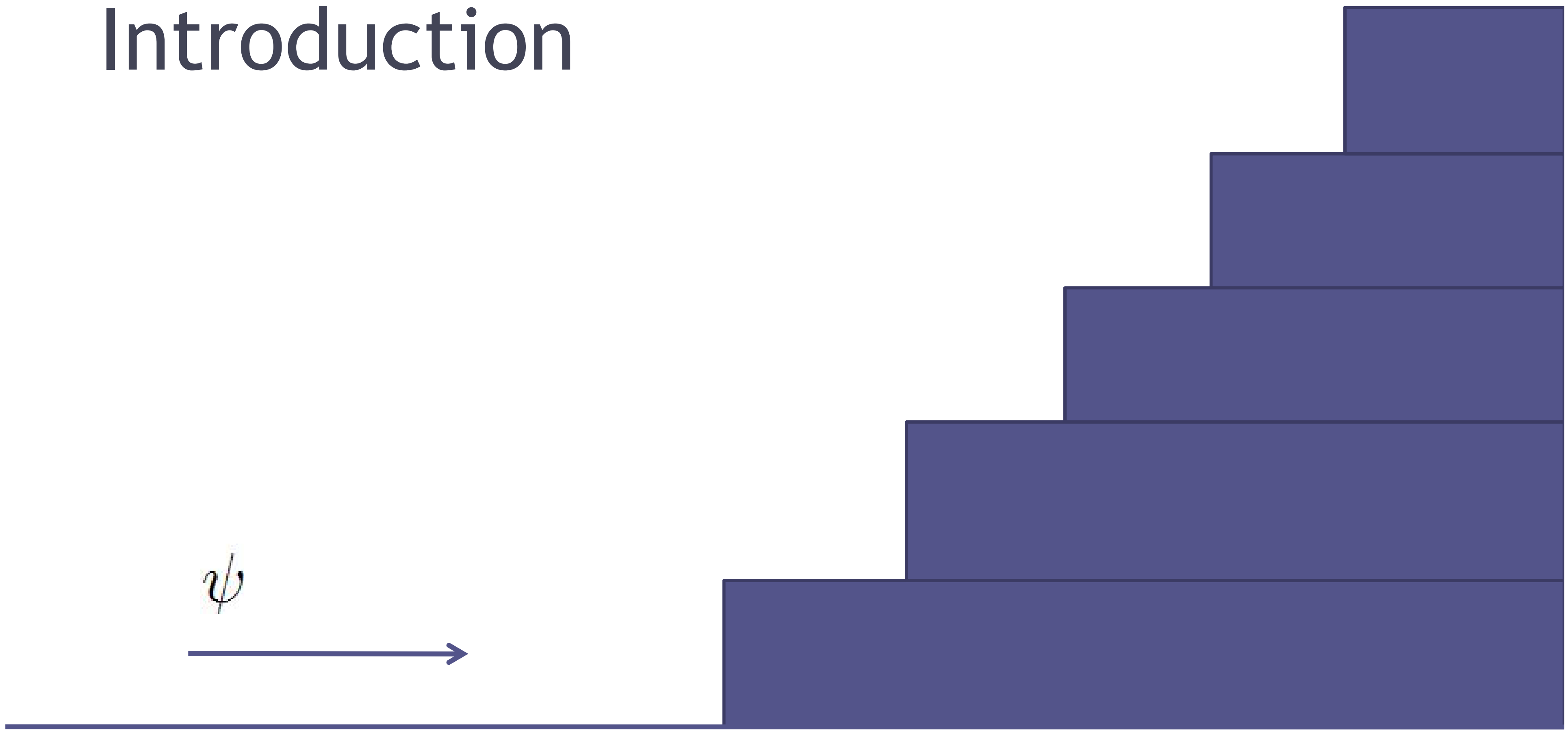
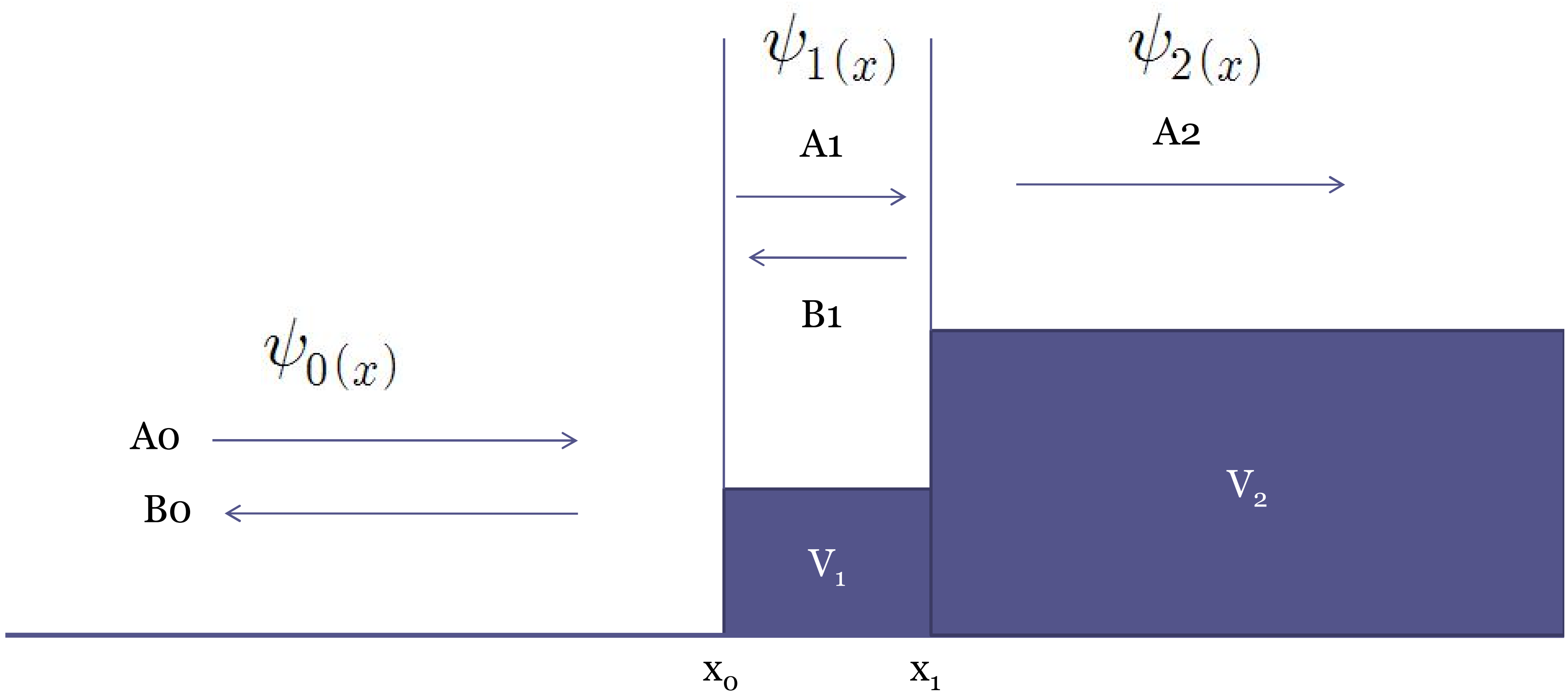
Transfer Matrix Approach for the 1-dim Schrödinger equation

Introduction



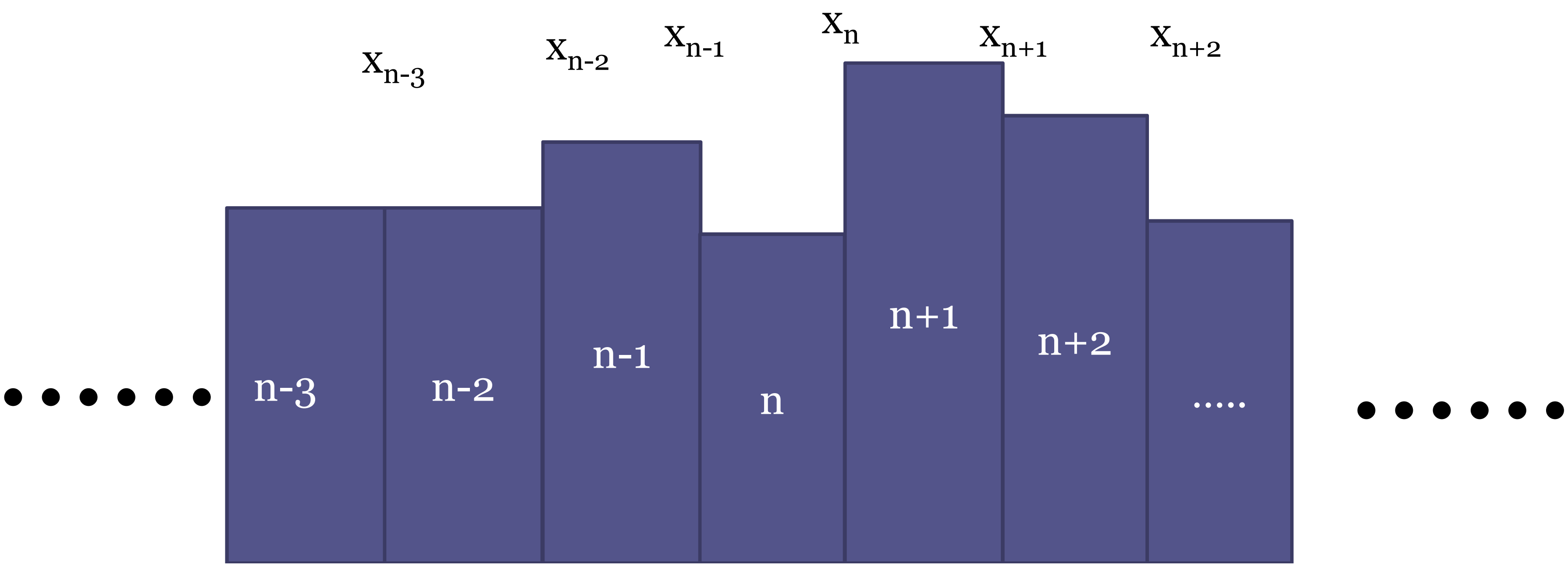
Dividing Regions



$$\begin{bmatrix} \psi_0(x_0) \\ \psi'_0(x_0) \end{bmatrix} = \begin{bmatrix} \psi_1(x_0) \\ \psi'_1(x_0) \end{bmatrix} \qquad \begin{bmatrix} \psi_1(x_1) \\ \psi'_1(x_1) \end{bmatrix} = \begin{bmatrix} \psi_2(x_2) \\ \psi'_2(x_2) \end{bmatrix}$$

Boundary Condition

$$\begin{bmatrix} \psi_n(x_n) \\ \psi'_n(x_n) \end{bmatrix} = \begin{bmatrix} \psi_{n+1}(x_n) \\ \psi'_{n+1}(x_n) \end{bmatrix}$$



Time-Independent 1-dim Shcrödinger Equation

$$[\frac{\hat{p}^2}{2m} + V]\psi(x) = E\psi(x)$$

(V is constant)

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

$$\frac{d\psi(x)}{dx} = ikAe^{ikx} - ikBe^{-ikx}$$

$$k = \sqrt{E - V}$$

$$\begin{bmatrix} \psi(x) \\ \psi'(x) \end{bmatrix} = \begin{bmatrix} e^{ikx} & e^{-ikx} \\ ke^{ikx} & -ke^{-ikx} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix}$$

Transfer Matrix

$$\begin{bmatrix} \psi_n(x_n) \\ \psi'_n(x_n) \end{bmatrix} = \begin{bmatrix} \psi_{n+1}(x_n) \\ \psi'_{n+1}(x_n) \end{bmatrix}$$

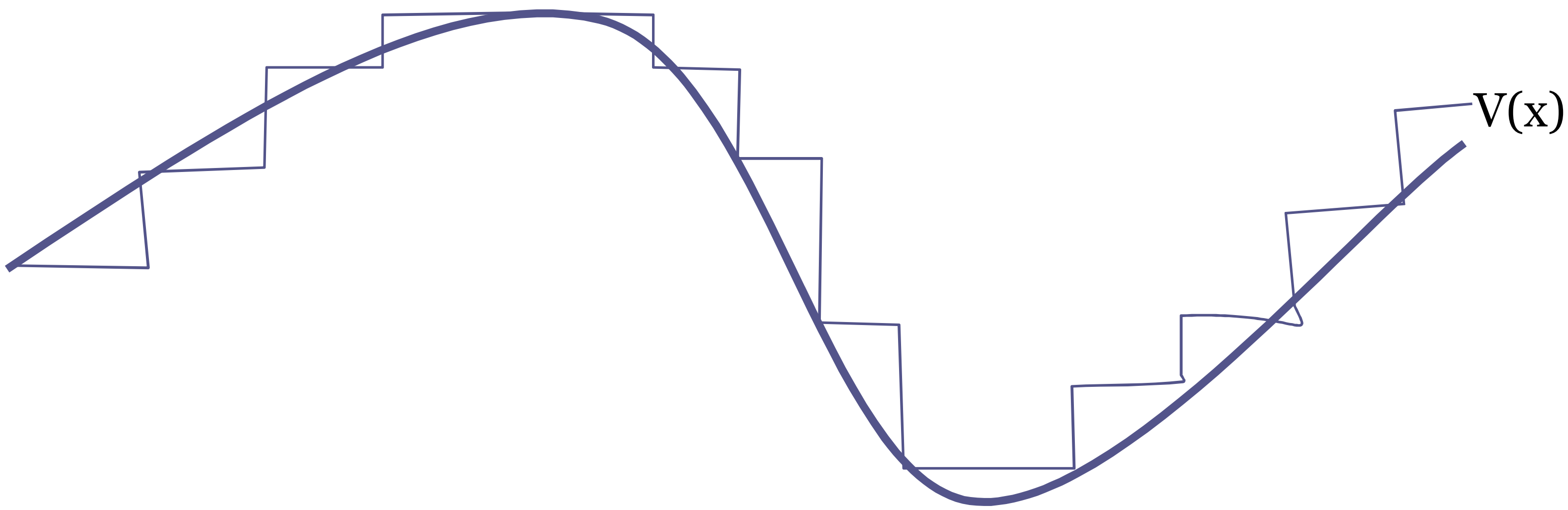
$$\begin{bmatrix} \psi(x_n) \\ \psi'(x_n) \end{bmatrix} = \begin{bmatrix} e^{ik_n x_n} & e^{-ik_n x_n} \\ ik_n e^{ik_n x_n} & -ik_n e^{-ik_n x_n} \end{bmatrix} \begin{bmatrix} A_n \\ B_n \end{bmatrix} = \begin{bmatrix} e^{ik_{n+1} x_n} & e^{-ik_{n+1} x_n} \\ ik_{n+1} e^{ik_{n+1} x_n} & -ik_{n+1} e^{-ik_{n+1} x_n} \end{bmatrix} \begin{bmatrix} A_{n+1} \\ B_{n+1} \end{bmatrix}$$

$$\begin{bmatrix} A_{n+1} \\ B_{n+1} \end{bmatrix} = \begin{bmatrix} \frac{k_{n+1}+k_n}{2k_{n+1}} e^{i(k_n-k_{n+1})x_n} & \frac{k_{n+1}-k_n}{2k_{n+1}} e^{i(-k_n-k_{n+1})x_n} \\ \frac{k_{n+1}-k_n}{2k_{n+1}} e^{i(k_n+k_{n+1})x_n} & \frac{k_{n+1}+k_n}{2k_{n+1}} e^{i(-k_n+k_{n+1})x_n} \end{bmatrix} \begin{bmatrix} A_n \\ B_n \end{bmatrix}$$

$$\begin{bmatrix} A_{n+1} \\ B_{n+1} \end{bmatrix} = M_{n+1,n} \begin{bmatrix} A_n \\ B_n \end{bmatrix}$$

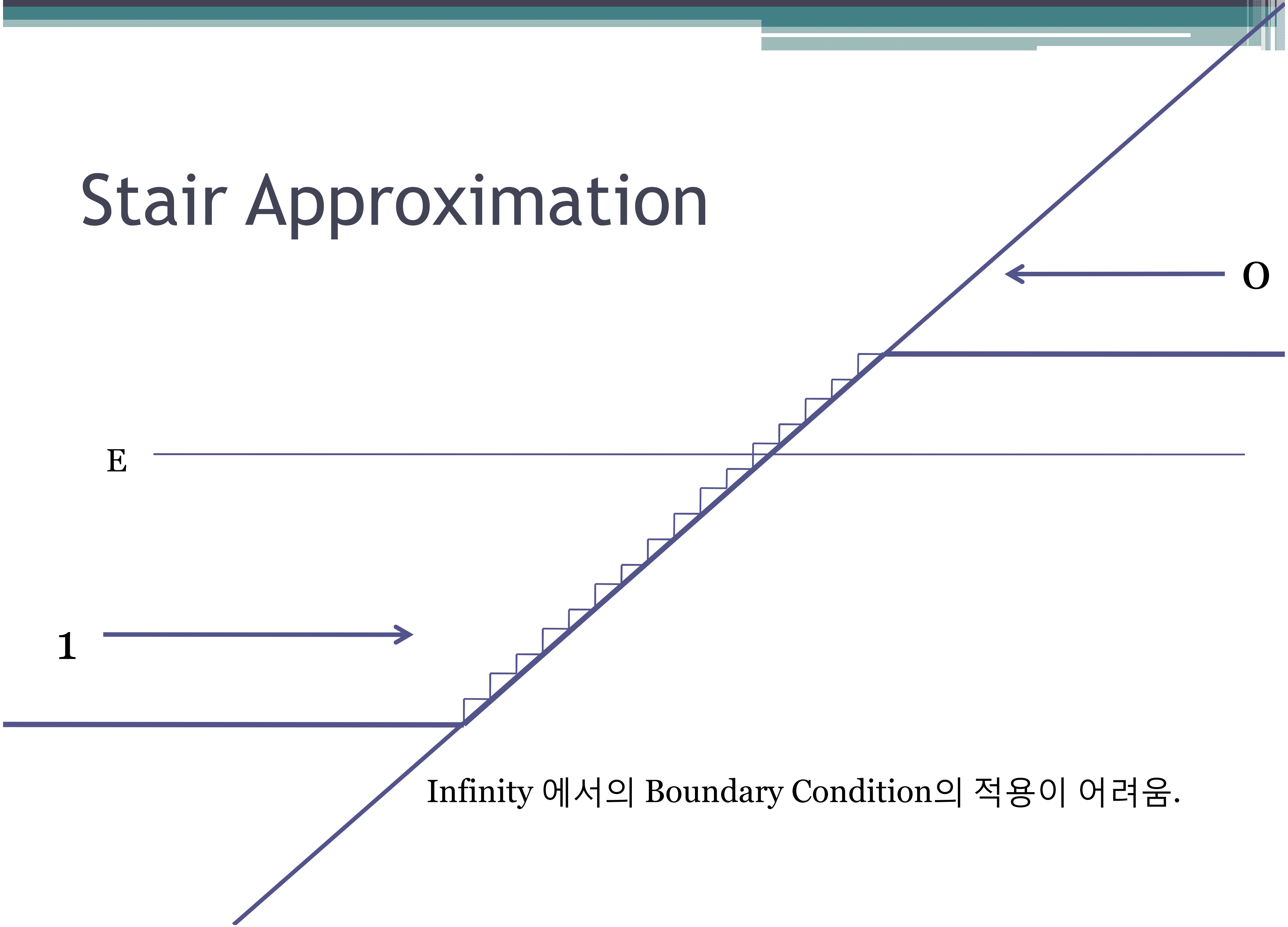
Application

$$\begin{bmatrix} A_n \\ B_n \end{bmatrix} = M_{n,n-1} M_{n-1,n-2} \ldots\ldots M_{4,3} M_{3,2} M_{2,1} M_{1,0} \begin{bmatrix} A_0 \\ B_0 \end{bmatrix}$$



Can it be universal?

Stair Approximation



Infinity 에서의 Boundary Condition의 적용이 어려움.

Note that, $M_{n+1,n}^{-1} = M_{n,n+1}$

$$\begin{bmatrix} A_n \\ B_n \end{bmatrix} = M_{n,n-1} M_{n-1,n-2} \cdots\cdots M_{4,3} M_{3,2} M_{2,1} M_{1,0} \begin{bmatrix} A_0 \\ B_0 \end{bmatrix}$$

E가 V(x) 보다 작아지기 시작하는 점에서는

$$k = \sqrt{E - V} = i\kappa$$

$$\psi(x) = Ae^{-\kappa x} + Be^{+\kappa x}$$

발산하는 두번째 항은 nonphysical , zero

이때가 n=N일 때라 하면

$$\begin{bmatrix} A_N \\ B_N \end{bmatrix} = M_{N,N-1} M_{N-1,N-2} \cdots\cdots M_{4,3} M_{3,2} M_{2,1} M_{1,0} \begin{bmatrix} A_0 \\ B_0 \end{bmatrix}$$

$$\begin{bmatrix} A_N \\ B_N \end{bmatrix} = \begin{bmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{bmatrix} \begin{bmatrix} A_0 \\ B_0 \end{bmatrix}$$

왼쪽에서 오른쪽으로 지속적으로 펄스가 공급되는 경우를
Infinity 에서의 Boundary Condition으로 정하면

$$\begin{bmatrix} T \\ 0 \end{bmatrix} = \begin{bmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{bmatrix} \begin{bmatrix} 1 \\ R \end{bmatrix}$$

$$R = -\frac{q_{21}}{q_{22}} \qquad T = q_{11} - q_{12} \frac{q_{21}}{q_{22}}$$

$$\begin{bmatrix} A_n \\ B_n \end{bmatrix} = M_{n,n-1} M_{n-1,n-2} \cdots\cdots M_{4,3} M_{3,2} M_{2,1} M_{1,0} \begin{bmatrix} 1 \\ -\dfrac{q_{21}}{q_{22}} \end{bmatrix}$$

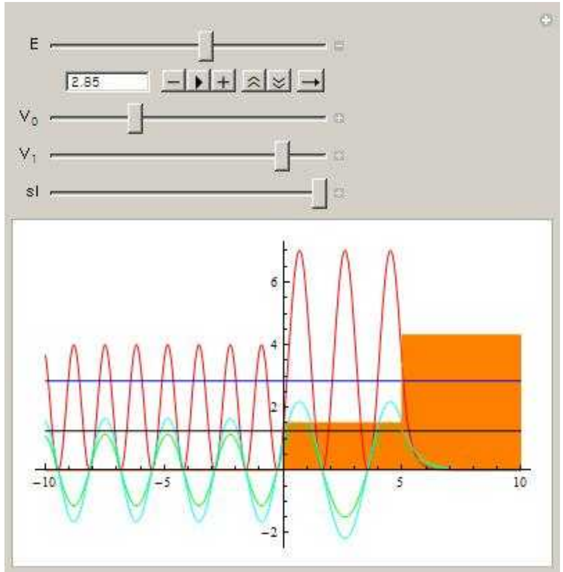
두 개의 step이 있는 경우

- 윗 계단에서의 amplitude가 아랫 계단에서의 amplitude보다 항상 크거나 같다.

- 실수부와 허수부의 진폭은 다르나 위상은 같다.

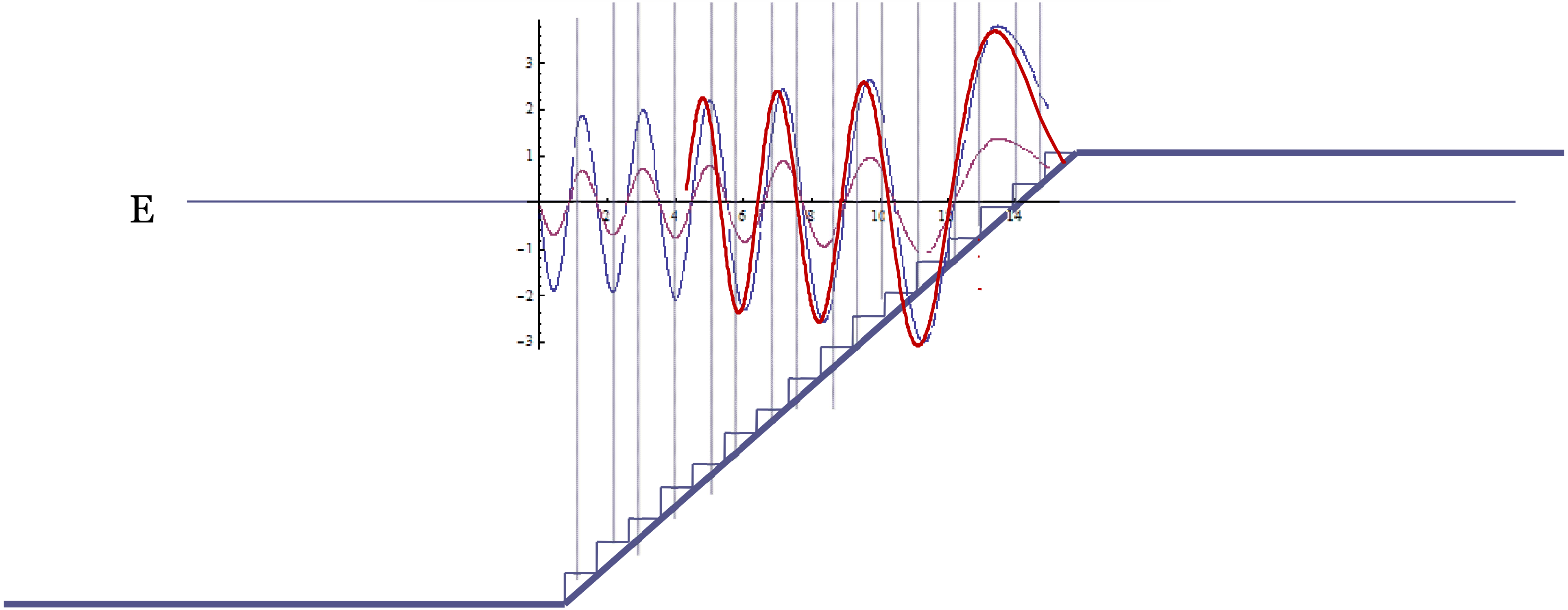
-> Standing Wave

$$(a+bi)\cos(kx+\phi)$$

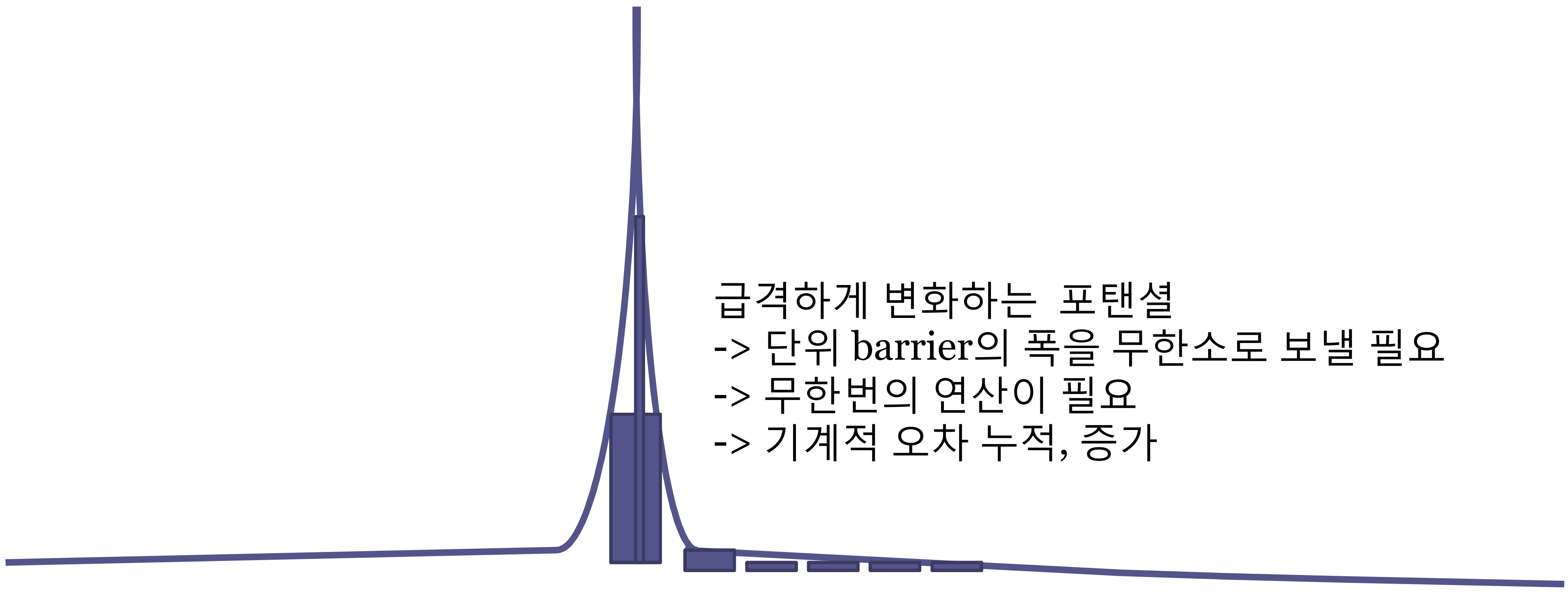


Numeric Result

$$\psi(x) = C_E M(x)\cos(k_x x + \phi_x)$$



Not suitable cases



Time-Dependent solution

- Eigenfunction :

standing wave, Time-independent solution 에서 진폭만 변한다.