Simulations of Photonic Crystal Structures

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Abstract

This document is intended to serve as a manual for electromagnetic simulations of photonic crystal structures, i.e. structures that possess periodicity in their material dielectric response, or permittivity. When an electromagnetic wave propagates through such a structure, it experiences periodic scattering events. Since these scattering events are *coherent* (i.e. phase information is preserved), periodicity-dependent interference effects are seen. These effects can be quite dramatic–including a slowing down of wave propagation, to the creation of a forbidden-frequency region–very different from wave propagation in a bulk material. The physical concepts underlying wave propagation in such structures will be introduced, along with instructions in the use of open-source software for validating and further exploring these concepts. *Note*: The theoretical sections of this manual are largely inspired by the elegant exposition on the subject by J D Joannopoulos et al. in their book [1]. Some theoretical explanations and simulation results are reproduced from the author's doctoral thesis [2].

I. Propagation through bulk media

Let us start with the simplest of electromagnetic waves, a plane wave, that is travelling through the simplest of materials, a bulk material of relative permittivity $\epsilon_r(r) = \epsilon_r$, relative permeability, $\mu_r(r) = \mu_r$. It is easy to see that the electric field of such a wave given by $\vec{E}(\vec{r}, t) = \vec{E}_0\, e^{j(\vec{k}\cdot\vec{r}-\omega t)}$, satisfies our beloved Maxwell's equations

$$\nabla \times \vec{E}(r) = -\frac{\partial B(r)}{\partial t} = j\omega\mu_0\mu_r(r)\vec{H}(r), \quad \nabla \times \vec{H}(r) = \frac{\partial D(r)}{\partial t} = -j\omega\epsilon_0\epsilon_r(r)\vec{E}(r) \tag{1}$$

where $\vec{k}$ is the wavevector (which corresponds to the direction of propagation of the plane wave), and $\vec{E}_0$ is some constant vector in the plane orthogonal to $\vec{k}$. Without loss of generality, assume that the wave is travelling along the $x-$direction, i.e. $\hat{k} = \hat{x}$. Plugging in the field into the above equations, we get the following relation

$$\omega = \frac{c}{\sqrt{\epsilon_r\mu_r}}\, k \tag{2}$$

This relation between frequency and wavevector, is called a dispersion relation for the material. It is common to use a system of units where the speed of light, $c \equiv 1$, in which case the dispersion relation for vacuum is a 45° line through the origin. Since the refractive index, $n = \sqrt{\epsilon_r\mu_r} > 1$, the dispersion relation for any other material has lower slope than that for vacuum.

II. Propagation in periodic structures

A. Master Equation

In a periodic structure, by definition the permittivity, ϵ_r, is a function of space. In such a case, the simple dispersion relation derived above doesn't hold. By combining the equations in (1) above, we get the vector wave equation

$$\nabla \times \left(\frac{1}{\epsilon(r)}\nabla \times \vec{H}(r)\right) = \left(\frac{\omega}{c}\right)^2 \vec{H}(r), \text{ or}$$
$$\Theta\vec{H}(r) = \left(\frac{\omega}{c}\right)^2 \vec{H}(r) \tag{3}$$

where the eigen operator, Θ, is defined as $\Theta \equiv \nabla \times \left(\frac{1}{\epsilon(r)}\nabla \times\right)$, and $\left(\frac{\omega}{c}\right)^2$ are the eigenvalues. The above equation is commonly referred to as the *master equation* [1]. The operator Θ has certain nice mathematical properties (which will not be derived here); it is a linear, positive semi-definite, Hermitian operator, as a consequence of which, its eigenvalues are real, non-negative, i.e. $\omega^2 > 0$. Further, non-degenerate eigenfunctions are orthogonal to each other.

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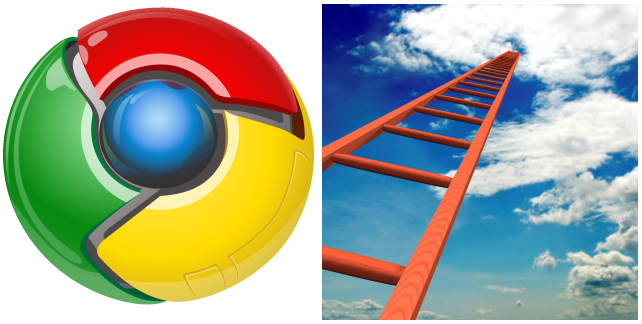

Fig. 1. Left panel: 3-fold rotational symmetry. Right panel: discrete translational symmetry.

B. Symmetries

Consider a spatial direction $\hat{s}$ in which the permittivity is periodic (with period s) such that

$$\epsilon(\vec{r}) = \epsilon(\vec{r} + n\, s\, \hat{s}), \quad n \in \mathbb{Z} \tag{4}$$

The above equation describes a discrete translation, which can be formally denoted by an operator T_s which acts in the following way: $T_s\, \epsilon(\vec{r}) = \epsilon(\vec{r} + \vec{s}) = \epsilon(\vec{r})$. Since the system is invariant under the application of the operator, it must be a symmetry of the system. Stated differently, the discrete translation operator T_s must commute with the operator Θ in the master equation (3) (i.e., the order of application of T, Θ should not matter). As a result, the eigenfunctions of the master equation must be simultaneous eigenfunctions of both operators (See Appendix A for a proof).

One might wonder, why bother with all these intricacies? The simple reason is that it is much easier to find eigenfunctions for a simple operator such as T_s, than for a complicated one such as Θ. Using the property of simultaneous eigenfunctions, we can classify the overall eigenfunction according to the simpler eigenfunctions of T_s.

Fig. 1 shows some examples of discrete rotational and translational symmetry. Consider the logo of the Google Chrome. The symmetry axes are placed 120° apart. So, this an example of a 3-fold rotational symmetry (In general, if the axes are placed apart by an angle of θ we call it a n-fold symmetry, where $n = 360/\theta$). A ladder which is infinitely long is an example of discrete translational symmetry in 1-dimension. Here, the periodicity is the spacing between the steps of the ladder. Note that if someone is making the ladder finite by truncating it after a certain step the symmetry wouldn't be preserved anymore (i.e. symmetry would be broken).

C. Bloch's theorem

Now, the discrete translation operator, T_s, clearly admits exponential-type eigenfunctions, since

$$T_s\, e^{j\vec{k}\cdot\vec{r}} = \left(e^{j\,\vec{k}\cdot\vec{s}}\right) e^{j\,\vec{k}\cdot\vec{r}} \tag{5}$$

Note that if $\vec{k}$ in the above equation (5) is replaced by $\vec{k} + (2\pi/s)\,\hat{s}$, a degenerate eigenfunction is generated whose eigenvalue, by definition, is the same. Thus, it is sufficient to restrict $\vec{k}$ to say, $|k| < \pi/s$. This vector $\vec{s} = (2\pi/s)\hat{s}$ is referred to as the *reciprocal lattice vector*. This general concept of a reciprocal lattice vector is very important when calculating the dispersion diagram.

Let us take a concrete example of a medium having periodicity in the x-direction. Since the eigenfunction must be a simultaneous eigenfunction of the translational operator as well, we can write an eigenfunction as

$$\vec{H}(x,y,z) = \vec{H}_0(y,z)\, e^{j\vec{k}\cdot\vec{x}}, \quad \text{which is generalized by } \vec{k} \to \vec{k} + n\vec{s} \tag{6}$$

$$\vec{H}(x,y,z) = \{\vec{H}_0(y,z)\, e^{j\vec{k}\cdot\vec{x}}\}\{\sum_{n\in\mathbb{Z}} \kappa_n(y,z)\, e^{jn(2\pi/s)\hat{s}\cdot\vec{x}}\} \tag{7}$$

where $\kappa_n(y,z)$ is the coefficient of the n^{th} eigenfunction (constant w.r.t. x). Thus, by simply using symmetry arguments, we have arrived at a very powerful result, known as Bloch's theorem, that expresses the eigenfunction as a plane wave expansion (left term in curly brackets in RHS of (7)) modulated by a periodic function (right term in curly brackets in RHS of (7)), also called a Bloch state. Note the immediate difference between this relation and that for a bulk medium; in a bulk medium the eigenfunctions of the master function are simply plane waves. Adding periodicity to the system has now resulted in the plane wave being modulated by a periodic function.

D. Reciprocal Lattice Space

In the case of the system having x-periodicity, we have $\hat{s} = \hat{x}$. Since the translation operator only translates along the x-direction, it is sufficient to restrict only the x-component of the wavevector, i.e. $\vec{k} \cdot \hat{x} = k_x$, $|k_x| < \pi/s$, where as the other components of the wavevector face no such restriction. It can be thought that k_x belongs to a restricted space of reciprocal lattice vectors. This space is referred to as the *Brillouin* zone (In order to construct the Brillouin zones for different lattices one can follow the procedure given in this tutorial: http://www.doitpoms.ac.uk/tlplib/brillouin_zones/zone_construction.php).

Analogous to the manner in which the discrete translational symmetry of the dielectric structure reduced the set of reciprocal wave vectors, k_x to the Brillouin zone, additional symmetries that might exist in the structure (rotations or reflections) further reduce the Brillouin zone to what is known as the irreducible Brillouin zone.

As an example, we note that for a loss-less material the operator Θ in (1) is real. By taking the complex conjugate of (1), we realize that $\vec{H}(r)$ and $\vec{H}^*(r)$ share the same eigenvalues. Further, given the form of (6) we see that $\vec{H}^*(r)$ is a Bloch state at wavevector $-\vec{k}$, and thus $\omega(\vec{k}) = \omega(-\vec{k})$. As a result, we have reduced the Brillouin zone to $0 < k_x < \pi/s$. Note that in this case complex conjugating is equivalent to reversing the direction of time in Maxwell's equations ($t \to -t$), therefore this effect of Brillouin zone reduction is a consequence of time-reversal symmetry.

E. Dispersion relations

Given the dielectric structure $\epsilon(r)$ of a photonic crystal, the eigenmodes (of the form in (7)) can be found by solving the master equation (1) and each mode can be labelled by its eigenfrequency ω and its wave vector $\vec{k}$ from the irreducible Brillouin zone. This leads to the dispersion relation $\omega(\vec{k})$ for a photonic crystal; each $(\omega, \vec{k})$ point is called a *guided* mode of the system.

A consequence of the periodic nature of the eigenfunctions in (7) is that the spectrum of eigenvalues of the Hermitian operator, Θ, is discontinuous. That is, at each given $\vec{k}$ point, the set of eigenvalues form a discrete set, i.e. at a fixed $\vec{k}$ we have a discrete set of frequencies. Graphically viewed, we pick a point $\vec{k}$ on the x-axis, and corresponding to this point we have a set of discrete ω points along the y-axis. Now, $\vec{k}$ enters into (7) (and hence in (1)), in a continuous sense within the irreducible Brilluoin zone, which, along with the previous observation leads to discrete bands of eigenfrequencies. Graphically viewed, as we slide $\vec{k}$ along the x-axis, the discrete ω points trace out a line, or 'band.' As $\vec{k}$ approaches the edges of the Brillouin zone, the band structure is continued by a "folding" of the bands. See Figure (2) for an illustration of a band structure for a 2D photonic crystal.

F. Photonic Band Gap

An important property of photonic crystals, the photonic band-gap, can now be explained. We find from energy minimization arguments, that it is preferable for *most* of the electric field to be concentrated in a region of *high* $\epsilon(r)$[1]. Now, as a mode in a particular band approaches an edge of the Brillouin zone with increasing $|\vec{k}|$, it gets folded and creates a second band. As noted previously, modes (and hence bands) with different eigenvalues are orthogonal. As a result of all the above, at an edge of the Brillouin zone, orthogonality between the two bands can only be maintained if the two bands differ in frequency. The mode in the lower band (called the dielectric band) concentrates its energy in regions of high $\epsilon(r)$, while remaining orthogonal to the mode in the higher band (called the air band), which concentrates its energy in the regions of lower $\epsilon(r)$. It is this splitting in frequency that creates a photonic band-gap: a spectral region that does not contain any eigenmodes of the system. The width of this band-gap is correlated with the dielectric contrast $(\epsilon_{max}/\epsilon_{min})$ in the structure.

Within the photonic band gap, there are no electromagnetic modes allowed. But, hypothetically speaking, if an electromagnetic excitation within the band gap is launched in a photonic crystal, what is it's nature? It turns out that the wavevector in this case happens to be complex, i.e. the modes are evanescent. Thus, in the simple case of a 1D photonic crystal, (6) becomes of the form $\vec{H}(x, y, z) = \vec{H}_0(y, z)\, e^{jkx}\, e^{-\kappa x}$, thus decaying as a function of x.

The presence of a photonic band-gap in one or more dimensions makes photonic crystals very elegant structures for constructing resonators. Such resonators, called photonic crystal cavities, are based on the principle that if an electromagnetic excitation (light) within the band-gap can be excited in the crystal, its

[1]We must take this on faith for now. The curious can look up the Electromagnetic Variational theorem for a rigourous derivation.

propagation within the crystal is inhibited, and it remains spatially localized in the neighborhood of the excitation.

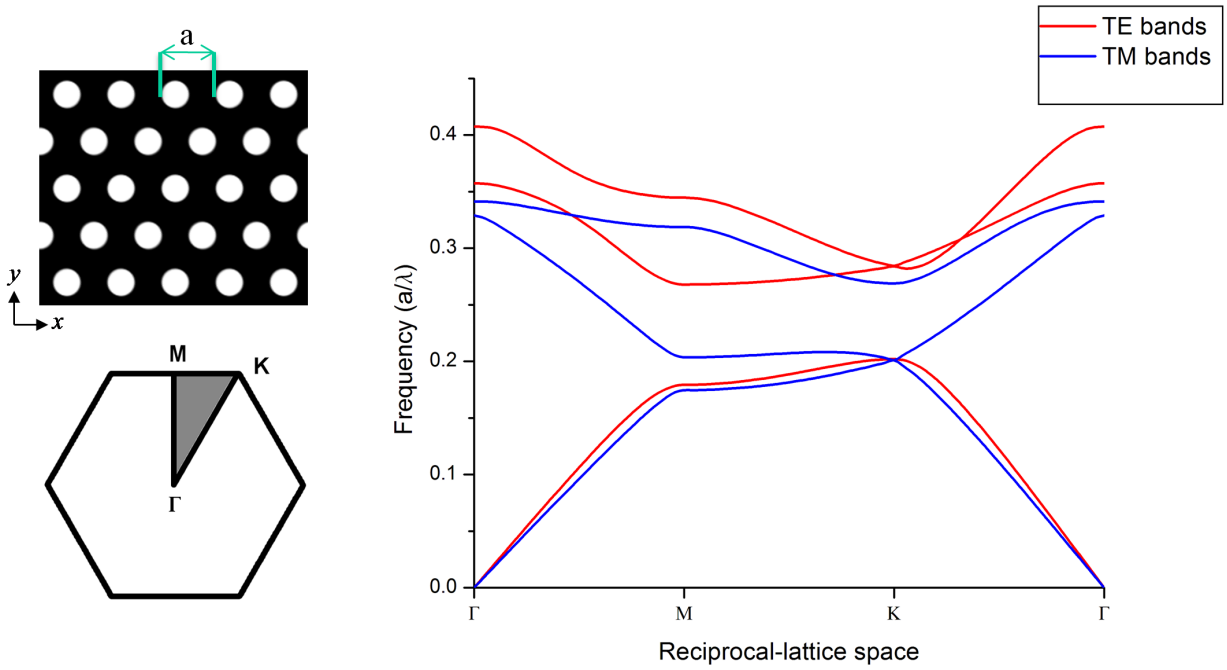

Fig. 2. (Left) Real-space and reciprocal-space representation of triangular lattice of air holes (radius $r = 0.30\ a$) in an infinitely thick structure ($\epsilon_r = 12.605$). (Right) Corresponding dispersion relation showing transverse electric (TE) and transverse magnetic (TM) eigenmodes. Reproduced from [2].

G. Example of a 2D photonic crystal

As a concrete example, consider a two-dimensional photonic crystal of air holes in a dielectric substrate. The software MPB [3] is used to generate the dispersion relation in Figure (2). An image of the real-space lattice is shown in the top left of the same figure. Here, a triangular lattice of air holes with periodicity 'a' (also called the lattice constant) is considered. The irreducible Brilouin zone is shown in the bottom left pane of the Figure. The Γ point refers to the origin of the zone, ($\Gamma = \vec{0}$), i.e. with no in-plane wavevector. The x-axis of the dispersion diagram is derived by walking from $\Gamma\,(0,0)$ to $M\,(0,1)\pi/a$ to $K\,(1/2,\sqrt{3}/2)\pi/a$ and back to Γ. Any arbitrary wavevector can be constructed by linear combinations of these basis vectors. It is evident that different polarizations show different properties. For instance, TE modes show a complete band gap, where as TM modes do not, and so on.

H. Example of a 2D photonic crystal slab

So far, the photonic crystal structure we have considered has infinite extent in the third dimension (z). Obviously, such a structure is not practically realizable. While it would be ideal to have a 3-dimensional photonic band-gap, its fabrication is a major challenge (but possible!). If a planar fabrication sequence is adopted instead (the same fabrication technology used to fabricate most electronic devices), we are naturally led to devices which use the photonic bandgap principle in one or two dimensions alone. Such devices are called photonic crystal slabs.

As mentioned previously, the extent of the band-gap depends on the dielectric contrast ($\epsilon_{max}/\epsilon_{min}$) in the structure. A larger band-gap results in a tighter confinement of light to the resonator, and allows room for some device imperfections that are inevitable during fabrication. A maximum dielectric contrast is possible when a high index material is surrounded by air ($\epsilon_r = 1$).

Frequency domain simulations of a photonic crystal slab consisting of a triangular lattice of air holes reveal the extent of the photonic band-gap as a function of the in-plane Bloch wave vectors, as seen in Figure 4. An important point here: Since the structure only has 2D periodicity, light is (incompletely) confined in the vertical direction by total-internal-reflection. Any mode (designated by $[\omega, k]$) lying above the light line (defined as, $\omega = c\,k$) will always couple to the continuum of electromagnetic modes (called radiation modes).

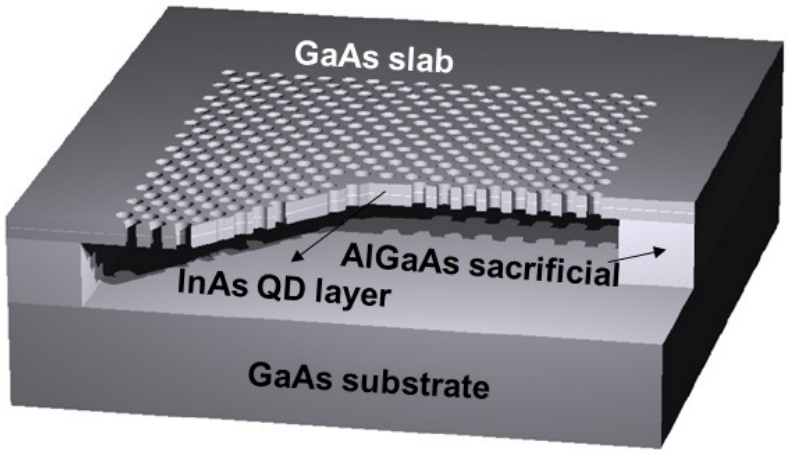

Fig. 3. Schematic of a realistic air-suspended 2D photonic crystal slab made out of a triangular lattice of air holes in Galium Arsenide (GaAs). Embedding quantum dots (QD) in between the slab allows the creation of 'active' devices such as lasers.

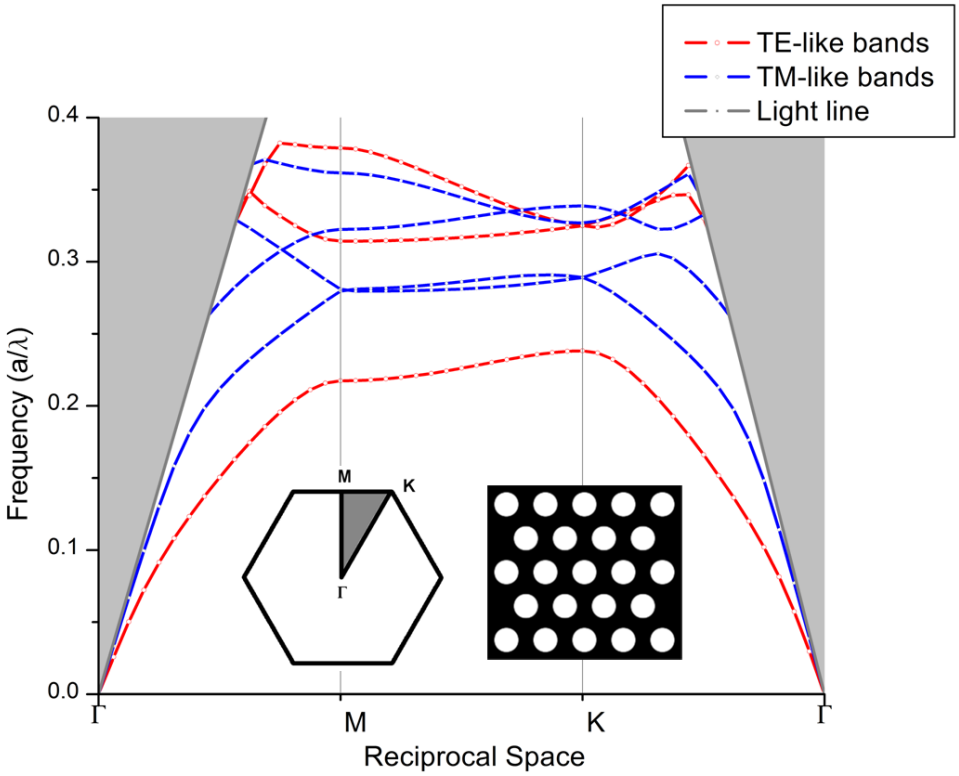

Fig. 4. Dispersion diagram for a photonic crystal slab. TE-like and TM-like eigenmodes are shown for a triangular lattice photonic crystal slab (thickness $d = 0.75\ a$, radius $r = 0.30\ a$, $\epsilon_r = 12.605$). Insets show real-space and reciprocal-space representation of the photonic crystal.

Why is this? Consider a mode of the photonic crystal and some plane wave far away from the device. We know that for a plane wave the following relation always holds, $\omega = c\|k\| = c\sqrt{k_\perp^2 + k_\|^2}$, where $k_\|$ is an in-plane wavevector, and $k_\perp$ is the perpendicular component of the wavevector. Within a photonic crystal structure, $k_\|$ is restricted to belong to the Brillouin zone (which corresponds to picking a point from the x-axis of Figure 2 or 4). Thus, for a photonic crystal mode with $\omega > ck_\|$, a suitable amount of $k_\perp$ (which is unrestricted) can be added to make it resemble a plane wave ($\omega = ck$) and hence couple to it. Correspondingly, no real value of $k_\perp$ exists for a mode below the light line, i.e. modes below the light line can not couple to radiation modes.

As a result of the above, the photonic band-gap in this case is defined as the frequency range that is devoid of any *guided* modes [4] below the light line (i.e., for $\omega < ck$). Radiation modes, of course, exist at all frequencies. These are typically masked out of the dispersion relation (note the grey cones in Figure 4).

It should be noted that all guided bands can be divided into two groups depending on the E-field symmetry with respect to the plane in the middle of the slab; even and odd (or equivalently, transverse electric [TE]-like or transverse magnetic [TM]-like, to invoke the similarities to their 2D counterparts). In case of the triangular lattice of air holes, it is well known that a band-gap exists only for TE-like modes, and this can be seen in Figure 4. Due to its resemblance to a cone, these regions are often called the light cones of the dispersion relation.

III. Computing band structures

Having being introduced to the theory of wave propagation in photonic crystal structures, we can now simulate these structures in the open source MIT Photonic Bands (MPB) software[3]. The native language in which the tool is used is Scheme, which is not a compiled language. This language has its peculiarities, particularly for users more accustomed to C-like languages. For example, consider a relation between two variables, say, $a = b/2$, and note the order in which the operator is specified in Scheme.

C-like	Scheme
`a=b/2`	`a (/ b 2)`

Navigate to the MPB user tutorial here: http://ab-initio.mit.edu/wiki/index.php/MPB_User_Tutorial and read through it to familiarize yourself with the language and band structure calculations (till section 4, "Bands of a triangular lattice"). Once done, read the first section ("Triangular Lattice of Rods") of the MPB data analysis tutorial to understand how to produce field plots, etc., http://ab-initio.mit.edu/wiki/index.php/MPB_Data_Analysis_Tutorial.
Update: there is now a Python version available.

A. On units

It is important to understand the correct the units used in MPB. All quantities are expressed in terms of the lattice constant of the structure, 'a', which we usually fix at unity. The speed of light is chosen to be 1. Since Maxwell's equations are scale-invariant, any calculations done at a single frequency simply need to be scaled to any other frequency of interest as long as the dielectric properties of the medium (ϵ_r, μ_r) remain unchanged. For example, say that we are interested in simulating a 1D photonic crystal with lattice-constant 2 cm in real units. In MPB, we set this lattice constant to be 1. If the wavelength of interest is say $\lambda = a/2 = 1$ cm, then in MPB the wavelength becomes 0.5, and the frequency $f = c/\lambda$ becomes 2 in MPB ($= 30$ GHz in real units).

Appendix
Simultaneous eigenfunctions of commuting operators

Let ψ be an eigenfunction of the operator T with eigenvalue t, i.e. $T\psi = t\psi$. Given that operators Θ and T commute, i.e. $T\Theta\,\psi = \Theta T\,\psi$, we get that $T\Theta\,\psi = t\Theta\,\psi$, implying that $\Theta\,\psi$ is an eigen function of T with the *same* eigenvalue, t. Assuming that none of the eigenfunctions are degenerate (i.e. no two eignefunctions produce the same eigenvalue), the only possibility is that $\Theta\,\psi$ and ψ, both of which have the same eigenvalue for the operator T, must be scalar multiples of each other. This is easy to see: if ψ has eigenvalue t, then $k\psi$ (where k is a scalar) also has the same eignevalue t for the operator T. We thus get: $\Theta\,\psi = k\psi$, which proves that ψ is also an eigenvalue of Θ.
In the context of Section II-B, the implication is that we can find the eigenfunctions of the master operator Θ by finding the eigenfunctions of simpler operators, like translation and reflection operators that commute with the master operator.

References

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