Lecture 8:
Scattering from an infinite number of obstacles (2)

In the previous lecture we reviewed the basics of wave propagation in periodic media, developing the concept of reciprocal space based on the symmetry properties of the Helmholtz equation. We also introduced a couple of approaches to solving wave propagation in one dimensional periodic media.

Because of the relevance of the theory of periodic media to metamaterials research, we shall spend a second lecture on this topic. Here we'll show how perturbation theory can be applied to understand when a band gap is opened at the Brillouin zone boundary. Following this we'll show a simple semi–analytic method for solving wave propagation problems in arbitrarily complicated periodic media.

1 Band gaps and perturbation theory:

In my opinion one of the main problems with a reliance on numerical modelling is revealed when we tackle the problem of wave propagation in periodic media. Typically we try to solve a wave equation in some complicated geometry that closely models an experiment. The software spits out $\omega(\boldsymbol{K})$ and the best we can do is stare at a graph and some pictures. Unless we have a good deal of prior experience we can just wonder at the magic of COMSOL and go home, having learned nothing about physics. The numerical results are 'too much too soon', because we haven't followed Shockley's advice and taken 'simplest cases first'. We can't hope to get any understanding if we don't break the complicated experiment down into simple parts.

1.1 The empty unit cell:

With this ethos in mind, let's try to build up an understanding of wave propagation in arbitrary periodic media, from the ground up. Where's the simplest place to start? Free space. We'll first consider the dispersion relation of a lattice where the unit cell is empty. You might complain that this is rubbish because free space doesn't have such a periodicity. But this isn't true: *free space has every possible periodicity*, and we're just artificially singling out one of these. We can imagine that what we're doing is taking the limit as the objects making up the lattice are taken to a vanishingly small size, making the scattering so weak that all diffractive features such as band gaps become too small to care about.

Let's assume a periodic structure with lattice vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ and $\boldsymbol{a}_3$. Given this periodicity, the wave satisfies Bloch's theorem

$$\phi(\boldsymbol{x}) = e^{i\,\boldsymbol{K}\cdot\boldsymbol{x}}\phi_{\boldsymbol{K}}(\boldsymbol{x}) \tag{1}$$

where $\phi_{\boldsymbol{K}}(\boldsymbol{x})$ is periodic when the position coordinate is shifted by some multiple of the lattice vectors $\boldsymbol{x} \to \boldsymbol{x} + n\,\boldsymbol{a}_1 + m\,\boldsymbol{a}_2 + p\,\boldsymbol{a}_3$. We can expand this periodic function as a Fourier series

$$\phi_{\boldsymbol{K}}(\boldsymbol{x}) = \sum_{n,m,p} \phi_{n,m,p} e^{i(n\,\boldsymbol{b}_1 + m\,\boldsymbol{b}_2 + p\,\boldsymbol{b}_3)} \tag{2}$$

where the three reciprocal lattice vectors are given by (see lecture 7)

$$\begin{aligned} \boldsymbol{b}_1 &= \frac{2\pi(\boldsymbol{a}_2 \times \boldsymbol{a}_3)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} \\ \boldsymbol{b}_2 &= \frac{2\pi(\boldsymbol{a}_3 \times \boldsymbol{a}_1)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} \\ \boldsymbol{b}_3 &= \frac{2\pi(\boldsymbol{a}_1 \times \boldsymbol{a}_2)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} \end{aligned} \tag{3}$$

where $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}$. Inserting the representation (1) into the free space Helmholtz equation we find the Helmholtz equation for the function $\phi_{\boldsymbol{K}}$

$$\begin{aligned} [\boldsymbol{\nabla}^2 + k_0^2]\phi(\boldsymbol{x}) &= 0 \\ \rightarrow \quad [(\boldsymbol{\nabla} + i\,\boldsymbol{K})^2 + k_0^2]\phi_{\boldsymbol{K}}(\boldsymbol{x}) &= 0. \end{aligned} \tag{4}$$

into which we substitute our Fourier expansion (2)

$$\sum_{n,m,p} \phi_{n,m,p}[-\boldsymbol{K}_{n,m,p}^2 + k_0^2] e^{i(n\,\boldsymbol{b}_1 + m\,\boldsymbol{b}_2 + p\,\boldsymbol{b}_3)} = 0 \tag{5}$$

where $\boldsymbol{K}_{n,m,p} = \boldsymbol{K} + n\,\boldsymbol{b}_1 + m\,\boldsymbol{b}_2 + p\,\boldsymbol{b}_3$. The functions in the sum are orthogonal to one another when integrated over the unit cell. This can be shown quite simply

$$\begin{aligned} \int_{\text{Unit cell}} d^3\boldsymbol{x} e^{i[(n-q)\,\boldsymbol{b}_1 + (m-r)\,\boldsymbol{b}_2 + (p-s)\,\boldsymbol{b}_3]\cdot\boldsymbol{x}} &= V\int_{-1/2}^{1/2} d\zeta \int_{-1/2}^{1/2} d\xi \int_{-1/2}^{1/2} d\chi\, e^{2\pi i[(n-q)\,\zeta + (m-r)\,\xi + (p-s)\chi]} \\ &= V\delta_{nq}\delta_{mr}\delta_{ps} \end{aligned} \tag{6}$$

where I introduced the volume of the unit cell $V = \boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)$ and changed the integration variable $\boldsymbol{x} = x\hat{\boldsymbol{x}} + y\hat{\boldsymbol{y}} + z\hat{\boldsymbol{z}}$ to

$$\boldsymbol{x} = \zeta\boldsymbol{a}_1 + \xi\boldsymbol{a}_2 + \chi\boldsymbol{a}_3 \tag{7}$$

so that the volume element is $d^3\boldsymbol{x} = V d\zeta d\xi d\chi$. The Kronecker deltas on the right hand side of (6) show that the functions are orthogonal. Multiplying (5) by $\exp(-i[q\,\boldsymbol{b}_1 + r\,\boldsymbol{b}_2 + s\,\boldsymbol{b}_3])$ and integrating over a unit cell (using (6)) we find the dispersion relation of free space cut up into a periodic lattice

$$k_0^2 = k_{q,r,s}^2 = \boldsymbol{K}_{q,r,s}^2 \tag{8}$$

and we also find the Fourier components of $\phi_{\boldsymbol{K}}$

$$\phi_{n,m,p} = \delta_{nq}\delta_{mr}\delta_{ps}. \tag{9}$$

Of course, we haven't done anything except view free space in the strange light of a periodic lattice: equation (8) is just the usual $k_0^2 = \boldsymbol{k}^2$, but with the wave–vector $\boldsymbol{k}$ written in a funny way.

So what does (8) tell us? It tells us that the periodicity of the lattice breaks the continuous free–space dispersion relation into discrete bands labelled by the three indices q, r and s. In free space two or more of these bands are joined together at the Brillouin zone boundary, representing the fact that we are wrapping the *continuous* conical dispersion $k_0^2 = \boldsymbol{k}^2$ (that extends out to infinite values of $\boldsymbol{k}$) as a set of discrete bands within a finite region of $\boldsymbol{K}$ space. As soon as we introduce something into the unit cell, the bands will break apart at the zone boundary and propagation becomes forbidden over a range of frequencies (this is the band gap).

This peculiar representation of the free space dispersion relation is far from trivial, and many of the odd features that one sees in periodic media are simply due to this folding of free space into a finite region of $\boldsymbol{K}$ space. In my opinion it is best to understand the empty unit cell of your structure before you do anything else (after all, it's really easy!). In the jupyter notebook that goes with this lecture '*dispersion-empty-unit-cell.ipynb*' you can calculate the dispersion relation in an empty unit cell for any set of lattice vectors, exploring how the dispersion of free space waves can look very weird, just by imposing an artificial periodicity.

1.2 Introducing a refractive index profile into the unit cell:

Having understood how periodicity affects a wave in the absence of anything else, let's consider adding something into the unit cell. The problem of calculating the change in the dispersion relation due to this additional refractive index is very similar to the problem of a spatially varying shift in the potential energy in time independent quantum mechanics. As in that case, to make progress we apply time independent perturbation theory.

We look to solve (4) for the periodic function $\phi_{\boldsymbol{K}}(\boldsymbol{x})$

$$(\boldsymbol{\nabla} + i\,\boldsymbol{K})^2\phi_{\boldsymbol{K}}(\boldsymbol{x}) + k_0^2[1+\chi(\boldsymbol{x})]\phi_{\boldsymbol{K}}(\boldsymbol{x}) = 0 \tag{10}$$

where the refractive index squared is written as $n^2(\boldsymbol{x}) = 1+\chi(\boldsymbol{x})$. We assume that the change in the refractive index is small $\chi \ll 1$ so that we can apply perturbation theory. In what follows we use the set of orthonormal functions given by

$$|n,m,p\rangle = \frac{1}{\sqrt{V}} e^{i(n\,\boldsymbol{b}_1 + m\,\boldsymbol{b}_2 + p\,\boldsymbol{b}_3)} \tag{11}$$

where for simplicity we have used the Dirac bra-ket notation. We have already proved in equation (6) these states are orthonormal

$$\langle q,r,s|n,m,p\rangle = \frac{1}{V}\int_{\text{Unit cell}} d^3\boldsymbol{x} e^{i[(n-q)\,\boldsymbol{b}_1 + (m-r)\,\boldsymbol{b}_2 + (p-s)\,\boldsymbol{b}_3]\cdot\boldsymbol{x}} = \delta_{q,n}\delta_{r,m}\delta_{s,p}.$$

1.2.1 Non–degenerate modes (well separated bands):

Let's consider a mode of the empty unit cell with frequency $k_0 = k_{q,r,s} = |\boldsymbol{K}_{q,r,s}|$. We now ask how this frequency changes after the refractive index $n^2 = 1+\chi$ has been introduced into the unit cell. The wave is written as the mode of the empty unit cell plus some small change $\delta\phi_{\boldsymbol{K}}$

$$\phi_{\boldsymbol{K}}(\boldsymbol{x}) = |q,r,s\rangle + \delta\phi_{\boldsymbol{K}}(\boldsymbol{x}) \tag{12}$$

Writing the frequency k_0 as the value for the empty unit cell κ_0 plus a shift δk_0 due to the presence of the refractive index

$$k_0 = k_{q,r,s} + \delta k_0$$

We find that the Helmholtz equation (10) for $\phi_{\boldsymbol{K}}$ becomes (to leading order in small quantities)

$$(\boldsymbol{\nabla} + i\,\boldsymbol{K})^2\delta\phi_{\boldsymbol{K}}(\boldsymbol{x}) + k_{q,r,s}^2\delta\phi_{\boldsymbol{K}}(\boldsymbol{x}) + 2k_{q,r,s}\delta k_0|q,r,s\rangle + k_{q,r,s}^2\chi(\boldsymbol{x})|q,r,s\rangle = 0 \tag{13}$$

Expanding the change in the wave $\delta\phi_{\boldsymbol{K}}$ as a sum over the functions (11)

$$\delta\phi_{\boldsymbol{K}}(\boldsymbol{x}) = \sum_{\substack{n,m,p \\ \neq q,r,s}} c_{n,m,p}|n,m,p\rangle$$

the Helmholtz equation (13) takes the form

$$\sum_{\substack{n,m,p \\ \neq q,r,s}} (k_{q,r,s}^2 - k_{n,m,p}^2)c_{n,m,p}|n,m,p\rangle + 2k_{q,r,s}\delta k_0|q,r,s\rangle + k_{q,r,s}^2\chi(\boldsymbol{x})|q,r,s\rangle = 0 \tag{14}$$

Performing the inner product on the left by the state $\langle q,r,s|$ we find the shift in the frequency δk_0

$$\delta k_0 = -\frac{k_{q,r,s}}{2}\langle q,r,s|\chi(\boldsymbol{x})|q,r,s\rangle = -\frac{k_{q,r,s}}{2}\frac{1}{V}\int_{\text{Unit cell}} d^3\boldsymbol{x}\,\chi(\boldsymbol{x})$$

which shows that to leading order the frequency of the mode is shifted by the volume average of the change in the refractive index $\chi(\boldsymbol{x}) = n^2(\boldsymbol{x}) - 1$.

Similarly, an inner product on the left of (14) with the state $\langle n, m, p|$ $(n, m, p \neq q, r, s)$ gives us the change in the wave $\delta\phi_{\boldsymbol{K}}$

$$c_{n,m,p} = -k^2_{q,r,s}\frac{\langle n,m,p|\chi(\boldsymbol{x})|q,r,s\rangle}{k^2_{q,r,s} - k^2_{n,m,p}} \rightarrow \delta\phi_{\boldsymbol{K}}(\boldsymbol{x}) = -\sum_{\substack{n,m,p \\ \neq q,r,s}} k^2_{q,r,s}\frac{\langle n,m,p|\chi(\boldsymbol{x})|q,r,s\rangle}{k^2_{q,r,s} - k^2_{n,m,p}}|n,m,p\rangle$$

i.e. the spread of the wave from its original state $|q, r, s\rangle$ into the state $|n, m, p\rangle$ is determined by the ratio of the Fourier components of the refractive index profile $\chi(\boldsymbol{x})$, $\langle n, m, p|\chi(\boldsymbol{x})|q, r, s\rangle$, to the distance in frequency $k^2_{q,r,s} - k_{n,m,p}$. The approximation of $\delta\phi_{\boldsymbol{K}}$ being a small perturbation to the original wave $|q,\ r,\ s\rangle$ is very bad when this ratio takes a large value. This problem is especially severe at values of $\boldsymbol{K}$ close to the Brillouin zone boundary, where two or more of the values of $k_{n,m,p}$ become equal (see the jupyter notebook '*dispersion-empty-unit-cell.ipynb*'). This causes the coefficients $c_{n,m,p}$ to become infinite and our perturbation theory fails. Such a problem is because our periodic system has degeneracies at the zone boundary, forcing us to use *degenerate perturbation theory*.

1.2.2 Degenerate modes (at the zone centre or boundary):

If we want to predict the form of the wave and the dispersion relation for values of $\boldsymbol{K}$ close to the Brillouin zone boundary then we must use *degenerate perturbation theory*. This is because several different modes meet at the zone boundary. As in quantum mechanics, the introduction of the refractive index profile $\chi(\boldsymbol{x})$ will lift this degeneracy, creating a gap (a band gap) between the frequencies of the different modes.

Suppose we have N different modes that meet at the Brillouin zone boundary (all with frequency κ_0). Our above perturbation theory broke down because we implicitly assumed that at the zone boundary the wave was of the form $\phi_{\boldsymbol{K}} = |q, r, s\rangle + \delta\phi_{\boldsymbol{K}}$. However, in this region of $\boldsymbol{K}$ space we have—even for weak variations of the refracive index—a large amount of scattering that couples some of the modes $|n, m, p\rangle$ very strongly: the physics is fundamentally changed when $\boldsymbol{K}$ is close to the Brillouin zone boundary.

Because of this strong coupling at the zone boundary we write $\phi_{\boldsymbol{K}}$ as some linear combination of the N degenerate modes

$$\phi_{\boldsymbol{K}} = \sum_{n=1}^{N} c_n|n\rangle \tag{15}$$

where for brevity the single index n labels the N degenerate modes. We now determine the values of these coefficients c_n. Substituting (15) into (10) (with $k_0 = \kappa_0 + \delta k_0$) and using the fact that for all $|n\rangle$ we have $(\boldsymbol{\nabla} + i\,\boldsymbol{K})^2|n\rangle + k_0^2|n\rangle = 0$, to leading order we have

$$[2\kappa_0\delta k_0 + \kappa_0^2\chi(\boldsymbol{x})]\sum_{n=1}^{N} c_n|n\rangle = 0$$

Taking the inner product of the left hand side with respect to one of the degenerate modes $|m\rangle$

$$-\frac{1}{2}\sum_{n=1}^{N}\langle m|\chi(\boldsymbol{x})|n\rangle c_n = \frac{\delta k_0}{\kappa_0}\,c_m \tag{16}$$

which is simply an eigenvalue equation for the N eigenvectors $\boldsymbol{c} = (c_1,\ c_2,\ ...c_N)$ of the matrix $\boldsymbol{M} = -\frac{1}{2}\langle m|\chi(\boldsymbol{x})|n\rangle$, with eigenvalue $\delta k_0\,/\,\kappa_0$. The eigenvalues $\delta k_0\,/\,\kappa_0$ will in general all be different, indicating that the N modes will be split in frequency by the introduction of the refractive index profile. Thus one generally has a set of gaps in frequency at the Brillouin zone boundary, between the end of one band and the beginning of the next.

1.2.3 Example: a single delta function scatterer in a hexagonal unit cell

I've tried to keep this general so far, so that you can apply the results to any relevant problems you meet. But it's all a bit non–specific—only cowards study the general case. Let's apply the above results to the problem of wave propagation in a 2D hexagonal lattice containing a delta function scatterer in each unit cell.

A 2D hexagonal lattice can be generated from two lattice vectors of equal length, with a relative angle of 60°

$$\begin{aligned}\boldsymbol{a}_1 &= a\hat{\boldsymbol{x}}\\ \boldsymbol{a}_2 &= a[\cos(\pi/3)\hat{\boldsymbol{x}}+\sin(\pi/3)\hat{\boldsymbol{y}}] = a\left[\frac{1}{2}\hat{\boldsymbol{x}}+\frac{\sqrt{3}}{2}\hat{\boldsymbol{y}}\right]\end{aligned}$$

which (using formulae (3)) correspond to the following pair of reciprocal space lattice vectors

$$\begin{aligned}\boldsymbol{b}_1 &= \frac{2\pi}{a}\left[\hat{\boldsymbol{x}}-\frac{1}{\sqrt{3}}\hat{\boldsymbol{y}}\right]\\ \boldsymbol{b}_2 &= \frac{4\pi}{\sqrt{3}a}\hat{\boldsymbol{y}}\end{aligned} \tag{17}$$

When the unit cell is empty the solutions to the Helmholtz equation are simple plane waves

$$\phi(\boldsymbol{x}) = \phi_{\boldsymbol{K}}(\boldsymbol{x})e^{i\,\boldsymbol{K}\cdot\boldsymbol{x}} = \frac{1}{\sqrt{A}}e^{i\,(n\,\boldsymbol{b}_1+m\,\boldsymbol{b}_2)\cdot\boldsymbol{x}}e^{i\,\boldsymbol{K}\cdot\boldsymbol{x}}$$

where A is the area of the unit cell. The frequency of each of these empty–cell modes is given by

$$\kappa_0 = |\boldsymbol{K}+n\,\boldsymbol{b}_1+m\,\boldsymbol{b}_2|$$

Let's now consider values of $\boldsymbol{K}$ that lie on the Brillouin zone boundary. First we need to describe a bit about our Brillouin zone. A hexagonal lattice in real space is also hexagonal in reciprocal space (see the jupyter notebook '*dispersion-empty-unit-cell.ipynb*'), and the Brillouin zone boundary is in the shape of a hexagon. For the reciprocal lattice vectors (17) the centres of the flat sides of this hexagon are at e.g. $\boldsymbol{K}=\boldsymbol{b}_2/2=2\pi/\sqrt{3}a\hat{\boldsymbol{y}}$, and corresponding vectors rotated 60° to this (these are known as the M points on the zone boundary). The corners of the Brillouin zone boundary can be found through breaking up the hexagon into six equilateral triangles with these M points half way along their bases, and the origin of reciprocal space at their tips. We already know the height of each of these triangles is $2\pi/\sqrt{3}a$. Therefore each of the sides of these equilateral triangles has length $\left(2\pi/\sqrt{3}a\right)/\cos(\pi/6) = 4\pi/3a$. The corners of the Brillouin zone are therefore at $\boldsymbol{K}=(4\pi/3a)(\cos(\pi/2-\pi/6)\hat{\boldsymbol{x}}+\sin(\pi/2-\pi/6)\hat{\boldsymbol{y}})$ or

$$\text{Corners of BZ boundary:}\qquad \boldsymbol{K} = \left(\frac{4\pi}{3a}\right)\left(\frac{1}{2}\hat{\boldsymbol{x}}+\frac{\sqrt{3}}{2}\hat{\boldsymbol{y}}\right)\qquad \text{(and vectors at 60° to this)}$$

At one of these corners the frequency of the different modes is given by

$$\begin{aligned}\kappa_0 &= \left|\left(\frac{4\pi}{3a}\right)\left(\frac{1}{2}\hat{\boldsymbol{x}}+\frac{\sqrt{3}}{2}\hat{\boldsymbol{y}}\right)+\frac{2\pi n}{a}\left[\hat{\boldsymbol{x}}-\frac{1}{\sqrt{3}}\hat{\boldsymbol{y}}\right]+\frac{4\pi m}{\sqrt{3}a}\hat{\boldsymbol{y}}\right|\\ &= \frac{2\pi}{a}\left|\left(\frac{1}{3}+n\right)\hat{\boldsymbol{x}}+\left(\frac{1-n+2m}{\sqrt{3}}\right)\hat{\boldsymbol{y}}+\right|\\ &= \frac{2\pi}{a}\sqrt{\left(\frac{1}{3}+n\right)^2+\left(\frac{1-n+2m}{\sqrt{3}}\right)^2}\end{aligned}$$

Considering the $n=0$, $m=0$ mode, we see that there are two other modes with the same frequency $\kappa_0 = 4\pi/3a$ at the corners of the Brillouin zone

$$\begin{array}{cc} n=0 & m=0 \\ n=0 & m=-1 \\ n=-1 & m=-1 \end{array}$$

These three degenerate modes are

$$\begin{aligned} |0\rangle &= \frac{1}{\sqrt{A}} \\ |1\rangle &= \frac{1}{\sqrt{A}} e^{-i\,\boldsymbol{b}_2\cdot\boldsymbol{x}} \\ |2\rangle &= \frac{1}{\sqrt{A}} e^{-i\,(\boldsymbol{b}_1+\boldsymbol{b}_2)\cdot\boldsymbol{x}} \end{aligned}$$

We now consider breaking the degeneracy between these modes through introducing a point scatterer into the unit cell. To be explicit we assume that the function $\chi(\boldsymbol{x}) = n^2(\boldsymbol{x}) - 1$ is proportional to a delta function

$$\chi(\boldsymbol{x}) = \chi_0\, \delta^{(2)}(\boldsymbol{x} - \boldsymbol{x}_0)$$

To understand the effect of this scatterer on the modes of the lattice we apply formula (16) from degenerate perturbation theory, constructing the matrix

$$-\frac{1}{2}\langle m|\chi(\boldsymbol{x})|n\rangle = -\frac{\chi_0}{2A}\begin{pmatrix} 1 & e^{-i\,\boldsymbol{b}_2\cdot\boldsymbol{x}_0} & e^{-i\,(\boldsymbol{b}_1+\boldsymbol{b}_2)\cdot\boldsymbol{x}_0} \\ e^{i\,\boldsymbol{b}_2\cdot\boldsymbol{x}_0} & 1 & e^{-i\,\boldsymbol{b}_1\cdot\boldsymbol{x}} \\ e^{i\,(\boldsymbol{b}_1+\boldsymbol{b}_2)\cdot\boldsymbol{x}_0} & e^{i\,\boldsymbol{b}_1\cdot\boldsymbol{x}} & 1 \end{pmatrix}$$

The eigenvalues and eigenvectors of this matrix give respectively the shift of the frequencies of the three modes due to the scatterer, and the combinations of modes $|0\rangle$, $|1\rangle$ and $|2\rangle$ that must be summed to give the eigenfunctions at this point on the zone boundary. The eigenvalues λ are given by

$$\det\begin{pmatrix} 1+\frac{2A\lambda}{\chi_0} & e^{-i\,\boldsymbol{b}_2\cdot\boldsymbol{x}_0} & e^{-i\,(\boldsymbol{b}_1+\boldsymbol{b}_2)\cdot\boldsymbol{x}_0} \\ e^{i\,\boldsymbol{b}_2\cdot\boldsymbol{x}_0} & 1+\frac{2A\lambda}{\chi_0} & e^{-i\,\boldsymbol{b}_1\cdot\boldsymbol{x}_0} \\ e^{i\,(\boldsymbol{b}_1+\boldsymbol{b}_2)\cdot\boldsymbol{x}_0} & e^{i\,\boldsymbol{b}_1\cdot\boldsymbol{x}_0} & 1+\frac{2A\lambda}{\chi_0} \end{pmatrix} = 0$$

$$\rightarrow \left(1+\frac{2A\lambda}{\chi_0}\right)\left[\left(1+\frac{2A\lambda}{\chi_0}\right)^2 - 1\right] + 2\left[1-\left(1+\frac{2A\lambda}{\chi_0}\right)\right] = 0$$

$$\rightarrow \qquad \left(1+\frac{2A\lambda}{\chi_0}\right)^2 + \left(1+\frac{2A\lambda}{\chi_0}\right) - 2 = 0$$

$$\text{or} \qquad \left(1+\frac{2A\lambda}{\chi_0}\right) = 1$$

so that the frequency shifts of the three modes are given by

$$\lambda = \frac{\delta k_0}{\kappa_0} = \frac{\chi_0}{2A} \times \begin{cases} 0 & \text{Eigenvalue 1} \\ 0 & \text{Eigenvalue 2} \\ -3 & \text{Eigenvalue 3} \end{cases}$$

Meanwhile the corresponding three normalized eigenvectors are

$$\boldsymbol{c} = \begin{cases} \sqrt{\frac{2}{3}} \begin{pmatrix} 1 \\ -\frac{e^{i\,\boldsymbol{b}_2\cdot\boldsymbol{x}_0}}{2} \\ -\frac{e^{i\,(\boldsymbol{b}_1+\boldsymbol{b}_2)\cdot\boldsymbol{x}_0}}{2} \end{pmatrix} & \text{Eigenvector 1} \\ \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ e^{i\,\boldsymbol{b}_2\cdot\boldsymbol{x}_0} \\ -e^{i\,(\boldsymbol{b}_1+\boldsymbol{b}_2)\cdot\boldsymbol{x}_0} \end{pmatrix} & \text{Eigenvector 2} \\ \sqrt{\frac{1}{3}} \begin{pmatrix} 1 \\ e^{i\,\boldsymbol{b}_2\cdot\boldsymbol{x}_0} \\ e^{i\,(\boldsymbol{b}_1+\boldsymbol{b}_2)\cdot\boldsymbol{x}_0} \end{pmatrix} & \text{Eigenvector 3} \end{cases}$$

The form of these three waves at the Brillouin zone boundary is plotted in the jupter notebook "*degenerate-perturbation-theory.ipynb*" that goes with this lecture.

In our results (17) and (17) we have found an approximation to the behaviour of waves in a hexagonal lattice of point scatterers, for the case where $\boldsymbol{K}$ takes a value at the corner of the Brillouin zone. For weak point scatterers we can therefore expect the first three modes to have frequencies

$$k_0 = \frac{4\pi}{3a} + \begin{cases} 0 \\ 0 \\ -\frac{3\chi_0}{2A} \end{cases}$$

Two of the three empty–cell modes is unaffected by the presence of the scatterer, and the third is shifted either above or below the first two, depending on the sign of χ_0. This is a generic feature of lattices with hexagonal symmetry, and we shall return to it when we discuss the honeycomb lattice below. We can understand the lack of any frequency shift for modes 1 and 2 in terms of the spatial form of the eigenmodes (17): the first two modes have nodes at the position of the scatterer and therefore cannot interact with it (see the notebook "*degenerate-perturbation-theory.ipynb*").

2 An accurate soluton for any periodic index profile:

Let's now try to do better than perturbation theory. I'm going to show how to find the form of the wave and $\omega(\boldsymbol{K})$ without any approximations. The catch is that we're going to end up with the problem of finding the eigenvalues and eigenvectors of a big matrix, which we'll have to do numerically. We start from the Helmholtz equation for propagation through a periodic refractive index profile $n(\boldsymbol{x})$

$$[\boldsymbol{\nabla}^2 + k_0^2 n^2(\boldsymbol{x})]\phi(\boldsymbol{x}) = 0 \tag{18}$$

and we use Bloch's theorem (see lecture 7) to write the wave as $\phi(\boldsymbol{x}) = e^{i\,\boldsymbol{K}\cdot\boldsymbol{x}}\phi_{\boldsymbol{K}}(\boldsymbol{x})$. Substituting this form into (18) we obtain the equation governing the behaviour of $\phi_{\boldsymbol{K}}(\boldsymbol{x})$

$$[(\boldsymbol{\nabla} + i\,\boldsymbol{K})^2 + k_0^2 n^2(\boldsymbol{x})]\phi_{\boldsymbol{K}}(\boldsymbol{x}) = 0$$

or equivalently (provided that the refractive index is not zero anywhere)

$$-\frac{1}{n^2(\boldsymbol{x})}(\boldsymbol{\nabla} + i\,\boldsymbol{K})^2\phi_{\boldsymbol{K}}(\boldsymbol{x}) = k_0^2\phi_{\boldsymbol{K}}(\boldsymbol{x}) \tag{19}$$

We now look to solve equation (19). To do this we use the general form of $\phi_{\boldsymbol{K}}(\boldsymbol{x})$ as a sum over the allowed set of waves in reciprocal space (see lecture 7)

$$\phi_{\boldsymbol{K}}(\boldsymbol{x}) = \sum_{n,m,p} \phi_{n,m,p} e^{i(n\,\boldsymbol{b}_1 + m\,\boldsymbol{b}_2 + p\,\boldsymbol{b}_3)\cdot\boldsymbol{x}} \tag{20}$$

The problem is now to determine the coefficients $\phi_{n,m,p}$ and the relationship between ω and $\boldsymbol{K}$ (i.e. between k_0 and $\boldsymbol{K}$). Inserting the expansion (20) into (19)

$$\sum_{n,m,p} \phi_{n,m,p}\boldsymbol{K}_{n,m,p}^2 \frac{1}{n^2(\boldsymbol{x})} e^{i(n\,\boldsymbol{b}_1 + m\,\boldsymbol{b}_2 + p\,\boldsymbol{b}_3)\cdot\boldsymbol{x}} = k_0^2 \sum_{n,m,p} \phi_{n,m,p} e^{i(n\,\boldsymbol{b}_1 + m\,\boldsymbol{b}_2 + p\,\boldsymbol{b}_3)\cdot\boldsymbol{x}}$$

where $\boldsymbol{K}_{n,m,p} = \boldsymbol{K} + n\,\boldsymbol{b}_1 + m\,\boldsymbol{b}_2 + p\,\boldsymbol{b}_3$. Using the orthogonality of the exponentials (6) we can write this as

$$\sum_{n,m,p} \phi_{n,m,p}\boldsymbol{K}_{n,m,p}^2 \frac{1}{V}\int_{\text{Unit cell}} d^3\boldsymbol{x} \frac{1}{n^2(\boldsymbol{x})} e^{i[(n-q)\,\boldsymbol{b}_1 + (m-r)\,\boldsymbol{b}_2 + (p-s)\,\boldsymbol{b}_3]\cdot\boldsymbol{x}} = k_0^2\phi_{q,r,s}$$

which is of the form matrix$\times\phi = k_0^2\phi$ which is a standard eigenvalue problem. To simplify the form of this eigenvalue problem we redefine our eigenvectors $\phi_{n,m,p}$ so that the matrix is Hermitian when $n^2(\boldsymbol{x})$ is real valued, i.e. we introduce the quantities $v_{n,m,p}$

$$v_{n,m,p} \quad = \phi_{n,m,p}|\boldsymbol{K}_{n,m,p}|$$

and the matrix $M_{q,r,s;n,m,p}$

$$M_{q,r,s;n,m,p}(\boldsymbol{K}) \;\; = |\boldsymbol{K}_{n,m,p}||\boldsymbol{K}_{q,r,s}|\frac{1}{V}\int_{\text{Unit cell}} d^3\boldsymbol{x} \frac{1}{n^2(\boldsymbol{x})} e^{i[(n-q)\,\boldsymbol{b}_1 + (m-r)\,\boldsymbol{b}_2 + (p-s)\,\boldsymbol{b}_3]\cdot\boldsymbol{x}}$$

so that our problem becomes one of simply finding the eigenvalues and eigenvectors of the Hermitian matrix $\boldsymbol{M}$:

$$\sum_{n,m,p} M_{q,r,s;n,m,p}(\boldsymbol{K})\; v_{n,m,p} \; = k_0^2\; v_{q,r,s} \tag{21}$$

This equation may look a bit odd because we have these triple of indices n, m, p. How then is it equivalent to an ordinary problem involving matrices? To make this into an ordinary matrix problem we simply 'flatten' the three indices into a single one. For eaxmple if each index ranges between $-N$ and N then we can replace n, m, p with the single index $q = (n+N) + (m+N)(2\,N + 1) + (p+N)(\,2N+1)^2$ which ranges from 0 to $(2N+1)^3 - 1$. Doing this 'flattening' operation we find that (21) simplifies to

$$\sum_{n,m,p} M_{q;n}(\boldsymbol{K})\; v_n \; = k_0^2\; v_q$$

or

$$\boldsymbol{M}(\boldsymbol{K}) \cdot \boldsymbol{v} = k_0^2 \boldsymbol{v}$$

Therefore the eigenvalues of the Hermitian matrix $\boldsymbol{M}(\boldsymbol{K})$ give the frequencies (squared) of the various bands in the periodic medium, and the eigenvectors give the Fourier components of the solution. This is known as the plane wave expansion method of solving problems in periodic media. It can be a bit slow compared to some more optimized techniques, but it is simple and has a simple physical interpretation. In the notebook that goes with this lecture "*plane-wave-expansion-solution.ipynb*", this method is implemented in two dimensions.