ECE 595, Section 10
Numerical Simulations
Lecture 27: S-Matrix Methods

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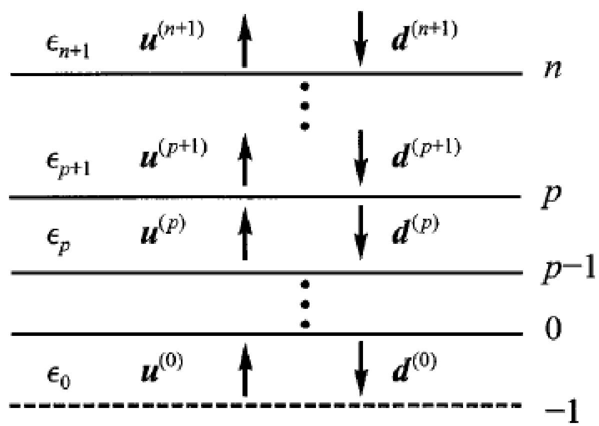
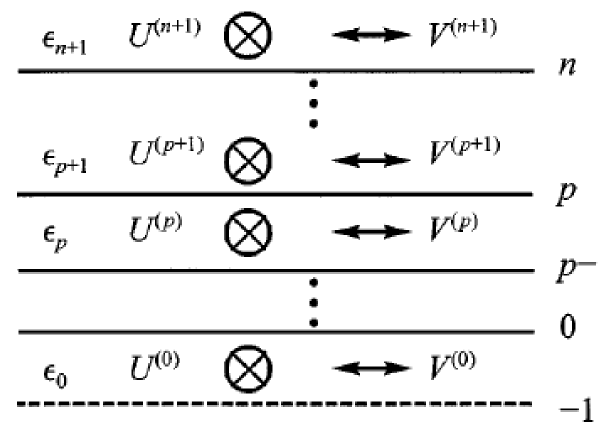
Recap from Monday

- Ray-optics transfer matrix
- Wave-optics matrix methods:
  - T-matrix
  - R-matrix
  - S-matrix



S-matrix problem for inputs + outputs



R-matrix problem for 2 polarizations

S-Matrices

- For S-matrix, connect incoming to outgoing fields from boundaries of region
- Mathematically,

$$\begin{bmatrix} u^{(p+1)} \\ d^{(0)} \end{bmatrix} = \begin{bmatrix} T_{uu}^{(p)} & R_{ud}^{(p)} \\ R_{du}^{(p)} & T_{dd}^{(p)} \end{bmatrix} \begin{bmatrix} u^{(0)} \\ d^{(p+1)} \end{bmatrix}$$

- For input from below:
  - transmission from bottom to top given by $T_{uu}^{(p)}$
  - reflection at bottom given by $R_{du}^{(p)}$

S-Matrices: Key Properties

- In absence of loss, S matrices are unitary, i.e.: $S^{\dagger}S = 1$
- Result is no exponentially growing terms – mathematically, all exponentials in denominators
- Greater numerical stability vis-a-vis *T*-matrices

S-Matrix Construction

- If we already know answer from T-matrix:

$$\begin{bmatrix} u^{(p+1)} \\ d^{(p+1)} \end{bmatrix} = \begin{bmatrix} A^{(p)} & B^{(p)} \\ C^{(p)} & D^{(p)} \end{bmatrix} \begin{bmatrix} u^{(0)} \\ d^{(0)} \end{bmatrix}$$

- Then we can rearrange equations:

$$D^{(p)}\, d^{(0)} = d^{(p+1)} - C^{(p)} u^{(0)}$$

$$u^{(p+1)} = \left[A^{(p)} - B^{(p)} C^{(p)} / D^{(p)}\right] u^{(0)} + \left[B^{(p)} / D^{(p)}\right] d^{(p+1)}$$

- Thus, we have:

$$\begin{bmatrix} T_{uu}^{(p)} & R_{ud}^{(p)} \\ R_{du}^{(p)} & T_{dd}^{(p)} \end{bmatrix} = \begin{bmatrix} A^{(p)} - B^{(p)} C^{(p)} / D^{(p)} & B^{(p)} / D^{(p)} \\ -C^{(p)} / D^{(p)} & 1 / D^{(p)} \end{bmatrix}$$

S-Matrix Construction

- For p layers, can construct p+1th layer using the following relations:
- First, match fields with boundary conditions:

$$W^{(p+1)} \begin{bmatrix} u^{(p+1)}(y_p) \\ d^{(p+1)}(y_p) \end{bmatrix} = W^{(p)} \begin{bmatrix} u^{(p)}(y_p) \\ d^{(p)}(y_p) \end{bmatrix}$$

- Second, construct layer *t*-matrix:

$$\begin{bmatrix} u^{(p+1)}(y_p) \\ d^{(p+1)}(y_p) \end{bmatrix} = \tilde{t}^{(p)} \begin{bmatrix} u^{(p)}(y_{p-1}) \\ d^{(p)}(y_{p-1}) \end{bmatrix}$$

S-Matrix Construction

- Layer *t*-matrix consists of product of two terms:

$$\tilde{t}^{(p)} = t^{(p)}\phi^{(p)}$$

- Interface *t*-matrix:

$$t^{(p)} = \frac{W^{(p)}}{W^{(p+1)}}$$

- Propagation matrix:

$$\phi^{(p)} = \begin{bmatrix} \exp\left(j\beta_{m,+}^{(p)}\Delta y_p\right) & 0 \\ 0 & \exp\left(j\beta_{m,-}^{(p)}\Delta y_p\right) \end{bmatrix}$$

S-Matrix Construction

- By analogy, can define s-layer matrix such that:

$$\begin{bmatrix} u^{(p+1)}(y_p) \\ d^{(p)}(y_{p-1}) \end{bmatrix} = \tilde{s}^{(p)} \begin{bmatrix} u^{(p)}(y_{p-1}) \\ d^{(p+1)}(y_p) \end{bmatrix}$$

- Can then express in terms of s-interface matrix:

$$\tilde{s}^{(p)} = \begin{bmatrix} 1 & 0 \\ 0 & \exp\left(-j\beta_{m,-}^{(p)}\Delta y_p\right) \end{bmatrix} s^{(p)} \begin{bmatrix} \exp\left(j\beta_{m,+}^{(p)}\Delta y_p\right) & 0 \\ 0 & 1 \end{bmatrix}$$

S-Matrix Construction

- We can relate the *s*-interface matrix to the *t*-interface matrix from before:

$$s^{(p)} = \begin{bmatrix} t_{11}^{(p)} - t_{12}^{(p)} t_{22}^{(p)\,-1} t_{21}^{(p)} & t_{12}^{(p)} t_{22}^{(p)\,-1} \\ -t_{22}^{(p)\,-1} t_{21}^{(p)} & t_{22}^{(p)\,-1} \end{bmatrix}$$

- Then iteratively construct next S-matrix via:

$$\begin{bmatrix} T_{uu}^{(p)} & R_{ud}^{(p)} \\ R_{du}^{(p)} & T_{dd}^{(p)} \end{bmatrix} = \begin{bmatrix} \tilde{t}_{uu}^{(p)} \left[1 - R_{ud}^{(p-1)} \tilde{r}_{du}^{(p)}\right]^{-1} T_{uu}^{(p-1)} & \tilde{r}_{ud}^{(p)} + \tilde{t}_{uu}^{(p)} R_{ud}^{(p-1)} \left[1 - \tilde{r}_{du}^{(p)} R_{ud}^{(p-1)}\right]^{-1} \tilde{t}_{dd}^{(p)} \\ R_{ud}^{(p-1)} + T_{dd}^{(p-1)} \tilde{r}_{du}^{(p)} \left[1 - R_{ud}^{(p-1)} \tilde{r}_{du}^{(p)}\right]^{-1} T_{uu}^{(p-1)} & T_{dd}^{(p-1)} \left[1 - \tilde{r}_{du}^{(p)} R_{ud}^{(p-1)}\right]^{-1} \tilde{t}_{dd}^{(p)} \end{bmatrix}$$

S-Matrices: Periodicity

- What happens if one or more layers are periodic?
- Then there are two types of coupling:
  - Layer-to-layer (refractive)
  - Mode-to-mode (diffractive)
- Can both be treated in a single framework?

S-Matrices: Periodic Solution Strategy

- Divide into layers, uniform in z-direction
- Find Bloch states in each layer
- Calculate transfer function for field amplitudes
- Iteratively develop S-matrix
- Choose inputs from both sides
- Calculate resulting outputs (transmission and reflection) and losses (absorption $A=1-T-R$)

Whittaker & Culshaw, *Phys. Rev. B* **60**, 2610 (1999)
Tikhodeev *et al.*, *Phys. Rev. B* **66**, 045102 (2002)

S-Matrices: Periodic Solution Strategy

- Can use a Fourier series expansion in real space of the H-fields:

$$\mathbf{H}(\mathbf{r},z) = \sum_{\mathbf{G}} \left(\phi_x(\mathbf{G}) \left[\hat{\mathbf{x}} - \frac{1}{q}(k_x + G_x)\hat{\mathbf{z}} \right] + \phi_y(\mathbf{G}) \left[\hat{\mathbf{y}} - \frac{1}{q}(k_y + G_y)\hat{\mathbf{z}} \right] \right) e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r} + iqz}$$

- In momentum space, can represent as:

$$h(z) = e^{iqz} \left\{ \phi_x \hat{\mathbf{x}} + \phi_y \hat{\mathbf{y}} - \frac{1}{q}(\hat{k}_x \phi_x + \hat{k}_y \phi_y)\hat{\mathbf{z}} \right\}$$

- And then the electric field as:

$$e(z) = \frac{1}{q} e^{iqz} \hat{\eta} \{ [\hat{k}_y \hat{k}_x \phi_x + (q^2 + \hat{k}_y \hat{k}_y)\phi_y]\hat{\mathbf{x}}$$

$$- [\hat{k}_x \hat{k}_y \phi_y + (q^2 + \hat{k}_x \hat{k}_x)\phi_x]\hat{\mathbf{y}} + q[\hat{k}_y \phi_x - \hat{k}_x \phi_y]\hat{\mathbf{z}} \}$$

S-Matrices: Periodic Solution Strategy

- Eigenvalue equation becomes

$$\left\{ \begin{pmatrix} \hat{\eta} & 0 \\ 0 & \hat{\eta} \end{pmatrix} \left[q^2 + \begin{pmatrix} \hat{k}_x \hat{k}_x & \hat{k}_x \hat{k}_y \\ \hat{k}_y \hat{k}_x & \hat{k}_y \hat{k}_y \end{pmatrix} \right] + \begin{pmatrix} \hat{k}_y \hat{\eta} \hat{k}_y & -\hat{k}_y \hat{\eta} \hat{k}_x \\ -\hat{k}_x \hat{\eta} \hat{k}_y & \hat{k}_x \hat{\eta} \hat{k}_x \end{pmatrix} \right\} \times \begin{pmatrix} \phi_x \\ \phi_y \end{pmatrix} = \omega^2 \begin{pmatrix} \phi_x \\ \phi_y \end{pmatrix}$$

- More compactly represented as:

$$[\mathcal{H}(q^2 + K) + \mathcal{K}]\phi = \omega^2 \phi$$

- Where the eigenvectors ϕ have a unique orthonormality condition:

$$\phi_n^T (\omega^2 - \mathcal{K}) \phi_{n'} = \delta_{nn'}$$

S-Matrix Method: Advantages

- No *ad hoc* assumptions regarding structures
- Applicable to wide variety of problems
- Suitable for eigenmodes or high-*Q* resonant modes at single frequency
- Can treat layers with large difference in length scales
- Computationally tractable enough on single core machines

S-Matrix Method: Disadvantages

- Accurate solutions obtained more slowly as the following increase:
  - Number of layers
  - Absolute magnitude of Fourier components (especially for metals)
  - Number of plane-wave components (~N^3)
- Relatively slow for broad-band problems (time-domain is a good alternative)

Next Class

- Is on Friday, March 22
- Will continue developing S-matrix simulation approach
- Read Whittaker & Culshaw, *Phys. Rev. B* **60**, 2610 (1999)