Due giorni di Algebra Lineare Numerica

Structured matrices in the computation of band spectra of photonic crystals

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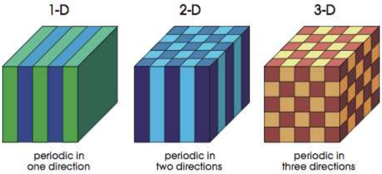
Photonic Crystal: What is it?



- Photonic crystals are dielectric media whose dielectric constant $\varepsilon(\mathbf{x})$, with $\mathbf{x} \in \mathbb{R}^3$, satisfies the periodicity condition

$$\varepsilon(\mathbf{x} + m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + m_3\mathbf{a}_3) = \varepsilon(\mathbf{x})$$

  for certain linearly independent vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3 \in \mathbb{R}^3$, where m_1, m_2 and m_3 are arbitrary integers.
- The periodicity of the dielectric constant $\varepsilon(\mathbf{x})$ causes optical properties which are similar to the electronic properties for semiconductor crystals with a periodic potential.
- Photonic crystals exhibit frequency intervals where incident light can propagate (**bands**) and frequency intervals in which incident light cannot propagate (**band-gaps**).

Physical Assumptions

In order to study photonic crystals we have to refer to **Maxwell's equations** and cast them into the photonic crystals frame.

- Isotropy and linearity yield:

$$\mathbf{D} = \varepsilon(\mathbf{r})\mathbf{E}, \qquad \mathbf{B} = \mu(\mathbf{r})\mathbf{H} \ . \tag{1}$$

- Magnetic permeability constant ($\mu(\mathbf{r}) \simeq 1$): $\mathbf{B} = \mathbf{H}$.
- Lossless media: $\varepsilon(\mathbf{r}) : \mathbb{R}^3 \to \mathbb{R}$.
- In a photonic crystal we don't have free charge ($\rho = 0$) and free current ($\mathbf{J} = 0$).
- We seek time-harmonic modes:

$$\mathbf{H}(\mathbf{r}, t) = \mathbf{H}(\mathbf{r})e^{i\omega t} \ , \qquad \mathbf{E}(\mathbf{r}, t) = \mathbf{E}(\mathbf{r})e^{i\omega t} \ . \tag{2}$$

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Maxwell's Equations for photonic crystals

Maxwell equations, which govern light transmission in photonic crystals, reduce to the following system of equations:

$$\begin{aligned} \nabla \cdot [\varepsilon \mathbf{E}] &= 0, && \text{[Coulomb's law]} \\ \nabla \times \mathbf{H} - i\sqrt{\eta}\varepsilon \mathbf{E} &= 0, && \text{[Ampère's law]} \\ \nabla \times \mathbf{E} + i\sqrt{\eta}\mathbf{H} &= 0, && \text{[Faraday's law]} \\ \nabla \cdot \mathbf{H} &= 0, && \text{[Absence of free magnetic poles]} \end{aligned}$$

where $\sqrt{\eta} = \frac{\omega}{c}$.

We apply **Bloch's theorem**: $\mathbf{E}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}\mathcal{E}(\mathbf{x})$, $\mathbf{H}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}\mathcal{H}(\mathbf{x})$, where $\mathcal{E}(\mathbf{x} + m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + m_3\mathbf{a}_3) = \mathcal{E}(\mathbf{x})$ and $\mathcal{H}(\mathbf{x} + m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + m_3\mathbf{a}_3) = \mathcal{H}(\mathbf{x})$, we get:

$$\begin{aligned} \nabla \cdot [\varepsilon(\mathbf{x})\mathcal{E}(\mathbf{x})] + i\mathbf{k} \cdot [\varepsilon(\mathbf{x})\mathcal{E}(\mathbf{x})] &= 0, \\ \nabla \times \mathcal{H}(\mathbf{x}) + i[\mathbf{k} \times \mathcal{H}(\mathbf{x})] - i\sqrt{\eta}\varepsilon(\mathbf{x})\mathcal{E}(\mathbf{x}) &= 0, \\ \nabla \times \mathcal{E}(\mathbf{x}) + i[\mathbf{k} \times \mathcal{E}(\mathbf{x})] + i\sqrt{\eta}\varepsilon(\mathbf{x})\mathcal{H}(\mathbf{x}) &= 0, \\ \nabla \cdot [\mathcal{H}(\mathbf{x})] + i\mathbf{k} \cdot \mathcal{H}(\mathbf{x}) &= 0. \end{aligned}$$

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\begin{aligned}
&\nabla \cdot [\varepsilon(\mathbf{x})\mathcal{E}(\mathbf{x})] + i\mathbf{k} \cdot [\varepsilon(\mathbf{x})\mathcal{E}(\mathbf{x})] = 0, \\
&\nabla \times \mathcal{H}(\mathbf{x}) + i[\mathbf{k} \times \mathcal{H}(\mathbf{x})] - i\sqrt{\eta}\varepsilon(\mathbf{x})\mathcal{E}(\mathbf{x}) = 0, \\
&\nabla \times \mathcal{E}(\mathbf{x}) + i[\mathbf{k} \times \mathcal{E}(\mathbf{x})] + i\sqrt{\eta}\varepsilon(\mathbf{x})\mathcal{H}(\mathbf{x}) = 0, \\
&\nabla \cdot [\mathcal{H}(\mathbf{x})] + i\mathbf{k} \cdot \mathcal{H}(\mathbf{x}) = 0.
\end{aligned}
$$

2D: TE and TM Modes

When $k_z = 0$, the modes of every two-dimensional photonic crystal can be classified into two distinct polarizations: either (H_x, H_y, E_z) or (E_x, E_y, H_z).

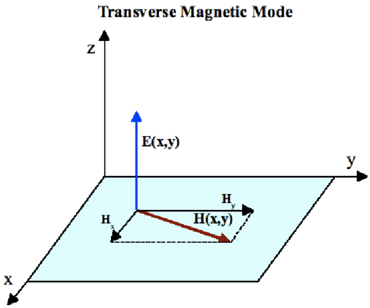


Figura: TM mode: the magnetic field is confined to the xy plane.

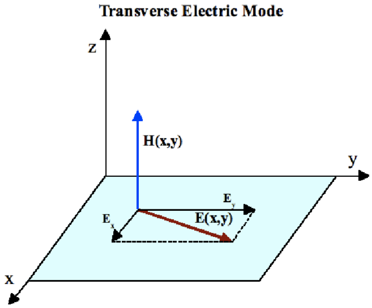


Figura: TE mode: the electric field is confined to the xy plane.

2D: TE and TM Eigenvalue Equations

In the **TM mode** we have to study spectral eigenvalue problem for the Helmholtz equation

$$-\left(\frac{\partial^2\psi}{\partial^2 x}+\frac{\partial^2\psi}{\partial^2 y}\right)=\eta\varepsilon(x,y)\psi \tag{3}$$

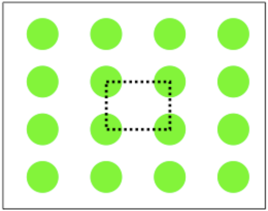
and in the **TE mode** we have to solve the following

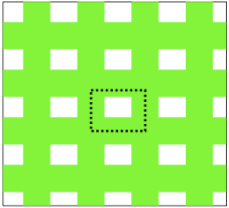
$$-\nabla\cdot\left(\frac{1}{\varepsilon(x,y)}\nabla\psi\right)=\eta\psi \tag{4}$$

(where $\varepsilon(x,y)=n^2(x,y)$). In (3) the electric field is given by $(0,0,\psi(x,y))^T$, whereas in (4) the magnetic field is given by $(0,0,\psi(x,y))^T$. The main goal is to find the eigenvalues η.

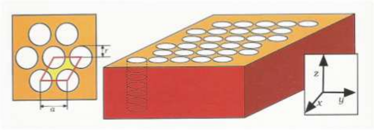
Photonic Crystals in 2 Dimensions

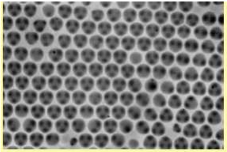
Basically, we study two numerical methods for the following two cases:





As an example, in the connected case:





Prevailing Numerical Methods

Time Domain Methods

1) Plane Wave Expansion (**PWE**) Method;
2) Finite Difference Time Domain (**FDTD**) Method.

Frequency Domain Methods

1) Finite difference frequency domain (**FDFD**) method;
2) Fourier expansion (**FE**) method;
3) Finite element frequency domain (**FEFD**) method.

FDFD Method

- We get the 2-D (modified) Helmholtz equations for **TE modes**

$$-\nabla\cdot\left(\frac{1}{\varepsilon}\nabla\phi\right)-i\nabla\cdot\left(\frac{1}{\varepsilon}\mathbf{k}\phi\right)-i\frac{1}{\varepsilon}\mathbf{k}\cdot\nabla\phi+\frac{\|\mathbf{k}\|^2}{\varepsilon}\phi=\eta\phi, \quad (5)$$

and for **TM modes**

$$-\nabla^2\phi-2i\mathbf{k}\cdot\nabla\phi+\|\mathbf{k}\|^2\phi=\eta\varepsilon\phi, \quad (6)$$

under the following periodicity conditions

$$\phi(x,0)=\phi(x,b), \quad \phi(0,y)=\phi(a,y),$$
$$\frac{\partial\phi}{\partial y}(x,0)=\frac{\partial\phi}{\partial y}(x,b), \quad \frac{\partial\phi}{\partial x}(0,y)=\frac{\partial\phi}{\partial x}(a,y).$$

FDFD Method

Let us introduce the grid points

$$\mathbf{x}_{j,l} = \left(\frac{ja}{n}, \frac{lb}{m}\right),$$

where $j = 0, 1, \ldots, n, n+1$ and $l = 0, 1, \ldots, m, m+1$.
Then finite differencing Eq. (5) (TE modes) and Eq. (6) (TM modes) yields, for $h_x = a/n$ and $h_y = b/m$,

$$\begin{aligned}
&\tfrac{1}{2}\left(\frac{1}{\varepsilon_{j+1,l}} + \frac{1}{\varepsilon_{j,l}}\right)\left[-\frac{1}{h_x^2} - \frac{ik_x}{h_x}\right]\phi_{j+1,l} + \tfrac{1}{2}\left(\frac{1}{\varepsilon_{j,l}} + \frac{1}{\varepsilon_{j-1,l}}\right)\left[-\frac{1}{h_x^2} + \frac{ik_x}{h_x}\right]\phi_{j-1,l} \\
&+ \tfrac{1}{2}\left(\frac{1}{\varepsilon_{j,l+1}} + \frac{1}{\varepsilon_{j,l}}\right)\left[-\frac{1}{k_y^2} - \frac{ik_y}{h_y}\right]\phi_{j,l+1} + \tfrac{1}{2}\left(\frac{1}{\varepsilon_{j,l}} + \frac{1}{\varepsilon_{j,l-1}}\right)\left[-\frac{1}{h_y^2} + \frac{ik_y}{h_y}\right]\phi_{j,l-1} \\
&+ \left\{\tfrac{1}{4}\left(\frac{1}{\varepsilon_{j+1,l}} + \frac{2}{\varepsilon_{j,l}} + \frac{1}{\varepsilon_{j-1,l}}\right)\left[\frac{2}{h_x^2} + k_x^2\right]\right. \\
&\left. + \tfrac{1}{4}\left(\frac{1}{\varepsilon_{j,l+1}} + \frac{2}{\varepsilon_{j,l}} + \frac{1}{\varepsilon_{j,l-1}}\right)\left[\frac{2}{h_y^2} + k_y^2\right]\right\}\phi_{j,l} = \eta\phi_{j,l}, \qquad (7)
\end{aligned}$$

FDFD Method

$$-\frac{\phi_{j+1,l}-2\phi_{j,l}+\phi_{j-1,l}}{h_x^2}-\frac{\phi_{j,l+1}-2\phi_{j,l}+\phi_{j,l-1}}{h_y^2}$$
$$-2ik_x\frac{\phi_{j+1,l}-\phi_{j-1,l}}{2h_x}-2ik_y\frac{\phi_{j,l+1}-\phi_{j,l-1}}{2h_y}+[k_x^2+k_y^2]\phi_{j,l}$$
$$=\eta\varepsilon_{j,l}\phi_{j,l}, \quad (8)$$

Equations (8) and (17) can both be written in the form

$$(C-\eta D)\Psi = 0$$

Modi TE

- C positive semidefinite sparse hermitian matrix;
- D identity matrix of order mn.

Modi TM

- C two-index sparse circulant matrix;
- D diagonal matrix with positive entries.

FDFD Method

$$
\begin{aligned}
&-\frac{\phi_{j+1,l}-2\phi_{j,l}+\phi_{j-1,l}}{h_x^2}-\frac{\phi_{j,l+1}-2\phi_{j,l}+\phi_{j,l-1}}{h_y^2}\\
&-2ik_x\frac{\phi_{j+1,l}-\phi_{j-1,l}}{2h_x}-2ik_y\frac{\phi_{j,l+1}-\phi_{j,l-1}}{2h_y}+[k_x^2+k_y^2]\phi_{j,l}\\
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FDFD Method

$$
C = \left(\begin{array}{cccc|cccc|cccc|cccc}
\alpha & \beta & 0 & \bar{\beta} & \gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\gamma} & 0 & 0 & 0 \\
\bar{\beta} & \alpha & \beta & 0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\gamma} & 0 & 0 \\
0 & \bar{\beta} & \alpha & \beta & 0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\gamma} & 0 \\
\beta & 0 & \bar{\beta} & \alpha & 0 & 0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\gamma} \\
\hline
\bar{\gamma} & 0 & 0 & 0 & \alpha & \beta & 0 & \bar{\beta} & \gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \bar{\gamma} & 0 & 0 & \bar{\beta} & \alpha & \beta & 0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \bar{\gamma} & 0 & 0 & \bar{\beta} & \alpha & \beta & 0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \bar{\gamma} & \beta & 0 & \bar{\beta} & \alpha & 0 & 0 & 0 & \gamma & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & \bar{\gamma} & 0 & 0 & 0 & \alpha & \beta & 0 & \bar{\beta} & \gamma & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \bar{\gamma} & 0 & 0 & \bar{\beta} & \alpha & \beta & 0 & 0 & \gamma & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \bar{\gamma} & 0 & 0 & \bar{\beta} & \alpha & \beta & 0 & 0 & \gamma & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\gamma} & \beta & 0 & \bar{\beta} & \alpha & 0 & 0 & 0 & \gamma \\
\hline
\gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\gamma} & 0 & 0 & 0 & \alpha & \beta & 0 & \bar{\beta} \\
0 & \gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\gamma} & 0 & 0 & \bar{\beta} & \alpha & \beta & 0 \\
0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\gamma} & 0 & 0 & \bar{\beta} & \alpha & \beta \\
0 & 0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\gamma} & \beta & 0 & \bar{\beta} & \alpha
\end{array}\right),
$$

FDFD Method

where

$$\alpha = \left(\frac{2}{h_x^2} + \frac{2}{h_y^2} + k^2 \right),$$

$$\beta = \left(-\frac{1}{h_x^2} + i\frac{k_x}{h_x} \right), \qquad \bar{\beta} = \left(-\frac{1}{h_x^2} - i\frac{k_x}{h_x} \right),$$

$$\gamma = \left(-\frac{1}{h_y^2} + i\frac{k_y}{h_y} \right), \qquad \bar{\gamma} = \left(-\frac{1}{h_y^2} - i\frac{k_y}{h_y} \right).$$

The eigenvalues of C are the numbers

$$\begin{aligned} \hat{c}(z, w; \mathbf{k}) = \frac{2}{h_x^2} + k_x^2 + k_y^2 + \left(-\frac{1}{h_x^2} + \frac{ik_x}{h_x} \right) z + \left(-\frac{1}{h_x^2} - \frac{ik_x}{h_x} \right) z^{-1} \\ + \frac{2}{h_y^2} + \left(-\frac{1}{h^2} + \frac{ik_y}{h_y} \right) w + \left(-\frac{1}{h_y^2} - \frac{ik_y}{h_y} \right) w^{-1}, \end{aligned}$$

where $z^n = 1$ and $w^m = 1$.

FDFD Method

Writing $z = e^{i\theta_j}$ with $\theta_j = \frac{2\pi j}{n}$ and $w = e^{i\varphi_l}$ with $\varphi_l = \frac{2\pi l}{m}$, we can write the eigenvalues in the form

$$\hat{c}(z, w; \mathbf{k}) = k_x^2 + k_y^2 + \frac{2}{h_x^2}(1 - \cos\theta_j) - \frac{2k_x}{h_x}\sin\theta_j + \frac{2}{h_y^2}(1 - \cos\varphi_l) - \frac{2k_y}{h_y}\sin\varphi_l,$$

where $j = 0, 1, \ldots, n-1$ and $l = 0, 1, \ldots, m-1$.

$$\begin{aligned} E_{\text{abs}} = & -\frac{1}{3}\left(\frac{\pi j}{n}\right)^2\left[\left(\frac{2\pi j}{a} + k_x\right)^2 - k_x^2\right]\left\{1 + O\left(\left(\frac{j}{n}\right)^2\right)\right\} \\ & -\frac{1}{3}\left(\frac{\pi l}{m}\right)^2\left[\left(\frac{2\pi l}{b} + k_y\right)^2 - k_y^2\right]\left\{1 + O\left(\left(\frac{l}{m}\right)^2\right)\right\}, \end{aligned}$$

For the relative error we then get the following upper bound:

$$E_{\text{rel}} = \max\left[\frac{1}{3}\left(\frac{\pi j}{n}\right)^2\left\{1 + O\left(\left(\frac{j}{n}\right)^2\right)\right\}, \frac{1}{3}\left(\frac{\pi l}{m}\right)^2\left\{1 + O\left(\left(\frac{l}{m}\right)^2\right)\right\}\right].$$

FDFE Method

Putting $\mathbf{A} = \{t_1\mathbf{a}_1 + t_2\mathbf{a}_2 : 0 \leq t_1, t_2 < 1\}$, we define the complex Hilbert spaces H_{per} and H^1_{per} consisting of those measurable complex-valued functions ϕ on $\mathbb{R}^2$ which satisfy the periodicity condition $\phi(\mathbf{x} + m_1\mathbf{a}_1 + m_2\mathbf{a}_2, \mathbf{k}) = \phi(\mathbf{x}, \mathbf{k})$ and are finite with respect to the following respective squared norms:

$$\|\phi\|^2_{H_{\text{per}}} = \iint_{\mathbf{A}} dxdy\, |\phi(x,y)|^2,$$
$$\|\phi\|^2_{H^1_{\text{per}}} = \iint_{\mathbf{A}} dxdy\, \left(|\phi(x,y)|^2 + \|\nabla\phi(x,y)\|^2\right).$$

As a consequence of the first Green identity and the periodicity condition, we see that $\phi \in H^1_{\text{per}}$ is a variational solution to (6) (TM mode) if

$$\iint_{\mathbf{A}} dxdy\, \left\{\nabla\phi \cdot \nabla v^* - 2i[\mathbf{k}\cdot\nabla\phi]v^* + \|\mathbf{k}\|^2\phi v^* - \eta\varepsilon\phi v^*\right\} = 0, \qquad (9)$$

for every $v \in H^1_{\text{per}}$.

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FDFE Method

Analogously, we call $\phi \in H^1_{\text{per}}$ a distributional solution to (5) (TE mode) if

$$\iint_{\mathbf{A}} dxdy \left\{ \frac{1}{\varepsilon} \nabla\phi \cdot \nabla v^* - iv^* \mathbf{k} \cdot \nabla \left(\frac{1}{\varepsilon}\phi \right) - \frac{i}{\varepsilon} v^* \mathbf{k} \cdot \nabla\phi + \frac{\|\mathbf{k}\|^2}{\varepsilon} \phi v^* - \eta\phi v^* \right\} = 0, \tag{10}$$

for every $v \in H^1_{\text{per}}$. Putting $h_x = (a/n)$, $h_y = (b/m)$, we introduce the bivariate functions

$$\varphi_{(j_1,j_2)}(x,y) = \left(1 - \frac{|x - x_{j_1}|}{h_1}\right)\left(1 - \frac{|y - y_{j_2}|}{h_2}\right), \quad (j_1, j_2) \in \mathbb{Z}^2,$$

extended periodically to $(x, y) \in \mathbb{R}^2$. Here, for $(j, l) \in \mathbb{Z}^2$, we have $x_j = j_1 h_1 = (j_1/n)a_1$ and $y_l = j_2 h_2 = (j_2/m)a_2$ and we interpolate $\phi \in H^1_{\text{per}}$ as follows:

$$\phi(x,y) = \sum_{j_1=0}^{n-1} \sum_{j_2=0}^{m-1} \phi_{(j_1,j_2)} \varphi_{(j_1,j_2)}(x,y)$$

and take $v = \varphi_{(l_1,l_2)}$ for every $l_1 \in \{0, 1, \ldots, n-1\}$ and $l_2 \in \{0, 1, \ldots, m-1\}$.

FDFE Method

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$$\iint_{\mathbf{A}} dxdy \left\{ \frac{1}{\varepsilon} \nabla\phi \cdot \nabla v^* - i v^* \mathbf{k} \cdot \nabla \left(\frac{1}{\varepsilon} \phi \right) - \frac{i}{\varepsilon} v^* \mathbf{k} \cdot \nabla\phi + \frac{\|\mathbf{k}\|^2}{\varepsilon} \phi v^* - \eta \phi v^* \right\} = 0, \tag{10}$$

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FDFE Method

Bivariate functions

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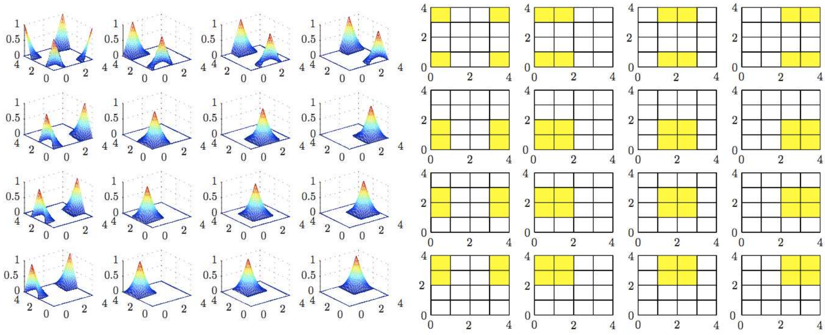
and their support:



FDFE Method

We obtain the linear system (TM mode) of order nm

$$\sum_{j'=0}^{n-1}\sum_{l'=0}^{m-1}\phi_{(j',l')}\int_0^a dx\int_0^b dy\ \{(\nabla\varphi_{(j',l')}+i\varphi_{(j',l')}\mathbf{k})\cdot(\nabla\varphi_{(j,l)}-i\varphi_{(j,l)}\mathbf{k})\}$$
$$=\eta\sum_{j'=0}^{n-1}\sum_{l'=0}^{m-1}\phi_{(j',l')}\int_0^a dx\int_0^b dy\,\varepsilon(x,y)\varphi_{(j',l')}(x,y)\varphi_{(j,l)}(x,y), \tag{11}$$

whose unknowns are the values of $\phi(x,y)$ at the interpolation points of the photonic cell $0\le x\le a$, $0\le x\le b$. From (10) (TE mode) we obtain instead

$$\sum_{j'=0}^{n-1}\sum_{l'=0}^{m-1}\phi_{(j',l')}\int_0^a\int_0^b\frac{dx\,dy}{\varepsilon(x,y)}\{(\nabla\varphi_{(j',l')}+i\varphi_{(j',l')}\mathbf{k})\cdot(\nabla\varphi_{(j,l)}-i\varphi_{(j,l)}\mathbf{k})\}$$
$$=\eta\sum_{j'=0}^{n-1}\sum_{l'=0}^{m-1}\phi_{(j',l')}\int_0^a dx\int_0^b dy\,\varphi_{(j',l')}(x,y)\varphi_{(j,l)}(x,y). \tag{12}$$

FDFE Method

The linear systems (11) and (12) constitute the finite element schemes to compute the eigenvalues η for fixed wavevector **k** for the TM and TE modes, respectively.

$$A\psi = \eta B\psi.$$

$$A = \left(\begin{array}{cccc|cccc|cccc|cccc}
\alpha & \beta_2 & 0 & \bar{\beta}_2 & \beta_1 & \gamma_1 & 0 & \gamma_2 & 0 & 0 & 0 & 0 & \bar{\beta}_1 & \bar{\gamma}_2 & 0 & \bar{\gamma}_1 \\
\bar{\beta}_2 & \alpha & \beta_2 & 0 & \gamma_2 & \beta_1 & \gamma_1 & 0 & 0 & 0 & 0 & 0 & \bar{\gamma}_1 & \bar{\beta}_1 & \bar{\gamma}_2 & 0 \\
0 & \bar{\beta}_2 & \alpha & \beta_2 & 0 & \gamma_2 & \beta_1 & \gamma_1 & 0 & 0 & 0 & 0 & 0 & \bar{\gamma}_1 & \bar{\beta}_1 & \bar{\gamma}_2 \\
\beta_2 & 0 & \bar{\beta}_2 & \alpha & \gamma_1 & 0 & \gamma_2 & \beta_1 & 0 & 0 & 0 & 0 & \bar{\gamma}_2 & 0 & \bar{\gamma}_1 & \bar{\beta}_1 \\
\hline
\bar{\beta}_1 & \bar{\gamma}_2 & 0 & \bar{\gamma}_1 & \alpha & \beta_2 & 0 & \bar{\beta}_2 & \beta_1 & \gamma_1 & 0 & \gamma_2 & 0 & 0 & 0 & 0 \\
\bar{\gamma}_1 & \bar{\beta}_1 & \bar{\gamma}_2 & 0 & \bar{\beta}_2 & \alpha & \beta_2 & 0 & \gamma_2 & \beta_1 & \gamma_1 & 0 & 0 & 0 & 0 & 0 \\
0 & \bar{\gamma}_1 & \bar{\beta}_1 & \bar{\gamma}_2 & 0 & \bar{\beta}_2 & \alpha & \beta_2 & 0 & \gamma_2 & \beta_1 & \gamma_1 & 0 & 0 & 0 & 0 \\
\bar{\gamma}_2 & 0 & \bar{\gamma}_1 & \bar{\beta}_1 & \beta_2 & 0 & \bar{\beta}_2 & \alpha & \gamma_1 & 0 & \gamma_2 & \beta_1 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & \bar{\beta}_1 & \bar{\gamma}_2 & 0 & \bar{\gamma}_1 & \alpha & \beta_2 & 0 & \bar{\beta}_2 & \beta_1 & \gamma_1 & 0 & \gamma_2 \\
0 & 0 & 0 & 0 & \bar{\gamma}_1 & \bar{\beta}_1 & \bar{\gamma}_2 & 0 & \bar{\beta}_2 & \alpha & \beta_2 & 0 & \gamma_2 & \beta_1 & \gamma_1 & 0 \\
0 & 0 & 0 & 0 & 0 & \bar{\gamma}_1 & \bar{\beta}_1 & \bar{\gamma}_2 & 0 & \bar{\beta}_2 & \alpha & \beta_2 & 0 & \gamma_2 & \beta_1 & \gamma_1 \\
0 & 0 & 0 & 0 & \bar{\gamma}_2 & 0 & \bar{\gamma}_1 & \bar{\beta}_1 & \beta_2 & 0 & \bar{\beta}_2 & \alpha & \gamma_1 & 0 & \gamma_2 & \beta_1 \\
\hline
\beta_1 & \gamma_1 & 0 & \gamma_2 & 0 & 0 & 0 & 0 & \bar{\beta}_1 & \bar{\gamma}_2 & 0 & \bar{\gamma}_1 & \alpha & \beta_2 & 0 & \bar{\beta}_2 \\
\gamma_2 & \beta_1 & \gamma_1 & 0 & 0 & 0 & 0 & 0 & \bar{\gamma}_1 & \bar{\beta}_1 & \bar{\gamma}_2 & 0 & \bar{\beta}_2 & \alpha & \beta_2 & 0 \\
0 & \gamma_2 & \beta_1 & \gamma_1 & 0 & 0 & 0 & 0 & 0 & \bar{\gamma}_1 & \bar{\beta}_1 & \bar{\gamma}_2 & 0 & \bar{\beta}_2 & \alpha & \beta_2 \\
\gamma_1 & 0 & \gamma_2 & \beta_1 & 0 & 0 & 0 & 0 & \bar{\gamma}_2 & 0 & \bar{\gamma}_1 & \bar{\beta}_1 & \beta_2 & 0 & \bar{\beta}_2 & \alpha
\end{array}\right)$$

FDFE Method

where

$$\alpha = \frac{4}{3}\frac{h_y}{h_x} + \frac{4}{3}\frac{h_x}{h_y} + k^2\frac{4}{9}h_x h_y,$$

$$\beta_1 = -\frac{1}{3} + k^2\frac{1}{9}h_x h_y - ik_y\frac{2}{3}h_x, \quad \bar{\beta}_1 = -\frac{1}{3} + k^2\frac{1}{9}h_x h_y + ik_y\frac{2}{3}h_x,$$

$$\beta_2 = -\frac{1}{3} + k^2\frac{1}{9}h_x h_y - ik_x\frac{2}{3}h_y, \quad \bar{\beta}_2 = -\frac{1}{3} + k^2\frac{1}{9}h_x h_y + ik_x\frac{2}{3}h_y,$$

$$\gamma_1 = -\frac{1}{3} + k^2\frac{1}{36}h_x h_y - i\frac{k_x h_y + k_y h_x}{6}, \quad \bar{\gamma}_1 = -\frac{1}{3} + k^2\frac{1}{36}h_x h_y + i\frac{k_x h_y + k_y h_x}{6},$$

$$\gamma_2 = -\frac{1}{3} + k^2\frac{1}{36}h_x h_y + i\frac{k_x h_y - k_y h_x}{6}, \quad \bar{\gamma}_2 = -\frac{1}{3} + k^2\frac{1}{36}h_x h_y - i\frac{k_x h_y - k_y h_x}{6}.$$

$$B = \left(\begin{array}{cccc|cccc|cccc|cccc}
a & b & 0 & b & b & c & 0 & c & 0 & 0 & 0 & 0 & b & c & 0 & c \\
b & a & b & 0 & c & b & c & 0 & 0 & 0 & 0 & 0 & c & b & c & 0 \\
0 & b & a & b & 0 & c & b & c & 0 & 0 & 0 & 0 & 0 & c & b & c \\
b & 0 & b & a & c & 0 & c & b & 0 & 0 & 0 & 0 & c & 0 & c & b \\
\hline
b & c & 0 & c & a & b & 0 & b & b & c & 0 & c & 0 & 0 & 0 & 0 \\
c & b & c & 0 & b & a & b & 0 & c & b & c & 0 & 0 & 0 & 0 & 0 \\
0 & c & b & c & 0 & b & a & b & 0 & c & b & c & 0 & 0 & 0 & 0 \\
c & 0 & c & b & b & 0 & b & a & c & 0 & c & b & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & b & c & 0 & c & a & b & 0 & b & b & c & 0 & c \\
0 & 0 & 0 & 0 & c & b & c & 0 & b & a & b & 0 & c & b & c & 0 \\
0 & 0 & 0 & 0 & 0 & c & b & c & 0 & b & a & b & 0 & c & b & c \\
0 & 0 & 0 & 0 & c & 0 & c & b & b & 0 & b & a & c & 0 & c & b \\
\hline
b & c & 0 & c & 0 & 0 & 0 & 0 & b & c & 0 & c & a & b & 0 & b \\
c & b & c & 0 & 0 & 0 & 0 & 0 & c & b & c & 0 & b & a & b & 0 \\
0 & c & b & c & 0 & 0 & 0 & 0 & 0 & c & b & c & 0 & b & a & b \\
c & 0 & c & b & 0 & 0 & 0 & 0 & c & 0 & c & b & b & 0 & b & a
\end{array}\right),$$

where

$$a = \frac{4}{9}h_x h_y, \quad b = \frac{1}{9}h_x h_y, \quad c = \frac{1}{36}h_x h_y.$$

FDFE Method

Eigenvalues in the homogenous case ($\varepsilon(x,y) = 1$)

$$\eta(\mathbf{k}) = \frac{\hat{a}(z,w;\mathbf{k})}{\hat{b}(z,w;\mathbf{k})},$$

where

$$\begin{aligned}
\hat{a}(z,w;\mathbf{k}) &= a\big(\phi_{(j_1,j_2)},\phi_{(j_1,j_2)}\big) + a\big(\phi_{(j_1,j_2)},\phi_{(j_1+1,j_2)}\big)z + \bar{a}\big(\phi_{(j_1,j_2)},\phi_{(j_1+1,j_2)}\big)z^{-1} \\
&+ a\big(\phi_{(j_1,j_2)},\phi_{(j_1,j_2+1)}\big)w + \bar{a}\big(\phi_{(j_1,j_2)},\phi_{(j_1,j_2+1)}\big)w^{-1}, \\
\hat{b}(z,w;\mathbf{k}) &= b\big(\phi_{(j_1,j_2)},\phi_{(j_1,j_2)}\big) + b\big(\phi_{(j_1,j_2)},\phi_{(j_1+1,j_2)}\big)z + \bar{b}\big(\phi_{(j_1,j_2)},\phi_{(j_1+1,j_2)}\big)z^{-1} \\
&+ b\big(\phi_{(j_1,j_2)},\phi_{(j_1,j_2+1)}\big)w + \bar{b}\big(\phi_{(j_1,j_2)},\phi_{(j_1,j_2+1)}\big)w^{-1},
\end{aligned}$$

with $z^n = 1$ and $w^m = 1$.

FDFE Method

As in the FDFD method we can easily prove that:

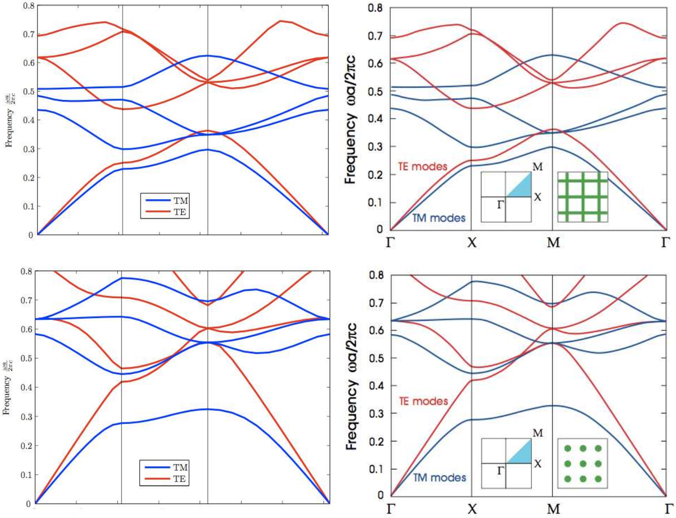
$$E_{\text{abs}} = \text{const}_1 \left[\left(\frac{2\pi j}{a} + k_x \right)^2 - k_x^2 \right] \left\{ 1 + O\left(\left(\frac{j}{n} \right)^2 \right) \right\} + \text{const}_2 \left[\left(\frac{2\pi l}{b} + k_y \right)^2 - k_y^2 \right] \left\{ 1 + O\left(\left(\frac{l}{m} \right)^2 \right) \right\},$$

and for the relative error we then get the following upper bound:

$$E_{\text{rel}} = -\max \left[\text{const}_1 \left\{ 1 + O\left(\left(\frac{j}{n} \right)^2 \right) \right\}, \text{const}_2 \left\{ 1 + O\left(\left(\frac{l}{m} \right)^2 \right) \right\} \right],$$

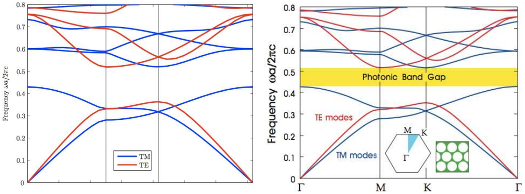
n and m being the number of mesh points along the x and y axes, respectively.

Numerical Results



Numerical Results

In the **nonrectangular** 2D case we use the basis vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ to convert the Helmholtz equation to cartesian coordinates and both FDFD and FDFE methods work successfully:



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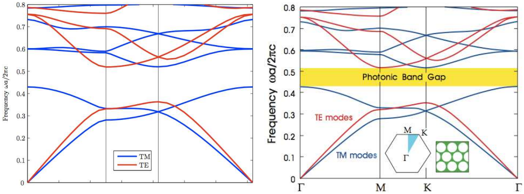

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FDFD method for 3D PC

Let us now introduce the $3n_1n_2n_3$-dimensional (real or complex) vector space H_{n_1,n_2,n_3} of columns vectors indexed by $(j_1, j_2, j_3, s) \in \mathbb{Z}[n_1] \times \mathbb{Z}[n_2] \times \mathbb{Z}[n_3] \times \{1, 2, 3\}$, where (j_1, j_2, j_3) is a lower index and s is an upper index.
We define the *discrete divergence*:

$$[\nabla \cdot \mathbf{F}]_{j_1,j_2,j_3} = \frac{F^1_{j_1+1,j_2,j_3} - F^1_{j_1-1,j_2,j_3}}{2h_1} + \frac{F^2_{j_1,j_2+1,j_3} - F^2_{j_1,j_2-1,j_3}}{2h_2} + \frac{F^3_{j_1,j_2,j_3+1} - F^3_{j_1,j_2,j_3-1}}{2h_3},$$

and the *discrete curl* $\nabla\times : \mathrm{H}_{n_1,n_2,n_2} \to \mathrm{H}_{n_1,n_2,n_3}$ as follows:

$$\begin{aligned}
(\nabla \times \mathbf{F})^1_{j_1,j_2,j_3} &= (\partial_2 F^3 - \partial_3 F^2)_{j_1,j_2,j_3},\\
(\nabla \times \mathbf{F})^2_{j_1,j_2,j_3} &= (\partial_3 F^1 - \partial_1 F^3)_{j_1,j_2,j_3},\\
(\nabla \times \mathbf{F})^3_{j_1,j_2,j_3} &= (\partial_1 F^2 - \partial_2 F^1)_{j_1,j_2,j_3}.
\end{aligned}$$

FDFD Method for 3D PC

We have to solve the spectral problem under periodicity conditions:

$$\nabla \cdot [\varepsilon(\mathbf{x})\mathcal{E}(\mathbf{x})] + i\mathbf{k} \cdot [\varepsilon(\mathbf{x})\mathcal{E}(\mathbf{x})] = 0, \tag{13}$$

$$\nabla \times \mathcal{H}(\mathbf{x}) + i[\mathbf{k} \times \mathcal{H}(\mathbf{x})] - i\sqrt{\eta}\varepsilon(\mathbf{x})\mathcal{E}(\mathbf{x}) = 0, \tag{14}$$

$$\nabla \times \mathcal{E}(\mathbf{x}) + i[\mathbf{k} \times \mathcal{E}(\mathbf{x})] + i\sqrt{\eta}\varepsilon(\mathbf{x})\mathcal{H}(\mathbf{x}) = 0, \tag{15}$$

$$\nabla \cdot [\mathcal{H}(\mathbf{x})] + i\mathbf{k} \cdot \mathcal{H}(\mathbf{x}) = 0. \tag{16}$$

Proposition

For $\sqrt{\eta} > 0$, any solution to the equations (14) and (15) satisfies the discrete divergence equations

$$\nabla \cdot [\varepsilon(\mathbf{x})\mathcal{E}(\mathbf{x})] + i\mathbf{k} \cdot [\varepsilon(\mathbf{x})\mathcal{E}(\mathbf{x})] = 0,$$

$$\nabla \cdot [\mathcal{H}(\mathbf{x})] + i\mathbf{k} \cdot \mathcal{H}(\mathbf{x}) = 0.$$

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$$\nabla \times \mathcal{H}(\mathbf{x}) + i[\mathbf{k} \times \mathcal{H}(\mathbf{x})] - i\sqrt{\eta}\varepsilon(\mathbf{x})\mathcal{E}(\mathbf{x}) = 0, \tag{14}$$

$$\nabla \times \mathcal{E}(\mathbf{x}) + i[\mathbf{k} \times \mathcal{E}(\mathbf{x})] + i\sqrt{\eta}\varepsilon(\mathbf{x})\mathcal{H}(\mathbf{x}) = 0, \tag{15}$$

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$$\nabla \cdot [\mathcal{H}(\mathbf{x})] + i\mathbf{k} \cdot \mathcal{H}(\mathbf{x}) = 0.$$

FDFD Method for 3D PC

Finite Differencing Eqs. (14) and (15) we get a linear system of order $6n_1n_2n_3 \times 6n_1n_2n_3$, where n_1, n_2 and n_3 are the numbers of grid points along the x, y and z axes, respectively:

$$\frac{1}{2h_2}(H^3_{j_1,j_2+1,j_3} - H^3_{j_1,j_2-1,j_3}) - \frac{1}{2h_3}(H^2_{j_1,j_2,j_3+1} - H^2_{j_1,j_2,j_3-1}) + i(k_2H^3_{j_1,j_2,j_3} - k_3H^2_{j_1,j_2,j_3})$$
$$= i\sqrt{\eta}\varepsilon_{j_1,j_2,j_3}E^1_{j_1,j_2,j_3},$$
$$\frac{1}{2h_3}(H^1_{j_1,j_2,j_3+1} - H^1_{j_1,j_2,j_3-1}) - \frac{1}{2h_1}(H^3_{j_1+1,j_2,j_3} - H^3_{j_1-1,j_2,j_3}) + i(k_3H^1_{j_1,j_2,j_3} - k_1H^3_{j_1,j_2,j_3})$$
$$= i\sqrt{\eta}\varepsilon_{j_1,j_2,j_3}E^2_{j_1,j_2,j_3},$$
$$\frac{1}{2h_1}(H^2_{j_1+1,j_2,j_3} - H^2_{j_1-1,j_2,j_3}) - \frac{1}{2h_2}(H^1_{j_1,j_2+1,j_3} - H^1_{j_1,j_2-1,j_3}) + i(k_1H^2_{j_1,j_2,j_3} - k_2H^1_{j_1,j_2,j_3})$$
$$= i\sqrt{\eta}\varepsilon_{j_1,j_2,j_3}E^3_{j_1,j_2,j_3},$$
$$\frac{1}{2h_2}(E^3_{j_1,j_2+1,j_3} - E^3_{j_1,j_2-1,j_3}) - \frac{1}{2h_3}(E^2_{j_1,j_2,j_3+1} - E^2_{j_1,j_2,j_3-1}) + i(k_2E^3_{j_1,j_2,j_3} - k_3E^2_{j_1,j_2,j_3})$$
$$= i\sqrt{\eta}H^1_{j_1,j_2,j_3},$$
$$\frac{1}{2h_3}(E^1_{j_1,j_2,j_3+1} - E^1_{j_1,j_2,j_3-1}) - \frac{1}{2h_1}(E^3_{j_1+1,j_2,j_3} - E^3_{j_1-1,j_2,j_3}) + i(k_3E^1_{j_1,j_2,j_3} - k_1E^3_{j_1,j_2,j_3})$$
$$= i\sqrt{\eta}H^2_{j_1,j_2,j_3},$$
$$\frac{1}{2h_1}(E^2_{j_1+1,j_2,j_3} - E^2_{j_1-1,j_2,j_3}) - \frac{1}{2h_2}(E^1_{j_1,j_2+1,j_3} - E^1_{j_1,j_2-1,j_3}) + i(k_1E^2_{j_1,j_2,j_3} - k_2E^1_{j_1,j_2,j_3})$$
$$= i\sqrt{\eta}H^3_{j_1,j_2,j_3},$$

FDFD Method for 3D PC

The $6n_1n_2n_3 \times 6n_1n_2n_3$ linear system can be written in a more compact form:

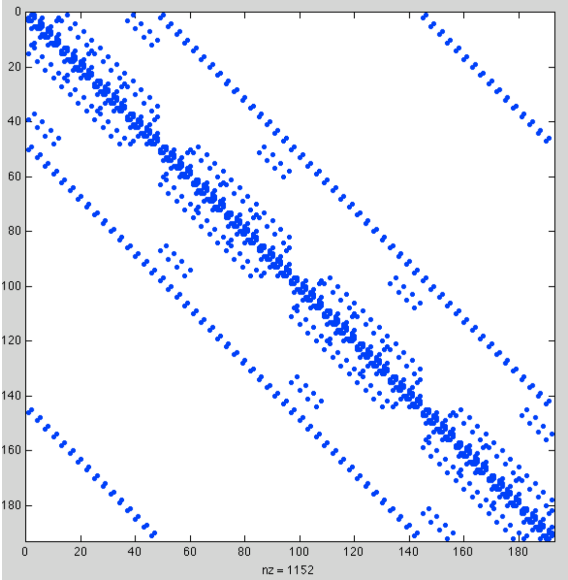
$$\begin{pmatrix} \mathbf{C} & i\sqrt{\eta}\,\mathbf{I} \\ -i\sqrt{\eta}\,\boldsymbol{\varepsilon} & \mathbf{C} \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} = 0 \qquad (18)$$

where $\boldsymbol{\varepsilon} = \varepsilon \otimes \mathbb{I}_3$ is a diagonal matrix with positive entries and $\mathbf{C}$ is a block circulant matrix with 3×3 blocks:

$$C_{0,0,0} = \begin{pmatrix} 0 & -ik_3 & ik_2 \\ ik_3 & 0 & -ik_1 \\ -ik_2 & ik_1 & 0 \end{pmatrix}, \quad C_{\pm1,0,0} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \mp\frac{1}{2h_1} \\ 0 & \pm\frac{1}{2h_1} & 0 \end{pmatrix},$$

$$C_{0,\pm1,0} = \begin{pmatrix} 0 & 0 & \pm\frac{1}{2h_2} \\ 0 & 0 & 0 \\ \mp\frac{1}{2h_2} & 0 & 0 \end{pmatrix}, \quad C_{0,0,\pm1} = \begin{pmatrix} 0 & \mp\frac{1}{2h_3} & 0 \\ \pm\frac{1}{2h_3} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

FDFD Method for 3D PC



FDFD Method for 3D PC

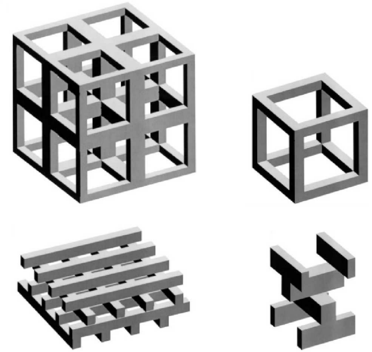
Writing the two equations (18) in the form $\mathbf{CH} = i\sqrt{\eta}\mathbf{E}$ and $\mathbf{CE} = -i\sqrt{\eta}\mathbf{H}$, we get after one iteration

Eigenvalue problem for E

- $\mathbf{C}^2\ \mathbf{E} = \eta\ \varepsilon\ \mathbf{E}$

Eigenvalue problem for H

- $\mathbf{C}\ \frac{1}{\varepsilon}\mathbf{C}\ \mathbf{H} = \eta\ \mathbf{H}$



Conclusions

- FDFD method for 3D photonic crystal is in progress;
- Generalized eigenvalue problems appear in the study of photonic devices in optoelectronics;
- Algorithms which study multi-index circulant+diagonal eigenvalue problems, in particular for large matrix orders, have to be properly implemented.

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Time Domain Methods

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Frequency Domain Methods

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