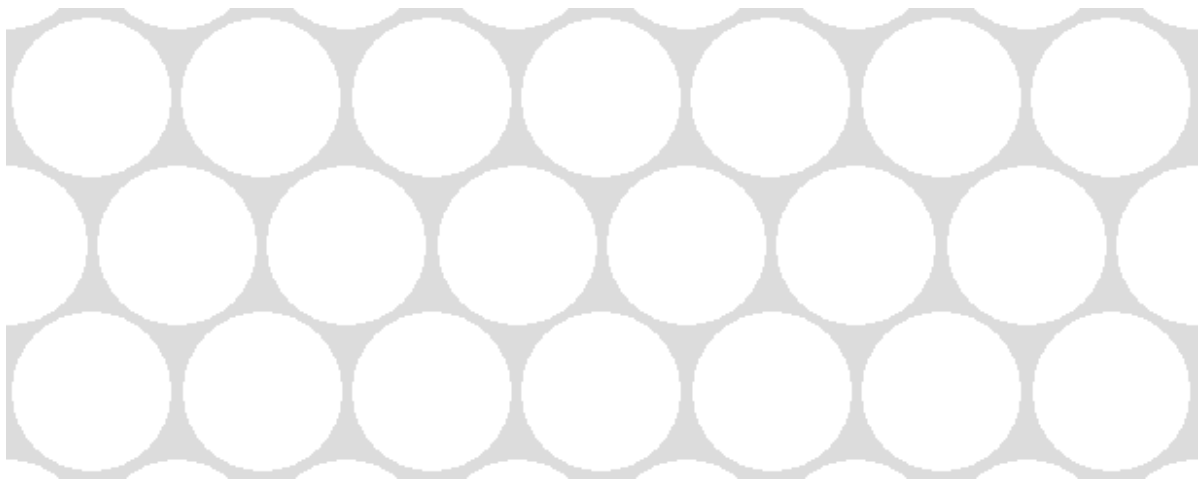


APPLICATION OF THE PLANE WAVE EXPANSION METHOD TO A TWO-DIMENSIONAL, HEXAGONAL PHOTONIC CRYSTAL



a Student Project for the Course Advanced Solid State Physics (513.804)



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1. Introduction

Photonic crystals are composed of periodic, dielectric structures that affect the propagation of electromagnetic waves. As in forbidden electronic energy bands in semiconductors there are certain frequencies for which electromagnetic waves can not travel through those crystals. These disallowed frequency regions are called photonic band gaps. The physical basis for this phenomenon is diffraction. In nature photonic crystals appear for example in structural colouration of butterfly wings or in algae as protection against ultraviolet radiation. There's a broad range of technical applications for artificially produced photonic crystals, for example in thin-film optics, photonic-crystal fibers and in future maybe even in optical computers.

There are several methods to calculate the dispersion relation and therewith the range of the band gaps. In this document we will apply the plane wave expansion method on a specific photonic crystal: a two-dimensional, hexagonal arrangement of air holes in a dielectric material. By doing so we will derive the dispersion relation and the density of states and thus the photonic band gaps. From the density of states finally we will be able to determine some thermodynamic properties.

2. Properties of the Considered Photonic Crystal

2.1. Dielectric Properties and Structure in Real Space

The photonic crystal that we consider is a hexagonal arrangement of air-holes in a dielectric material with a dielectric constant $\epsilon_M = 13$. We'll approximate the phase-velocity of the electromagnetic waves in air as the speed of light and we'll take into account that $\frac{c_M^2}{c^2} = \frac{1}{\epsilon_M}$. The ratio of the radius of the holes R to the lattice constant $a = 0.5 \mu m$ should be $\frac{R}{a} = 0.48$. Thus every plot in this document will be calculated with those properties. The primitive basis vectors for a hexagonal lattice in real space can be written as:

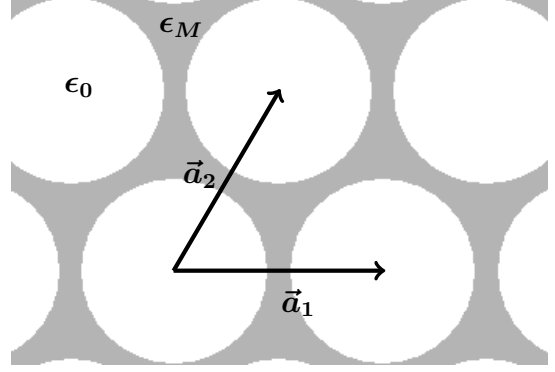


Figure 1: Structure of the photonic crystal in real space.

$$\vec{a}_1 = a \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (1a)$$

$$\vec{a}_2 = a \begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix} \quad (1b)$$

2.2. Reciprocal Lattice Vectors and Brillouin zone

If we assume that the photonic crystal is distributed over an infinitely big plane, then due to its periodicity a Fourier transformation of the physical properties is possible. This approach is the basis for the plane wave expansion method in which we additionally assume that the propagating electromagnetic waves are plane waves. For the Fourier transformation thus we will need the reciprocal lattice vectors:

$$\vec{G} = m\vec{b}_1 + n\vec{b}_2, \quad m, n \in \mathbb{Z} \quad (2)$$

Those are constructed by the reciprocal basis vectors \vec{b}_1 and \vec{b}_2 which result as:

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{e}_z}{\vec{a}_1(\vec{a}_2 \times \vec{e}_z)} = \frac{2\pi}{a} \begin{pmatrix} 1 \\ -\frac{1}{\sqrt{3}} \end{pmatrix} \quad (3a)$$

$$\vec{b}_2 = 2\pi \frac{\vec{e}_z \times \vec{a}_1}{\vec{a}_1(\vec{a}_2 \times \vec{e}_z)} = \frac{2\pi}{a} \begin{pmatrix} 0 \\ \frac{2}{\sqrt{3}} \end{pmatrix} \quad (3b)$$

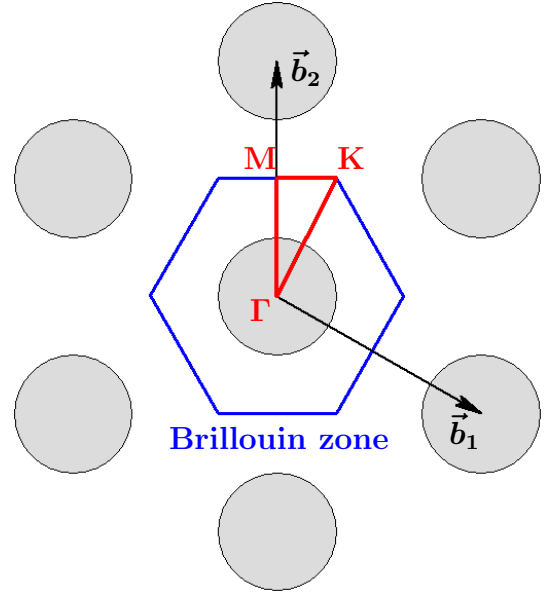


Figure 2: First Brillouin zone and high symmetric directions.

With those basis vectors the Brillouin zone can be constructed – see figure 2. We will need the wave vectors \vec{k} inside this zone for the calculation of the density of states. For the depiction of the dispersion relation just certain directions of high symmetry ($\overline{\Gamma\text{M}}$, $\overline{\text{MK}}$ and $\overline{\text{KT}}$) will be used.

3. Application of the Plane Wave Expansion Method

3.1. Starting from Maxwell's Equations

The propagation of electromagnetic waves can be described by Maxwell's equations. From those we will derive a set of equations, whose solutions can be approximated by the plane wave expansion method.

Due to the dielectric material two of Maxwell's equations – namely Faraday's and Ampère's law – can be written as:

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \quad (4a) \quad \vec{\nabla} \times \vec{B} = \mu_0 \epsilon(\vec{r}) \frac{\partial \vec{E}}{\partial t} \quad (4b)$$

For two dimensional problems the dispersion relation contains two types of solutions: transversal magnetic (TM) and electric (TE) modes. In TM modes the magnetic field of the propagating electromagnetic wave lies completely in the considered two-dimensional plane, whereat the electric field is perpendicular to that plane. For the TE modes the magnetic field is perpendicular to the plane. With the assumption of plane waves latter can be expressed as:

$$\vec{E}_{TM} = \vec{e}_z E(\vec{r}) e^{i(\vec{k} \cdot \vec{r} - \omega t)} \quad (5a) \quad \vec{B}_{TE} = \vec{e}_z B(\vec{r}) e^{i(\vec{k} \cdot \vec{r} - \omega t)} \quad (5b)$$

Because the time derivation then yields to a factor $-i\omega$, equation (4b) can be substituted into (4a) and vice-versa, what gives with $\mu_0 \epsilon(\vec{r}) = c(\vec{r})^{-2}$:

$$c(\vec{r})^2 \vec{\nabla} \times \vec{\nabla} \times \vec{E}_{TM} = \omega^2 \vec{E}_{TM} \quad (6a) \quad \vec{\nabla} \times (c(\vec{r})^2 \vec{\nabla} \times \vec{B}_{TE}) = \omega^2 \vec{B}_{TE} \quad (6b)$$

On the right hand side of latter equations just the z-component is non-zero. Hence just the last line will contain ω and can be used for the calculation of the dispersion relation. After writing out the differential operators for equations (6a) and (6b) the line that contains ω can be written as:

$$c(\vec{r})^2 \left[-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} \right] E(\vec{r}) e^{i(\vec{k} \cdot \vec{r})} = \omega^2 \vec{E}(\vec{r}) e^{i(\vec{k} \cdot \vec{r})} \quad (7a)$$

$$\left[-\frac{\partial c(\vec{r})^2}{\partial x} \frac{\partial}{\partial y} - \frac{\partial c(\vec{r})^2}{\partial y} \frac{\partial}{\partial x} - c(\vec{r})^2 \left[\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} \right] \right] B(\vec{r}) e^{i(\vec{k} \cdot \vec{r})} = \omega^2 \vec{B}(\vec{r}) e^{i(\vec{k} \cdot \vec{r})} \quad (7b)$$

3.2. Derivation of the Central Equations by Fourier Expansion

Due to the assumed periodic arrangement of the holes over an infinitely big two-dimensional plane it can be assumed that the phase velocity and the components of the electric and magnetic field can be expanded as a Fourier series:

$$c(\vec{r})^2 = \sum_{\vec{G}} c_{\vec{G}}^2 e^{i(\vec{G} \cdot \vec{r})} \quad (8a) \quad E(\vec{r}) = \sum_{\vec{G}} E_{\vec{G}} e^{i(\vec{G} \cdot \vec{r})} \quad (8b) \quad B(\vec{r}) = \sum_{\vec{G}} B_{\vec{G}} e^{i(\vec{G} \cdot \vec{r})} \quad (8c)$$

We already assumed that the electromagnetic field propagates through the crystal in form of a plane wave – see equation (5a) and (5b). The reciprocal lattice vector \vec{G} is determined by two indices m and n and can be expressed in certain ways:

$$\vec{G} = \vec{G}_{mn} = m\vec{b}_1 + n\vec{b}_2 = G_x^{mn} \vec{e}_x + G_y^{mn} \vec{e}_y \quad (9)$$

For the Fourier expansion of $c(\vec{r})^2$ in the following the indices l and m will be used – so $c_{\vec{G}}^2 = c_{lm}^2$. The Fourier expansions of the electric and magnetic field will be expressed by indices n and o on the left and p and q on the right hand side of equations. Then the differential equations (7a) and (7b) can be transformed into algebraic equations:

$$\sum_{lm} \sum_{no} c_{lm}^2 e^{i\vec{G}_{lm} \cdot \vec{r}} \underbrace{\left[-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} \right]}_{=(G_x^{no}+k_x)^2 + (G_y^{no}+k_y)^2} E_{no} e^{i[(\vec{G}_{no}+\vec{k}) \cdot \vec{r}]} = \sum_{pq} \omega^2 E_{pq} e^{i[(\vec{G}_{pq}+\vec{k}) \cdot \vec{r}]} \quad (10a)$$

$$\begin{aligned} \sum_{lm} \sum_{no} c_{lm}^2 \overbrace{\left[-\frac{\partial e^{i\vec{G}_{lm} \cdot \vec{r}}}{\partial x} \frac{\partial}{\partial y} - \frac{\partial e^{i\vec{G}_{lm} \cdot \vec{r}}}{\partial y} \frac{\partial}{\partial x} - e^{i\vec{G}_{lm} \cdot \vec{r}} \left[\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} \right] \right]}^{=e^{i\vec{G}_{lm} \cdot \vec{r}} [G_x^{lm}(G_x^{no}+k_x) + G_y^{lm}(G_y^{no}+k_y) + (G_x^{no}+k_x)^2 + (G_y^{no}+k_y)^2]} B_{no} e^{i[(\vec{G}_{no}+\vec{k}) \cdot \vec{r}]} = \\ = \sum_{pq} \omega^2 B_{pq} e^{i[(\vec{G}_{pq}+\vec{k}) \cdot \vec{r}]} \quad (10b) \end{aligned}$$

By comparing the arguments of the exponential functions on the right and left we find that $l + n = p$ and $m + o = q$. With those index transformations we can compare the coefficients of the exponential functions and get the following eigenvalue problems:

$$\sum_{lm} \left[(G_x^{(p-l)(q-m)} + k_x)^2 + (G_y^{(p-l)(q-m)} + k_y)^2 \right] c_{lm}^2 E_{(p-l)(q-m)} = \omega^2 E_{pq} \quad (11a)$$

$$\begin{aligned} \sum_{lm} \left[G_x^{lm} (G_x^{(p-l)(q-m)} + k_x) + G_y^{lm} (G_y^{(p-l)(q-m)} + k_y) + \right. \\ \left. + (G_x^{(p-l)(q-m)} + k_x)^2 + (G_y^{(p-l)(q-m)} + k_y)^2 \right] c_{lm}^2 B_{(p-l)(q-m)} = \omega^2 B_{pq} \quad (11b) \end{aligned}$$

Those equations that are called the central equation can be solved numerically, if we restrict the number of reciprocal lattice vectors \vec{G} . So we have to set an upper bound $O_{pq} = \sup\{p + q\}$ for the indices p and q .

For demonstration of the numerical calculations we set $O_{pq} = 1$. In the algebraic equations (11a) and (11b) we can substitute the square brackets as:

$$\Xi_{lm}^{pq} = \left[(G_x^{(p-l)(q-m)} + k_x)^2 + \dots \right] \quad (12)$$

Then (11a) and (11b) lead to linear systems of equations that can be expressed similarly by the matrix:

$$\begin{pmatrix} c_{00}^2 \Xi_{00}^{01} & c_{11}^2 \Xi_{11}^{01} & c_{01}^2 \Xi_{01}^{01} & c_{11}^2 \Xi_{11}^{01} & c_{02}^2 \Xi_{02}^{01} \\ c_{1\bar{1}}^2 \Xi_{1\bar{1}}^{10} & c_{00}^2 \Xi_{00}^{10} & c_{10}^2 \Xi_{10}^{10} & c_{20}^2 \Xi_{20}^{10} & c_{11}^2 \Xi_{11}^{10} \\ c_{0\bar{1}}^2 \Xi_{0\bar{1}}^{01} & c_{10}^2 \Xi_{10}^{01} & c_{00}^2 \Xi_{00}^{01} & c_{10}^2 \Xi_{10}^{01} & c_{01}^2 \Xi_{01}^{01} \\ c_{1\bar{1}}^2 \Xi_{1\bar{1}}^{10} & c_{20}^2 \Xi_{20}^{10} & c_{10}^2 \Xi_{10}^{10} & c_{00}^2 \Xi_{00}^{10} & c_{11}^2 \Xi_{11}^{10} \\ c_{02}^2 \Xi_{02}^{01} & c_{11}^2 \Xi_{11}^{01} & c_{0\bar{1}}^2 \Xi_{0\bar{1}}^{01} & c_{1\bar{1}}^2 \Xi_{1\bar{1}}^{01} & c_{00}^2 \Xi_{00}^{01} \end{pmatrix} \begin{pmatrix} A_{01} \\ A_{10} \\ A_{00} \\ A_{1\bar{0}} \\ A_{0\bar{1}} \end{pmatrix} = \omega^2 \begin{pmatrix} A_{01} \\ A_{10} \\ A_{00} \\ A_{1\bar{0}} \\ A_{0\bar{1}} \end{pmatrix} \quad (13)$$

Because we set $O_{pq} = 1$, in the following we can neglect all matrix elements with index pairs 02, 0 $\bar{2}$, 11, ... :

$$\begin{pmatrix} c_{00}^2 \Xi_{00}^{01} & 0 & c_{01}^2 \Xi_{01}^{01} & 0 & 0 \\ 0 & c_{00}^2 \Xi_{00}^{10} & c_{10}^2 \Xi_{10}^{10} & 0 & 0 \\ c_{0\bar{1}}^2 \Xi_{0\bar{1}}^{01} & c_{10}^2 \Xi_{10}^{01} & c_{00}^2 \Xi_{00}^{01} & c_{10}^2 \Xi_{10}^{01} & c_{01}^2 \Xi_{01}^{01} \\ 0 & 0 & c_{10}^2 \Xi_{10}^{10} & c_{00}^2 \Xi_{00}^{10} & 0 \\ 0 & 0 & c_{0\bar{1}}^2 \Xi_{0\bar{1}}^{01} & 0 & c_{00}^2 \Xi_{00}^{01} \end{pmatrix} \begin{pmatrix} A_{01} \\ A_{10} \\ A_{00} \\ A_{1\bar{0}} \\ A_{0\bar{1}} \end{pmatrix} = \omega^2 \begin{pmatrix} A_{01} \\ A_{10} \\ A_{00} \\ A_{1\bar{0}} \\ A_{0\bar{1}} \end{pmatrix} \quad (14)$$

If we know the Fourier expansion coefficients c_{lm}^2 , we can solve the eigenvalue problem (14) for the TM and TE modes. A formula for those is derived in the following chapter.

3.3. Fourier Coefficients of the Phase Velocity

As already mentioned, we can expand $c^2(\vec{r})$ in a Fourier-series – see equation (8a) – with the coefficients c_{lm}^2 , that can be calculated in the following way:

$$c_{lm}^2 = \frac{1}{A_{cell}} \int_{cell} c(\vec{r})^2 e^{-i(l\vec{b}_1 + m\vec{b}_2) \cdot \vec{r}} d^2r \quad (15)$$

When we consider that

$$c(\vec{r})^2 = \begin{cases} c_M^2, & r \geq R \dots \text{phase velocity in dielectric material} \\ c^2, & r < R \dots \text{phase velocity in vacuum} \end{cases}, \quad (16)$$

where R is the radius of the holes, we can split up the integral in equation (11) and we get:

$$c_{lm}^2 = \frac{c_M^2}{A_{cell}} \int_{cell} e^{-i(l\vec{b}_1 + m\vec{b}_2) \cdot \vec{r}} d^2r + \frac{c^2 - c_M^2}{A_{cell}} \int_{hole} e^{-i(l\vec{b}_1 + m\vec{b}_2) \cdot \vec{r}} d^2r \quad (17)$$

If $l = m = 0$ latter equation gives:

$$c_{lm}^2 = \frac{c_M^2}{A_{cell}} \int_{cell} d^2r + \frac{c^2 - c_M^2}{A_{cell}} \int_{hole} d^2r = c_M^2 + (c^2 - c_M^2) \frac{A_{hole}}{A_{cell}} \quad (18)$$

For $l \neq 0$ or $m \neq 0$ we change the second term to polar coordinates due to the symmetry of the holes:

$$c_{lm}^2 = \frac{c_M^2}{A_{cell}} \int_0^a \int_0^{\frac{\sqrt{3}}{2}a} e^{-i(l\vec{b}_1 + m\vec{b}_2) \cdot \vec{r}} dy dx + \frac{c^2 - c_M^2}{A_{cell}} \int_{-\pi}^{\pi} \int_0^R e^{-i(l\vec{b}_1 + m\vec{b}_2) \cdot \vec{r}} dr d\varphi \quad (19)$$

When we integrate the first term over the rectangular unit cell in real space, we find that this term vanishes:

$$\begin{aligned} \int_0^a \int_0^{\frac{\sqrt{3}}{2}a} e^{-i[l\vec{b}_1 + m\vec{b}_2] \cdot \vec{r}} dy dx &= \int_0^a \int_0^{\frac{\sqrt{3}}{2}a} e^{-i\frac{2\pi}{a} \left[l \left(-\frac{1}{\sqrt{3}} \right) + m \left(\frac{0}{\sqrt{3}} \right) \right] \cdot \begin{pmatrix} x \\ y \end{pmatrix}} dy dx = \\ &= \underbrace{\int_0^a e^{-i\frac{2\pi}{a} l x} dx}_{\propto e^{-i2\pi l} - e^{-0} = 1 - 1 = 0} \cdot \int_0^{\frac{\sqrt{3}}{2}a} e^{-i\frac{2\pi}{a} \frac{(2m-l)y}{\sqrt{3}}} dy = 0 \quad (20) \end{aligned}$$

When we use the relationship $(l\vec{b}_1 + m\vec{b}_2) \cdot \vec{r} = \vec{G}_{lm} \cdot \vec{r} = G_{lm} r \cos \varphi$, we obtain a Bessel function of the first kind for the remaining integral:

$$\begin{aligned} c_{lm}^2 &= 0 + \frac{c^2 - c_M^2}{A_{cell}} \int_{-\pi}^{\pi} \int_0^R e^{-i \underbrace{G_{lm} r}_{=x} \cos \varphi} r dr d\varphi = \frac{c^2 - c_M^2}{A_{cell} G_{lm}^2} \int_0^{G_{lm} R} u \underbrace{\int_{-\pi}^{\pi} e^{-iu \cos \varphi} d\varphi}_{=\frac{j_0(u)}{2\pi} \dots \text{Bessel function}} du = \\ &= \frac{c^2 - c_M^2}{A_{cell} G_{lm}^2} 2\pi \int_0^{G_{lm} R} u j_0(u) du = \frac{c^2 - c_M^2}{A_{cell}} 2\pi \frac{R}{G_{lm}} j_1(G_{lm} R) \quad (21) \end{aligned}$$

In the last step we used the following integral identity for Bessel functions of the first kind:

$$\int_0^U u j_0(u) du = U j_1(U) \quad (22)$$

So finally we get:

$$\frac{c_{lm}^2}{c^2} = \delta_{l,0} \delta_{m,0} \left[\frac{c_M^2}{c^2} + \left(1 - \frac{c_M^2}{c^2} \right) \frac{A_{hole}}{A_{cell}} \right] + \Theta(|l+m| > 0) \left[\frac{(1 - \frac{c_M^2}{c^2})}{A_{cell}} \frac{2\pi R}{G_{lm}} j_1(G_{lm} R) \right], \quad (23)$$

where $\delta_{A,B}$ is the Kronecker delta and $\Theta(L)$ is the Heaviside step function.

4. Results

With a Matlab script – see appendix A – the central equations (11a) and (11b) were solved numerically for a discrete set of wave vectors \vec{k} inside the first Brillouin zone of the two-dimensional, hexagonal photonic crystal. With the solutions it was possible to calculate the dispersion relation, the density of states and thermodynamic properties.

4.1. Dispersion Relation and Density of States

In the dispersion relation the solutions for ω of the central equations (11a) and (11b) are usually plotted along directions of high symmetry (ΓM , MK and $\text{K}\Gamma$). In the density of states the number of solutions inside the first Brillouin zone and a frequency interval $[\omega, \omega + \Delta\omega]$ is counted. The resulting dispersion relation and density of states for the considered two-dimensional, hexagonal photonic crystal are depicted in figure 5.

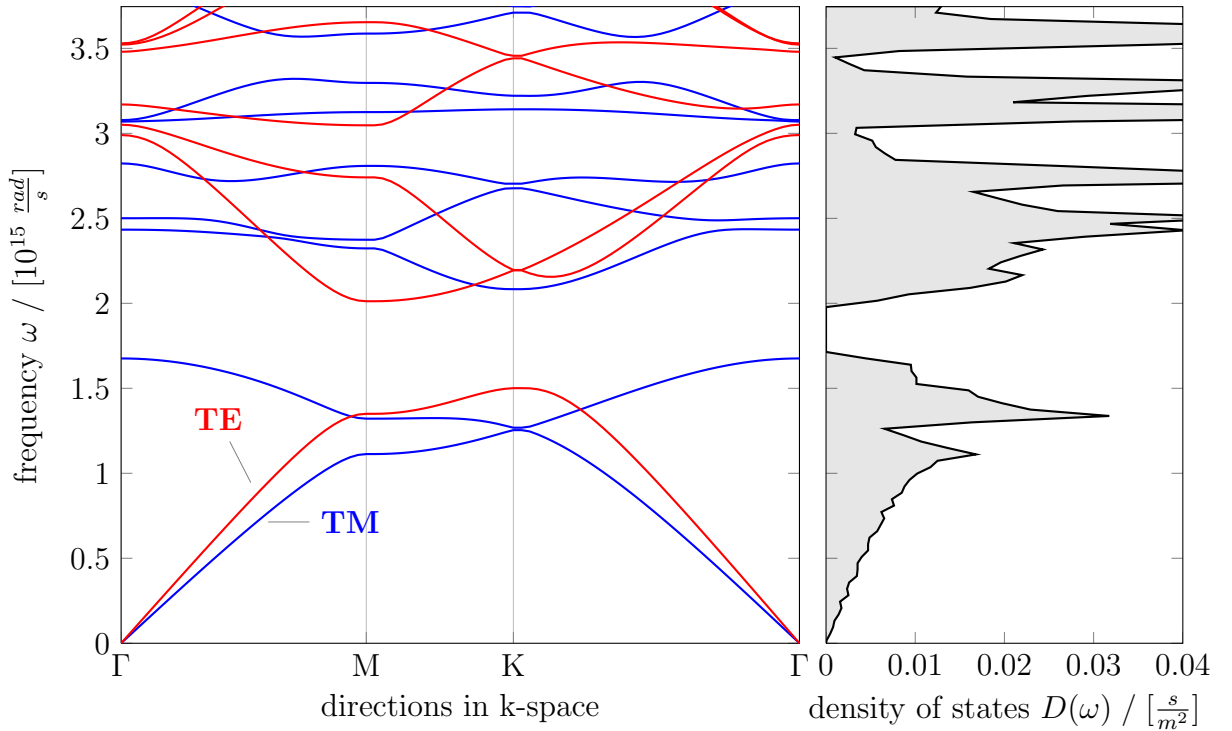


Figure 3: Dispersion relation (left) and density of states (right) for a hexagonal arrangement of air holes in a dielectric material. The calculations were done by the plane wave expansion method in Matlab – see code in appendix A. The red lines are solutions that belong to the transversal electric modes (TE), whereat the blue lines belong to the transversal magnetic modes (TM).

In those plots a photonic band gap occurs in the interval $\frac{\omega a}{2\pi c} \in [0.46, 0.52]$ where no solutions exist. In this frequency range the electromagnetic waves are reflected for any direction of arrival.

4.2. Thermodynamic Properties

With the density of states $D(\omega)$ it was possible to calculate thermodynamic properties by equations (24a) - (24e).

$$\text{Energy Spectral Density:} \quad u(\omega) = \hbar\omega \cdot D(\omega) \cdot \frac{1}{\exp(\frac{\hbar\omega}{k_B T}) - 1} \quad (24a)$$

$$\text{Internal energy density:} \quad u(T) = \int_0^\infty u(\omega) d\omega \quad (24b)$$

$$\text{Specific heat:} \quad c_V(T) = \left. \frac{\partial u(T)}{\partial T} \right|_{V=\text{const.}} \quad (24c)$$

$$\text{Helmholtz free energy:} \quad f(T) = k_B T \int_0^\infty D(\omega) \cdot \ln \left(1 - \exp(-\frac{\hbar\omega}{k_B T}) \right) d\omega \quad (24d)$$

$$\text{Entropy density} \quad s(T) = - \left. \frac{\partial f(T)}{\partial T} \right|_{N,V=\text{const.}} \quad (24e)$$

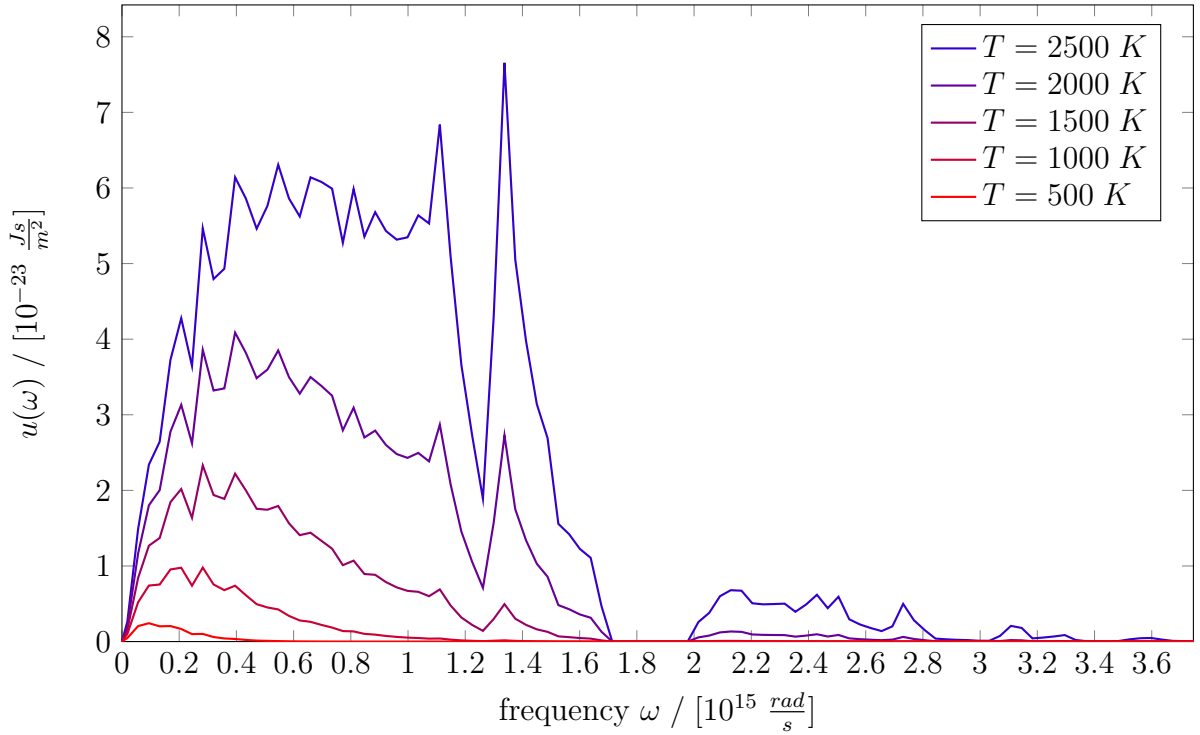


Figure 4: Energy spectral density $u(\omega)$ for a set of temperatures.

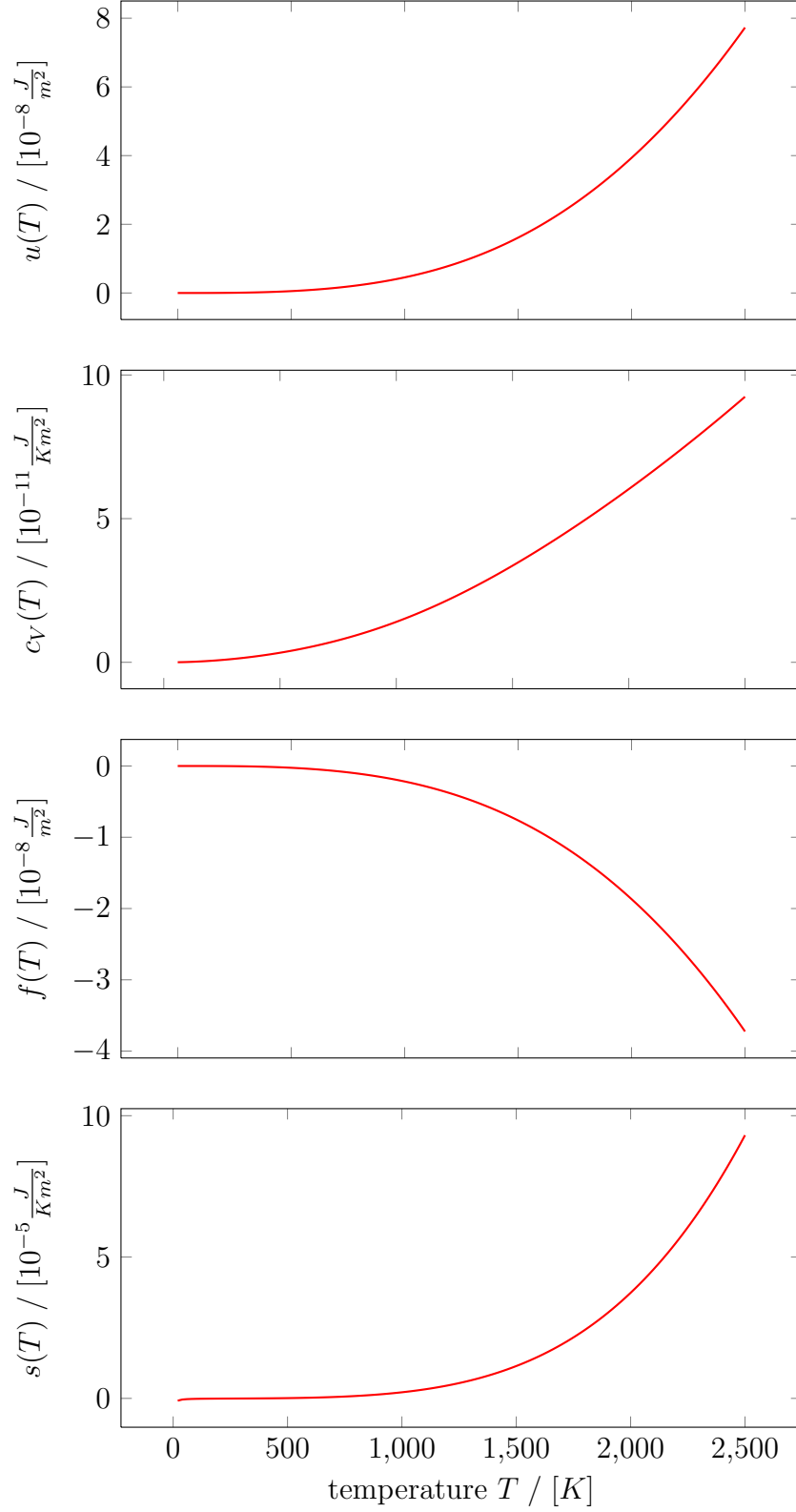


Figure 5: Thermodynamic properties: internal energy $u(T)$, heat capacity $c_V(T)$, Helmholtz free energy $f(T)$ and entropy density $s(T)$.

A. Matlab Code

```

1 %% This program calculates the dispersion relation and the
   density of states with the plane wave expansion method for a
   hexagonal arrangement of air holes in a dielectric material
   (2D photonic crystal).
2 k_B = 1.380658*10^-23; h_bar = 1.05457266*10^-34; c =
   2.99792458*10^8;
3 %% k-space in units of 2*pi/a:
4 N_gm = 30; N_mk = floor(N_gm/sqrt(3)); % number of wave vectors
   for different directions in k-space
5 D_gm = (2/sqrt(3)) / 2; % distance from Gamma to M in k-space (
   half of reciprocal lattice vector b_2)
6 D_mk = D_gm/sqrt(3); % distance from M to K
7 [k_xx, k_yy] = meshgrid(D_mk*(-2*N_mk:2*N_mk)/N_mk, D_gm*(-N_gm:
   N_gm)/N_gm); % those variables will get the k-states inside
   of the Wigner-Seitz cell (hexagon)
8 for i=1:N_mk % in this loop the hexagon is "cut" into a
   rectangle
9     j=floor(N_gm-N_gm/N_mk*i+2);
10    k_xx(1:j, 4*N_mk-i+2)=NaN; k_yy(1:j, 4*N_mk-i+2)=NaN;
11    k_xx(1:j, i)=NaN; k_yy(1:j, i)=NaN;
12    k_xx(N_gm+j:end, N_mk-i+1)=NaN; k_yy(N_gm+j:end, N_mk-i+1)=
        NaN;
13    k_xx(N_gm+j:end, 3*N_mk+i+1)=NaN; k_yy(N_gm+j:end, 3*N_mk+i
        +1)=NaN;
14 end;
15 k_xx = k_xx(~isnan(k_xx(:))); k_yy = k_yy(~isnan(k_yy(:))); %
   dispose NaN values
16 ind_gm = find(k_xx==0); ind_gm(1:ceil(numel(ind_gm)/2)-1)
   =[]; % Gamma -> M
17 ind_mk = find(k_yy==D_gm); ind_mk(1:ceil(numel(ind_mk)/2)-1)
   =[]; % M -> K
18 ind_kg = find(k_yy==0); ind_kg(ceil(numel(ind_kg)/2)+1:end)
   =[]; % K -> Gamma
19 ind = [ind_gm; ind_mk; ind_kg]; % indices for dispersion
   relation plot
20 N_disp = numel(ind); N_dos = numel(k_xx); % total number of
   wave vectors for the dispersion relation and the density of
   states
21 %% properties of the problem:
22 c_sq_rat = 1/13; % ratio of the quadratic phase velocities (
   hole/material)
23 O_pq = 25; % order of reciprocal lattice vectors (G=m*b1+n*b2
   => ord_G = m_max + n_max)
24 N_pq = (O_pq-1)*O_pq/2 + (O_pq+1)*(O_pq+2)/2; % number of
   reciprocal lattice vectors (arithmetic series)

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```

25 dim = 2*N_pq-1; % dimension of the matrix from the
    Eigenwertproblem
26 a = 500*10^-9; A_cell = a^2*sqrt(3)/2; % distance between the
    holes and area of the cell
27 R = 0.48*a; A_hole = R^2*pi; % radius and area of the holes
28 beta_TM=zeros(dim,dim); beta_TE=zeros(dim,dim); % factors due
    to differential operations
29 vec_TM=zeros(N_dos,dim); vec_TE=zeros(N_dos,dim); %
    eigenvectors for transversal magnetic and transv. electric
    modes
30 %% index transformation due to coefficient comparison
31 u=0; tic
32 p = zeros(dim,1); q = zeros(dim,1); % indices G that belongs to
    the electric or magnetic field
33 for i=0:N_pq
34     for j=0:i
35         if (i>0), t=((i+1)*i)/2+1+j; else t=1; end;
36         p(t)=j; q(t)=i-j;
37         if (j>0 && j<i)
38             p(N_pq-u)=-p(t); q(N_pq-u)=q(t); u=u+1;
39         end;
40     end;
41 end;
42 p = [flipud(p(2:N_pq));-p(1:N_pq)]; q = [flipud(q(2:N_pq));-q
    (1:N_pq)];
43 [nn1, nn2] = meshgrid(p); [oo1, oo2] = meshgrid(q);
44 l = nn2-nn1; m = oo2-oo1;
45 %% setting up and solving the system of algebraic equations (
    Eigenwertproblem) - calculating the dispersion relation
46 G = 2*pi/a*sqrt(1.^2+(2*m-1).^2/3);
47 c_sq_G = (1-c_sq_rat)/A_cell*2*pi*R./G.*besselj(1,G*R); %
    expansion coefficients for the speed of light
48 c_sq_G(l==0 & m==0) = c_sq_rat+(1-c_sq_rat)*A_hole/A_cell; %
    diagonal elements of the expansion coefficients
49 G_x = nn2 - l; G_y = (2*(oo2-m)-(nn2-1))/sqrt(3); % x- and y-
    components of the reciprocal lattice vectors corresponding
    to the E- or B-field
50 wb = waitbar(0,['working ... ',num2str(ceil(0/N_dos*100)),' %
    done']);
51 pool = 10;
52 matlabpool(pool)
53 for i=1:pool:numel(k_xx)
54     vec_tm = zeros(pool,dim); vec_te = zeros(pool,dim);
55     parfor j=0:pool-1
56         p = i + j;
57         if p<=numel(k_xx)

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58         k_x = k_xx(p); k_y = k_yy(p); % x- and y-components
           for the different directions in k-space
59         beta_TM = (G_x+k_x).^2+(G_y+k_y).^2; % factor due
           to differential operators from  $\text{rot}(\text{rot}(E))=w^2E$ 
           , where  $E_x = E_y = 0$ 
60         beta_TE = 1.*(G_x+k_x) + (2*m-1)/sqrt(3).*(G_y+k_y)
           + beta_TM; % factor due to differential
           operators from  $\text{rot}(c^2\text{rot}(B))=w^2B$ , where  $B_x$ 
           =  $B_y = 0$ 
61         ewp_TM = c_sq_G.*beta_TM; % setting up the
           Eigenwertproblems for the TM and TE modes
62         ewp_TE = c_sq_G.*beta_TE; % expansion coefficients
           times the factor from the differential operators
63         %solving the TM and TE eigenvalue problems
64         vec_tm(j+1,:) = sort(sqrt(eig(ewp_TM(:,:))));
65         vec_te(j+1,:) = sort(sqrt(eig(ewp_TE(:,:))));
66     end;
67 end;
68     vec_TM(i:i+pool-1,:) = vec_tm; vec_TE(i:i+pool-1,:) =
           vec_te;
69     t = toc; waitbar(i/N_dos,wb,['Working ',num2str(floor(t
           /60^2)), ' h, '...
70         ,num2str(floor(t/60)), ' min and ',num2str(rem(t,60)), '
           sec ... ',num2str(ceil(i/N_dos*100)), ' % done!']);
71 end;
72 matlabpool close
73 vec_TM(N_dos+1:end,:) = []; vec_TE(N_dos+1:end,:) = [];
74 bands = 1:9; % energy bands of interest
75 dispersion_relation = [vec_TM(ind,bands),vec_TE(ind,bands)]*(2*
           pi*c)/a;
76 %% calculation of the density of states
77 n_w = 100; [dos,w_] = hist([vec_TE(vec_TE<1);vec_TM(vec_TM<1)
           ]*(2*pi*c)/a,n_w);
78 dos=dos/(w_(2)-w_(1))/N_dos/A_cell; % normalize density of
           states to  $[s/m^2]$ 
79 %% calculation of the thermodynamic properties:
80 T_max = 2500; n_T = 126; T_ = ceil(linspace(0,T_max,n_T));
81 T = repmat(T_,n_w,1);
82 w = repmat(w_',1,n_T);
83 bose_einstein = 1./(exp(h_bar*w/k_B./T)-1);
84 DOS = repmat(dos',1,n_T);
85 u_spectral = h_bar*w.*bose_einstein.*DOS;
86 du_spectral_dT = -(h_bar*w./T).^2/k_B.*DOS.*exp(h_bar*w/k_B./T)
           .*bose_einstein.^2;
87 u_internal = trapz(w(:,1),u_spectral);
88 c_V = -trapz(w(:,1),du_spectral_dT);
89 f = trapz(w(:,1),k_B*T.*DOS.*log(1-exp(-h_bar*w/k_B./T)));

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90 s = -f.*T_ - trapz(w(:,1),DOS./(1-exp(-h_bar*w/k_B./T)).*h_bar
    .*w./T);
91 close(wb);
92 %% writing the results to files
93 fname = '2Dhex_dispersion_info.txt';
94 dlmwrite(fname, [num2str(numel(ind_gm)), ' ', num2str(numel(
    ind_gm)+numel(ind_mk)), ' ', num2str(N_disp)], 'delimiter', '');
95 fname = '2Dhex_dispersion_TM.txt'; dlmwrite(fname, ['k', sprintf
    (' TM%i ', bands)], 'delimiter', '');
96 dlmwrite(fname, [(1:N_disp)', vec_TM(ind, bands)*(2*pi*c)/a
    *10^-15], '-append', 'delimiter', '');
97 fname = '2Dhex_dispersion_TE.txt'; dlmwrite(fname, ['k', sprintf
    (' TE%i ', bands)], 'delimiter', '');
98 dlmwrite(fname, [(1:N_disp)', vec_TE(ind, bands)*(2*pi*c)/a
    *10^-15], '-append', 'delimiter', '');
99 fname = '2Dhex_density_of_states.txt'; dlmwrite(fname, 'w dos',
    'delimiter', '');
100 dlmwrite(fname, [0,0;w_*10^-15,dos';w_(end)*10^-15,0], '-
    append', 'delimiter', '');
101 fname = '2Dhex_spectral_energy_density.txt'; ind_T=mod(T_,500)
    ==0;
102 dlmwrite(fname, ['w', sprintf(' T%i ', T_(ind_T))], 'delimiter', '')
    ;
103 dlmwrite(fname, [zeros(1,sum(ind_T)+1);w_*10^-15,u_spectral(:,
    ind_T)*10^23], '-append', 'delimiter', '');
104 fname = '2Dhex_thermo_prop.txt'; dlmwrite(fname, 'T u_int c_V f
    s', 'delimiter', '');
105 dlmwrite(fname, [T_', u_internal '*10^8, c_V '*10^11, f '*10^8, s
    '*10^5], '-append', 'delimiter', '');

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