# Study of EM waves in Periodic Structures

with addenda: "Study of EM waves in Periodic Structures (mathematical details)"

Massachusetts Institute of Technology
6.635 lecture notes

## 1  Introduction

We will study here the distribution of electromagnetic fields in dielectric periodic media. The main difference with the previous topic comes from the word "dielectric". Obviously, even a 2D periodic dielectric medium cannot be studied with the Green's functions presented in a previous lecture, since the Green's function was for periodic metallic structures.

In this topic, we will study the EM fields in media where:

- The material is *macroscopic* and *isotropic.*

- Since the material is constituted of real dielectric, we suppose we work in a small enough frequency band such that we can ignore the frequency dispersive behavior of $\epsilon$.

- The dielectric are lossless, so that $\epsilon$ is purely real.

## 2  Wave equations

### 2.1  Wave equations for $\bar{H}$

Starting from Maxwell's equations and using a permittivity $\epsilon = \epsilon(\bar{r})$, it is straightforward to show that we can write the following equations:

$$\nabla \times \left[ \frac{1}{\epsilon(\bar{r})} \nabla \times \bar{H}(\bar{r}) \right] = \left( \frac{\omega}{c} \right)^2 \bar{H}(\bar{r}) \,, \tag{1a}$$

$$\nabla \cdot \bar{H}(\bar{r}) = 0 \,. \tag{1b}$$

In this approach, the strategy is therefore:

1. Find the modes of $\bar{H}(\bar{r})$.

2. Find those of $\bar{E}(\bar{r})$ by solving Maxwell's equations.

Note that we can rewrite Eq. (1a) as an eigenvalue problem:

$$\Theta\,\bar{H}(\bar{r}) = \left(\frac{\omega}{c}\right)^2 \bar{H}(\bar{r})\,, \tag{2}$$

where

$$\Theta = \nabla \times \left[\frac{1}{\epsilon(\bar{r})}\nabla\times\right]. \tag{3}$$

Upon solving, we get the eigenvectors which correspond to the field patterns of the harmonic modes, and the eigenvalues which are proportional to the squared frequencies of these modes.

Note that $\Theta$ is a linear operator and that it is Hermitian. The demonstration of the last property is straightforward:

> Define a scalar product $< \bar{F}, \bar{G} >= \int d\bar{r}\ \bar{F}^\star(\bar{r}) \cdot \bar{G}(\bar{r})$ and show that (by integration by part for example): $< \bar{F}, \Theta\bar{G} >=< \Theta\bar{F}, \bar{G} >$, which is the definition of a Hermitian operator. The consequence of this property is of course that $\Theta$ has real eigenvalues.

## 2.2   Wave equations for $\bar{E}$

Another approach to get the fields would be of course to write the wave equation for $\bar{E}$ instead of for $\bar{H}$:

$$\nabla \times \nabla \times \bar{E}(\bar{r}) = \left(\frac{\omega}{c}\right)^2 \epsilon(\bar{r})\bar{E}(\bar{r})\,. \tag{4}$$

However, this system cannot be cast in a simple eigenvalue problem. Although it can still be solved for, it is far more complicated to get accurate results since the operator we would have to define would not be Hermitian. For this reason, this approach is in general avoided.

## 2.3   Bloch states

In a periodic medium, we know that the fields can be written as:

$$\bar{H}_k(\bar{r}) = e^{i\bar{k}\cdot\bar{r}}\bar{u}_k(\bar{r}), \qquad \bar{u}_k(\bar{r} + \bar{R}) = \bar{u}_k(\bar{r})\,. \tag{5}$$

Inserting into Eq. (2) yields:

$$(i\bar{k} + \nabla) \times \left[\frac{1}{\epsilon(\bar{r})}\,(i\bar{k} + \nabla) \times \bar{u}_k(\bar{r})\right] = \left(\frac{\omega(\bar{k})}{c}\right)^2 \bar{u}_k(\bar{r})\,, \tag{6}$$

so that the operator becomes:

$$\Theta = (i\bar{k} + \nabla) \times \left[\frac{1}{\epsilon(\bar{r})}\,(i\bar{k} + \nabla)\times\right] \tag{7}$$

Note that because $\bar{u}_k(\bar{r} + \bar{R}) = \bar{u}_k(\bar{r})$, the eigenvalue problem can be restricted to a small zone in space, which would necessarily imply a discrete spectrum of eigenvalues. Therefore, we expect a set of discrete modes for each $\bar{k}$.

# 3 Fundamentals of photonic crystals

We shall briefly explain some terminology here related essentially to solid state physics, but which is of prime importance for the study of the structures we are dealing with here.

## 3.1 Direct lattice (some details are given in the "mathematical details" addenda)

A photonic crystal is a periodic structure (that we will take to be dielectric here) in 1D, 2D or 3D.

Any vector $\bar{r}'$ in space can be written as

$$\bar{r}' = \bar{r} + \bar{R}, \tag{8}$$

where $\bar{R}$ is the translational vector in space defined by

$$\bar{R} = \alpha_1 \bar{a}_1 + \alpha_2 \bar{a}_2 + \alpha_3 \bar{a}_3, \tag{9}$$

where $\alpha_{1,2,3} \in \{\ldots, -2, -1, 0, 1, 2, 3, \ldots\}$ and $\bar{a}_1$, $\bar{a}_2$ and $\bar{a}_3$ are the lattice vectors.

From the lattice, we can construct the Wigner-Seitz cell as shown in Fig. 1.
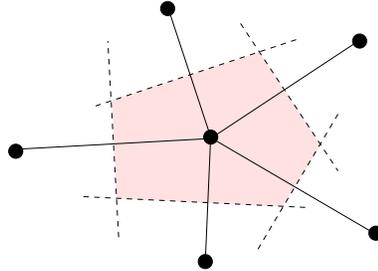


**Figure 1:** Wigner-Seitz cell for an arbitrary position of points: the cell is constructed by joining the center element to its closest neighbors and drawing perpendicular lines from to the center of these segments. The polygon thus created is the smallest repeatable cell of the periodic lattice, and is defined as the Wigner-Seitz cell.

Note that there exist only one type of lattice for a 1D photonic crystal, five distinct types for 2D photonic crystals (rectangular, square, hexagonal or triangle, centered rectangular and oblique), and fourteen for 3D photonic crystals.

## 3.2 Reciprocal lattice (some details are given in the "mathematical details" addenda)

We will use here the same notation as [Joannopoulos, Meade, and Winn, "*Photonic Crystals*"] and write the reciprocal translational vector as $\bar{G}$:

$$\bar{G} = \beta_1 \bar{b}_1 + \beta_2 \bar{b}_2 + \beta_3 \bar{b}_3, \tag{10}$$

where $\beta_{1,2,3} \in \{\ldots, -2, -1, 0, 1, 2, 3, \ldots\}$ and $\bar{b}_1$, $\bar{b}_2$ and $\bar{b}_3$ are the lattice vectors in the spectral domain.

For the sake of illustration, Tab. 1 gives the definition of vectors $\bar{a}$ and $\bar{b}$ for square and triangular lattices.

| Square lattice | $\bar{a}_1 = a\hat{x}$ | $\bar{b}_1 = 2\pi/a\,\hat{x}$ |
|---|---|---|
| | $\bar{a}_2 = a\hat{y}$ | $\bar{b}_2 = 2\pi/a\,\hat{y}$ |
| Triangular lattice | $\bar{a}_1 = a\hat{x}$ | $\bar{b}_1 = 2\pi/a\,(\hat{x} - \sqrt{3}/3\,\hat{y})$ |
| | $\bar{a}_2 = (\hat{x} + \sqrt{3}\hat{y})$ | $\bar{b}_2 = 2\pi/a\,2\sqrt{3}/3\,\hat{y}$ |

**Table 1:** Definition of $\bar{a}$ and $\bar{b}$ vectors for square and triangular (or hexagonal) lattice.

### 3.3    Bloch-Floquet theorem

From Bloch-Floquet theorem, we know that we can write the electric and magnetic fields as a summation over reciprocal vectors $\bar{G}$ (see the "mathematical details" part of the notes). This means that different $\bar{k}$ do not necessarily correspond to different modes and that therefore there is a redundancy in the label $\bar{k}$: we can therefore reduce the study to what is called the *first Brillouin zone* (which is the Wigner-Seitz cell in the reciprocal lattice). Some examples of Brillouin zones are given in Fig. 2 and Fig. 3.
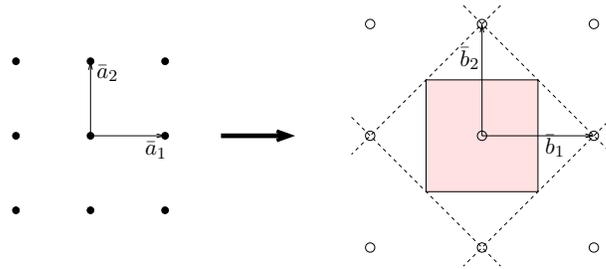


**Figure 2:** Direct square lattice and corresponding reciprocal lattice with highlighted Brillouin zone.
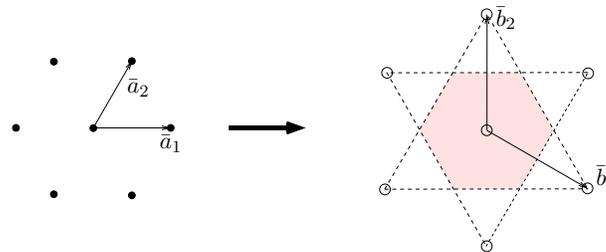


**Figure 3:** Direct triangular (or hexagonal) lattice and corresponding reciprocal lattice with highlighted Brillouin zone.

## 4    Bragg-like diffraction

The standard Bragg diffraction is illustrated in Fig. 4. Here, we will derive another diffraction condition, equivalent to Bragg, and shall see that the diffraction is entirely governed by the reciprocal vector $\bar{G}$.
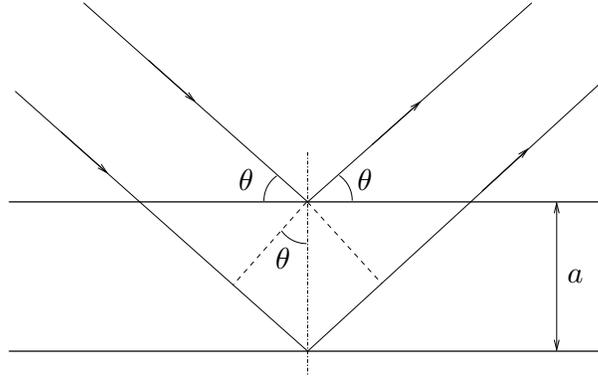
**Figure 4:** Schematic representation of Bragg diffraction. Maximal diffraction occurs at $2a\sin\theta = n\lambda$ where $\lambda$ is the wavelength of the electromagnetic wave and $n$ is an integer.

Referring to Fig. 5, we can write the scattering amplitude in terms of the reflection coefficient $\Gamma$ at position $\bar{r}$ times a phase factor.
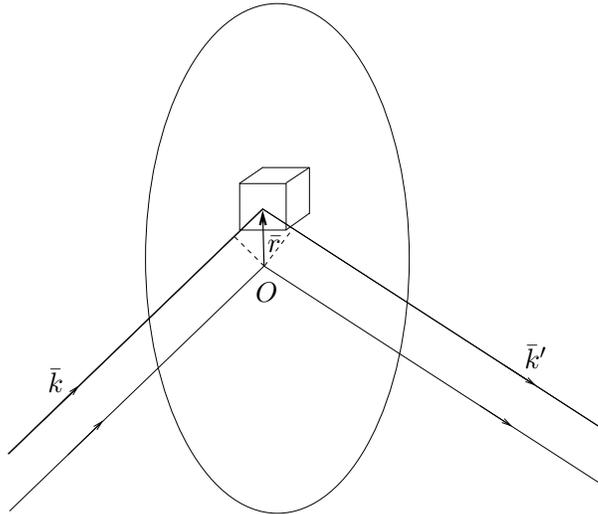


**Figure 5:** Diffraction from an elementary volume of a periodic medium: $\bar{k}$ is the wavevector of the incident wave whereas $\bar{k}'$ is the wavevector of the diffracted wave.

Upon integrating over the whole volume, we get:

$$F(\bar{k}, \bar{k}') = \int \Gamma(\bar{r}) e^{i(\bar{k}-\bar{k}')\cdot\bar{r}} \mathrm{d}v \,. \tag{11}$$

Since the medium is periodic, we can write:

$$\Gamma(\bar{r} + \bar{R}) = \Gamma(\bar{r}) = \sum_{\bar{G}} \tilde{\Gamma}(\bar{G}) e^{i\bar{G}\cdot\bar{r}} \,, \tag{12}$$

such that

$$F(\bar{k}, \bar{k}') = \sum_{\bar{G}} \int \tilde{\Gamma}(\bar{G}) e^{i(\bar{G}-\Delta\bar{k})\cdot\bar{r}} \mathrm{d}v \,, \tag{13}$$

where $\Delta\bar{k} = \bar{k}' - \bar{k}$. This amplitude is maximal when $\bar{G} - \Delta\bar{k} = 2m\pi$ or, when $m = 0$,

$$\bar{G} = \Delta\bar{k}. \tag{14}$$

This is an important relation which, again, is a condition for maximal diffraction. Upon expanding back in terms of $\bar{k}$ and $\bar{k}'$ and rising to the square, we write (noting that $|\bar{k}| = |\bar{k}'| = k$):

$$k^2 = k^2 + 2\bar{k} \cdot \bar{G} + G^2 , \tag{15}$$

or (taking $-\bar{k}$ instead of $\bar{k}$):

$$2\bar{k} \cdot \bar{G} = G^2 . \tag{16}$$

As an exercise, it is interesting to show that this condition is equivalent to the standard Bragg diffraction.

Upon dividing both terms of Eq. (16) by 4, we eventually write

$$\bar{k} \cdot (\frac{\bar{G}}{2}) = (\frac{\bar{G}}{2})^2 . \tag{17}$$

This last equation has a nice geometrical interpretation shown in Fig. 6 which shows that the vectors $\bar{k}$ that satisfy the maximum diffraction condition are actually those which lie on the edge of the Brillouin zone.
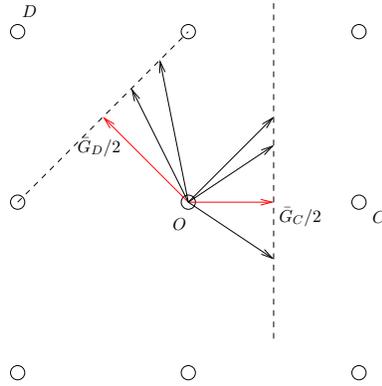


**Figure 6:** Graphical representation of Eq. (17): each vector $\bar{k}$ (black vector) with its tip on a dashed line (not all represented) will satisfy the equation. Graphically: all those $\bar{k}$ have the same projection on the generating vector $\bar{G}/2$ (red vector).

Therefore:

**The edge of the Brillouin zone plus its center ($\bar{G} = 0$) satisfy the maximum diffraction condition.**

This condition can also be rewritten in terms of group velocity: for those $\bar{k}$ which tip lie on the edge of the Brillouin zone and $\bar{k} = 0$, the component of the group velocity normal to the

Bragg diffraction planes tends to zero since the electromagnetic wave tends to be completely reflected for these $\bar{k}$:

$$v_g^{\text{norm}}(\bar{k} \in \text{BZ tip}) = \left(\nabla_k \omega(\bar{k})\right)^{\text{norm}} (\bar{k} \in \text{BZ tip}) \to 0 \,. \tag{18}$$

For the symmetry points, the diffracted wave is reflected in the direction of the incident wave so that for these points, the total group velocity is zero. This can be directly seen on the dispersion curves where, at the symmetry points of the crystal, the tangent to the curve is horizontal (except possibly for those points corresponding to a zero frequency).

# 5   Mathematical details

Using all the principles shown before, we can construct the eigenvalue system for $\bar{H}$ and then solve for $\bar{E}$. The detailed mathematical manipulations are given in the annex document "Study of EM waves in Periodic Structures (mathematical details)".

Note that to build the system, we need to evaluate the Fourier coefficients of the permittivity (or the inverse of the permittivity, $\kappa$). We shall show how to get these coefficients for the case of infinite dielectric rods $\epsilon_a$ of circular cross-section organized in a square lattice, embedded in a background of $\epsilon_b$. We therefore place ourselves in a 2D situation where the $\bar{G}$ vector will be written $\bar{G}_\rho$ to denote that it does not depend on $z$ (and similarly $\bar{R}$ will be noted $\bar{R}_\rho$).

As a reminder, we write the permittivity as:

$$\epsilon(\rho) = \sum_{\bar{G}_\rho} \tilde{\epsilon}(\bar{G}_\rho)e^{i\bar{G}_\rho \cdot \rho}, \qquad \tilde{\epsilon}(\bar{G}_\rho) = \frac{1}{\Omega}\int_\Omega \epsilon(\rho)e^{-i\bar{G}_\rho \cdot \rho} \,, \tag{19}$$

where $\Omega$ denotes the surface of the elementary cell.

The idea is to write the permittivity as

$$\epsilon(\rho) = \epsilon_b + (\epsilon_a - \epsilon_b)\sum_{\bar{R}_\rho} S(R_c - |\rho - \bar{R}_\rho|) \,, \tag{20}$$

where again the subscript $\rho$ in $\bar{R}_\rho$ denotes a dependency on $x$ and $y$ only, $R_c$ is the radius of the dielectric rods and $S$ denotes the step function. Merging these two equations, we get:

$$\tilde{\epsilon}(\bar{G}_\rho) = \frac{1}{\Omega}\int_\Omega \left[\epsilon_b + (\epsilon_a - \epsilon_b)\sum_{\bar{R}_\rho} S(R_c - |\rho - \bar{R}_\rho|)\right]e^{-i\bar{G}_\rho \cdot \rho}\mathrm{d}\rho \,,$$

$$= \frac{1}{\Omega}\int_\Omega \epsilon_b e^{-i\bar{G}_\rho \cdot \rho}\mathrm{d}\rho \, + \, \frac{1}{\Omega}\int_\Omega (\epsilon_a - \epsilon_b)\sum_{\bar{R}_\rho} S(R_c - |\rho - \bar{R}_\rho|)e^{-i\bar{G}_\rho \cdot \rho}\mathrm{d}\rho \,. \tag{21}$$

Let us call the first integral $I_1(\bar{G}_\rho)$ and the second integral $I_2(\bar{G}_\rho)$, and evaluate them separately.

*Evaluation of $I_1(\rho)$*

The first integral is easily evaluated as:

$$I_1(\bar{G}_\rho) = \begin{cases} \epsilon_b & \text{if } \bar{G}_\rho = 0 \\ 0 & \text{elsewhere} \end{cases} \tag{22}$$

*Evaluation of $I_2(\rho)$*

For the second integral, we can make the change of variable $\rho' = \rho - \bar{R}_\rho$. Since $\rho$ spans the whole domain $\Omega$ and $\bar{R}_\rho$ is the translational vector, $\rho'$ spans the whole space. We can therefore replace the sum of integrals over $\Omega$ by a single integral over the whole 2D space. We write then:

*If $\bar{G}_\rho = 0$:*

$$I_2(\bar{G}_\rho) = \frac{\epsilon_a - \epsilon_b}{\Omega} \iint \mathrm{d}\rho' S(R_c - |\rho - \bar{R}_\rho|) = (\epsilon_a - \epsilon_b) \frac{\pi R_c^2}{\Omega} = f_r(\epsilon_a - \epsilon_b), \tag{23}$$

where $f_r = \frac{\pi R_c^2}{\Omega}$ is the fractional volume.

*If $\bar{G}_\rho \neq 0$:*

$$\begin{aligned} I_2(\bar{G}_\rho) &= \frac{1}{\Omega}(\epsilon_a - \epsilon_b) \iint_{-\infty}^{\infty} \mathrm{d}\rho' \, S(R_c - |\rho - \bar{R}_\rho|) \, e^{-i\bar{G}_\rho \cdot \rho'} \\ &= \frac{\epsilon_a - \epsilon_b}{\Omega} \int_0^{R_c} \mathrm{d}\rho' \rho' \int_0^{2\pi} \mathrm{d}\phi e^{-iG_\rho \rho' \cos(\phi - \theta)} \\ &= \frac{\epsilon_a - \epsilon_b}{\Omega} 2\pi \int_0^{R_c} \mathrm{d}\rho' \rho' J_0(\rho' G_\rho), \end{aligned} \tag{24}$$

where we have used the change of variable (now standard) $x' = \rho' \sin\phi$, $y' = \rho' \cos\phi$, $G_x = G_\rho \sin\theta$, $G_y = G_\rho \cos\theta$, and the well-known identity for the Bessel function. Upon using $\int x J_0(\alpha x) \mathrm{d}x = x/\alpha \, J_1(\alpha x)$, we continue with

$$\begin{aligned} I_2(\bar{G}_\rho) &= \frac{2\pi}{\Omega}(\epsilon_a - \epsilon_b) \left[ \frac{\rho'}{G_\rho} J_1(G_\rho \rho') \right]_0^{R_c} \\ &= f_r(\epsilon_a - \epsilon_b) \frac{2 J_1(G_\rho R_c)}{G_\rho R_c}. \end{aligned} \tag{25}$$
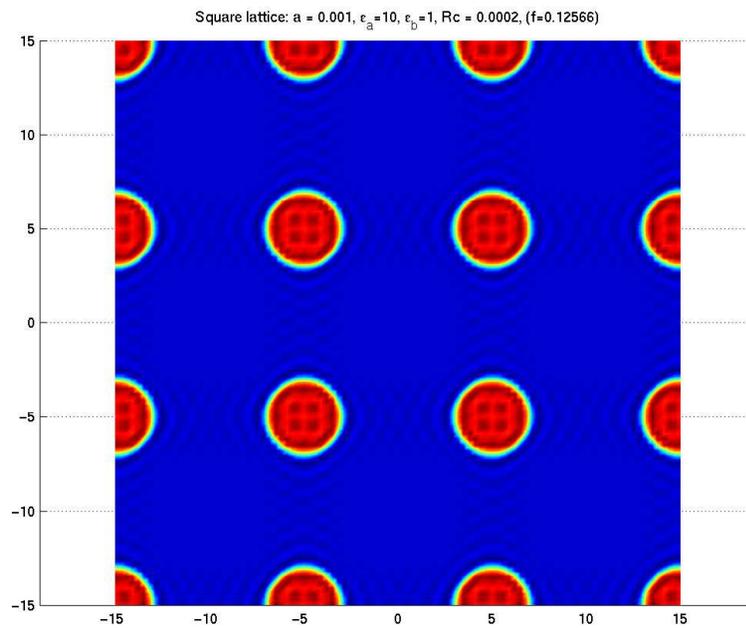
This lead to the final result that:

$$\tilde{\epsilon}(G_\rho) = \begin{cases} \epsilon_a f_r + \epsilon_b(1 - f_r) & \text{if } G_\rho = 0 \\ (\epsilon_a - \epsilon_b) f_r \frac{2J_1(G_\rho R_c)}{G_\rho R_c} & \text{elsewhere.} \end{cases} \tag{26}$$

The reconstruction of the permittivity is then straightforward, and examples of two lattice are given in Fig. 7.
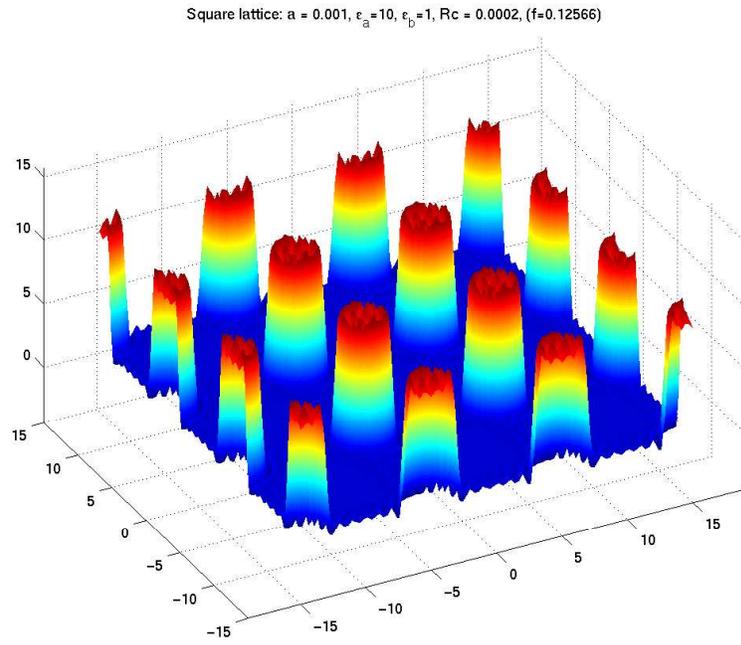
**(a)** Side view.



**(b)** Top view.

**Figure 7:** Reconstruction of the permittivity for cylindrical rods in a square lattice $\epsilon_a = 10$, $\epsilon_b = 1$, $R_c/a = 0.2$ (yielding a fractional volume $f_r = 12.5\%$).

# 6   Dispersion curves

At this point, we have everything to build the eigensystem (34) given in the additional document "Study of EM waves in periodic structures (mathematical details)". Solving it gives a set of eigenvalues that are directly related to the dispersion curve of the material. An example is given in Fig. 8.
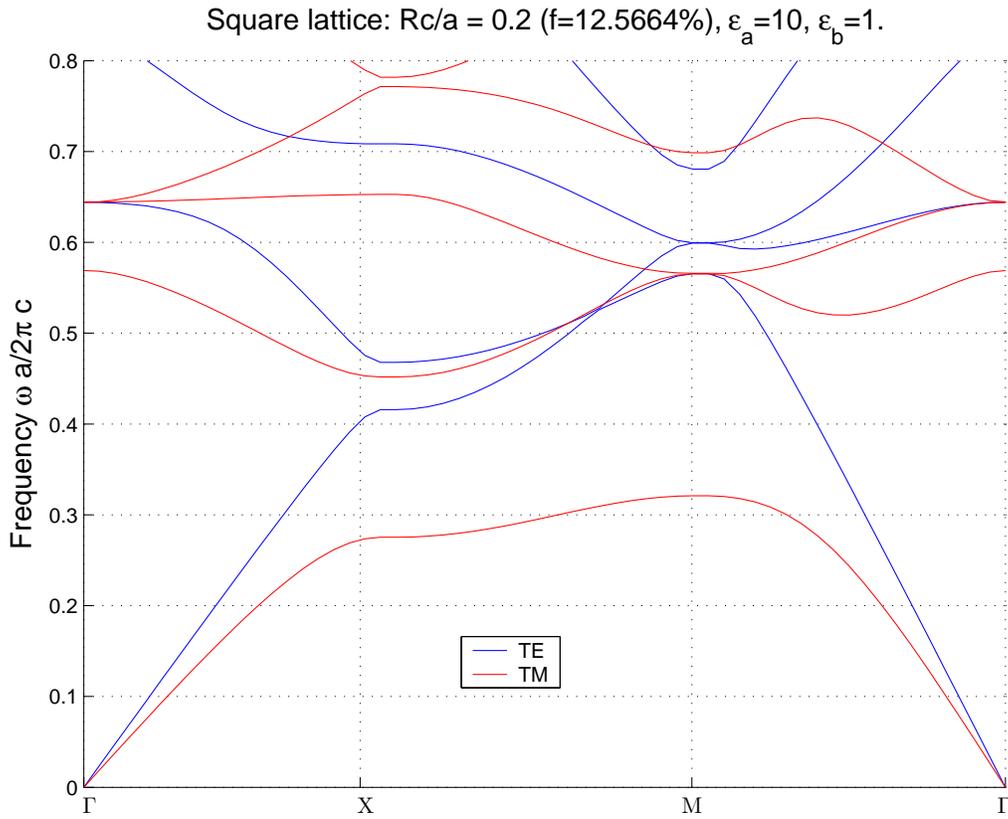
**Figure 8:** Dispersion diagram for the photonic crystal of Fig. 7.