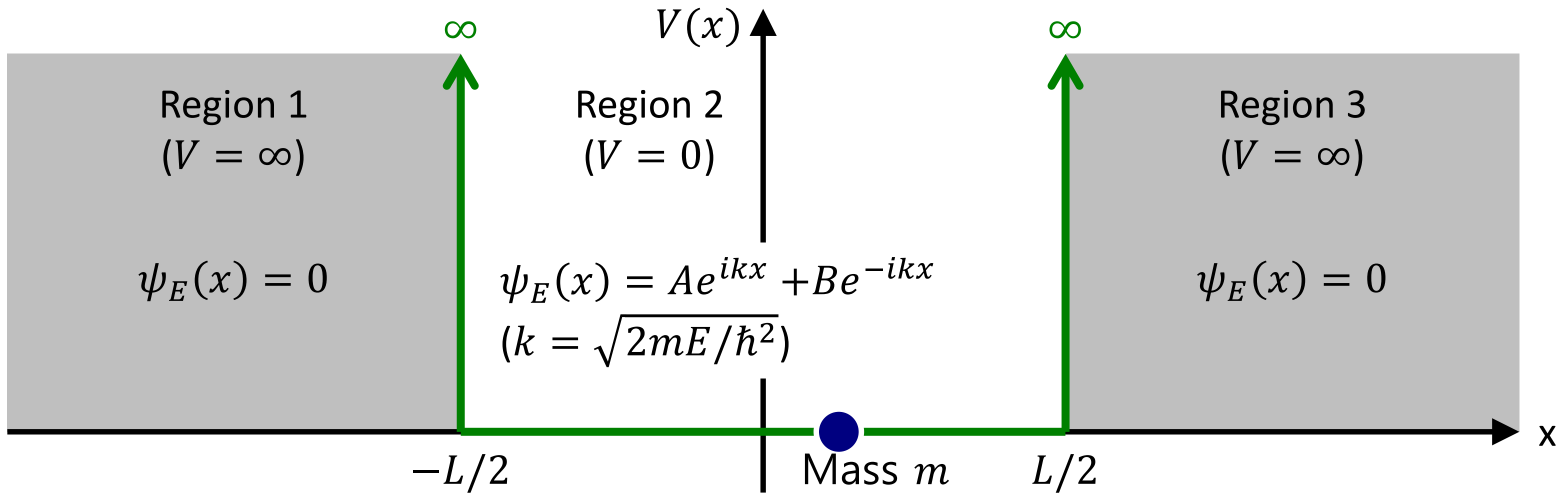
Further examples of 1-dimensional problem

(Ex2) Particle in a box



$H = \dfrac{p^2}{2m} + V(x)$ (Classical) Hamiltonian $\qquad \hat{H} = \dfrac{\hat{P}^2}{2m} + V(\hat{X})$ (Quantum) Hamiltonian operator

$\hat{H}|E\rangle = \left[\dfrac{\hat{P}^2}{2m} + V(\hat{X})\right]|E\rangle = E|E\rangle$ Time-independent Schrödinger equation (TISE)

$\left[-\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2} + V(x)\right]\psi_E(x) = E\psi_E(x)$ Representation of TISE in the X basis

$\psi_E(x)$ is continuous at the two boundaries, $x = -L/2$ & $x = L/2$

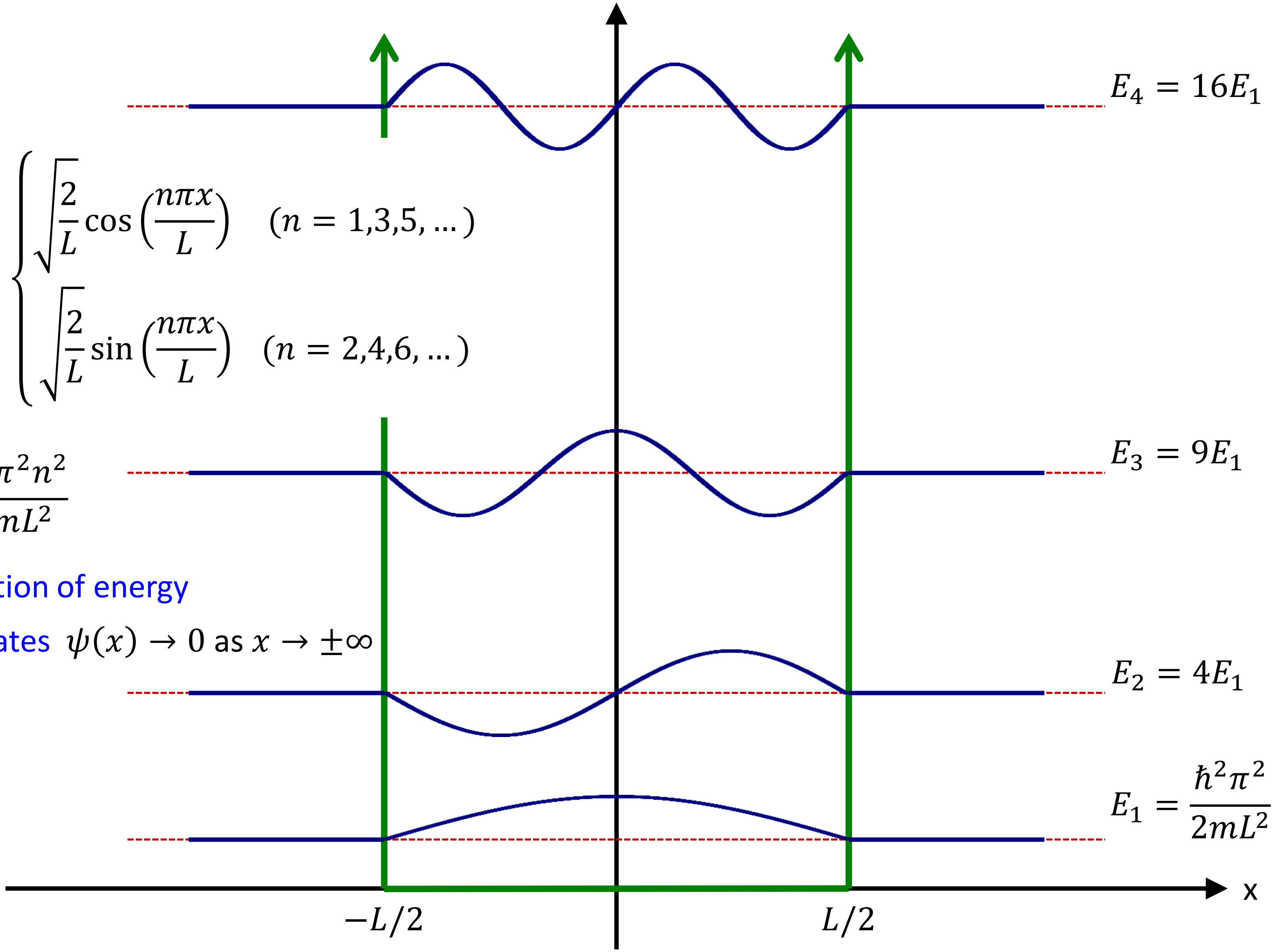
(Ex2) Particle in a box

$$\psi_n(x) = \begin{cases} \sqrt{\dfrac{2}{L}}\cos\left(\dfrac{n\pi x}{L}\right) & (n = 1,3,5,\dots) \\ \sqrt{\dfrac{2}{L}}\sin\left(\dfrac{n\pi x}{L}\right) & (n = 2,4,6,\dots) \end{cases}$$

$$E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2}$$

Quantization of energy

Bound states $\psi(x) \to 0$ as $x \to \pm\infty$



(Ex2) Particle in a box

Parity operation on a state

Classical	Quantum
$x \rightarrow -x$ $p \rightarrow -p$	Parity operator $\hat{\Pi}$ $\hat{\Pi}\vert x\rangle = \vert -x\rangle$ $\hat{\Pi}\vert p\rangle = \vert -p\rangle$

For any state $|\psi\rangle$,

$\langle x|\psi\rangle = \psi(x) \rightarrow \langle x|\hat{\Pi}|\psi\rangle = \psi(-x)$

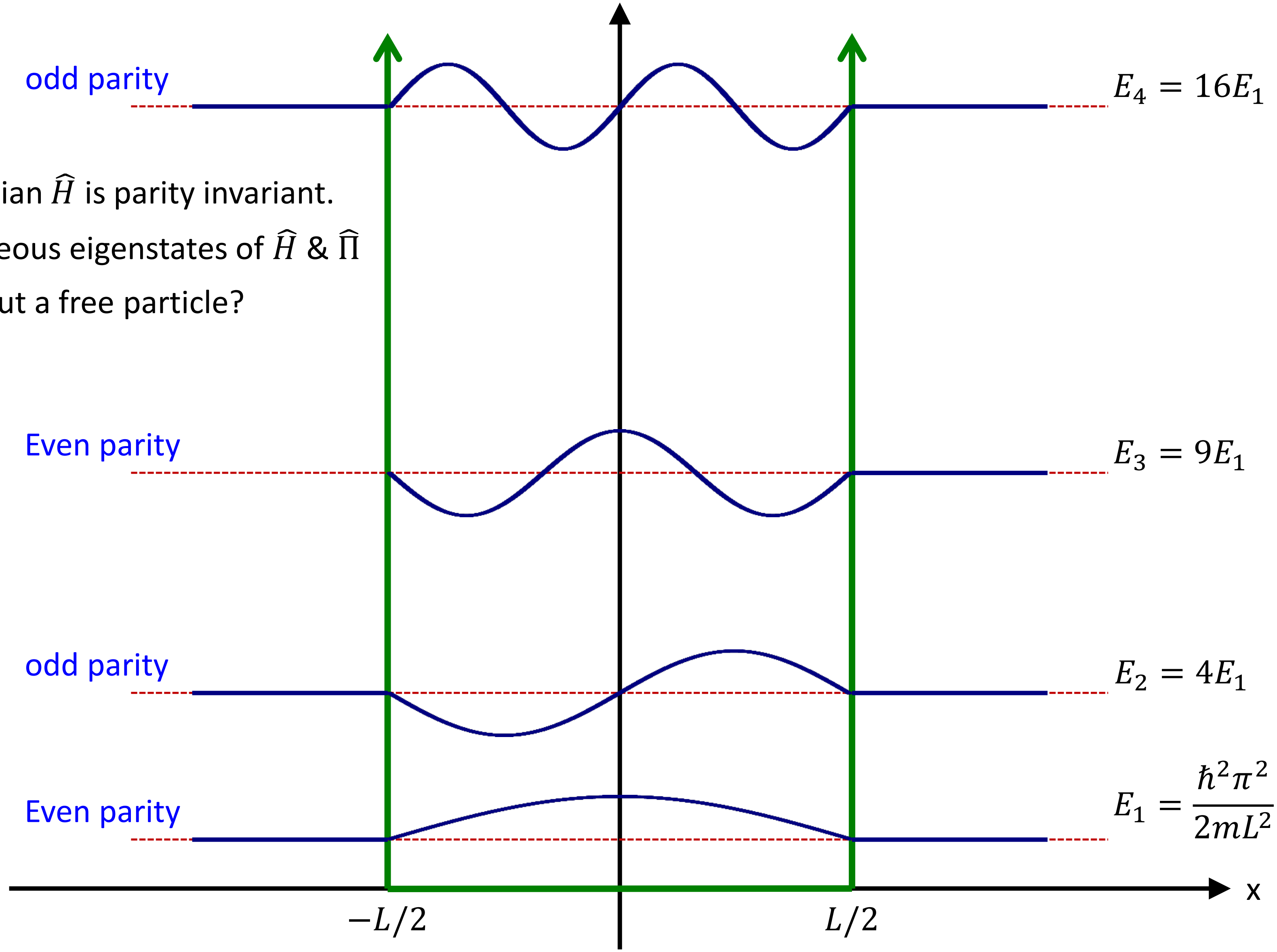
$\langle p|\psi\rangle = \psi(p) \rightarrow \langle p|\hat{\Pi}|\psi\rangle = \psi(-p)$

(Can you derive these relations using the completeness relation?)

Properties

- Eigenvalues ± 1 (eigenstates having even/odd parity)
- Hermitian & unitary ($\hat{\Pi}^\dagger = \hat{\Pi}^{-1} = \hat{\Pi}$)
- If $\hat{H}(-\hat{X}, -\hat{P}) = \hat{H}(\hat{X}, \hat{P})$,
  - the Hamiltonian $\hat{H}$ is said to be parity invariant.
  - $[\hat{\Pi}, \hat{H}] = 0$

(Ex2) Particle in a box



Hamiltonian $\hat{H}$ is parity invariant.

Simultaneous eigenstates of $\hat{H}$ & $\hat{\Pi}$

How about a free particle?

(Ex2) Particle in a box

Bound states

- The energy levels are always quantized.
- No degeneracy in 1D bound states
  (How about a free particle?)

Expectation value of momentum $\langle P \rangle = 0$

Ground-state energy $E_1 \neq 0$ (why?)

Can you quickly make an order-of-magnitude estimation of the ground-state energy of a particle in an (infinite) box?

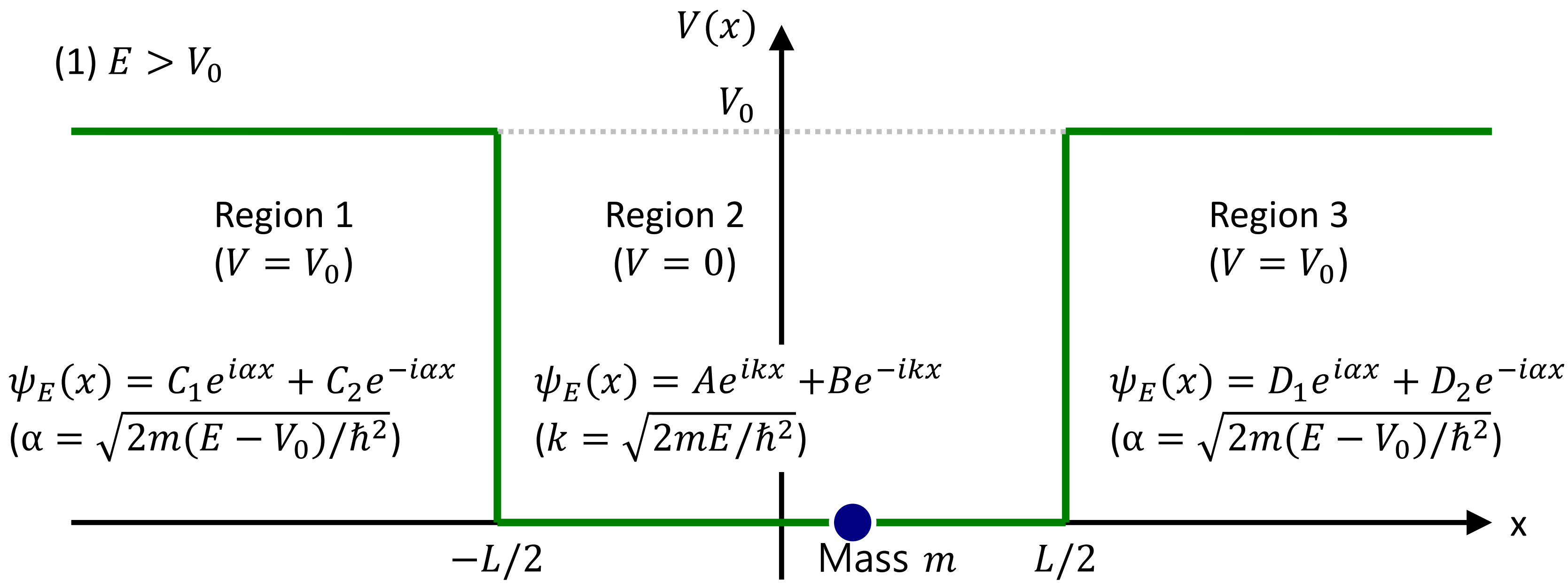
Evolution of a state with time

- All the eigenstates are stationary.
- How will the state $|\psi(0)\rangle = \frac{1}{\sqrt{2}}[|1\rangle + |2\rangle]$ evolve with time?
- How will the state $|\psi(0)\rangle = \frac{1}{\sqrt{2}}[|1\rangle + |3\rangle]$ evolve with time?
- How do they look in the X basis?

(Ex3) (Finite) potential well

(The mathematical detail left as your homework)

(1) $E > V_0$



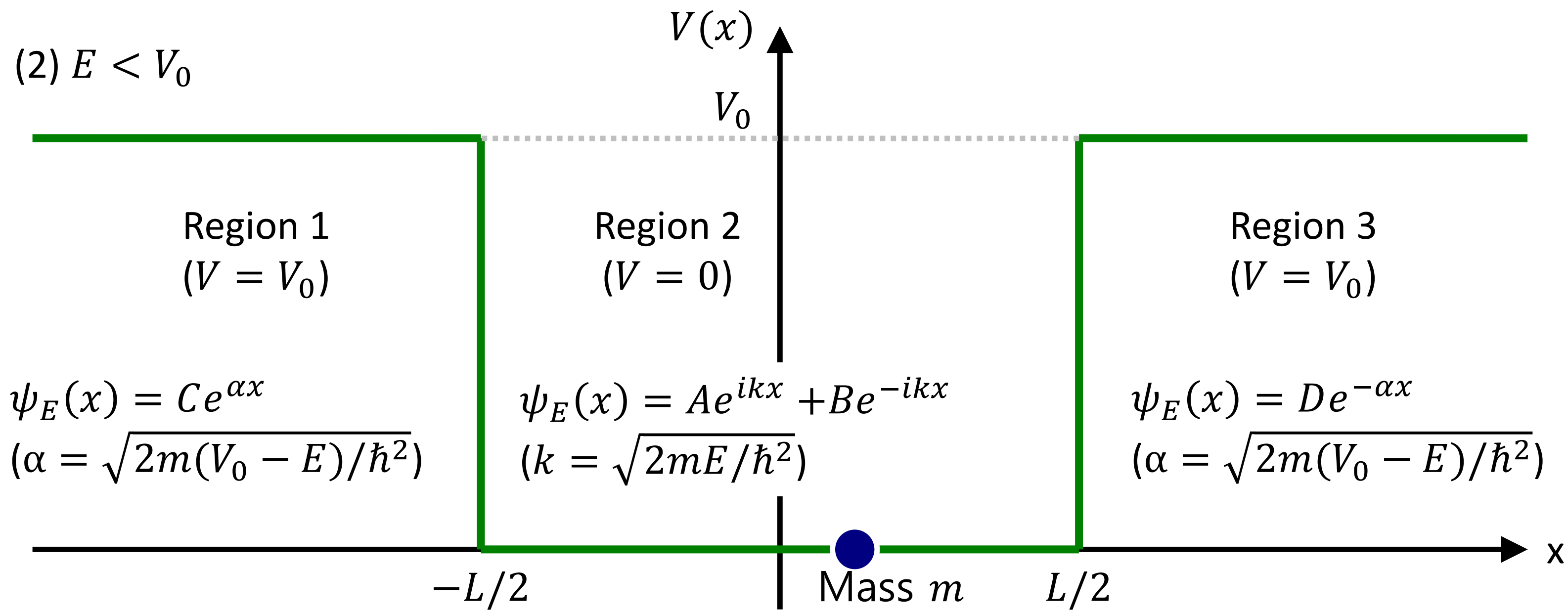
$\psi_E(x)$ & $\psi_E{}'(x)$ are continuous at the two boundaries, $x = -L/2$ & $x = L/2$

E is continuous.

(Ex3) (Finite) potential well

(The mathematical detail left as your homework)

(2) $E < V_0$



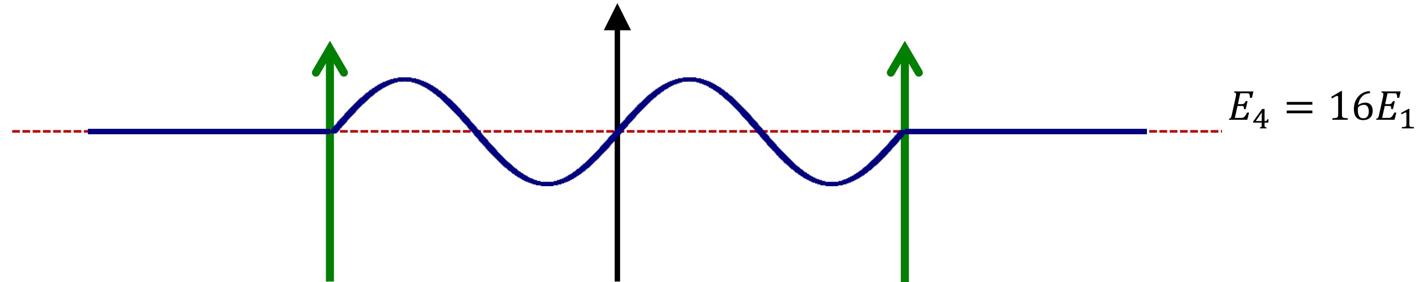
$\psi_E(x)$ & $\psi_E'(x)$ are continuous at the two boundaries, $x = -L/2$ & $x = L/2$

E is quantized (discrete).

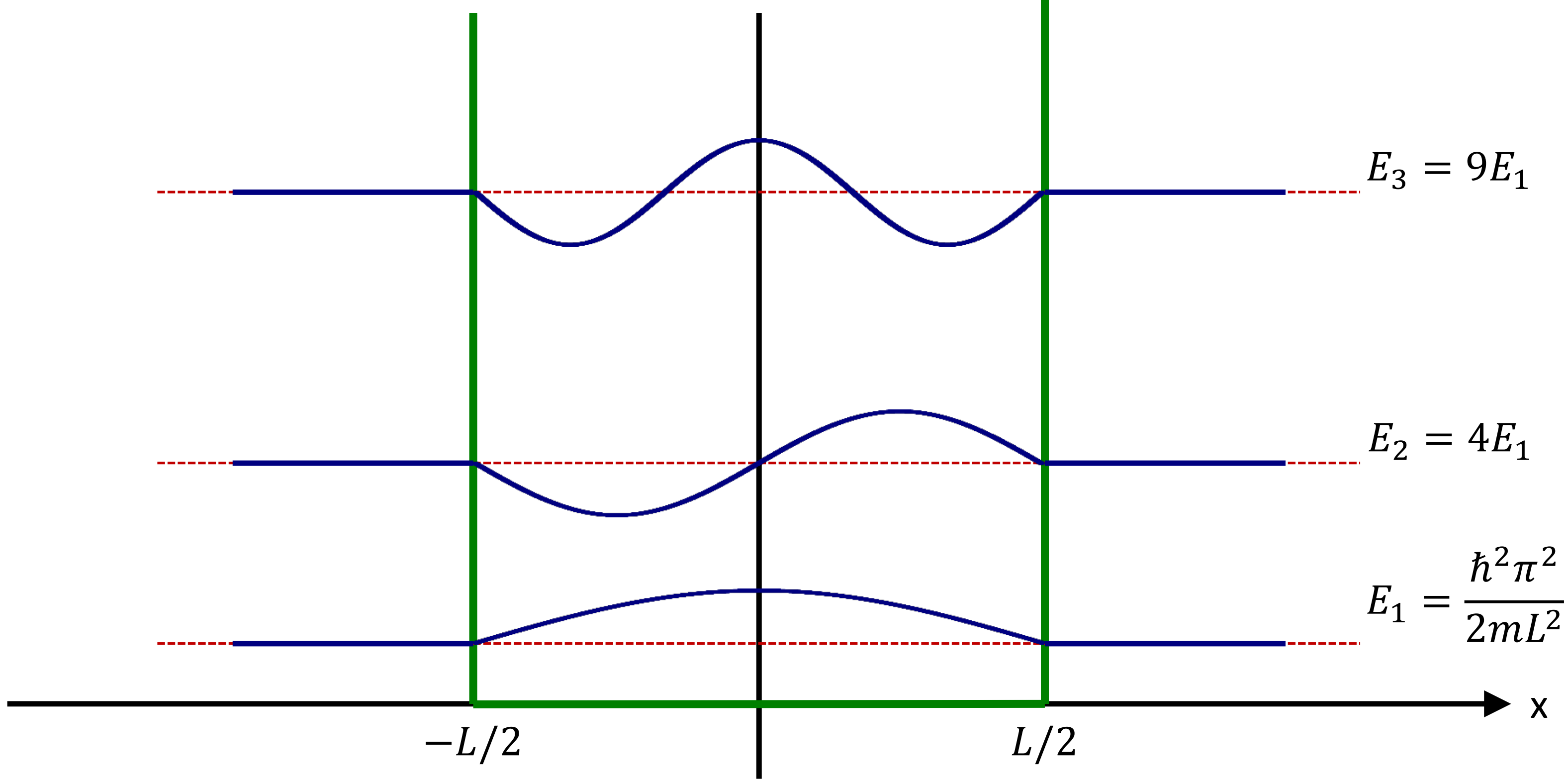
# of bound states are finite.

- More bound states for higher V_0 and/or longer L
- There exists at least 1 bound state (for 1D potential well).

(Ex3) (Finite) potential well

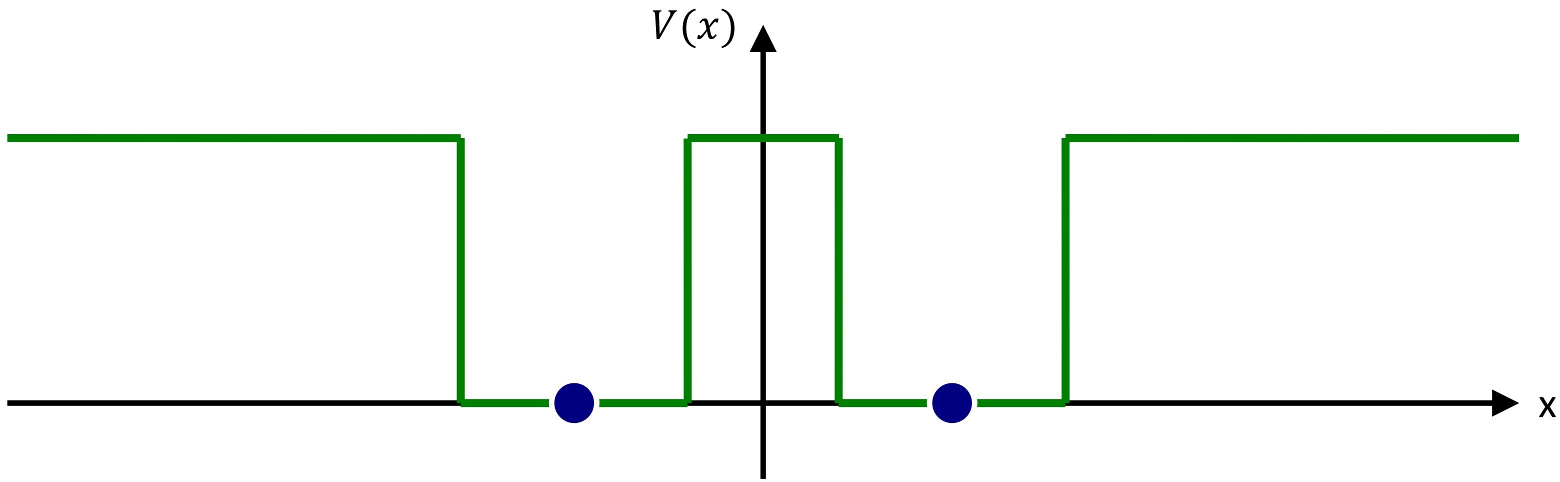


Can you adjust these wavefunctions in a box (infinite potential well) into those of bound states in a finite potential well?

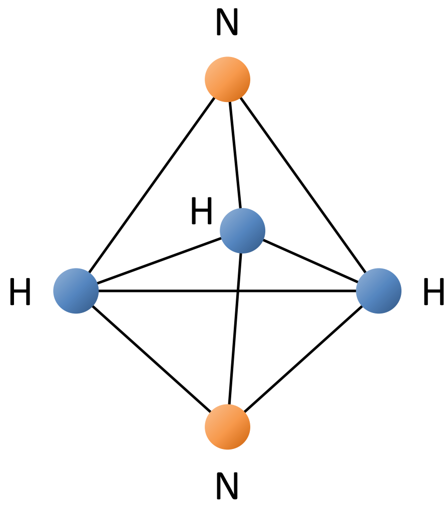


(Ex3) (Finite) potential well

Double potential wells
Two potential wells placed closely (coupled) to each other



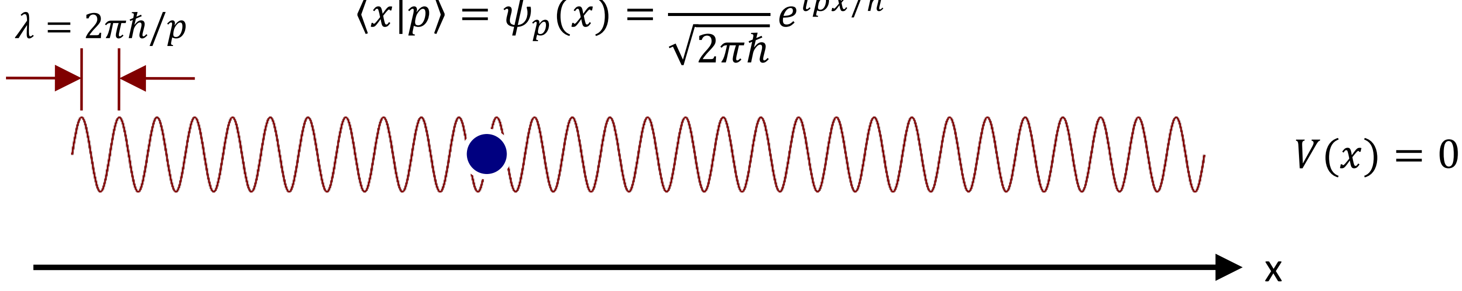
- Parity invariance & eigenstates of $\hat{H}$
- Tunneling through the barrier
- Inversion doubling of an NH_3 molecule (24 GHz)
- NH_3 maser (by Charles Townes)

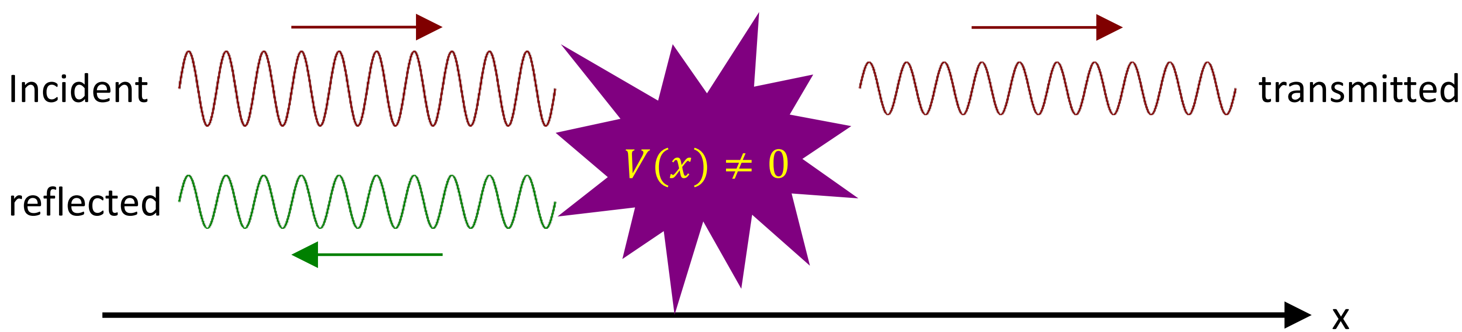


1D scattering problem

(Quasi) plane wave propagating along the +x direction

$$\langle x|p\rangle = \psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$





What are the probabilities of reflection & transmission?

Probability current

The rate of change of probability density $P(x,t) = |\psi(x,t)|^2$ at x

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial \psi^*}{\partial t}\psi + \psi^* \frac{\partial \psi}{\partial t}$$

$$= -\frac{\partial}{\partial x}\left[\frac{\hbar}{2im}\left(\psi^*\frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right)\right]$$

$$= -\frac{\partial}{\partial x}\left[\underline{\frac{\hbar}{m}\mathrm{Im}\left(\psi^*\frac{\partial \psi}{\partial x}\right)}\right]$$

$\equiv j(x,t)$ probability current (flux)

Substitution $\longleftarrow$

$$i\hbar\frac{\partial \psi(x,t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x,t)$$

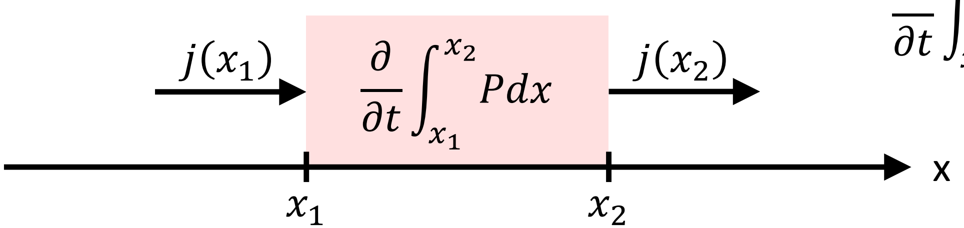
(Representation of Schrödinger equation in the X basis)

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial j(x,t)}{\partial x}$$

Continuity equation

$$\frac{\partial}{\partial t}\int_{x_1}^{x_2} P\,dx = -\int_{x_1}^{x_2}\frac{\partial j}{\partial x}dx$$

$$= j(x_1) - j(x_2) \quad \text{for arbitrary } (x_1, x_2)$$



$$\psi(x) = Ae^{ipx/\hbar} + Be^{-ipx/\hbar} \quad \rightarrow \quad j(x) = \frac{p}{m}(|A|^2 - |B|^2)$$

$$\psi(x) = A\tilde{\psi}(x),\ \tilde{\psi}(x) \text{ is real} \quad \rightarrow \quad j(x) = 0$$

1D scattering problem

(Quasi) plane wave propagating along the +x direction

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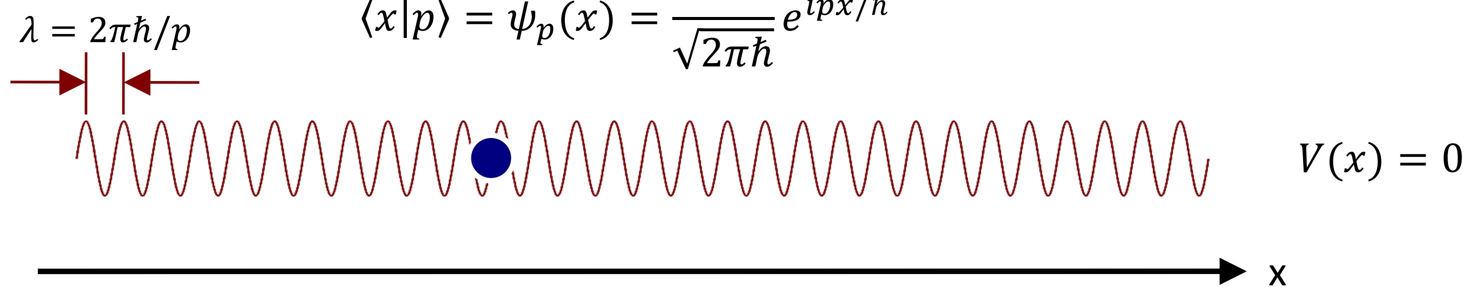
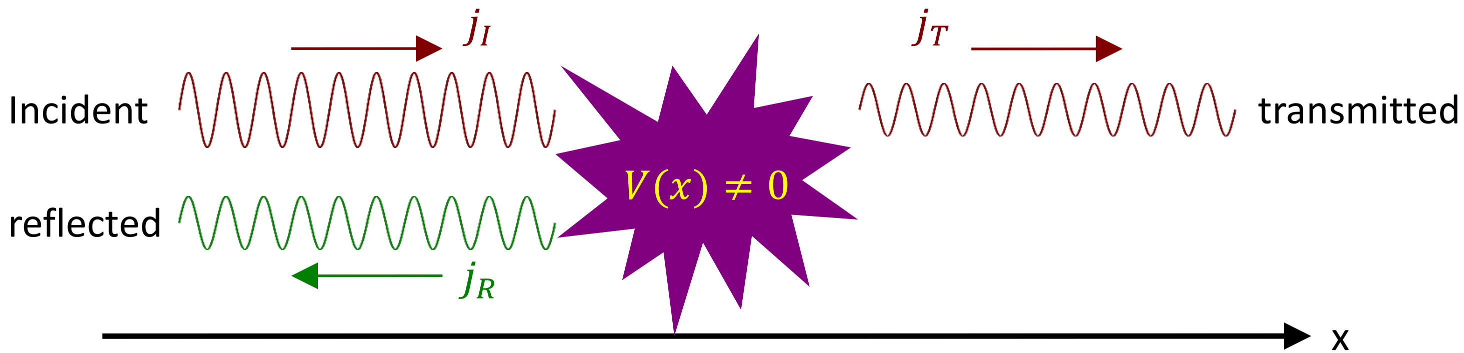


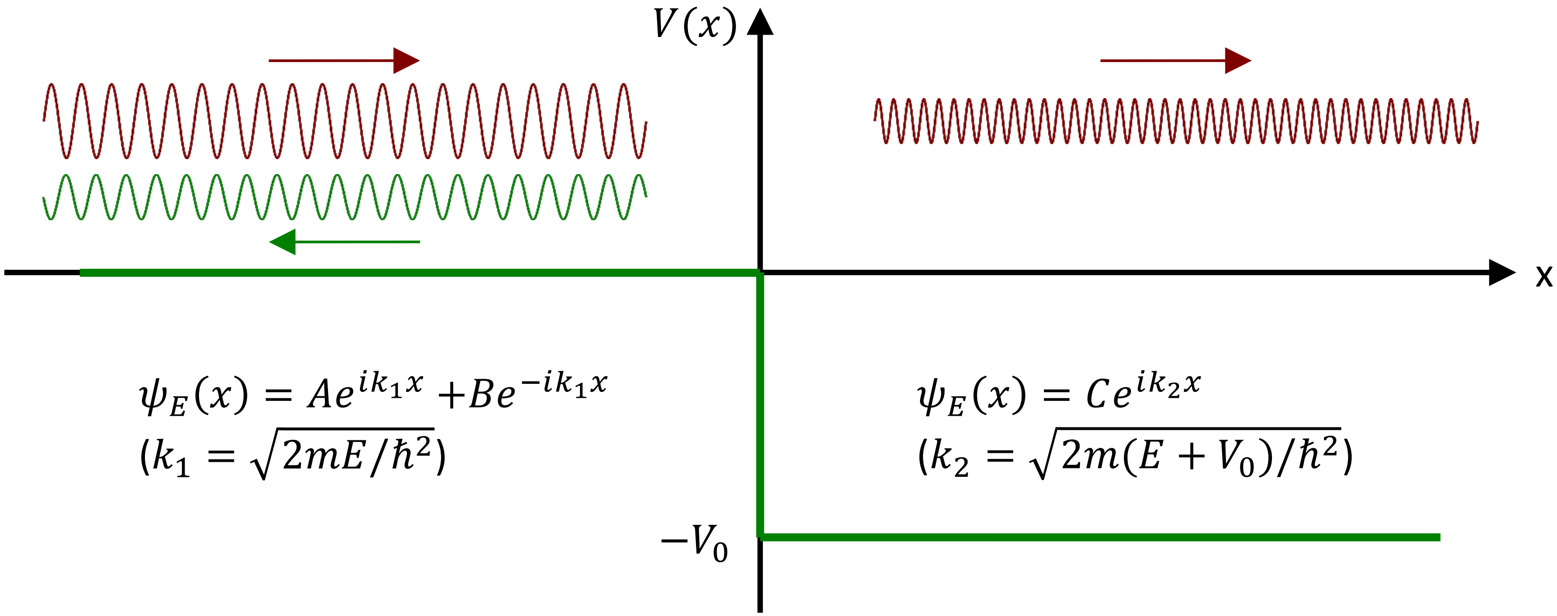


What are the probabilities of reflection & transmission?

Reflection coefficient $R = j_R/j_I$

Transmission coefficient $T = j_T/j_I$

(Ex4) Negative potential step



$\psi_E(x) = Ae^{ik_1x} + Be^{-ik_1x}$
$(k_1 = \sqrt{2mE/\hbar^2})$

$\psi_E(x) = Ce^{ik_2x}$
$(k_2 = \sqrt{2m(E+V_0)/\hbar^2})$

$\psi_E(x)$ & $\psi_E{}'(x)$ are continuous at the boundary $x = 0$.

$$B = \frac{k_1 - k_2}{k_1 + k_2}A$$

$$C = \frac{2k_1}{k_1 + k_2}A$$

$\longrightarrow$

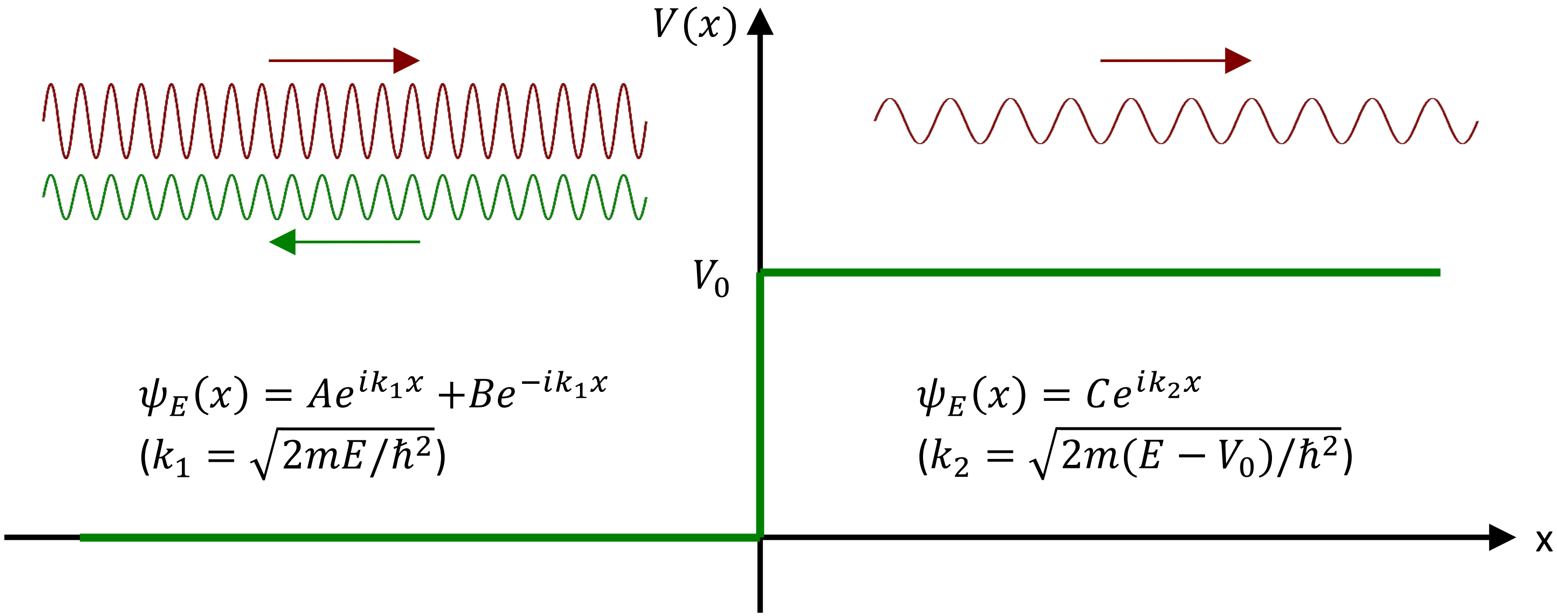
$$R = \frac{j_R}{j_I} = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$$

$$T = \frac{j_T}{j_I} = \frac{4k_1k_2}{(k_1 + k_2)^2}$$

$R + T = 1$
(Conservation of probability)

Partial reflection & partial transmission

(Ex5) Positive potential step



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(1) $E > V_0$

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$$\longrightarrow$$

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Partial reflection & partial transmission

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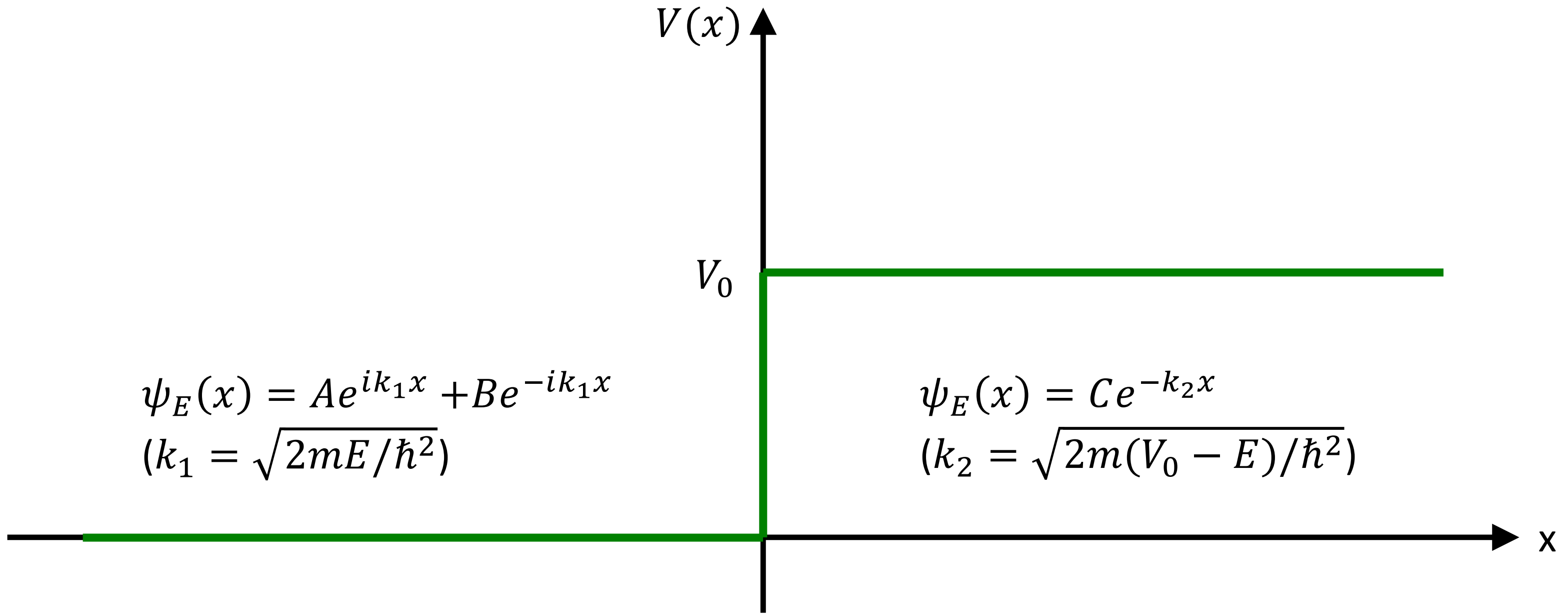

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$(k_1 = \sqrt{2mE/\hbar^2})$

$\psi_E(x) = Ce^{-k_2x}$
$(k_2 = \sqrt{2m(V_0 - E)/\hbar^2})$

(2) $E < V_0$

$\psi_E(x)$ & $\psi_E{}'(x)$ are continuous at the boundary $x = 0$.

$$B = \frac{k_1 - ik_2}{k_1 + ik_2}A \qquad C = \frac{2k_1}{k_1 + ik_2}A \quad \longrightarrow \quad R = \frac{j_R}{j_I} = 1 \qquad T = \frac{j_T}{j_I} = 0$$

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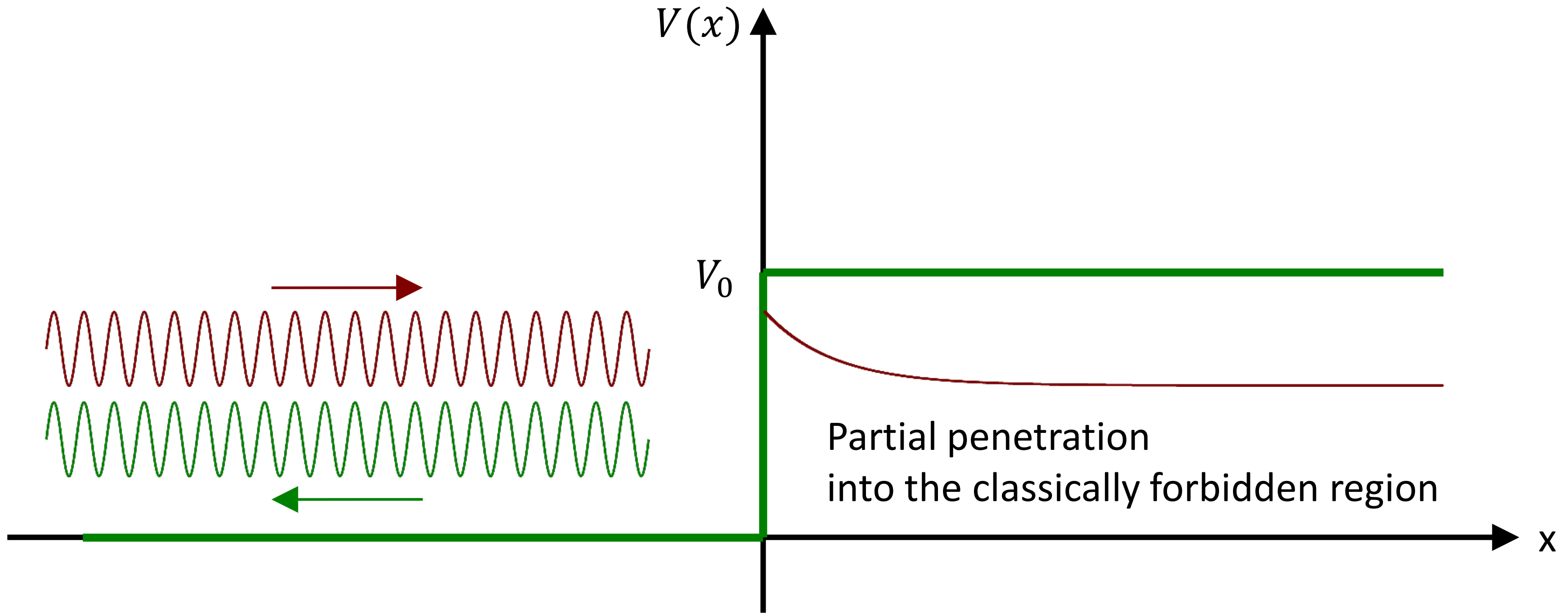
(Ex5) Positive potential step



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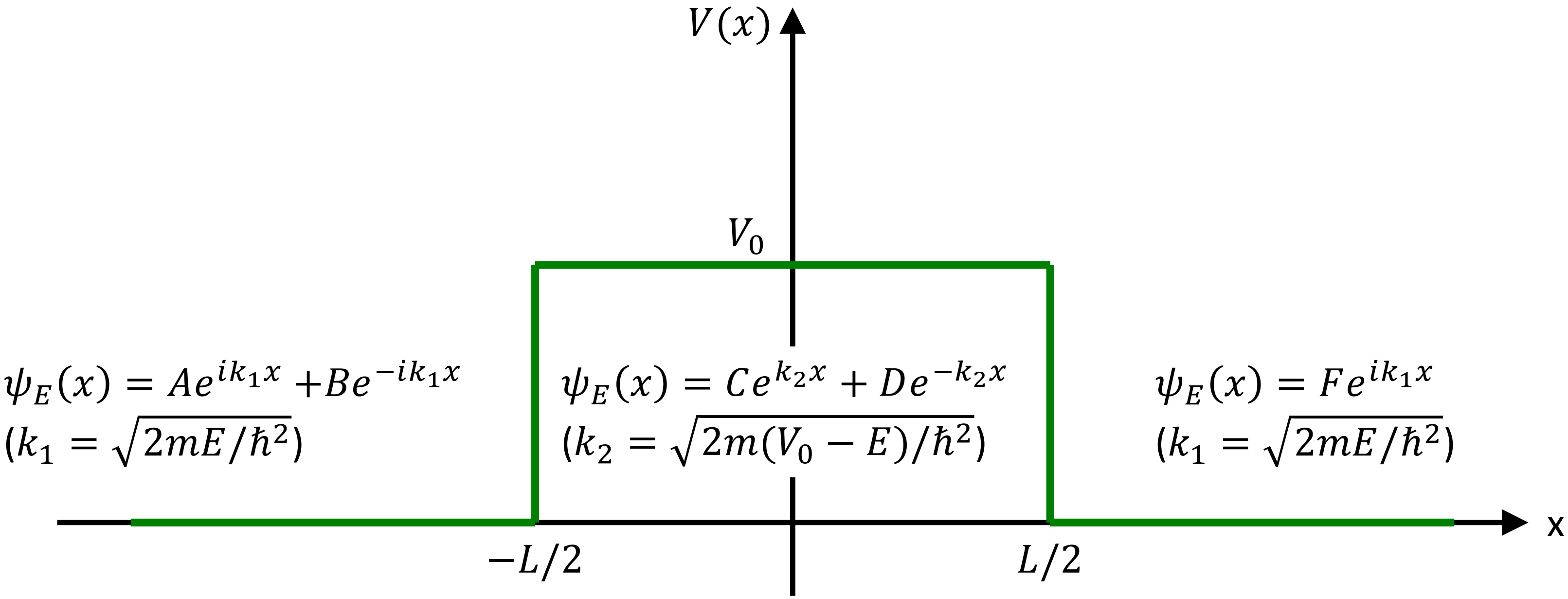
$$\longrightarrow$$

$$R = \frac{j_R}{j_I} = 1 \qquad T = \frac{j_T}{j_I} = 0$$

$R + T = 1$
(Conservation of probability)

(Ex6) Potential barrier



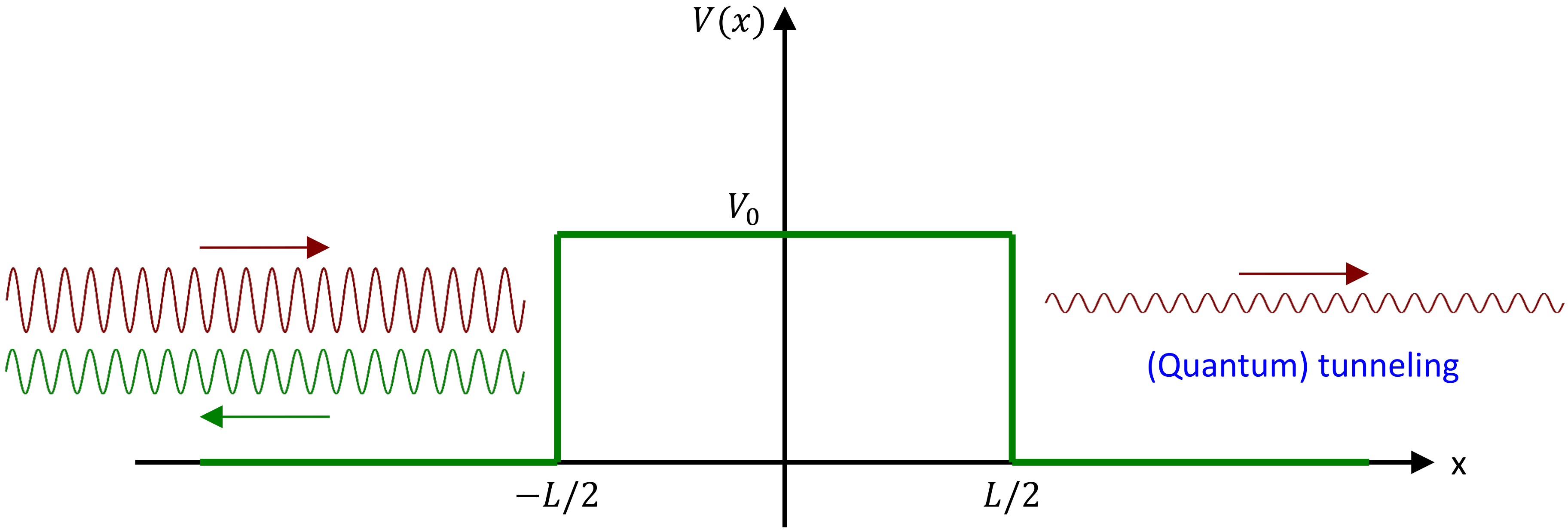
(1) $E < V_0$

$\psi_E(x)$ & $\psi_E{}'(x)$ are continuous at the boundaries $x = \pm L/2$.

$$T = \frac{j_T}{j_I} = \left[1 + \left(\frac{k_1^2 + k_2^2}{2k_1 k_2}\sinh(k_2 L)\right)^2\right]^{-1}$$

$R + T = 1$
(Conservation of probability)

(Ex6) Potential barrier



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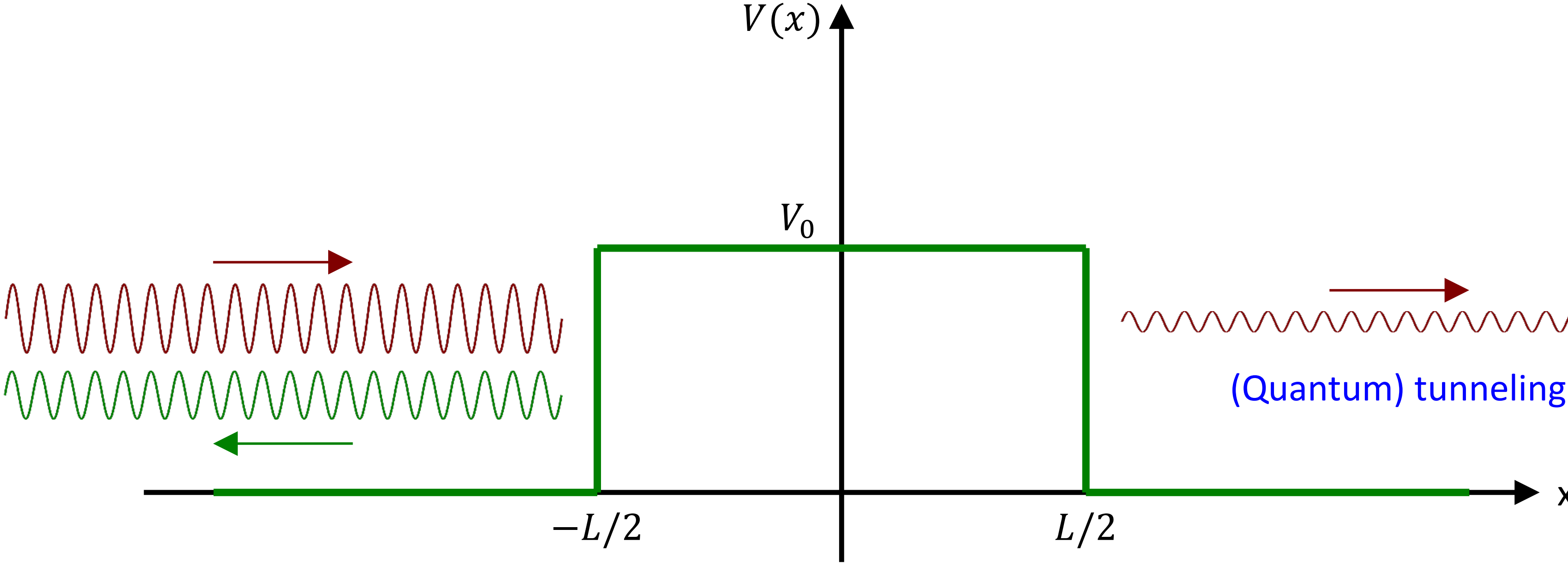
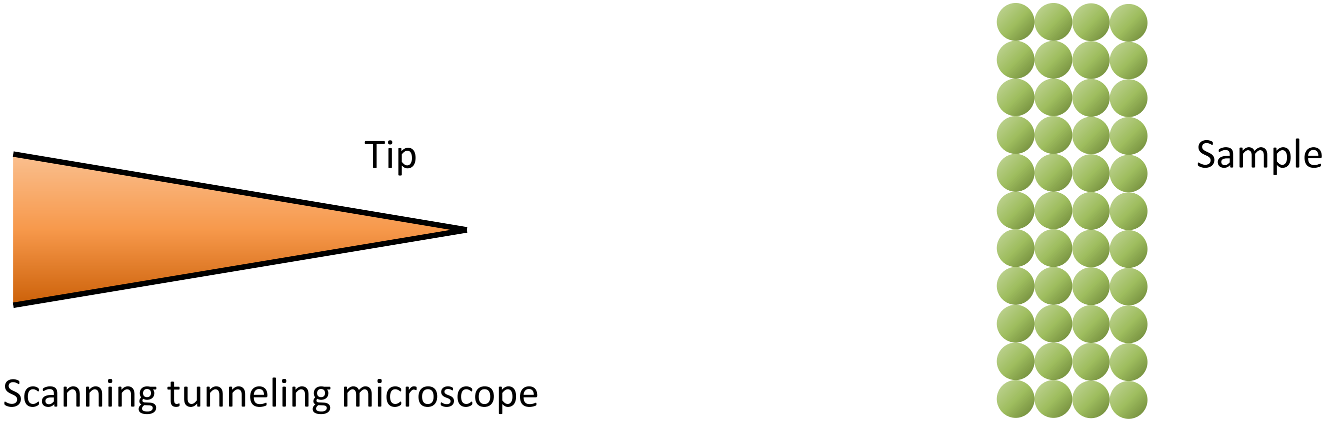
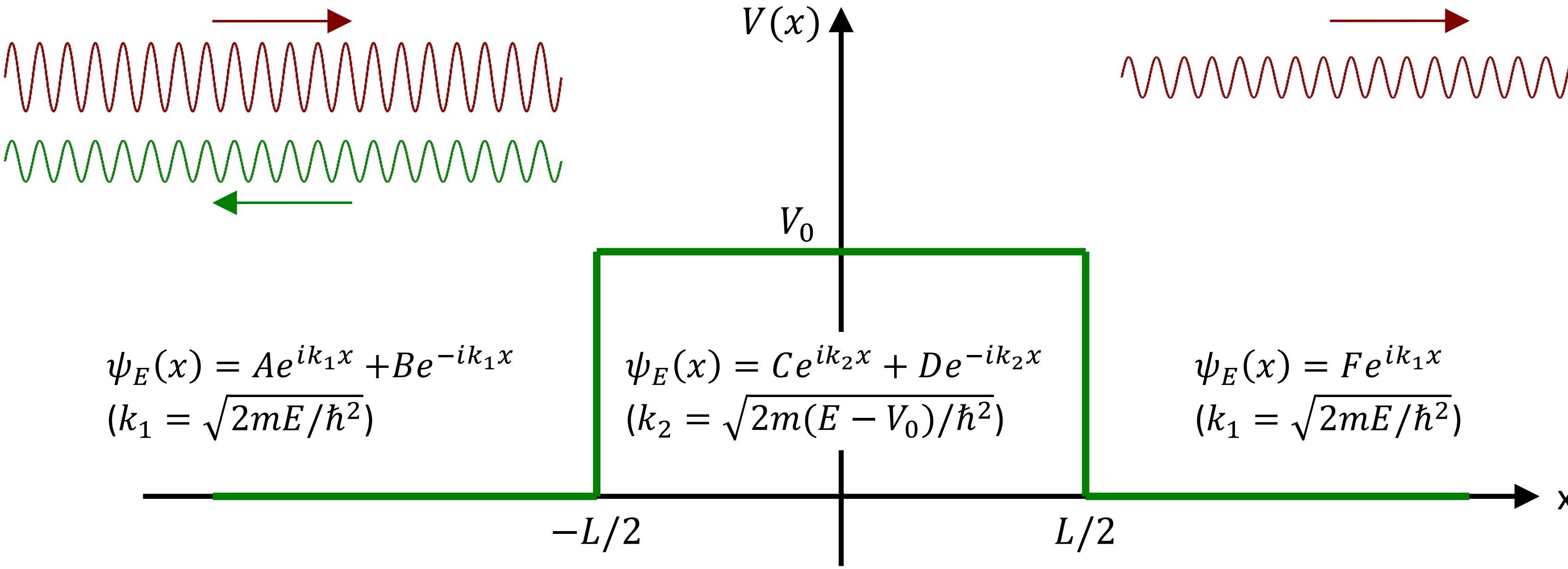
(Ex6) Potential barrier





Scanning tunneling microscope
(STM, by Gerd Binnig & Heinrich Rohrer)

(Ex6) Potential barrier



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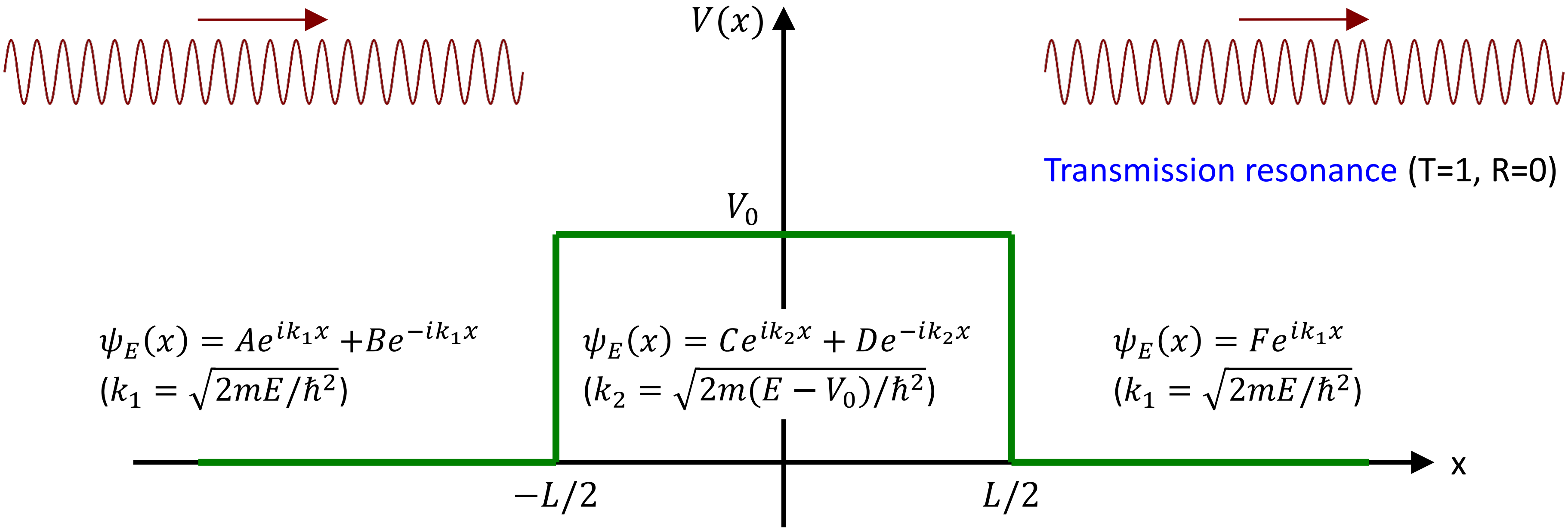
$R + T = 1$
(Conservation of probability)

Perfect transmission (T=1, R=0) can happen. When does it take place?

(Ex6) Potential barrier



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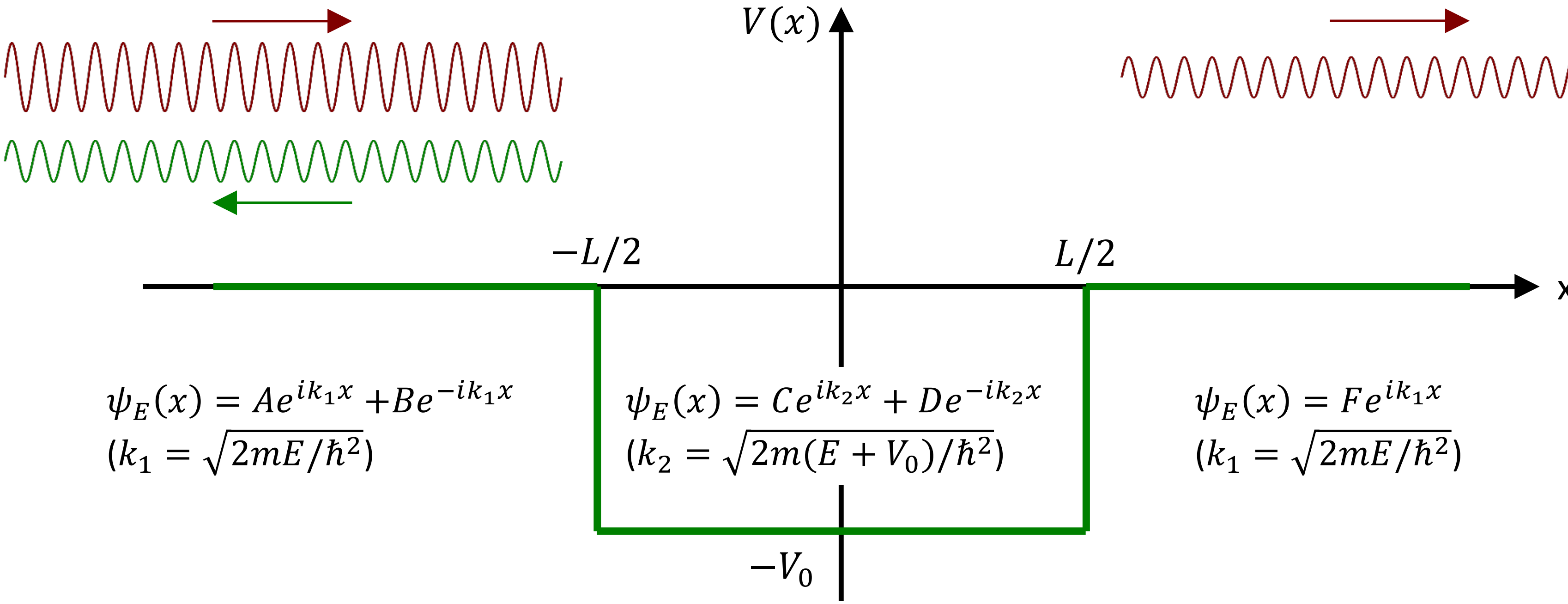
Perfect transmission (T=1, R=0) can happen. When does it take place?

(Ex7) Potential well



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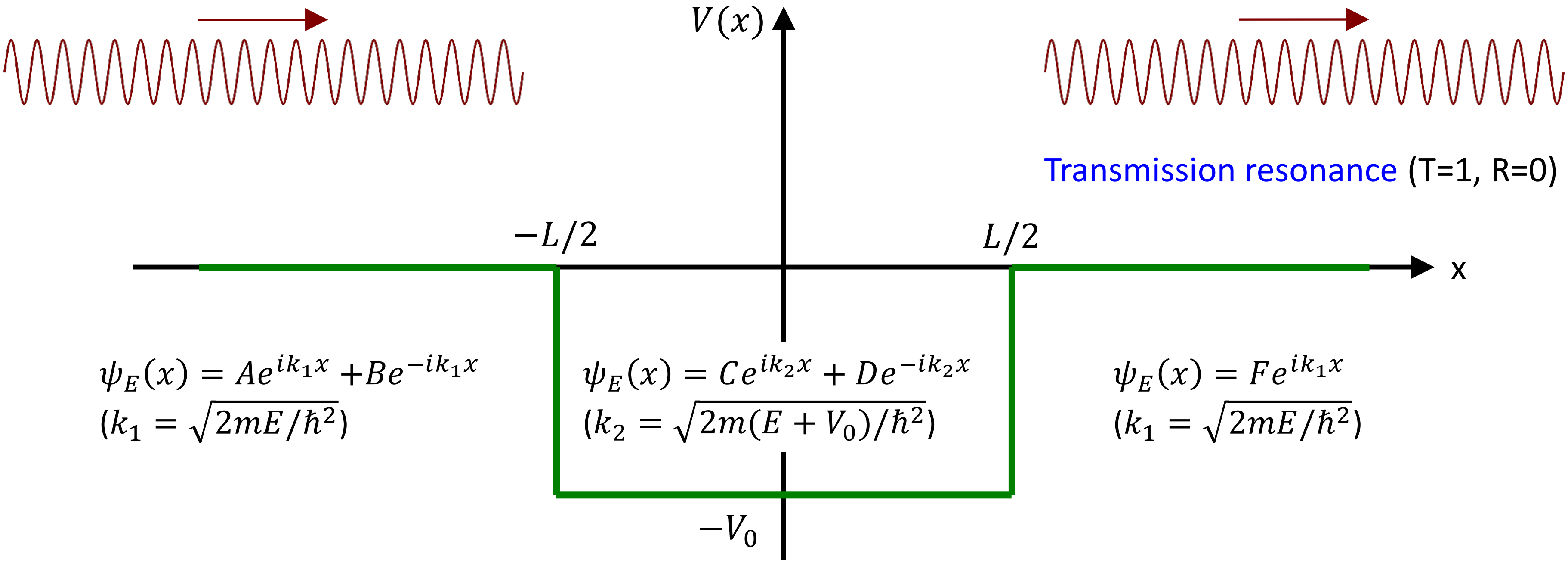
(Ex7) Potential well



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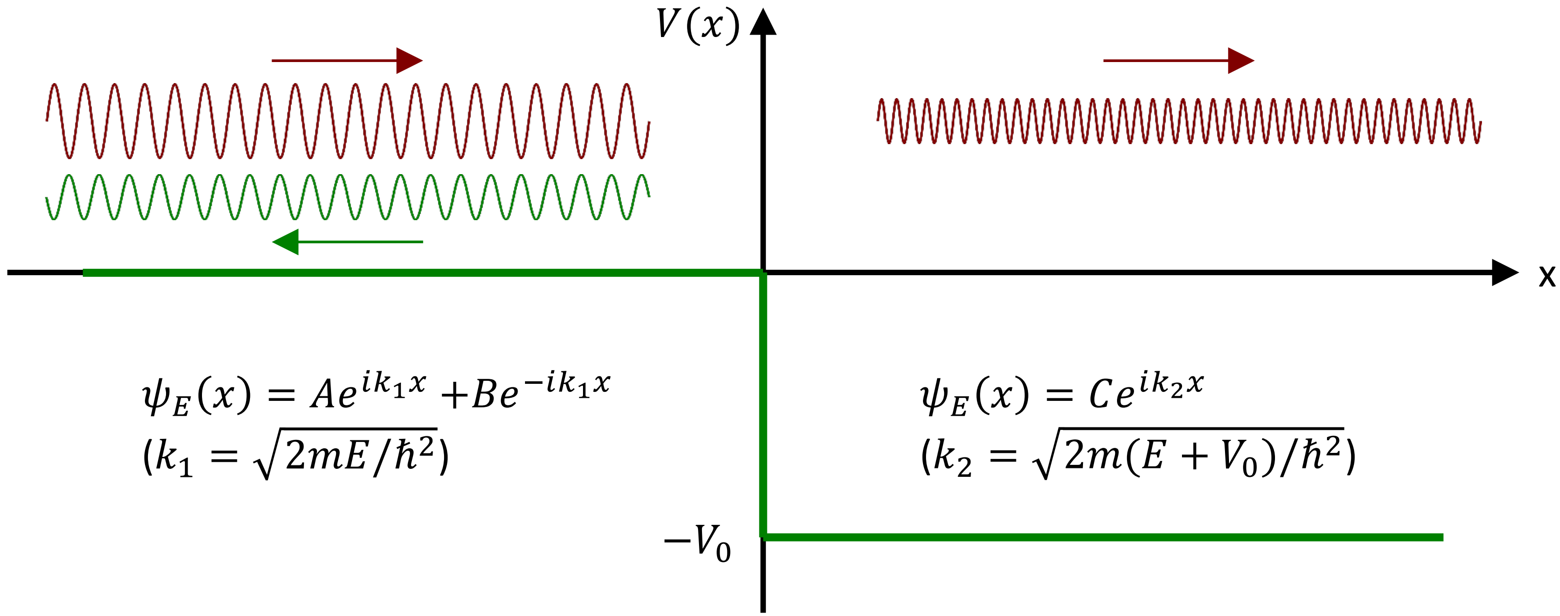
$R + T = 1$
(Conservation of probability)

Perfect transmission (T=1, R=0) can happen. When does it take place?

(Ex4) Negative potential step



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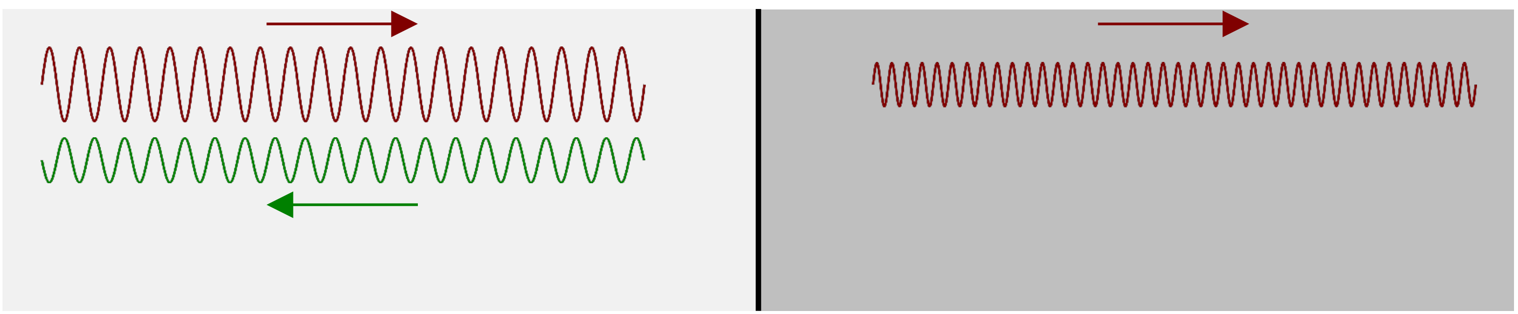
Can you devise a "photonic" system corresponding to this case?



How about the other cases?

Can you find out similarity between the TISE in the X basis & the 1D EM wave equation?