Square Well Potentials

* review of Wave mechanics

1) $\hat{H}\Psi = \hat{E}\Psi$ where $\hat{H} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$ "hamiltonian"

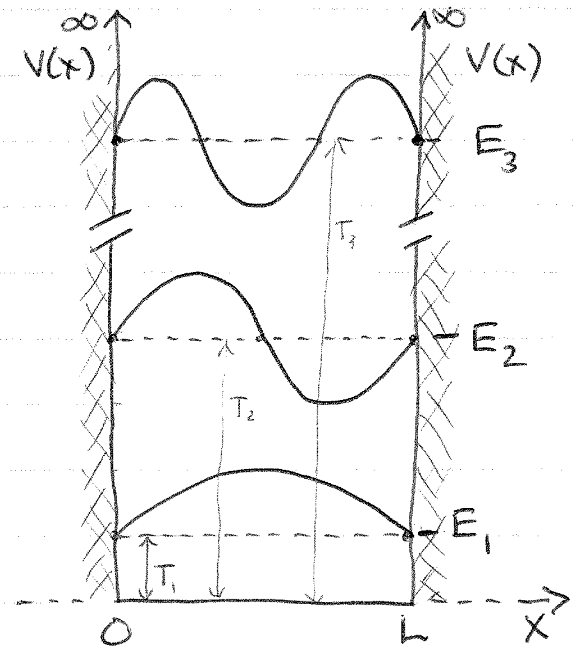
$\hat{E} = \underbrace{i\hbar\frac{\partial}{\partial t}}_{\text{TDSE}}$ or $\underbrace{E}_{\text{TISE}}$ "energy"

2) $\int_{-\infty}^{\infty} dx\, |\Psi|^2 = 1$ "probability density"

3) $\Psi(x), \frac{\partial\Psi}{\partial x}$ are a) continuous b) finite c) single-valued d) $\to 0$ as $x \to \pm\infty$

"normalizable" "well-behaved"

* infinite square well



a) at $x<0$ or $x>L$:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \underbrace{\infty\cdot\psi(x) = E\cdot\psi(x)}_{\psi(x)=0\ !}$$

b) between $0<x<L$

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

$$\psi(x) = e^{ikx} = \cos(kx) + i\sin(kx)$$

$$\Rightarrow A\cos(kx) + B\sin(kx)$$

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \boxed{\frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2} = \hbar\omega_n$$

$$p_n = \hbar k_n = \frac{\hbar n\pi}{L}$$

c) boundary conditions.

$0 = \psi(0) = A$ (LHS)

$0 = \psi(L) = B\sin(kL)$ $\quad k_nL = n\pi$

d) normalization:

$$\int_{-\infty}^{\infty} dx\, |\psi|^2 = \int_0^L B^2\sin^2(k_nx) = B^2\cdot\frac{L}{2} = 1$$

e) solution: $\boxed{\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)}$

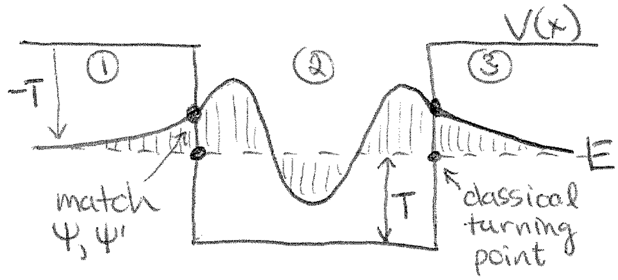
time-dependence: $\Psi_n(x,t) = \underbrace{\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)}_{\psi(x)}\underbrace{e^{-i\omega_n t}}_{\phi(t)} = \frac{1}{2i}\sqrt{\frac{2}{L}}\left\{e^{i(k_nx-\omega_nt)} - e^{i(k_nx+\omega_nt)}\right\}$

standing "skipping rope" wave

= counterpropagating travelling waves.

* <u>finite square well</u>

$$\underbrace{\frac{-\hbar^2}{2m}\overbrace{\frac{\partial^2}{\partial x^2}}^{ik}}_{\frac{\hbar^2k^2}{2m}=\frac{p^2}{2m}}\psi = \underbrace{\left[E-V(x)\right]}_{T}\psi$$



- find the solution for ψ in each region of constant V: ①②③

  ②: $\boxed{\psi = e^{ikx}}$ $\quad k = \sqrt{2mT}/\hbar = \sqrt{2m(E-V)}/\hbar$

  oscillatory, spatial frequency $k \sim \sqrt{T}$

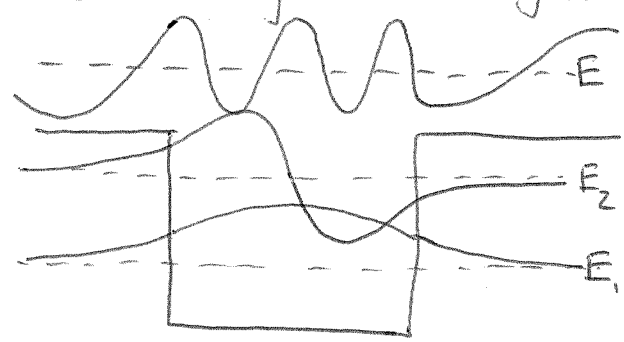
  ①,③: $E-V(x) < 0$! classically forbidden.

  $$k = \sqrt{2m(E-V)}/\hbar = \sqrt{-2m\underbrace{(V-E)}_{\text{positive}}}/\hbar$$

  $\boxed{\psi = e^{-\kappa}}$

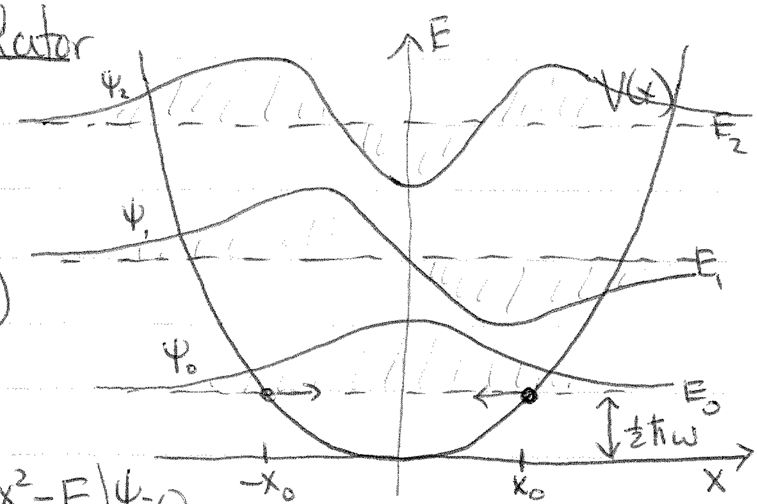
  $$= i\sqrt{2m(V-E)}/\hbar \equiv i\kappa$$

  exponential decay in classically forbidden region "evanescent wave"



- final wave function:
  - match up $\psi(x)$, $\psi'(x)$ on the boundary.
  - $\psi(x) \to 0$ as $x \to \pm\infty$
  - still get a quantization of "n" oscillations in the well.
  - only a finite number of bound states.

Simple Harmonic Oscillator



classical: $ma = F = -kx$

$$m\ddot{x} + kx = 0$$
$$-m\omega^2 + k = 0 \quad (x = e^{i\omega t})$$
$$\omega^2 = k/m$$

quantum: $\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + \left(\frac{1}{2}m\omega^2 x^2 - E\right)\psi = 0$

$$V = \tfrac{1}{2}kx^2 = \tfrac{1}{2}m\omega^2 x^2$$

ground state: $E_0 = \frac{1}{2}\hbar\omega$ at $x_0 = \sqrt{\frac{\hbar}{m\omega}}$

so let $\epsilon = E/E_0$ and $\xi = x/x_0$

$$\frac{\partial^2\psi}{\partial\xi^2} + (\varepsilon - \xi^2)\psi = 0$$

now, let $\psi = h(\xi)e^{-\frac{1}{2}\xi^2}$

then $\frac{\partial^2\psi}{\partial\xi^2} = \frac{\partial}{\partial\xi}\left[h'\cdot e^{-\frac{1}{2}\xi^2} + h\cdot(-\xi)\cdot e^{-\frac{1}{2}\xi^2}\right]$

$$= h''\cdot e^{-\frac{1}{2}\xi^2} + \underbrace{h'(-\xi)e^{-\frac{1}{2}\xi^2} + h'(-\xi)e^{-\frac{1}{2}\xi^2}} - he^{-\frac{1}{2}\xi^2} + h\xi^2 e^{-\frac{1}{2}\xi^2}$$
$$= \left(h'' - 2\xi h' + (\xi^2 - 1)h\right)e^{-\frac{1}{2}\xi^2}$$

so $\boxed{h'' - 2\xi h' + (\varepsilon - 1)h = 0}$ differential equation for Hermite polynomials.

$$\varepsilon = 2n + 1$$

n	ε	$h(\xi)$	$\psi(x)$	E_n
0	1	1	$A_0 e^{-m\omega x^2/2\hbar}$	$\frac{1}{2}\hbar\omega$
1	3	2ξ	$A_1\sqrt{\frac{m\omega}{\hbar}}\, x\, e^{-m\omega x^2/2\hbar}$	$3/2\ \hbar\omega$
2	5	$4\xi^2 - 2$	$A_2\left(1 - \frac{2m\omega x^2}{\hbar}\right)e^{-m\omega x^2/2\hbar}$	$5/2\ \hbar\omega$
3	7	$8\xi^3 - 12\xi$	$A_3\left(3x - 2\frac{m\omega}{\hbar}x^3\right)\sqrt{\frac{m\omega}{\hbar}}\, e^{-\frac{m\omega x^2}{2\hbar}}$	$7/2\ \hbar\omega$
4	9	$16\xi^4 - 48\xi^2 + 12$	$A_4 \cdots$	$9/2\ \hbar\omega$