Lecture 7: Scattering from an infinite number of obstacles (1)

In the previous lecture we discussed the scattering of a wave from a single obstacle, focussing on the Born approximation. The next problem in order of difficulty is not scattering from two or three obstacles, but scattering from an *infinite* number of objects that are arranged into a periodic lattice. This is the subject of this lecture and the next. The reason this is a comparatively simple problem has its origins in *Bloch's theorem*, which we shall briefly review. This result reduces the problem of understanding the interaction with an infinite lattice of objects, to a slightly complicated version of the interaction with a single object.

A typical 'metamaterial' is a periodic arrangement of scatterers, with the effective medium properties (e.g. the refractive index, the bulk modulus, the permittivity) emerging in the limit where the spacing between the scatterers is much smaller than the spatial period of the wave. Because of the relevance to metamaterials, we'll devote two lectures to wave propagation in periodic structures. In this first lecture we'll focus on some simple examples in one dimension.

1 Bloch's theorem—how symmetry makes life easier:

The reason that wave propagation through an infinite lattice of scatterers is much simpler to understand than say the interaction with (say) ten scatterers is one of symmetry. The lattice has a discrete translational symmetry (the operation of moving the lattice by one spatial period), whereas there is no such symmetry for arrangements of a few objects. We'll start by explaining how one can use symmetry to make progress towards solving the wave equation (or the Helmholtz equation), even in quite complicated systems.

1.1 Symmetry groups:

Suppose we have a system where some operation $\hat{T}$ leaves the system unchanged. For example, if our system has translational symmetry then $\hat{T}$ is a shift of the spatial coordinates by any distance a, and the result of $\hat{T}$ acting on the wave ϕ would be $\hat{T}_a\phi(x)=\phi(x+a)$ (I use a subscript on the $\hat{T}$ to distinguish between the different symmetry operations). Similarly, if the system has n–fold rotational symmetry around the z–axis then $\hat{T}$ is a rotation of the coordinate system by $2\pi/n$ and changes the wave to $\hat{T}_{\frac{2\pi}{n}}\phi(r,\theta,z)=\phi(r,\theta+2\pi/n,z)$.

Now let's see what we can use these symmetry operators $\hat{T}$ for. Consider the wave equation in some general material described by a spatially varying refractive index $n(\boldsymbol{x})$. Ignoring the effects of dispersion (see lecture 3) the wave equation takes the form

$$\left[\boldsymbol{\nabla}^2-\frac{n^2(\boldsymbol{x})}{c^2}\frac{\partial^2}{\partial t^2}\right]\phi(\boldsymbol{x},t)=0 \tag{1}$$

At the moment the only symmetry this system has is that it looks the same at all times. If we change the time coordinate by a infinitesimal amount δt then the system looks identical (infinitesimal because any time translation can be built out of many small translations). Performing such a translation on equation (1) we find

$$\begin{aligned}\hat{T}_{\delta t}\left[\boldsymbol{\nabla}^2-\frac{n^2(\boldsymbol{x})}{c^2}\frac{\partial^2}{\partial t^2}\right]\phi(\boldsymbol{x},t) &=\left[\boldsymbol{\nabla}^2-\frac{n^2(\boldsymbol{x})}{c^2}\frac{\partial^2}{\partial t^2}\right]\hat{T}_{\delta t}\phi(\boldsymbol{x},t)\\ &=\left[\boldsymbol{\nabla}^2-\frac{n^2(\boldsymbol{x})}{c^2}\frac{\partial^2}{\partial t^2}\right]\phi(\boldsymbol{x},t+\delta t)\\ &=0\end{aligned} \tag{2}$$

where the symmetry operator $\hat{T}_{\delta t}$ could be taken to the right of the operator in the square brackets because nothing in the square brackets depends on the value of the time coordinate t (which is another way of saying the system looks the same at all times). What equation (2) tells us is that both $\phi(\boldsymbol{x},t)$ and $\phi(\boldsymbol{x},t+\delta t)$ are solutions to the same wave equation, for any value of δt. Because there is no explicit time dependence in the wave operator, we free to choose the time dependence of ϕ, so long as (2) holds. We make this choice such that $T_{\delta t}\phi(\boldsymbol{x},t)$ is proportional to $\phi(\boldsymbol{x},t)$: i.e. we choose the time dependence such that ϕ is an eigenfunction of the symmetry operator

$$\hat{T}_{\delta t}\phi(\boldsymbol{x},t)=\lambda\phi(\boldsymbol{x},t) \tag{3}$$

Having made this choice (2) is automatically satisfied. What are the eigenfunctions of the time translation operator? Given that δt is infinitesimal, the time translation is $\phi(\boldsymbol{x},t+\delta t)=\phi(\boldsymbol{x},t)+\delta t\partial\phi(\boldsymbol{x},t)/\partial t$, and (3) is equivalent to

$$\left(1+\delta t\frac{\partial}{\partial t}\right)\phi(\boldsymbol{x},t)=\lambda\phi(\boldsymbol{x},t)\rightarrow\frac{\partial\phi(\boldsymbol{x},t)}{\partial t}=\frac{1}{\delta t}(\lambda-1)\phi(\boldsymbol{x},t) \tag{4}$$

which has the solution (labelled by ω)

$$\phi(\boldsymbol{x},t)=\phi_{\omega}(\boldsymbol{x})e^{-i\omega t} \tag{5}$$

where I wrote $\lambda=1-i\omega\delta t$. In other words the harmonic time dependence we often assume, that turns the wave equation into the Helmholtz equation is equivalent to choosing a set of solutions (labelled by the frequency ω) that are eigenfunctions of the time translation operator.

An analogous argument also applies when a system has spatial translation symmetry (i.e. if the refractive index in (2) is independent of one or more of the spatial coordinates, but now possibly depends on time). Then we can choose $\phi(\boldsymbol{x},t)$ such that it is an eigenfunction of infinitesimal spatial translations $\boldsymbol{x}\rightarrow\boldsymbol{x}+\delta x\hat{\boldsymbol{n}}$ (where $\hat{\boldsymbol{n}}$ is a unit vector in some direction where the system doesn't change)

$$(1+\delta\boldsymbol{x}\cdot\boldsymbol{\nabla})\phi(\boldsymbol{x},t)=\lambda\phi(\boldsymbol{x},t)\rightarrow\hat{\boldsymbol{n}}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x},t)=\frac{1}{\delta x}(\lambda-1)\phi(\boldsymbol{x},t) \tag{6}$$

which has solutions (labelled by k)

$$\phi(\boldsymbol{x},t)=\phi_{k}(\overline{\boldsymbol{x}},t)e^{ik\hat{\boldsymbol{n}}\cdot\boldsymbol{x}} \tag{7}$$

where I wrote $\lambda=1+ik\delta x$, and $\overline{\boldsymbol{x}}$ are all the coordinates orthogonal to the symmetry direction $\hat{\boldsymbol{n}}$ (for example if $\hat{\boldsymbol{n}}$ points along $\hat{\boldsymbol{x}}$ then $\overline{\boldsymbol{x}}=y\,\hat{\boldsymbol{y}}+z\,\hat{\boldsymbol{z}}$). Again, we are familiar with choosing an $\exp(i\,\boldsymbol{k}\cdot\boldsymbol{x})$ dependence for our field in cases where we have translational symmetry, but perhaps are not aware that we are doing this so that each of the waves in the system is an eigenfunction of the symmetry operator $\hat{T}$. Of course the above examples are rather basic, but the same approach can be used for other more complicated symmetries.

The symmetry operators $\hat{T}$ that we have introduced form something mathematicians call a *group*, and the study of their properties is known as *group theory*. As far as a mathematician is concerned, a group is an abstract set of elements (for example the set of elements in our case could be all the $\hat{T}$ operators for translations along the x axis) obeying the following rules:

1. **The product of any two elements in the set equals another element in the set** (e.g. a translation by distance a followed by a translation by a distance b is the same as a single translation by a distance $a+b$).

2. **The elements obey the law of association** $\left(\hat{T}_a\hat{T}_b\right)\hat{T}_c=\hat{T}_a\left(\hat{T}_b\hat{T}_c\right)$ (e.g. for translation we'll get $\hat{T}_{a+b+c}$, however we evaluate the product).

3. **In the set there is an identity element I that leaves all elements in the set unchanged** (e.g. for the case of translation this is the operator corresponding to translation by zero distance: $\hat{T}_0 = I$, and $\hat{T}_0\hat{T}_a = \hat{T}_a\hat{T}_0 = \hat{T}_a$).

4. **For every element in the set $\hat{T}_a$ there is an inverse $\hat{T}_a^{-1}$, such that $\hat{T}_a\hat{T}_a^{-1} = I$** (e.g. for the case of translation this is translation by the negative of the original distance $\hat{T}_a\hat{T}_{-a} = I$)

As mathematicians have been studying this abstract notion of groups for a long time, they know a lot about their properties. Having realised that the symmetry operations of physics are actually groups, we can therefore use these hard–won results to help us solve the problems of physics. This general approach (using group theory to study symmetry) has been very successful in physics and forms the basis of our current theories of the strong and weak nuclear force (first it was recognised that Maxwell's equations could be understood as a particular symmetry of the wave–function, and the generalization of the groups of this symmetry led to the theories of the strong and weak nuclear force). For more information about group theory I recommend the chapter in Arfken and Weber as well as "*Group theory and quantum mechanics*" by M. Tinkham (see references at the end of lecture 1).

Before moving on to Bloch's theorem we should note that in the above cases we are dealing with *continuous symmetry groups*. That is, the symmetry is one where—for example—we can translate by any distance however big or small. There are also *discrete symmetry groups*, where there are only a finite number of operations that leave the system unchanged.

For example, consider a two dimensional system where we have a refractive index profile $n(\boldsymbol{x})$ that is invariant under rotations by an angle $2\pi/N$ (N–fold symmetry—this symmetry group is known as C_N). Suppose we expand the solution to the Helmholtz equation as a sum of waves with an $\exp(in\theta)$ dependence (any function can be expanded like this)

$$\phi(r,\theta) = \sum_{n=-\infty}^{\infty} c_n(r)e^{in\theta} \tag{8}$$

We now require ϕ to be an eigenfunction of the symmetry operation $\theta \to \theta + 2\pi/N$. This is equivalent to demanding that

$$\phi(r,\theta+2\pi/N) = \sum_{n=-\infty}^{\infty} c_n(r)e^{in\theta}e^{\frac{2\pi i n}{N}} = \lambda\sum_{n=-\infty}^{\infty} c_n(r)e^{in\theta} \tag{9}$$

In general we can only do this if we restrict the possible value of n in the sum (8) to

$$n = m + pN$$

where m is any fixed integer, and the summation now runs over p. With these values of n, the eigenvalue λ appearing in (9) is labelled by m and equals $\exp(2\pi i m/N)$. The eigenfunctions of the symmetry operator for rotations by $2\pi/N$ thus take a form analogous to that of the continuous symmetries (7)

$$\phi(r,\theta) = e^{im\theta}\sum_{p=-\infty}^{\infty} c_p(r)e^{ipN\theta} = e^{im\theta}\phi_m(r,\theta) \tag{10}$$

where ϕ_m is invariant under a rotation by $2\pi/N$. We have thus established the form of the solution to the Helmholtz equation in a system with N–fold symmetry through finding the eigenfunctions of the symmetry group.

1.2 Bloch's theorem

In a system where we have a periodic array of objects that can scatter waves, we also have a discrete symmetry group. In general this is a symmetry under translation by any multiple of three possible lattice vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ or $\boldsymbol{a}_3$ (e.g. in a cubic lattice with lattice spacing a these would be $\boldsymbol{a}_1 = a\hat{\boldsymbol{x}}$, $\boldsymbol{a}_2 = a\hat{\boldsymbol{y}}$ and $\boldsymbol{a}_3 = a\hat{\boldsymbol{z}}$). Our symmetry operation is thus

$$\hat{T}_{n,m,p}\phi(\boldsymbol{x}) = \phi(\boldsymbol{x} + n\,\boldsymbol{a}_1 + m\,\boldsymbol{a}_2 + p\,\boldsymbol{a}_3) \tag{11}$$

Again we look for eigenfunctions of this symmetry operation. To do this we expand ϕ as a Fourier integral

$$\phi(\boldsymbol{x}) = \int \frac{d^3\boldsymbol{k}}{(2\pi)^3}\tilde{\phi}(\boldsymbol{k})e^{i\,\boldsymbol{k}\cdot\boldsymbol{x}} \tag{12}$$

inserting (12) into (11) we require

$$\hat{T}_{n,m,p}\phi(\boldsymbol{x}) = \int \frac{d^3\boldsymbol{k}}{(2\pi)^3}\tilde{\phi}(\boldsymbol{k})e^{i\,\boldsymbol{k}\cdot(\boldsymbol{x}+n\,\boldsymbol{a}_1+m\,\boldsymbol{a}_2+p\,\boldsymbol{a}_3)} = \lambda\phi(\boldsymbol{x})$$

The only way to achieve this is if we restrict the allowed values of $\boldsymbol{k}$ to

$$\boldsymbol{k} = \boldsymbol{K} + \frac{2\pi q(\boldsymbol{a}_2\times\boldsymbol{a}_3)}{\boldsymbol{a}_1\cdot(\boldsymbol{a}_2\times\boldsymbol{a}_3)} + \frac{2\pi r(\boldsymbol{a}_3\times\boldsymbol{a}_1)}{\boldsymbol{a}_1\cdot(\boldsymbol{a}_2\times\boldsymbol{a}_3)} + \frac{2\pi s(\boldsymbol{a}_1\times\boldsymbol{a}_2)}{\boldsymbol{a}_1\cdot(\boldsymbol{a}_2\times\boldsymbol{a}_3)} = \boldsymbol{K} + \boldsymbol{k}_{q,r,s} \tag{13}$$

so that the field becomes a sum over discrete values of wave–vector

$$\phi(\boldsymbol{x}) = e^{i\,\boldsymbol{K}\cdot\boldsymbol{x}}\sum_{p,q,r}\phi_{p,q,r}e^{i\,\boldsymbol{k}_{p,q,r}\cdot\boldsymbol{x}} = e^{i\,\boldsymbol{K}\cdot\boldsymbol{x}}\phi_{\boldsymbol{K}}(\boldsymbol{x}). \tag{14}$$

where $\phi_{\boldsymbol{K}}$ is periodic under any translation by a multiple of the lattice vectors. The three vectors appearing in this sum

$$\begin{aligned}\boldsymbol{b}_1 &= \frac{2\pi(\boldsymbol{a}_2\times\boldsymbol{a}_3)}{\boldsymbol{a}_1\cdot(\boldsymbol{a}_2\times\boldsymbol{a}_3)}\\ \boldsymbol{b}_2 &= \frac{2\pi(\boldsymbol{a}_3\times\boldsymbol{a}_1)}{\boldsymbol{a}_1\cdot(\boldsymbol{a}_2\times\boldsymbol{a}_3)}\\ \boldsymbol{b}_3 &= \frac{2\pi(\boldsymbol{a}_1\times\boldsymbol{a}_2)}{\boldsymbol{a}_1\cdot(\boldsymbol{a}_2\times\boldsymbol{a}_3)}\end{aligned} \tag{15}$$

are known as the *reciprocal lattice vectors*. The periodicity in real space automatically implies that the Fourier transform of ϕ only contains discrete values of wave–vector $\boldsymbol{k}$, also on a lattice, and spaced by multiples of the three reciprocal lattice vectors (15). In the Jupyter notebook "*the-reciprocal-lattice.ipynb*" you can play with the relationship between two dimensional real and reciprocal space lattices, choosing any two real space vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$.

The above form of the wave in a periodic medium (14) is known as *Bloch's theorem*, and is the statement that in a periodic medium the solutions can be written as a periodic function $\phi_{\boldsymbol{K}}$ times a phase factor $\exp(i\,\boldsymbol{K}\cdot\boldsymbol{x})$ (note the similarity between this and the discrete rotational symmetry (10)). If we substitute the form of the wave (14) into the Helmholtz equation within a periodic refractive index profile

$$[\boldsymbol{\nabla}^2 + k_0^2n^2(\boldsymbol{x})]\phi(\boldsymbol{x}) = 0 \tag{16}$$

we find a modified Helmholtz equation

$$[(\boldsymbol{\nabla} + i\,\boldsymbol{K})^2 + k_0^2n^2(\boldsymbol{x})]\phi_{\boldsymbol{K}}(\boldsymbol{x}) = 0 \tag{17}$$

Typically we solve this equation (within a single unit cell of the periodic lattice, imposing periodic boundary conditions at the boundaries of the cell) to determine the frequency k_0 as a function of $\boldsymbol{K}$, thus finding how waves propagate through the periodic medium.

Note that changing the value of $\boldsymbol{K}$ in (17) only corresponds to distinct eigenfunctions of the translation operator for values of $\boldsymbol{K}$ which cannot be transformed into one another through translation by a reciprocal lattice vector $\boldsymbol{K}\rightarrow\boldsymbol{K}+j\,\boldsymbol{b}_1+k\,\boldsymbol{b}_2+l\,\boldsymbol{b}_3$. This is because a translation by a reciprocal lattice vector can always be subsumed into the function $\phi_{\boldsymbol{K}}$, and thus the value of $\boldsymbol{K}$ is only defined up to a multiple of the three reciprocal lattice vectors. These distinct values of $\boldsymbol{K}$ form what is known as the *first Brillouin zone*.

2 Scattering from a 1D array of delta functions:

You may have met this example before (it is known as the Kronig–Penney model), but I think it is worth repeating. It is probably the simplest exactly solvable model of wave propagation through a periodic medium and illustrates most of the important physical phenomena that occur in a periodic medium. In one dimension the first Brillouin zone is simple and is for the range of K values $[-\pi/a,\pi/a]$.

We consider the 1D Helmholtz equation for a wave propagating through a infinite series of delta function scatterers (of strength α) spaced by a distance a

$$\frac{d^2\phi}{dx^2}+k_0^2\left[1+\alpha\sum_{n=-\infty}^{\infty}\delta(x-na)\right]\phi=0 \tag{18}$$

We can solve this using the Green function, first taking the sum of delta functions over to the right hand side of this equation

$$\frac{d^2\phi}{dx^2}+k_0^2\phi=-k_0^2\alpha\sum_{n=-\infty}^{\infty}\delta(x-na)\phi(na) \tag{19}$$

Applying the 1D version of Bloch's theorem (14), $\phi(na)=e^{iKna}\phi(0)$ and using the one dimensional Green function we can solve (19) in one step

$$\phi(x)=-k_0^2\alpha\phi(0)\sum_{n=-\infty}^{\infty}G(x-na)e^{iKna} \tag{20}$$

2.1 The dispersion relation:

In order that this equation be self consistent we must have

$$\phi(0)=-k_0^2\alpha\phi(0)\sum_{n=-\infty}^{\infty}G(-na)e^{iKna}\rightarrow 1+k_0^2\alpha\sum_{n=-\infty}^{\infty}G(-na)e^{iKna}=0$$

which is the dispersion relation connecting k_0 and K. The sum is a bit awkward to use, so we insert the expression for the 1D Green function (lecture 2)

$$G(x-x')=\frac{e^{ik_0|x-x'|}}{2ik_0} \tag{21}$$

and evaluate the sum as a pair of geometric series

$$1+\frac{k_0\alpha}{2i}\sum_{n=-\infty}^{\infty}e^{ik_0|na|}e^{iKna}=1+\frac{k_0\alpha}{2i}\left[\sum_{n=0}^{\infty}e^{i(K+k_0)na}+\sum_{n=-\infty}^{-1}e^{i(K-k_0)na}\right]=0 \tag{22}$$

To evaluate the series we imagine taking the limit of zero loss, inserting factors of $i\eta$ to make the sums vanish at the limits,

$$\begin{aligned}\sum_{n=0}^{\infty} e^{i\,(K+k_0+i\eta)\,n\,a} &= \frac{1}{1-e^{i\,(K+k_0+i\eta)a}} \\ \sum_{n=-\infty}^{-1} e^{i(K-k_0-i\eta)\,n\,a} &= \frac{-1}{1-e^{i(K-k_0-i\eta)\,a}}\end{aligned} \tag{23}$$

which simplifies the dispersion relation to

$$1+\frac{k_0\alpha}{2i}\left[\frac{1}{1-e^{i\,(K+k_0)a}}-\frac{1}{1-e^{i(K-k_0)\,a}}\right]=0$$

which after a few steps becomes

$$\cos(Ka)=\cos(k_0a)-\frac{k_0\alpha}{2}\sin(k_0a) \tag{24}$$

This is the exact dispersion relation that relates the wave–vector and the frequency in an infinite 1D lattice of point scatterers. As mentioned at the outset in quantum mechanics this is known as the *Kronig–Penney model*, but as we've seen many times, this is a model that can be applied in many areas of wave physics. The dispersion relation (24) is plotted in the notebook associated with this lecture "*1d-lattice-of-scatterers.ipynb*".

The modulus of the right hand side of (24) is not restricted to be less than unity. In the regions of frequency where the right hand side has a modulus greater than unity there is only a solution for complex values of K. In these regions of frequency the wave is extinguished as it progresses through the material; the strong reflection from the lattice inhibits propagation. This region of frequency is known as a *band gap* or sometimes a *stop band*. Note that depending on the sign of the right hand side of (24), the real part of this complex value of K is either 0 or $\pm\pi/a$; i.e. the complex value of K starts from either the centre of the Brillouin zone, or the edges.

2.2 The group velocity:

We can also use (24) to calculate the group velocity of a wave propagating through such a system, differentiating with respect to k_0

$$\begin{aligned}&\frac{dK}{dk_0}\sin(Ka)=-\left[\sin(k_0a)+\frac{k_0\alpha}{2}\cos(k_0a)\right]\\ \rightarrow\ &\frac{d\omega}{dK}=-\frac{c\sin(Ka)}{\sin(k_0a)+\frac{k_0\alpha}{2}\cos(k_0a)}\\ \rightarrow\ &\frac{d\omega}{dK}=-\frac{c\sqrt{1-\left[\cos(k_0a)-\frac{k_0\alpha}{2}\sin(k_0a)\right]^2}}{\sin(k_0a)+\frac{k_0\alpha}{2}\cos(k_0a)}\end{aligned} \tag{25}$$

Notice that when $K=0,\pm\pi/a$ (which is the Brillouin zone boundary or the centre of the zone in 1D) the group velocity vanishes. This is a generic feature of propagation when K is at the centre of the zone, or the zone boundary; no power can propagate in the direction of strong scattering.

2.3 Summing the series to simplify the solution:

Just as we summed the infinite series (22) to obtain the dispersion relation in our 1D lattice, we can also sum the series (20) to simplify the solution $\phi(x)$. Inserting the expression for the 1D Green function (21) and restricting x to lie in a unit cell $x\in[-a/2,a/2]$ the solution to the Helmholtz equation can be written as

$$\phi(x)=-\frac{k_0\alpha}{2i}\left[e^{ik_0|x|}+e^{-ik_0x}\sum_{n=1}^{\infty}e^{i\,(K+k_0)na}+e^{ik_0x}\sum_{n=-\infty}^{-1}e^{i\,(K-k_0)\,na}\right]$$

(I set the arbitrary value $\phi(0)=1$) which contains the same sums we faced before (23). Inserting these previous results, the above expression for the field can be reduced to

$$\phi(x)=\frac{ik_0\alpha}{2}\left[e^{ik_0|x|}+e^{-ik_0x}\frac{e^{i\,(K+k_0)a}}{1-e^{i\,(K+k_0)a}}+e^{ik_0x}\frac{e^{i(k_0-K)\,a}}{1-e^{i(k_0-K)\,a}}\right] \tag{26}$$

The three terms in the square brackets have a simple physical interpretation. The first is the wave scattered by the delta that lies within the unit cell centred around the origin; the second is the wave scattered by all of the objects to the right of the origin (resulting in a left going reflected wave); and the third is the wave scattered by all the objects to the left of the origin (resulting in a right going reflected wave). Notice that when $K=0$ or $K=\pm\pi/a$ the amplitudes of the waves coming from the left hand and right hand half of the lattice (the second and thrid terms in the square brackets) are equal. This indicates that there is no net power flow in either direction, as we expect from the vanishing group velocity (25). You can explore the dependence of this solution on the strength of the scatterers α and the frequency in the notebook associated with this lecture "*1d-lattice-of-scatterers.ipynb*".

3 Band structure and the transfer matrix:

A more general way to find the dispersion relation between the frequency ω and the Bloch vector K in a 1D system is to construct something known as the transfer matrix. This object connects the wave amplitudes on the left and on the right of any unit cell and contains all the information about wave propagation through the system.

To motivate the introduction of the transfer matrix suppose we have some periodic variation of the refractive index $n(x)$ and we want to solve the Helmholtz equation

$$\frac{d^2\phi}{dx^2}+k_0^2n^2(x)\phi=0$$

Say the spatial period is a, so that we can forget about nearly all of the medium, and focus on a unit cell $x\in[-a/2,a/2]$. Without changing the physics we can imagine that at the two edges of the unit cell we introduce fictional layers of infinitesimal width where the medium is locally homogeneous (the refractive index of these fictional layers equals the index at the edge of the unit cell $n(\pm a/2)$). Within these homogeneous layers the wave takes the form

$$\phi=\begin{cases}A_L\,e^{in(-a/2)\,k_0(x+a/2)}+B_Le^{-in(-a/2)k_0(x+a/2)} & \text{left hand layer}\\ A_R\,e^{in(a/2)\,k_0(x-a/2)}+B_Re^{-in(a/2)k_0(x-a/2)} & \text{right hand layer}\end{cases}$$

The transfer matrix $\boldsymbol{T}$ connects the amplitudes on the right (A_R and B_R) to those on the left (A_L and B_L) of the unit cell

$$\begin{pmatrix}A_R\\B_R\end{pmatrix}=\begin{pmatrix}T_{11}&T_{12}\\T_{21}&T_{22}\end{pmatrix}\begin{pmatrix}A_L\\B_L\end{pmatrix} \tag{27}$$

The elements of the transfer matrix T_{ij} are functions of the refractive index profile within the unit cell and the frequency of the wave k_0. We can write (27) more compactly as

$$\boldsymbol{\phi}_R = \boldsymbol{T} \cdot \boldsymbol{\phi}_L$$

Of course, at the moment we don't know the elements of the matrix $\boldsymbol{T}$ but we'll come to that. If the medium is periodic with spatial period a then from Bloch's theorem (14) we know that $\boldsymbol{\phi}_R = \boldsymbol{\phi}_L e^{iKa}$. Therefore

$$\boldsymbol{T} \cdot \boldsymbol{\phi}_L = e^{iKa} \boldsymbol{\phi}_L \tag{28}$$

which implies that the eigenvectors of the transfer matrix are the combinations of left and right–going waves making up the solution ϕ, and the eigenvalues of the transfer matrix tell us relationship between K and k_0. Because $\boldsymbol{T}$ is a 2×2 matrix these eigenvalues and eigenvectors are easy to find. The eigenvalues are given by the condition that $\det(\boldsymbol{T} - e^{iKa}\mathbf{1}) = 0$,

$$\begin{aligned}\det\begin{pmatrix} T_{11} - e^{iKa} & T_{12} \\ T_{21} & T_{22} - e^{iKa} \end{pmatrix} &= (T_{11} - e^{iKa})(T_{22} - e^{iKa}) - T_{12}T_{21} \\ &= \det(\boldsymbol{T}) - \mathrm{Tr}[\boldsymbol{T}]e^{iKa} + e^{2iKa} \\ &= 0\end{aligned}$$

which is a quadratic equation in e^{iKa} with the solution

$$e^{iKa} = \frac{\mathrm{Tr}[\boldsymbol{T}]}{2} \pm \sqrt{\left(\frac{\mathrm{Tr}[\boldsymbol{T}]}{2}\right)^2 - \det(\boldsymbol{T})} \tag{29}$$

This is the general expression connecting K to k_0 in one dimension: if we know the transfer matrix then we know the dispersion relation. The two possible signs correspond to left or right–going propagation through the lattice. In cases where the modulus of the right hand side is smaller or larger than unity, the value of K is complex and the propagation through the lattice will be damped. When the medium is lossless, these regions of frequency where K is complex are the band gaps already mentioned in the section on the lattice of delta function scatterers.

3.1 The elements of the transfer matrix:

We have a general expression for the dispersion relation in a 1D periodic medium (29). But clearly the problem is now shifted to that of finding the transfer matrix. For a continuously varying $n(x)$, one option is to split the unit cell up into N strips of homogeneous refractive index n_i (approximating the continuous function $n(x)$). We can then calculate the transfer matrix for the whole unit cell as the product of the many different matrices each associated with crossing between neighbouring layers $\boldsymbol{T}_{i\to i+1}$

$$\boldsymbol{T} = \boldsymbol{T}_{N-1\to N} \ldots \boldsymbol{T}_{1\to 2} \cdot \boldsymbol{T}_{0\to 1} = \prod_{i=0}^{N-1} \boldsymbol{T}_{i\to i+1}$$

This procedure is done in detail, and the derivation of the individual $T_{i\to i+1}$ is given in the notebook "*bragg-mirror.ipynb*" that goes with this lecture.

We can also find the elements of $\boldsymbol{T}$ if we know the reflection and transmission coefficients for a single unit cell: i.e. if one unit cell was placed in a homogeneous background medium of refractive index n_b (equal to the index at the boundaries of the unit cell), then what are its reflection and transmission properties? If we know these then we know the elements of the transfer matrix.

To see how they are related consider a wave of unit amplitude incident from the left. On the left and the right of the unit cell the wave has the form (r_L and t_L are the reflection and transmission coefficients for incidence from the left)

$$\phi = \begin{cases} e^{in_b k_0(x+a/2)} + r_L e^{-in_b k_0(x+a/2)} & \text{left hand side} \\ t_L e^{in_b k_0(x-a/2)} & \text{right hand side} \end{cases}$$

which means that

$$\begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} 1 \\ r_L \end{pmatrix} = \begin{pmatrix} t_L \\ 0 \end{pmatrix} \tag{30}$$

Similarly for a wave incident from the right (r_R and t_R are the reflection and transmission coefficients for incidence from the right)

$$\phi = \begin{cases} t_R e^{-in_b k_0(x+a/2)} & \text{left hand side} \\ r_R e^{in_b k_0(x+a/2)} + e^{-in_b k_0(x+a/2)} & \text{right hand side} \end{cases}$$

implying that

$$\begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} 0 \\ t_R \end{pmatrix} = \begin{pmatrix} r_R \\ 1 \end{pmatrix} \tag{31}$$

Combining (30) and (31) we find that

$$\begin{aligned} T_{11} &= \frac{t_L t_R - r_L r_R}{t_R} \\ T_{12} &= \frac{r_R}{t_R} \\ T_{21} &= -\frac{r_L}{t_R} \\ T_{22} &= \frac{1}{t_R} \end{aligned} \tag{32}$$

Most 'normal' materials that can be characterized in terms of a simple refractive index $n(x)$ are reciprocal, meaning that transmission from left to right is the same as from right to left $t_R = t_L = t$, a relationship which simplifies the above formulae (32) to

$$\begin{aligned} T_{11} &= \frac{t^2 - r_L r_R}{t} \\ T_{12} &= \frac{r_R}{t} \\ T_{21} &= -\frac{r_L}{t} \\ T_{22} &= \frac{1}{t} \end{aligned} \tag{33}$$

Having made this assumption we find that

$$\det(\boldsymbol{T}) = T_{11}T_{22} - T_{12}T_{21} = \frac{t^2 - r_L r_R}{t^2} + \frac{r_L r_R}{t^2} = 1$$

and

$$\frac{\mathrm{Tr}[\boldsymbol{T}]}{2} = \frac{1 + t^2 - r_L r_R}{2t}$$

Therefore in terms of the reflection and transmission coefficients of a unit cell, the dispersion relation is simplified to

$$1-\mathrm{Tr}[\boldsymbol{T}]e^{iKa}+e^{2iKa}=0\rightarrow\cos(Ka)=\frac{\mathrm{Tr}[\boldsymbol{T}]}{2} \tag{34}$$

This relationship between the transfer matrix and the reflection and transmission coefficients of a single unit cell is useful if—for example—we have an experimental characterization of a single element of a periodic medium. It is similarly useful if we have an exact solution for wave propagation through a region of varying refractive index that we want to translate into a solution for propagation through a periodic variation of index.

4 Application—transparent mirrors:

When you think of a mirror, you probably think of a metal sheet. Why does it act as a mirror? It's because the metal contains electrons that are quite easy to move and this makes it very easy to polarize. The large polarization of the metal causes the wave to be extinguished as it propagates into the material, leading to a large amount of reflection. However, it is also possible to construct mirrors out of periodic layers of material that are not so easy to polarize, using the fact that within a band gap the wave will be extinguished and therefore there will be a large amount of reflection. In this section we shall derive the theory of such mirrors (typically called '*Bragg mirrors*').

Suppose we have a planar material that we make out of N periods of some unit cell. We might for instance have a unit cell made out of two layers of different refractive indicies, and then construct N such unit cells stacked together. If the unit cell has the transfer matrix

$$\boldsymbol{t}=\begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \tag{35}$$

then the transfer matrix associated with the stack of N such cells is

$$\boldsymbol{T}=\boldsymbol{t}^N \tag{36}$$

We might think at this point that we can't make any progress, because a matrix to the N^{th} power does not seem like an easy think to evaluate. However the N^{th} power of a 2×2 matrix can actually be computed analytically. First we note that the square of a 2×2 matrix $\boldsymbol{t}$ can be written entirely in terms of $\boldsymbol{t}$ and the identity matrix $\mathbf{1}$

$$\begin{aligned}\boldsymbol{t}^2 &=\begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix}\begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix}=\begin{pmatrix} t_{11}^2+t_{12}t_{21} & t_{11}t_{12}+t_{12}t_{22} \\ t_{21}t_{11}+t_{22}t_{21} & t_{22}^2+t_{12}t_{22} \end{pmatrix}\\ &=(t_{11}+t_{22})\boldsymbol{t}-(t_{11}t_{22}-t_{12}t_{21})\mathbf{1}\\ &=\mathrm{Tr}(\boldsymbol{t})\boldsymbol{t}-\det(\boldsymbol{t})\mathbf{1}\\ &=\mathrm{Tr}(\boldsymbol{t})\boldsymbol{t}-\mathbf{1}\end{aligned} \tag{37}$$

(where I assumed reciprocity (33) so that $\det(\boldsymbol{t})=1$). This implies that the N^{th} power of $\boldsymbol{t}$ can also be written in terms of only $\boldsymbol{t}$ and $\mathbf{1}$. Writing

$$\boldsymbol{t}^N=\alpha_N\boldsymbol{t}+\beta_N\mathbf{1}$$

and multiplying by $\boldsymbol{t}$ and applying (37) this becomes

$$\begin{aligned}\boldsymbol{t}^{N+1} &= \alpha_N \boldsymbol{t}^2 + \beta_N \boldsymbol{t} \\ &= [\beta_N + \alpha_N \mathrm{Tr}(\boldsymbol{t})]\boldsymbol{t} - \alpha_N \mathbf{1} \\ &= \alpha_{N+1}\boldsymbol{t} + \beta_{N+1}\mathbf{1}\end{aligned}$$

Therefore

$$\begin{aligned}\beta_{N+1} &= -\alpha_N \\ \alpha_{N+1} &= \alpha_N \mathrm{Tr}(\boldsymbol{t}) - \alpha_{N-1} = 2\alpha_N \cos(Ka) - \alpha_{N-1}\end{aligned} \tag{38}$$

where I applied (34). Notice that the wave–vector K (which is derived for the infinite system) automatically enters the expression for a finite number of periods of the medium. We can find α_N through recognising that $\sin(NKa)/\sin(Ka)$ obeys the same recursion relation as the α_N and also has the correct limiting values $\alpha_0 = 0$ and $\alpha_1 = 1$

$$\begin{aligned}\frac{\sin((N+1)\,Ka)}{\sin(Ka)} &= \frac{\sin(NKa)\cos(Ka) + \cos(NKa)\sin(Ka)}{\sin(Ka)} \\ &= \cos(Ka)\frac{\sin(NKa)}{\sin(Ka)} + \frac{[\cos((N-1)\,Ka)\cos(Ka) - \sin((N-1)\,Ka)\sin(Ka)]\sin(Ka)}{\sin(Ka)} \\ &= 2\cos(Ka)\frac{\sin(NKa)}{\sin(Ka)} - \frac{\sin((N-1)\,Ka)}{\sin(Ka)}\end{aligned} \tag{39}$$

Therefore the transfer matrix $\boldsymbol{T}$ for our N period planar material is generally

$$\begin{aligned}\boldsymbol{T} &= \boldsymbol{t}^N = \frac{\sin(NKa)}{\sin(Ka)}\boldsymbol{t} - \frac{\sin((N-1)\,Ka)}{\sin(Ka)}\mathbf{1} \\ &= \begin{pmatrix} \frac{\sin(NKa)}{\sin(Ka)}t_{11} - \frac{\sin((N-1)\,Ka)}{\sin(Ka)} & \frac{\sin(NKa)}{\sin(Ka)}t_{12} \\ \frac{\sin(NKa)}{\sin(Ka)}t_{21} & \frac{\sin(NKa)}{\sin(Ka)}t_{22} - \frac{\sin((N-1)\,Ka)}{\sin(Ka)} \end{pmatrix}.\end{aligned}$$

which connects wave amplitudes on the left and on the right of the planar medium. From this we can calculate the reflection and transmission coefficients from our N layered slab, using the formulae (33)

$$\begin{aligned}r_R &= \frac{T_{12}}{T_{22}} &&= \frac{\frac{\sin(NKa)}{\sin(Ka)}t_{12}}{\frac{\sin(NKa)}{\sin(Ka)}t_{22} - \frac{\sin((N-1)\,Ka)}{\sin(Ka)}} \\ r_L &= -\frac{T_{21}}{T_{22}} &&= -\frac{\frac{\sin(NKa)}{\sin(Ka)}t_{21}}{\frac{\sin(NKa)}{\sin(Ka)}t_{22} - \frac{\sin((N-1)\,Ka)}{\sin(Ka)}} \\ t &= \frac{1}{T_{22}} &&= \frac{1}{\frac{\sin(NKa)}{\sin(Ka)}t_{22} - \frac{\sin((N-1)\,Ka)}{\sin(Ka)}}\end{aligned}$$

And now we can see that our layered medium can act as a mirror. At frequencies where the infinite system exhibits a band gap (where K is complex) then the sine functions will become hyperbolic sine functions, which are very large when $\mathrm{Im}[NKa]$ is large. This implies that the transmission coefficient becomes very small, and the reflection coefficient is close to unit magnitude. This is explored in the notebook "*bragg-mirror.ipynb*" that goes with this lecture.