Open 1d Systems: The Transfer Matrix Method

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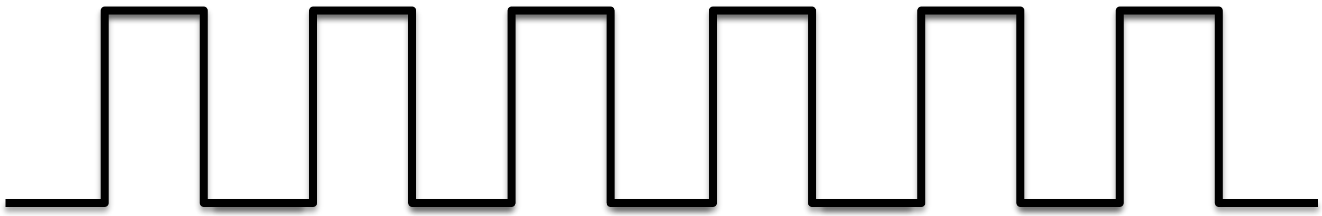
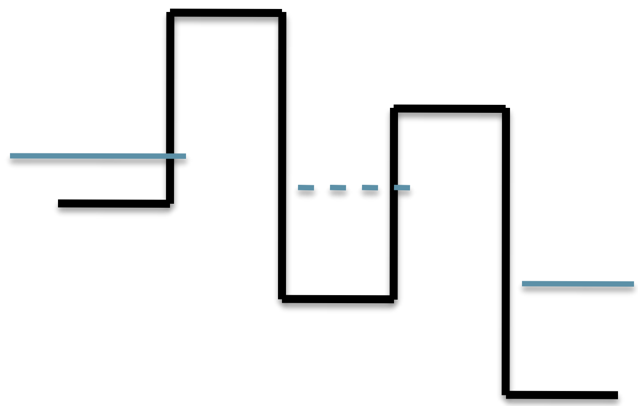
Transfer Matrix (TM) Approach Application Targets

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

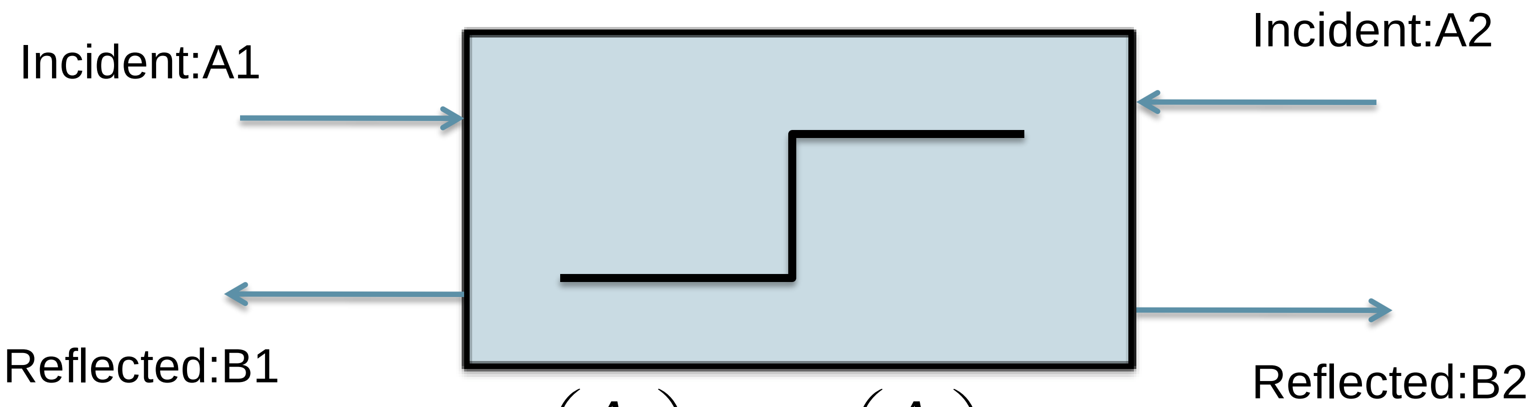


  - » Resonant Tunneling Diode

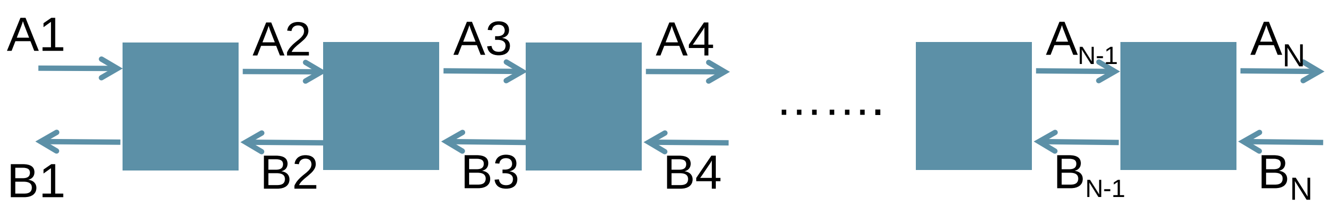


- TM is conceptually simple
- **TM has severe numerical limitations**

TM Principles



$$\begin{pmatrix}A_2\\B_2\end{pmatrix} = T_1 * \begin{pmatrix}A_1\\B_1\end{pmatrix}$$

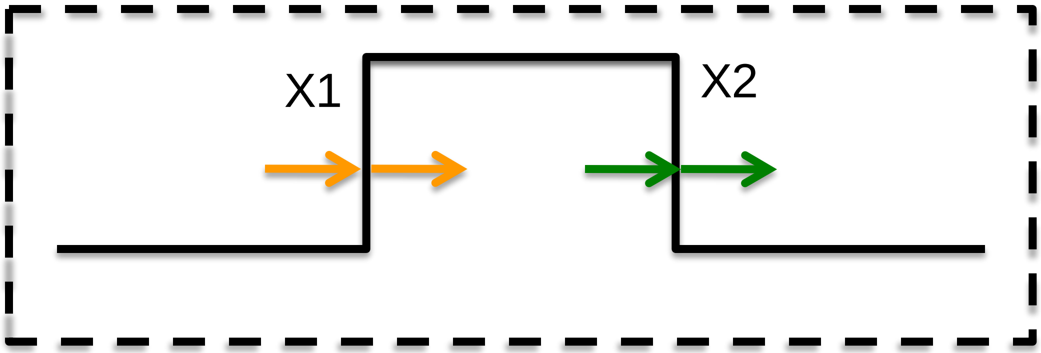


$$\begin{pmatrix}A_N\\B_N\end{pmatrix} = \prod_{j=2..N} T_j \begin{pmatrix}A_1\\B_1\end{pmatrix} .$$

Wave functions and derivatives are matched at each interface

Layering of a device

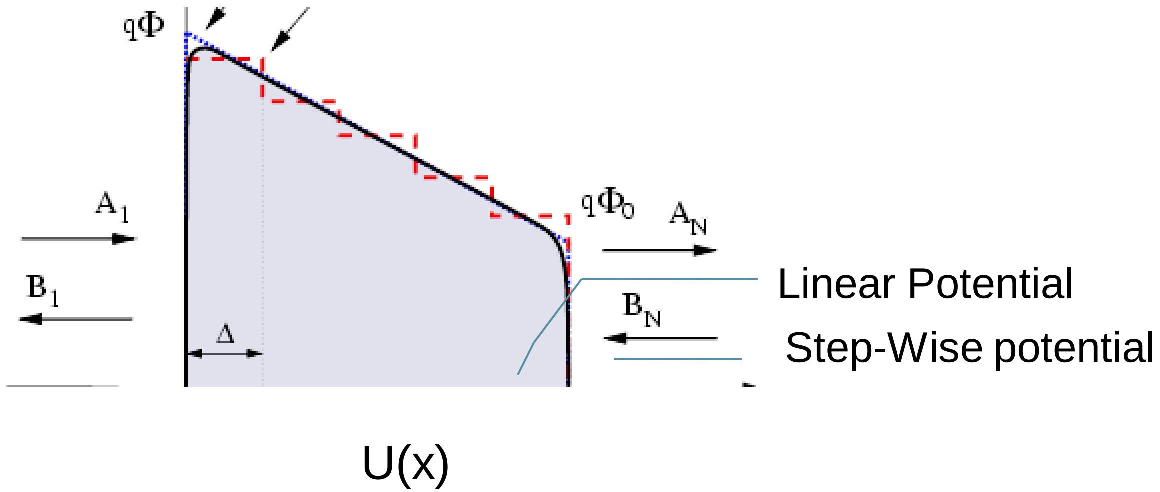
A slice of a device after division is shown



One set of conditions for each interface

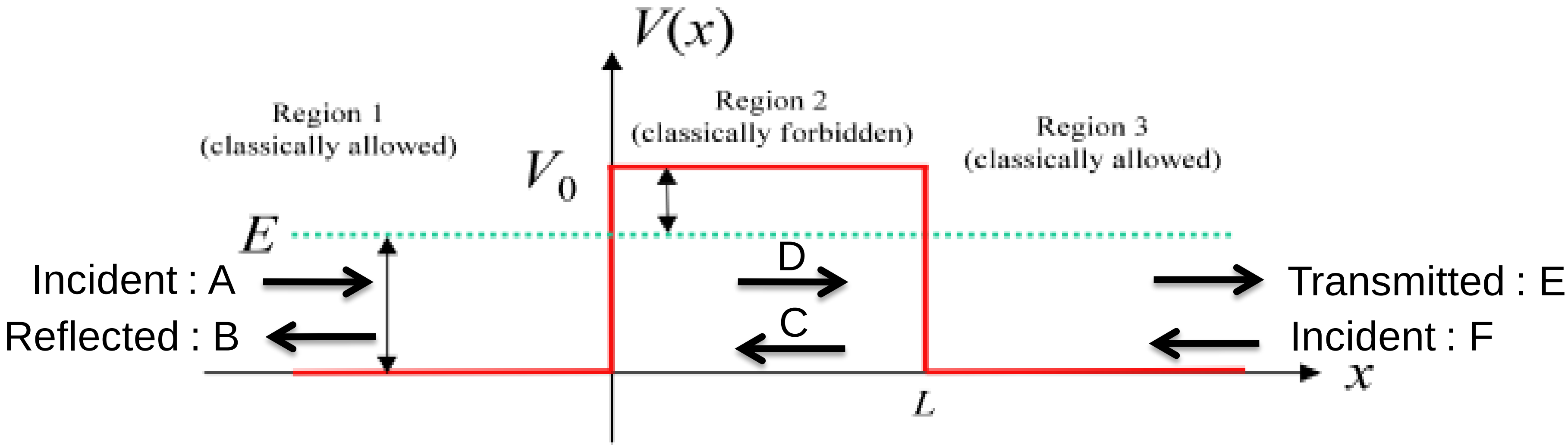
- Incoming wave and outgoing waves at edge X1 and X2 are matched
- Device is split in to several such layers to give a chain-like topology

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,

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

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

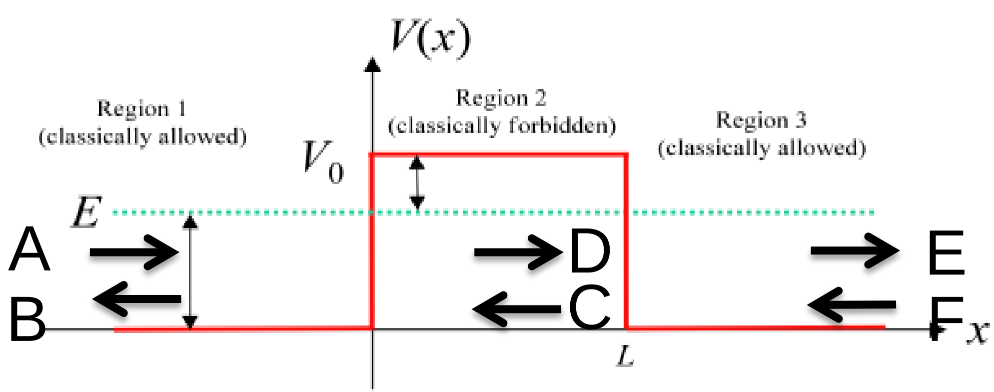
$$\psi_3(x) = Ee^{ikx} + Fe^{-ikx}$$

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

Boundary Conditions

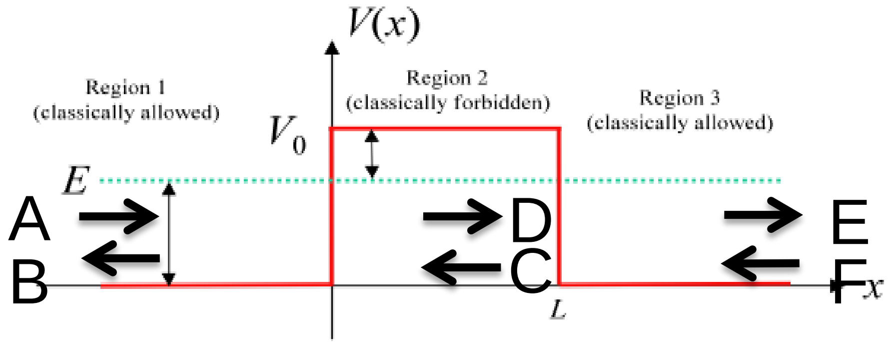
Applying boundary conditions at each interface x=0 and x=L gives the following

$$\psi_1(0)=\psi_2(0) \quad\rightarrow\quad A+B=C+D$$
$$\psi_1'(0)=\psi_2'(0) \quad\rightarrow\quad ik(A-B)=-\gamma(C-D)$$
$$\psi_2(L)=\psi_3(L) \quad\rightarrow\quad Ce^{-\gamma L}+De^{\gamma L}=Ee^{ikL}+Fe^{-ikL}$$
$$\psi_2'(L)=\psi_3'(L) \quad\rightarrow\quad -\gamma\left(Ce^{-\gamma L}-De^{\gamma L}\right)=ik\left(Ee^{ikL}-Fe^{-ikL}\right)$$



Complete Transfer Matrix

Complete transfer matrix is given as product of the interface matrices



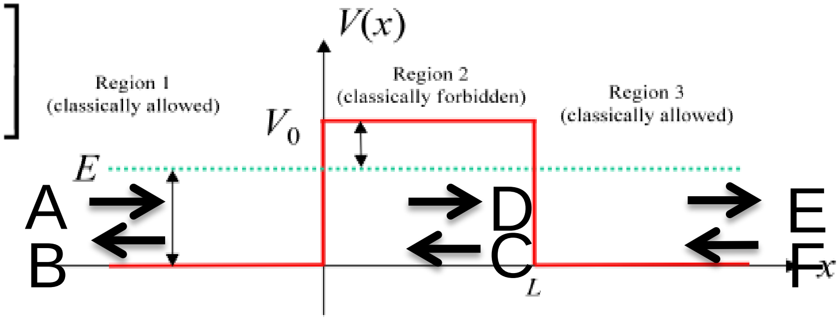
$$\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} \frac{1}{2}\left(1 + i\frac{\gamma}{k}\right) & \frac{1}{2}\left(1 - i\frac{\gamma}{k}\right) \\ \frac{1}{2}\left(1 - i\frac{\gamma}{k}\right) & \frac{1}{2}\left(1 + i\frac{\gamma}{k}\right) \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} =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

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

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:

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

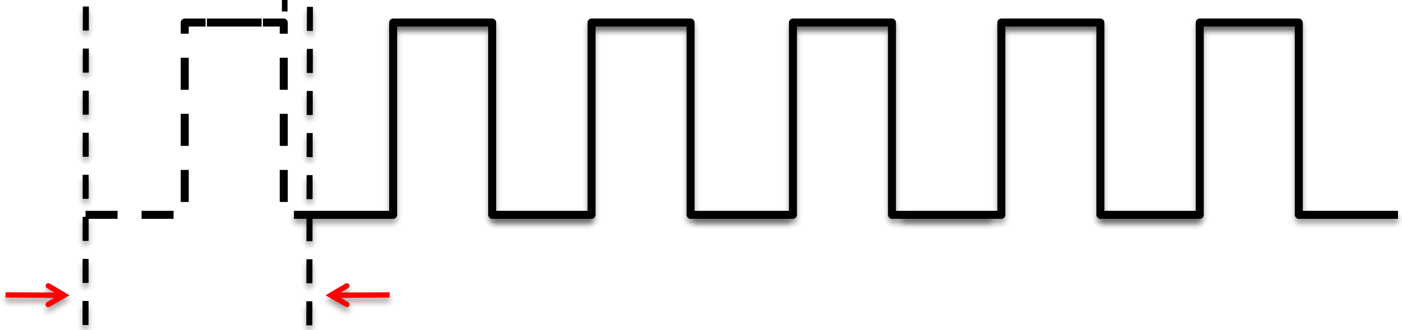
- For multiple layers the overall transfer matrix will be

$$\begin{pmatrix} A_{\mathrm{N}} \\ B_{\mathrm{N}} \end{pmatrix} = \prod_{j=2..\mathrm{N}} \underline{T}_j \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} .$$

- Looks conceptually very simple and analytically pleasing

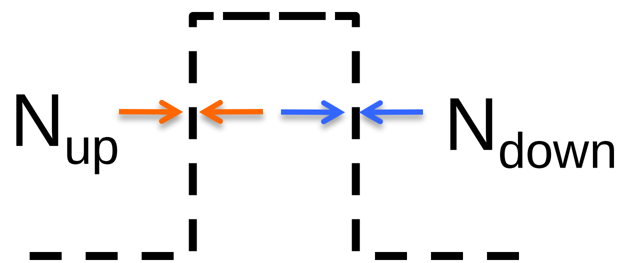
Numerical Validity of TMM

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

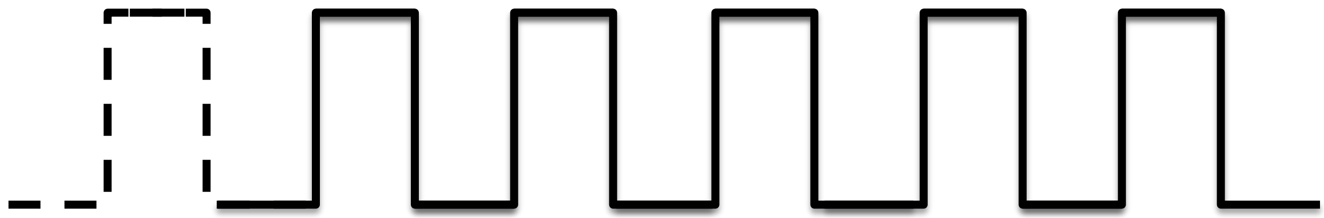
$$\begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} \frac{1}{2}\left(1 - i\frac{k}{\gamma}\right) e^{(ik+\gamma)L} & \frac{1}{2}\left(1 + i\frac{k}{\gamma}\right) e^{-(ik-\gamma)L} \\ \frac{1}{2}\left(1 + i\frac{k}{\gamma}\right) e^{(ik-\gamma)L} & \frac{1}{2}\left(1 - i\frac{k}{\gamma}\right) e^{-(ik+\gamma)L}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

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

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

Loss in Accuracy

$$N_{down} = \begin{bmatrix} Big & Big \\ Small & Small \end{bmatrix} \qquad N_{up} = \begin{bmatrix} Small & Big \\ Small & Big \end{bmatrix}$$

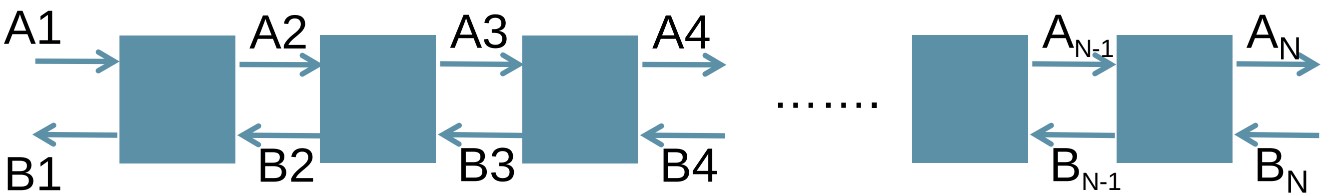


Continued product: $(N_{up})*(N_{down})*(N_{up})*(N_{down})*(N_{up})*(N_{down})*\ldots$

- 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.

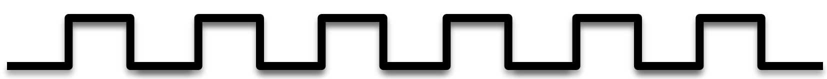
Key Summary

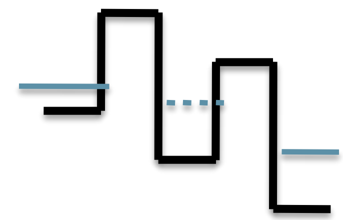
- Transfer Matrix Method appears analytically as very appealing



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

- Any heterostructure can be cascaded





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