Study of EM waves in Periodic Structures (mathematical details)

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6.635 partial lecture notes

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1 Introduction: periodic media nomenclature

1. The space domain is defined by a basis,$(\overline{a}_1, \overline{a}_2, \overline{a}_3)$, where any vector can be written as

$$\overline{r}' = \overline{r} + \overline{R} = \overline{r} + \alpha_1 \overline{a}_1 + \alpha_2 \overline{a}_2 + \alpha_3 \overline{a}_3 \,, \tag{1}$$

   where $\overline{R}$ is the translation vector, with $\alpha_1, \alpha_2, \alpha_3$ integers.

2. The spectral domain is defined by a basis, $(\overline{b}_1, \overline{b}_2, \overline{b}_3)$, and similarly, the translational vector is written as

$$\overline{G} = \beta_1 \overline{b}_1 + \beta_2 \overline{b}_2 + \beta_3 \overline{b}_3 \,, \tag{2}$$

   where $\beta_1, \beta_2, \beta_3$ are integers.

3. The two basis are linked since the functions (fields, permittivity) are periodic. For example, if we write the permittivity:

$$\text{Fourier expansion:} \quad \epsilon(\overline{r}) = \sum_{\overline{G}} \tilde{\epsilon}(\overline{G})\, e^{i\overline{G}\cdot\overline{r}} \quad \text{where } \tilde{\epsilon}(\overline{G}) = \frac{1}{V_{\text{cell}}} \iiint \mathrm{d}\overline{r}^3 \epsilon(\overline{r})\, e^{-i\overline{G}\cdot\overline{r}} \,. \tag{3}$$

$$\begin{aligned} \text{Periodicity:} \quad \epsilon(\overline{r} + \overline{R}) &= \sum_{\overline{G}} \tilde{\epsilon}(\overline{G})\, e^{i\overline{G}\cdot(\overline{r}+\overline{R})} \\ &= \sum_{\overline{G}} \tilde{\epsilon}(\overline{G})\, e^{i\overline{G}\cdot\overline{r}}\, e^{i\overline{G}\cdot\overline{R}} = \epsilon(\overline{r}) \end{aligned} \tag{4}$$

   so that $e^{i\overline{G}\cdot\overline{R}} = 1$ and

$$\overline{G} \cdot \overline{R} = 2\text{m}\pi \qquad \text{where m} \in \{\ldots, -1, 0, 1, 2, \ldots\} \,. \tag{5}$$

   We can see that condition (5) is immediately verified if we impose:

$$\overline{b}_j \cdot \overline{a}_i = 2\pi \delta_{ij} \,. \tag{6}$$

4. Bloch-Floquet theorem:

   Since EM fields are periodic, we can write them as a propagating function times a function with the same periodicity as the medium:

$$\overline{\xi}_{\overline{k}}(\overline{r}) = e^{i\overline{k}\cdot\overline{r}}\,\overline{\zeta}_{\overline{k}}(\overline{r}) \qquad \text{where} \qquad \overline{\zeta}_{\overline{k}}(\overline{r}+\overline{R}) = \overline{\zeta}_{\overline{k}}(\overline{r}), \tag{7}$$

   and where $\overline{\xi}$ can represent either the electric or magnetic fields, $\overline{E}$ or $\overline{H}$.

   Since $\overline{\zeta}(\overline{r})$ is periodic, we can Fourier expand it:

$$\overline{\zeta}_{\overline{k}}(\overline{r}) = \sum_{\overline{G}} \tilde{\overline{\zeta}}_{\overline{G}}\, e^{i\overline{G}\cdot\overline{r}}, \tag{8}$$

   so that we shall write:

$$\overline{E}_{\overline{k}}(\overline{r}) = \sum_{\overline{G}} \overline{e}_{\overline{G}}\, e^{i(\overline{k}+\overline{G})\cdot\overline{r}}, \tag{9a}$$

$$\overline{H}_{\overline{k}}(\overline{r}) = \sum_{\overline{G}} \overline{h}_{\overline{G}}\, e^{i(\overline{k}+\overline{G})\cdot\overline{r}}. \tag{9b}$$

5. Wave equation in source-free region:

   From Maxwell's equation, we can easily obtain the following wave equations in source-free regions (with $\epsilon = \epsilon(\overline{r})$):

$$\nabla\times\nabla\times\overline{E}(\overline{r}) = \left(\frac{\omega}{c}\right)^2 \mu_r\epsilon_r(\overline{r})\,\overline{E}(\overline{r}), \tag{10a}$$

$$\nabla\times\left[\frac{1}{\epsilon_r(\overline{r})}\nabla\times\overline{H}(\overline{r})\right] = \left(\frac{\omega}{c}\right)^2 \mu_r\,\overline{H}(\overline{r}), \tag{10b}$$

   To make these equations more symmetrical, we shall work with $1/\epsilon_r(\overline{r})$ instead of $\epsilon_r(\overline{r})$ directly, so that we define

$$\kappa_r(\overline{r}) = \frac{1}{\epsilon_r(\overline{r})} = \sum_{\overline{G}} \tilde{\kappa}_r(\overline{G})\, e^{i\overline{G}\cdot\overline{r}}. \tag{11}$$

   The wave equations are rewritten as:

$$\kappa_r(\overline{r})\nabla\times\nabla\times\overline{E}(\overline{r}) = \left(\frac{\omega}{c}\right)^2 \mu_r\,\overline{E}(\overline{r}), \tag{12a}$$

$$\nabla\times\left[\kappa_r(\overline{r})\nabla\times\overline{H}(\overline{r})\right] = \left(\frac{\omega}{c}\right)^2 \mu_r\,\overline{H}(\overline{r}). \tag{12b}$$

2 Treatment of the $\overline{E}$ field

2.1 Method 1: direct expansion of the permittivity

We want to write Eq. (10a) with the decomposition of Eq. (9a). First, let us compute the first curl (taking $\overline{G}'$ as the variable for the expansion):

$$\nabla \times \overline{E}_k(\overline{r}) = \sum_{\overline{G}'} \nabla \times \left[\overline{e}_{\overline{G}'}\, e^{i(\overline{k}+\overline{G}')\cdot\overline{r}} \right] = i \sum_{\overline{G}'} (\overline{k}+\overline{G}') \times \overline{e}_{\overline{G}'}\, e^{i(\overline{k}+\overline{G}')\cdot\overline{r}} \,. \tag{13}$$

Taking the curl one more time gives

$$\nabla \times \nabla \times \overline{E}_{\overline{k}}(\overline{r}) = -\sum_{\overline{G}'} (\overline{k}+\overline{G}') \times \left[(\overline{k}+\overline{G}') \times \overline{e}_{\overline{G}'} \right] e^{i(\overline{k}+\overline{G}')\cdot\overline{r}} \,. \tag{14}$$

Upon using Eq. (3) but changing the index $\overline{G}$ into $\overline{G}''$, we write

$$\epsilon_r(\overline{r})\overline{E}(\overline{r}) = \sum_{\overline{G}'} \sum_{\overline{G}''} \tilde{\epsilon}_r(\overline{G}'')\, \overline{e}_{\overline{G}'}\, e^{i(\overline{k}+\overline{G}'+\overline{G}'')\cdot\overline{r}} \,. \tag{15}$$

By changing the variables $\overline{G} = \overline{G}' + \overline{G}''$:

$$\epsilon_r(\overline{r})\overline{E}(\overline{r}) = \sum_{\overline{G}} \sum_{\overline{G}'} \tilde{\epsilon}_r(\overline{G}-\overline{G}')\, \overline{e}_{\overline{G}'}\, e^{i(\overline{k}+\overline{G})\cdot\overline{r}} \,. \tag{16}$$

The wave equation (see Eq. (10a)) can therefore be rewritten as:

$$-\sum_{\overline{G}'} (\overline{k}+\overline{G}') \times \left[(\overline{k}+\overline{G}') \times \overline{e}_{\overline{G}'} \right] e^{i(\overline{k}+\overline{G}')\cdot\overline{r}} = \left(\frac{\omega}{c}\right)^2 \mu_r \sum_{\overline{G}} \sum_{\overline{G}'} \tilde{\epsilon}_r(\overline{G}-\overline{G}')\, \overline{e}_{\overline{G}'}\, e^{i(\overline{k}+\overline{G})\cdot\overline{r}} \,. \tag{17}$$

We can simplify by $\exp(i\overline{k}\cdot\overline{r})$ and multiply by $\exp(-i\overline{G}''\cdot\overline{r})$ to get:

$$-\sum_{\overline{G}'} (\overline{k}+\overline{G}') \times \left[(\overline{k}+\overline{G}') \times \overline{e}_{\overline{G}'} \right] e^{i(\overline{G}'-\overline{G}'')\cdot\overline{r}} = \left(\frac{\omega}{c}\right)^2 \mu_r \sum_{\overline{G}} \sum_{\overline{G}'} \tilde{\epsilon}_r(\overline{G}-\overline{G}')\, \overline{e}_{\overline{G}'}\, e^{i(\overline{G}-\overline{G}'')\cdot\overline{r}} \,. \tag{18}$$

If we integrate this equation over the entire space, we can pull all the terms out of the integral, except $e^{i(\overline{G}'-\overline{G}'')\cdot\overline{r}}$ on the left-hand side and. $e^{i(\overline{G}-\overline{G}'')\cdot\overline{r}}$ on the right-hand side. Yet, we have

$$\iiint_V \mathrm{d}\overline{r}^3 e^{i(\overline{G}-\overline{G}'')\cdot\overline{r}} = \frac{1}{(2\pi)^3}\, \delta(\overline{G}-\overline{G}'') \,, \tag{19}$$

so that Eq. (18) becomes (upon substituting $\overline{G}''$ by $\overline{G}$ since these are dummy variables):

$$-(\overline{k}+\overline{G}) \times \left[(\overline{k}+\overline{G}) \times \overline{e}_{\overline{G}} \right] = \left(\frac{\omega}{c}\right)^2 \mu_r \sum_{\overline{G}'} \tilde{\epsilon}_r(\overline{G}-\overline{G}')\, \overline{e}_{\overline{G}'} \,, \qquad \forall \overline{G} \,. \tag{20}$$

2.2 Method 2: expansion of the inverse of the permittivity

Instead of working with Eq. (10a), we can also use Eq. (12a), which would need the expansion of Eq. (11).

Applying the same method (and transforming the index of Eq. (11) from $\overline{G}$ to $\overline{G}''$), we get:

$$-\sum_{\overline{G}''}\sum_{\overline{G}'}\tilde{\kappa}_r(\overline{G}'')(\overline{k}+\overline{G}')\times\left[(\overline{k}+\overline{G}')\times\overline{e}_{\overline{G}'}\right]e^{i(\overline{k}+\overline{G}'+\overline{G}'')\cdot\overline{r}} = \left(\frac{\omega}{c}\right)^2\mu_r\sum_{\overline{G}'}\overline{e}_{\overline{G}'}e^{i(\overline{k}+\overline{G}')\cdot\overline{r}}\,. \quad (21)$$

which, upon substituting $\overline{G} = \overline{G}' + \overline{G}''$, simplifying by $\exp(i\overline{k}\cdot\overline{r})$, multiplying by $\exp(-i\overline{G}''\cdot\overline{r})$, integrating over the whole space, using Eq. (19) and finally substituting $\overline{G}''$ by $\overline{G}$, becomes:

$$-\sum_{\overline{G}'}\tilde{\kappa}_r(\overline{G}-\overline{G}')(\overline{k}+\overline{G}')\times\left[(\overline{k}+\overline{G}')\times\overline{e}_{\overline{G}'}\right] = \left(\frac{\omega}{c}\right)^2\mu_r\,\overline{e}_{\overline{G}}\,,\qquad\forall\overline{G}\,. \quad (22)$$

3 Treatment of the $\overline{H}$ field

The $\overline{H}$ field is treated in an exactly similar way to eventually obtain very similar equations.

However, these equations can still be pushed further by using the fact that $\nabla\cdot\overline{H}_{\overline{k}}(\overline{r}) = 0$. Upon using this equality, we see from Eq. (9b) that (using $\overline{G}'$ for the expansion of the field):

$$(\overline{k}+\overline{G}')\cdot\overline{h}_{\overline{G}'} = 0\,. \quad (23)$$

We can therefore define three vectors $(\hat{e}_1,\hat{e}_2,\hat{e}_3)$ such that

$$\overline{k}+\overline{G}' = |\overline{k}+\overline{G}'|\,\hat{e}_3\,, \quad (24a)$$

$$\hat{e}_1\cdot\hat{e}_3 = \hat{e}_2\cdot\hat{e}_3 = 0\,, \quad (24b)$$

and $(\hat{e}_1,\hat{e}_2,\hat{e}_3)$ for an orthonormal tryad. In that case, we can decompose

$$\overline{h}_{\overline{G}'} = h_{1\overline{G}'}\hat{e}_1 + h_{2\overline{G}'}\hat{e}_2 = \sum_{\lambda=1,2}h_{\lambda\overline{G}'}\,\hat{e}_\lambda\,. \quad (25)$$

We need now to introduce this expression into Eq. (12b). First, we compute

$$\nabla\times\overline{H}_{\overline{k}}(\overline{r}) = i\sum_{\overline{G}'}\sum_{\lambda}h_{\lambda\overline{G}'}\left[(\overline{k}+\overline{G}')\times\hat{e}_\lambda\right]e^{i(\overline{k}+\overline{G}')\cdot\overline{r}}\,, \quad (26)$$

so that

$$\begin{aligned}\kappa_r(\overline{r})\nabla\times\overline{H}_{\overline{k}}(\overline{r}) &= i\sum_{\overline{G}''}\sum_{\overline{G}'}\sum_{\lambda}h_{\lambda\overline{G}'}\,\tilde{\kappa}_r(\overline{G}'')\left[(\overline{k}+\overline{G}')\times\hat{e}_\lambda\right]e^{i(\overline{k}+\overline{G}'+\overline{G}'')\cdot\overline{r}}\\ &= i\sum_{\overline{G}}\sum_{\overline{G}'}\sum_{\lambda}h_{\lambda\overline{G}'}\,\tilde{\kappa}_r(\overline{G}-\overline{G}')\left[(\overline{k}+\overline{G}')\times\hat{e}_\lambda\right]e^{i(\overline{k}+\overline{G})\cdot\overline{r}}\,. \quad (27)\end{aligned}$$

Taking the next curl, we write:

$$\nabla\times\Big[\kappa_r(\overline{r})\nabla\times\overline{H}_{\overline{k}}(\overline{r})\Big] = -\sum_{\overline{G}}\sum_{\overline{G}'}\sum_{\lambda} h_{\lambda\overline{G}'}\,\tilde{\kappa}_r(\overline{G}-\overline{G}')\,\Big[(\overline{k}+\overline{G})\times[(\overline{k}+\overline{G}')\times\hat{e}_\lambda]\Big]\,e^{i(\overline{k}+\overline{G})\cdot\overline{r}}\,, \quad (28)$$

so that the wave equation (see Eq. (12b)) becomes:

$$-\sum_{\overline{G}}\sum_{\overline{G}'}\sum_{\lambda} h_{\lambda\overline{G}'}\,\tilde{\kappa}_r(\overline{G}-\overline{G}')\,\Big[(\overline{k}+\overline{G})\times[(\overline{k}+\overline{G}')\times\hat{e}_\lambda]\Big]\,e^{i(\overline{k}+\overline{G})\cdot\overline{r}} = \left(\frac{\omega}{c}\right)^2\mu_r\sum_{\overline{G}'}\sum_{\lambda} h_{\lambda\overline{G}'}\,e^{i(\overline{k}+\overline{G}')\cdot\overline{r}}\hat{e}_\lambda\,. \quad (29)$$

Always by the same token (multiplying by the proper functions and integrating over whole space), we write:

$$-\sum_{\overline{G}'}\sum_{\lambda} h_{\lambda\overline{G}'}\,\tilde{\kappa}_r(\overline{G}-\overline{G}')\,\Big[(\overline{k}+\overline{G})\times[(\overline{k}+\overline{G}')\times\hat{e}_\lambda]\Big] = \left(\frac{\omega}{c}\right)^2\mu_r\sum_{\lambda''} h_{\lambda''\overline{G}}\,\hat{e}_{\lambda''} \qquad \forall\overline{G}\,. \quad (30)$$

We can further simplify this expression by dot-multiplying the equation by $\hat{e}_{\lambda'}$ and noting that (using $\overline{C}\cdot(\overline{A}\times\overline{B}) = \overline{B}\cdot(\overline{C}\times\overline{A})$)

$$\Big[(\overline{k}+\overline{G})\times[(\overline{k}+\overline{G}')\times\hat{e}_\lambda]\Big]\cdot\hat{e}_{\lambda'} = -\Big[(\overline{k}+\overline{G}')\times\hat{e}_\lambda\Big]\cdot\Big[(\overline{k}+\overline{G})\times\hat{e}_{\lambda'}\Big] \quad (31)$$

Therefore, dot-multiplying Eq. (30) by $\hat{e}_{\lambda'}$, we get the final result:

$$\sum_{\overline{G}'}\sum_{\lambda}\Big\{\Big[(\overline{k}+\overline{G}')\times\hat{e}_\lambda\Big]\cdot\Big[(\overline{k}+\overline{G})\times\hat{e}_{\lambda'}\Big]\Big\}\,\tilde{\kappa}_r(\overline{G}-\overline{G}')\,h_{\lambda\overline{G}'} = \left(\frac{\omega}{c}\right)^2\mu_r h_{\lambda'\overline{G}}\,. \quad (32)$$

Upon exchanging $\overline{G}$ and $\overline{G}'$ (transformations: $\overline{G}\to\overline{G}''$, $\overline{G}'\to\overline{G}$, $\overline{G}''\to\overline{G}'$), we obtain

$$\sum_{\overline{G}}\sum_{\lambda}\Big\{\Big[(\overline{k}+\overline{G})\times\hat{e}_\lambda\Big]\cdot\Big[(\overline{k}+\overline{G}')\times\hat{e}_{\lambda'}\Big]\Big\}\,\tilde{\kappa}_r(\overline{G}'-\overline{G})\,h_{\lambda\overline{G}} = \left(\frac{\omega}{c}\right)^2\mu_r h_{\lambda'\overline{G}'}\,. \quad (33)$$

which is the relation given in [Joannopoulos *et al.*, 1995, p. 129]. Upon using the same notation, we rewrite Eq. (33) as:

$$\sum_{\lambda\overline{G}}\Theta^{\overline{k}}_{(\lambda\overline{G}),(\lambda\overline{G})'}\,h_{(\lambda\overline{G})} = \left(\frac{\omega}{c}\right)^2\mu_r h_{(\lambda\overline{G})'}\,, \quad (34a)$$

where

$$\Theta^{\overline{k}}_{(\lambda\overline{G}),(\lambda\overline{G})'} = \tilde{\kappa}_r(\overline{G}'-\overline{G})\,\Big[(\overline{k}+\overline{G})\times\hat{e}_\lambda\Big]\cdot\Big[(\overline{k}+\overline{G}')\times\hat{e}_{\lambda'}\Big]\,. \quad (34b)$$

3.1 Matrix form

We can cast Eq. (33) in matrix form. First, we rewrite the kernel of the operator of Eq. (34b) as:

$$\left[(\overline{k}+\overline{G})\times\hat{e}_\lambda\right]\cdot\left[(\overline{k}+\overline{G}')\times\hat{e}_{\lambda'}\right]=\left|(\overline{k}+\overline{G})\right|\left|(\overline{k}+\overline{G}')\right|\left[\hat{e}_3\times\hat{e}_\lambda\right]\cdot\left[\hat{e}_3\times\hat{e}_{\lambda'}\right]. \tag{35}$$

Remembering that $\hat{e}_3\times\hat{e}_1=\hat{e}_2$ and $\hat{e}_3\times\hat{e}_2=-\hat{e}_1$, we can write:

$$[\hat{e}_3\times\hat{e}_\lambda]\cdot[\hat{e}_3\times\hat{e}_{\lambda'}]=\begin{pmatrix}\hat{e}_2\cdot\hat{e}_2 & -\hat{e}_2\cdot\hat{e}_1\\ -\hat{e}_1\cdot\hat{e}_2 & \hat{e}_1\cdot\hat{e}_1\end{pmatrix}, \tag{36}$$

so that we write the operator as:

$$\begin{aligned}\Theta^{\overline{k}}_{(\lambda\overline{G}),(\lambda\overline{G})'}&=\tilde{\kappa}_r(\overline{G}'-\overline{G})\left[(\overline{k}+\overline{G})\times\hat{e}_\lambda\right]\cdot\left[(\overline{k}+\overline{G}')\times\hat{e}_{\lambda'}\right]\\&=\tilde{\kappa}_r(\overline{G}'-\overline{G})\left|(\overline{k}+\overline{G})\right|\cdot\left|(\overline{k}+\overline{G}')\right|\begin{pmatrix}\hat{e}_2\cdot\hat{e}_2 & -\hat{e}_2\cdot\hat{e}_1\\ -\hat{e}_1\cdot\hat{e}_2 & \hat{e}_1\cdot\hat{e}_1\end{pmatrix},\end{aligned} \tag{37}$$

used in Eq. (34a).