Band structure of a 1D photonic crystal

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In this note, we review two different methods to calculate the band structure of a one dimensional (1D) photonic crystal (PhC). The emphasis is on the calculations but the tools required provide some physical insight into the system. We hope to add to the notes in the future to provide more physical insight.

Note that both methods below deal only with the simplest case where the electric field polarization is parallel with the PhC layers. More general calculations for the planewave method may be found in [1].

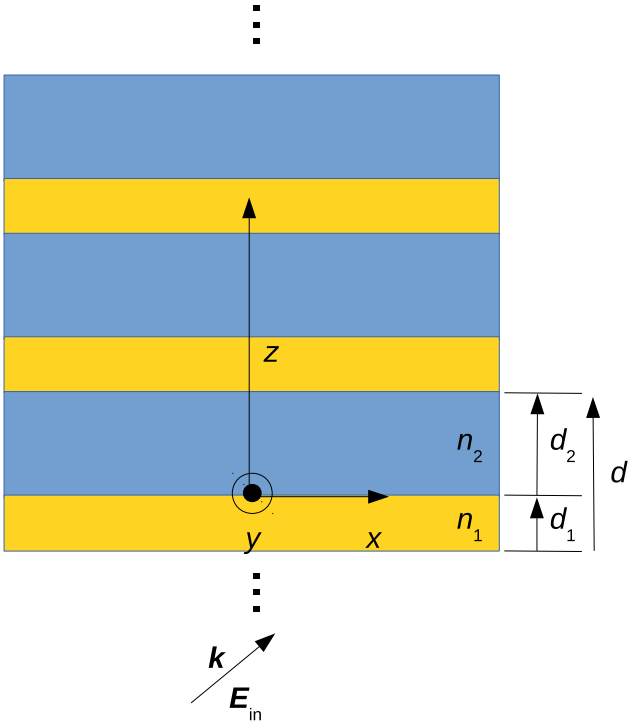

FIG. 1. Diagram of the 1D photonic crystal. Note that the crystal is assumed to extend infinitely in *all* three directions (i.e. x and y as well as in z. The angle of the incoming field $\mathbf{E}_{\text{in}}$ is meant to indicate the general case. However, in the derivations below, we will assume that the electric field is always parallel with the PhC layer boundaries.

I. METHOD 1: MATRIX TRANSFER METHOD)

A. Note on TM and TE polarizations

The following derivation of the bandstructure for a 1D (PhC) largely follows the outlines given in References [2, 3] with some extra details provided. Inspecting Fig. 1, it might seem unnecessary to define transverse magnetic (TM) and transverse electric (TE) polarizations for this problem since it is one dimensional. However, in general, we will not be assuming a true one dimensional problem. Rather, we assume infinite extent of the PhC layers in the x and y planes, and periodicity in the z plane. In this case, it is possible for an incident electromagnetic (EM) field to "enter" the crystal at an angle, or more precisely, since we are assuming that the PhC is infinite, for the EM field inside the crystal to have a wavevector with non-zero x and y components. In this case, the choice of TE or TM polarization is important, since in the TE (TM) case the magnetic (electric) field is not in general parallel to the PhC layers, assuming an arbitrary incident angle. For this reason is is reasonable to define TE (TM) polarization as the case where the electric (magnetic) field is polarized along the x axis.

B. Formal statement of the problem

In Method 1, we will not actually find it necessary to solve for the field explicitly, only to find the conditions for the existence or not of a solution. For this purpose, it is sufficient to consider only the z-propagating component of the incident EM field, although as discussed above, a transverse component also exists in general.

We begin, as always, with the wave equation:

$$\frac{\mathrm{d}^2}{\mathrm{d}z^2}E(z) - \frac{\omega^2}{c^2}n^2(z)E(z) = 0, \tag{1}$$

where E is the (x-polarized) electric field, ω is the frequency of the electromagnetic wave and c is the speed of light. $n(z)$ is the index of fraction which varies periodically along the z axis as shown in Fig. 1. We note from the outset that Eq. 1 will not be explicitly used to derive the results of this section. Rather, we write it down to remind us the equation that any solution we choose must ultimately satisfy. Indeed, rather than the wave equation itself, we will now see that the boundary conditions are all-important in deriving a useful form for the solutions and thus eventually the band structure of the PhC.

The assumed infinite extent of the periodic structure allows us to make use of the Bloch theorem for the field in the PhC, i.e.

$$E(z) = u(k_B, z)\exp(\mathrm{i}k_B z), \tag{2}$$

where $u(z) = u(z + D)$, and $D = d_1 + d_2$ is the spatial period of the PhC and k_B is the Bloch wave number which is yet to be determined. We note that the Bloch theorem describes our intuition that in an infinite crystal,

we should not be able to determine where in the crystal we are better than modulo D or, rather, the solution must look the same wherever we are in the crystal since by translational symmetry, there is no possible cause for it to vary.

Given the Bloch theorem, it is also necessary to constrain the solution in each layer of the PhC as follows:

$$E(z) = \begin{cases} E_1(z) & 0 \leq z \mod D \leq d_1 \\ E_2(z) & d_1 \leq z \mod D \leq d_2 \end{cases}. \tag{3}$$

Eq. 3 tells us that we can concentrate on finding a solution in the region $0 \leq z \leq D$ and use that to construct the solution anywhere in the PhC.

To flesh out the solution of Eq. 3, let's make the following assumptions which represent the simplest solutions which agree with Bloch's theorem. First, we assume a constant amplitude inside each layer which will definitely give a u function satisfying Eq. 2. Next, we recognize that forward and backward propagating solutions can exist. Putting these two ideas together, we get

$$E_1(z) = E_1^+ \exp(\mathrm{i}k_1 z) + E_1^- \exp(-\mathrm{i}k_1 z) \tag{4}$$
$$E_2(z) = E_2^+ \exp(\mathrm{i}k_2(z-d_1)) + E_2^- \exp(-\mathrm{i}k_2(z-d_1)) \tag{5}$$

The phase shift of E_2 by a complex exponential dependent on d_1 is in principle unnecessary, but it does not conflict with the Bloch boundary conditions and makes the solution neater. Essentially, introducing this term decides the overall phase of the solution by determinining that E_2 will have zero phase when $z = d_1$.

1. $E_1(z)$ and $E_2(z)$ - evaluation at layer boundaries

We now focus on the values of the solution at the layer boundaries to further pin down the solution. First, however, we expand the complex exponential terms and rewrite as follows:

$$E_1(z) = A_1 \cos(k_1 z) + \mathrm{i}B_1 \sin(k_1 z), \tag{6}$$

where $A_1 = E_1^+ + E_1^-$ and $B_1 = E_1^+ - E_1^-$. Similarly,

$$E_2(z) = A_2 \cos(k_2(z-d_1)) + \mathrm{i}B_2 \sin(k_2(z-d_1)), \tag{7}$$

where $A_2 = E_2^+ + E_2^-$ and $B_2 = E_2^+ - E_2^-$.

The equation for E_1 simplifies for $z = 0$ and that for E_2 when $z = d_1$. Specifically, substiution of these values gives, respectively

$$E(z=0) \equiv E_1(0) = A_1 \tag{8}$$
$$E'(z=0) \equiv E_1'(0) = k_1 B_1 \tag{9}$$

and

$$E(z=d_1) \equiv E_2(d_1) = A_2 \tag{10}$$
$$E'(z=d_1) \equiv E_2'(d_1) = k_2 B_2 \tag{11}$$

2. Application of continuity at layer boundaries

Gauss' law requires that the component of the electric field parallel to the dielectric layers is continuous at the boundary between the two layers. This allows us to further pin down the form of the solution. In particular, we can write

$$E_1(d_1) = E_2(d_1) = E(d_1) \tag{12}$$
$$E_1'(d_1) = E_2'(d_1) = E'(d_1) \tag{13}$$

Now let's put together Eqs. 10 and 12, then Eqs. 11 and 13 to write

$$E(0)\cos(k_1 d_1) + \frac{E'(0)}{k_1}\sin(k_1 d_1) = E_2(d_1) = E(d_1), \tag{14}$$
$$-E(0)k_1 \sin(k_1 d_1) + E'(0)\cos(k_1 d_1) = E_2(d_1) = E'(d_1). \tag{15}$$

These expressions can be written in matrix form as

$$\begin{pmatrix} \cos(k_1 d_1) & \sin(k_1 d_1)/k_1 \\ -k_1 \sin(k_1 d_1) & \cos(k_1 d_1) \end{pmatrix} \begin{pmatrix} E(0) \\ E'(0) \end{pmatrix} = \begin{pmatrix} E(d_1) \\ E'(d_1) \end{pmatrix} \tag{16}$$

or, in compact form,

$$\hat{M}_1 \mathbf{E}(0) = \mathbf{E}(d_1). \tag{17}$$

At this point we can pause and consider the goal of our analysis. As mentioned above, we do not need to produce a complete solution for E, only find a condition for its existence or not. It may be tempting to note that we can already do this as in general Eq. 16 can hold if and only if the matrix $\hat{M}_1$ has non-zero determinant. Therefore finding a condition for the non-existence of the determinant will allow us to identify the "band gaps" where no solutions exist. It is, however, still too early to apply this method since the equation we have so far only encodes information about half of the PhC, as is plainly seen by the lack of dependence on k_2 and d_2. To find an equation which fully defines the PhC over one unit cell, we apply the Bloch theorem.

3. Application of the Bloch theorem

By the assumption of the periodicity of u, the Bloch theorem guarantees that

$$E_2(d) = \exp(\mathrm{i}k_B d)E(0) \tag{18}$$
$$E_2'(d) = \exp(\mathrm{i}k_B d)E'(0). \tag{19}$$

Using Eqs. 10, 11 and Eq. 7 into the above equations, and substituting $d = d_1 + d_2$, we find

$$E(d_1)\cos(k_2 d_2) + \frac{E'(d_1)}{k_2}\sin(k_2 d_2) = \exp(\mathrm{i}k_B d)E(0), \tag{20}$$
$$-E(d_1)k_2\sin(k_2 d_2) + E'(d_1)\cos(k_2 d_2) = \exp(\mathrm{i}k_B d)E'(0). \tag{21}$$

As before, we write these equations in matrix form as follows:

$$\begin{pmatrix} \cos(k_2 d_2) & \sin(k_2 d_2)/k_2 \\ -k_2\sin(k_2 d_2) & \cos(k_2 d_2) \end{pmatrix} \begin{pmatrix} E(d_1) \\ E'(d_1) \end{pmatrix} = \exp(\mathrm{i}k_B d) \begin{pmatrix} E(0) \\ E'(0) \end{pmatrix} \tag{22}$$

or, in compact form,

$$\hat{M}_2 \mathbf{E}(d_1) = \exp(\mathrm{i}k_B d)\mathbf{E}(0). \tag{23}$$

By substituting Eq. 17 in Eq. 23 we arrive at the eigenvalue equation

$$\hat{M}\mathbf{E}(0) = \exp(\mathrm{i}k_B d)\mathbf{E}(0), \tag{24}$$

where

$$\begin{aligned}\hat{M} &= \hat{M}_2\hat{M}_1 \\ &= \begin{pmatrix} \cos(k_1 d_1)\cos(k_2 d_2) - \sin(k_1 d_1)\sin(k_2 d_2) & \cos(k_1 d_1)\sin(k_2 d_2)/k_2 - \sin(k_1 d_1)cos(k_2 d_2)/k_1 \\ -k_1\sin(k_1 d_1)\cos(k_2 d_2) - k_2\cos(k_1 d_1)\sin(k_2 d_2) & -\sin(k_1 d_1)\sin(k_2 d_2)/k_1 k_2 + \cos(k_1 d_1)\cos(k_2 d_2) \end{pmatrix}. \end{aligned} \tag{25}$$

4. Determining the existence of solutions from the eigenvalue equation

Linear algebra guarantees that the eigenvalue equation Eq. 24 has a solution if and only if

$$\det(\hat{M} - \exp(\mathrm{i}k_B d)\hat{I}) = 0, \tag{26}$$

where det indicates the determinant. (This is the so called characteristic equation associated with the eigenvalue equation). We will use the identity

$$\det(\hat{A} - \lambda\hat{I}) = \det(A) - \mathrm{Tr}(A)\lambda + \lambda^2 \tag{27}$$

to evaluate separately the real and imaginary parts of Eq. 26. We start with the imaginary part as it turns out to be simpler. If Eq. 26 is to hold, then by identity 27, we must have

$$\mathscr{I}m[-\mathrm{Tr}(\hat{M})\exp(\mathrm{i}k_B d) + \exp(2\mathrm{i}k_B d)] = 0. \tag{28}$$

Some rudimentary algebra establishes that this requires

$$\begin{aligned}\cos(k_B d) &= \frac{1}{2}\mathrm{Tr}(\hat{M}) \\ &= \cos(k_1 d_1)\cos(k_2 d_2) - \frac{1}{2}\frac{k_1^2 + k_2^2}{k_1 k_2}\sin(k_1 d_1)\sin(k_2 d_2).\end{aligned} \tag{29}$$

This result is, in fact, the equation that defines the bands of the PhC. However, it's not obvious that the real part of the characteristic equation will allow Eq. 29 to hold so it's necessary to check the real part as well. Using identity 27 again, the real part of Eq. 26 is given by

$$\mathscr{R}e[\det(\hat{M}) - \mathrm{Tr}(\hat{M})\exp(\mathrm{i}k_B d) + \exp(2\mathrm{i}k_B d)] = 0. \tag{30}$$

Simple manipulations show that this requires

$$\det(\hat{M}) - \mathrm{Tr}(\hat{M})\cos(k_B d) + 2\cos^2(k_B d) - 1 = 0, \quad (31)$$

but since Eq. 29 shows that $\cos(k_B d) = \frac{1}{2}\mathrm{Tr}(\hat{M})$ if the characteristic equation is to hold, the real part becomes simply

$$\det(\hat{M}) - 1 = 0. \quad (32)$$

A little algebra shows that this equation is always true given the definition of $\hat{M}$ in Eq. 25 and thus Eq 29 becomes the sole equation which determines the existence or not of solutions in the PhC and thus the existence or not of band gaps. It seems a little remarkable that the characteristic equation should hold for both real and imaginary parts even though its real and imaginary forms are different. However, it should be noted that this result can be arrived at without breaking the characteristic equation into real and imaginary parts as is done in the solutions to Ref. [3].

II. METHOD 2: PLANE WAVE EXPANSION

In this section, we again perform an analysis of the 1D photonic crystal considered above. This time we will use the method of planewave expansion, which can also be applied to periodic media outside of the context of photonic crystals (e.g., when analysing the near field diffraction pattern due to a plane wave incident on a grating structure). The treatment used here follows that of Danner [4]. Assuming that the time dependence of solutions is $\exp(-\mathrm{i}\omega t)$, we write Maxwell's wave equation for the electric field as

$$\frac{1}{n^2(z)}\nabla \times \nabla \times \mathbf{E} = \frac{\omega^2}{c^2}\mathbf{E}. \quad (33)$$

As in Method 1, We will assume that only the x component of the field is non-zero, which is equivalent to restricting ourselves to the TE component. Then Eq. 33 becomes

$$\frac{1}{n^2(z)}\left(\frac{\partial^2}{\partial x^2}E_x - \frac{\partial^2}{\partial z^2}E_x\right). \quad (34)$$

We proceed by making an ansatz for the solution in the form of a Fourier decomposition of E_x:

$$E_x = \sum_{n=-\infty}^{\infty} E_{x,n}\exp(\mathrm{i}(2\pi n/d + k_z)z), \quad (35)$$

where $E_{x,n}$ is the amplitude of the nth Fourier component and k_z is the wavenumber along the photonic crystal axis. Similarly, we expand the inverse, squared index to give

$$\frac{1}{n(z)^2} = \sum_{m=-\infty}^{\infty} n_m \exp(-\mathrm{i}2\pi m/d). \quad (36)$$

Some algebra shows that the Fourier coefficients are given by $n_m = (d_1/d)\mathrm{sinc}(md_1/d)[1/n_2^2 - 1/n_1^2]$.

Substituting Eqs.35 and 36 into Eq. 34, and omitting the sum limits for brevity, we get

$$\sum_m \sum_n \left(\frac{2\pi n}{d} + k_z\right) n_m E_{x,n}\exp[-\mathrm{i}(2\pi m/)z]\exp[-\mathrm{i}(2\pi n/)z] = \frac{\omega^2}{c^2}\sum_n E_{x,n}\exp[-\mathrm{i}(2\pi n/)z], \quad (37)$$

where we have removed the common factor of $\exp(-\mathrm{i}k_z z)$ from both sides.

To proceed, we define the inner product $< g(z), f(z) >= (1/d)\int_{-d/2}^{d/2} g(z)f(z)dz$. Taking the inner product of the LHS of Eq. 37, with $\exp[-\mathrm{i}(2pip/d)z]$ for integer p we find:

$$< \mathrm{LHS}, \exp[-\mathrm{i}(2pip/d)z] >= \sum_n \left(\frac{2\pi}{d}n + k_z\right) n_{p-n}E_{x,n}, \quad (38)$$

where orthgonality imposes the condition $m + n = p \Rightarrow m = p - n$. For the inner product with the RHS, we find simply

$$< \mathrm{RHS}, \exp[-\mathrm{i}(2pip/d)z] >= \frac{\omega^2}{c^2}E_{x,p}. \quad (39)$$

We can now write Eq. 37 as p independent equations:

$$\sum_n \left(\frac{2\pi}{d}n + k_z\right) n_{p-n}E_{x,n} = \frac{\omega^2}{c^2}E_{x,p} \quad (40)$$

All that remains is to recognize that Eq. 40 can be rewritten as a matrix equation

$$\hat{M}\mathbf{E} = \frac{w^2}{c^2}\mathbf{E}, \quad (41)$$

where $(\hat{M})_{n,p} = [(2\pi/d)m + k_z)n_{p-n}$, and $(\mathbf{E})_p = E_{x,p}$. For a given value of k_z, the value of ω/c can only take on discrete values defined by the eigenvalues of Eq. 41. These discrete values define the bands of the photonic crystal.

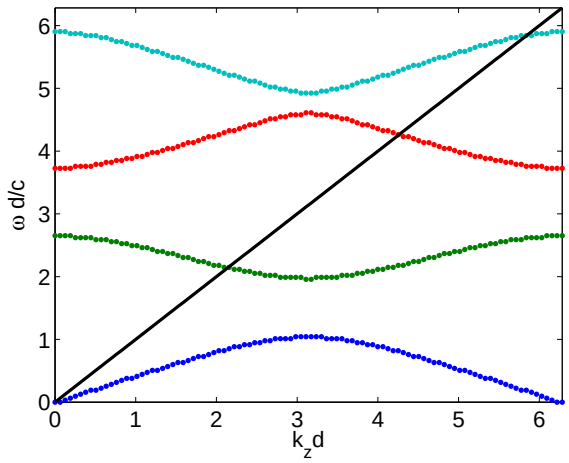

FIG. 2. Band structure calculated using method 1. The parameters are $d_1 = 0.4$, $d_2 = 0.6$, $n_1 = \sqrt{12}$ and $n_2 = 1$. The solid black line shows the light line.

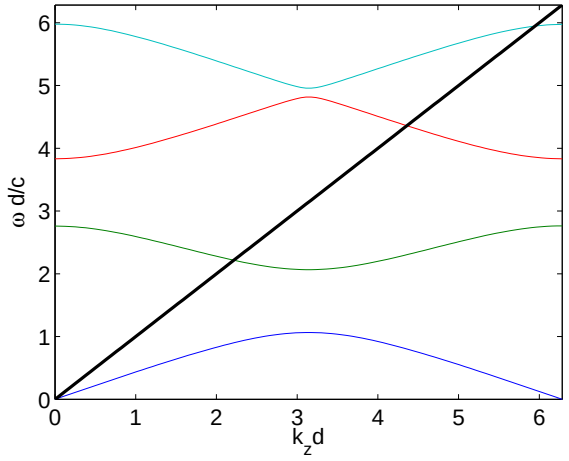

FIG. 3. Band structure calculated using method 1. The parameters are the same as for Fig. II. The solid black line shows the light line.

III. DISCUSSION

We have now reviewed two methods for finding the dispersion relation ω *vs.* k_z for a 1D photonic crystal. Calculated band diagrams using methods 1 and 2 are shown in Figs. II and II respectively. The code which generates the band diagrams is given in the Appendix. Of the two methods outlined above, the planewave expansion method seems to be superior. Apart from giving a shorter route to the band diagram, it also constructs a solution for the field distribution, which is not the case for Method 1. However, it is important to note that sufficient terms in the Fourier expansion must be taken in order for the correct band diagram to be obtained. Small differences seen in the band diagrams in Figs. II and II are due to the truncation of the Fourier series. Additionally, Method 1 allows us to use several different tools to arrive at the solution including Bloch's theorem. Finally, having two independent calculation methods allows us to check that the results are correct.

Appendix A: Code for plotting band diagrams

Code for plotting the band diagram using each of the methods covered above is given below. There is a notable difference between the two sets of code apart from their method. In the code for Method 1, scaled units are used from the start. In the code for Method 2, we use SI units and scale later. As noted in the code, the scale invariance of Maxwell's equations guarantees that the behaviour is universal, so that, for example, with the appropriate scaling, we could plot a photonic crystal band diagram for microwaves and one for visible light on the same axes.

1. Code for Method 1

```
% Clean up workspace
close all
clear all

% EM constants
c = 1; % In this example we will use normalized units
    % Due to the scale invariance of Maxwell's equations,
    % so long as we are consistent, the units we use don't matter.

% PhC constants
d1 = 4/10;
d2 = 6/10;
d = d1 + d2;
n1 = sqrt(12);
n2 = 1;
```

```
% Light constants
w = linspace(0,2*pi, 200);
D1 = w*n1 * d1;
D2 = w*n2 * d2;

% Right hand side of the characteristic equation is independent of k_z
RHS = cos(D1).*cos(D2) - 0.5*(n1^2+n2^2)/(n1*n2) * sin(D1) .* sin(D2);

% Define the wave number space
kz = linspace(0,2*pi,100);

% Calculate the bands, one point of kz at a time
for ll = 1:length(kz)

    LHS = cos(kz(ll)*d);

    [indw,zero] = crossing(LHS-RHS,w); % Zero finding algorithm

    if (length(indw)>=1)
            imin = sort(indw);
           Omegas = w(imin);


        if (ll == 1)
            figure(1)
            clf
            plot(kz(ll)*d,Omegas*d/c,'.','MarkerSize',10)
        else
            figure(1)
            hold on
            plot(kz(ll)*d,Omegas*d/c,'.','MarkerSize',10)
            hold off
        end

    end


end

% Add light line
figure(1)
hold on
plot(kz,abs(kz),'k-','LineWidth',2)
hold off
axis([min(kz*d),max(kz*d),min(w*d/c) max(w*d/c)])

set(gca,'FontSize',14)
xlabel('k_zd','FontSize',14)
ylabel('\omega d/c','FontSize',14)
ylim([0,2*pi])
```

2. Code for Method 2

```
% Band diagram from the plane wave decomposition method as
% per A. J. Danner's notes
% http://www.ece.nus.edu.sg/stfpage/eleadj/planewave.htm

% Clean up workspace
clear all
%close all

% PhC parameters
d1 = 400e-9;
d2 = 600e-9;
d = d1 + d2;
n1 = sqrt(12);
n2 = 1;

% Input light parameters
kz = linspace(0,2*pi/d,100);
c = 3e8;

% Decomposition constants
N = 12; % This chooses the number of bands
% NB: choosing this number too small will lead to
% an innacurate band diagram due to truncation of
% the Fourier series.

% Create matrix and solve eigenvalue equation
w2 = zeros(2*N+1,length(kz)); % Set up storage array

for kk = 1:length(kz)
    % Make matrix using for loop
    M =zeros(2*N+1,2*N+1)
    for nn = (-N):N
        for pp = (-N):N
            Fn = (d1/d) * (1/n1^2-1/n2^2) * sinc((pp-nn)*d1/d);
            if ((pp-nn)==0)
               Fn = Fn + 1/n2^2;
            end
            M(nn+N+1,pp+N+1) = (2*pi/d*nn + kz(kk))^2 * Fn ;

        end
    end
    w2(:,kk) = sort(eig(M)); % Find and sort the eigenvalues

end

% Plot band diagram
figure(2)
clf
plot(kz*d,sqrt(w2)*d)
hold on
plot(kz*d,abs(kz)*d,'k-','LineWidth',2)
hold off
axis tight
set(gca,'FontSize',14)
xlabel('k_zd','FontSize',14)
ylabel('\omega d/c','FontSize',14)
ylim([0,2*pi])
```

[1] John David Shumpert, "Modelling of periodic dielectric structures (electromagnetic crystals)", PhD Thesis, University of Michigan (2001).
[2] L. Novotny and B. Hecht, *Principles of nanophotonics*, Cambridge University Press (2012).
[3] J. O. Grepstad, "Excercise: 1D Photonic crystal and band gaps", `http://www.iet.ntnu.no/courses/tfe13/ovinger/PC_oving_2`.
[4] A. Danner, `http://www.ece.nus.edu.sg/stfpage/eleadj/planewave`