PHOT 301: Quantum Photonics

LECTURE 12B

Michaël Barbier, Fall semester (2024-2025)

INTRODUCTION TO DIFFERENT APPROXIMATIONS

APPROXIMATIONS

	Method	Approximates?
1	Transfer matrix method	piece-wise constant $V(x)$
2	Finite basis method	limited ψ_n, E_n: Matrix-formalism
3	Finite difference method	discretizes wave function
4	Perturbation theory (stat.)	small perturbation known solutions
5	Time-dependent perturbation	small perturbation known solutions
6	Tight-binding approx.	electrons strongly bound (covalent)
7	Variational method	finding energy minima

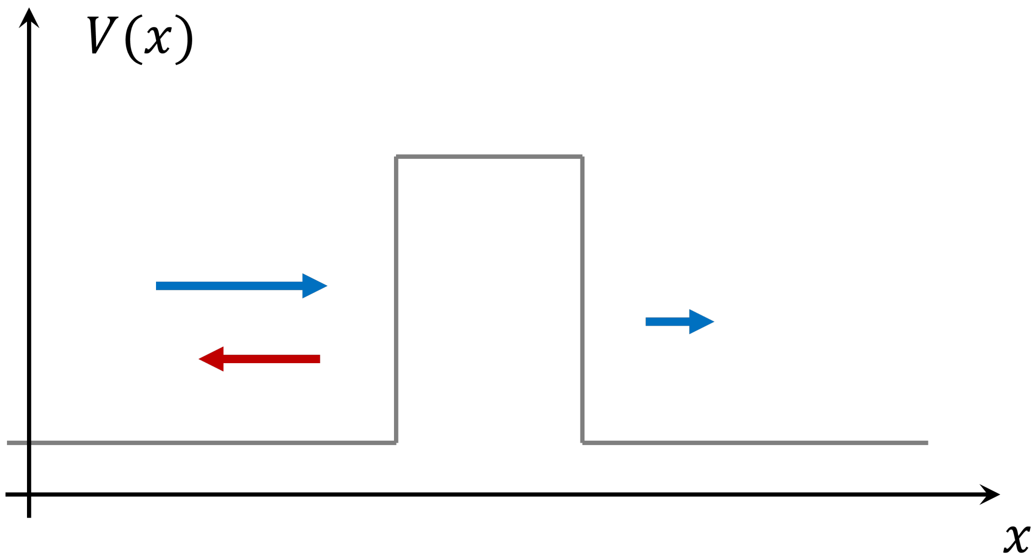
Usage of simple examples to compare over approximations

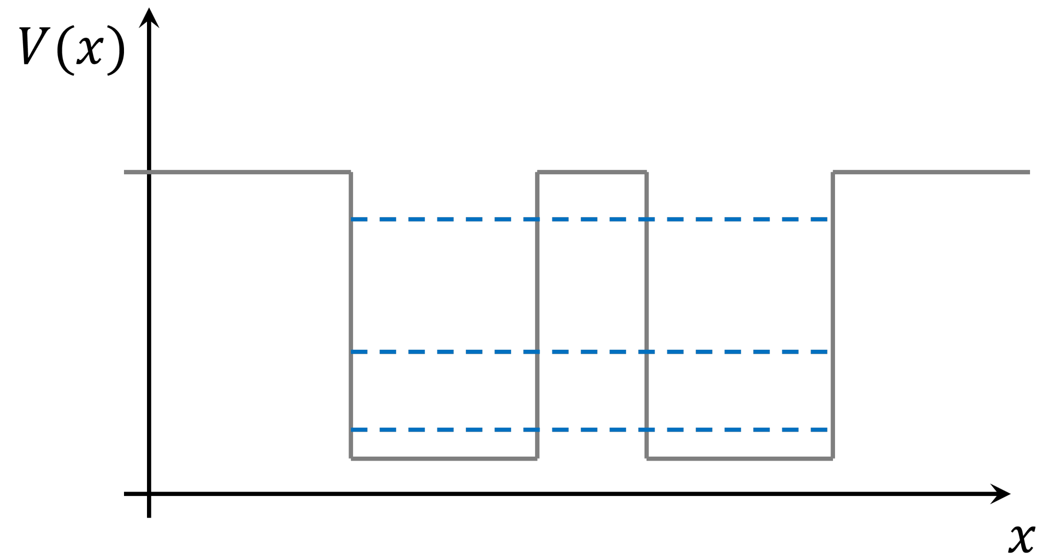
- Infinite square well with E-field (David Miller's book)
- Harmonic oscilator
- Transmission: Smoothed finite barrier

TRANSFER MATRIX METHOD IN 1D

INTRO: TRANSFER MATRIX METHOD

- For 1D potential energy functions $V(x)$ (here assume 1D systems)
- Approximation of potential energy $V(x)$ by piece-wise constant V_i
- Transmission or bound states





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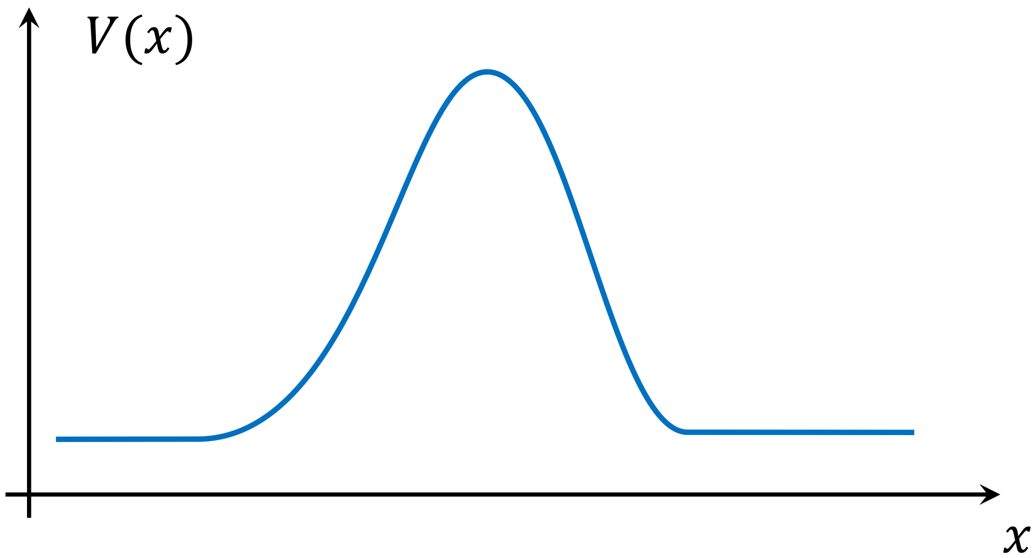

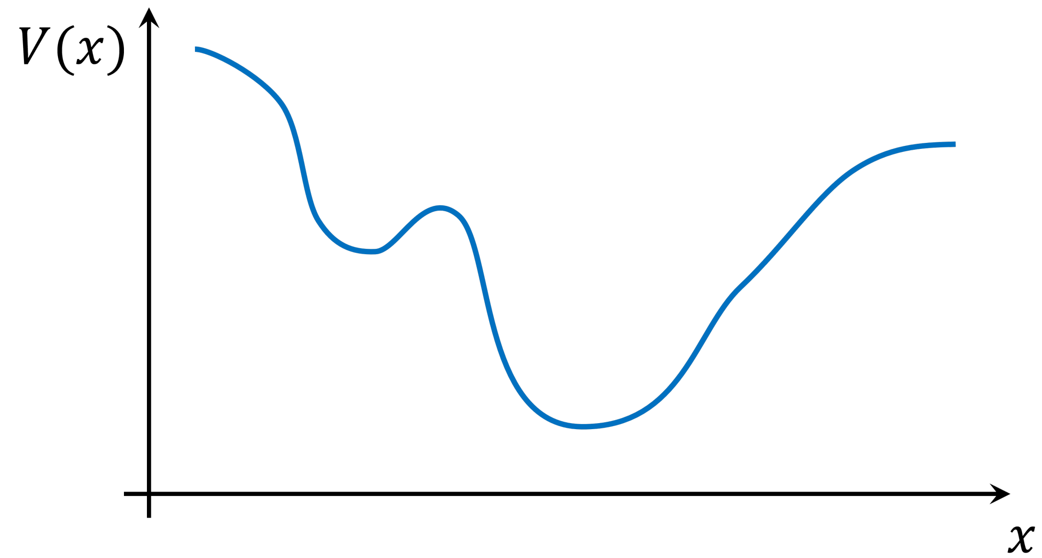

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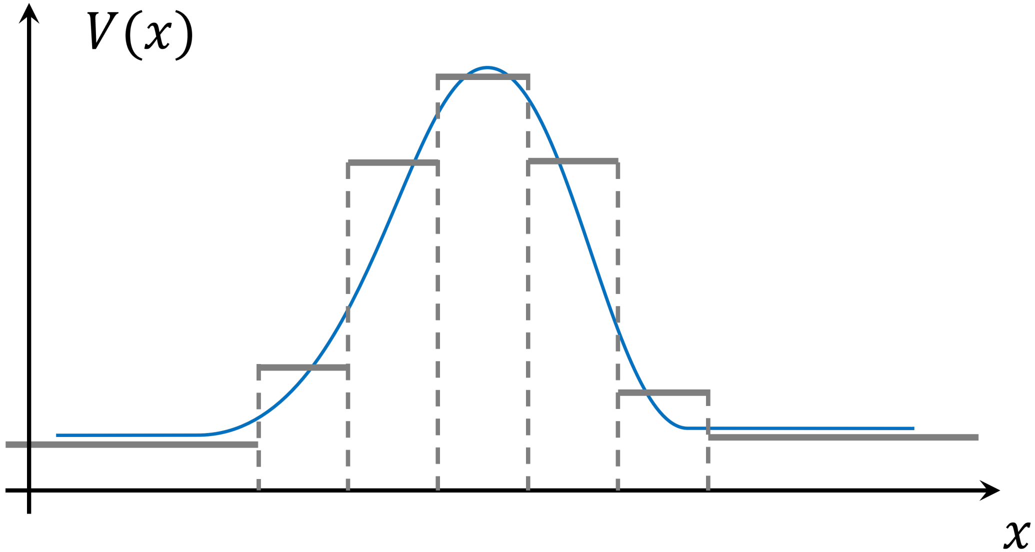

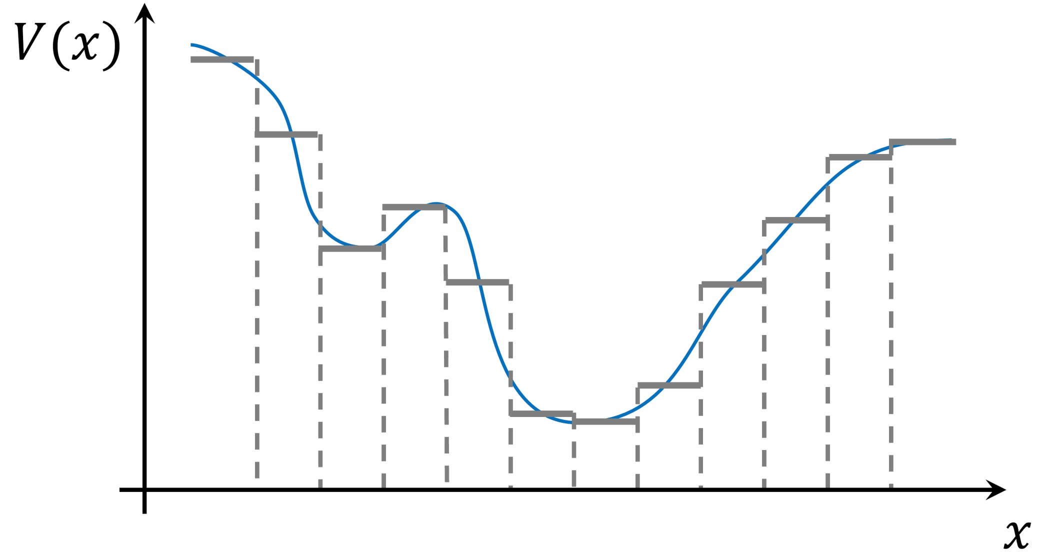

INTRO: TRANSFER MATRIX METHOD

- For 1D potential energy functions $V(x)$ (here assume 1D systems)
- Approximation of potential energy $V(x)$ by piece-wise constant V_i
- Schrodinger equation for constant $V(x) = V$

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2}(E - V)\psi(x)$$

- Solution depends on value of $E - V$:
- If energy is **larger than** the potential energy $E > V$, then we have propagating waves

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \qquad k^2 = \frac{2m}{\hbar^2}(E - V)$$

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- Solution depends on value of $E - V$:
- If energy is **less than** the potential $E < V$, then we have evanescent waves:

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x} \qquad \kappa^2 = \frac{2m}{\hbar^2}(V - E)$$

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$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2}(E - V)\psi(x)$$

- Solution depends on value of $E - V$:
- If energy is the **same** as the potential energy $E = V$, then:

$$\psi(x) = A + Bx$$

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$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2}(E - V)\psi(x)$$

- Solution depends on value of $E - V$:

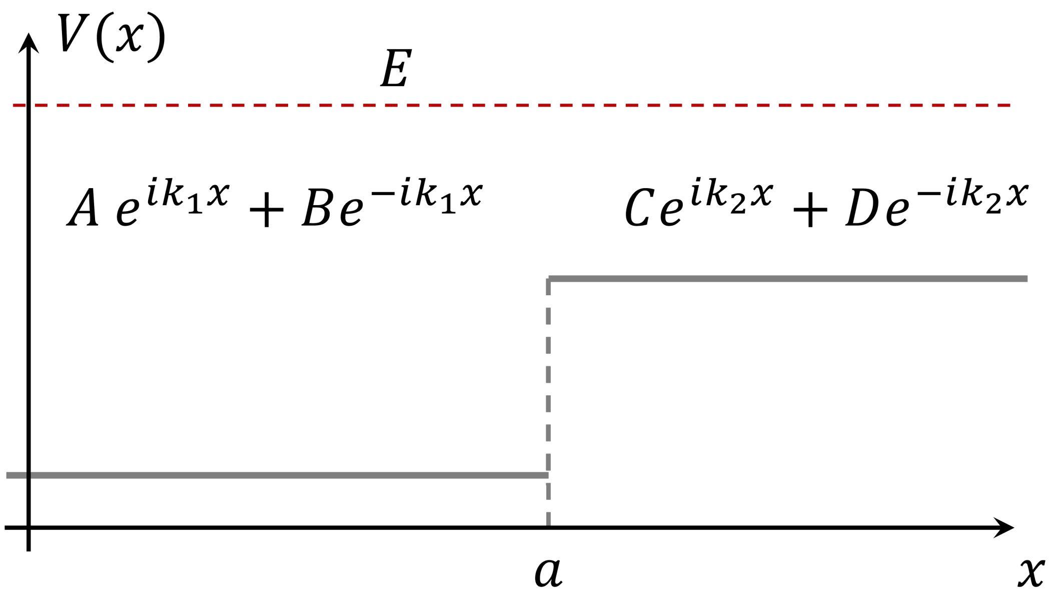
case	solutions	eigenvalue of $\hat{p}$	parameter
$E > V$	$e^{\pm ikx}$	$\pm\hbar k$	$k^2 = \frac{2m}{\hbar^2}(E - V)$
$E = V$	$1, x$	0, no e.v.	$E = V$
$E < V$	$e^{\mp\kappa x}$	$\pm i\hbar\kappa$	$\kappa^2 = \frac{2m}{\hbar^2}(V - E)$

BOUNDARY CONDITIONS ACROSS A STEP IN V(X)

- Suppose there is a step in the potential in $x = a$.
- **Boundary conditions:** Continuity of wave function $\psi(x)$ and derivative $\frac{d\psi(x)}{dx}$:

$$\psi_I(a) = \psi_{II}(a)$$
$$\frac{d\psi_I(a)}{dx} = \frac{d\psi_{II}(a)}{dx}$$

$$Ae^{ik_1 a} + Be^{-ik_1 a} = Ce^{ik_2 a} + De^{-ik_2 a}$$
$$ik_1 Ae^{ik_1 a} - ik_1 Be^{-ik_1 a} = ik_2 Ce^{ik_2 a} - ik_2 De^{-ik_2 a}$$



BOUNDARY CONDITIONS ACROSS A STEP IN V(X)

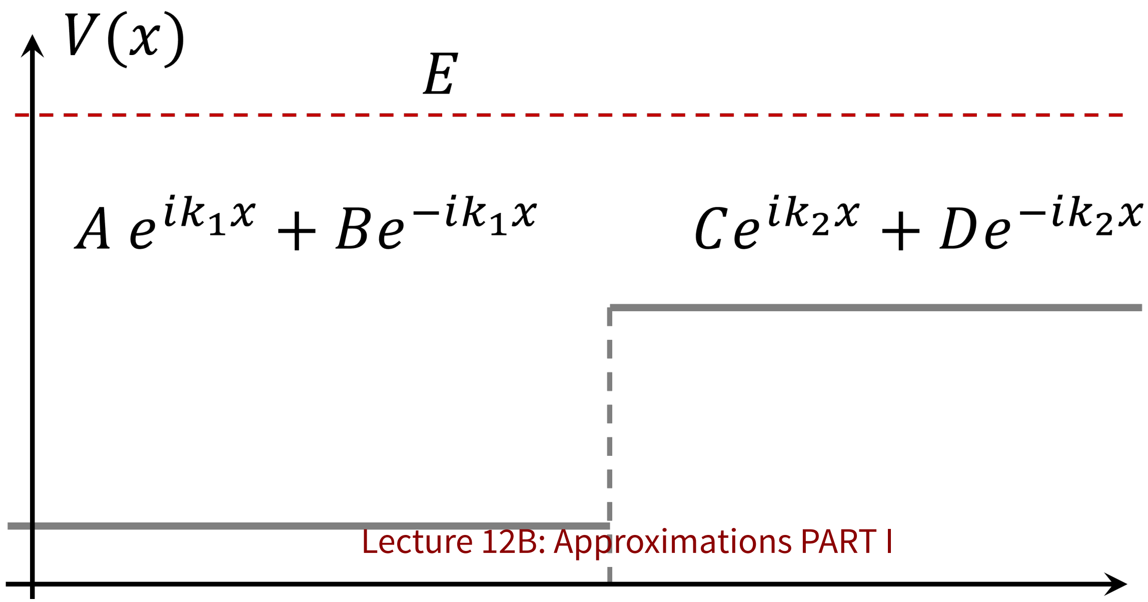
$$\psi_I(a) = \psi_{II}(a)$$

$$\frac{d\psi_I(a)}{dx} = \frac{d\psi_{II}(a)}{dx}$$

$$Ae^{ik_1 a} + Be^{-ik_1 a} = Ce^{ik_2 a} + De^{-ik_2 a}$$

$$ik_1 Ae^{ik_1 a} - ik_1 Be^{-ik_1 a} = ik_2 Ce^{ik_2 a} - ik_2 De^{-ik_2 a}$$

$$\begin{pmatrix} 1 & 1 \\ ik_1 & -ik_1 \end{pmatrix} \begin{pmatrix} e^{ik_1 a} & 0 \\ 0 & e^{-ik_1 a} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ ik_2 & -ik_2 \end{pmatrix} \begin{pmatrix} e^{ik_2 a} & 0 \\ 0 & e^{-ik_2 a} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}$$



BOUNDARY CONDITIONS ACROSS A STEP IN V(X)

$$\begin{pmatrix} 1 & 1 \\ ik_1 & -ik_1 \end{pmatrix} \begin{pmatrix} e^{ik_1 a} & 0 \\ 0 & e^{-ik_1 a} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ ik_2 & -ik_2 \end{pmatrix} \begin{pmatrix} e^{ik_2 a} & 0 \\ 0 & e^{-ik_2 a} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}$$

Express coefficient A, B in C, D:

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} e^{ik_1 a} & 0 \\ 0 & e^{-ik_1 a} \end{pmatrix}^{-1} \begin{pmatrix} 1 & 1 \\ ik_1 & -ik_1 \end{pmatrix}^{-1} \times \begin{pmatrix} 1 & 1 \\ ik_2 & -ik_2 \end{pmatrix} \begin{pmatrix} e^{ik_2 a} & 0 \\ 0 & e^{-ik_2 a} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}$$

Rename the matrices as function of V and a:

$$\begin{pmatrix} A \\ B \end{pmatrix} = E_1^{-1}(a) K_1^{-1} K_2 E_2(a) \begin{pmatrix} C \\ D \end{pmatrix}$$

TRANSFER MATRIX FOR A SINGLE STEP

$$E_j(a) = \begin{pmatrix} e^{ik_j a} & 0 \\ 0 & e^{-ik_j a} \end{pmatrix}, \qquad K_j \begin{pmatrix} 1 & 1 \\ ik_j & -ik_j \end{pmatrix}$$

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = E_1^{-1}(a) K_1^{-1} K_2 E_2(a) \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}$$

We can define the transfer matrix for a single step:

$$T_{12} = E_1^{-1}(a) K_1^{-1} K_2 E_2(a)$$

Connection between coefficient before/after step:

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = T_{12} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}$$

MULTIPLE POTENTIAL STEPS

Extending the relation over multiple steps:

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = T_{12} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = T_{12}\, T_{23} \begin{pmatrix} A_3 \\ B_3 \end{pmatrix}$$

In general, after N steps we obtain:

$$\begin{pmatrix} A_0 \\ B_0 \end{pmatrix} = T \begin{pmatrix} A_{N+1} \\ B_{N+1} \end{pmatrix} = T_{01}\, T_{12}\, \ldots\, T_{N,N+1} \begin{pmatrix} A_{N+1} \\ B_{N+1} \end{pmatrix}$$

Or renaming the indices on the left and right:

$$\begin{pmatrix} A_L \\ B_L \end{pmatrix} = \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix} \begin{pmatrix} A_R \\ B_R \end{pmatrix}$$

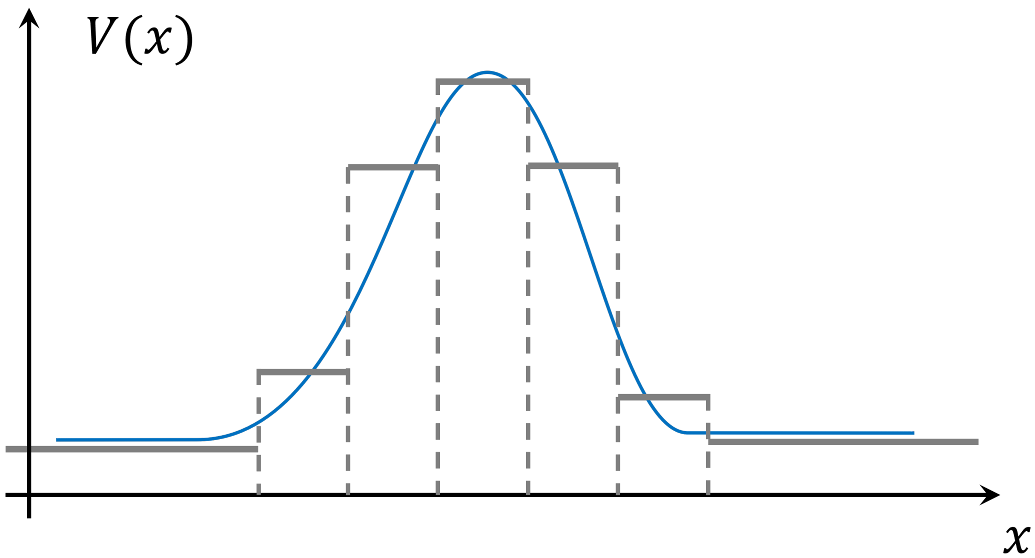
SCATTERING AND BOUND STATES

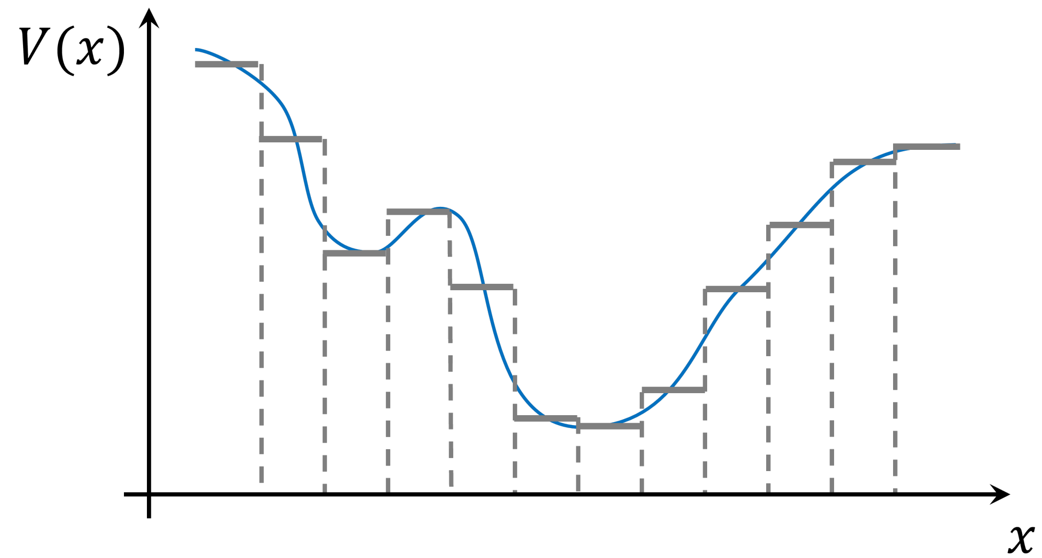
Scattering: $B_R = 0$

$$\begin{pmatrix} A_L \\ B_L \end{pmatrix} = \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix} \begin{pmatrix} A_R \\ 0 \end{pmatrix}$$

Therefore the transmission and reflection coefficients become:

$$\begin{aligned} \text{Transmission} \quad & T(E) = \left| A_R / A_L \right|^2 = 1 \,/\, \left| t_{11}(E) \right|^2 \\ \text{Reflection} \quad & R(E) = \left| B_L / A_L \right|^2 = \left| t_{21}(E) \right|^2 / \left| t_{11}(E) \right|^2 \end{aligned}$$


$V(x)$
x

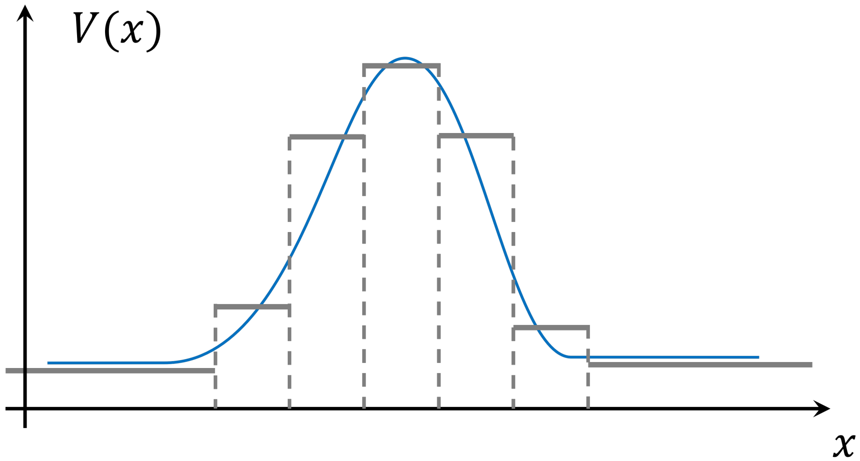

$V(x)$
x

SCATTERING AND BOUND STATES

Bound states: $A_L = 0, \quad B_R = 0$

$$\begin{pmatrix} 0 \\ B_L \end{pmatrix} = \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix} \begin{pmatrix} A_R \\ 0 \end{pmatrix} \Longrightarrow \begin{array}{l} A_L = t_{11}(E)\, A_R \\ B_L = t_{21}(E)\, A_R \end{array}$$

- Bound states are given by zeros of t_{11}
- The total wave function is defined upon the coefficients B_L and A_R. We can obtain these unknowns by
  - first using the second equation: $B_L = t_{21}(E)\, A_R$ to obtain B_L, and then
  - applying normalization to the whole wave function to fix A_R.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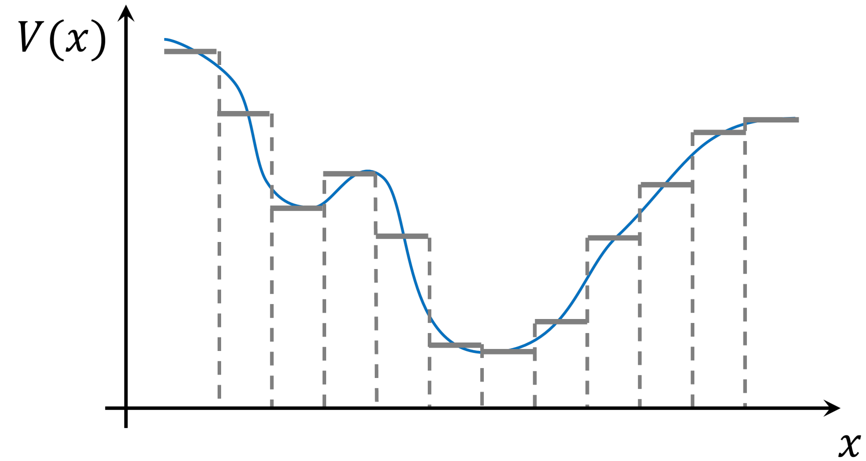
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