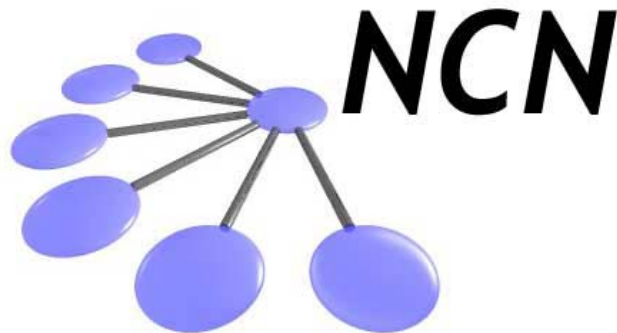


Network for Computational Nanotechnology (NCN)

UC Berkeley, Univ. of Illinois, Norfolk State, Northwestern, Purdue, UTEP

Open 1d Systems: The Transfer Matrix Method

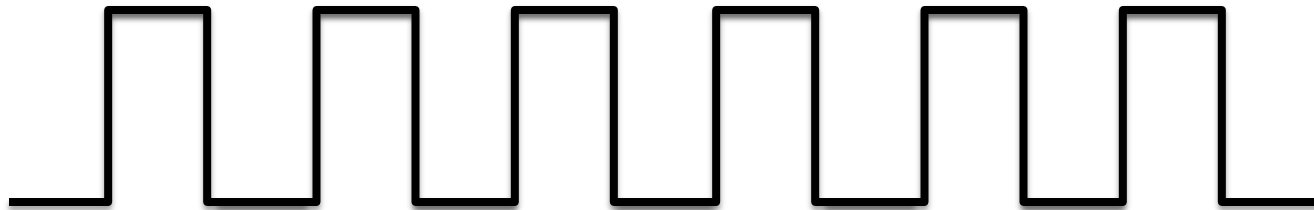


Gerhard Klimeck
Dragica Vasileska,
Parijat Sengupta, Samarth Agarwal

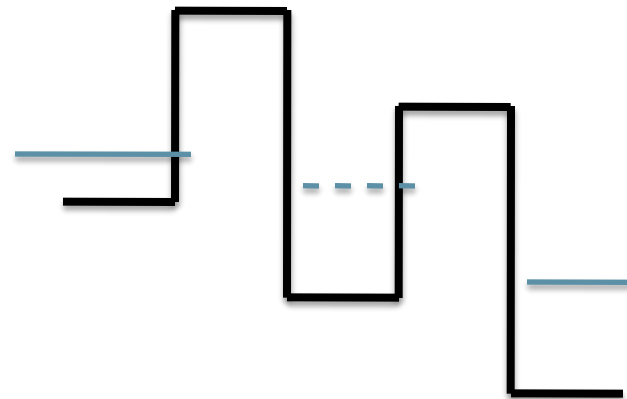
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Transfer Matrix (TM) Approach Application Targets

- TM can compute quantum transmission in electronic devices
 - » Super lattice structure

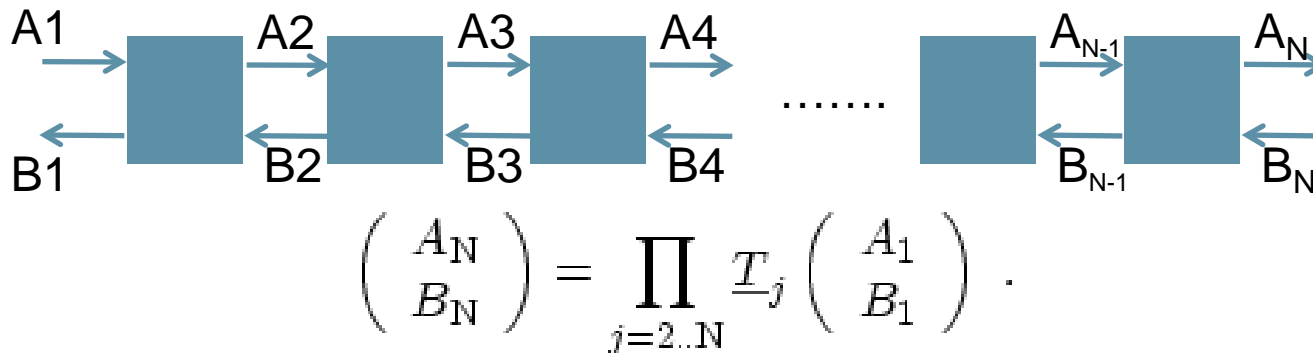
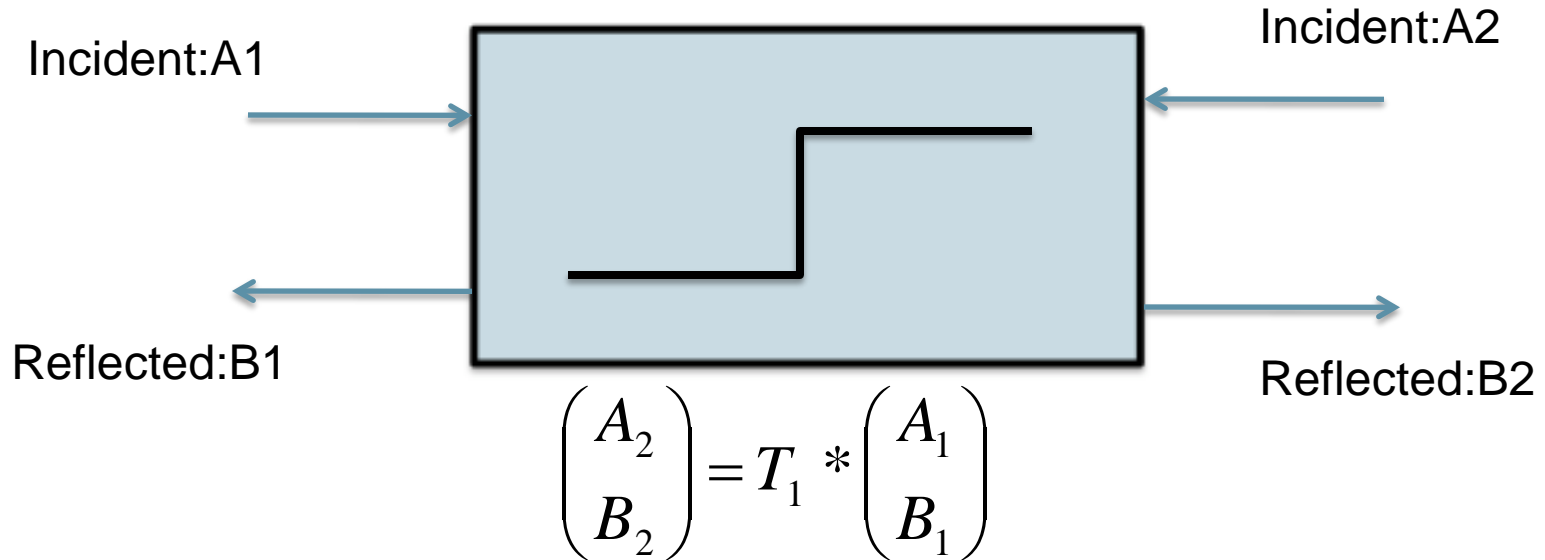


- » Resonant Tunneling Diode



- TM is conceptually simple
- **TM has severe numerical limitations**

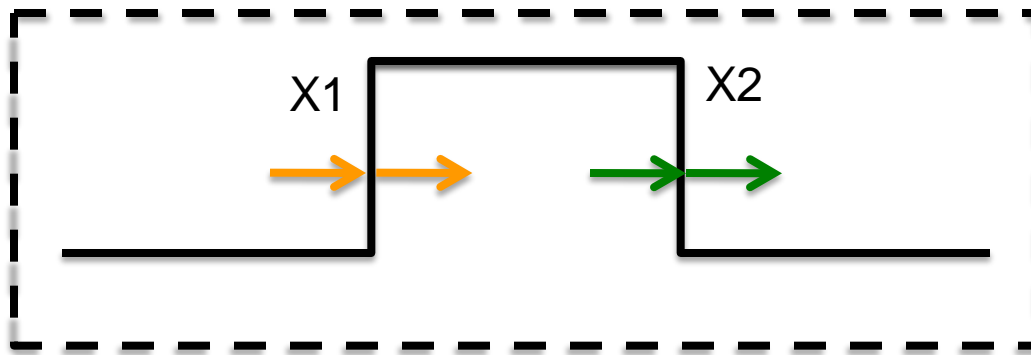
TM Principles



Wave functions and derivatives are matched at each interface

Layering of a device

A slice of a device after division is shown

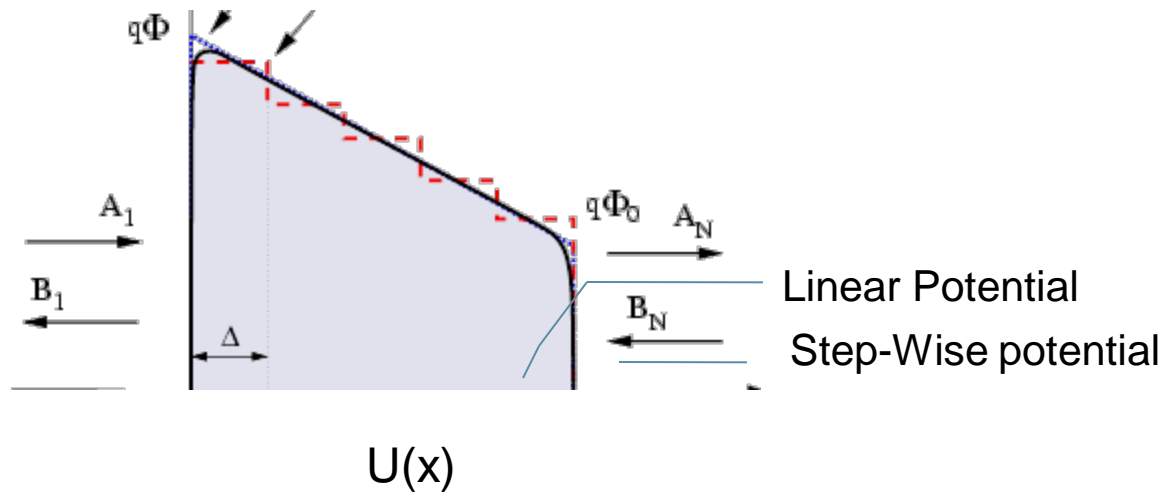


One set of conditions for each interface

Incoming wave and outgoing waves at edge X1 and X2 are matched

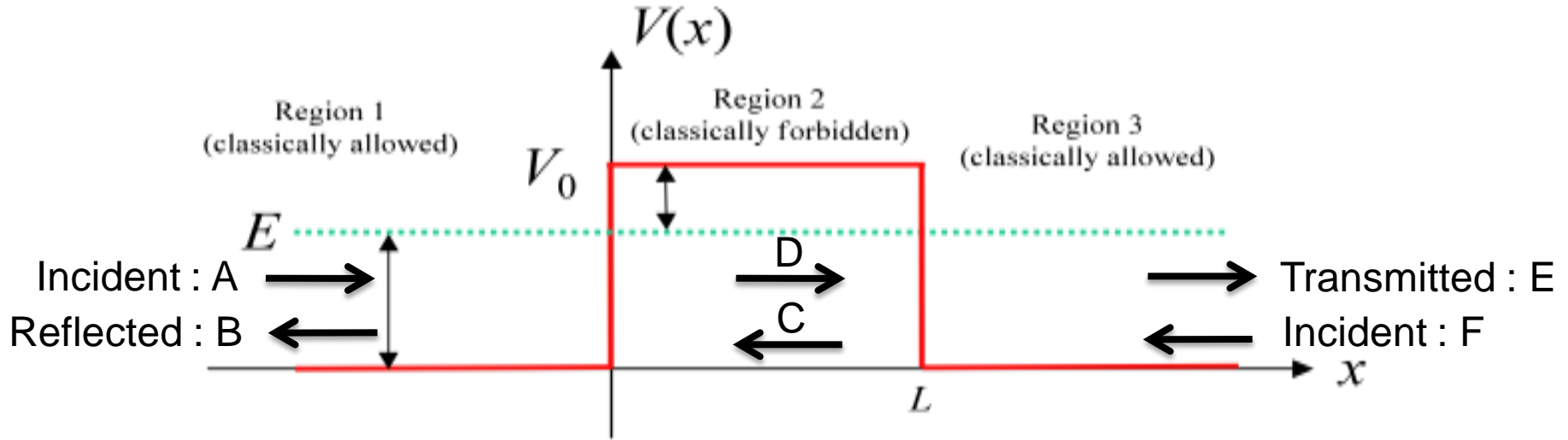
Device is split in to several such layers to give a chain-like topology

Step-Wise potential Approximation



- Transfer Matrix is “easy” for constant potentials
- Linear potentials may be approximated through linear steps
=> may need to have many steps for extended devices
=> implies many transfer matrix multiplications

Numerical Approach



Wave-function each region,

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx}$$

$$\psi_2(x) = Ce^{-\gamma x} + De^{\gamma x}$$

$$\psi_3(x) = Ee^{ikx} + Fe^{-ikx}$$

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad \gamma = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Boundary Conditions

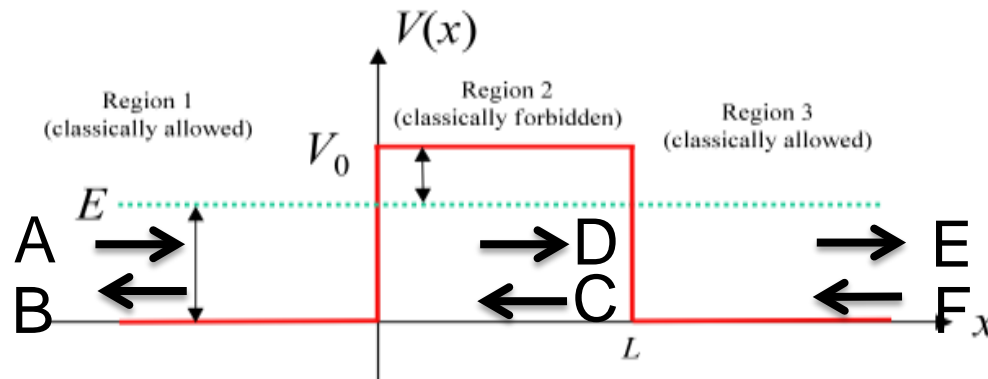
Applying boundary conditions at each interface $x=0$ and $x=L$ gives the following

$$\psi_1(0) = \psi_2(0) \rightarrow A + B = C + D$$

$$\psi_1'(0) = \psi_2'(0) \rightarrow ik(A - B) = -\gamma(C - D)$$

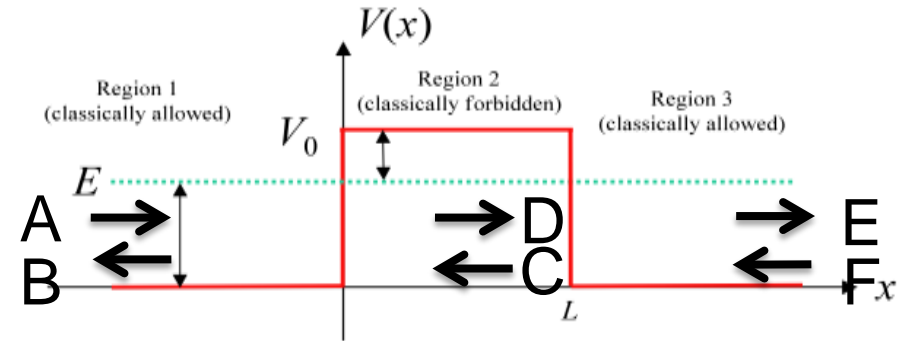
$$\psi_2(L) = \psi_3(L) \rightarrow Ce^{-\gamma L} + De^{\gamma L} = Ee^{ikL} + Fe^{-ikL}$$

$$\psi_2'(L) = \psi_3'(L) \rightarrow -\gamma(Ce^{-\gamma L} - De^{\gamma L}) = ik(Ee^{ikL} - Fe^{-ikL})$$



Complete Transfer Matrix

Complete transfer matrix is given as product of the interface matrices



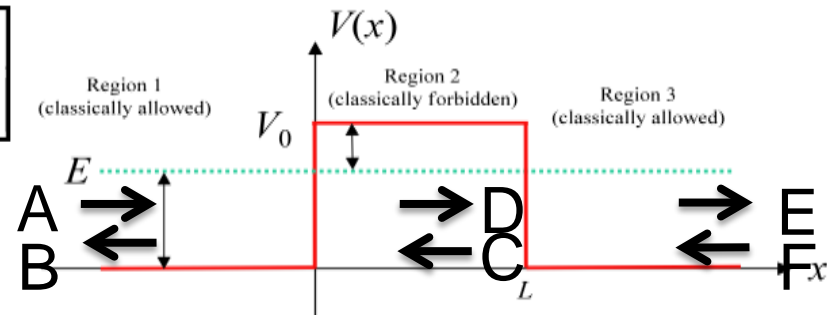
$$\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \left(1 + i \frac{\gamma}{k} \right) & \frac{1}{2} \left(1 - i \frac{\gamma}{k} \right) \\ \frac{1}{2} \left(1 - i \frac{\gamma}{k} \right) & \frac{1}{2} \left(1 + i \frac{\gamma}{k} \right) \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = M_1 \begin{bmatrix} C \\ D \end{bmatrix}$$

$$\begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \left(1 - i \frac{k}{\gamma} \right) e^{(ik+\gamma)L} & \frac{1}{2} \left(1 + i \frac{k}{\gamma} \right) e^{-(ik-\gamma)L} \\ \frac{1}{2} \left(1 + i \frac{k}{\gamma} \right) e^{(ik-\gamma)L} & \frac{1}{2} \left(1 - i \frac{k}{\gamma} \right) e^{-(ik+\gamma)L} \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix} = M_2 \begin{bmatrix} E \\ F \end{bmatrix}$$

Results with TMM

- The complete transfer matrix

$$\begin{bmatrix} A \\ B \end{bmatrix} = M_1 \begin{bmatrix} C \\ D \end{bmatrix} = M_1 M_2 \begin{bmatrix} E \\ F \end{bmatrix} = M \begin{bmatrix} E \\ F \end{bmatrix}$$



- In general for any intermediate set of layers, the TMM is expressed as:

$$\begin{pmatrix} A_{n-1}^+ \\ A_{n-1}^- \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} A_n^+ \\ A_n^- \end{pmatrix}$$

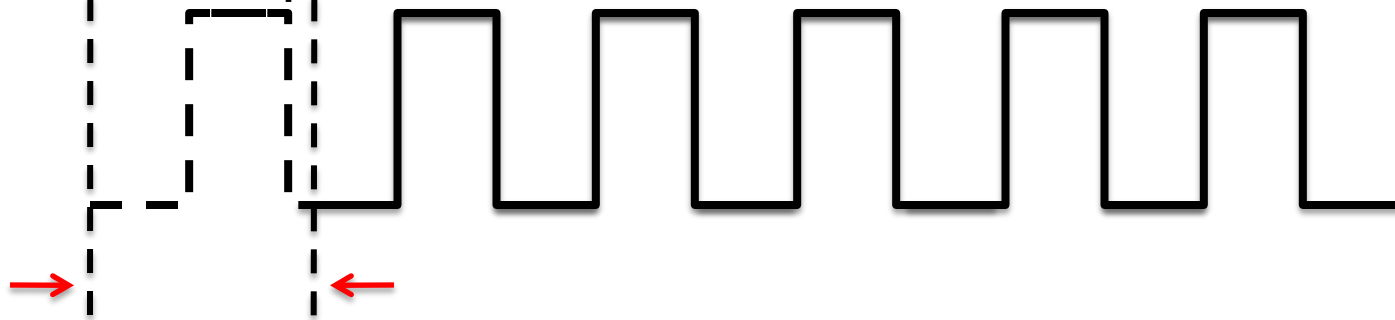
- For multiple layers the overall transfer matrix will be

$$\begin{pmatrix} A_N \\ B_N \end{pmatrix} = \prod_{j=2..N} \underline{T}_j \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} .$$

- Looks conceptually very simple and analytically pleasing

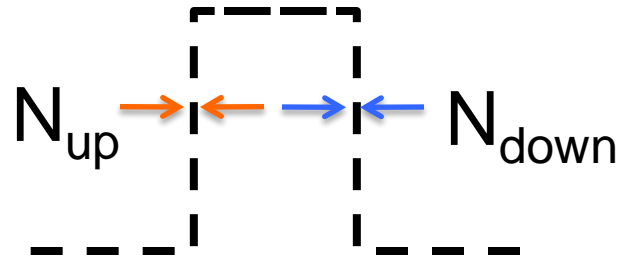
Numerical Validity of TMM

Consider a super lattice:



Repeating structure

One repeating unit:



N_{up} or N_{down} : Transfer matrix at interface.

Both contain evanescent and propagating states

Numerical instability in interface matrices

N_{down} has the form:

$e^{\gamma L}$: Large for increasing L

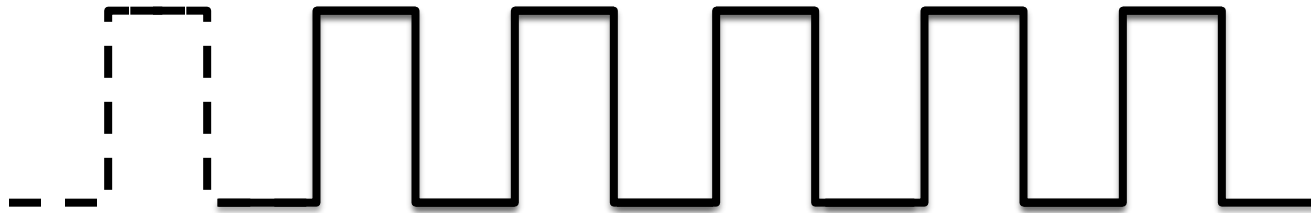
$$\begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \left(1 - i \frac{k}{\gamma} \right) e^{(ik+\gamma)L} & \frac{1}{2} \left(1 + i \frac{k}{\gamma} \right) e^{-(ik-\gamma)L} \\ \frac{1}{2} \left(1 + i \frac{k}{\gamma} \right) e^{(ik-\gamma)L} & \frac{1}{2} \left(1 - i \frac{k}{\gamma} \right) e^{-(ik+\gamma)L} \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix} = M_2 \begin{bmatrix} E \\ F \end{bmatrix}$$

$e^{-\gamma L}$: Diminishing for increasing L

N_{up} : Similar structure, beset with the same problem

Loss in Accuracy

$$N_{\text{down}} = \begin{bmatrix} \textit{Big} & \textit{Big} \\ \textit{Small} & \textit{Small} \end{bmatrix} \quad N_{\text{up}} = \begin{bmatrix} \textit{Small} & \textit{Big} \\ \textit{Small} & \textit{Big} \end{bmatrix}$$

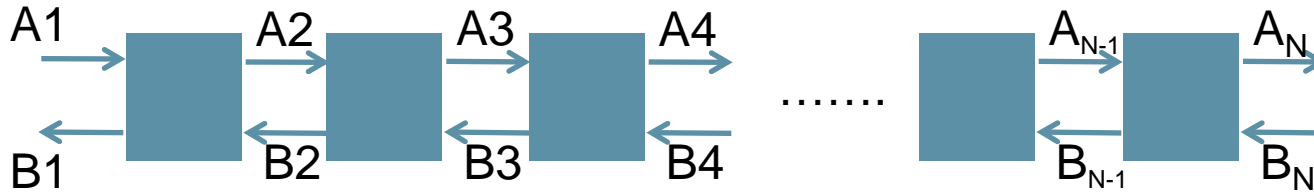


Continued product: $(N_{\text{up}})^*(N_{\text{down}})^*(N_{\text{up}})^*(N_{\text{down}})^*(N_{\text{up}})^*(N_{\text{down}})^* \dots$

- Elements span several orders of magnitude.
- Multiple multiplications and additions of (small*small), (small*big), (big*big)
- Machine precision limits accuracy.
- Repeated multiplication of such matrices give widely discrepant results.

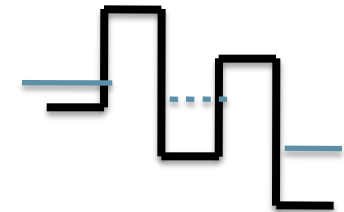
Key Summary

- Transfer Matrix Method appears analytically as very appealing



$$\begin{pmatrix} A_N \\ B_N \end{pmatrix} = \prod_{j=2..N} \underline{T}_j \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} .$$

- Any heterostructure can be cascaded



- Transfer matrix is numerically unstable
 - » realistic heterostructures with significant band bending
 - » large number of basis sets