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

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

   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):

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