Selected Topics in Computational Electromagnetics
Lecture Notes

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1 Preliminaries

1.1 Basic equations

Time harmonic Maxwell's equations with $\exp(-i\omega t)$ time dependence:

$$\begin{aligned} \nabla \times \boldsymbol{E} &= i\omega\mu\boldsymbol{H} \\ \nabla \times \boldsymbol{H} &= \boldsymbol{J} - i\omega\varepsilon\boldsymbol{E} \end{aligned} \tag{1}$$

Helmholtz equation either for the electric or magnetic field providing that the dielectric permittivity and the magnetic permeability are constants:

$$\nabla \times \nabla \times \boldsymbol{H} - \omega^2\varepsilon\mu\boldsymbol{H} = \nabla \times \boldsymbol{J} \tag{2}$$

$$\nabla \times \nabla \times \boldsymbol{E} - \omega^2\varepsilon\mu\boldsymbol{E} = i\omega\mu\boldsymbol{J} \tag{3}$$

Matching conditions and conditions at infinity define solutions of direct problems. Matching conditions imply the continuity of the tangential electric and magnetic field components at material interfaces. Conditions at infinity imply that the waves at large distances from scattering objects must be either outgoing spherical or plane waves depending on a particular problem formulation.

1.2 Plane waves

The electromagnetic fields can be represented in terms of the vector and scalar potentials – $\boldsymbol{A}$ and φ. Let they be related by the Lorentz gauge condition:

$$\begin{gathered} \varphi + \frac{i}{\omega\varepsilon_b\mu_b}\nabla\boldsymbol{A} = 0 \\ \boldsymbol{E} = -\nabla\varphi + i\omega\boldsymbol{A} = \frac{i}{\omega\varepsilon_b\mu_b}\left(\nabla\nabla\boldsymbol{A} + k_b^2\boldsymbol{A}\right) \\ \boldsymbol{H} = \frac{1}{\mu_b}\nabla \times \boldsymbol{A} \end{gathered} \tag{4}$$

Here constant material constants $\varepsilon = \varepsilon_b$, $\mu = \mu_b$ describe an infinite homogeneous "basis" medium. The Helmholtz equation for the vector potential appears to be

$$\Delta\boldsymbol{A} + k_b^2\boldsymbol{A} = -\mu_0\boldsymbol{J} \tag{5}$$

with $k_b^2 = \omega^2\varepsilon_b\mu_b$. In the absence of sources $\boldsymbol{J} = 0$ eigen solutions of the homogeneous isotropic medium are plane waves:

$$\boldsymbol{A} = \boldsymbol{A}_0 \exp\left(i\boldsymbol{k}\boldsymbol{r}\right), |\boldsymbol{k}| = k_b \tag{6}$$

Going back to the electric and magentic fields we get

$$\begin{gathered} \boldsymbol{E} = \frac{i}{\omega\varepsilon_b\mu_b}\left[k_b^2\boldsymbol{A}_0 - \boldsymbol{k}\left(\boldsymbol{k}\boldsymbol{A}_0\right)\right]\exp\left(i\boldsymbol{k}\boldsymbol{r}\right) \\ \boldsymbol{H} = \frac{1}{\mu_b}\boldsymbol{k} \times \boldsymbol{A}_0 \exp\left(i\boldsymbol{k}\boldsymbol{r}\right) \end{gathered} \tag{7}$$

which are transverse in the isotropic medium. It is convenient to introduce the TE and TM polarizations relative to some Cartesian coordinate system $(OXYZ)$. Correspoding unit vectors for these polarizations will be

$$\begin{aligned} \hat{\boldsymbol{e}}_e^{\pm} &= \frac{\boldsymbol{k}^{\pm} \times \hat{\boldsymbol{e}}_z}{\left|\boldsymbol{k}^{\pm} \times \hat{\boldsymbol{e}}_z\right|} = \frac{k_y}{\varkappa}\hat{\boldsymbol{e}}_x - \frac{k_x}{\varkappa}\hat{\boldsymbol{e}}_y \\ \hat{\boldsymbol{e}}_h^{\pm} &= \frac{\boldsymbol{k}^{\pm} \times \left(\boldsymbol{k}^{\pm} \times \hat{\boldsymbol{e}}_z\right)}{\left|\boldsymbol{k}^{\pm} \times \left(\boldsymbol{k}^{\pm} \times \hat{\boldsymbol{e}}_z\right)\right|} = \pm\frac{k_x k_z}{\varkappa k_b}\hat{\boldsymbol{e}}_x \pm \frac{k_y k_z}{\varkappa k_b}\hat{\boldsymbol{e}}_y - \frac{\varkappa}{k_b}\hat{\boldsymbol{e}}_z \end{aligned} \tag{8}$$

where $\varkappa = \sqrt{k_x^2 + k_y^2}$, the wavevectors $\boldsymbol{k}^{\pm} = (k_x, k_y, \pm k_z)$ correspond to plane waves propagating upwards and downwards with respect to axis Z, and the dispersion equation is $k_z = \sqrt{k_b^2 - \varkappa^2}$, $\Re k_z + \Im k_z \geq 0$. Also, $\boldsymbol{k}^{\pm} \times \hat{\boldsymbol{e}}_e^{\pm} = k_b \hat{\boldsymbol{e}}_h^{\pm}$, $\boldsymbol{k}^{\pm} \times \hat{\boldsymbol{e}}_h^{\pm} = -k_b \hat{\boldsymbol{e}}_e^{\pm}$, and $\hat{\boldsymbol{e}}_e^{\pm} \times \hat{\boldsymbol{e}}_h^{\pm} = \boldsymbol{k}^{\pm}/k_b$.

Field decomposition in a homogeneous isotropic medium is a continuum of plane waves propagating upwards and downwards with respect to the axis Z:

$$\begin{pmatrix} \boldsymbol{E}(\boldsymbol{r}) \\ \boldsymbol{H}(\boldsymbol{r}) \end{pmatrix} = \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} dk_x dk_y \exp\left(ik_x x + ik_y y\right) \left\{ \begin{pmatrix} \boldsymbol{E}_{\boldsymbol{\kappa}}^{+} \\ \boldsymbol{H}_{\boldsymbol{\kappa}}^{+} \end{pmatrix} \exp\left(ik_z z\right) + \begin{pmatrix} \boldsymbol{E}_{\boldsymbol{\kappa}}^{-} \\ \boldsymbol{H}_{\boldsymbol{\kappa}}^{-} \end{pmatrix} \exp\left(-ik_z z\right) \right\} \tag{9}$$

where $\kappa^2 = k_x^2 + k_y^2$, $k_z = \sqrt{\omega^2 \varepsilon\mu - \kappa_x^2}$.

1.3 Power flow

Time averaged power density (observable quantity)

$$\langle \boldsymbol{S} \rangle = \frac{1}{2} Re\left\{\boldsymbol{E} \times \boldsymbol{H}^*\right\} \tag{10}$$

When there is a distinguished axis Z one can relate the plane wave power density $\langle \boldsymbol{S} \rangle_z$ with TE and TM wave amplitudes

$$\begin{aligned} \langle \boldsymbol{S} \rangle_z &= \frac{1}{2}\Re\left\{\boldsymbol{E} \times \boldsymbol{H}^*\right\}_z = \frac{1}{2}\Re\left\{\left(a_e \hat{\boldsymbol{e}}_e - \frac{k_b}{\omega\varepsilon_b} a_h \hat{\boldsymbol{e}}_h\right) \times \left(a_h^* \hat{\boldsymbol{e}}_e + \frac{k_b}{\omega\mu_b} a_e^* \hat{\boldsymbol{e}}_h\right)\right\}_z \\ &= \frac{1}{2}\Re\left\{\left(\frac{1}{\omega\mu_b}\left|a_e\right|^2 \boldsymbol{k}^{\pm} + \frac{1}{\omega\varepsilon_b}\left|a_h\right|^2 \boldsymbol{k}^{\pm}\right)\right\}_z = \frac{1}{2}\left|a_e\right|^2 \Re\left(\frac{\pm k_z}{\omega\mu_b}\right) + \frac{1}{2}\left|a_h\right|^2 \Re\left(\frac{\pm k_z}{\omega\varepsilon_b}\right) \end{aligned} \tag{11}$$

1.4 Fresnel equations

Given a plane interface between two half-space homogeneous media with material parameters $\varepsilon_{1,2}$, μ_{12}, the tangential components of the electric and magnetic fields should be continuous across this interface. Suppose that axis Z is orthogonal to the interface, then

$$\begin{aligned} E_{x,y}\left(x, y, -0\right) &= E_{x,y}\left(x, y, +0\right) \\ H_{x,y}\left(x, y, -0\right) &= H_{x,y}\left(x, y, +0\right) \end{aligned} \tag{12}$$

For a plane wave field decomposition:

$$\begin{aligned} \boldsymbol{E}\left(x, y, +0\right) &= \textstyle\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dk_x dk_y \exp\left(ik_x x + ik_y y\right) \left(a_e^+ \hat{\boldsymbol{e}}_e^+ + a_e^- \hat{\boldsymbol{e}}_e^- - \frac{k_b}{\omega\varepsilon_b} a_h^+ \hat{\boldsymbol{e}}_h^+ - \frac{k_b}{\omega\varepsilon_b} a_h^- \hat{\boldsymbol{e}}_h^-\right) \\ \boldsymbol{E}\left(x, y, -0\right) &= \textstyle\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dk_x dk_y \exp\left(ik_x x + ik_y y\right) \left(b_e^+ \hat{\boldsymbol{e}}_e^+ + b_e^- \hat{\boldsymbol{e}}_e^- - \frac{k_b}{\omega\varepsilon_b} b_h^+ \hat{\boldsymbol{e}}_h^+ - \frac{k_b}{\omega\varepsilon_b} b_h^- \hat{\boldsymbol{e}}_h^-\right) \\ \boldsymbol{H}\left(x, y, +0\right) &= \textstyle\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dk_x dk_y \exp\left(ik_x x + ik_y y\right) \left(a_h^+ \hat{\boldsymbol{e}}_e^+ + a_h^- \hat{\boldsymbol{e}}_e^- + \frac{k_b}{\omega\mu_b} a_e^+ \hat{\boldsymbol{e}}_h^+ + \frac{k_b}{\omega\mu_b} a_e^- \hat{\boldsymbol{e}}_h^-\right) \\ \boldsymbol{H}\left(x, y, -0\right) &= \textstyle\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dk_x dk_y \exp\left(ik_x x + ik_y y\right) \left(b_h^+ \hat{\boldsymbol{e}}_e^+ + b_h^- \hat{\boldsymbol{e}}_e^- + \frac{k_b}{\omega\mu_b} b_e^+ \hat{\boldsymbol{e}}_h^+ + \frac{k_b}{\omega\mu_b} b_e^- \hat{\boldsymbol{e}}_h^-\right) \end{aligned} \tag{13}$$

Then, usung the orthogonality of exponential factors we find that in-plane wavevector projections preserve. Without loss of generality we can take $k_y = 0$ so that the boundary conditions become

$$\begin{aligned}
\frac{k_{z2}}{\varepsilon_2}\left(a_h^+ - a_h^-\right) &= \frac{k_{z1}}{\varepsilon_1}\left(b_h^+ - b_h^-\right) \\
a_e^+ + a_e^- &= b_e^+ + b_e^- \\
\frac{k_{z2}}{\mu_2}\left(a_e^+ - a_e^-\right) &= \frac{k_{z1}}{\mu_1}\left(b_e^+ - b_e^-\right) \\
a_h^+ + a_h^- &= b_h^+ + b_h^-
\end{aligned}
\Rightarrow
\begin{aligned}
a_e^+ &= \frac{2\mu_2 k_{z1}}{\mu_1 k_{z2} + \mu_2 k_{z1}} b_e^+ + \frac{\mu_1 k_{z2} - \mu_2 k_{z1}}{\mu_1 k_{z2} + \mu_2 k_{z1}} a_e^- \\
b_e^- &= \frac{\mu_2 k_{z1} - \mu_1 k_{z2}}{\mu_1 k_{z2} + \mu_2 k_{z1}} b_e^+ + \frac{2\mu_1 k_{z2}}{\mu_1 k_{z2} + \mu_2 k_{z1}} a_e^- \\
a_h^+ &= \frac{2\varepsilon_2 k_{z1}}{\varepsilon_1 k_{z2} + \varepsilon_2 k_{z1}} b_h^+ + \frac{\varepsilon_1 k_{z2} - \varepsilon_2 k_{z1}}{\varepsilon_1 k_{z2} + \varepsilon_2 k_{z1}} a_h^- \\
b_h^- &= \frac{\varepsilon_2 k_{z1} - \varepsilon_1 k_{z2}}{\varepsilon_1 k_{z2} + \varepsilon_2 k_{z1}} b_h^+ + \frac{2\varepsilon_1 k_{z2}}{\varepsilon_1 k_{z2} + \varepsilon_2 k_{z1}} a_h^-
\end{aligned} \tag{14}$$

Coefficients behind the amplitudes in the right-hand side are nothing that the Fresnel reflection and transmission coeffients:

$$\begin{aligned}
r_{22}^e &= \frac{\mu_1 k_{z2} - \mu_2 k_{z1}}{\mu_1 k_{z2} + \mu_2 k_{z1}} \\
t_{21}^e &= \frac{2\mu_2 k_{z1}}{\mu_1 k_{z2} + \mu_2 k_{z1}} = 1 - r_{22}^e \\
r_{11}^e &= \frac{\mu_2 k_{z1} - \mu_1 k_{z2}}{\mu_1 k_{z2} + \mu_2 k_{z1}} = -r_{22}^e \\
t_{12}^e &= \frac{2\mu_1 k_{z2}}{\mu_1 k_{z2} + \mu_2 k_{z1}} = 1 + r_{22}^e
\end{aligned} \tag{15}$$

2 S and T matrices

2.1 Definitions and properties

Reflection and transmission of plane wave at a planar interface is described in terms of the Fresnel reflection and transmission coefficients. For simulation of linear optical properties of multilayer structures it is convenient to group these coefficient into so called T and S-matrices. Consider a planar structure (one or several plane layers and interfaces) parallel to the XY of a Cartesian coordinate system (Fig. ...). Time-harmonic field of incoming and outgoing plane waves at boundaries of the structure $z = z_{1,2}$ have the form of a superposition of plane waves propagating upwards and downwards with respect to the axis Z:

$$F = a^+ \exp\left(ik_x x + ik_z z\right) + a^- \exp\left(ik_x x - ik_z z\right) \tag{16}$$

with $k_z = \sqrt{\omega\varepsilon\mu_0 - k_x^2}$ providing that $k_y = 0$. Then, the T and S-matrices of the structure are defined as

$$\begin{pmatrix} a_2^+ \\ a_2^- \end{pmatrix} = \begin{pmatrix} T^{++} & T^{+-} \\ T^{-+} & T^{--} \end{pmatrix} \begin{pmatrix} a_1^+ \\ a_1^- \end{pmatrix} \tag{17}$$

$$\begin{pmatrix} a_1^- \\ a_2^+ \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} a_1^+ \\ a_2^- \end{pmatrix} \tag{18}$$

Obviously, components of the S-matrix are nothing that the reflection and transmission coefficients, Eq. (15):

$$S = \begin{pmatrix} r_{11} & t_{12} \\ t_{21} & r_{22} \end{pmatrix} \tag{19}$$

The T-matrix can be derived from the Eqs. (2), (3) and explicitly is

$$T = \frac{1}{t_{21}} \begin{pmatrix} t_{12}t_{21} - r_{11}r_{22} & r_{22} \\ -r_{11} & 1 \end{pmatrix} \tag{20}$$

Given a structure surrounded by a homogeneous isotropic medium, the energy conservation law brings:

$$\left|a_1^+\right|^2 + \left|a_2^-\right|^2 = \left|a_1^-\right|^2 + \left|a_2^+\right|^2 \Rightarrow S^\dagger S = I \tag{21}$$

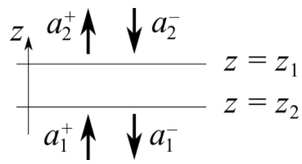

Figure 1: To the definition of scattering and transmission matrices.

i.e., in this case S is a unitary matrix. Upon changing the time $t \to -t$ (time reversal) we get $a^+ \to (a^-)^*$, $a^- \to (a^+)^*$, so that

$$\begin{pmatrix} a_1^+ \\ a_2^- \end{pmatrix}^* = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} a_1^- \\ a_2^+ \end{pmatrix}^* \Rightarrow \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}^{-*} \begin{pmatrix} a_1^+ \\ a_2^- \end{pmatrix} = \begin{pmatrix} a_1^- \\ a_2^+ \end{pmatrix} \Rightarrow S = S^{-*} \tag{22}$$

When there are two adjacent structures with known matrices (4), (5) (Fig. (2)), S- and T-matrices of the corresponding composite structure are found through compositions rules for these matrices. It follows from the definition (2) that the composition of the T-matrices is simply the matrix multiplication

$$T = T^{(1)} T^{(2)} \tag{23}$$

In case of S-matrices one can derive that

$$\begin{aligned} S_{11} &= S_{11}^{(1)} + S_{12}^{(1)} \left[1 - S_{11}^{(2)} S_{22}^{(1)}\right]^{-1} S_{11}^{(2)} S_{21}^{(1)} \\ S_{12} &= S_{12}^{(1)} \left[1 - S_{11}^{(2)} S_{22}^{(1)}\right]^{-1} S_{12}^{(2)} \\ S_{21} &= S_{21}^{(1)} \left[1 - S_{11}^{(2)} S_{22}^{(1)}\right]^{-1} S_{21}^{(2)} \\ S_{22} &= S_{22}^{(2)} + S_{21}^{(2)} \left[1 - S_{11}^{(2)} S_{22}^{(1)}\right]^{-1} S_{22}^{(1)} S_{12}^{(2)} \end{aligned} \tag{24}$$

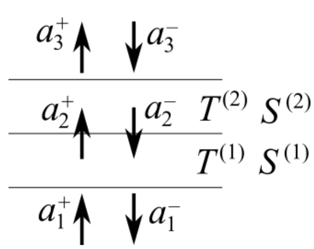

Figure 2: To the composition rules for S- and T-matrices

To simulate reflection and transmission of a plane wave through a medium with continuously varying refractive index $n(z)$, the function $n(z)$ can be approximated by a piecewise continuous function as Fig. 3 shows. Such function corresponds to a multilayer structure which reflection and transmission coefficients can be attained by successive composition of corresponding matrices of interfaces and homogeneous layers. Interface matrices are written directly as (4) and (5) when r and t mean the Fresnel coefficients. Homogeneous layer matrices should only add a phase difference to the complex wave amplitudes, and write

$$S_L = \begin{pmatrix} 0 & \exp(ik_z h) \\ \exp(ik_z h) & 0 \end{pmatrix} \tag{25}$$

$$T_L = \begin{pmatrix} \exp(ik_z h) & 0 \\ 0 & \exp(-ik_z h) \end{pmatrix} \tag{26}$$

Due to the presence of the negative sign exponent in (9) multiplication of the T-matrix become numerically unstable for evanescent waves which have pure imaginary k_z, and using S-matrices in such situations is preferable.

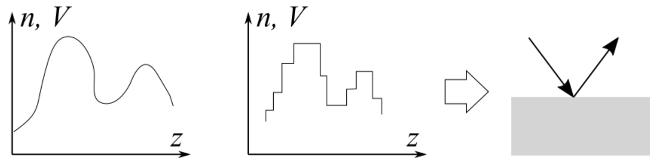

Figure 3: Approximation of a medium with continuously varying refractive index $n(z)$ by a set homogeneous plane layers with constant permittivity.

2.2 Fabry-Perot resonator

An ideal Fabry-Perot resonator is a plane parallel plate. Once a monochromatic beam is incident on this plate, the transmitted wave is a sum of all waves reflected inside the resonator:

$$a_t = a_{inc}\left(t_{12}t_{21}e^{ik_zh} + t_{12}r_{22}r_{22}e^{3ik_zh}t_{21} + t_{12}r_{22}r_{22}r_{22}r_{22}t_{21}e^{5ik_zh} + \dots\right) = \frac{t_{12}t_{21}e^{ik_zh}}{1 - r_{22}^2 e^{2ik_zh}} \tag{27}$$

Instead we can use the S-matrix formalism. Consider a slab (parallel plate) in the region $-h/2 \le z \le h/2$. S-matrix of the lower interface

$$S_L = \begin{pmatrix} -r_L & 1 + r_L \\ 1 - r_L & r_L \end{pmatrix} \tag{28}$$

S-matrix of the lower interface and the homogeneous slab is

$$S = \begin{pmatrix} -r_L & (1 + r_L)\exp(ik_zh) \\ (1 - r_L)\exp(ik_zh) & r_L \exp(2ik_zh) \end{pmatrix} \tag{29}$$

S-matrix of the upper interface is

$$S_U = \begin{pmatrix} r_U & 1 - r_U \\ 1 + r_U & -r_U \end{pmatrix} \tag{30}$$

Thus, the S-matrix of the whole slab is

$$S_{slab} = \begin{pmatrix} r_U - \dfrac{\left(1 - r_U^2\right) r_L \exp(2ik_zh)}{1 - r_U r_L \exp(2ik_zh)} & \dfrac{(1 + r_L)(1 - r_U)\exp(ik_zh)}{1 - r_U r_L \exp(2ik_zh)} \\ \dfrac{(1 - r_L)(1 + r_U)\exp(ik_zh)}{1 - r_U r_L \exp(2ik_zh)} & r_L - \dfrac{\left(1 - r_L^2\right) r_U \exp(2ik_zh)}{1 - r_U r_L \exp(2ik_zh)} \end{pmatrix} \tag{31}$$

If $r_L = r_U = r_{22}$

$$S_{slab} = \begin{pmatrix} r_{22}\dfrac{1 - \exp(2ik_zh)}{1 - r_{22}^2 \exp(2ik_zh)} & \dfrac{\left(1 - r_{22}^2\right)\exp(ik_zh)}{1 - r_{22}^2 \exp(2ik_zh)} \\ \dfrac{\left(1 - r_{22}^2\right)\exp(ik_zh)}{1 - r_{22}^2 \exp(2ik_zh)} & r_{22}\dfrac{1 - \exp(2ik_zh)}{1 - r_{22}^2 \exp(2ik_zh)} \end{pmatrix} \tag{32}$$

In case of propagating wave $r_{22}$is purely real, and the power transmission coefficient

$$T \sim \left|\frac{\left(1 - r_{22}^2\right)\exp(ik_zh)}{1 - r_{22}^2 \exp(2ik_zh)}\right|^2 = \frac{(1 - R_{22})^2}{1 - 2R_{22}\cos(2k_zh) + R_{22}^2} = \frac{(1 - R_{22})^2}{(1 - R_{22})^2 + 4R_{22}\sin^2(k_zh)} \tag{33}$$

where $R_{22} = r_{22}^2$. A typical dependence of $T(\lambda)$ is a periodic set of maxima correspoding to points $k_zh = \pi k$. The quality factor is

$$Q = \frac{\omega}{\delta\omega_{1/2}} = \frac{2nh}{\lambda}\frac{\pi\sqrt{R}}{1 - R} \tag{34}$$

2.3 Planar waveguide

Consider guided modes of a homogeneous slab. They can be derived from different considerations. First, it is the phase-matching condition based on the geometric optical interpretation:

$$2k_z h + \varphi_1 + \varphi_2 = 2\pi k,\ k \in \mathbb{Z} \tag{35}$$

where h is the slab thickness, and $\varphi_{1,2}$ are phases of the Fresnel reflection coefficients for waves reflected at the slab plane interfaces. This equation holds both for the Fabry-Pero resonances and waveguide modes, so in the case of the waveguide modes one should require the plane wave to be evanescent in the media which surround the slab.

The second derivation is based on the plane wave solutions of the Maxwell's equations. In case of the TE polarization, Maxwell's equations for the plane wave read:

$$\begin{gathered} -\frac{\partial E_y}{\partial z} = i\omega\mu H_x \\ \frac{\partial E_y}{\partial x} = i\omega\mu H_z \\ \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} = -i\omega\varepsilon E_y \end{gathered} \tag{36}$$

Inside the waveguide we search for a propagating solutions

$$E_y = \exp\left(ik_x x\right)\left[C_1 \sin\left(k_{2z} z\right) + C_2 \cos\left(k_{2z} z\right)\right];\ H_x = -\frac{1}{i\omega\mu_2}\frac{\partial E_y}{\partial z};\ H_z = \frac{k_x}{\omega\mu_2}E_y,\ |z| \le \frac{h}{2} \tag{37}$$

while outside – for evanescent solutions:

$$E_y = C_3 \exp\left(ik_x x\right)\exp\left(-\kappa_{1z}\left(z - \frac{h}{2}\right)\right);\ H_x = -\frac{1}{i\omega\mu_1}\frac{\partial E_y}{\partial z};\ H_z = \frac{k_x}{\omega\mu_1}E_y,\ z > \frac{h}{2} \tag{38}$$

$$E_y = C_4 \exp\left(ik_x x\right)\exp\left(\kappa_{1z}\left(z + \frac{h}{2}\right)\right);\ H_x = -\frac{1}{i\omega\mu_1}\frac{\partial E_y}{\partial z};\ H_z = \frac{k_x}{\omega\mu_1}E_y,\ z < -\frac{h}{2} \tag{39}$$

where $\kappa_{1z} = \sqrt{k_x^2 - \omega^2\varepsilon_1\mu_1} = ik_{1z}$. The interface conditions write

$$\begin{gathered} C_1 \sin\left(k_{2z}\frac{h}{2}\right) + C_2 \cos\left(k_{2z}\frac{h}{2}\right) = C_3 \\ -C_1 \sin\left(k_{2z}\frac{h}{2}\right) + C_2 \cos\left(k_{2z}\frac{h}{2}\right) = C_4 \\ -\frac{k_{2z}}{\mu_2}\left[C_1 \cos\left(k_{2z}\frac{h}{2}\right) - C_2 \sin\left(k_{2z}\frac{h}{2}\right)\right] = \frac{\kappa_{1z}}{\mu_1}C_3 \\ -\frac{k_{2z}}{\mu_2}\left[C_1 \cos\left(k_{2z}\frac{h}{2}\right) + C_2 \sin\left(k_{2z}\frac{h}{2}\right)\right] = -\frac{\kappa_{1z}}{\mu_1}C_4 \end{gathered} \tag{40}$$

It is easy to see that this system splits in two independent pairs:

$$\begin{gathered} 2C_1 \sin\left(k_{2z}\frac{h}{2}\right) = C_3 - C_4 \\ -2\frac{\mu_1}{\mu_2}\frac{k_{2z}}{\kappa_{1z}}C_1 \cos\left(k_{2z}\frac{h}{2}\right) = C_3 - C_4 \\ 2C_2 \cos\left(k_{2z}\frac{h}{2}\right) = C_3 + C_4 \\ 2\frac{\mu_1}{\mu_2}\frac{k_{2z}}{\kappa_{1z}}C_2 \sin\left(k_{2z}\frac{h}{2}\right) = C_3 + C_4 \end{gathered} \Rightarrow \begin{gathered} \tan\left(k_{2z}\frac{h}{2}\right) = -\frac{\mu_1}{\mu_2}\frac{k_{2z}}{\kappa_{1z}} \\ \cot\left(k_{2z}\frac{h}{2}\right) = \frac{\mu_1}{\mu_2}\frac{k_{2z}}{\kappa_{1z}} \end{gathered} \tag{41}$$

The latter equations are the dispersion equations for the even and odd modes.

The third derivation of the dispersion equation comes from the poles of the scattering matrix:

$$\boldsymbol{a}_{out} = S\boldsymbol{a}_{inc} \Rightarrow S^{-1}\boldsymbol{a}_{out} = \boldsymbol{a}_{inc} \Rightarrow S^{-1}\boldsymbol{a}_{eig} = 0 \Rightarrow \frac{1}{\det S} = 0 \tag{42}$$

For the slab this condition means

$$1 - r_{22}^2 \exp\left(2ik_{z2}h\right) = 0 \tag{43}$$

Take the square root:

$$\frac{\mu_1 k_{z2} - i\mu_2\kappa_{1z}}{\mu_1 k_{z2} + i\mu_2\kappa_{1z}} \exp\left(ik_{z2}h\right) = \pm 1 \tag{44}$$

where $\kappa_{1z} = \sqrt{k_x^2 - \omega^2\varepsilon_1\mu_1} = ik_{1z}$. Expanding the complex exponent into the sine and cosine functions, and equalizing the real and imaginary parts brings

$$\begin{array}{c} \mu_1 k_{z2}\cos\left(k_{z2}h\right) + \sin\left(k_{z2}h\right)\mu_2\kappa_{1z} = \pm\mu_1 k_{z2} \\ -\mu_2\kappa_{1z}\cos\left(k_{z2}h\right) + \sin\left(k_{z2}h\right)\mu_1 k_{z2} = \pm\mu_2\kappa_{1z} \end{array} \tag{45}$$

Using the trigonometric equalities for double argument it is straightforwardly to see, that these equations yield only two independent conditions:

$$\begin{array}{c} \sin\left(\dfrac{k_{z2}h}{2}\right)\left[\mu_1 k_{z2}\sin\left(\dfrac{k_{z2}h}{2}\right) - \mu_2\kappa_{1z}\cos\left(\dfrac{k_{z2}h}{2}\right)\right] = 0 \\ \cos\left(\dfrac{k_{z2}h}{2}\right)\left[\mu_1 k_{z2}\cos\left(\dfrac{k_{z2}h}{2}\right) + \mu_2\kappa_{1z}\sin\left(\dfrac{k_{z2}h}{2}\right)\right] = 0 \end{array} \tag{46}$$

or

$$\begin{array}{c} \dfrac{\mu_1 k_{z2}}{\mu_2\kappa_{1z}} = \cot\left(\dfrac{k_{z2}h}{2}\right) \\ \dfrac{\mu_1 k_{z2}}{\mu_2\kappa_{1z}} = -\tan\left(\dfrac{k_{z2}h}{2}\right) \end{array} \Rightarrow \begin{array}{c} \dfrac{\mu_1}{\mu_2}k_{z2}\tan\left(\dfrac{k_{z2}h}{2}\right) = \sqrt{\omega^2\left(\varepsilon_2\mu_2 - \varepsilon_1\mu_1\right) - k_{z2}^2} \\ \dfrac{\mu_1}{\mu_2}k_{z2}\cot\left(\dfrac{k_{z2}h}{2}\right) = -\sqrt{\omega^2\left(\varepsilon_2\mu_2 - \varepsilon_1\mu_1\right) - k_{z2}^2} \end{array} \tag{47}$$

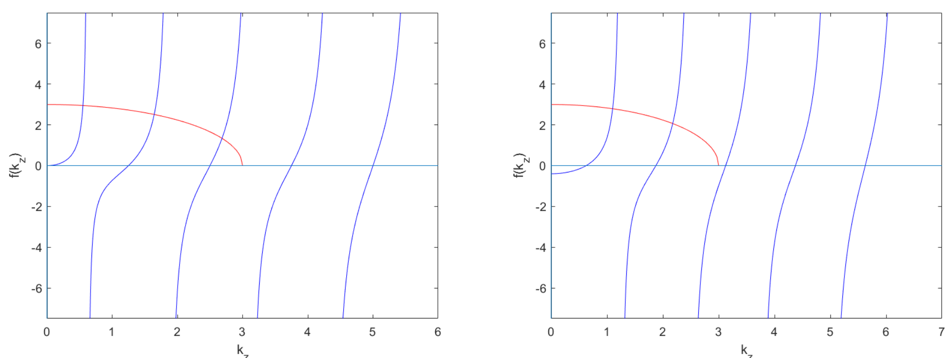

Figure 4: Graphical solution of the Eq. (47)

Discrete spectrum of a slab waveguide is a set of modes in the region $\omega\sqrt{\varepsilon_1\mu_1} < k_x < \omega\sqrt{\varepsilon_2\mu_2}$. At leas one TE mode exists for any thickness. Cut-off frequency for the first TM mode is $k_{z2}h/2 = \pi/2$, $k_{z2} = \omega_c\sqrt{\varepsilon_2\mu_2 - \varepsilon_1\mu_1}$.

3 1D photonic crystals

1D photoinc crystal is an infinite periodic set of plane layers of different permittivity (and permeability). Such structure admit an almost analytical treatment, so it is convenient to derive important properties of photonic crystals by considering the 1D case.

In the following derivations we will use the Floquet-Bloch theorem: solutions of the wave equation in a periodic potential with period Λ can be represented as products $\Phi\left(x,z\right) = \varphi\left(x,z\right)\exp\left(ikz\right)$ where $\varphi\left(x,z\right)$ is the z-periodic function with period Λ, and k is the Bloch wavevector modulo.

3.1 Dispersion

The homogeneous Helmholtz equation

$$\nabla \times \frac{1}{\varepsilon} \nabla \times \boldsymbol{H} = \omega^2 \mu_0 \boldsymbol{H} \tag{48}$$

is an eigenvalue equation for each fixed Bloch wavenumber k. The solutions should also be eigenstates of the translation operator – Bloch wavefunctions. The corresponding eigenvalues

$$T_{z\rightarrow z+n\Lambda} \Phi(x, z) = \Phi(x, z + n\Lambda) = \exp(ikn\Lambda) \Phi(x, z) \tag{49}$$

The eigenvalues are the same for any $k + mG$ with $G = 2\pi/\Lambda$. This is called reciprocal lattice. The eigenstate appears to be degenerate for the set of Bloch wavenumbers $k+mG$. Therefore, for a complete description of wave dispersion in 1D photonic crystals it is sufficient to consider $-G/2 \leq k \leq G/2$ region only: $\omega(k) = \omega(k + mG)$. This region is called the first Brillouen zone. Also in case of pure dielectric materials form time-reversal symmetry $\omega(-k) = \omega(k)$: since eigenvalues of an Hermitial operator are real and positive

$$\nabla \times \frac{1}{\varepsilon} \nabla \times \boldsymbol{H}^* = (\omega^*)^2 \mu_0 \boldsymbol{H}^* \Rightarrow \boldsymbol{H}^* = \boldsymbol{h}^*(x, z) \exp(-ikz) \Rightarrow \omega(-k) = \omega(k) \tag{50}$$

In the vicinity of $k = 0$ the dispersion is linear as the wavelentgh is much larger than the period in the empty-lattice model. So the light propagates in some effective medium. At the edge of the Brillouin zone two counter-propagating waves $\exp(\pm ikz)$ meet and form a standing wave. Thus, the group velocity $d\omega/dk \approx 0$.

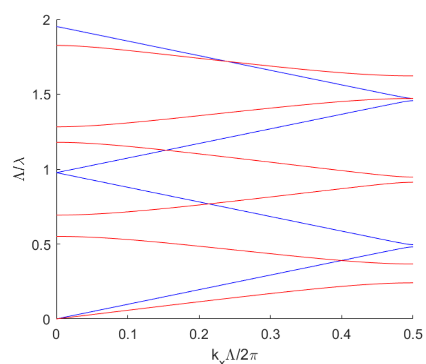

Figure 5: Disperison of 1D PhC for wave propagation perpendicular to the layers. Blue line – weak refractive index contrast; red line – high contrast.

3.2 1D PhC band diagram calculation example

Consider first a simple case case of wave propagation perpendicular to the layers of the 1D photonic crystal, and apply the Fourier method to solve the wave equation. Fourier decomposition of the periodic dielectric function:

$$\varepsilon(z) = \sum_{n=-\infty}^{\infty} \varepsilon_n \exp\left(2\pi i n \frac{z}{\Lambda}\right) \Rightarrow \varepsilon_n = \frac{1}{\Lambda} \int_0^{\Lambda} dz \varepsilon(z) \exp\left(-2\pi i n \frac{z}{\Lambda}\right) \tag{51}$$

$$\varepsilon_n = \begin{cases} \varepsilon_1 \dfrac{d_1}{\Lambda} + \varepsilon_2 \dfrac{d_2}{\Lambda} & n = 0 \\ (\varepsilon_1 - \varepsilon_2) \dfrac{\sin(\pi n d_1/\Lambda)}{\pi n} & n \neq 0 \end{cases} \tag{52}$$

The field E_y in case of the TE polarization in accordance with the Bloch theorem can also be represented as a series

$$E_x(z) = \sum_{n=-\infty}^{\infty} \varphi_n \exp\left[i\left(k + \frac{2\pi n}{\Lambda}\right)z\right] \tag{53}$$

This field satisfies the wave equation

$$\frac{d^2 E_x(z)}{dz^2} + \omega^2 \varepsilon(z)\mu_0 E_x(z) = 0 \tag{54}$$

Substitute the Fourier decompositions:

$$\begin{aligned} &-\left[\sum_{n=-\infty}^{\infty} \psi_n \left(k + \frac{2\pi n}{\Lambda}\right)^2 \exp\left(i\left(k + \frac{2\pi n}{\Lambda}\right)z\right)\right] \\ &+\omega^2\mu_0 \left[\sum_{m=-\infty}^{\infty} \varepsilon_m \exp\left(2\pi i m \frac{z}{\Lambda}\right)\right] \left[\sum_{p=-\infty}^{\infty} \psi_p \exp\left(i\left(k + \frac{2\pi p}{\Lambda}\right)z\right)\right] = 0 \end{aligned} \tag{55}$$

Let us multiply both parts of the equation by $\exp\left(-i\left(k + \frac{2\pi q}{\Lambda}\right)z\right)$, and integrate over the period. The first term is

$$\begin{aligned} &\sum_{n=-\infty}^{\infty} \left(k + \frac{2\pi n}{\Lambda}\right)^2 \psi_n \int_0^\Lambda dz \exp\left(i\left(k + \frac{2\pi n}{\Lambda}\right)z\right) \exp\left(-i\left(k + \frac{2\pi q}{\Lambda}\right)z\right) \\ &= \sum_{n=-\infty}^{\infty} \left(k + \frac{2\pi n}{\Lambda}\right)^2 \psi_n \int_0^\Lambda dz \exp\left(i\frac{2\pi}{\Lambda}(n-q)z\right) \\ &= \sum_{n=-\infty}^{\infty} \left(k + \frac{2\pi n}{\Lambda}\right)^2 \psi_n \Lambda \delta_{n-q} = \left(k + \frac{2\pi q}{\Lambda}\right)^2 \psi_q \Lambda \end{aligned} \tag{56}$$

The second term is

$$\begin{aligned} &\omega^2\mu_0 \sum_{m=-\infty}^{\infty} \sum_{p=-\infty}^{\infty} \varepsilon_m \psi_p \int_0^\Lambda dz \exp\left(i\left(k + \frac{2\pi m}{\Lambda} + \frac{2\pi p}{\Lambda}\right)z\right) \exp\left(-i\left(k + \frac{2\pi q}{\Lambda}\right)z\right) \\ &= \omega^2\mu_0 \sum_{m=-\infty}^{\infty} \sum_{p=-\infty}^{\infty} \varepsilon_m \psi_p \Lambda \delta_{m+p-q} = \Lambda \sum_{p=-\infty}^{\infty} \varepsilon_{q-p}\psi_p \end{aligned} \tag{57}$$

This is nothing that the convolution theorem for the Fourier series. Thus,

$$\left(k + \frac{2\pi q}{\Lambda}\right)^2 \psi_q - \omega^2\mu_0 \sum_{m=-\infty}^{\infty} \varepsilon_{q-m}\psi_m = 0 \tag{58}$$

This is the generalized eigenvalue equation. In the normalized form it writes

$$\left(\frac{k\Lambda}{2\pi} + q\right)^2 \psi_q = \left(\frac{k_0\Lambda}{2\pi}\right)^2 \sum_{m=-\infty}^{\infty} \varepsilon_{q-m}\psi_m \tag{59}$$

Eigenfrequencies are found upon truncation of infinite series and solving a finite matrix equation. Components ε_{q-m} constitute a matrix, which elements depends on the index difference only. Such matrices are called Toeplitz matrices.

3.3 Modal solutions

To generalize the results of the previous section let us construct the complete modal basis for a 1D PhC with material parameters being periodic functions of the coordinate x: $\varepsilon(z) = \varepsilon(z + n\Lambda)$, $\mu(z) = \mu(z + n\Lambda)$, $n \in \mathbb{Z}$. Maxwell's equations for the TE and TM polarizations split into two independent sets:

$$\begin{aligned} -\frac{\partial E_y}{\partial z} &= i\omega\mu H_x \\ \frac{\partial E_y}{\partial x} &= i\omega\mu H_z \\ \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} &= -i\omega\varepsilon E_y \end{aligned} \tag{60}$$

$$\begin{aligned}\frac{\partial H_y}{\partial z} &= i\omega\varepsilon E_x \\ \frac{\partial H_y}{\partial x} &= -i\omega\varepsilon E_z \\ \frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} &= i\omega\mu H_y\end{aligned} \tag{61}$$

Denote $\eta_e(z) = \mu(z)$, $\eta_h(z) = \varepsilon(z)$. Due to the translation invariance in the layer plane one can decompose $E_y = \psi^e(z)\exp(i\beta^e x)$ in the TE case, and $H_y = \psi^h(z)\exp\left(i\beta^h x\right)$ in the TM case. This result comes from the fact that a general solution appears to be separable:

$$\frac{\partial}{\partial z}\left(\frac{1}{\mu(z)}\frac{\partial E_y}{\partial z}\right) + \frac{\partial}{\partial x}\left(\frac{1}{\mu(z)}\frac{\partial E_y}{\partial x}\right) + \omega^2\varepsilon(z)E_y = 0 \Rightarrow E_y = \xi(x)\psi(z) \Rightarrow \tag{62}$$

$$\Rightarrow \frac{1}{\xi(x)}\frac{d^2\xi(x)}{dx^2} + \frac{\mu(z)}{\psi(z)}\frac{d}{dz}\left(\frac{1}{\mu(z)}\frac{\partial\psi(z)}{\partial z}\right) + \omega^2\varepsilon(z)\mu(z) = 0 \tag{63}$$

$$\Rightarrow \begin{cases} \dfrac{1}{\xi(x)}\dfrac{d^2\xi(x)}{dx^2} = -\beta^2 \\ \dfrac{\mu(z)}{\psi(z)}\dfrac{d}{dz}\left(\dfrac{1}{\mu(z)}\dfrac{\partial\psi(z)}{\partial z}\right) + \omega^2\varepsilon(z)\mu(z) - \beta^2 = 0 \end{cases} \Rightarrow \xi(x) \sim \exp(\pm i\beta x) \tag{64}$$

The Maxwell's equations yield an eigenvalue problem, which has the same form for both polarizations:

$$\eta(z)\frac{d}{dz}\left(\frac{1}{\eta(z)}\frac{d\psi(z)}{dz}\right) + \omega^2\varepsilon(z)\mu(z)\psi(z) = \beta^2\psi(z) \tag{65}$$

Denote the second order operator

$$\mathfrak{L}_{e,h} = \eta_{e,h}(z)\frac{d}{dz}\left(\frac{1}{\eta_{e,h}(z)}\frac{d}{dz}\right) + \omega^2\varepsilon(z)\mu(z) \Rightarrow \mathfrak{L}\psi(z) = \beta^2\psi(z) \tag{66}$$

In case of a pure dielectric material this operator is self-conjugate, having real eigenvalues and eigen functions which form a complete orthonormal set

$$\mathfrak{L}\psi_m(z) = \beta_m^2\psi_m(z) \tag{67}$$

$$\frac{1}{\Lambda}\int_0^\Lambda \frac{\psi_m(z)\overline{\psi}_n(z)}{\omega\eta(z)}dz = \delta_{mn} \tag{68}$$

In case of lossy materials one can also construct a complete set of solutions, and for this purpose bi-orhogonal bases should be used.

In each layer material parameters are constant, and the differential equation becomes

$$\frac{d^2\psi(z)}{dz^2} + \omega^2\varepsilon_{1,2}\mu_{1,2}\psi(z) = \beta^2\psi(z) \tag{69}$$

Solutions of this second order equation with constant coefficients are harmonic functions, so that the modal solutions can be written generally as

$$\psi_m(x,z) = \exp(i\beta_m x)\begin{cases} a_{1m}\exp(i\kappa_1 z) + a_{2m}\exp(-i\kappa_1 z) & 0 \le z \le d \\ b_{1m}\exp(i\kappa_2 z) + b_{2m}\exp(-i\kappa_2 z) & d \le z \le \Lambda \end{cases} \tag{70}$$

with $\kappa_{1,2} = \sqrt{\omega^2\varepsilon_{1,2}\mu_{1,2} - \beta^2}$. Second solution (magnetic field in the TE case and the electric field in the TM case):

$$\chi_m(z) = \mp\frac{1}{i\omega\eta_{1,2}}\frac{d\psi_m(z)}{dz} = \mp\exp(i\beta_m x)\begin{cases} \dfrac{i\kappa_1}{i\omega\eta_1}\left[a_{1m}\exp(i\kappa_1 z) - a_{2m}\exp(-i\kappa_1 z)\right] & 0 \le z \le d \\ \dfrac{i\kappa_2}{i\omega\eta_2}\left[b_{1m}\exp(i\kappa_2 z) - b_{2m}\exp(-i\kappa_2 z)\right] & d \le z \le \Lambda \end{cases} \tag{71}$$

where the sign $\mp$ corresponds to different polarizations in accordance with Maxwell's equations. Continuity of the solutions at the interface $z = 0$ yield an interface T-matrix:

$$\begin{gathered} a_{1m} + a_{2m} = b_{1m} + b_{2m} \\ \frac{\kappa_1}{\eta_1}\left(a_{1m} - a_{2m}\right) = \frac{\kappa_2}{\eta_2}\left(b_{1m} - b_{2m}\right) \\ \Rightarrow \begin{pmatrix} a_{1m} \\ a_{2m} \end{pmatrix} = T \begin{pmatrix} b_{1m} \\ b_{2m} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 + \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1} & 1 - \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1} \\ 1 - \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1} & 1 + \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1} \end{pmatrix} \begin{pmatrix} b_{1m} \\ b_{2m} \end{pmatrix} \end{gathered} \tag{72}$$

Using this expression we can evaluate a T-matrix of the PhC period. In accordance with the Bloch theorem for some Bloch wavenumber k_0

$$\begin{gathered} T_\Lambda = \begin{pmatrix} \exp\left(i\kappa_2 d_2\right) & 0 \\ 0 & \exp\left(-i\kappa_2 d_2\right) \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 + \frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2} & 1 - \frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2} \\ 1 - \frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2} & 1 + \frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2} \end{pmatrix} \\ \times \begin{pmatrix} \exp\left(i\kappa_1 d_1\right) & 0 \\ 0 & \exp\left(-i\kappa_1 d_1\right) \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 + \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1} & 1 - \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1} \\ 1 - \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1} & 1 + \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1} \end{pmatrix} = \exp\left(ik_0\Lambda\right) I \end{gathered} \tag{73}$$

Here $d_1 = d$, $d_2 = \Lambda - d_1$. Performing multiplications one finds that

$$\begin{gathered} T_{\Lambda 11} = \frac{1}{2} e^{i\kappa_2 d_2}\left(e^{i\kappa_1 d_1} + e^{-i\kappa_1 d_1}\right) + \frac{1}{4}\left(\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2} + \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1}\right) e^{i\kappa_2 d_2}\left(e^{i\kappa_1 d_1} - e^{-i\kappa_1 d_1}\right) \\ T_{\Lambda 12} = \frac{1}{4}\left(\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2} - \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1}\right) e^{i\kappa_2 d_2}\left(e^{i\kappa_1 d_1} - e^{-i\kappa_1 d_1}\right) \\ T_{\Lambda 21} = -\frac{1}{4}\left(\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2} - \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1}\right) e^{-i\kappa_2 d_2}\left(e^{i\kappa_1 d_1} - e^{-i\kappa_1 d_1}\right) \\ T_{\Lambda 22} = \frac{1}{2} e^{-i\kappa_2 d_2}\left(e^{i\kappa_1 d_1} + e^{-i\kappa_1 d_1}\right) - \frac{1}{4}\left(\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2} + \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1}\right) e^{-i\kappa_2 d_2}\left(e^{i\kappa_1 d_1} - e^{-i\kappa_1 d_1}\right) \end{gathered} \tag{74}$$

The determinant of the $\left[T_\Lambda - \exp\left(ik_0\Lambda\right) I\right]$ should be zero. Using the Euler's formula for complex exponents one attains

$$\begin{gathered} \left[4e^{i\kappa_2 d_2}\cos\left(\kappa_1 d_1\right) + 2i\left(\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2} + \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1}\right) e^{i\kappa_2 d_2}\sin\left(\kappa_1 d_1\right) - 4e^{ik_0\Lambda}\right] \times \\ \times \left[4e^{-i\kappa_2 d_2}\cos\left(\kappa_1 d_1\right) - 2i\left(\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2} + \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1}\right) e^{-i\kappa_2 d_2}\sin\left(\kappa_1 d_1\right) - 4e^{ik_0\Lambda}\right] - \\ -4\left(\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2} - \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1}\right)^2 \sin\left(\kappa_1 d_1\right)\sin\left(\kappa_1 d_1\right) = 0 \end{gathered} \tag{75}$$

where from

$$e^{2ik_0\Lambda} + 1 + e^{ik_0\Lambda}\left[\left(\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2} + \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1}\right)\sin\left(\kappa_1 d_1\right)\sin\left(\kappa_1 d_1\right) - 2\cos\left(\kappa_1 d_1\right)\cos\left(\kappa_1 d_1\right)\right] = 0 \tag{76}$$

Both real and imaginary parts yield the same dispersion equation:

$$\cos\left(k_0\Lambda\right) = \cos\left(\kappa_2 d_2\right)\cos\left(\kappa_1 d_1\right) - \frac{1}{2}\left(\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2} + \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1}\right)\sin\left(\kappa_1 d_1\right)\sin\left(\kappa_2 d_2\right) \tag{77}$$

If $k_0 = 0$ the dispersion equation splits into two equations for even and odd modes:

$$1 = \cos\left(\kappa_2 d_2\right)\cos\left(\kappa_1 d_1\right) - \frac{1}{2}\left(\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2} + \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1}\right)\sin\left(\kappa_1 d_1\right)\sin\left(\kappa_2 d_2\right) \Rightarrow \tag{78}$$

$$\Rightarrow \begin{gathered} \sin^2\left(\frac{\kappa_1 d_1}{2}\right)\cos^2\left(\frac{\kappa_2 d_2}{2}\right) + \frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2}\sin\left(\frac{\kappa_1 d_1}{2}\right)\cos\left(\frac{\kappa_1 d_1}{2}\right)\sin\left(\frac{\kappa_2 d_2}{2}\right)\cos\left(\frac{\kappa_2 d_2}{2}\right) \\ +\cos^2\left(\frac{\kappa_1 d_1}{2}\right)\sin^2\left(\frac{\kappa_2 d_2}{2}\right) + \frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1}\sin\left(\frac{\kappa_1 d_1}{2}\right)\cos\left(\frac{\kappa_1 d_1}{2}\right)\sin\left(\frac{\kappa_2 d_2}{2}\right)\cos\left(\frac{\kappa_2 d_2}{2}\right) = 0 \end{gathered} \Rightarrow \tag{79}$$

$$\Rightarrow \begin{array}{c}\left[\cos\left(\frac{\kappa_1 d_1}{2}\right)\sin\left(\frac{\kappa_2 d_2}{2}\right)+\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2}\sin\left(\frac{\kappa_1 d_1}{2}\right)\cos\left(\frac{\kappa_2 d_2}{2}\right)\right] \\ \times\left[\cos\left(\frac{\kappa_1 d_1}{2}\right)\sin\left(\frac{\kappa_2 d_2}{2}\right)+\frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1}\sin\left(\frac{\kappa_1 d_1}{2}\right)\cos\left(\frac{\kappa_2 d_2}{2}\right)\right]=0\end{array} \Rightarrow \tag{80}$$

$$\Rightarrow \left[\begin{array}{l}\cot\left(\frac{\kappa_1 d_1}{2}\right)\tan\left(\frac{\kappa_2 d_2}{2}\right)=-\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2} \\ \cot\left(\frac{\kappa_1 d_1}{2}\right)\tan\left(\frac{\kappa_2 d_2}{2}\right)=-\frac{\eta_1}{\eta_2}\frac{\kappa_2}{\kappa_1}\end{array}\right. \tag{81}$$

Solution of Eq. (77) maybe treaky, though, in case of the TE polarization and pure dielectric structure (consider $\varepsilon_2 > \varepsilon_1$) one can single out three regions: there are no solutions for $\beta^2 > \omega^2\varepsilon_2\mu_0$, there is at least one solution in the region $\omega^2\varepsilon_1\mu_0 < \beta^2 < \omega^2\varepsilon_2\mu_0$, and the right hand-part of Eq. (77) oscillates with maxima ≥ 1 and minima ≤ -1 (see the figure).

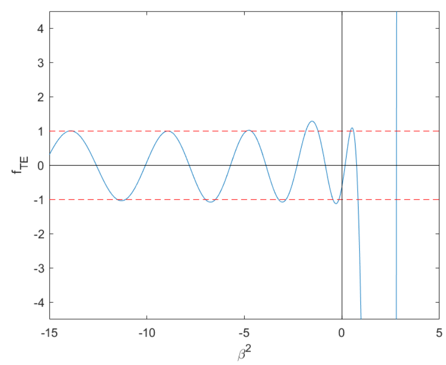

Figure 6: Right-hand part of Eq. (77) for a dielectric photonic crystal in TE polarization.

In order to construct the modal field let us take the derived functions in the following form:

$$\psi(x,z)=\exp(i\beta x)\begin{cases}a_1\cos(\kappa_1 z)+a_2\sin(\kappa_1 z) & 0\leq z\leq d \\ b_1\cos(\kappa_2 z)+b_2\sin(\kappa_2 z) & d\leq z\leq \Lambda\end{cases} \tag{82}$$

$$\chi(x,z)=\mp\exp(i\beta x)\begin{cases}\frac{\kappa_1}{i\omega\eta_1}\left[-a_1\sin(\kappa_1 x)+a_2\cos(\kappa_1 z)\right] & 0\leq z\leq d \\ \frac{\kappa_2}{i\omega\eta_2}\left[-b_1\sin(\kappa_2 x)+b_2\cos(\kappa_2 z)\right] & d\leq z\leq \Lambda\end{cases} \tag{83}$$

and relate the amplitudes via the boundary and periodic conditions. To simplify this procedure, first, let us neglect the periodic Bloch condition and assume either $a_1=1$, $a_2=0$ or $a_1=0$, $a_2=1$ (denote the corresponding functions as $\psi^{(1)}$, $\chi^{(1)}$, and $\psi^{(2)}$, $\chi^{(2)}$). In the first case the boundary conditions at $z=d_1$ yield

$$\begin{array}{c}\cos(\kappa_1 d_1)=b_1^{(1)}\cos(\kappa_2 d_1)+b_2^{(1)}\sin(\kappa_2 d_1) \\ \frac{\kappa_1}{\eta_1}\sin(\kappa_1 d_1)=\frac{\kappa_2}{\eta_2}\left[b_1^{(1)}\sin(\kappa_2 d_1)-b_2^{(1)}\cos(\kappa_2 d_1)\right]\end{array} \tag{84}$$

$$\Rightarrow \begin{array}{l}b_1^{(1)}=\cos(\kappa_1 d_1)\cos(\kappa_2 d_1)+\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2}\sin(\kappa_1 d_1)\sin(\kappa_2 d_1) \\ b_2^{(1)}=\sin(\kappa_2 d_1)\cos(\kappa_1 d_1)-\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2}\sin(\kappa_1 d_1)\cos(\kappa_2 d_1)\end{array} \tag{85}$$

In the second case when $a_1=0$:

$$\begin{array}{l}b_1^{(2)}=\sin(\kappa_1 d_1)\cos(\kappa_2 d_1)-\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2}\cos(\kappa_1 d_1)\sin(\kappa_2 d_1) \\ b_2^{(2)}=\sin(\kappa_1 d_1)\sin(\kappa_2 d_1)+\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2}\cos(\kappa_1 d_1)\cos(\kappa_2 d_1)\end{array} \tag{86}$$

So that

$$\psi^{(1)}(z) = \exp(i\beta x) \begin{cases} \cos(\kappa_1 z) & 0 \le z \le d \\ \cos(\kappa_1 d_1)\cos(\kappa_2(z-d_1)) - \dfrac{\eta_2}{\eta_1}\dfrac{\kappa_1}{\kappa_2}\sin(\kappa_1 d_1)\sin(\kappa_2(z-d_1)) & d \le z \le \Lambda \end{cases} \tag{87}$$

$$\psi^{(2)}(z) = \exp(i\beta x) \begin{cases} \sin(\kappa_1 z) & 0 \le z \le d \\ \sin(\kappa_1 d_1)\cos(\kappa_2(z-d_1)) + \dfrac{\eta_2}{\eta_1}\dfrac{\kappa_1}{\kappa_2}\cos(\kappa_1 d_1)\sin(\kappa_2(z-d_1)) & d \le z \le \Lambda \end{cases} \tag{88}$$

Now suppose that the full solution is a composition of the attained $\psi^{(1)}$, $\psi^{(2)}$ and $\chi^{(1)}$, $\chi^{(2)}$:

$$\begin{aligned} \psi(x,z) = C\left[\psi^{(1)}(z) + \alpha\psi^{(2)}(z)\right]\exp(i\beta x) \\ \chi(x,z) = C\left[\chi^{(1)}(z) + \alpha\chi^{(2)}(z)\right]\exp(i\beta x) \end{aligned} \tag{89}$$

The periodic Bloch condition allows finding the constant α:

$$\psi(x,+0) = \exp(ik_{x0}\Lambda)\,\psi(x,\Lambda-0)$$
$$\Rightarrow \alpha = \frac{\exp(-ik_{x0}\Lambda) - \psi^{(1)}(\Lambda)}{\psi^{(2)}(\Lambda)} = \frac{\exp(-ik_{x0}\Lambda) - \cos(\kappa_1 d_1)\cos(\kappa_2 d_2) + \dfrac{\eta_2}{\eta_1}\dfrac{\kappa_1}{\kappa_2}\sin(\kappa_1 d_1)\sin(\kappa_2 d_2)}{\sin(\kappa_1 d_1)\cos(\kappa_2 d_2) + \dfrac{\eta_2}{\eta_1}\dfrac{\kappa_1}{\kappa_2}\cos(\kappa_1 d_1)\sin(\kappa_2 d_2)} \tag{90}$$

Normalization constant C is found from the orthogonality condition

$$\frac{1}{\Lambda}\int_0^\Lambda \frac{\psi(z)\,\overline{\psi}(z)}{\omega\eta(z)}dz = 1$$
$$\Rightarrow C^2 = \frac{\Lambda}{\int_0^\Lambda \dfrac{\left[\psi^{(1)}(z) + \alpha\psi^{(2)}(z)\right]\left[\psi^{(1)}(z) + \overline{\alpha}\psi^{(2)}(z)\right]}{\omega\eta}dz} \tag{91}$$

3.4 Effective medium approximations for 1D photonic crystals

Consider the dispersion equation in the limit $k\Lambda \to 0$, $k_{x0} = 0$.

$$\cot\left(\frac{\kappa_1 d_1}{2}\right)\tan\left(\frac{\kappa_2 d_2}{2}\right) = -\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2} \tag{92}$$

For small arguments $\tan\alpha \approx \alpha$, hence,

$$\frac{\kappa_2 d_2}{\kappa_1 d_1} = -\frac{\eta_2}{\eta_1}\frac{\kappa_1}{\kappa_2} \Rightarrow \frac{d_2}{d_1}\kappa_2^2 = -\frac{\eta_2}{\eta_1}\kappa_1^2 \Rightarrow \omega^2\frac{d_2\eta_1\varepsilon_2\mu_2 + d_1\eta_2\varepsilon_1\mu_1}{d_1\eta_2 + d_2\eta_1} = \beta^2 \tag{93}$$

In case of the pure dielectric media and TE/TM polarizations we get

$$\omega^2\frac{d_2\varepsilon_2 + d_1\varepsilon_1}{d_1 + d_2}\mu_0 = (\beta^e)^2 \Rightarrow \varepsilon_{eff}^e = \frac{d_1\varepsilon_1 + d_2\varepsilon_2}{d_1 + d_2} \tag{94}$$

$$\omega^2\frac{d_2\varepsilon_1\varepsilon_2 + d_1\varepsilon_2\varepsilon_1}{d_1\varepsilon_2 + d_2\varepsilon_1}\mu_0 = \left(\beta^h\right)^2 \Rightarrow \varepsilon_{eff}^h = \left(\frac{\dfrac{d_1}{\varepsilon_1} + \dfrac{d_2}{\varepsilon_2}}{d_1 + d_2}\right)^{-1} \tag{95}$$

Then, one can see that in the limit of the small period the photonic crystal behaves as a uniaxial medium. Based on the S-matrix method an optical responce ofthe slab in such a case can be analyzed via simplified equations (see the Appendix).

4 1D photonic crystal slab

In the following methods the diffraction problem is solved in two steps. First the grating region $-h/2 < z < h/2$ is considered as a composite medium – photonic crystal, and one calculates Fourier decomposition of eigen waves in the corresponding infinite 1D photonic crystal. Then, owing these eigen solutions of the Maxwell's equations they should be stitched with the fields in the substrate ($z < -h/2$) and in the cover ($z > h/2$). The fields in the substrate and in the cover are represented in terms of sets of plane waves propagating upwards and downwards relative to axis Z.

The qualitative diespersion relation for the photonic crystal can be attined from the dispersion of a homogeneous slab waveguide by imposing the periodicity condition iand considering the first Brillouen zone, shematically shown in Figure 7.

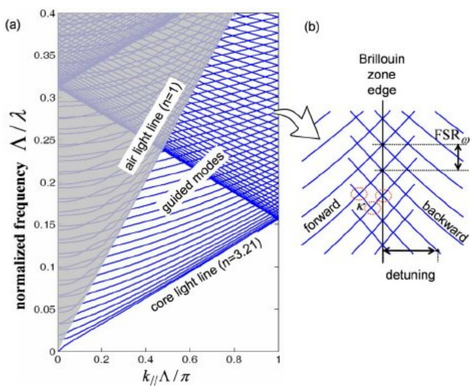

Figure 7: Qualitative explanation of the dispersion in a PhC slab (from H. Kurt, et. al., JOSA B, 25, C1 (2008))

4.1 True Modal Method

Consider a photonic crystal slab parallel to $z = 0$ plane, with axis X being the periodicity direction. Owing to the modal decomposition for an infinite 1D photonic crystal, e.g., for the TE polarization

$$E_y = \sum_m \left[a_m^+ \exp(i\beta_m z) + a_m^- \exp(-i\beta_m z)\right] \psi_m(x) \tag{96}$$

$$H_x = -\sum_m \frac{\beta_m}{\omega\mu_0} \left[a_m^+ \exp(i\beta_m z) - a_m^- \exp(-i\beta_m z)\right] \psi_m(x) \tag{97}$$

we can use the boundary conditions to relate the plane wave decomposition in the homogeneous space which surrounds the slab with the modal decomposition inside the slab via reflection and transmission matrices.

Let us start with calculating a scattering matrix of a single interface $z = 0$ between 1D PhC and a homogeneous medium. Below the interface the field is expanded into the modal solutions with coefficients $a_m^\pm$ and the above – into the plane waves with coefficients $b_n^\pm$:

$$\left\{ \begin{array}{c} E_y(-0) = E_y(+0) \\ H_y(-0) = H_y(+0) \end{array} \right. \Rightarrow$$

$$\Rightarrow \left\{ \begin{array}{c} \sum_m \left(a_m^+ + a_m^-\right) \psi_m(x) = \sum_n \left(b_n^+ + b_n^-\right) \exp(ik_{xn}x) \\ \sum_m \dfrac{\beta_m}{\omega\mu_0} \left(a_m^+ - a_m^-\right) \psi_m(x) = \sum_n \dfrac{k_{zn}}{\omega\mu_0} \left(b_n^+ - b_n^-\right) \exp(ik_{xn}x) \end{array} \right. \tag{98}$$

Denote coefficient vectors $\boldsymbol{a}^\pm = \{a_m^\pm\}$, $\boldsymbol{b}^\pm = \{b_m^\pm\}$. Multiply the latter equations by $\psi_q^*(x)$, integrate along the period, and apply the orthogonality of modal functions in the TE polarization

$\int_0^\Lambda \psi_m(x)\,\psi_n^*(x)\,dx = \omega\mu_0\Lambda\delta_{n-m}$:

$$\left\{\begin{array}{l} a_m^+ + a_m^- = \sum_n \left(b_n^+ + b_n^-\right) M_{mn} \\ a_m^+ - a_m^- = \sum_n N_{mn}\left(b_n^+ - b_n^-\right) \end{array}\right. \Rightarrow \left\{\begin{array}{l} \boldsymbol{a}^+ = \frac{1}{2}\left(M+N\right)\boldsymbol{b}^+ + \frac{1}{2}\left(M-N\right)\boldsymbol{b}^- \\ \boldsymbol{a}^- = \frac{1}{2}\left(M-N\right)\boldsymbol{b}^+ + \frac{1}{2}\left(M+N\right)\boldsymbol{b}^- \end{array}\right. \tag{99}$$

where the matrix elements $M_{mn} = \frac{1}{\omega\mu_0\Lambda}\int_0^\Lambda \exp\left(ik_{xn}x\right)\psi_m^*(x)\,dx$, $N_{mn} = \frac{k_{zn}}{\beta_m}M_{mn}$. This is the T-matrix relation. It can be transformed to an S-matrix relation:

$$\left\{\begin{array}{c} \boldsymbol{b}^+ = 2\left(M+N\right)^{-1}\boldsymbol{a}^+ - \left(M+N\right)^{-1}\left(M-N\right)\boldsymbol{b}^- \\ \boldsymbol{a}^- = \left(M-N\right)\left(M+N\right)^{-1}\boldsymbol{a}^+ + \left[\frac{1}{2}\left(M+N\right) - \frac{1}{2}\left(M-N\right)\left(M+N\right)^{-1}\left(M-N\right)\right]\boldsymbol{b}^- \end{array}\right. \tag{100}$$

or

$$S = \begin{pmatrix} -\left(M+N\right)^{-1}\left(M-N\right) & 2\left(M+N\right)^{-1} \\ \frac{1}{2}\left(M+N\right) - \frac{1}{2}\left(M-N\right)\left(M+N\right)^{-1}\left(M-N\right) & \left(M-N\right)\left(M+N\right)^{-1} \end{pmatrix} \tag{101}$$

The same steps can be used to derive a scattering matrix of a photonic crystal slab:

1. write down the field plane wave expansion in the half-infinite media above and below the slab, and the modal expansion within the slab
2. apply the boundary conditions at the upper and lower interfaces of the slab ($z = \pm h/2$)
3. express the amplitude vectors for outgoing plane waves above and below the slab via amplitude vectors of incoming plane waves

4.2 Fourier modal method

The idea of the Fourier modal method (FMM) is just the same as in the modal method, but instead of the true modal field solutions of the 1D photonic crystal one seeks for the eigen solutions in the Fourier space. Consider a photonic crystal slab parallel to $z = 0$ plane, with axis X being the periodicity direction. First, we start with an infinite photonic crystal, invoke the Bloch theorem, and decompose the periodic part of the field into the Fourier series

$$\Phi(x,z) = \exp(ikx)\,\varphi(x,z) = \sum_m \varphi_m(z)\exp\left(ik_{xm}x\right) \tag{102}$$

where $k_{xm} = k_0 + \frac{2\pi}{\Lambda}m$. Also, for the periodic permittivity $\varepsilon(x) = \sum_m \varepsilon_m \exp\left(im\frac{2\pi}{\Lambda}x\right)$. A special attention should be payed to the Fourier decomposition of products $D_{x,z} = \varepsilon E_{x,z}$. It has to be taken into account that since the function $\varepsilon(x)$ is discontinuous, solutions to the diffraction problem lie in the set of distributions (generalized functions). Due to the boundary conditions at vertical interfaces separating different materials of the photonic crystal E_z is continuous along the X direction whereas E_x is not. Formally, the electric displacement field should meet the equation $\nabla\mathbf{D} = 0$. However, a derivative of a product of two discontinuous distributions with coincident points of discontinuities, as εE_x, does not exist. Therefore, one may expect that the Fourier decomposition of $D_x = \varepsilon E_x$ would yield a poor convergence to the method. To overcome this issue it was proposed to, first, rewrite this equality as $\frac{1}{\varepsilon}D_x = E_x$, second, perform the Fourier transform $\sum_n (1/\varepsilon)_{mn} D_{xn} = E_{xm}$, third, truncate the series to get finite vectors and matrices, and then express the required amplitude vector $\boldsymbol{D}_x = [\![1/\varepsilon]\!]^{-1}\boldsymbol{E}_x$, where $[\![1/\varepsilon]\!]^{-1}$ is inverse of the truncated Fourier matrix, and $\boldsymbol{D}_x = \{D_{xm}\}$, $\boldsymbol{E}_x = \{E_{xm}\}$. This said, substitution of Fourier decomposed field and permittivity into Maxwell's equations (60) and (61) yields

$$\begin{array}{c} -\frac{\partial}{\partial z}\boldsymbol{E}_y(z) = i\omega\mu_0\boldsymbol{H}_x(z) \\ iK\boldsymbol{E}_y(z) = i\omega\mu_0\boldsymbol{H}_z(z) \\ \frac{\partial}{\partial z}\boldsymbol{H}_x(z) - iK\boldsymbol{H}_z(z) = -i\omega\,[\![\varepsilon]\!]\,\boldsymbol{E}_y(z) \end{array} \tag{103}$$

for the TE polarization, and

$$\begin{array}{c} \frac{\partial}{\partial z}\boldsymbol{H}_y(z) = i\omega\,[\![1/\varepsilon]\!]^{-1}\boldsymbol{E}_x(z) \\ iK\boldsymbol{H}_y(z) = -i\omega\,[\![\varepsilon]\!]\,\boldsymbol{E}_z(z) \\ \frac{\partial}{\partial z}\boldsymbol{E}_x(z) - iK\boldsymbol{E}_z(z) = i\omega\mu_0\boldsymbol{H}_y(z) \end{array} \tag{104}$$

for the TM polarization. The diagonal matrix $K = \{k_{xm}\}$. After rearranging the terms one obtains the corresponding differential equations for the Fourier components of the fields (the the TE and TM polarization):

$$\frac{d^2}{\partial z^2}\boldsymbol{E}_y(z) + \left(\omega^2\mu_0 [\![\varepsilon]\!] - K^2\right)\boldsymbol{E}_y(z) = 0 \tag{105}$$

$$\frac{\partial}{\partial z}\begin{pmatrix}\boldsymbol{H}_y(z)\\ \boldsymbol{E}_x(z)\end{pmatrix} = i\omega\begin{pmatrix} 0 & [\![1/\varepsilon]\!]^{-1} \\ \mu_0\left(I - \frac{1}{\omega^2\mu_0}K[\![\varepsilon]\!]^{-1}K\right) & 0\end{pmatrix}\begin{pmatrix}\boldsymbol{H}_y(z)\\ \boldsymbol{E}_x(z)\end{pmatrix} \tag{106}$$

Solutions of these differential equations can be searched in form $\varphi_m(z) = \varphi_m \exp(i\beta z)$. Denote the field coefficient vectors with small letters $\boldsymbol{e}$, and $\boldsymbol{h}$. This yields the following matrix eigenvalue problems:

$$\beta^2\boldsymbol{e}_y = \left(\omega^2\mu_0[\![\varepsilon]\!] - K^2\right)\boldsymbol{e}_y = M^e\boldsymbol{e}_y \tag{107}$$

and:

$$\begin{gathered} i\beta\begin{pmatrix}\boldsymbol{h}_y\\ \boldsymbol{e}_x\end{pmatrix} = i\omega\begin{pmatrix} 0 & [\![1/\varepsilon]\!]^{-1} \\ \mu_0\left(I - \frac{1}{\omega^2\mu_0}K[\![\varepsilon]\!]^{-1}K\right) & 0\end{pmatrix}\begin{pmatrix}\boldsymbol{h}_y\\ \boldsymbol{e}_x\end{pmatrix} \Rightarrow \\ \Rightarrow \beta^2\begin{pmatrix}\boldsymbol{h}_y\\ \boldsymbol{e}_x\end{pmatrix} = M^h\begin{pmatrix}\boldsymbol{h}_y\\ \boldsymbol{e}_x\end{pmatrix}, \\ M^h = \omega^2\mu_0\begin{pmatrix}[\![1/\varepsilon]\!]^{-1}\left(I - \frac{1}{\omega^2\mu_0}K[\![\varepsilon]\!]^{-1}K\right) & 0 \\ 0 & \left(I - \frac{1}{\omega^2\mu_0}K[\![\varepsilon]\!]^{-1}K\right)[\![1/\varepsilon]\!]^{-1}\end{pmatrix}\end{gathered} \tag{108}$$

Numerical solution of these two eigenvalue problems yields vectors of propagation constants $\boldsymbol{\beta} = \left\{\beta_m^{e,h}\right\}$ and corresponding eigenvectors $\boldsymbol{e_y}$, and $\boldsymbol{h}_y$, $\boldsymbol{e}_x$.

Analogously to the true modal method, at the second step one has to apply the boundary conditions at the slab interfaces $z = \pm d/2$ on the continuity of the tangential field components

$$\begin{gathered} E_{x,y}\left(z = \pm\tfrac{d}{2} - 0\right) = E_{x,y}\left(z = \pm\tfrac{d}{2} + 0\right) \\ H_{x,y}\left(z = \pm\tfrac{d}{2} - 0\right) = H_{x,y}\left(z = \pm\tfrac{d}{2} + 0\right)\end{gathered} \tag{109}$$

The general field decomposition for the periodic problem under consideration in a homogeneous isotropic medium is (compare with Eq. (13))

$$\begin{gathered} \boldsymbol{E}(x,y,z) = \sum_m \exp(ik_{xm}x)\left[\begin{array}{c}\left(a_m^{e+}\hat{\boldsymbol{e}}_m^{e+} - \dfrac{k}{\omega\varepsilon}a_m^{h+}\hat{\boldsymbol{e}}_m^{h+}\right)\exp(ik_{zm}z) \\ +\left(a_m^{e-}\hat{\boldsymbol{e}}_m^{e-} - \dfrac{k}{\omega\varepsilon}a_m^{h-}\hat{\boldsymbol{e}}_m^{h-}\right)\exp(-ik_{zm}z)\end{array}\right] \\ \boldsymbol{H}(x,y,z) = \sum_m \exp(ik_{xm}x)\left[\begin{array}{c}\left(a_m^{h+}\hat{\boldsymbol{e}}_m^{e+} + \dfrac{k}{\omega\mu}a_m^{e+}\hat{\boldsymbol{e}}_m^{h+}\right)\exp(ik_{zm}z) \\ +\left(a_m^{h-}\hat{\boldsymbol{e}}_m^{e-} + \dfrac{k}{\omega\mu}a_m^{e-}\hat{\boldsymbol{e}}_m^{h-}\right)\exp(-ik_{zm}z)\end{array}\right]\end{gathered} \tag{110}$$

Consider for simplicity the TE polarization (treatment of the TM case is quite similar). The explicit decomposition of the field in the lower half-space (with $\varepsilon = \varepsilon_1$, and $k_{zm}^{(1)} = \sqrt{\omega^2\varepsilon_1\mu_0 - k_{xm}^2}$) when $z \le h/2$ is

$$\begin{pmatrix}E_y\\ H_x\end{pmatrix} = \sum_m \exp(ik_{xm}x)\left[\begin{pmatrix}a_m^{e+}\\ \dfrac{k_{zm}^{(1)}}{\omega\mu_0}a_m^{e+}\end{pmatrix}\exp\left[ik_{zm}^{(1)}\left(z + \frac{d}{2}\right)\right] + \begin{pmatrix}a_m^{e-}\\ -\dfrac{k_{zm}^{(1)}}{\omega\mu_0}a_m^{e-}\end{pmatrix}\exp\left[-ik_{zm}^{(1)}\left(z + \frac{d}{2}\right)\right]\right] \tag{111}$$

Here we used explicit components of the polarization unit vectors given by Eq. (8). Analogously, for the upper homogeneous medium (with $\varepsilon = \varepsilon_2$, and $k_{zm}^{(2)} = \sqrt{\omega^2 \varepsilon_2 \mu_0 - k_{xm}^2}$), $z \geq h/2$:

$$\left(\begin{array}{c} E_y \\ H_x \end{array} \right) = \sum_m \exp\left(ik_{xm}x\right) \left[\left(\begin{array}{c} b_m^{e+} \\ \frac{k_{zm}^{(2)}}{\omega\mu_0} b_m^{e+} \end{array} \right) \exp\left[ik_{zm}^{(2)}\left(z - \frac{d}{2}\right)\right] + \left(\begin{array}{c} b_m^{e-} \\ -\frac{k_{zm}^{(2)}}{\omega\mu_0} b_m^{e-} \end{array} \right) \exp\left[-ik_{zm}^{(2)}\left(z - \frac{d}{2}\right)\right] \right] \tag{112}$$

Within the slab the modal decomposition writes

$$\left(\begin{array}{c} E_y \\ H_x \end{array} \right) = \sum_m \exp\left(ik_{xm}x\right) \sum_q \left[c_q^+ \exp\left(i\beta_q z\right) + c_q^- \exp\left(-i\beta_q z\right)\right] \left(\begin{array}{c} e_{yqm} \\ h_{xqm} \end{array} \right) \tag{113}$$

Then, the interface conditions (109) yield (here one shoud use the orthogonality of factors $\exp\left(ik_{xm}x\right)$):

$$\left(\begin{array}{cc} 1 & 1 \\ \frac{k_{zm}^{(1)}}{\omega\mu_0} & -\frac{k_{zm}^{(1)}}{\omega\mu_0} \end{array} \right) \left(\begin{array}{c} a_m^{e+} \\ a_m^{e-} \end{array} \right) = \sum_q \left(\begin{array}{cc} e_{yqm} & e_{yqm} \\ h_{xqm} & h_{xqm} \end{array} \right) \left(\begin{array}{cc} \exp\left(-i\beta_q \frac{d}{2}\right) & 0 \\ 0 & \exp\left(i\beta_q \frac{d}{2}\right) \end{array} \right) \left(\begin{array}{c} c_q^+ \\ c_q^- \end{array} \right) \tag{114}$$

$$\left(\begin{array}{cc} 1 & 1 \\ \frac{k_{zm}^{(2)}}{\omega\mu_0} & -\frac{k_{zm}^{(2)}}{\omega\mu_0} \end{array} \right) \left(\begin{array}{c} b_m^{e+} \\ b_m^{e-} \end{array} \right) = \sum_q \left(\begin{array}{cc} e_{yqm} & e_{yqm} \\ h_{xqm} & h_{xqm} \end{array} \right) \left(\begin{array}{cc} \exp\left(i\beta_q \frac{d}{2}\right) & 0 \\ 0 & \exp\left(-i\beta_q \frac{d}{2}\right) \end{array} \right) \left(\begin{array}{c} c_q^+ \\ c_q^- \end{array} \right) \tag{115}$$

The matrices in the left-had parts can be inverted, and the equations can be rearranged to give

$$\begin{array}{c} \left(\begin{array}{c} a_m^{e+} \\ b_m^{e-} \end{array} \right) = \frac{1}{2} \left(\begin{array}{cc} 1 & \omega\mu_0/k_{zm}^{(1)} \\ 1 & -\omega\mu_0/k_{zm}^{(2)} \end{array} \right) \sum_q \exp\left(-i\beta_q \frac{d}{2}\right) \left(\begin{array}{cc} e_{yqm} & 0 \\ 0 & h_{xqm} \end{array} \right) \left(\begin{array}{cc} 1 & \exp\left(i\beta_q d\right) \\ \exp\left(i\beta_q d\right) & 1 \end{array} \right) \left(\begin{array}{c} c_q^+ \\ c_q^- \end{array} \right) \\ \left(\begin{array}{c} a_m^{e-} \\ b_m^{e+} \end{array} \right) = \frac{1}{2} \left(\begin{array}{cc} 1 & -\omega\mu_0/k_{zm}^{(1)} \\ 1 & \omega\mu_0/k_{zm}^{(2)} \end{array} \right) \sum_q \exp\left(-i\beta_q \frac{d}{2}\right) \left(\begin{array}{cc} h_{yqm} & 0 \\ 0 & e_{xqm} \end{array} \right) \left(\begin{array}{cc} 1 & \exp\left(i\beta_q d\right) \\ \exp\left(i\beta_q d\right) & 1 \end{array} \right) \left(\begin{array}{c} c_q^+ \\ c_q^- \end{array} \right) \end{array} \tag{116}$$

In the matrix-vector form they give the S-matrix

$$\begin{array}{l} \left(\begin{array}{c} \boldsymbol{a}^{e+} \\ \boldsymbol{b}^{e-} \end{array} \right) = Q^e \left(\begin{array}{c} \boldsymbol{c}^+ \\ \boldsymbol{c}^- \end{array} \right) \\ \left(\begin{array}{c} \boldsymbol{a}^{e-} \\ \boldsymbol{b}^{e+} \end{array} \right) = R^e \left(\begin{array}{c} \boldsymbol{c}^+ \\ \boldsymbol{c}^- \end{array} \right) \end{array} \Rightarrow \left(\begin{array}{c} \boldsymbol{a}^{e-} \\ \boldsymbol{b}^{e+} \end{array} \right) = R^e \left(Q^e\right)^{-1} \left(\begin{array}{c} \boldsymbol{a}^{e+} \\ \boldsymbol{b}^{e-} \end{array} \right) = S^e \left(\begin{array}{c} \boldsymbol{a}^{e+} \\ \boldsymbol{b}^{e-} \end{array} \right) \tag{117}$$

4.3 Emission from 1D photonic crystal

To describe luminescence in a complex structure one can use the FMM together with the reciprocity conditions. We start with deriving the reciprocity theorem for time-harmonic Maxwell's equations

$$\begin{array}{c} \nabla \times \boldsymbol{E} = i\omega \boldsymbol{B} \\ \nabla \times \boldsymbol{H} = \boldsymbol{J} - i\omega \boldsymbol{D} \end{array} \tag{118}$$

with linear relations

$$\begin{array}{c} \boldsymbol{D} = \varepsilon \boldsymbol{E} \\ \boldsymbol{B} = \mu \boldsymbol{H} \end{array} \tag{119}$$

defined by symmetric tensors. Consider two different monochromatic sources having equal frequencies ω: $\boldsymbol{J}_{1,2}$.

$$\begin{array}{c} \nabla \times \boldsymbol{E}_1 = i\omega \boldsymbol{B}_1 \\ \nabla \times \boldsymbol{H}_1 = \boldsymbol{J}_1 - i\omega \boldsymbol{D}_1 \end{array} \left| \begin{array}{c} \cdot \boldsymbol{H}_2 \\ \cdot \boldsymbol{E}_2 \end{array} \right. \Rightarrow \begin{array}{c} \boldsymbol{H}_2 \cdot \nabla \times \boldsymbol{E}_1 = i\omega \boldsymbol{H}_2 \cdot \boldsymbol{B}_1 \\ \boldsymbol{E}_2 \cdot \nabla \times \boldsymbol{H}_1 = \boldsymbol{E}_2 \cdot \boldsymbol{J}_1 - i\omega \boldsymbol{E}_2 \cdot \boldsymbol{D}_1 \end{array} \tag{120}$$

$$\begin{array}{c} \nabla \times \boldsymbol{E}_2 = i\omega \boldsymbol{B}_2 \\ \nabla \times \boldsymbol{H}_2 = \boldsymbol{J}_2 - i\omega \boldsymbol{D}_2 \end{array} \left| \begin{array}{c} \cdot (-\boldsymbol{H}_1) \\ \cdot (-\boldsymbol{E}_1) \end{array} \right. \Rightarrow \begin{array}{c} -\boldsymbol{H}_1 \cdot \nabla \times \boldsymbol{E}_2 = -i\omega \boldsymbol{H}_1 \cdot \boldsymbol{B}_2 \\ -\boldsymbol{E}_1 \cdot \nabla \times \boldsymbol{H}_2 = -\boldsymbol{E}_1 \cdot \boldsymbol{J}_2 + i\omega \boldsymbol{E}_1 \cdot \boldsymbol{D}_2 \end{array} \tag{121}$$

Sum up all the equations:

$$\boldsymbol{H}_2 \cdot \nabla \times \boldsymbol{E}_1 - \boldsymbol{H}_1 \cdot \nabla \times \boldsymbol{E}_2 + \boldsymbol{E}_2 \cdot \nabla \times \boldsymbol{H}_1 - \boldsymbol{E}_1 \cdot \nabla \times \boldsymbol{H}_2 = \boldsymbol{E}_2 \cdot \boldsymbol{J}_1 - \boldsymbol{E}_1 \cdot \boldsymbol{J}_2 \tag{122}$$

Where we used the fact that

$$\begin{gathered} \boldsymbol{H}_2 \cdot \boldsymbol{B}_1 = H_{2\alpha}\mu_{\alpha\beta}H_{1\beta} = H_{2\alpha}\mu_{\beta\alpha}H_{1\beta} = \boldsymbol{H}_1 \cdot \boldsymbol{B}_2 \\ \boldsymbol{E}_2 \cdot \boldsymbol{D}_1 = \boldsymbol{E}_1 \cdot \boldsymbol{D}_2 \end{gathered} \tag{123}$$

Then, apply $\nabla\left(\boldsymbol{A} \times \boldsymbol{B}\right) = \boldsymbol{B} \cdot \nabla \times \boldsymbol{A} - \boldsymbol{A} \cdot \nabla \times \boldsymbol{B}$:

$$\nabla\left[\left(\boldsymbol{E}_1 \times \boldsymbol{H}_2\right) + \left(\boldsymbol{H}_1 \times \boldsymbol{E}_2\right)\right] = \boldsymbol{E}_2 \cdot \boldsymbol{J}_1 - \boldsymbol{E}_1 \cdot \boldsymbol{J}_2 \tag{124}$$

Integrate over the total space:

$$\int d^3\boldsymbol{r}\nabla\left[\left(\boldsymbol{E}_1 \times \boldsymbol{H}_2\right) + \left(\boldsymbol{H}_1 \times \boldsymbol{E}_2\right)\right] = \int d^3\boldsymbol{r}\left(\boldsymbol{E}_2 \cdot \boldsymbol{J}_1 - \boldsymbol{E}_1 \cdot \boldsymbol{J}_2\right) \tag{125}$$

$$\int d^3\boldsymbol{r}\nabla\left[\left(\boldsymbol{E}_1 \times \boldsymbol{H}_2\right) + \left(\boldsymbol{H}_1 \times \boldsymbol{E}_2\right)\right] = \int\limits_{\infty} d\boldsymbol{\sigma} \cdot \left[\left(\boldsymbol{E}_1 \times \boldsymbol{H}_2\right) + \left(\boldsymbol{H}_1 \times \boldsymbol{E}_2\right)\right] = 0 \tag{126}$$

Thus,

$$\int d^3\boldsymbol{r}\left(\boldsymbol{E}_2 \cdot \boldsymbol{J}_1\right) = \int d^3\boldsymbol{r}\left(\boldsymbol{E}_1 \cdot \boldsymbol{J}_2\right) \tag{127}$$

Now consider a PhC slab with local incoherent sources. To find the field they emit at infinity at a given direction (θ_0, φ_0) we can apply the reciprocity theorem, where $\boldsymbol{J}_1 \equiv \boldsymbol{J}_{loc}\left(\boldsymbol{r}\right)$ is a local dipole source, $\boldsymbol{E}_1 = \boldsymbol{E}_{emi}\left(\theta_0, \varphi_0\right) = \boldsymbol{E}_{emi}\exp\left(i\boldsymbol{k}_0\boldsymbol{r}\right)$ – the (unknown) plane wave field emitted by this source at infinity, $\boldsymbol{J}_2 \equiv \boldsymbol{J}_{ext}\left(\theta_0, \varphi_0\right)$ is a dipole source at infinity, and $\boldsymbol{E}_2 = \boldsymbol{E}_{exc}\left(\boldsymbol{r}\right)$ is the local field excited by an incident plane wave. The monochromatic local dipole source

$$\boldsymbol{J}_{loc}\left(\boldsymbol{r}\right) = -i\omega\boldsymbol{p}_{loc}\delta\left(\boldsymbol{r} - \boldsymbol{r}_d\right) \tag{128}$$

Then,

$$-i\omega\int d^3\boldsymbol{r}\boldsymbol{E}_{exc}\left(\boldsymbol{r}\right)\boldsymbol{p}_d\delta\left(\boldsymbol{r} - \boldsymbol{r}_d\right) = \int d^3\boldsymbol{r}\boldsymbol{E}_{emi}\exp\left(i\boldsymbol{k}_{inc}\boldsymbol{r}\right)\boldsymbol{J}_{ext}\left(\theta_0, \varphi_0\right) \tag{129}$$

Suppose the external source is also a dipole source of unit amplitude $|\boldsymbol{p}_{exc}| = 1$, where $\boldsymbol{p}_{exc} \perp \boldsymbol{k}_0$, $\boldsymbol{E}_{exc}||\boldsymbol{p}_{exc}$:

$$\boldsymbol{p}_{loc} \cdot \boldsymbol{E}_{exc}\left(\boldsymbol{r}_d\right) = \boldsymbol{p}_{exc} \cdot \boldsymbol{E}_{emi}\exp\left(i\boldsymbol{k}_0\boldsymbol{r}_\infty\right) \tag{130}$$

$$\left|\boldsymbol{E}_{emi}^{TE,TM}\right|^2 = \left|\boldsymbol{p}_{loc} \cdot \boldsymbol{E}_{exc}^{TE,TM}\left(\boldsymbol{r}_d\right)\right|^2 \tag{131}$$

Power flow of the TE and TM polarizations:

$$P_z\left(\boldsymbol{p}_{loc}, \boldsymbol{r}_d\right) = \frac{1}{2}\left[\left|\boldsymbol{E}_{emi}^{TE}\right|^2 \Re\left(k_0\right) + \left|\boldsymbol{E}_{emi}^{TM}\right|^2 \Re\left(\frac{k_0}{\varepsilon_b}\right)\right] \tag{132}$$

Averaging over dipole orientations:

$$P_z\left(\boldsymbol{p}_{loc}, \boldsymbol{r}_d\right) = \frac{1}{2N_o}\sum_{k=1}^{N_o}\left[\left|\boldsymbol{p}_{loc}^{(k)} \cdot \boldsymbol{E}_{exc}^{TE,TM}\left(\boldsymbol{r}_d\right)\right|^2 \Re\left(k_0\right) + \left|\boldsymbol{p}_{loc}^{(k)} \cdot \boldsymbol{E}_{exc}^{TE,TM}\left(\boldsymbol{r}_d\right)\right|^2 \Re\left(\frac{k_0}{\varepsilon_b}\right)\right] \tag{133}$$

or

$$P_z\left(\boldsymbol{p}_{loc}, \boldsymbol{r}_d\right) = \frac{1}{8\pi}\int d\Omega_d\left[\left|\boldsymbol{p}_{loc} \cdot \boldsymbol{E}_{exc}^{TE,TM}\left(\boldsymbol{r}_d\right)\right|^2 \Re\left(k_0\right) + \left|\boldsymbol{p}_{loc} \cdot \boldsymbol{E}_{exc}^{TE,TM}\left(\boldsymbol{r}_d\right)\right|^2 \Re\left(\frac{k_0}{\varepsilon_b}\right)\right] \tag{134}$$

5 Resonant effects in 1D photonic crystal slabs

Consider calculation of the reflectance spectrum from a 1D PhC subwavelength dielectric slab by the FMM (slab parameters are $h = 0.255\mu m$, $\Lambda = 1.15\mu m$, $d/\Lambda = 0.4$, $\varepsilon_1 = 3.17^2$, $\varepsilon_2 = 1$) for $\theta_0 = 0°$ and $\theta_0 = 1°$ angles of incidence [...]. The result is given in figure ... . One can distinguish a sharp asymmetric resonance at 1° angle of incidence which cannot be found at normal incidence (when $k_{x0} = 0$ – at Γ point). This resonance is due to an excitation of the slab mode, which has an odd (asymmetric) field profie. Since the field of the incident plane wave at $k_{x0} = 0$ is purely symmetric, it cannot be coupled to this mode. At small angles the coupling is very small, so the quality factor of the resonance is very high.

5.1 Symmetric and asymmetric resonance shape

In this section consider simple resonant systems, which exhibit either symmetric or asymmetric resonance lineshape. An example of a simple resonant system is a 1D oscillator, which motion is governed by the wave equation

$$\frac{d^2x}{dt^2} + 2\gamma\frac{dx}{dt} + \omega_0^2 x = f \tag{135}$$

For the external harmonic force $f = f_0 \exp(i\omega t)$ a general solution for sustained oscillations can be searched in form $x = C(\omega)\exp(i\omega t)$. Substitution into the wave equation yields

$$C(\omega) = \frac{f_0}{\omega_0^2 - \omega^2 + 2i\omega\gamma} \Rightarrow \left\{ \begin{array}{l} |C(\omega)| = \dfrac{f_0}{\sqrt{\left(\omega_0^2 - \omega^2\right)^2 + 4\omega^2\gamma^2}} \\ \arg C(\omega) = \arctan\left(\dfrac{2\omega\gamma}{\omega^2 - \omega_0^2}\right) \end{array} \right. \tag{136}$$

For sufficiently small losses in the vicinity of the resonance $|\omega - \omega_0| \ll \omega_0$ the lineshape can be approximated by the Lorentzian

$$|C(\omega)| \approx \frac{f_0}{2\omega\gamma\left[1 + \dfrac{1}{2}\dfrac{(\omega_0+\omega)^2(\omega_0-\omega)^2}{4\omega^2\gamma^2}\right]} \approx \frac{\gamma f_0}{\omega_0\left[(\omega-\omega_0)^2 + 2\gamma^2\right]} \tag{137}$$

This lineshape has a symmetric profile, which is generally the case when an exciting field interacts with a resonant system. Resonance position of the latter equation is determined by the poles of function $|C(\omega)|$:

$$(\omega - \omega_0)^2 + 2\gamma^2 = 0 \Rightarrow \omega_{res} = \omega_0 \pm i\sqrt{2}\gamma \tag{138}$$

Here one should choose the sign +, which corresponds to the damping. The quality factor, which is equal to the ratio between the stored and lost energy by one period of oscillations (or the relation of the resonant frequency to the half-width of the resonance line) can be related to the imaginry part of the resonance frequency:

$$Q = \frac{W_{stored}}{W_{lost}} = \frac{\omega_0}{2\gamma} \sim \frac{\Re(\omega_{res})}{\Im(\omega_{res})} \tag{139}$$

A model, which gives an asymmetric lineshape is more sophysticated. Let us consider two coupled oscillators with an external force exciting one of them:

$$\left\{ \begin{array}{l} \dfrac{d^2x_1}{dt^2} + 2\gamma_1\dfrac{dx_1}{dt} + \omega_{01}^2 x_1 + v x_2 = f_0 \exp(i\omega t) \\ \dfrac{d^2x_2}{dt^2} + 2\gamma_2\dfrac{dx_2}{dt} + \omega_{02}^2 x_2 + v x_1 = 0 \end{array} \right. \tag{140}$$

For simplicity suppose that $\omega_{01} \approx \omega_{02}$, $\gamma_2 = 0$, and $\gamma_1, v \ll \omega_{01}$. Then one can search for solutions $x_{1,2} = c_{1,2}\exp(i\omega t)$. Substitution yields:

$$\left\{ \begin{array}{l} c_1\left(\omega_{01}^2 - \omega^2 + 2i\gamma_1\omega\right) + vc_2 = f_0 \\ vc_1 + c_2\left(\omega_{02}^2 - \omega^2\right) = 0 \end{array} \right. \tag{141}$$

In the absence of the external force one gets the dispersion equation

$$\left(\omega_{01}^2 - \omega^2 + 2i\gamma_1\omega\right)\left(\omega_{02}^2 - \omega^2\right) - v^2 = 0 \tag{142}$$

which solutions define the eigenfrequencies of the system. Solution of Eq. (141) is

$$\begin{aligned} c_1 &= \frac{f_0\left(\omega_{02}^2 - \omega^2\right)}{\left(\omega_{01}^2 - \omega^2 + 2i\gamma_1\omega\right)\left(\omega_{02}^2 - \omega^2\right) - v^2} \\ c_2 &= -\frac{vf_0}{\left(\omega_{01}^2 - \omega^2 + 2i\gamma_1\omega\right)\left(\omega_{02}^2 - \omega^2\right) - v^2} \end{aligned} \tag{143}$$

For the first power coefficient in case $\omega \approx \omega_{02}$ (hence, $\left(\omega_{02}^2 - \omega^2\right) \approx 2\omega_{02}\left(\omega_{02} - \omega\right)$)

$$\begin{aligned} |c_1|^2 &= \frac{f_0^2\left(\omega_{02}^2 - \omega^2\right)^2}{\left[\left(\omega_{01}^2 - \omega^2\right)\left(\omega_{02}^2 - \omega^2\right) - v^2\right]^2 + 4\gamma_1^2\omega^2\left(\omega_{02}^2 - \omega^2\right)^2} \\ &\approx \frac{4f_0^2\omega_{02}^2\left(\omega_{02} - \omega\right)^2}{\left[2\omega_{02}\left(\omega_{01}^2 - \omega_{02}^2\right)\left(\omega_{02} - \omega\right) - v^2\right]^2 + 16\gamma_1^2\omega_{02}^4\left(\omega_{02} - \omega\right)^2} = |c_{01}|^2\frac{(\epsilon + q)^2}{\epsilon^2 + 1} \end{aligned} \tag{144}$$

with

$$\begin{aligned} \epsilon &= \frac{\left(\omega_{01}^2 - \omega_{02}^2\right)^2 + 4\gamma_1^2\omega_{02}^2}{v^2\gamma_1}\left(\omega - \omega_{02}\right) - \frac{\omega_{02}^2 - \omega_{01}^2}{2\gamma_1\omega_{02}} \\ q &= \frac{\omega_{02}^2 - \omega_{01}^2}{2\gamma_1\omega_{02}} \\ |c_{01}|^2 &= \frac{f_0^2}{v^4\gamma_1^2}\frac{v^4\gamma_1^2}{\left[\left(\omega_{01}^2 - \omega_{02}^2\right)^2 + 4\gamma_1^2\omega_{02}^2\right]} \end{aligned} \tag{145}$$

The asymmetry of the responce can be seen by taking $\omega = \omega_{02}$ – in this case $|c_1| = 0$. The latter of Eq. (144) is a general form for the asymmetric Fano lineshape profile. If considering a particle having two scattering chennels: one is directly to the continuum, and the second is to a bound state with a further tunneling to the continuum, then, variable ϵ has the meaning of the energy, and the parameter q characterizes the relation of the probabilitites for the paricle to scatter through each channel. In the normalized form

$$\sigma = \frac{1}{q^2 + 1}\frac{(\epsilon + q)^2}{\epsilon^2 + 1},\ \sigma_{max} = 1 \tag{146}$$

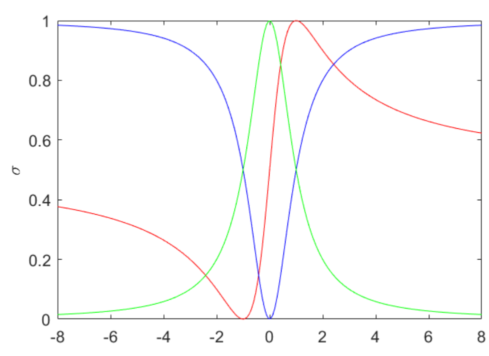

Figure 8: Fano formula lineshapes, Eq. (146). Red line – for $q = 1$, blue line – for $q = 0$, green line – for $q = \infty$.

5.2 Calculation of zeros and poles

In physical problems the equation for eigenmodes or resonances

$$\det S^{-1} = 0 \tag{147}$$

can be a transcendental equation like in case of the slab waveguide, a polynomial equation like in case of a simple resonator, a matrix equation, or even be defined by a numerical algorithm. There is no universal method to solve it, so in each case one has to search for a most appropriate way. The equation is equivalent to a search for poles of the scattering matrix.

In case when the dispersion relation is defined by a polynomial or transcendental function $f(x)$ one apply the Newton root-finging method: given an inital approximation x_0 do until convergence:

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} \tag{148}$$

This is the consequence of the Taylor series decomposition:

$$0 \approx f(x_k + \Delta x) = f(x_k) + f'(x_k)\,\Delta x \Rightarrow \Delta x = x_{k+1} - x_k = -\frac{f(x_k)}{f'(x_k)} \tag{149}$$

When function f is complex-valued one should take care when searching for all zeros since a set of initial approximations which converge to a given root is a fractal set (called Newton bassin) (see Figure 9). Sometimes it is useful to search for roots with a higher order approximation, e.g., the third order Halley method:

$$\begin{aligned} 0 \approx f(x_k + \Delta x) = f(x_k) + f'(x_k)\,\Delta x + \frac{1}{2} f''(x_k)\,(\Delta x)^2 \\ \Rightarrow \Delta x = -\frac{f'(x_k)}{f''(x_k)}\left(1 - \sqrt{1 - 2\frac{f''(x_k)\,f(x_k)}{[f'(x_k)]^2}}\right) \approx -\frac{f'(x_k)}{f''(x_k)}\left(\frac{f''(x_k)\,f(x_k)}{[f'(x_k)]^2} - \frac{1}{2}\left(\frac{f''(x_k)\,f(x_k)}{[f'(x_k)]^2}\right)^2\right) \\ = -\frac{f(x_k)}{f'(x_k)}\left(1 + \frac{1}{2}\frac{f''(x_k)\,f(x_k)}{[f'(x_k)]^2}\right) \end{aligned} \tag{150}$$

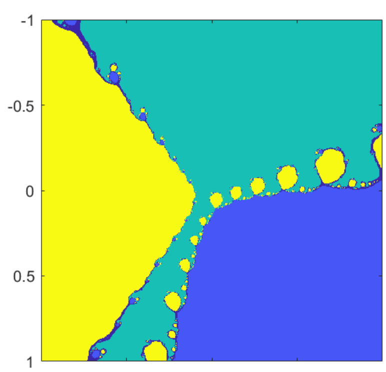

Figure 9: Newton bassin for a third order polynomial.

If one faces the matrix equation $S^{-1}\boldsymbol{a} = 0$, analogs for the Newton and Halley methods can be derived. First, given an approximation for the root ω_n, consider a decomposition of the inverse scattering matrix aroun zero:

$$S^{-1}(\omega) \approx S^{-1}(\omega_n) + (\omega - \omega_n)\left[\frac{dS^{-1}}{d\omega}\right]_{\omega=\omega_n} \tag{151}$$

Then let us multiply this matrix equation by a scattered amplitude vector $\boldsymbol{a}$, and evaluate the equality in the pole:

$$\begin{aligned} 0 = S^{-1}(\omega_p)\,\boldsymbol{a} \approx S^{-1}(\omega_n)\,\boldsymbol{a} + (\omega_p - \omega_n)\left[\frac{dS^{-1}}{d\omega}\right]_{\omega=\omega_n}\boldsymbol{a} \\ \Rightarrow (\omega_n - \omega_p)\left[\frac{dS^{-1}}{d\omega}\right]_{\omega=\omega_n}\boldsymbol{a} \approx S^{-1}(\omega_n)\,\boldsymbol{a} \end{aligned} \tag{152}$$

We attain the generalized eigenvalue problem, and once it is solved the minimal eigenvalue can be used to get a new approximation ω_{n+1}:

$$\omega_{n+1} = \omega_n - \min\operatorname{eig}\left(S^{-1}(\omega_n),\left[\frac{dS^{-1}}{d\omega}\right]_{\omega=\omega_n}\right) \tag{153}$$

Usually this methods leads to a rapid loss of accuracy due to the inversion operation with the incresing matrix dimension.

To avoid matrix inversion consider a resonant decomposition of the scattering matrix

$$S(\omega) = A(\omega) + \sum_m \frac{B_m}{\omega - \omega_{pm}} \tag{154}$$

with slowly varying matrix function $A(\omega)$, and pole amplitude matrices B_m. Since $S^{-1}(\omega_{pm})\,\boldsymbol{a} = 0$, then $\ker S^{-1}$ describes eigen fields, and $\mathrm{Im}B_m = \ker S^{-1}$. If $\mathrm{rank}B_m = r$, then there exists a decomposition $B_m = L_m R_m$ with $L_m \subset \mathbb{C}^{n\times r}$, $R_m \subset \mathbb{C}^{r\times n}$, so that

$$S(\omega) = A(\omega) + \sum_m L_m \frac{1}{\omega - \omega_{pm}} R_m = A(\omega) + L\,(I\omega - \Omega_p)^{-1} R \tag{155}$$

One can take the derivatives

$$\begin{aligned} S'(\omega) &= -L\,(I\omega - \Omega_p)^{-2} R \\ S''(\omega) &= 2L\,(I\omega - \Omega_p)^{-3} R \end{aligned} \tag{156}$$

When $\omega = \omega_n$ (some approximation of the pole), these are the equation for unknown diagonal matrix Ω_p. Consider a singular value decomposition of the second derivative:

$$S''(\omega) = U\Sigma V^{\dagger} \tag{157}$$

with unitary matrices U and V ($U^{\dagger}U = I$, $V^{\dagger}V = I$) and the diagonal matrix of singular values $\Sigma \subset \mathbb{C}^{r\times r}$,. Then, $\Sigma = U^{\dagger}S''(\omega)\,V$, and

$$\begin{aligned} &\begin{cases} U^{\dagger}S'(\omega)\,V = -U^{\dagger}L\,(I\omega - \Omega_p)^{-2} RV \\ \Sigma = 2U^{\dagger}L\,(I\omega - \Omega_p)^{-3} RV \end{cases} \Rightarrow \begin{cases} (I\omega - \Omega_p)^{-2} = -\left(U^{\dagger}L\right)^{-1} U^{\dagger}S'(\omega)\,V\,(RV)^{-1} \\ (I\omega - \Omega_p)^{-3} = \frac{1}{2}\left(U^{\dagger}L\right)^{-1}\Sigma\,(RV)^{-1} \end{cases} \\ &\Rightarrow (I\omega - \Omega_p) = (I\omega - \Omega_p)^{-2}(I\omega - \Omega_p)^{3} = -2\left(U^{\dagger}L\right)^{-1} U^{\dagger}S'(\omega)\,V\,(RV)^{-1}(RV)\,\Sigma^{-1}\left(U^{\dagger}L\right) \\ &\qquad = -2\left(U^{\dagger}L\right)^{-1}\left(U^{\dagger}S'(\omega)\,V\Sigma^{-1}\right)\left(U^{\dagger}L\right) \\ &\Rightarrow U^{\dagger}S'(\omega)\,V\Sigma^{-1} = \frac{1}{2}\left(U^{\dagger}L\right)(\Omega_p - I\omega)\left(U^{\dagger}L\right)^{-1} \end{aligned} \tag{158}$$

The latter relation is an eigenvalue decomposition of the left hand part matrix. Thus,

$$\Omega_p - I\omega = 2\mathrm{diageig}\left(U^{\dagger}S'(\omega)\,V\Sigma^{-1}\right) \tag{159}$$

and the algorithm can be constructed as follows

$$\omega_{n+1} = \omega_n + 2\min\operatorname{eig}\left(U^{\dagger}S'(\omega_n)\,V\Sigma^{-1}\right),\ S''(\omega_n) = U\Sigma V^{\dagger} \tag{160}$$

The derivatives can be calculated via the finite differences as

$$\begin{aligned} S'(\omega_n) &\approx \frac{S(\omega_n + \Delta_\omega) - S(\omega_n - \Delta_\omega)}{2\Delta_\omega} \\ S''(\omega_n) &\approx \frac{S(\omega_n + \Delta_\omega) - 2S(\omega_n) + S(\omega_n - \Delta_\omega)}{(\Delta_\omega)^2} \end{aligned} \tag{161}$$

where the step Δ_ω should be taken to be small enough to resolve the resonance. The S-matrix for these resonant frequency search can be calculated, e.g., by the FMM or TMM described above.

In case there is only one resonance in the region of interest, $\mathrm{rank}B = r = 1$, Σ has only one nonzero element σ in the first row and the first column. Therefore,

$$S''(\omega) = U\Sigma V^\dagger = U_1 \Sigma V_1^\dagger \Rightarrow \begin{cases} S''(\omega) U_1 = \sigma \left(V_1^\dagger U_1\right) U_1 \\ S''^\dagger(\omega) V_1 = \sigma \left(U_1^\dagger V_1\right) V_1 \end{cases} \tag{162}$$

i.e., U_1 is an eigenvector of $S''(\omega)$, and V_1 is an eigenvector of $S''^\dagger(\omega)$. Hence, $\sigma = \max\mathrm{eig}\left(S''(\omega)\right) / \left(V_1^\dagger U_1\right)$ where $\max\mathrm{eig}\left(S''(\omega)\right)$ is the only nonzero eigenvalue of $S''(\omega)$. So,

$$S''(\omega) = U_1 \frac{\max\mathrm{eig}\left(S''(\omega)\right)}{\left(V_1^\dagger U_1\right)} V_1^\dagger \tag{163}$$

Also U_1 and V_1 are also eigenvectors of S', since

$$\begin{gathered} U^\dagger S'(\omega) V\Sigma^{-1} = \frac{1}{2}\left(U^\dagger L\right)(\omega_p - \omega)\left(U^\dagger L\right)^{-1} \\ \Rightarrow S'(\omega) = \frac{1}{2}(\omega_p - \omega) U\Sigma V^\dagger = U_1 \frac{\max\mathrm{eig}\left(S'(\omega)\right)}{\left(V_1^\dagger U_1\right)} V_1^\dagger \end{gathered} \tag{164}$$

and

$$U^\dagger S'(\omega) V\Sigma^{-1} = \frac{\max\mathrm{eig}\left(S'(\omega)\right)}{\left(V_1^\dagger U_1\right)} U^\dagger U_1 V_1^\dagger V \Sigma^{-1} = \frac{\max\mathrm{eig}\left(S'(\omega)\right)}{\left(V_1^\dagger U_1\right)} \frac{1}{\sigma} = \frac{\max\mathrm{eig}\left(S'(\omega)\right)}{\max\mathrm{eig}\left(S''(\omega)\right)} \tag{165}$$

so the iteration algorithm reduces to

$$\omega_{n+1} = \omega_n + 2\frac{\max\mathrm{eig}\left(S'(\omega_n)\right)}{\max\mathrm{eig}\left(S''(\omega_n)\right)} \tag{166}$$

5.3 Modal description of resonant reflection

If one calcultes the quality factors of the leaky mode resonance of a 1D photonic crystal slab, the appear points with infinitely large quality factor (Fig. 10, 11). These are so called boud states in the continuum (BIC). They are of two types. The first type states are due the symmetry mismatch at Γ point, whereas the second type are due to the interference effects.

The appearence of the second type resonances can be qualitatively (and quantitatively also) rationalized by considering propagating Bloch modes in the slab. Bloch modes were derived above while considering an infinite photonic crystal. For a rather small period there exists only one solution $\beta^2 > 0$ of Eq. (77) which corresponds to a single propagating mode. Owing an interface with a homogeneous medium this mode can be reflected and transmitted at this interface (Fig. 12). For larger period there appear several modes (say, N modes). Let us denote their reflection coefficients at the slab interfaces as r_{mn}. Then the equation for the self-consistent modal amplitudes inside the slab is

$$\begin{cases} a_m^+ = \sum_{n=1}^N r_{mn} a_n^- \exp(i\beta_m h) \\ a_m^- = \sum_{n=1}^N r_{mn} a_n^+ \exp(i\beta_m h) \end{cases} \tag{167}$$

Writing this equation in the form $R\boldsymbol{a} = 0$ yields the disperison equaion for the leaky modes $\det R = 0$. Transmitted wave amplitude for the leackage radiation is

$$b^t = \sum_{m=1}^N t_m a_m^+ \exp(i\beta_m h) \tag{168}$$

Within the single mode approximation $N=1$, and the dispersion equation gives resonance condition

$$1 - r_{11}^2 \exp\left(2i\beta_1 h\right) = 0 \Rightarrow \beta_1 h + \arg r_{11} = \pi l \tag{169}$$

This is similar to the Fabry-Perot resonator and a slab waveguide equation. Amplitude of the transmitted wave is

$$b^t = t_1 a_1^+ \exp\left(i\beta_1 h\right) \tag{170}$$

Since $t_1 \neq 0$, no BIC can appear under the single mode approximation, since the first mode is even.

Consider two modes. At Γ point ($k_{x0}=0$) the two modes are not coupled due to the symmetry (the mode is even, and the second is odd, see Fig. 12): $r_{12}=r_{21}=0$. Also for the odd mode we have $r_{22}=1$, $t_2=0$, and attain the symmetry-protected BIC metioned above. When $k_{x0}\neq 0$

$$\left\{\begin{array}{ll} a_1^+ & = r_{11}a_1^- \exp\left(i\beta_1 h\right) + r_{12}a_2^- \exp\left(i\beta_2 h\right) \\ a_2^+ & = r_{21}a_1^- \exp\left(i\beta_1 h\right) + r_{22}a_2^- \exp\left(i\beta_2 h\right) \\ a_1^- & = r_{11}a_1^+ \exp\left(i\beta_1 h\right) + r_{12}a_2^+ \exp\left(i\beta_2 h\right) \\ a_2^- & = r_{21}a_1^+ \exp\left(i\beta_1 h\right) + r_{22}a_2^+ \exp\left(i\beta_2 h\right) \end{array}\right. \Rightarrow 1 - \left(r_{eff}^{(12)}\right)^2 \exp\left(2i\beta_2 h\right) = 0 \tag{171}$$

with the effective reflection coefficient

$$r_{eff}^{(12)} = \frac{r_{22} + \alpha r_{11} r_{21} r_{12} \exp\left(2i\beta_1 h\right)}{1 - \alpha r_{21} r_{12} \exp\left[i\left(\beta_1+\beta_2\right)h\right]},\ \alpha = \frac{1}{1 - r_{11}^2 \exp\left(2i\beta_1 h\right)} \tag{172}$$

So the behaviour of two coupled modes can be described as in the case of the Fabry-Perot resonator. The radiated plane wave amplitude can be also described via an effective transmission coefficient

$$b^t = t_1 a_1^+ \exp\left(i\beta_1 h\right) + t_2 a_2^+ \exp\left(i\beta_2 h\right) = t_{eff}^{(12)} a_2^+ \exp\left(i\beta_2 h\right) \tag{173}$$

$$t_{eff}^{(12)} = t_2 + \alpha t_1 r_{21} \exp\left(i\beta_1 h\right)\left[r_{eff}^{(12)} \exp\left(i\beta_2 h\right) + r_{11}\exp\left(i\beta_1 h\right)\right] \tag{174}$$

The dependence of $t_{eff}^{(12)}$ from the Bloch wavenumber shown in Fig. 13 reveals that for certain values of k_{x0} where the effective transmission goes to zeros. This also corresponds to states with infinite quality factor, and these states are called accidental BIC. Therefore we can conclude that the nature of these accidental BIC-s is the destructive interference of leaky states.

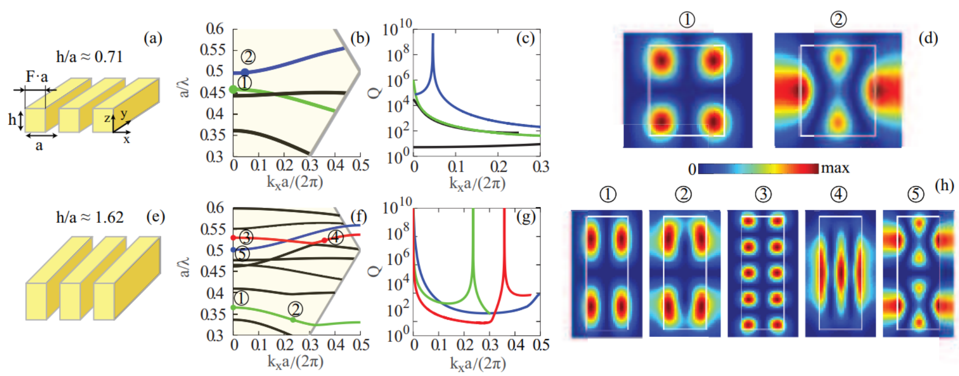

Figure 10: Several leaky modes of 1D PhC slab and their quality factors (from arXiv:1907.09330v1).

6 2D and 2D Photonic crystals

Similarly to the 1D case of photonic crystals the reciprocal space splits into equivalen Brillouin zones, so the physical properties of a crystal are defined by modal behavior in the first Brillouin zone. Three non-complanar Bravais lattice vectors of elementary cell $\boldsymbol{p}_{1,2,3}$ and the condition (see Eq. (49))

$$\exp\left(i\boldsymbol{G}_n\boldsymbol{R}_m\right) = 1,\ \boldsymbol{G}_n = n_1\boldsymbol{b}_1 + n_2\boldsymbol{b}_2 + n_3\boldsymbol{b}_3 \tag{175}$$

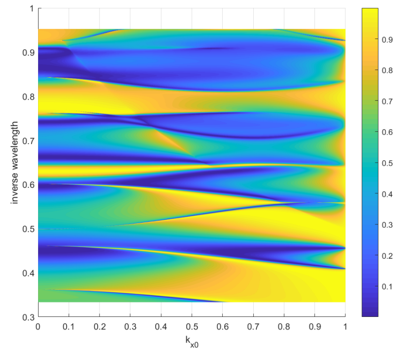

Figure 11: Dependence of the power reflection coefficient from the inverse wavelength and angle of incidence for a photonic crystal slab in the air with period $\Lambda = 1\mu m$, thickness 0.7Λ, pitch width 0.6Λ, and permittivity 3.5^2. One can distinguish poits at which some resonance lines become infinitely thin.

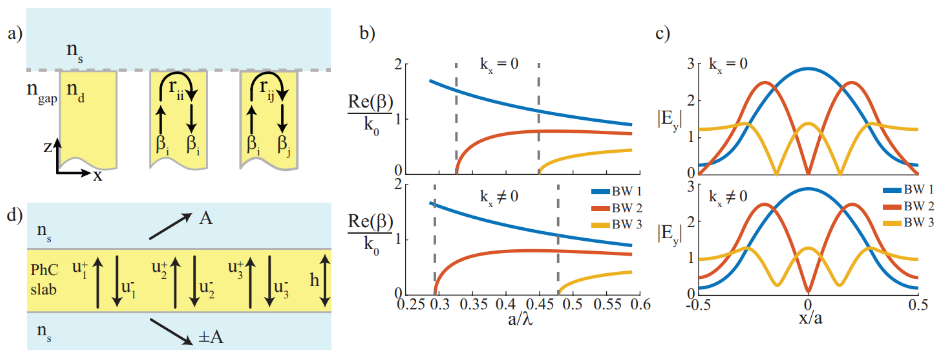

Figure 12: First, second and third propagating modes in 1D PhC and their reflection at the slab interfaces (from arXiv:1907.09330v1).

where $\boldsymbol{R}_m = m_1\boldsymbol{p}_1 + m_2\boldsymbol{p}_2 + m_3\boldsymbol{p}_3,$, yield the basis reciprocal lattice vectors

$$\begin{aligned} \boldsymbol{b}_1 &= 2\pi\frac{\boldsymbol{p}_2 \times \boldsymbol{p}_3}{\boldsymbol{p}_1 \cdot (\boldsymbol{p}_2 \times \boldsymbol{p}_3)} \\ \boldsymbol{b}_2 &= 2\pi\frac{\boldsymbol{p}_3 \times \boldsymbol{p}_1}{\boldsymbol{p}_1 \cdot (\boldsymbol{p}_2 \times \boldsymbol{p}_3)} \\ \boldsymbol{b}_3 &= 2\pi\frac{\boldsymbol{p}_1 \times \boldsymbol{p}_2}{\boldsymbol{p}_1 \cdot (\boldsymbol{p}_2 \times \boldsymbol{p}_3)} \end{aligned} \tag{176}$$

In 2D and 3D the Brilloin zone can have different shapes. Its characteristic points are denoted with capital Greek characters, e.g. see Fig. ...

The Floquet-Bloch theorem reads in vector form:

$$\Phi(\boldsymbol{r}) = \varphi(\boldsymbol{r})\exp(i\boldsymbol{k}\boldsymbol{r}),\ \varphi(\boldsymbol{r} + \boldsymbol{R}_m) = \varphi(\boldsymbol{r}),\ m_\alpha \in \mathbb{Z} \tag{177}$$

6.1 Plane wave expansion method in 2D

Analogously to the previous consideration of 1D PhC eigen solutions of the Maxwell's equations can be searched for by means of the Fourier method. Being written for the time-harmonic fields with time dependence factor $\exp(-i\omega t)$ the vector Helmholtz equation for the magnetic field reads

$$\nabla \times \frac{1}{\varepsilon(\boldsymbol{r})}\nabla \times \boldsymbol{H}(\boldsymbol{r}) = \omega^2\mu_0\boldsymbol{H}(\boldsymbol{r}) \tag{178}$$

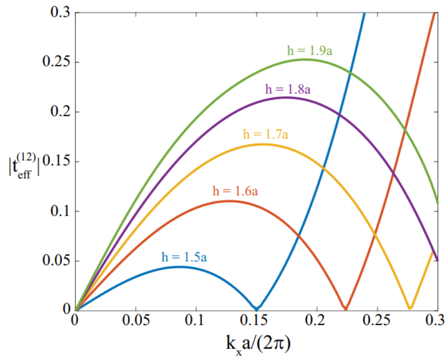

Figure 13: Effective transmission coefficient for the two-mode approximation

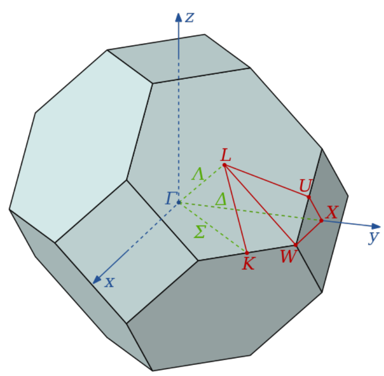

Figure 14: Example of the Brillouin zone for FCC lattice (wikipedia)

In case of 2D crystals the function $\varepsilon(\boldsymbol{r})$ is periodic in the XY plane and independent of the third coordinate z:

$$\varepsilon(\boldsymbol{r}) = \varepsilon(\boldsymbol{\rho}, z) = \varepsilon(\boldsymbol{\rho} + \boldsymbol{R}_m, z), \ \boldsymbol{\rho} = (x, y)^T \tag{179}$$

with the Bravais lattice vectors $\boldsymbol{R}_m = m_1\boldsymbol{p}_1 + m_2\boldsymbol{p}_2$, $m_{1,2}$ are integers and $\boldsymbol{p}_{1,2}$ are lattice constants. Eq. (178) is an eigenvalue problem which will be solved for unknown eigen frequencies ω providing that the dielectric permittivity is real and dispersionless in a frequency range under consideration (the case of dispersive materials will be discussed below). The Bloch theorem states

$$\boldsymbol{H}(\boldsymbol{r}) = \exp(i\boldsymbol{k}\boldsymbol{r})\,\boldsymbol{H}_{\boldsymbol{k}}(\boldsymbol{r}) \tag{180}$$

so that the function $\boldsymbol{H}_{\boldsymbol{k}}(\boldsymbol{r}) = \boldsymbol{H}_{\boldsymbol{k}}(\boldsymbol{r} + \boldsymbol{R}_m)$ is purely periodic with lattice periodicity. The Bloch vector $\boldsymbol{k} = (k_x, k_y, 0)^T$ This periodic vector function can be decomposed into two polarization states, TE, and TM (see Eq. (8)),

$$\boldsymbol{H}_{\boldsymbol{k}}(\boldsymbol{r}) = \hat{\boldsymbol{e}}^e_{\boldsymbol{k}} H^e_{\boldsymbol{\kappa}}(\boldsymbol{r}) + \hat{\boldsymbol{e}}^h_{\boldsymbol{k}} H^h_{\boldsymbol{\kappa}}(\boldsymbol{r}) \tag{181}$$

where $\hat{\boldsymbol{e}}^{e,h}_{\boldsymbol{k}}$ are unit plane wave polarization vectors. Explicitly for the 2D problem under investigation $\hat{\boldsymbol{e}}^{TM}_{\boldsymbol{k}} = \hat{\boldsymbol{e}}_z$, $\hat{\boldsymbol{e}}^{TE}_{\boldsymbol{k}} = \frac{1}{k}(\boldsymbol{k} \times \hat{\boldsymbol{e}}_z)$.

Periodic functions in Eqs. (178) and (181) can be decomposed into their Fourier series

$$\begin{array}{c} 1/\varepsilon(\boldsymbol{r}) = \sum_m f_m \exp(i\boldsymbol{G}_m\boldsymbol{r}) \\ H^{e,h}_{\boldsymbol{k}}(\boldsymbol{r}) = \sum_m H^{e,h}_{\boldsymbol{k}m} \exp(i\boldsymbol{G}_m\boldsymbol{r}) \end{array} \tag{182}$$

with $\boldsymbol{G}_m = m_1\boldsymbol{b}_1 + m_2\boldsymbol{b}_2$ being the reciprocal lattice vectors, $\boldsymbol{b}_1 = \frac{2\pi}{\Lambda}(\boldsymbol{p}_2 \times \hat{\boldsymbol{e}}_z) / (\hat{\boldsymbol{e}}_z \cdot [\boldsymbol{p}_1 \times \boldsymbol{p}_2])$, $\boldsymbol{b}_2 = \frac{2\pi}{\Lambda}(\hat{\boldsymbol{e}}_z \times \boldsymbol{p}_1) / (\hat{\boldsymbol{e}}_z \cdot [\boldsymbol{p}_1 \times \boldsymbol{p}_2])$, which lie in the plane XY. Substitution of (180)-(182) into (178) gives

$$\begin{aligned}\nabla \times \textstyle\sum_n f_n \exp\left(i\boldsymbol{G}_n\boldsymbol{r}\right) \nabla \times \sum_p \left(\hat{\boldsymbol{e}}_p^e H_{\boldsymbol{k}p}^e + \hat{\boldsymbol{e}}_p^h H_{\boldsymbol{k}p}^h\right) \exp\left(i\boldsymbol{k}_p\boldsymbol{r}\right) \\ = \omega^2\mu_0 \textstyle\sum_m \left(\hat{\boldsymbol{e}}_p^e H_{\boldsymbol{k}m}^e + \hat{\boldsymbol{e}}_p^h H_{\boldsymbol{k}m}^h\right) \exp\left(i\boldsymbol{k}_m\boldsymbol{r}\right)\end{aligned} \tag{183}$$

where $\boldsymbol{k}_m = \boldsymbol{k} + \boldsymbol{G}_m$, and the unit vectors $\hat{\boldsymbol{e}}_m^{e,h}$ correspond to the wavevector $\boldsymbol{k}_m$. Index m here is a two-dimensional index. Curl operators transform to vector products

$$\begin{aligned}\textstyle\sum_n \sum_p f_n \left[\left(\boldsymbol{k}_p + \boldsymbol{G}_n\right) \times \boldsymbol{k}_p \times \left(\hat{\boldsymbol{e}}_p^e H_{\boldsymbol{k}p}^e + \hat{\boldsymbol{e}}_p^h H_{\boldsymbol{k}p}^h\right)\right] \exp\left[i\left(\boldsymbol{k}_p + \boldsymbol{G}_n\right)\boldsymbol{r}\right] \\ = -\omega^2\mu_0 \textstyle\sum_m \left(\hat{\boldsymbol{e}}_m^e H_{\boldsymbol{k}m}^e + \hat{\boldsymbol{e}}_m^h H_{\boldsymbol{k}m}^h\right) \exp\left(i\boldsymbol{k}_m\boldsymbol{r}\right)\end{aligned} \tag{184}$$

To simplify the equation the orthogonality of exponential functions can be used. Multiplication of the both parts by $\exp\left(-i\boldsymbol{k}_m\boldsymbol{r}\right)$ and integration over the period yields

$$\sum_n f_n \left[\boldsymbol{k}_m \times \left(\boldsymbol{k}_m - \boldsymbol{G}_n\right) \times \left(\hat{\boldsymbol{e}}_{m-n}^e H_{\boldsymbol{k},m-n}^e + \hat{\boldsymbol{e}}_{m-n}^h H_{\boldsymbol{k},m-n}^h\right)\right] = -\omega^2\mu_0 \left(\hat{\boldsymbol{e}}_m^e H_{\boldsymbol{k}m}^e + \hat{\boldsymbol{e}}_m^h H_{\boldsymbol{k}m}^h\right) \tag{185}$$

Note that $\boldsymbol{G}_m - \boldsymbol{G}_n = \left(m_1 - n_1\right)\boldsymbol{b}_1 + \left(m_1 - n_1\right)\boldsymbol{b_2}$. Then, substitution $\boldsymbol{G}_p = \boldsymbol{G}_m - \boldsymbol{G}_n$ and a change of the summation index yield

$$\sum_n f_{m-n} \left[\boldsymbol{k}_m \times \boldsymbol{k}_n \times \left(\hat{\boldsymbol{e}}_n^e H_{\boldsymbol{k},n}^e + \hat{\boldsymbol{e}}_n^h H_{\boldsymbol{k},n}^h\right)\right] = -\omega^2\mu_0 \left(\hat{\boldsymbol{e}}_m^e H_{\boldsymbol{k}m}^e + \hat{\boldsymbol{e}}_m^h H_{\boldsymbol{k}m}^h\right) \tag{186}$$

Since $\boldsymbol{k} \cdot \hat{\boldsymbol{e}}_z = 0$, the latter equation splits into two independent equations for the TM and the TE polarizations. By multiplying both parts by either $\hat{\boldsymbol{e}}_m^e$ or $\hat{\boldsymbol{e}}_m^h$ one attains

$$\sum_n f_{m-n} \left|\boldsymbol{k}_m\right| \left|\boldsymbol{k}_n\right| H_{\boldsymbol{k}n}^e = \omega^2\mu_0 H_{\boldsymbol{k}m}^e \tag{187}$$

for the TE polarization, and

$$\sum_n f_{m-n} \left(\boldsymbol{k}_m \cdot \boldsymbol{k}_n\right) H_{\boldsymbol{k}n}^h = \omega^2\mu_0 H_{\boldsymbol{k}m}^h \tag{188}$$

for the TM polarization.

Eigen solutions of Eqs. (187) and (188) yield frequencies of waves, which can propagate in the photonic crystal for a given direction and modulo of the Bloch wavevector $\boldsymbol{k}$.

6.2 Plane wave expansion method in 3D

In order to generalize the results of the previous section here we consider a 3D infinitely periodic structure – 3D photonic crystal:

$$\nabla \times \frac{1}{\varepsilon\left(\boldsymbol{r}\right)} \nabla \times \boldsymbol{H}\left(\boldsymbol{r}\right) = \omega^2\mu_0 \boldsymbol{H}\left(\boldsymbol{r}\right) \tag{189}$$

$$\boldsymbol{H}\left(\boldsymbol{r}\right) = \exp\left(i\boldsymbol{k}\boldsymbol{r}\right) \boldsymbol{H}_{\boldsymbol{k}}\left(\boldsymbol{r}\right) \tag{190}$$

so that the function $\boldsymbol{H}_{\boldsymbol{k}}\left(\boldsymbol{r}\right) = \boldsymbol{H}_{\boldsymbol{k}}\left(\boldsymbol{r} + \boldsymbol{R}_m\right)$ is purely periodic with lattice periodicity, $\boldsymbol{R}_m = m_1\boldsymbol{p}_1 + m_2\boldsymbol{p_2} + m_2\boldsymbol{p}_3$, and the Bloch vector $\boldsymbol{k} = \left(k_x, k_y, k_z\right)^T$. Fourier decomposition:

$$\begin{aligned}1/\varepsilon\left(\boldsymbol{r}\right) = \textstyle\sum_m f_m \exp\left(i\boldsymbol{G}_m\boldsymbol{r}\right) \\ \boldsymbol{H}_{\boldsymbol{k}}\left(\boldsymbol{r}\right) = \textstyle\sum_m \boldsymbol{h}_{\boldsymbol{k}m} \exp\left(i\boldsymbol{G}_m\boldsymbol{r}\right)\end{aligned} \tag{191}$$

where $m = \left(m_1, m_2, m_3\right)^T \in \mathbb{Z}^3$.

$$\sum_p \sum_n f_p \left[\left(\boldsymbol{k}_n + \boldsymbol{G}_p\right) \times \boldsymbol{k}_n \times \boldsymbol{h}_{\boldsymbol{k}n}\right] \exp\left[i\left(\boldsymbol{k}_n + \boldsymbol{G}_p\right)\boldsymbol{r}\right] = -\omega^2\mu_0 \sum_m \boldsymbol{h}_{\boldsymbol{k}m} \exp\left(i\boldsymbol{k}_m\boldsymbol{r}\right) \tag{192}$$

with $\boldsymbol{k}_m = \boldsymbol{k} + \boldsymbol{G}_m$. Orthogonality gives

$$\sum_n f_{m-n} \left(\boldsymbol{k}_m \times \boldsymbol{k}_n \times \boldsymbol{h}_{\boldsymbol{k}n} \right) = -\omega^2 \mu_0 \boldsymbol{h}_{\boldsymbol{k}m} \tag{193}$$

The eigenvalue problem of Eq. (193) can be solved directly by the QR algorithm. Ones sorted, the solutions ω_n will correspond to the energy bands in the ascending order. However, when the geometrical shape of a photonic crystal unit cell is complex, one should take a sufficiently large number of Fourier components of the function $1/\varepsilon$ in each dimension, so the size of the linear system (193) would be too large to apply the QR algorithm (as its numerical complexity grows cubically $O\left(N^3\right)$ relative to the matrix size). From the other hand, one usually needs to calculate only several lowest bands where the largest gaps may appear, therefore, only several smallest eigen solutions are of interest. To conform these restrictions in practice one usually applies iterative methods, like the method of inverse iteration or Krylov subspace methods. Iterative procedures used within these approaches require performing a matrix-vector multiplication at each iteration, thus, the computational complexity reduces approximately to $O\left(N^2\right)$.

Further reduction of the computational complexity can be done by exploiting the special structure of the left-hand part matrix in (193). Multiplications by wavevector projections $k_{mx,y,z}$ are diagonal, and can be done with $O\left(N\right)$ operations. Multiplication by the three-dimensional block-Toeplitz matrix can be done via the Fast Fourier Transform. In order to explain the algorithm let us start with one-dimensional multiplication of a Toeplitz matrix T of size $N \times N$ by a vector $\boldsymbol{x}$ of size N:

$$y_m = \left(T\boldsymbol{x}\right)_m = \sum_n t_{m-n} x_n \Leftrightarrow \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \dots \end{pmatrix} = \begin{pmatrix} t_0 & t_{-1} & t_{-2} & \dots \\ t_1 & t_0 & t_{-1} & \dots \\ t_2 & t_1 & t_0 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \dots \end{pmatrix} \tag{194}$$

The size of the matrix can be increased up to $2N-1$ so as to make the product to have a form of a convolution:

$$\tilde{T} = \begin{pmatrix} t_0 & t_{-1} & t_{-2} & \dots & t_{-N+1} & t_{N-1} & \dots & t_2 & t_1 \\ t_1 & t_0 & t_{-1} & \dots & t_{-N+2} & t_{-N+1} & \dots & t_3 & t_2 \\ t_2 & t_1 & t_0 & \dots & t_{-N+3} & t_{-N+2} & \dots & t_4 & t_3 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ t_{N-1} & t_{N-2} & t_{N-3} & \dots & t_0 & t_{-1} & \dots & t_{-N+1} & t_{N-1} \end{pmatrix} \Rightarrow \tag{195}$$

$$\Rightarrow \tilde{y}_m = \left(\tilde{T}\tilde{\boldsymbol{x}}\right)_m = \sum_n t_{(m-n) \mod N} \tilde{x}_n \tag{196}$$

where $\tilde{\boldsymbol{x}} = \left(\boldsymbol{x}^T, 0, \dots, 0\right)^T$. Matrix $\tilde{T}$ is called the circulant matrix as its multiplication by a vector is a convolution product. From the latter equation it can be seen that the first N elements of $\tilde{\boldsymbol{y}}$ equal to $\boldsymbol{y}$. The advantage of such transformation is that the discrete Fourier image $\mathcal{F}$ of a convolution product is an element-by-element multiplication:

$$\left(\mathcal{F}\tilde{\boldsymbol{y}}\right)_m = \left(\mathcal{F}\left(\tilde{T}\tilde{\boldsymbol{x}}\right)\right)_m = \mathcal{F}\left(\tilde{\boldsymbol{t}}\right)_m \mathcal{F}\left(\tilde{\boldsymbol{x}}\right)_m \tag{197}$$

with vector $\tilde{\boldsymbol{t}} = \left(t_0, t_1, t_2, \dots, t_{-N+1}, t_{N-1}, \dots, t_2, t_1\right)^T$. Since the Fourier transform of a vector, which size is power of 2 or factorizes into a product of powers of small prime numbers, can be calculated by the Fast Fourier Transform algorithm, the product $\boldsymbol{y} = T\boldsymbol{x}$ can be evaluated with $O\left(N \log N\right)$ operations.

A generalization of the fast multiplication approach to three dimensions is straightforward, so the net cost of calculating several small eigenvalues of Eq. (193) can be as small as $O\left(N \log N\right)$ with N being the total number of Fourier harmonics in all three dimensions.

7 Coupled dipole lattices

For some physical problems it is also meaningful to consider periodic lattices of small scattering particles, so that each particle can be modeled by its dipole response. In this section we consider the coupled dipole problem and a related Discrete Dipole Approximation (DDA) used for large scattering particle simulations.

7.1 Coupled Dipole Method

Consider N_d dipoles with moments $\boldsymbol{p}_m$ located at points $\boldsymbol{r}_m$, $m = 1, \dots, N_d$ and surrounded by a homogeneous isotropic medium of permittivity ε. Electric field of each dipole at point $\boldsymbol{r}$ is

$$\begin{aligned} \boldsymbol{E}_m\left(\boldsymbol{r}, \boldsymbol{p}_m\right) = \frac{\exp\left(ik_0\left|\boldsymbol{r}-\boldsymbol{r}_m\right|\right)}{4\pi\varepsilon} \Bigg[& \hat{\boldsymbol{r}}_m\left(\hat{\boldsymbol{r}}_m\boldsymbol{p}_m\right)\left(\frac{3}{\left|\boldsymbol{r}-\boldsymbol{r}_m\right|^3} - \frac{3ik_0}{\left|\boldsymbol{r}-\boldsymbol{r}_m\right|^2} - \frac{k_0^2}{\left|\boldsymbol{r}-\boldsymbol{r}_m\right|}\right) + \\ & + \boldsymbol{p}_m\left(-\frac{1}{\left|\boldsymbol{r}-\boldsymbol{r}_m\right|^3} + \frac{ik_0}{\left|\boldsymbol{r}-\boldsymbol{r}_m\right|^2} + \frac{k_0^2}{\left|\boldsymbol{r}-\boldsymbol{r}_m\right|}\right)\Bigg] \end{aligned} \tag{198}$$

where $k_0 = \omega\sqrt{\varepsilon\mu_0}$, and $\hat{\boldsymbol{r}}_m = \left(\boldsymbol{r}-\boldsymbol{r}_m\right)/\left|\boldsymbol{r}-\boldsymbol{r}_m\right|$. Each dipole moment depends from the self-consistent field at its location:

$$\boldsymbol{p}_m = \chi_m \boldsymbol{E}\left(\boldsymbol{r}_m\right) \tag{199}$$

This field is a sum of fields of the rest of dipoles and, possibly, some external field $\boldsymbol{E}^{inc}$ (vector Foldy-Lax equations):

$$\boldsymbol{E}\left(\boldsymbol{r}_m\right) = \boldsymbol{E}^{inc}\left(\boldsymbol{r}_m\right) + \sum_{n\neq m} \boldsymbol{E}_n\left(\boldsymbol{r}_m, \boldsymbol{p}_n\right) \tag{200}$$

For the m-th dipole multiplication by the polarizability χ_m yields the system of linear equations on unknown self-consistent dipole moments:

$$\boldsymbol{p}_m = \chi_m \boldsymbol{E}^{inc} + \sum_{n\neq m} \chi_m \boldsymbol{E}_n\left(\boldsymbol{r}_m, \boldsymbol{p}_n\right) \Rightarrow \left(\mathbb{I} - \Gamma\mathcal{A}\right)\mathcal{P} = \Gamma\mathcal{E}^{inc} \tag{201}$$

where $\mathbb{I}$ is the identity matrix, $\Gamma = \operatorname{diag}\left\{\chi_1, \chi_2, \dots, \chi_{N_d}\right\}$, vector $\mathcal{P} = \left(\boldsymbol{p}_1^T, \boldsymbol{p}_2^T, \dots, \boldsymbol{p}_{N_d}^T\right)^T$, and $\mathcal{E}^{inc} = \left(\left[\boldsymbol{E}^{inc}\left(\boldsymbol{r}_1\right)\right]^T, \left[\boldsymbol{E}^{inc}\left(\boldsymbol{r}_2\right)\right]^T, \dots, \left[\boldsymbol{E}^{inc}\left(\boldsymbol{r}_{N_d}\right)\right]^T\right)^T$. The overall size of the linear system is $3N_d \times 3N_d$. The elements of matrix can be enumerated with two types of indices – dipole number m, and Cartesian coordinate index $\alpha = x, y, z$:

$$\begin{aligned} \mathcal{A}_{nm,\alpha\beta} = \frac{\exp\left(ik_0\left|\boldsymbol{r}_n-\boldsymbol{r}_m\right|\right)}{4\pi\varepsilon} \Bigg[& \hat{r}_{mn,\alpha}\hat{r}_{mn,\beta}\left(\frac{3}{\left|\Delta\boldsymbol{r}_{mn}\right|^3} - \frac{3ik_0}{\left|\Delta\boldsymbol{r}_{mn}\right|^2} - \frac{k_0^2}{\left|\Delta\boldsymbol{r}_{mn}\right|}\right) + \\ & + \delta_{\alpha\beta}\left(-\frac{1}{\left|\Delta\boldsymbol{r}_{mn}\right|^3} + \frac{ik_0}{\left|\Delta\boldsymbol{r}_{mn}\right|^2} + \frac{k_0^2}{\left|\Delta\boldsymbol{r}_{mn}\right|}\right)\Bigg] \end{aligned} \tag{202}$$

where $\Delta\boldsymbol{r}_{mn} = \boldsymbol{r}_m - \boldsymbol{r}_n$.

If the number of dipoles N_d is small, than the system (201) can be solved directly by matrix inversion, which has the asymptotic complexity $O\left(N^3\right)$. For large coupled dipole ensembles one has to apply an iterative procedure, which requires only matrix-vector multiplications with complexity $O\left(N^2\right)$. This complexity can be further reduced if all dipoles are arranged in a regular 3D lattice. Denote the lattice constants d_α, and let the dipole indices be triples corresponding to indices for each Cartesian coordinate: $m = (m_x, m_y, m_z)$. Then, $\left|\boldsymbol{r}_m - \boldsymbol{r}_n\right| = \sqrt{\sum_\alpha d_\alpha^2\left(m_\alpha - n_\alpha\right)^2}$, and one can see, that matrix $\mathcal{A}$ is a 3D block-Toeplitz matrix. The technique for fast multiplications of matrices of this kind by vectors was explained above.

Once the polarizabilities are found, one can calculate the far field amplitude in any direction by a direct summation of fields from each dipole, Eq. (198). In the limit $r \to \infty$ only the terms $\sim 1/r$

remain, so

$$\boldsymbol{E}^{far}(\boldsymbol{r}) = \boldsymbol{E}^{inc}(\boldsymbol{r}) + k_0^2 \frac{\exp(ik_0 r)}{4\pi\varepsilon r} \sum_m \left[\boldsymbol{p}_m - \hat{\boldsymbol{r}}_m(\hat{\boldsymbol{r}}_m \boldsymbol{p}_m)\right] \exp\left[ik_0(\hat{\boldsymbol{r}} \cdot \boldsymbol{r}_m)\right] \tag{203}$$

For the plane wave incidence the extinction cross-section is given by the optical theorem

$$C_{ext} = \frac{4\pi}{k_0 \left|\boldsymbol{E}^{inc}\right|^2} \Im\left[\boldsymbol{E}^{sca}\left(\hat{\boldsymbol{r}}^{inc}\right) \cdot \boldsymbol{E}^{inc}\right] \tag{204}$$

7.2 Discrete Dipole Approximation

A related approach, which is often used for calculation of the light scattering by non-spherical particles of various scales is the Discrete Dipole Approximation (DDA). The derivation starts from the volume integral solution of the Helmholtz equation (3):

$$\boldsymbol{E}(\boldsymbol{r}) = \boldsymbol{E}^{inc}(\boldsymbol{r}) + i\omega\mu_0 \int_V \boldsymbol{G}_0(\boldsymbol{r} - \boldsymbol{r}') \boldsymbol{J}(\boldsymbol{r}') d^3\boldsymbol{r}' \tag{205}$$

where the free-space dyadic Green's function satisfies equation

$$\nabla \times \nabla \times \boldsymbol{G}_0(\boldsymbol{r} - \boldsymbol{r}') - k_0^2 \boldsymbol{G}_0(\boldsymbol{r} - \boldsymbol{r}') = \mathbb{I}\delta(\boldsymbol{r} - \boldsymbol{r}') \tag{206}$$

Explicitly in the Cartesian coordinates

$$\boldsymbol{G}_0(\boldsymbol{r} - \boldsymbol{r}') = \left(\mathbb{I} + \frac{1}{k_0^2}\nabla\nabla\right) g_0(\boldsymbol{r} - \boldsymbol{r}') = \left(\mathbb{I} + \frac{1}{k_0^2}\nabla\nabla\right) \frac{\exp(ik_0|\boldsymbol{r} - \boldsymbol{r}'|)}{4\pi|\boldsymbol{r} - \boldsymbol{r}'|} \tag{207}$$

The operator behind the scalar Green's function g_0 yields the dipole response of the form of Eq. (198). Taking the source to be polarization currents due to inhomogeneous permittivity $\boldsymbol{J} = -i\omega(\varepsilon(\boldsymbol{r}) - \varepsilon_0)\boldsymbol{E}$ results in the Lippmann-Schwinger equation

$$\boldsymbol{E}(\boldsymbol{r}) = \boldsymbol{E}^{inc}(\boldsymbol{r}) + \omega^2\mu_0 \int_V \boldsymbol{G}_0(\boldsymbol{r} - \boldsymbol{r}') \left[\varepsilon(\boldsymbol{r}') - \varepsilon_0\right] \boldsymbol{E}(\boldsymbol{r}') d^3\boldsymbol{r}' \tag{208}$$

The dyadic $\boldsymbol{G}_0(\boldsymbol{r} - \boldsymbol{r}')$ becomes singular at $\boldsymbol{r} = \boldsymbol{r}'$, and $\boldsymbol{G}_0(\boldsymbol{r} - \boldsymbol{r}') \sim 1/|\boldsymbol{r} - \boldsymbol{r}'|^3$ around this point. In order to treat the singularity consider a small volume V_0 bounded by the surface S_0 containing the point $\boldsymbol{r} = \boldsymbol{r}'$ so that

$$\begin{aligned} \textstyle\int_V \boldsymbol{G}_0(\boldsymbol{r} - \boldsymbol{r}') \boldsymbol{J}(\boldsymbol{r}') d^3\boldsymbol{r}' &= \textstyle\int_{V \setminus V_0} \boldsymbol{G}_0(\boldsymbol{r} - \boldsymbol{r}') \boldsymbol{J}(\boldsymbol{r}') d^3\boldsymbol{r}' \\ + \textstyle\int_{V_0} \left[\boldsymbol{G}_0(\boldsymbol{r} - \boldsymbol{r}') - \boldsymbol{G}_s(\boldsymbol{r} - \boldsymbol{r}')\right] \boldsymbol{J}(\boldsymbol{r}') d^3\boldsymbol{r}' &- \frac{1}{k_0^2} \oint_{S_0} \boldsymbol{n}_s \frac{(\boldsymbol{r} - \boldsymbol{r}') \cdot \boldsymbol{J}(\boldsymbol{r}')}{4\pi|\boldsymbol{r} - \boldsymbol{r}'|^3} d^2\boldsymbol{r}' \end{aligned} \tag{209}$$

where $\boldsymbol{n}_s$ is the external unit normal to S_0, and

$$\boldsymbol{G}_s(\boldsymbol{r} - \boldsymbol{r}') = \frac{1}{k_0^2}\nabla\nabla \frac{1}{4\pi|\boldsymbol{r} - \boldsymbol{r}'|} \tag{210}$$

The equation was also transformed in accordance with the Gauss-Ostrogradsky theorem

$$\begin{aligned} \textstyle\int_{V_0} G_{s,\alpha\beta}(\boldsymbol{r} - \boldsymbol{r}') J_\beta(\boldsymbol{r}') d^3\boldsymbol{r}' &= \frac{1}{k_0^2} \textstyle\int_{V_0} \frac{d}{dx_\alpha} \frac{d}{dx_\beta} \frac{J_\beta(\boldsymbol{r}')}{4\pi|\boldsymbol{r} - \boldsymbol{r}'|} = \frac{1}{k_0^2} \oint_{S_0} n_{s,\alpha} \frac{d}{dx_\beta} \frac{J_\beta(\boldsymbol{r}')}{4\pi|\boldsymbol{r} - \boldsymbol{r}'|} \\ &= -\frac{1}{k_0^2} \oint_{S_0} n_{s,\alpha} \frac{\left(x_\beta - x'_\beta\right) J_\beta(\boldsymbol{r}')}{4\pi|\boldsymbol{r} - \boldsymbol{r}'|^3} \end{aligned} \tag{211}$$

In the following we will use the long wavelength approximation $\boldsymbol{J}(\boldsymbol{r}') \approx \boldsymbol{J}(\boldsymbol{r})$ for any $\boldsymbol{r} \in V$. Then, the integral becomes

$$\begin{gathered}\int_V \boldsymbol{G}_0(\boldsymbol{r}-\boldsymbol{r}')\,\boldsymbol{J}(\boldsymbol{r}')\,d^3\boldsymbol{r}' \approx \int_{V\setminus V_0} \boldsymbol{G}_0(\boldsymbol{r}-\boldsymbol{r}')\,\boldsymbol{J}(\boldsymbol{r})\,d^3\boldsymbol{r}' \\ + \int_{V_0} \left[\boldsymbol{G}_0(\boldsymbol{r}-\boldsymbol{r}') - \boldsymbol{G}_s(\boldsymbol{r}-\boldsymbol{r}')\right]\boldsymbol{J}(\boldsymbol{r})\,d^3\boldsymbol{r}' - \frac{1}{k_0^2}\oint_{S_0} \boldsymbol{n}_s \frac{(\boldsymbol{r}-\boldsymbol{r}')\cdot\boldsymbol{J}(\boldsymbol{r})}{4\pi\left|\boldsymbol{r}-\boldsymbol{r}'\right|^3} d^2\boldsymbol{r}'\end{gathered} \tag{212}$$

Since V is electrically small we can further associate V with V_0 to get

$$\int\limits_V \boldsymbol{G}_0(\boldsymbol{r}-\boldsymbol{r}')\,\boldsymbol{J}(\boldsymbol{r}')\,d^3\boldsymbol{r}' \approx \left[\boldsymbol{M} - \frac{1}{k_0^2}\boldsymbol{L}\right]\cdot\boldsymbol{J}(\boldsymbol{r}) \tag{213}$$

with

$$\begin{gathered}\boldsymbol{M} = \int_{V_0}\left[\boldsymbol{G}_0(\boldsymbol{r}-\boldsymbol{r}') - \boldsymbol{G}_s(\boldsymbol{r}-\boldsymbol{r}')\right] d^3\boldsymbol{r}' \\ \boldsymbol{L} = \oint_{S_0} \boldsymbol{n}_s \frac{(\boldsymbol{r}-\boldsymbol{r}')}{4\pi\left|\boldsymbol{r}-\boldsymbol{r}'\right|^3} d^2\boldsymbol{r}'\end{gathered} \tag{214}$$

Evaluation of these terms can be done analytically or numerically for volumes of different shapes.

Going back to the Lippmann-Schwinger equation (208) written for a large scattering particle, one can divide the scattering volume into a set of electrically small volumes $V = \bigcup V_m$:

$$\begin{gathered}\boldsymbol{E}(\boldsymbol{r}) = \boldsymbol{E}^{inc}(\boldsymbol{r}) + \omega^2\mu_0 \sum_n \int_{V_n} \boldsymbol{G}_0(\boldsymbol{r}-\boldsymbol{r}')\left[\varepsilon(\boldsymbol{r}') - \varepsilon_0\right]\boldsymbol{E}(\boldsymbol{r}')\,d^3\boldsymbol{r}' \Rightarrow \\ \Rightarrow \boldsymbol{E}(\boldsymbol{r}_m) = \boldsymbol{E}^{inc}(\boldsymbol{r}_m) + \omega^2\mu_0 \sum_{n\neq m} \boldsymbol{G}_0(\boldsymbol{r}_m-\boldsymbol{r}_n)\,\Delta\varepsilon_n \boldsymbol{E}(\boldsymbol{r}_n)\,\Delta V_n - i\omega\Delta\varepsilon_m\left[\boldsymbol{M}_m - \frac{1}{k_0^2}\boldsymbol{L}_m\right]\cdot\boldsymbol{E}(\boldsymbol{r}_m)\end{gathered} \tag{215}$$

where $\boldsymbol{r}_m \in V_m$. This is the linear equation system for unknown fields $\boldsymbol{E}(\boldsymbol{r}_m)$, which has the form similar to the case of CDA, Eq. (201), but with a different block diagonal terms defined in Eq. (214).