Chapter 2

The plane wave expansion method

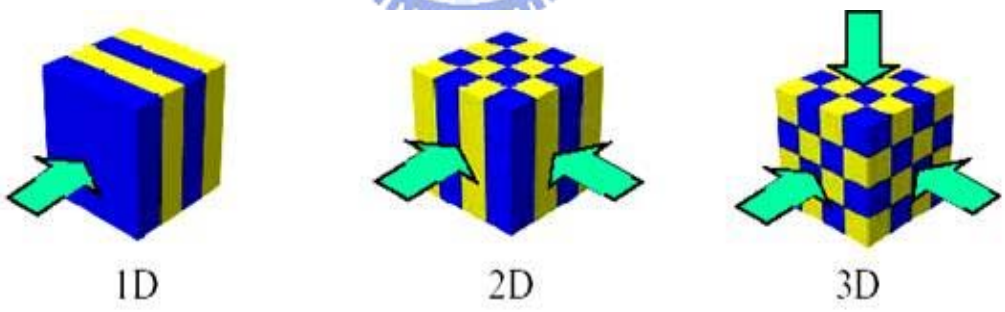
2.1 Plane wave expansion concept

In principle, plane wave expansion (PWE) can be applied to find the time-independent modes of any lossless photonic structure. For the most part, however, it is intended to be applied to structures with some degree of periodicity in the refractive index distribution. Indeed, even when applied to non-periodic structures, the calculation is performed by introducing an artificial periodicity.

To begin with, we introduce a number of standard concepts common to all periodic systems, electromagnetic or not. Subsequently, we derive some basic results for the vector Helmholtz equation as applied to periodic dielectric systems.

2.1.1 Geometry of periodic structures

PWE method can find the optical modes of photonic structures with periodic dielectric constants. For instance, in one, two and three dimensions the refractive index distribution $\varepsilon(R)$ can be pictured schematically like Fig. 2.1:



2.1 One, two and three dimensions photonic crystal structures.

It is a basic property of all periodic systems, photonic or not, that a periodic function f (R) can be expressed in terms of a lattice. A lattice is a set of discrete points in space that repeats periodically. Mathematically, we say that there are fixed vectors a_1, a_2 and a_3 such that for all points R in the lattice, $R= la_1+ma_2+na_3$, for some integers *l*, *m* and *n*. The points **R** are known as *lattice vectors*, while the basis vectors, a_1, a_2 and a_3 are termed *primitive lattice vectors*. (In one- or two-dimensional problems, we naturally need only one or two primitive lattice

vectors.) Note that the primitive lattice vectors are not unique. The connection between the *continuous* periodic function f (R) and the *discrete* lattice is provided by the *unit cell*. A unit cell is any region of space which, when translated by every lattice vector in the lattice, maps out the entire function.

2.1.2 The first Brillouin zone

When we study the optical modes of conventional photonic structures such as optical fibers or other waveguides, one of the central aims is to determine the dispersion relation $k = k(\omega)$ connecting the wavevector or *propagation constant* k of a given mode with the frequency ω. The propagation constant of course determines the phase velocity of the mode according to

$$E(x,t) = E(x,y)\exp(i\omega(t - z/v_p)) \quad (2.1)$$

where we have chosen a mode propagating along the z axis, and the phase velocity is $v_p=\omega/k$. If we invert the dispersion relation to obtain $\omega = \omega(k)$, then typically we find a different solution for every value of the wave vector k. So for example in an optical fiber, as we increase k without limit, the mode profile E(x,y) becomes ever more tightly bound to the core, and the effective index of the mode asymptotically approaches the core refractive index. For sufficiently large k, the system will support multiple modes and there are several solutions ω_i for each value of *k*. This kind of behavior may seem odd to treat the wavevector as the independent variable, since experimentally we have direct control over the frequency of the optical source, rather than the propagation constant.

2.1.3 Theory of band Structure

We now proceed to the calculation of band structures themselves. For technical reasons, we express the problem in terms of the magnetic field H(x) (see [1] for details). PWE solves for time independent solutions so we express the magnetic field as $\mathbf{H(x,t)=H(x)}\exp(-i\omega t)$. We first show that the magnetic field in a periodic system possesses a specific form.

The modes of the photonic crystal must of course be solutions of Maxwell's equations. However, symmetry considerations place restrictions on the possible form of the solutions. In

particular, the modes must satisfy the appropriate *translation symmetry*. Since the refractive index distribution is identical in every unit cell, a mode must remain unchanged if it is shifted in space by any lattice vector **R**. At most, the solution can change by a constant phase factor. We express the translation in terms of an operator $\hat{T}_R = \exp(iR \cdot \nabla)$ and seek solutions which are eigenvalues of $\hat{T}_R$—solutions which differ only by a change of phase under operation by $\hat{T}_R$.

Consider the form

$$H(x) = \exp(ikx)\sum_j c_j \hat{\varepsilon}_j \exp(iGx)$$

(2.2)

which represents an arbitrary plane wave multiplied by a Fourier series in the reciprocal lattice vectors. The c_j are expansion coefficients and the $\hat{\varepsilon}_j$ are polarization vectors chosen to guarantee that the field is transverse. Applying the translation operator to H(x), we obtain

$$\hat{T}_R H(x) = \sum_j c_j \hat{\varepsilon}_j \exp[i(k+G_j)\cdot R]\exp[i(k+G_j)\cdot x]$$
$$= \sum_j c_j \hat{\varepsilon}_j \exp[ik\cdot R]\exp[i(k+G_j)\cdot x]$$
$$= \exp[ik\cdot R][\exp(ik\cdot x]\sum_j c_j \hat{\varepsilon}_j \exp[iG_j \cdot x]$$
$$= \exp[ik\cdot R]H(x)$$

(2.3)

Thus, this form for the magnetic field changes by only a phase factor under translation by a lattice vector, and indeed satisfies the required symmetry. In fact, it can be shown that this is the most general form of solution possible, a result known as *Bloch's Theorem*--the magnetic field must take the form of a plane wave multiplied by a function with the periodicity of the lattice:

$$H(x) = \exp(ikx)u_k(x) \quad ,$$

(2.4)

where $u_k(x) = u_k(x+R)$ for all vector R. Note that Bloch's theorem justifies our earlier claim that in mapping the band structure, we only need to consider wavevectors **k** inside the 1BZ. For consider a wavevector k'outside the 1BZ. Then there is a reciprocal lattice vector G

such that k’ =k+G and **k** is inside the 1BZ. Therefore

$$H(x) = \exp(ik'x)u_{k'}(x)$$
$$= [\exp(ikx)\exp(iGx]u_{k'}(x)]$$
$$\exp(ikx)[\exp(iGx)u_{k'}(x)]$$
$$= \exp(ikx)u_k^{'}(x)$$

(2.5)

where we have used the fact that exp(iGx) is a function with the periodicity of the lattice. So any solution for a wavevector outside the 1BZ simply corresponds to a solution in a different band inside the 1BZ.

Since it relies only on symmetry arguments, Bloch’s Theorem applies far beyond photonics to problems of waves of all types in periodic systems.

We now derive the governing equation solved by PW*E*, which is based on the vector Helmholtz equation. Starting from the Maxwell curl equations in SI units:

$$\nabla \times E(x,t) = -\frac{\partial B}{\partial t},$$
$$\nabla \times H(x,t) = \frac{\partial D}{\partial t}$$

(2.6)

we assume for now that all materials are linear, lossless and isotropic, so that

$$D = \varepsilon_0 \varepsilon(x)E, B = \mu_0 H$$

(2.7)

where the dielectric function $\varepsilon(x)$ is the square of the refractive index. Taking time-independent solutions

$$E(x) = E(x)\exp(-i\omega t)$$
$$H(x) = H(x)\exp(-i\omega t) \qquad (2.8)$$

we can combine the Maxwell equations to obtain the vector Helmholtz equation

$$\nabla \times (\frac{1}{\varepsilon(x)} \nabla \times) H(x) = \frac{\omega^2}{c^2} H(x) \tag{2.9}$$

In the photonic crystal literature, this equation is sometimes referred to as the "master equation", though we shall not use this term here. Using Bloch's theorem, we write, $H(x) = \exp(ik \cdot x) u_k(x)$ where $u_k(x)$ is a function with the periodicity of the lattice. Inserting this expression in the Helmholtz equation we obtain

$$\hat{L} u_k = (ik + \nabla) \times (\frac{1}{\varepsilon(x)} (ik + \nabla) \times u_k = \varpi^2 u_k$$

(2.10)

where we have defined the operator $\hat{L}$ and the normalized frequency $\varpi = \omega / c$. This is the fundamental equation solved by PWE. It is to be viewed as an eigenvalue equation for the unknown eigenvalue ϖ and eigenvector u_k, with the wavevector k as a free parameter. This justifies our earlier discussion of dispersion relations using the wavevector as the independent variable. We emphasize again that is "back-to-front" to the normal picture for waveguide modes in which the frequency is the independent variable and the wavevector or propagation constant is the eigenvalue. In essence, this "back-to-frontness" is the price to be paid for exploiting periodic boundary conditions in the solution.

Our method of solution for Eq. (2.10) is discussed below.

For each value of **k**, Eq. (2.10) has an infinite number of solutions $\varpi_{k,n}$ labeled by the *band number n* in order of increasing frequency. In PWE, we use the convention that the lowest band is labeled by *n=0*. As we vary **k** over all possible values, the set of solutions $\varpi_{k,m}$ for a fixed integer m constitute a *band*, and the *band structure* of the crystal is the collection of all these bands. Thus a complete description of the band structure consists of finding all the solutions $\varpi_{k,m}$ for all values of **k** in the 1BZ. (For a numerical description, we of course discretize **k** at a suitable resolution and solve the problem at all the discrete values.) For any reasonable index distribution, the frequencies in a particular band , $\varpi_{k,m}$ vary smoothly as the wavevector varies, forming a curve in k-space in 1D problems, a surface in 2D problems

or a hypersurface in 3D problems.

The concept of a *band gap* arises by considering the relationship of adjacent bands, say m and m+1. In most cases, there are one or more points in **k**-space where the adjacent bands touch.

However, if the index distribution is chosen correctly, there can be adjacent bands which do not touch at any point. In this case, there is a range of frequencies between the two bands for which there are no solutions at all. Such a range comprises the *band gap*, and it is impossible for radiation of a frequency inside the gap to propagate in the crystal.

2.2. Problems with the Plane Wave Expansion Method

The PWE has the twin advantages of accuracy and efficiency. However, the approach has two drawbacks: (1) Inability to treat loss : The operator $\hat{L}$ is only Hermitian if the material is assumed to be lossless. The PWE method can therefore not account for materials with loss, or obtain complex eigenvalues representing decaying modes. (2) Inability to treat dispersion : As we have seen, the method solves for a number of frequency eigenvalues at a given wavevector k. In order for the minimization algorithm to make sense, the refractive index distribution must be assumed to be identical at all the frequencies of the modes being found. Consequently, it is not possible to account for material dispersion.

Reference

[1]. J. D. Joannapolous, R. D. Meade and J. N. Winn, *Photonic Crystals—Molding the Flow of Light*, (Princeton University Press, 1995).

[2] K. Sakoda, *Optical Properties of Photonic Crystals*, (Springer-Verlag, 2001).