the two; see Askar (1985) for the derivations. For example, here is the result for a mass defect.

$$R = \frac{1}{2} \left(1 - \frac{m'}{m} \right) (1 - e^{-iqa}) \quad (24)$$

and

$$T = \frac{1}{2} \left(\left(1 + \frac{m'}{m} \right) + \left(1 - \frac{m'}{m} \right) e^{-iqa} \right) \quad (25)$$

where m' is the mass of the defect and m is the mass of the elements of the perfect lattice. When $m' = m$, $T = 1$ and $R = 0$, as they must.

3.2 Random Lattices

It is straightforward to compute the normal modes and their frequencies for arbitrarily disordered 1D lattices. The problem still reduces to finding the eigenvalues and eigenvectors of a symmetric tridiagonal matrix. The eigenvalues of such a matrix can be efficiently calculated via Sturm bisection (Wilkinson, 1963), while the eigenvectors can be calculated by inverse iteration or by a generalization of the recursion formula in Equation 16.

In Figure 8 a selection of normal modes is shown from a lattice with constant masses but whose spring constants are given by $1 + \xi$, where ξ is a random variable with uniform distribution on $[0, 1]$. The particular realization used is shown at the top. Pronounced localization of the higher modes is evident. Exactly the same sort of result would apply if we have perturbed the masses or the masses and spring constants simultaneously. The most common quantitative measure of the degree of this localization is in terms of the exponential decay of the mode away from its maximum value. On the other hand, it is useful to measure the number of mass/oscillators that participate in the collective motion. For the homogenous lattice, all the mass points except those at nodes participate.

The onset of localization is gradual in 1D. Later it will be seen to be rigorously true that even very small amounts of disorder result in (small amounts of) localization. We can demonstrate this numerically by adding ϵ times a particular pseudorandom realization to the homogeneous lattice. Thus as ϵ is varied from zero to, say, one, a smooth transition is made from a homogeneous lattice, no localization, to a lattice exhibiting the same degree of localization as shown in Figure 8. Figure 9 shows a particular mode during this transition.

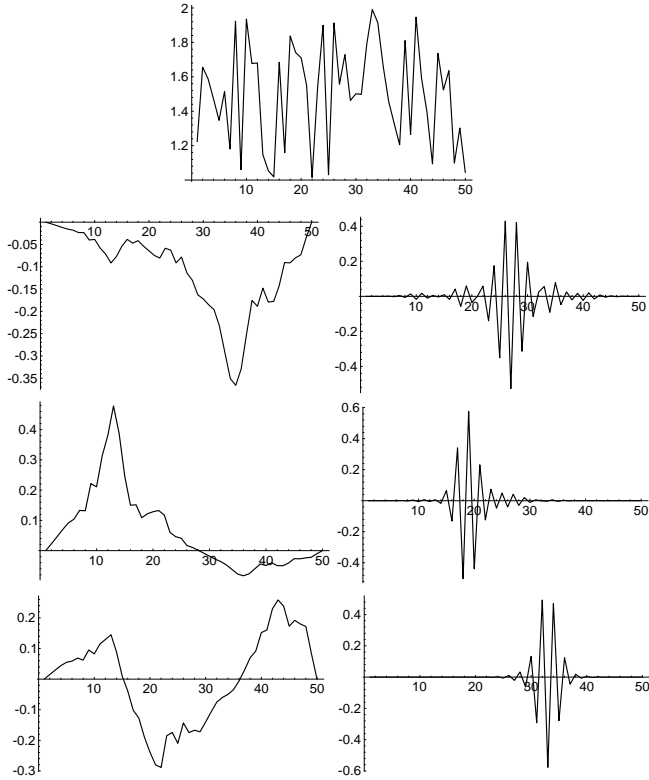


Figure 8. Typical free oscillations of a force-disordered lattice. The spring constants are all equal to $1 + \xi$, where ξ is a random variable with uniform distribution on $[0, 1]$. The particular realization used is shown at the top. On the left are the lowest frequency three modes, on the right are the highest frequency three modes. The high frequency modes are localized exponentially in space.

3.3 Products of Random Matrices

The first systematic study of the 1D disordered chain was published by Freeman Dyson (1952). Dyson developed a method for calculating the distribution of eigenfrequencies (the phonon spectrum in the quantum theoretical treatment) in the $N \rightarrow \infty$ limit as a continued fraction. If the oscillators themselves are distributed according to an exponential law, Dyson's result is analytic. This work was simplified and extended by Helmut Schmidt (1957) who developed the recursive method of computing the eigenfunctions.

The eigenvector recursion formula extends readily to arbitrarily disordered chains. In this case the equations of motion are

$$z_{\ell+1} = \frac{k_{\ell+1} + k_{\ell} - m_{\ell}\omega^2}{k_{\ell+1}} z_{\ell} - \frac{k_{\ell}}{k_{\ell+1}} z_{\ell-1} \quad (26)$$

which we can rewrite as

$$\begin{pmatrix} z_{\ell} \\ z_{\ell+1} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\frac{k_{\ell}}{k_{\ell+1}} & \frac{k_{\ell+1} + k_{\ell} - m_{\ell}\omega^2}{k_{\ell+1}} \end{pmatrix} \begin{pmatrix} z_{\ell-1} \\ z_{\ell} \end{pmatrix}. \quad (27)$$

Defining the matrix

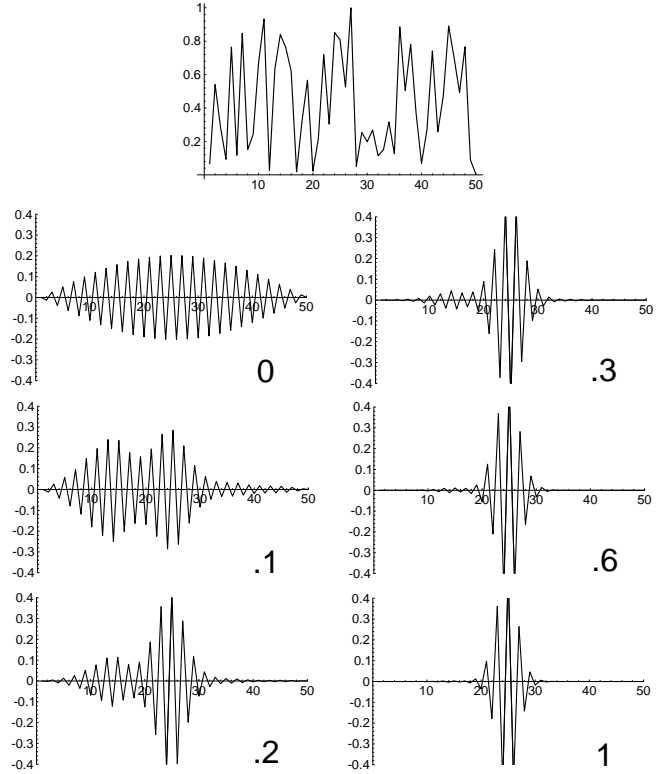


Figure 9. The highest frequency mode as the amplitude of the disorder is varied. The spring constants for this experiment are one plus ϵ times the particular pseudorandom realization shown at the top of the figure. As ϵ is varied from zero to one, a smooth transition is made from a homogeneous lattice, to one of the same degree of disorder shown in Figure 8

$$B_{\ell} = \begin{pmatrix} 0 & 1 \\ -\frac{k_{\ell}}{k_{\ell+1}} & \frac{k_{\ell+1} + k_{\ell} - m_{\ell}\omega^2}{k_{\ell+1}} \end{pmatrix} \quad (28)$$

it follows by induction that

$$\begin{pmatrix} z_{\ell} \\ z_{\ell+1} \end{pmatrix} = B_{\ell} \cdot B_{\ell-1} \cdots B_1 \begin{pmatrix} z_0 \\ z_1 \end{pmatrix} \equiv P_{\ell} \begin{pmatrix} z_0 \\ z_1 \end{pmatrix}. \quad (29)$$

In this way we have managed to reduce the study of transport in disordered 1D media to the problem of the products of random matrices, which has an extensive literature (for example, cf. Crisanti *et al.* (1993)). Further, if we think of the index of the matrices B_{ℓ} as representing time rather than distance, then Equation 29 can be thought of as a stochastic dynamical system. Localization then, the exponential decay of energy in wave propagation, is completely analogous to the exponential growth or decay of trajectories of the dynamical system as sketched in Figure 10. Thus, if one is used to thinking in terms of dynamical systems it is immediately apparent that the localization length is nothing more than the reciprocal of the largest Lyapunov exponent of the matrix P_N in Equation 29. (See Collet (1992) for the basic definitions of the Lyapunov exponents.)

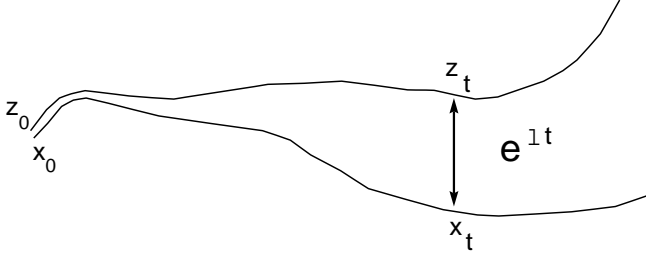


Figure 10. Sensitive dependence on initial conditions in a dynamical system is measured in terms of the exponential divergence of initially near-by trajectories. The exponent is called the Lyapunov exponent.

So there are two mathematical/computational issue that must be addressed. First, what is known or can be said about the asymptotic properties of products of random matrices, such as Equation 29. Secondly, how can the Lyapunov spectrum of P_N be computed.

3.4 Asymptotic Properties of Products of Random Matrices

If the problem involved asymptotic behavior of products of ordinary random variables, then the path would be straightforward. Assuming the random variables were independent and identically distributed one could appeal to the law of large numbers and the central limit theorem to show that for large N the product was lognormally distributed. But the non-commutativity of matrices makes life a good deal more complicated. The details are mathematically intricate and the interested reader should consult Crisanti *et al.* (1993) for details. The upshot is two fundamental theorems. The first, due to Furstenberg (1963), states that

$$\lambda_1 = \lim_{N \rightarrow \infty} \frac{1}{N} \ln \|P_n\| \quad (30)$$

exists almost surely. And further, that the maximum Lyapunov exponent λ_1 is a non-random quantity; in other words that

$$\lambda_1 = \lim_{N \rightarrow \infty} \frac{1}{N} \langle \ln \|P_n\| \rangle \quad (31)$$

where the angled brackets refer to the average under the distribution associated with the B_ℓ , which are assumed to be independent and identically distributed. As expected, the Lyapunov exponent measures the growth rate associated with *typical* vectors z

$$\lim_{N \rightarrow \infty} \frac{1}{N} \ln \|P_n z\| \quad (32)$$

although this does not preclude different growth rates for improbable choices of z .

The second basic result, due to Oseledec (1968), is called the multiplicative ergodic theorem. It states that

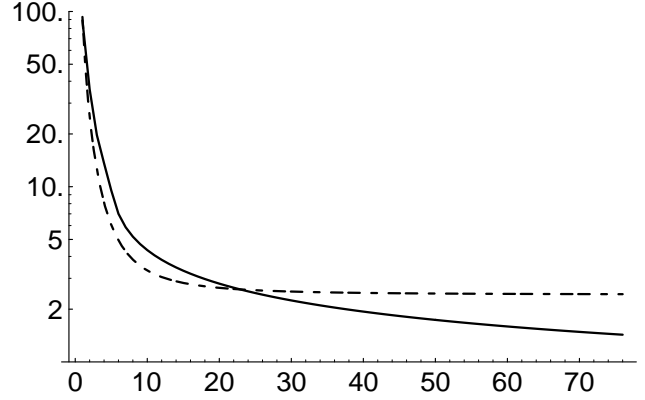


Figure 11. Reciprocal Lyapunov exponent of the matrix product $B^N \cdot B^{N-1} \cdots B^1$, for the isotropically disordered lattice ($k_i = k$, $m_i = \text{random}$) of length 200 as a function of frequency (in arbitrary units). The dashed curve is the best fitting curve of the form $c_1 + c_2/f^2$. The similarity seems reasonable except at high frequencies.

the $2N$ -th root of the symmetrized product matrix P_N

$$(P_N^T P_N)^{1/2N}$$

converges to a matrix Γ whose eigenvalues are e^{λ_i} , where λ_i are the Lyapunov exponents of P_N . Now in the case of the 1D lattice, the product matrix is just 2×2 . Oseledec's theorem gives a straightforward method to compute the Lyapunov spectrum, albeit not without numerical risks due to the exponential growth. Further, Furstenberg's theorem ensures that the estimate of localization length that results will be independent of the particular realization used.

The localization length is equal to one over the largest Lyapunov exponent of the n -fold matrix product

$$P_N \equiv B_N \cdot B_{N-1} \cdots B_1.$$

An example of the calculation of the characteristic Lyapunov exponent of a 200 element isotropically disordered lattice is shown in Figure 11. The random perturbations to mass are uniformly distributed and independent. The frequency units are arbitrary. The low frequencies were cut off when the localization length reached half the length of the lattice. Also shown in a dashed line style is the best fitting curve of the form $c_1 + c_2/f^2$. The similarity is reasonable except at high frequencies. And the smooth dependence of localization length on frequency is encouraging on purely numerical grounds.

3.5 Localization in Higher Dimensions

The 1D problem turns out to be peculiar from the standpoint of multiple scattering. Because of the lack of geometrical spreading, even a small amount of randomness is sufficient to cause (a small amount of) local-

ization. This has been proven rigorously by Ishii (1973). In higher dimensions, we can rely on the original work of Anderson, who showed that in 2D and 3D, provided the degree of disorder of the lattice spins was greater than some critical value, and provided the interparticle potential fell off sufficiently fast with distance, then the electron wavefunction was localized in space for arbitrarily large values of time.

Now in the frequency domain, the harmonic lattice equations (for constant k) are identical to the lattice Schroedinger equation of a particle moving in a potential:

$$i \frac{da_n}{dt} = \epsilon_n a_n + a_{n+1} + a_{n-1} \quad (33)$$

where a_n is the electron wavefunction at the n -th site and ϵ_n is the energy at the n -th site. The stationary Schroedinger equation is therefore

$$Ea_n = \epsilon_n a_n + a_{n+1} + a_{n-1} \quad (34)$$

which differs only by a slight change of variables from the isotropically (mass) disordered harmonic chain. And since the spring constants in the harmonic lattice act only on their nearest neighbor, there is no problem with them decaying fast enough.

We can expect, therefore, that for isotropically disordered lattices the existence of localization would be governed by the same principles as the spin diffusion problem. There are important differences, of course. The localization length for a quantum mechanical particle in a disordered medium generally decreases with decreasing energy. The analogy in wave propagation would be the long wavelength limit, in which case, as we have already seen, the localization length becomes unbounded. At the other extreme, as the frequency of a classical wave goes to infinity, there appears to be a minimum localization length (the constant c_2 in the theory of Sheng *et al.* (1986a)). Nevertheless, the analogy between the disordered mechanical lattice and Anderson's model of electron spin diffusion is sufficiently close mathematically to demonstrate the existence of localization of classical waves as a critical phenomenon in higher dimensions.

4 CONCLUSIONS

Classical waves scattering from heterogeneities in elastic solids excite vibrational modes which are localized about the heterogeneity. With a random distribution of such heterogeneities, it is possible for a propagating wave to become trapped altogether, with all its energy in some band of frequencies being converted into essentially random fluctuations of the medium. A model of this localization phenomenon has been presented using

a dynamical system of coupled masses and springs on a 1D chain.

The extension of the dynamical system approach to higher dimensional lattices is straightforward. The theory of the products of random matrices (PRM) still applies to some extent, although to more complicated matrices. It is difficult to untangle the effects of using non-infinite lattices (finite N effects), although there seems to be some hope of quantifying these using the existing theory of PRM. Also, only a rudimentary numerical analysis of the calculation of the Lyapunov exponents has been attempted here. More sophisticated methods are available in the literature on dynamical systems. Reasonable finite N uncertainties and accurate calculation of the Lyapunov exponents will be essential to making this theory useful on in-situ measurements of elastic parameters such as given by well logs.

5 ACKNOWLEDGEMENTS

I should like to thank Martin Smith for helping me understand normal modes and for his generous supply of ideas and time.

This work was partially supported by the sponsors of the Consortium Project on Seismic Inverse Methods for Complex Structures at the Center for Wave Phenomena, Colorado School of Mines, and the Shell Foundation.

References

- Anderson, P.W. 1958. Absence of diffusion in certain random lattices. *Physical Review*, **109**, 1492–1505.
- Asch, M., Kohler, W., Papanicolaou, G., Postel, M., & White, B. 1991. Frequency content of randomly scattered signals. *SIAM Review*, **33**, 519–625.
- Askar, Attila. 1985. *Lattice dynamical foundations of continuum theories*. World Scientific.
- Collet, P. 1992. Regular and chaotic behaviour of dynamical systems. *In: Goles, E., & Martinez, S. (eds), Statistical physics, automata networks and dynamical systems*. Kluwer.
- Crisanti, Andrea, Paladin, Giovanni, & Vulpiani, Angelo. 1993. *Products of random matrices*. Springer.
- Dyson, Freeman J. 1952. The dynamics of a disordered linear chain. *Physical Review*, **92**, 1331–1338.
- Furstenberg, H. 1963. Noncommuting random products. *Transactions American Mathematical Society*, **108**, 377.
- Gellermann, W., Kohmoto, M., Sutherland, B., & Taylor, P.C. 1994. Localization of light waves in Fibonacci dielectric multilayers. *Physical Review Letters*, 633–636.

- Ishii, K. 1973. Localization of eigenstates and transport phenomena in the one-dimensional disordered system. *Suppl. Progress of Theoretical Physics*, **53**, 77–138.
- Lifshitz, I.M. 1944. *J. Phys. USSR*, **8**, 89.
- Maradudin, A.A., Montroll, E.W., Weiss, G.H., & Ipatova, I.P. 1971. *Theory of lattice dynamics in the harmonic approximation*. Academic.
- Oseledec, V.I. 1968. *Transactions Moscow Mathematical Society*, **19**, 197.
- Rayleigh, J.W.S. 1945. *Theory of sound*. Dover.
- Scales, J.A. 1993. On the use of localization theory to characterize elastic wave propagation in randomly stratified 1-D media. *Geophysics*, **58**, 177–179.
- Schmidt, Helmut. 1957. Disordered one-dimensional crystals. *Physical Review*, **105**, 425–441.
- Sheng, Ping, Zhang, Zhao-Qing, White, Benjamin, & Papanicolaou, George. 1986a. Minimum wave-localization length in a one-dimensional random medium. *Physical Review*, **B34**, 4757–4761.
- Sheng, Ping, Zhang, Zhao-Qing, White, Benjamin, & Papanicolaou, George. 1986b. Multiple scattering noise in one dimension: universality through localization length scaling. *Physical Review Letters*, **57**, 1000–1003.
- Smith, G.D. 1978. *Numerical solution of partial differential equations: finite difference methods*. Oxford.
- White, Benjamin, Sheng, Ping, Postel, Marie, & Papanicolaou, George. 1989. Probing through cloudiness: theory of statistical inversion for multiply scattered data. *Physical Review Letters*, **63**, 2228–2231.
- White, Benjamin, Sheng, Ping, & Nair, Balan. 1990. Localization and backscattering spectrum of seismic waves in stratified lithology. *Geophysics*, **55**, 1158–1165.
- Wilkinson, J.H. 1963. *The algebraic eigenvalue problem*. Oxford.