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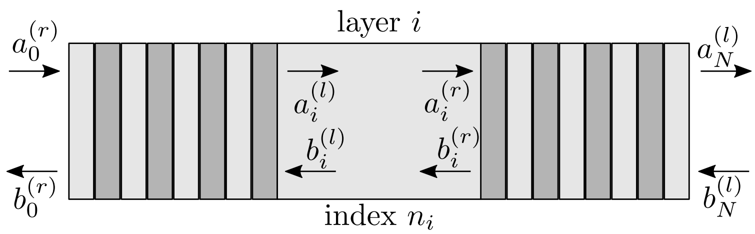
Computational Physics: Problem Set 1

Discussion: 15/02/2023

1 Transfer matrix method for scattering problems

Consider a stack of material layers through which light propagates. This works basically with any type of wave, but we chose light as an example. Each layer has a potentially complex refractive index n_i and thickness D_i, where $0 < i < N$ labels the layers. The propagating wave has the vaccum wave number k_0 (corresponds to the frequency) and its distribution is described by right-propagating amplitudes a and left-propagating amplitudes b in each layer:



This type of system appears in practice in ellipsometry, as anti-reflection coatings, dielectric mirrors, mechanical dampeners isolating equipment from narrow-band vibrations in the floor or as stripline-filters in microwave communication equipment. The transfer matrix method is a popular way to design them.

a) In each layer, the amplitudes accumulate a phase factor $\exp(\mathrm{i} n_i D_i k_0)$ in the respective direction of propagation. Formulate a matrix $P^{(i)}$ that relates the amplitudes $(a_i^{(r)}, b_i^{(r)})^T$ at the right end of a layer to the amplitudes $(a_i^{(l)}, b_i^{(l)})^T$ at the left end:

$$\begin{pmatrix} a_i^{(r)} \\ b_i^{(r)} \end{pmatrix} = \begin{pmatrix} P_{aa}^{(i)} & 0 \\ 0 & P_{bb}^{(i)} \end{pmatrix} \begin{pmatrix} a_i^{(l)} \\ b_i^{(l)} \end{pmatrix}.$$

Write a piece of MATLAB code (e.g. a function handle) that returns the matrix $P^{(i)}(n_i, D_i, k_0)$ as a function of the layer's index, thickness and of the vacuum wave number.

b) At each interface, some light is transmitted and some is back-reflected. This can be expressed as a matrix I_i that relates the amplitudes $(a_i^{(l)}, b_i^{(l)})$ right of a material interface to the amplitudes $(a_{i-1}^{(r)}, b_{i-1}^{(r)})$ left of the interface:

$$\begin{pmatrix} a_i^{(l)} \\ b_i^{(l)} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 + \frac{n_i}{n_{i-1}} & 1 - \frac{n_i}{n_{i-1}} \\ 1 - \frac{n_i}{n_{i-1}} & 1 + \frac{n_i}{n_{i-1}} \end{pmatrix} \begin{pmatrix} a_{i-1}^{(r)} \\ b_{i-1}^{(r)} \end{pmatrix} = I_i \begin{pmatrix} a_{i-1}^{(r)} \\ b_{i-1}^{(r)} \end{pmatrix}.$$

Derive this expression from the continuity conditions of the electric and magnetic fields assuming $\mu_r = 1, \varepsilon_r = n^2$ in each material. Write a piece of MATLAB code (e.g. a function handle) that returns the matrix $I^{(i)}(n_{i-1}, n_i)$ as a function of the indices of the two adjacent materials.

c) The total transfer matrix T of a stack of layers can be composed from the individual phase and interface matrices by simple multiplication:

$T = I^{(N)} P^{(N-1)} I^{(N-1)} \times \ldots \times I^{(2)} P^{(1)} I^{(1)}$.

It relates the amplitudes $(a_0^{(r)}, b_0^{(r)})$ just left to the first interface to the amplitudes $(a_N^{(l)}, b_N^{(l)})$ just right of the last interface:

$$\begin{pmatrix} a_0^{(r)} \\ b_0^{(r)} \end{pmatrix} = \begin{pmatrix} T_{aa} & T_{ab} \\ T_{ba} & T_{bb} \end{pmatrix} \begin{pmatrix} a_N^{(l)} \\ b_N^{(l)} \end{pmatrix},$$

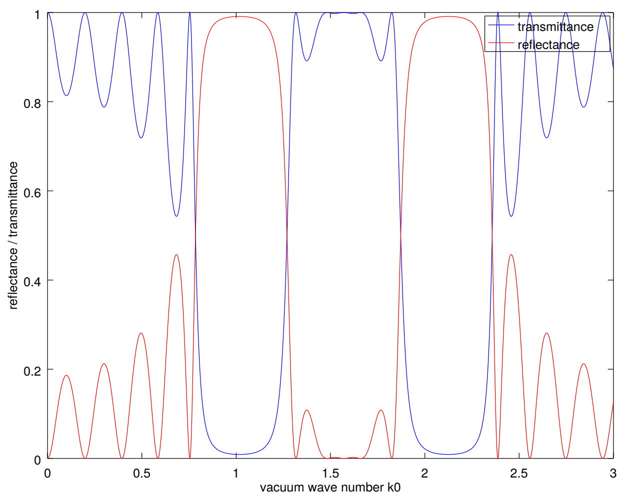
Why can T be represented as this product of individual matrices and why is it "backward" (smaller layer indices i to the right)? Write a piece of MATLAB code that generates the transfer matrix for a given set of layer indices and thicknesses as a function of the vacuum wave number k_0.

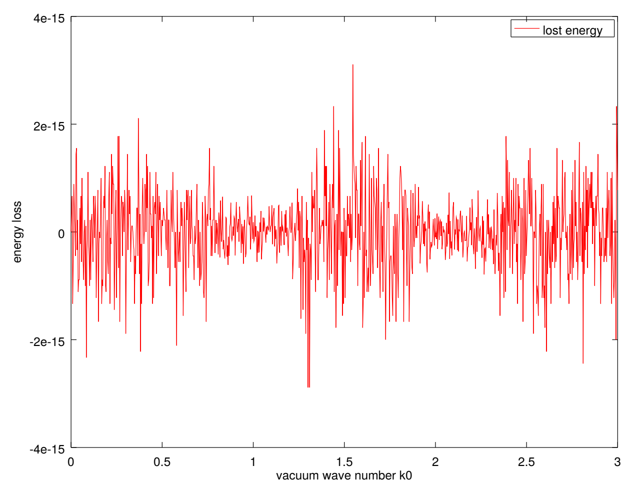
d) The total transmittance and reflectance coefficients (transmission/reflection of energy rather than amplitudes) are given as:

$$\mathcal{T} = \left| T_{aa} - \frac{T_{ab}T_{ba}}{T_{bb}} \right|^2, \qquad \mathcal{R} = \left| \frac{T_{ba}}{T_{bb}} \right|^2,$$

Assume that the system consists of layers of equal thickness $D = 1$ with alternating index $n = 1$ for even i and $n = 2$ for odd i.

Plot the transmission and reflection spectra in the range $0 \le k_0 \le 3$ for stacks with 5, 10 and 20 high-low-index pairs (9, 19, 39 layers overall). Plot also the lost energy $1 - \mathcal{T} - \mathcal{R}$. How does the error evolve as more and more layers are added? In the case of 5 layer pairs the transmittance/reflectance spectra should look something like this:





Feel free to play with layer indices and thicknesses. For example, replace the central layer with another index and observe how the rejection band develops a narrow transmission resonance. Alternatively, optimize the minima of the transmittance (use as a band-rejection filter) or reflectance (use as an anti-reflection coating).

e) In the example with 5 pairs, replace the central high index layer with a lossy layer (positive imaginary part in n) and plot reflection, transmission and energy mismatch. Try these values: $n = 2+5\mathrm{i}$, $n = 2+10\mathrm{i}$, and $n = 2+15\mathrm{i}$. What is happening and why? Try to identify the fundamental problem in the very design of the transfer matrix method for systems with strong absorption. Why is it good practice to inspect numerical results on a log scale, even if the "customer" only wants it on a linear scale?

Students are encouraged to solve these problems in groups. They should be able to informally present their solution in the problem class on 15/02/2023 at the white board (no PowerPoint slides to be prepared).