Modelling microstructured media: periodic systems and effective media

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Abstract My aim in these lectures is to give a broad overview of the Mathematics and Physics of perfectly periodic systems, drawing heavily upon the literature of solid-state physics: it is essential to understand how structure on a micro-scale affects longer scale macro-scale behaviour and periodic systems are a naturally place to begin. Periodic systems are, on one hand, quite special and the constructive interference created by periodicity leads to strong effects that we shall see later, but on the other hand many natural and man-made structures exhibit, at least some, general periodic structure. After developing the language of periodic systems we will turn our attention to the development of asymptotic "effective" media that are posed entirely upon the macro-scale. Importantly we will develop asymptotic theories valid at high frequencies. A general approach valid for continua, semi-discrete (frame) and fully discrete (mass-spring) systems will be developed. If time allows we will then look further into some of the remarkable physics that can be seen when waves move through structured media: defect states, all-angle negative refraction and ultra-refraction.

1 Motivation

Periodic, or almost periodic, structures surround us and are of considerable technological importance. One of the most talked about materials at the moment is graphene, an almost perfect material constructed from a hexagonal lattice and graphene has truly remarkable properties some of which are related to the properties of the waves that pass through it. Many atomistic systems are remarkably regular in their structure mainly due to the energetic arguments that force the material to adopt such regular patterns. The attraction of one atom to its neighbour, or neighbours, can be modelled by discrete mass-string models with the physics of the attraction lumped into some effective string constants. Historically the study of perfect lattice-like systems originated in solid-state physics and a huge amount of effort and

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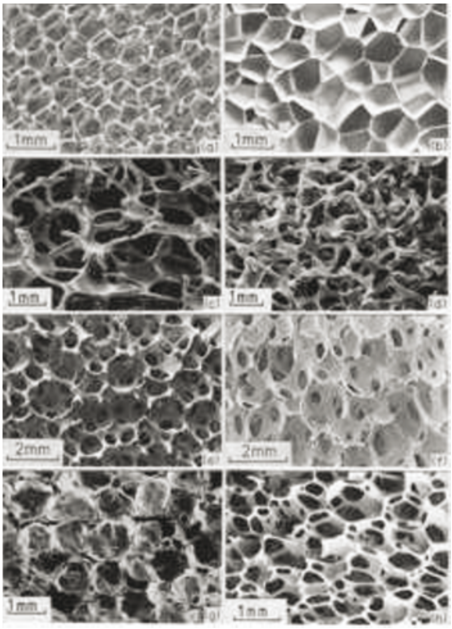

Figure 1: Photographs of cellular solids: (a) open-cell polyurethane (b) closed-cell polyurethane (c) nickel (d) copper (e) zirconia (f) mullite (g) glass (h) a polyether foam with both open and closed cells. Taken from the book of Gibson and Ashby [8].

scientific progress was made in that area: This is fortunate as we can then use that accumulated knowledge! The books of Kittel [11] and Brillouin [4] are the classical texts in this area and we will draw upon them in these lectures. It is also notable that considerable effort went into the properties of atomic systems with defects, i.e extra atoms or disruption/ disorder in the atomic structure [1].

Shifting to, yet, another area, that is, structural mechanics and designer materials one finds that the subjects of solid mechanics also abound with structured media. Cellular solids, engineering foams, or panels, created from honeycomb lattices are popular in industry for their lightweight, but strong, properties. A typical range of engineering foams are shown in Fig. 1, taken from [8], and although not perfectly regular, they still retain some periodic and regular structure. Once again waves passing through such a

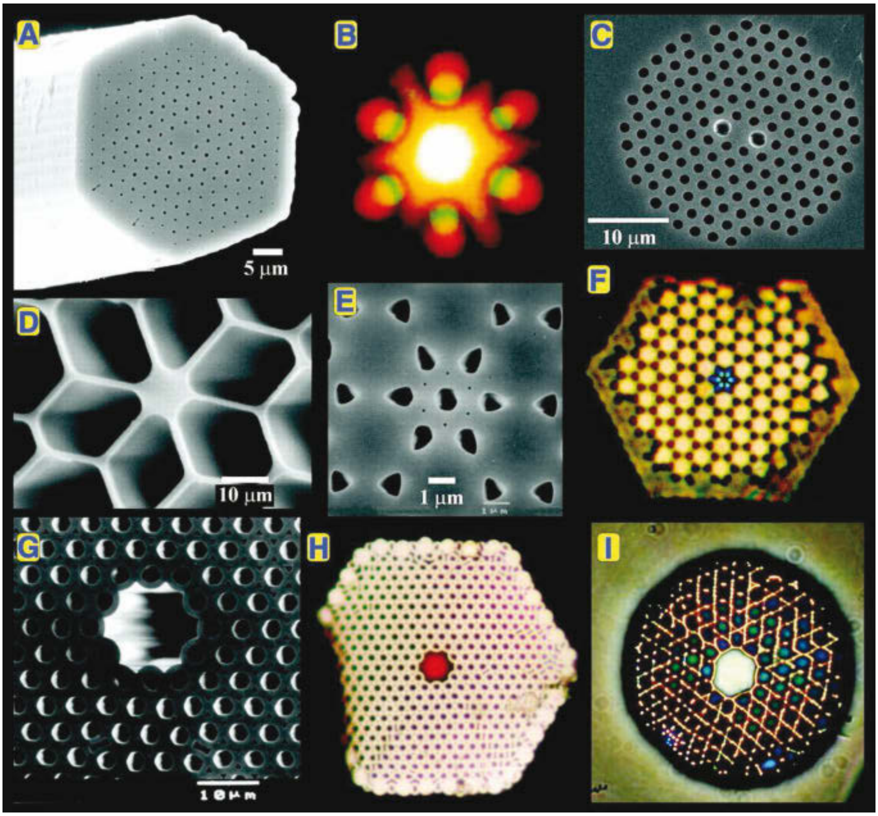

Figure 2: Micrographs of various Photonic Crystal Fibre structures taken from the review of Russell et al [15]. The regular array of holes allow for excellent (low-loss) waveguides in optics and have a host of applications: sensors, high bandwidth guides, optical filters.

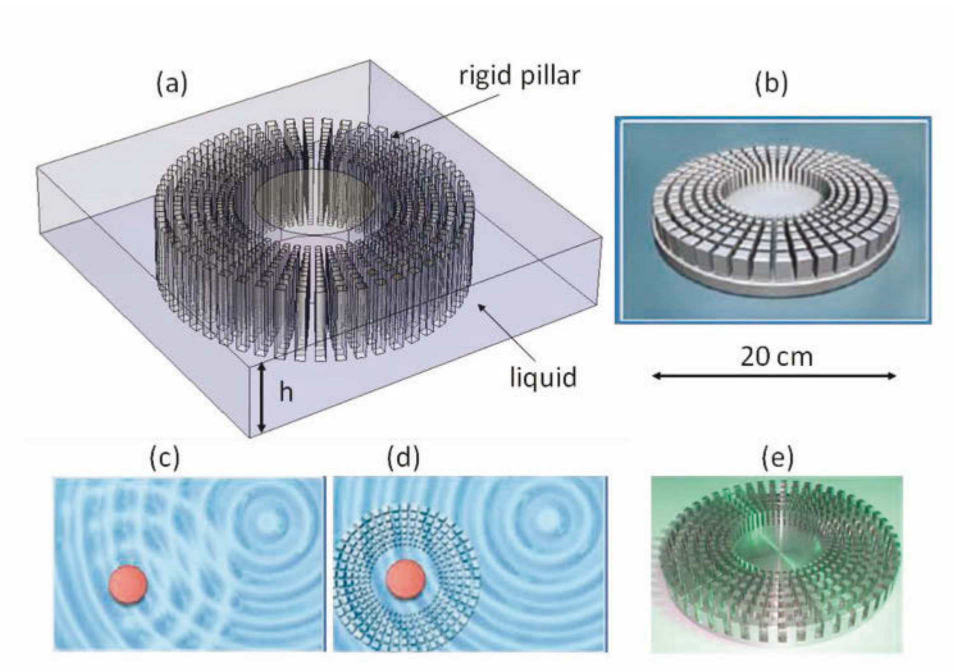

Figure 3: A water wave cloak: (a) Geometry of the structured cloak consisting of concentric arrays of rigid pillars immersed in a vessel of liquid of depth h; (b) Diagrammatic view of the cloak; (c-d) Scattering of water waves on a rigid obstacle (red disc) without (c) and with (d) the water wave cloak; (e) Photo of the micro-structured cloak used in experiments around 10 Hertz. Figure taken from [9].

structure are of interest, for instance, can one determine where or whether the honeycomb has sustained damage or whether some ligaments are broken. Similarly many buildings, bridges, roofs and other structures are created from a frame of beams or trusses, a famous example is the Eiffel tower and a common Civil Engineering task is to find the modes of vibration of such a structure in, for instance, Earthquake resistant design. Cellular microstructures also underlie many continuum models in micromechanics [14].

Modern physics and the new subjects of photonics and metamaterials utilise the properties of structured media to create the remarkable effects of cloaking, negative refraction, subwavelength imaging and almost perfect guiding, optical filtering, designer surfaces and much more. A selection of photonic crystal fibres are shown in Fig. 2, taken from [15], and interestingly, from our point of view, they consist of a large number of holes in a matrix material - all equally spaced - but with one or more holes filled, moved, or removed. So the structure is certainly not infinitely periodic, but has some features that are clearly regular. Later we will see that there exist, so-called, stop-bands which are windows of frequencies in which waves do not propagate through a perfect material: However, the destruction of perfect periodicity through the introduction, or removal, of additional features can create defect or localised modes. These modes only occur for single frequencies within the stop-band and thereby allow only specific waves to propagate. This striking result allows one to create very precise guiding structures which allow light to be controlled accurately - the books [10; 17] contain considerable discussion and demonstration of this.

Metamaterials are similarly dominated by the optics of structured media, actually it does not have to limited to optics as similar effects can be engineered in other wave systems such as acoustics or in water-waves. In the latter system, recent experiments have verified the efficacy of these cloaking systems and a recent example is shown in figure 3 taken from the book [9]. Quite incredibly one can make a piece of space, and whatever is enclosed by it, invisible to incoming waves - the lectures by Sebastien Guenneau will be covering this, and other exciting areas of metamaterials, and I do not want to encroach upon this, bar to say that clearly that understanding and modelling structured media is clearly important in that setting too.

There are three classes of structure of increasing technical difficulty and complexity: Completely discrete media created from point masses connected by conceptual springs, then semi-discrete frames, nets or trusses joined at points but these points are connected via strings or elastic beams that satisfy ordinary differential equations and finally fully continuum systems where, say, for holes in a photonic crystal the electromagetic waves obey Maxwell's

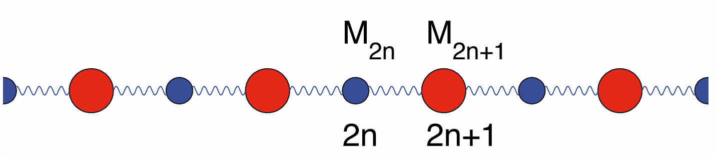

Figure 4: A chain of masses - the classical linear diatomic chain.

equations. In terms of the physics associated with microstructure one can go a long way in understanding the techniques and how the dominant physics can be encapsulated in a model by using the simplest, discrete, systems as "toy" problems. In these lectures I will endeavour to keep the Mathematics simple, and not obfuscate the physical ideas, and therefore the discrete systems are the toys of choice.

A key observation for all the motivational examples chosen is that there is a very regular structure on a small-scale, and that one might be interested in hundreds, thousands or even millions or repeating elementary cells, but that one would ideally be interested in modelling behaviour on some macro-scale. There is a potentially huge disparity in length-scales which one would wish to exploit in any asymptotic modelling. Another key observation is that there are actually three lengthscales in the problem: the micro-scale of the elementary cell, the macro-scale of the whole structure and finally the wavelength of oscillations we are interested in. Considerations of whether the waves are long relative to the elementary cell or short, so multiple scattering occurs, are important.

2 Perfect, infinite, systems

We begin by exploring the properties of the simplest periodic structures: linear chains, of which the diatomic chain is shown Figure 4 with the atoms interacting via nearest neighbour interactions; this is an oversimplification of the real atomic situation but rather good as a toy model that describes the essential features one expects to see. This is a toy model of salt, NaCl, in which there are two alternating atoms, Sodium and Chlorine, and one can label the displacements of each atom by y_{2n}, y_{2n+1} with the even and odd masses M_{2n}, M_{2n+1} taking values M_2, M_1 respectively. Scaling out the spring constants, and assuming nearest neighbour interactions one arrives at a model system:

$$y_{2n-1} + y_{2n+1} - 2y_{2n} = -\Omega^2 M_2 y_{2n} \tag{1}$$

$$y_{2n} + y_{2n+2} - 2y_{2n+1} = -\Omega^2 M_1 y_{2n+1} \tag{2}$$

where Ω is the wave frequency. Note that it is implicit that the time dependence of the system is $\exp(-i\Omega t)$. The difference equations simplify even further if we consider equal masses and then there is a single difference equation to consider:

$$y_{n+1} + y_{n-1} - 2y_n = -M\Omega^2 y_n. \tag{3}$$

Provided the lattice is infinite, and perfectly periodic, one can sidestep the explicit solution of the difference equation and instead pose quasi-periodic conditions. We simply consider one mass and say that as a wave moves from one mass to the next it undergoes a phase-shift, κ, so that

$$y_{n+1} = \exp(i\kappa) y_n. \tag{4}$$

This phase-shift can be interpreted as a wavenumber and it is often called the Bloch wavenumber and the quasi-periodic condition (4) is called a Bloch condition: It is more historically fair to call these Floquet-Bloch conditions, as a digresion Floquet proved one-dimensional results later generalised to three-dimensions by Bloch and often in one-dimension Floquet's name is used. The wave frequency Ω is related to the Bloch wavenumber κ via a dispersion relation

$$\Omega = \frac{2}{\sqrt{M}} \sin\left(\frac{\kappa}{2}\right). \tag{5}$$

Just to recall: dispersionless waves have the phase and group velocities equal and most linear wave systems such as those of acoustics, electromagnetism and elasticity have this property. One can see that in the limit of small wavenumber, long waves and low frequencies that equation (5) reduces to

$$\Omega \sim \frac{\kappa}{\sqrt{M}} \tag{6}$$

which is a linear relation and therefore the waves, in that limit, are dispersionless.

For the simple chain the dispersion relation is shown in Figure 5(a) from which we can see the relation is clearly non-linear - also shown are the asymptotics from homogenization theories.

To whet your appetite for how an "effective" medium would describe a large number of masses let us generate a continuum description of the discrete system in the long-wave, low frequency limit. We begin by introducing a long-scale continuous variable $\eta = \varepsilon n$ where ε is some small parameter, if

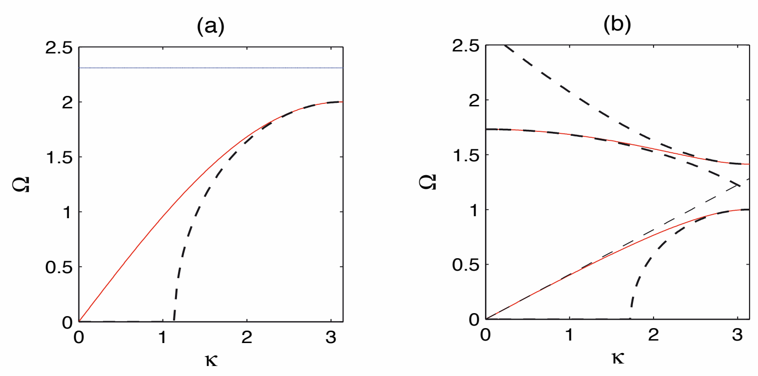

Figure 5: Dispersion curves for the one-dimensional uniform lattice, (a) and the diatomic lattice (b). The exact dispersion curves are the solid lines whilst the asymptotics in (a) and from [7] in (b)) of the perfect lattice are the dashed lines. In panel (a) the dashed line above the exact curve shows the frequency associated to the localised defect state. In panel (a) the mass value $M = 1$ whilst in (b) $M_1 = 2$ and $M_2 = 1$. Taken from [12].

we were practical people this could be found by considering the frequency, and the frequency is $\Omega = \varepsilon\hat{\Omega}$ (where $\hat{\Omega}$) is an order one quantity. Let us set

$$y_n = y(\eta), \quad y_{n\pm1} = y(\eta \pm \varepsilon) \tag{7}$$

and then the difference equation becomes, in this new language, that

$$y(\eta + \varepsilon) + y(\eta - \varepsilon) - 2y(\eta) - M\varepsilon^2\hat{\Omega}^2 y(\eta) = 0. \tag{8}$$

An expansion in a Taylor series

$$y(\eta + \varepsilon) \sim y(\eta) + \varepsilon y'(\eta) + \frac{\varepsilon^2}{2}y''(\eta) + \dots \tag{9}$$

yields, to leading order,

$$y_{\eta\eta} + M\hat{\Omega}^2 y = 0. \tag{10}$$

This is simply the wave equation (in one dimension with harmonic time dependence assumed) for a string and suggests (as we would expect) that, if the wave was long enough, it would see the collection of masses as being smeared out to produce an effective string. One could go to higher orders in the expansion and gradually dispersive effects would become evident. But

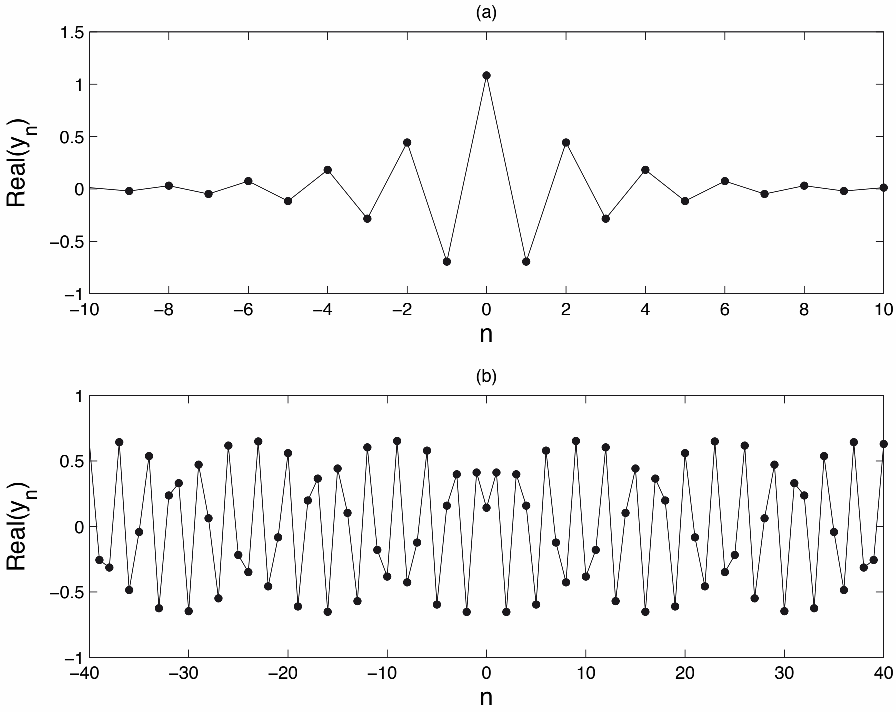

Figure 6: Forced lattice at origin. (a) Forcing frequency $\Omega = 2.05$ and (b) $\Omega = 1.8$.

going to higher orders tends, in general, to be a fair amount of effort for a reducing amount of increased knowledge (in my opinion). Notably the dispersion relation one obtains from the effective string is

$$\kappa = \sqrt{M}\Omega \tag{11}$$

when one replaces η with εn. Therefore this does indeed tie back in with (5) as one would hope.

If one forces the lattice close to the band-gap edge at $\Omega = 2$ (assuming $M = 1$) then one sees two distinct types of behaviour, as shown in figure

6, with spatially decaying solutions for frequencies within the stop-band, and oscillatory propagating solutions otherwise. Notably in figure 6(a) the masses are, at least roughly, out-of-phase from their neighbours and the decay appears exponential and in figure 6(b) the masses are, again, roughly out-of-phase and there is an apparent longer scale oscillation. Both the local behaviour and the long-scale features suggest that some asymptotic progress can be made.

As we have just witnessed some solutions are propagating within the system, a natural question is how, numerically, to mimic "infinity". In continuum systems a method due to Berenger [3] called perfectly matched layers is highy popular and widely used. Oddly, in discrete systems there does not appear to have been an analogous development. It is possible to generate a discrete PML (DPML) by following the arguments of, say, Turkel in the continuous case and discretise (after a further approximation) one gets

$$y_{n+1} + y_{n-1} - 2y_m + M\Omega^2 \left(1 - \frac{\sigma(n)}{i\Omega}\right)^2 y_n = \delta_{n,0} \qquad (12)$$

[12] on a lattice $-N \leq n \leq N$ with $\sigma(n) = 0$ for $|n| < N_{pml}$. In PML computations it is often observed, and indeed proved [16], that nonlinear dependence in σ is advantageous. Here we take $\sigma(n) = (N_{pml} - n)^q/N$ for $n > N_{pml}$ and a symmetric formula for $n < -N_{pml}$; in computations $q = 2$ unless otherwise indicated. Physically the masses are taken to have a frequency dependent damping.

Also shown in Fig. 5 is the dispersion curve from the classical example of the diatomic chain of masses and springs. Notably there are two dispersion curves (the upper/lower ones called optical and acoustic branches respectively) separated by a so-called stop band, the stop-band of frequencies is one in which propagation is disallowed and even in this simple system one can use it as a filter. The Bloch wavenumber κ again plays a vital role as it is the phase shift across a cell - and is related to the frequency via a dispersion relation

$$M_1 M_2 \Omega^4 - 2(M_1 + M_2)\Omega^2 + 2(1 - \cos\kappa) = 0. \qquad (13)$$

Note the range of κ (for 0 to π) caused by the periodicity of the system, and that there exist standing waves at end of Brillouin zone (the points $\kappa = 0$ and π.

2.1 Two-dimensions

There are naturally higher dimensional periodic structures, these are of more interest than one-dimensional chains, and the prototypical two-

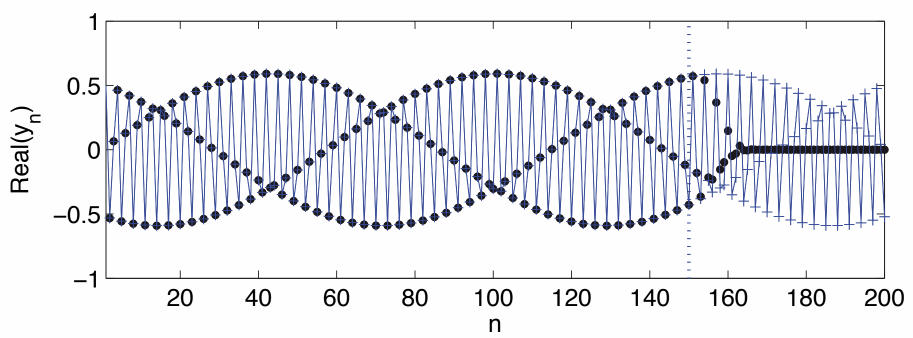

Figure 7: Comparing discrete PML with the exact solution for frequency $\lambda = 1.75$. The real part of y_n is shown with the exact solution as the crosses connected by lines, the PML numerics are solid circles; these are visually indistinguishable until we enter the PML region for $n > N_{pml} = 150$. Similar accuracy occurs for the imaginary part. Figure taken from [12].

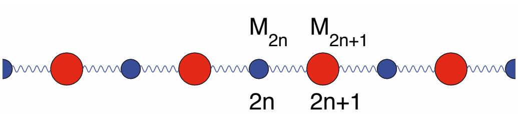

Figure 8: A schematic of the diatomic chain.

dimensional lattice is

$$y_{n+1,m} + y_{n-1,m} + y_{n,m+1} + y_{n,m-1} - 4y_{n,m} + \Omega^2 M y_{n,m} = 0 \tag{14}$$

and now the scalar (in 1D) Bloch wavenumber is replaced by a vector $\kappa = (\kappa_1, \kappa_2)$ where

$$y_{n+\hat{N},m+\hat{M}} = \exp(i[\hat{N}\kappa_1 + \hat{M}\kappa_2])y_{n,m} \tag{15}$$

for integer N, M and the resulting dispersion relation is

$$M\Omega^2 = 4 - 2(\cos\kappa_1 + \cos\kappa_2). \tag{16}$$

The Brillouin zone [4] is no longer a simple line (as in 1D) but now a square in κ space. More conventionally one just plots the dispersion relation around

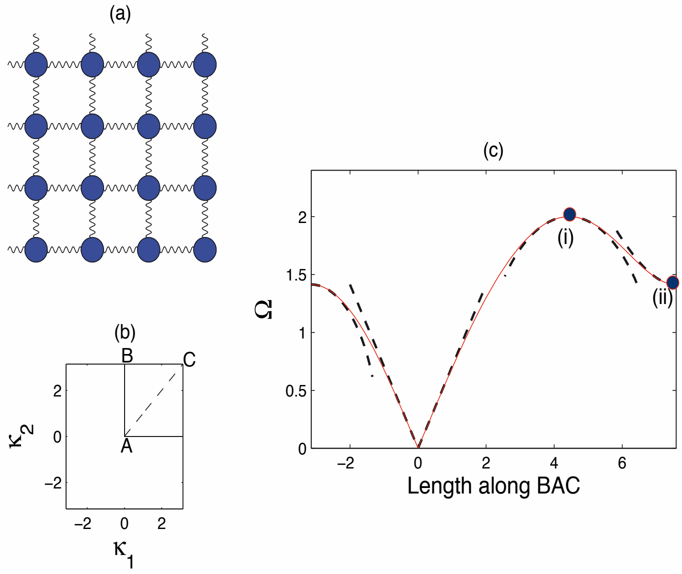

Figure 9: A uniform square lattice is shown in (a), with the irreducible Brillouin zone is the triangle A,B,C in (b). $M = 2$ in the dispersion curve (c); the dashed lines are from the HFH asymptotics. Figure taken from [12]

the edges of the irreducible Brillouin zone although that does carry some implications regarding the full iso-frequency surfaces [5]. The dispersion relation (16) is plotted in Fig. 9 and immediate observation is that the dispersion curves are linear near the origin, and a simple Taylor expansion then recovers an effective acoustic equation that can be obtained also by conventional homogenization. Another key observation is that standing waves occur at the wavenumber vector positions identified by A, B and C where they are perfectly in-phase/ out-of-phase in oscillation across the structure.

2.2 Homogenization

The homogenisation technique involves the confluence of two ideas: One mathematical, the idea of using a long-scale and a short-scale separation which is called the method of multiple scales. The other, physical, is that there exist standing wave frequencies, and associated eigenmodes, that encode the multiple scattering of near and far members of the periodic structure. This latter step is the key modification of standard homogenisation theory allowing one to model high frequency oscillations in periodic or nearly periodic structures. The full theory for lattices is in [7] and it can be extended to continuous systems [6].

In the simplest example of the diatomic lattice in one dimension (the basic idea carries across to higher dimensions with additional algebra) we introduce two scales: a long-scale, on the scale of the grid, characterised by $N \gg 1$ where N could be the number of lattice points and introduce a small parameter $\varepsilon = 1/N \ll 1$; the small parameter is crucial to the whole procedure. We introduce a new long-scale coordinate $\eta = 2n/N$ and take η to be a continuous, not discrete, variable. The other scale, the short-scale is taken to be the elementary cell and we specify an integer m that takes the values $m = -1, 0, 1, 2$; the elementary cell corresponds to the masses at $2n$, $2n + 1$ and their immediate neighbours. The two-scales are considered as independent variables, which is the standard multiple scales trick [2], and we take

$$y_{2n+m} = y(\eta+m\varepsilon, m) \sim y(\eta, m)+m\varepsilon y_\eta(\eta, m)+\frac{(m\varepsilon)^2}{2}y_{\eta\eta}(\eta, m)+\dots \quad (17)$$

as $\varepsilon \ll 1$. In particular the four displacements used in equations (1),(2) in this notation are $y_{2n-1} = y(\eta - \varepsilon, -1)$, $y_{2n} = y(\eta, 0)$, $y_{2n+1} = y(\eta + \varepsilon, 1)$ and $y_{2n+2} = y(\eta + 2\varepsilon, 2)$.

The asymptotic analysis only uses the displacements at y_{2n} and y_{2n+1}; their neighbouring displacements are related to these two via

$$[y_{2n-1}, y_{2n+2}] = [y(\eta - \varepsilon, -1), y(\eta + 2\varepsilon, 2)] = (-1)^J[y(\eta - \varepsilon, 1), y(\eta + 2\varepsilon, 0)] \quad (18)$$

as we assume that the motion, on the microscale of the elementary cell, is that of locally standing waves oscillating in-phase or out-of-phase ($J = 0, 1$ respectively) across the cell.

Equations (1),(2) to order ε^2 in matrix form become,

$$[A_0 - \lambda^2 M(1 + \varepsilon^2\alpha g(\eta)) + \varepsilon A_1(\partial, \lambda) + \varepsilon^2 A_2(\partial^2, \lambda)]\mathbf{y}(\eta) = 0, \quad (19)$$

where ∂ denotes $\partial/\partial\eta$, $\mathbf{y}(\eta) = [y(\eta, 0),\ y(\eta, 1)]^T$ is the displacement vector, M is a diagonal matrix $M = \text{diag}\ [M_2,\ M_1]$, A_0 is a constant matrix and A_1 and A_2 are matrix differential operators. These matrices depend on periodicity conditions and, therefore, are different for in-phase and out-of-phase cases.

The natural separation of scales leads to a hierarchy of equations in powers of ε where the ansatz

$$\mathbf{y}(\eta) = \mathbf{y}_0(\eta) + \varepsilon\mathbf{y}_1(\eta) + \varepsilon^2\mathbf{y}_2(\eta) + \dots \quad (20)$$

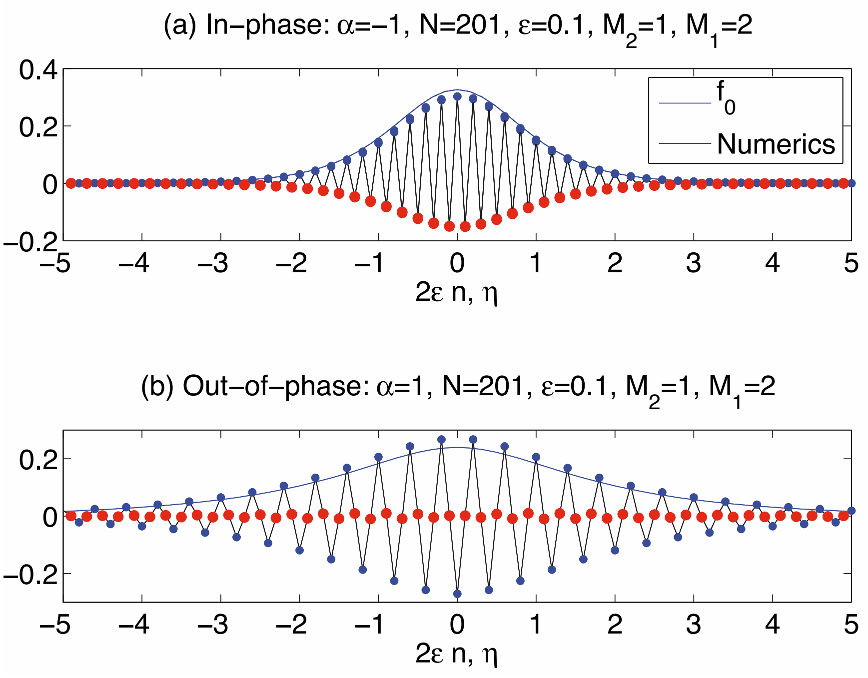

Figure 10: Localised modes for $M_1 = 2$, $M_2 = 1$ showing the numerical solution of (1,2) versus the f_0 from the asymptotic equations24), and its in-phase analogue, with the $g(\eta)$ =sech$^2(\eta)$. Panel (a) shows a localised in-phase solution for which the numerics give $\lambda^2 \sim 3.01896$ and the asymptotics give $\lambda^2 \sim 3.01880$ that differ in the fourth decimal place. Panel (b) shows the localised out-of-plane eigensolution for $\alpha = 1$ and the numerics give $\lambda^2 = 1.99239$ with the asymptotics as $\lambda^2 = 1.99236$. This figure is taken from [7].

$$\lambda^2 = \lambda_0^2 + \varepsilon\lambda_1^2 + \varepsilon^2\lambda_2^2 + \dots \tag{21}$$

is adopted. Substituting the ansatz into the lattice equations (19) gives differential-difference equations that are treated order-by-order in ε.

Let us now look at an example in detail: Standing waves with complete phase-shift across the structure lead to periodic conditions for the masses which are $y(\eta, -1) = -y(\eta, 1)$ and $y(\eta, 0) = -y(\eta, 2)$ (c.f. (18)) at each order. Matrices A_0, A_1 and A_2 become

$$A_0 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}, \; A_1 = \begin{pmatrix} 0 & -2\partial \\ 2\partial & (2-\lambda^2 M_1)\partial \end{pmatrix}, \; A_2 = \begin{pmatrix} 0 & 0 \\ 2\partial^2 & (1-\frac{1}{2}\lambda^2 M_1)\partial^2 \end{pmatrix}. \tag{22}$$

At leading order, the separation of scales, and lack of explicit dependence upon η, leads to $y_0(\eta) = f_0(\eta) Y_0$. The vector Y_0 is defined on the scale of the elementary cell and displacements of the masses are chosen that lead to standing waves:

$$\mathbf{Y}_0 = (1, 0)^T, \qquad \lambda_0^2 = \frac{2}{M_2} \tag{23}$$

and solutions at first and second order lead to the differential eigenvalue problem that determines $f_0(\eta)$ and λ_2^2 as

$$\frac{2}{(M_1 - M_2)} f_{0\eta\eta} + \lambda_2^2 f_0 = 0. \tag{24}$$

For $\alpha = 0$ the Bloch relation yields the local behaviour as $\varepsilon k \to \pi$ that

$$\lambda^2 \sim \frac{2}{M_2} + \frac{(\varepsilon k - \pi)^2}{2(M_1 - M_2)} + \ldots \tag{25}$$

which also follows from expanding the explicit dispersion relation. The main point though is that this is a systematic way of deriving the long-scale behaviour.

One can extend these ideas to non-periodic systems where, say, the masses vary slowly as

$$M_{2n} = M_2(1 + \varepsilon^2 \alpha g(\eta)), \qquad M_{2n+1} = M_1(1 + \varepsilon^2 \alpha g(\eta)) \tag{26}$$

and (24)

$$\frac{2}{(M_1 - M_2)} f_{0\eta\eta} + [\lambda_2^2 + \alpha \lambda_0^2 g(\eta)] f_0 = 0. \tag{27}$$

This is a differential-eigenvalue problem that allows one to identify localized defect states, these are non-zero eigensolutions that exponentially decay at infinity; typically these occur at frequencies within the stop-bands of the perfect system. An example, taken from [7], is shown in Fig. 10. It is notable that the details such as the local oscillation from one mass to the next emerge naturally through the asmyptotic theory. Another nice detail is that the asymptotic ODE is just Schroedinger's equation and so one can take the entire (and considerable) theory from Physics and apply it to show when localised defect tates occur and to find estimates.

Extending all this to two-dimensions (and indeed three) is certainly possible [12; 7] and the asymptotic ODE for f_0 gets replaced by a PDE that captures the long-scale effective anisotropy of the system in its simplest manner.

3 Conclusions

These lectures have concentrated upon the toy system of masses and springs, but the underlying ideas are relevant to continuous periodic, or near periodic, systems [6] and frame structures [13]. One can take any periodic system, not necessarily on a square lattice, and homogenize it to create effective equations that encapsulate the essential physics within just long-scale equations.

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