What is a photonic band gap material?

See book by Joannopoulos on Photonic Band Gap Materials

Basically, we know that for a homogeneous dielectric, the electromagnetic eigenstates satisfy

\[ \bar{E}(x,t) = \bar{E}_0 e^{i \mathbf{k} \cdot \mathbf{x} - i \omega t} \]

where \( \omega = c k / \varepsilon_0 \)

(assuming \( \varepsilon \) is indep. of frequency)

So the dispersion relation is very simple:

\[ \omega(k) = c |k| \]

Photonic band gap materials have a different kinds of dielectrics: specifically

\[ \varepsilon = \varepsilon(\tilde{x}) \]

and \( \varepsilon(\tilde{x}) \) is a periodic function of \( \tilde{x} \)

(defined below)

The property which has created a lot of experimental interests is the discovery that some periodic materials can have "photonic band gaps" (see next page)
Density of photonic states looks like this:

\[ \rho(\omega) \]

- Photonic band gaps = regions where there are no allowed photonic states.
- Now, how can we treat these states? First, must define periodic materials.
- First, in 1D. We mean
  \[ \varepsilon(x + n\alpha) = \varepsilon(x) \]  \[ \alpha = \text{cell size constant.} \]
- E.g. alternating layers of \( \varepsilon_1 \) and \( \varepsilon_2 \):
  \[
  \begin{array}{cccccccc}
    \varepsilon_1 & \varepsilon_2 & \varepsilon_1 & \varepsilon_2 & \varepsilon_1 & \varepsilon_2 & \varepsilon_1 & \varepsilon_2 \\
    a_1 & a_2 & a_1 & a_2 & a_1 & a_2 & a_1 & a_2
  \end{array}
  \]

We even discussed this during write qns.
- But it is only one-dimensional periodicity.
How do we treat these periodic systems in 3d?

If we have a simple cubic lattice, we would have

$$\varepsilon(\vec{x} + \vec{R}) = \varepsilon(\vec{x})$$

where

$$\vec{R} = n_1 a^\hat{x} + n_2 a^\hat{y} + n_3 a^\hat{z}$$

This is called a Bravais lattice vector, which is defined more carefully below.

Slide Side remarks: Mathematical description of periodic systems, and periodic functions.

(a) First, let's do 1D dimension:

Suppose we have $$\varepsilon(x) = \varepsilon(x + na)$$

where $$a$$ is called the lattice constant.

E.g. suppose $$\varepsilon$$ looks as below:

\[ \begin{array}{c}
| & a \\
\hline
| & a \\
| & a \\
| & a \\
\end{array} \]

$$0 < x < a$$ is primitive cell.
Primitive cell because can repeat entire solid by
primitive cells displaced by $a, 2a, \ldots$

Bravais lattice vectors:
the set of vectors $
\mathbf{R} = n\mathbf{a}\%
\text{ such that }
\mathbf{a} \cdot e(x + n\mathbf{a}) = e(x)$

Many choices of primitive cell, e.g.
region from $0 < x < a$:
region between $-\frac{a}{2} < x < \frac{a}{2}$, etc.
The one closest to the lattice site vector $\mathbf{R} = 0$
110. from $-\frac{a}{2} < x < \frac{a}{2}$, is called the
Wigner-Seitz cell

Now, how to describe periodic function on a
lattice?

Well, we know that only certain functions any
function $e(x)$ can in 1d can be expressed
as a Fourier transform, viz.:

$$e(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e(k) e^{ikx} \, dk$$

But in the case being considered
$e(x) = e(x + Na)$ so only certain $k$'s
are allowed. We can then therefore

What are these $k$'s?
Can write sum as
\[ e(x) = \sum_k e_k e^{ikx} \]

What are allowed \( k \)'s? Must have
\[ e^{ik(x+na)} = e^{ikx} \]
or \( e^{i k a} = 1 \) for any \( n \).
This must mean \( e^{i k a} = 1 \) or
\[ k = \frac{2\pi p}{a} = kp \quad p = 0, \pm 1, \pm 2, \ldots \]
Thus we have
\[ e(x) = \sum_{p=-\infty}^{\infty} e_p e^{i\frac{2\pi p x}{a}} \]

What are the \( e_p \)'s? Write down
\[ \int_{-\frac{a}{2}}^{\frac{a}{2}} e(x) e^{-i2\pi p' x/a} \, dx = \sum_{p=-\infty}^{\infty} e_p \int_{-\frac{a}{2}}^{\frac{a}{2}} e^{i\frac{2\pi (p-p') x}{a}} \, dx \]

If \( p \neq p' \) this integral is \( \frac{a}{2\pi(p-p')} (e^{i\frac{2\pi(p-p')}{a} \frac{a}{2}} - e^{-i\frac{2\pi(p-p')}{a} \frac{a}{2}}) = 0 \)

If \( p = p' \) it equals \( a \).
Therefore \( \text{rhs} = \sum_{p=-\infty}^{\infty} e_p a \delta_{pp'} = 6_p \).
True,
\[ e_p = \frac{1}{a} \int_{-a/2}^{a/2} \epsilon(x) e^{-i2\pi p x/a} \, dx \]

More conventional to write: the allowed Fourier components as \( K = \frac{\pm \pi}{a} p \)

and say
\[ \epsilon(x) = \sum_{K} \epsilon_K e^{iKx} \]

\[ \epsilon_K = \frac{1}{a/2} \int_{-a/2}^{a/2} \epsilon(x) e^{-iKx} \, dx \]

Thus we get:

Note that the \( K \)'s also form a Bravais lattice, called the reciprocal lattice.

Lattice constant \( \frac{2\pi}{a} \)

Wigner-Seitz cell \( \frac{-\pi}{a} < K \leq \frac{\pi}{a} \)

called the first Brillouin zone

What about \( 3D? \) (or \( 2D \))\n
The simplest case is simple cubic:
\[ \mathbf{R} = n_1 a \mathbf{a}_x + n_2 a \mathbf{a}_y + n_3 a \mathbf{a}_z \]
Then \( e(\mathbf{x} + \mathbf{R}) = e(\mathbf{x}) \)  
for a periodic dielectric

Can again write 
\[
e(\mathbf{x}) = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{x}}
\]

where \( \mathbf{k} = \frac{2\pi}{a} (m_x, m_y, m_z) \) with
\[
\epsilon_{\mathbf{k}} = \frac{1}{V_C} \int_{V_C} e^{-i\mathbf{k} \cdot \mathbf{x}} e(\mathbf{x}) \, d^3x
\]

\( V_C = \) volume of primitive cell

(\( \mathbf{R} \) is a lattice which could be Wigner–Seitz cell = cell centered around \( \mathbf{R} = 0 \))

A Bravais lattice in 3d is a set of points \( \mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3 \)

where here \( \mathbf{a}_1 = a\hat{\mathbf{x}} \)
\( \mathbf{a}_2 = a\hat{\mathbf{y}} \)
\( \mathbf{a}_3 = a\hat{\mathbf{z}} \)

The corresponding reciprocal lattice vectors are 
\( \mathbf{k} = 2\pi \sum m_i \mathbf{b}_i + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3 \)

where \( \mathbf{b}_1 = \frac{2\pi}{a} \hat{\mathbf{x}} \), \( \mathbf{b}_2 = \frac{2\pi}{a} \hat{\mathbf{y}} \), \( \mathbf{b}_3 = \frac{2\pi}{a} \hat{\mathbf{z}} \)
Central values:
\( \vec{a}_1, \vec{a}_2, \vec{a}_3 \) called primitive vectors
\( \vec{b}_1, \vec{b}_2, \vec{b}_3 \) are primitive vectors of reciprocal lattice

Definition: A Bravais lattice is defined by three primitive vectors (noncoplanar)
\( \vec{a}_1, \vec{a}_2, \vec{a}_3 \).

Such that the Bravais lattice vectors consist of the complete set
\( \vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 \)

Photonic materials have
\( \varepsilon (\vec{x}) = \varepsilon (\vec{x} + \vec{R}) \).

Reciprocal lattice. Consists of all points
\( \vec{R} = m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3 \)

where
\( \vec{b}_1 = \frac{2\pi \vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \)
\( \vec{b}_2 = \frac{2\pi \vec{a}_3 \times \vec{a}_1}{\vec{a}_2 \cdot \vec{a}_2 \times \vec{a}_3} \)
\( \vec{b}_3 = \frac{2\pi \vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \)

= primitive vectors of the reciprocal lattice.

Properties:
\( \vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij} \)

\( e^{i \vec{K} \cdot \vec{R}} = 1 \) for any \( \vec{K} \) and \( \vec{R} \)

\( = \exp \left\{ i \sum (m_1 \vec{a}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3) \cdot (n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3) \right\} = 1 \)
\[ e^{i\mathbf{k} \cdot \mathbf{x}} \]

Then

\[ e(\mathbf{x}) = \sum_{\mathbf{k}} e_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{x}} \]

where

\[ \nu_{\mathbf{K}} = \frac{1}{\nu_{c}} \int e^{-i\mathbf{k} \cdot \mathbf{x}} d^3x \]

and

\[ \nu_{c} = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)| \]

Easy to see:

\[ \nu_{c} = \text{vol. of reciprocal lattice primitive cell} \]

Comment:

\[ \nu_{c}^* = \frac{(2\pi)^3}{\nu_{c}} \]
Examples of Bravais Lattices

1. sc (simple cubic)

2. bcc (body-centered cubic)

3. fcc. (face-centered cubic)

4. Simple tetragonal
Wave eq. for EM wave in a periodic medium:

\[ \nabla \times E = -\frac{1}{c} \frac{\partial B}{\partial t} = \frac{i \omega}{c} B \]

\[ \nabla \times B = +\frac{1}{c} \frac{\partial E}{\partial t} = -\frac{i \omega}{c} D = -\frac{i \omega}{c} \varepsilon E \]

or \[ \nabla \times \left( \frac{1}{\varepsilon(x)} \nabla \times B \right) = -\frac{i \omega}{c} \nabla \times E = \frac{\omega^2}{c^2} B \]

or \[ +\nabla \times \left( \frac{1}{\varepsilon(x)} \nabla \times B \right) = \frac{\omega^2}{c^2} B = 0 \]

Like Schrödinger eq. (sort of):

\[ \vec{B} \text{ is like wave function} \]

\[ \frac{\omega^2}{c^2} \text{ is like eigenvalue} \]

\[ \vec{E} \text{ is like } \nabla \times \frac{1}{\varepsilon(x)} \nabla \times \text{ is like the Hamiltonian} \]

This "H" is actually hermitian (if \( \varepsilon \) is real).

So if \( \vec{B}_1 \) and \( \vec{B}_2 \) are two fields corresponding to two modes with different \( \omega^2 \),

then \[ \oint \vec{B}_1 \cdot \vec{B}_2 \, d^3x = 0 \]
Proof:
\[
\int \mathbf{B}_1^* \cdot \nabla \times \left( \frac{1}{e} \mathbf{\nabla} \times \mathbf{B}_2 \right) \, d^3x = \frac{\omega_2^2}{c^2} \int \mathbf{B}_1^* \cdot \mathbf{B}_2 \, d^3x
\]

\[
= \int \mathbf{\nabla} \times \mathbf{B}_1 \cdot \frac{1}{e(x)} \mathbf{\nabla} \times \mathbf{B}_2(x) \, d^3x \quad \text{(integrating by parts)}
\]

But also
\[
\int \mathbf{\nabla} \times \left( \frac{1}{e} \mathbf{\nabla} \times \mathbf{B}_1^* \right) \cdot \mathbf{B}_2 \, d^3x = \frac{\omega_1^2}{c^2} \int \mathbf{B}_1^* \cdot \mathbf{B}_2 \, d^3x \quad \text{(taking } \omega_1^2 \text{ and } \omega_2^2 \text{ to be real)}
\]

\[
= \int \mathbf{\nabla} \times \mathbf{B}_1^* \cdot \frac{1}{e} \mathbf{\nabla} \times \mathbf{B}_2 \, d^3x = \frac{\omega_2^2}{c^2} \int \mathbf{B}_1^* \cdot \mathbf{B}_2 \, d^3x
\]

So
\[
\frac{\omega_1^2 - \omega_2^2}{c^2} \int \mathbf{B}_1^* \cdot \mathbf{B}_2 \, d^3x = 0
\]

\[
\Rightarrow \int \mathbf{B}_1^* \cdot \mathbf{B}_2 \, d^3x = 0 \quad \text{if } \omega_1 \neq \omega_2 \quad \text{QED}
\]

Bloch's theorem:

Suppose \( \epsilon(x) = \epsilon(x + \mathbf{R}) \) periodic function.

Then \( \mathbf{B}(x) \) satisfies
\[
\mathbf{B}(x) = e^{i\mathbf{k} \cdot \mathbf{x}} \mathbf{u}(x)
\]
where \( \tilde{u}(x) = u(x + \vec{R}) \)

Proof: (there are several):

Let us write the wave equation as:

\[
\ddot{B} = \lambda \dot{B}
\]

where \( \lambda = \frac{\omega^2}{c^2} \) and \( H(x) = \nabla \times \frac{1}{\epsilon(x)} \nabla \times B(x) \)

Now introduce the operator \( T_{\vec{R}} \) defined by

\[
T_{\vec{R}} \dot{f}(x) = f(x + \vec{R})
\]

Some properties of \( T_{\vec{R}} \):

\[
T_{\vec{R}} T_{\vec{R}'} = T_{\vec{R} + \vec{R}'} = T_{\vec{R}'} T_{\vec{R}}.
\]

Now let \( \dot{B} \) be a non-degenerate eigenvector of \( H \) with eigenvalue

\[
\lambda = \frac{\omega^2}{c^2}
\]

Then we have:

\[
T_{\vec{R}} \dot{B}(H \dot{B}) = \lambda T_{\vec{R}} \dot{B}
\]

\[
= \lambda \dot{B}(x + \vec{R})
\]

\[
= T_{\vec{R}} \left[ \nabla \times \nabla \frac{1}{\epsilon(x)} \nabla \times B(x) \right]
\]
\[ \nabla \times \left( \frac{1}{\nabla \cdot \mathbf{B}(\mathbf{r} + \mathbf{R})} \nabla \times \mathbf{B}(\mathbf{r} + \mathbf{R}) \right) \]

\[ = \nabla \times \frac{1}{\nabla \cdot \mathbf{B}} \nabla \times \mathbf{B}(\mathbf{r} + \mathbf{R}) \]

\[ = \nabla \left( \mathbf{H}(\mathbf{T}_R \mathbf{B}) \right) = \mathbf{A}(\mathbf{T}_R \mathbf{B}) \]

Therefore, \( \mathbf{T}_R \mathbf{B} \) is also an eigenfunction of \( \mathbf{H} \) with the same eigenvalue as \( \mathbf{B} \).

But \( \mathbf{B} \) is assumed to be non-degenerate. Thus, we must have \( \mathbf{T}_R \mathbf{B} \) is just a multiple of \( \mathbf{B} \).

Say \( \mathbf{T}_R \mathbf{B} = c_R \mathbf{B} \) where \( c_R \) is just a number.

Evidently, \( \mathbf{F} \mathbf{R} \mathbf{G} = (c_R + c_R^*) \), etc.
Let \( \phi_{\vec{R}} = e^{i \phi_{\vec{R}}^k} \)

\( \phi_{\vec{R}} + \phi_{\vec{R}'} = \phi_{\vec{R} + \vec{R}'} \)

Thus \( \phi \) varies linearly with \( \vec{R} \).

We can write it as

\( \phi = i \vec{k} \cdot \vec{R} \)

most general linear homogeneous function

\( \vec{k} \) does not necessarily have to be real.

But we now have

\( \phi_{\vec{R}} = e^{i \vec{k} \cdot \vec{R}} \)

and thus

\( T_{\vec{R}} \vec{B} = e^{i \vec{k} \cdot \vec{R}} \vec{B} \)

or

\[ \vec{B}(\vec{x} + \vec{R}) = e^{i \vec{k} \cdot \vec{R}} \vec{B}(\vec{x}) \]

If we write \( \vec{B}(\vec{x}) = e^{i \vec{k} \cdot \vec{x}} \vec{u}(\vec{x}) \) then

\( e^{i \vec{k} \cdot (\vec{x} + \vec{R})} \vec{u}(\vec{x} + \vec{R}) = e^{i \vec{k} \cdot \vec{R}} \vec{u}(\vec{x}) \)

or

\( \vec{u}(\vec{x} + \vec{R}) = \vec{u}(\vec{x}) \)

Therefore \( \vec{B}(\vec{x}) \) can be written

\[ \vec{B}(\vec{x}) = e^{i \vec{k} \cdot \vec{x}} \vec{u}(\vec{x}) \]

where \( \vec{u}(\vec{x}) \) is a periodic function of \( \vec{x} \)

which is Bloch's theorem (QED)
Example: Layered medium:

\[
\begin{array}{c|c|c|c|c}
\epsilon_1 & \epsilon_2 & \vdots & \vdots & \epsilon_n \\
\hline
\mathbf{a} & & & & \mathbf{x}
\end{array}
\]

\[\kappa_1 \rightarrow (\kappa_2 \rightarrow) \]
\[k < a \rightarrow 1\]

Let's consider wave propagating in x direction.

In medium 1,

\[
\frac{1}{\epsilon_1} \nabla \times (\nabla \times \vec{B}) - \frac{\omega^2}{c^2} \vec{B} = 0
\]

\[= \frac{1}{\epsilon_1} \left[ \nabla (\nabla \cdot \vec{B}) - \nabla^2 \vec{B} \right] - \frac{\omega^2}{c^2} \vec{B}
\]

But \( \nabla \cdot \vec{B} = 0 \) so we have

\[
\frac{1}{\epsilon_1} \nabla^2 \vec{B} + \frac{\omega^2}{c^2} \vec{B} = 0
\]

\[
\vec{B}(x) = \vec{B}_1 e^{iK_1 x} + \vec{B}_2 e^{-iK_1 x}
\]

where \( K_1 = \sqrt{\epsilon_1 \frac{\omega}{c}} \)

Also \( \nabla \cdot \vec{B} = 0 \Rightarrow \vec{B}_1^\wedge \)

Take \( \vec{B}_1 = B_1^\wedge \hat{z} \)

\( \vec{B}_2 = B_2^\wedge \hat{z} \)
Thus, we have

\[ \mathbf{B}(x) = B_1 e^{iK_1 x} \quad \text{in region} \quad x < 0 \]

\[ = B_3 e^{iK_2 x} + B_4 e^{-iK_2 x} \quad \text{in region} \quad 0 < x < a_1 \]

\[ = B_5 e^{iK_2 x} + B_6 e^{-iK_2 x} \quad \text{in region} \quad a_1 < x < a_2 \]

where \( K_1 = \sqrt{\varepsilon_1 \frac{w}{c}} \) and \( K_2 = \sqrt{\varepsilon_2 \frac{w}{c}} \).

Now, use Bloch condition to write, for \( a < x < a + a_1 \)

\[ \mathbf{B}(x) = e^{ika} \mathbf{B}(x-a) \]

\[ = e^{ika} \left[ B_1 e^{iK_1 (x-a)} + B_2 e^{-iK_2 (x-a)} \right] \]

where \( k \) can be anything.

Boundary conditions: at \( x = a_1 \) and \( x = a \),

we have \( \mathbf{E} \) and \( \mathbf{E} \) continuous.

Well, \( \mathbf{E} = E_y \mathbf{e}_y \) and \( \mathbf{E} \) satisfies

\[ \nabla \times \mathbf{B} = -\frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} = \frac{\mu_0}{c} \mathbf{E} \; \text{so} \]

\[ \mathbf{E} = -i \frac{c}{\omega} \nabla \times \mathbf{B} = -i \frac{c}{\omega} \left[ \begin{array}{c} \frac{\partial}{\partial x} \frac{\partial}{\partial y} \frac{\partial}{\partial z} \\ 0 \end{array} \right] \]

\[ \left[ \begin{array}{c} E_x \\ E_y \\ E_z \\ B_y \\ B_z \end{array} \right] \]

\[ = i \frac{c}{\omega} \frac{\partial B_2}{\partial x}. \]
This gives, for any $k$, conditions on the $4$ coeffs.

$B_1, B_2, B_3, B_4.$

\[
\Rightarrow \text{ Determinantal equation (matrix of coeffs) for } W(k)
\]

\[
-\frac{\pi}{a} < k \leq \frac{\pi}{a}
\]

Comment: only need consider

\[
e^{ika} = e^{i(k + \frac{2\pi n}{a})a}
\]

$n = 0, \pm 1, \pm 2,$
For 1d wave, we have a matrix eq. determining \( \omega \) in terms of \( k \) (actually, determines \( \omega^2 \) in terms of \( k \))

The form of the wave is

\[
\hat{\mathbf{B}}(x) = e^{ikx} \beta(x)
\]

where \( \beta(x+a) = \beta(x) \)

Now, claim we only need consider

\[-\frac{\pi}{a} < k \leq \frac{\pi}{a}\]

Why is that?

Let \( \hat{\mathbf{B}}(x) = e^{ikx} \left[ e^{i2\pi n x/a} \beta(x) \right] \)

where \(-\frac{\pi}{a} < k \leq \frac{\pi}{a}\)

Then we can always write

\[
\hat{\mathbf{B}}(x) = e^{ikx} \left[ e^{i2\pi n x/a} \beta(x) \right]
\]

\[
= e^{ikx} \beta(x) \text{ where } \beta(x+a) = \beta(x)
\]

Thus, can always express \( \hat{\mathbf{B}}(x) \) as \( e^{ikx} \beta(x) \)

where \(-\frac{\pi}{a} < k \leq \frac{\pi}{a} \quad (k \in \text{1st Brillouin zone})\)
"Band structure":

\[ \frac{1}{ka} \text{ "band gap"} \]

\[ -\frac{\pi}{a} \quad 0 \quad \frac{\pi}{a} \]

If wave propagates \( L \) to layers, there is a forbidden region.

But actually, not really a band gap for layered system: can fill in this gap if waves propagate at an angle to the layers (i.e., not really 1D).

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Number of allowed modes:

Suppose our lattice has length \( Na \)
Assume periodic boundary conditions
Then \( \xi(x + Na) = \xi(x) \)
\[ e^{iNka} = 1 \]
\[ k = \frac{2\pi}{Na} \quad p = 0, \pm 1, \ldots \]

Density of states between modes is
\[
\frac{1}{2\pi/Na} = \frac{Na}{2\pi} = \frac{L}{2\pi}
\]

Therefore, in the 1st B.Z., there are a total of \( N \) orthogonal modes.

3D crystal "photonic crystal": Here
\[
\tilde{B}(\mathbf{x}) = e^{iK \cdot \mathbf{x}} \tilde{u}_K(\mathbf{x})
\]

where \( \tilde{u}_K(x + \frac{1}{2} \mathbf{R}) = \tilde{u}_K(x) \)

and \( \mathbf{R} \) = Bravais lattice vector

General principles still the same:
Can restrict attention to \( K \in \text{1st B.Z.} \)

Can define "photonic band structure"

B.Z. is a very irregular shape (e.g., 14-sided polyhedron for fcc lattices)
Now: how does one draw band structure.

Tend to draw because \( \omega = \frac{k^2}{2m} + 3 \) scalars: \( k_x, k_y, \) and \( k_z \).

Now what?

For certain structures, there is complete photonic band gap.

No allowed modes at all.

E.g. Si spheres arranged in a diamond structure — air host.

(For Si = 12.96 \((\text{at } \omega=0, T=300K)\))

How to make "diamond structure"?

Start with fcc lattice. With each

To each lattice point, associate two Si spheres,

located at \( \mathbf{R} \pm \left( \frac{a}{4}, \frac{a}{4}, \frac{a}{4} \right) \)

Radius of each sphere is \( \frac{a}{4} \)

So "packing fraction" of spheres is

\[
\frac{8 \cdot \frac{4\pi}{3} \left( \frac{a}{4} \right)^3}{\frac{8}{3}} \approx 0.524
\]
If one calculates the band structure, there is a forbidden gap.

The width of the gap is around $\Delta \omega / \omega \sim 0.1$

If $a \sim 0.5 \mu$, then

$$\Delta \omega \sim \frac{0.1 c}{a} \sim \frac{0.1 (3 \times 10^8)}{5 \times 10^{-5}}$$

$$\sim 0.06 \times 10^{15} \text{ sec}^{-1}$$

Physical meaning of gap: cannot get any waves through at these frequencies, even though $\omega \gamma$, there is no absorption.

Density of photonic states:

1. Discuss one of the last h.w. problems

We have $\omega = ck$.

Let cavity have volume $V$

There are is 2 modes per $\left( \frac{2\pi}{L} \right)^3$ of $k$-space

So $g(k) = 2 \frac{L^3}{(2\pi)^3} = \frac{V}{4\pi^3}$
How many modes between \( k \) and \( k + dk \)?
This equals \# between \( k \) and \( k + dk \),
where \( k = \frac{\omega}{c} \) and \( dk = \frac{d\omega}{c} \).

The total number of modes in this region of \( k \)-space is

\[
\frac{4\pi k^2 dk}{4\pi^3} = \frac{\sqrt{k^2 dk}}{4\pi^2}
\]

\[
= \frac{V}{c^3} \frac{\omega^2 dw}{4\pi^2} = n(\omega) dw
\]

So

\[
n(\omega) = \frac{V}{4\pi^2 c^3} \frac{\omega^2}{w^2}
\]

Energy per mode = \( \hbar \omega \) (stat. mech.)

\[
= \text{energy of harmonic oscillator at temp } T
\]

So

\[
U(\omega) = \frac{1}{4\pi^2 c^3} \frac{\omega^3}{\beta \hbar \omega - 1}
\]

\[\beta = \frac{1}{k_B T}\]

Peak in energy spectrum is given by

\[
\frac{dU}{d\omega} = 0 \quad \text{or} \quad \frac{3\omega^2}{\beta \hbar \omega - 1} - \frac{\omega^3 \beta \hbar \omega e^{\beta \hbar \omega}}{(e^{\beta \hbar \omega} - 1)^2} = 0
\]
or \[ 3\omega^2 (e^{\beta \hbar w} - 1) = \omega^2 \beta \hbar e^{\beta \hbar w} \]

or \[ 1 = \frac{\beta \hbar w e^{\beta \hbar w}}{3\omega(e^{\beta \hbar w} - 1)} \]

or \[ \beta \hbar w \approx 2.82 \quad \text{or} \quad \hbar w = 2.82 k_B T \]

= peak in blackbody spectrum.

Total energy is

\[ U = \int_0^\infty U(\omega) d\omega = \frac{V}{4\pi^2 c^3} \int_0^\infty \frac{\hbar w^3}{e^{\beta \hbar w} - 1} d\omega \]

Let \( x = \beta \hbar w \)

\[ w = \frac{x}{\beta \hbar} = \frac{x}{k_B T} \quad d\omega = \frac{dx}{k_B T} \]

\[ U = \frac{V}{4\pi^2 c^3} \left( \frac{k_B T}{\hbar} \right)^4 \int_0^\infty \frac{x^3}{e^x - 1} \alpha T^4 \]

(not counting zero-point energy)
Density of states for photonic crystal:

\[ n(\omega) = \frac{1}{n^k} \sum \delta \left( \omega \frac{k^*}{nk} - \omega \right) \]

\[ = \frac{V}{(2\pi)^3} \sum_n \int d^3k \delta \left( \omega \frac{k^*}{nk} - \omega \right) \]

For diamond structure photonic crystal made of Si

\[ n(\omega) \]

\[ \propto \omega^2 \]

If we have atom with high excitation energy in forbidden gap, atom cannot decay out of excited state.

Band extrema:

\[ \omega_n(\vec{k}) = \frac{1}{2} \sum_{i,j} c_{ij} (\vec{k}_i - \vec{k}_{0i}) (\vec{k}_j - \vec{k}_{0j}) + \omega_n(\vec{k}_0) \]
How to calculate photonic band structure?

"Schrodinger equation" is

$$\nabla \times \left[ \frac{1}{e(x)} \nabla \times \vec{B}(x) \right] = \frac{\omega^2}{c^2} \vec{B}(x)$$

Now $$\vec{B}(x) = \sum_{k} \vec{B}_k e^{\frac{i k \cdot x}{\hbar}} \vec{\Phi}_k(x)$$

But $$\vec{\Phi}_k(x)$$ is periodic.

Therefore, we can expand it as:

$$\vec{\Phi}_k(x) = \sum_{\vec{K}} \vec{B}_k e^{\frac{i \vec{K} \cdot x}{\hbar}}$$

and thus

$$\vec{B}(x) = \sum_{\vec{K}} \sum_{k} \vec{B}_k e^{\frac{i (\vec{k} + \vec{K}) \cdot x}{\hbar}}$$

Also, $$\epsilon(x)$$ is periodic, so we can write

$$\epsilon^{-1}(x) = \sum_{\vec{K}} \sum_{k} \epsilon(\vec{k} + \vec{K}) e^{\frac{i \vec{K} \cdot x}{\hbar}}$$

$$\epsilon^{-1}(\vec{k}) = \text{Fourier component of } \epsilon^{-1}(x).$$

(assumed known)

Then we have

$$\nabla \times \left[ \sum_{\vec{K}} \epsilon^{-1}(\vec{k}) e^{\frac{i \vec{K} \cdot x}{\hbar}} \right] \nabla \times \sum_{\vec{K}} \vec{B}_k e^{\frac{i \vec{K} \cdot x}{\hbar}}$$
Now
\[ \nabla \times \sum_{K} B_{K} e^{-i (K+\bar{K}) \cdot \mathbf{x}} \]
\[ = \sum_{K} i (K+\bar{K}) \times B_{K} e^{-i (K+\bar{K}) \cdot \mathbf{x}} \]

Then left-hand side is
\[ \nabla \times \sum_{K_1} \sum_{K} (e^{-i})_{K_1} (K+\bar{K}+K_1) \times [e^{i (K_1+\bar{K}) \cdot \mathbf{x}} B_{K} \hat{K}] \]
\[ = -\sum_{K_1} \sum_{K} (e^{-i})_{K_1} (K+\bar{K}+K_1) \times [e^{i (K_1+\bar{K}) \cdot \mathbf{x}} B_{K} \hat{K}] \]
\[ \times e^{i (K_1+\bar{K}) \cdot \mathbf{x}} = \frac{\omega^2}{c^2} \sum_{K} e^{-i (K_1+\bar{K}) \cdot \mathbf{x}} \]

Now, left-multiply by \( \frac{1}{\nu_c} e^{i \mathbf{G} \cdot \mathbf{x} - i \mathbf{\hat{K}} \cdot \mathbf{x}} \) and integrate over one unit cell.

Use \( \int_{\nu_c} e^{i (\mathbf{K}_1' - \mathbf{\bar{K}}') \cdot \mathbf{x}} d^3x = \nu_c \) if \( \mathbf{G} = \mathbf{K}_1' \)
\[ = 0 \) otherwise.

Finally, just get
\[ -\sum_{K_1} (e^{-i})_{K_1} (K+\bar{K}) \times \left[ e^{i (K+\bar{K}) \cdot \mathbf{x}} B_{K} \hat{K} \right] \]
\[ = \frac{\omega^2}{c^2} \frac{\mathbf{\hat{B}}}{\mathbf{\hat{B}}} \]
For each \( k \), gives large number of linear homog.
equations which for the \( B_k \)’s
which can be solved to give the bands
\[
\omega = \epsilon k.
\]
and corresponding magnetic
field \( \vec{B} \).
Given \( \vec{B} \), get \( \vec{E} \) from
\[
-\frac{\partial \vec{E}}{\partial t} = c \vec{\nabla} \times \vec{B} = \frac{\omega}{c} \vec{E}
\]
Given all the bands:

\underline{Phase and group velocity:}

I will concentrate on group velocity, since this
is velocity with which energy travels.
Recall that in a homogeneous medium,
the group velocity is
\[
\vec{v}_g = \frac{d\omega}{d\epsilon}
\]
The same is true here. So near bottom
of lowest band, \( \omega \propto |\vec{k}| \) and \( \vec{v}_g \approx \frac{d\omega}{d\epsilon} \)
is generally much lower than
the speed of light in vacuum.
In general $\omega$ is a function of $\vec{k}$, so can show that

$$J_g = \hat{\nabla}_k \omega(\vec{k})$$

for a particular band.

E.g. just above gap, $\omega$ must have some minimum. Suppose this occurs near at $\vec{k} = 0$.

Near $\vec{k} = 0$ we will have

$$\omega \sim \omega_0 + \frac{1}{2} \sum_{i=1}^{3} \frac{1}{2} \sum_{j=1}^{3} a_{ij} k_i k_j$$

So

$$\omega = \sum_{i=1}^{3} a_{ij} k_j$$

May not necessarily be isotropic.

Also, $J_g \to 0$ at band edge.

Rigorous energy moves very slowly.
Group velocity (again):

We have that the energy density is

\[ U_{av} = \frac{1}{8\pi} \int \left[ \epsilon(x) \mathbf{E}^*(x) \cdot \mathbf{E}(x) + \mathbf{B}^*(x) \cdot \mathbf{B}(x) \right] d^3x \]

and the energy current density is

\[ \mathbf{S}_{av} = \text{Re} \frac{c}{8\pi} \int \mathbf{E}^*(x) \times \mathbf{B}(x) d^3x \]

If we insert \( \mathbf{E} \) from

\[ -\epsilon(x) \frac{i\omega}{c} \mathbf{E}(x) = \nabla \times \mathbf{B}(x) \]

or \[ -i\omega \mathbf{E}(x) = \epsilon^{-1}(x) \nabla \times \mathbf{B}(x) \]

Compare \( \int \mathbf{S}_{av} d^3x \) and \( \frac{U_{av}}{c} \int \mathbf{S}_{av} d^3x \)

The first is \( \tilde{V}_g \) times the second.

And one can show that

\[ \tilde{V}_g = \tilde{V}_K \omega(k) \] just as in the

\[ \text{case of a free wave in free space} \]
2D photonic crystals:

\[ \nabla \times \frac{1}{\varepsilon(\mathbf{r})} \nabla \times \mathbf{B} = \frac{\omega^2}{c^2} \mathbf{B}(\mathbf{r}) \]

Suppose \( \mathbf{B} \) has \( \mathbf{k} \) vector in \( xy \) plane.
and that \( \mathbf{B} \) is also parallel to, say, \( z \) axis

\[ \mathbf{B}(\mathbf{r}) = \mathbf{B}(x,y) \hat{z} \, \tilde{u}(x,y) e^{i \mathbf{k} \cdot \mathbf{r}} \]

where \( \tilde{u}(x,y) \) is in \( xy \) plane and
\( \mathbf{k} = (k_x, k_y) \).

Then we have an entirely 2D problem
with a 2D band structure
This may have very
This structure could have full band gap

\[ \text{very slow light down here} \]

\[ \text{small group velocity} \]

\[ \text{fig. k} \]
Defects in photonic band gap materials: general concept; localized photonic states

Defect in photonic crystal — e.g., as shown below:

\[
\begin{array}{cccccc}
\circ & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ \\
\end{array}
\]

In region of missing cylinder, we have a homogeneous defective — no forbidden photonic gap — therefore, could have photonic states. But they can't propagate. As a result, can have defect states. Band structure is as below: