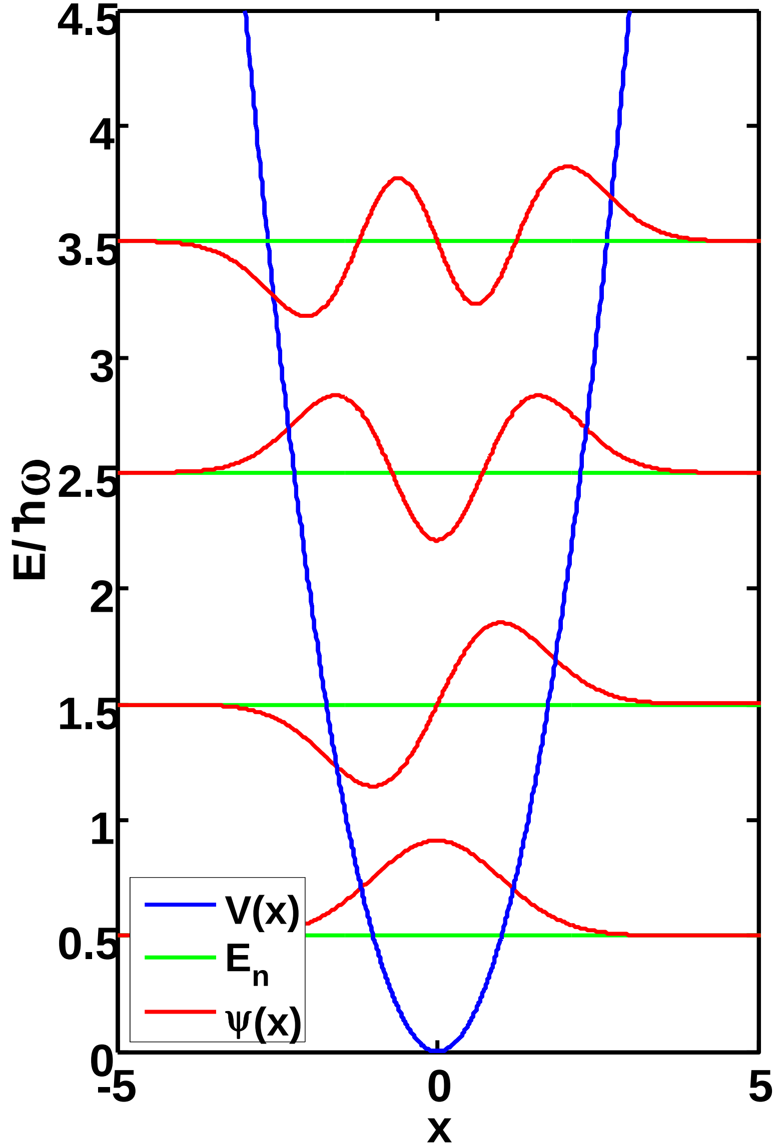
Lecture 18: 02/27/09

- Finite square well:
  - E_n, $\psi_n(x)$
- The simple harmonic oscillator potential:

$$V(x) = \frac{1}{2} C x^2$$



Recap

$II_{2,3}$ Qualitative Plots of Bound-State Wave Functions:

1) The amount of curvature increases with increasing $|V-E|$

1a) $\psi(x)$ oscillates when $E > V$

1b) $\psi(x)$ has curvature away from x-axis, when $E < V$

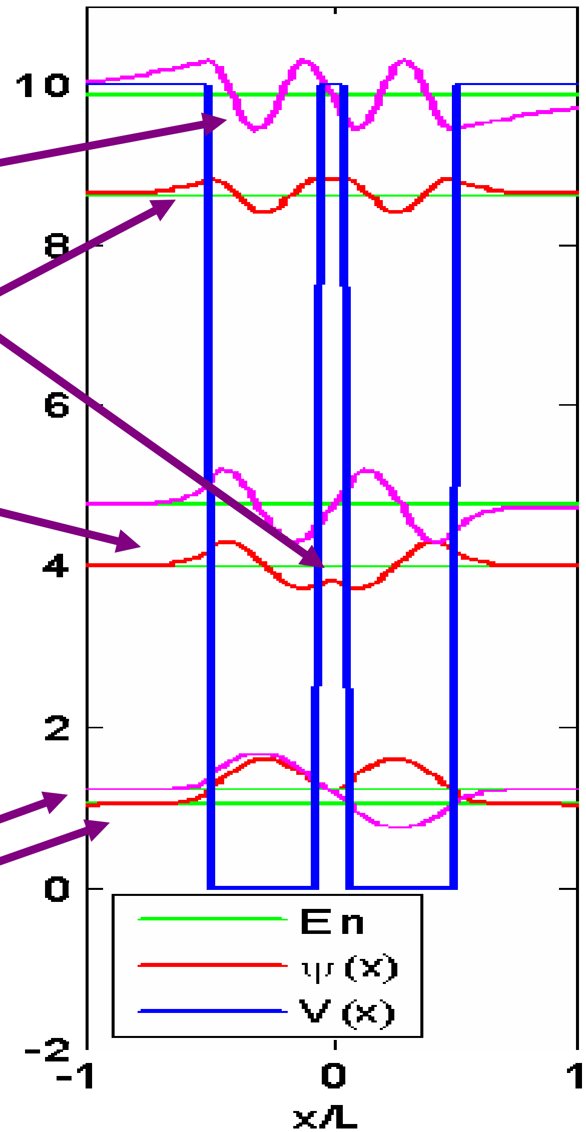
2) The n^{th} energy level has $n-1$ zero crossings

3) When $E > V$, larger $E-V$ gives smaller wave amplitude

4) symmetric potential $V(x)$: $\psi(x)$ is symmetric or antisymmetric

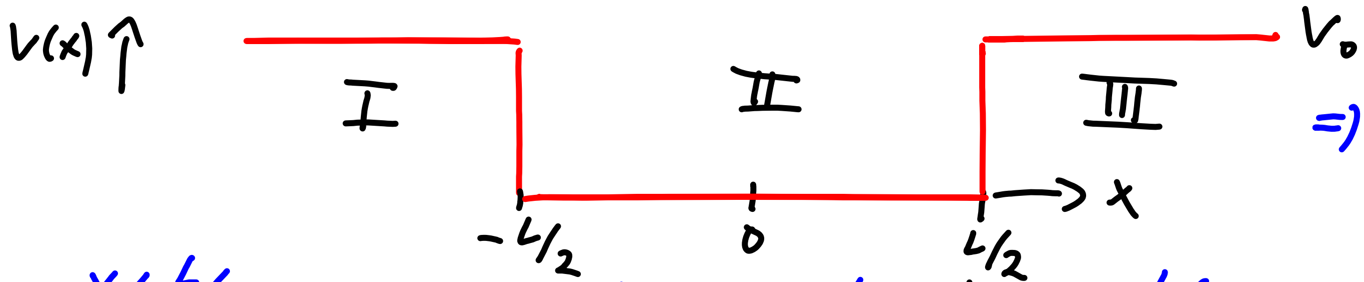
5) $\psi(x) \xrightarrow[x \to \pm\infty]{} 0$

n=3



$II_{2,4}$ Square Well of Finite Depth, part II :

Recap:



$\Rightarrow$ solve SE in 3 sections

$x < -L/2$	$-L/2 \le x \le L/2$	$x > L/2$	
even solutions: $\psi(x) = D\, e^{\alpha x}$	$\psi(x) = B \cos(kx)$	$\psi(x) = D\, e^{-\alpha x}$	$: \psi(x) = \psi(-x)$
odd solutions: $\psi(x) = -D\, e^{\alpha x}$	$\psi(x) = A \sin(kx)$	$\psi(x) = D\, e^{-\alpha x}$	$: \psi(x) = -\psi(-x)$
$\alpha = \dfrac{\sqrt{2m(V_0 - E)}}{\hbar}$	$k = \dfrac{\sqrt{2mE}}{\hbar}$	$\alpha = \dfrac{\sqrt{2m(V_0 - E)}}{\hbar}$	

Boundary conditions at $x = \pm L/2$
+ normalization $\left(\psi(x) \xrightarrow[x \to \pm\infty]{} 0\right)$

$\Rightarrow$ allowed energies

$\Rightarrow$ prefactors A_n (B_n) D_n of $\psi(x)$

- Even functions/states:

inside well: $-\frac{L}{2} \le x \le \frac{L}{2}$ $\quad \psi(x) = B\cos(kx)$ $\quad \frac{d\psi}{dx} = -BK\sin(kx)$

outside well: $x \ge L/2$ $\quad \psi(x) = D\, e^{-\alpha x}$ $\quad \frac{d\psi}{dx} = -\alpha D e^{-\alpha x}$

- continuity of $\frac{d\psi}{dx}$ at $x = L/2$: $\quad Bk\sin(k\frac{L}{2}) = \alpha D e^{-\alpha L/2}$

- continuity of $\psi(x)$ at $x = L/2$: $\quad B\cos(k\frac{L}{2}) = D e^{-\alpha \frac{L}{2}}$

- divide these equ. $\Rightarrow$ $\quad k\tan\left(\frac{kL}{2}\right) = \alpha$

$$\Rightarrow \quad \underline{\tan\left(\frac{kL}{2}\right) = \frac{\alpha}{k}}$$

insert k, α:

$$\tan\left[\frac{L}{2\hbar}\sqrt{2mE}\right] = \frac{\sqrt{2m(V_0-E)}}{\sqrt{2mE}} = \sqrt{\frac{V_0-E}{E}} = \sqrt{\frac{V_0}{E}-1}$$

$\Rightarrow$ get equation for allowed energies E_n of particle

$\Rightarrow$ get transcendental equation, can <u>not</u> be solved algebraically

$\Rightarrow$ solve numerically or graphically

$\Rightarrow$ for graphical solution:

introduce: $\theta \equiv \frac{kL}{2} = \frac{L}{2\hbar}\sqrt{2mE} \Leftrightarrow E = \frac{\left(\frac{2\hbar\theta}{L}\right)^2}{2m}$

$$\theta_0 \equiv \frac{L}{2\hbar}\sqrt{2mV_0}$$

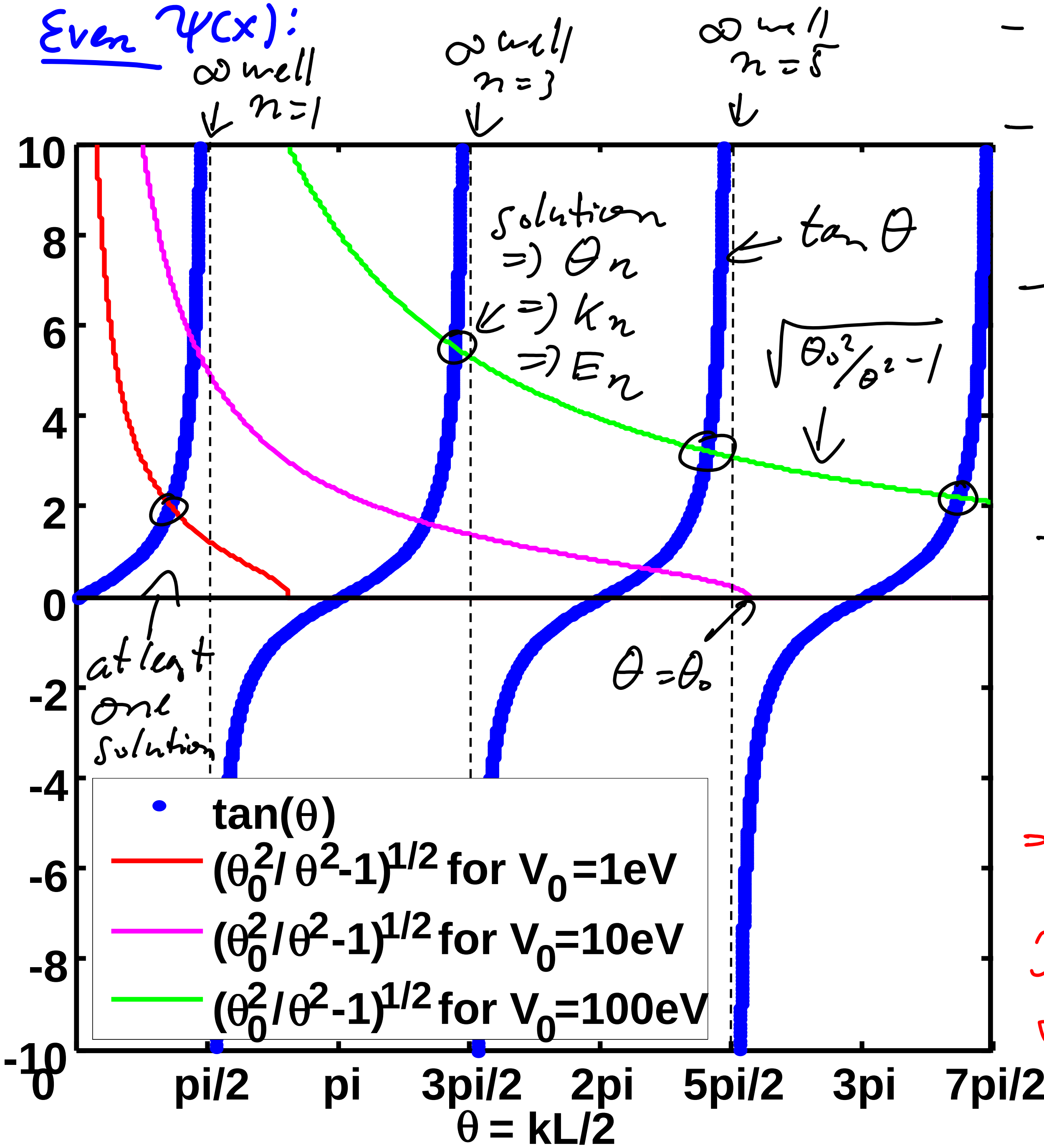
$$\Rightarrow \frac{V_0}{E} = \frac{V_0\, 2m}{\left(\frac{2\hbar\theta}{L}\right)^2} = \frac{V_0\, 2m\, \left(L/2\hbar\right)^2}{\theta^2} = \frac{\theta_0^2}{\theta^2}$$

$$\Rightarrow \tan(\theta) = \sqrt{\frac{\theta_0^2}{\theta^2}-1}$$

$\Rightarrow$ plot both sides of equ. as function of $\theta = kL/2$

$\Rightarrow$ when graphs intersect $\Rightarrow$ solution $\Rightarrow E_n$

Even $\psi(x)$:



- $\Theta_0 = \frac{L}{2\hbar}\sqrt{2mV_0} \propto \sqrt{V_0}$
- $\sqrt{\frac{\Theta_0^2}{\Theta^2}-1}$ goes to zero for $\Theta = \Theta_0 \propto \sqrt{V_0}$
- for 1-D well: no matter how small V_0, there is at least one solution (i.e. bound state!)
- for large V_0: solutions for $\theta = \frac{kL}{2} = \frac{2\pi}{\lambda}\frac{L}{2}$ is a little less than $\frac{\pi}{2}, \frac{3\pi}{2}, \ldots$ $= n\frac{\pi}{2}$ $n = 1, 3, 5, \ldots$

$\Rightarrow L \lesssim n\lambda/2$
$\lambda_n \gtrsim 2L/n$
λ is a little longer than for even solutions in the ∞ well!

- **Odd wave functions / bound states:**

inside well: $-\frac{L}{2} \leq x \leq \frac{L}{2}$: $\psi(x) = A\sin(kx) \Rightarrow \frac{d\psi}{dx} = kA\cos kx$

outside well: $x > \frac{L}{2}$: $\psi(x) = De^{-\alpha x}$ $\quad \frac{d\psi}{dx} = -\alpha D e^{-\alpha x}$

- continuity of $\frac{d\psi}{dx}$ at $x = L/2$: $kA\cos(k\frac{L}{2}) = -\alpha D e^{-\alpha L/2}$

- continuity of $\psi(x)$ at $x = L/2$: $A\sin(k\frac{L}{2}) = De^{-\alpha L/2}$

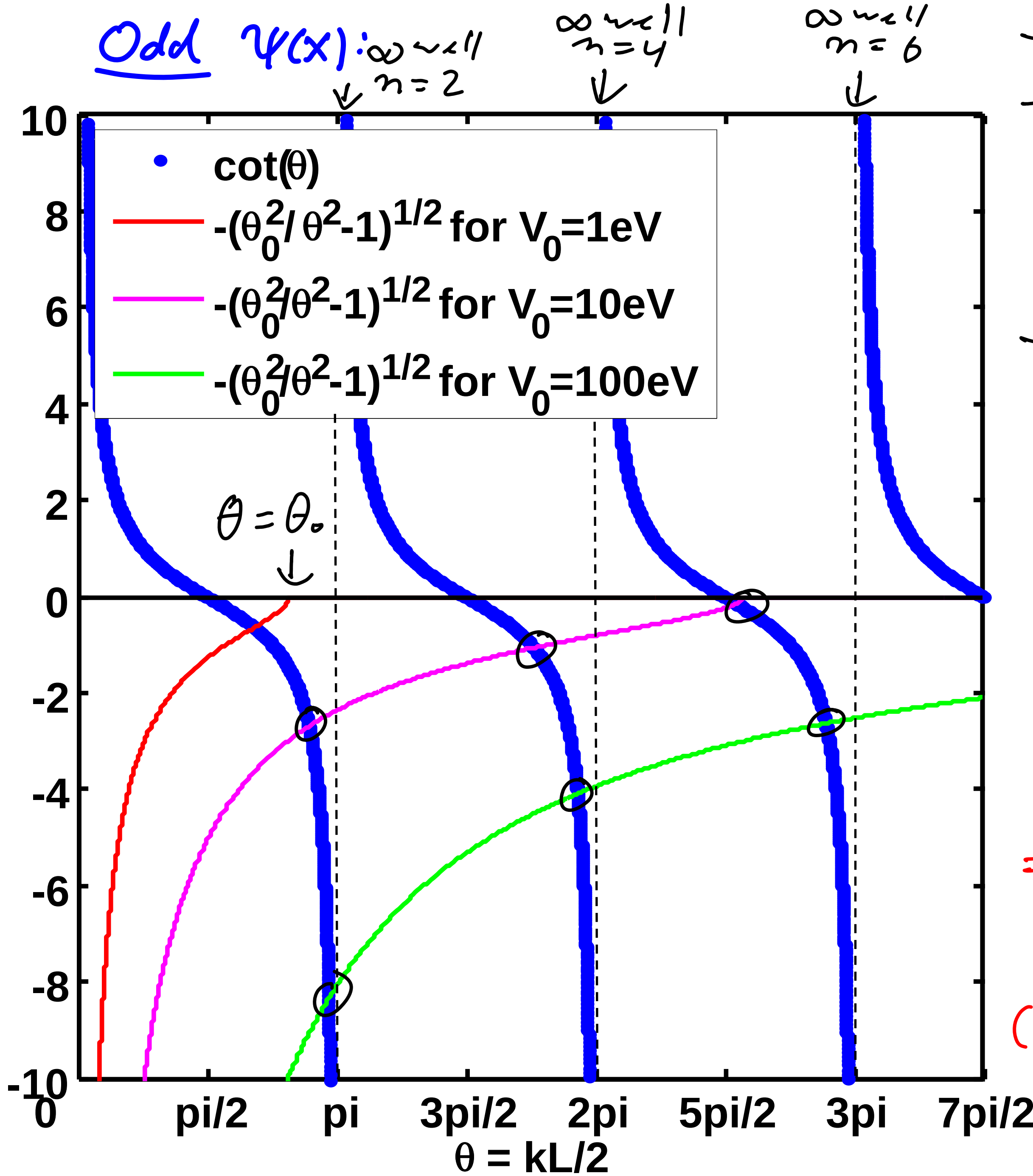
- divide: $k\cot(kL/2) = -\alpha$

$\Rightarrow \cot(kL/2) = -\alpha/k$

with $\theta = \frac{kL}{2}$, $\frac{\alpha}{k} = \sqrt{\frac{V_0}{E} - 1}$, $\theta_0 = \frac{L}{2\hbar}\sqrt{2mV_0}$ as before..

$$\Rightarrow \cot(\theta) = -\sqrt{\frac{\theta_0^2}{\theta^2} - 1}$$ $\Rightarrow$ solve graphically..

Odd $\psi(x)$:



– $\theta_0 \propto \sqrt{V_0}$

– for shallow well: <u>not</u> always an odd bound state solution (if $\theta_0 < \frac{\pi}{2}$)

– for large V_0: solutions for $\theta = \frac{kL}{2} = \pi \frac{L}{\lambda}$ are a little less than $n\frac{\pi}{2}$, if $n = 2, 4, 6, \ldots$

$\Rightarrow L \lesssim n\,\lambda/2$

$\Rightarrow \lambda \gtrsim 2L/n$

$\Rightarrow \lambda$ is a little <u>larger</u> than for odd solution of the infinite well (to fit smoothly to evanescent waves)

- Allowed particle energies E_n in finite square well:

- $k_n = \frac{\sqrt{2mE_n}}{\hbar}$ from graphs (from θ_n)

$\Rightarrow$ can calculate allowed energies $E_n = \frac{\hbar^2 k_n^2}{2m}$

$\Rightarrow$ from graphs: for large V_0, solutions for $\theta = \frac{kL}{2}$ are a little bit less than $n\frac{\pi}{2}$, $n = 1, 2, 3, \ldots$

$\Rightarrow$ $k_n \lesssim \frac{n\pi}{L}$

$\Rightarrow$ $E_n \lesssim \frac{\hbar^2 n^2 \pi^2}{2mL^2} = \underbrace{\frac{h^2 n^2}{8mL^2}}$

$\Rightarrow$ $E_n \lesssim$ E_n for infinite square well!

- Wave functions in finite square well:

  - Know $E_n \rightarrow k_n, \alpha_n$
  - what about $\psi(x)$ and the prefactors A (or B), D?

- for <u>even</u> $\psi(x)$ case:

  continuity of $\psi(x)$ at $x = L/2$: $B_n \cos\left(\frac{k_n L}{2}\right) = D_n e^{-\alpha_n \frac{L}{2}}$

  $$\Rightarrow D_n = B_n \frac{\cos(k_n L/2)}{e^{-\alpha_n L/2}}$$

  $\Rightarrow$ determine B_n by normalizing $\psi(x)$

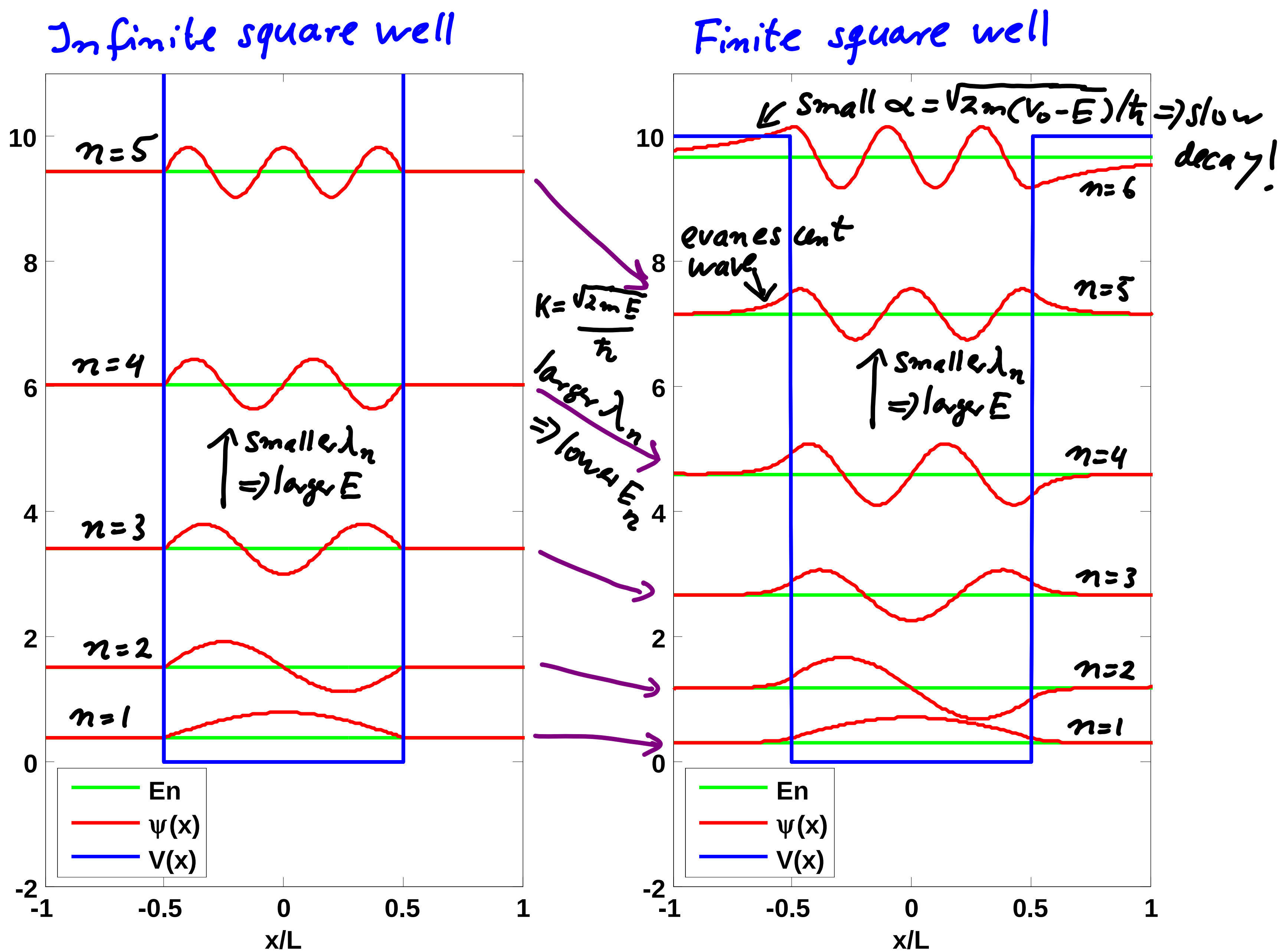
  $$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1$$

- for odd solutions:

  continuity of $\psi(x)$ at $x = L/2$

  $$\Rightarrow D_n = A_n \frac{\sin(k_n L/2)}{e^{-\alpha_n L/2}}$$

  $\Rightarrow A_n$ by normalizing $\psi(x)$



Infinite square well
Finite square well
n=5
n=4
n=3
n=2
n=1
smaller λ_n ⇒ larger E
$K=\frac{\sqrt{2mE}}{\hbar}$
larger λ_n ⇒ lower E_n
Small $\alpha=\sqrt{2m(V_0-E)}/\hbar$ ⇒ slow decay!
evanescent wave
n=6
n=5
n=4
n=3
n=2
n=1
smaller λ_n ⇒ larger E
En
ψ(x)
V(x)
x/L
-1
-0.5
0
0.5
1
-2
0
2
4
6
8
10

$II_{2,5}$ The simple harmonic oscillator potential $V(x)=1/2cx^2$:

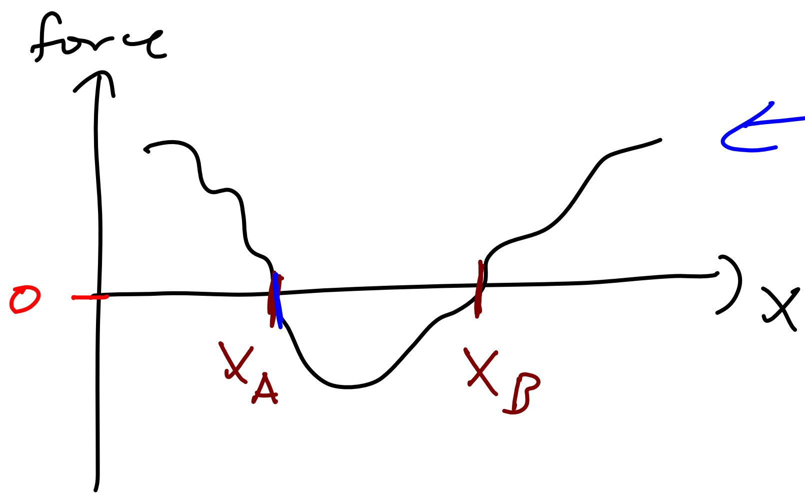
(not that simple...)

Potential: $V(x) = \frac{1}{2} c (x - x_0)^2 = \frac{1}{2} m \omega^2 (x - x_0)^2$ $\quad \omega = \sqrt{\frac{c}{m}}$

classical frequ.

Important! Basically any oscillatory motion is approximately simple harmonic, as long as the oscillation amplitude is small!

- Recall from mechanics:



arbitrary function of force vs. position

- at equilibrium: $F=0$
- stable equilibrium:
  $\Leftrightarrow$ need restoring force

$\Rightarrow$ x_A is stable, x_B is not

Near equilibrium point x_A: force is approximately linear with position

$\Rightarrow$ Formally, expand force $F(x)$ in a Taylor series about x_A:

$$F(x) = \underbrace{F(x_A)}_{0} + \underbrace{\left.\frac{dF}{dx}\right|_{x_A}}_{\equiv -c \; (c>0)} (x - x_A) + \underbrace{\text{higher order terms}}_{\text{drop for small } (x - x_A)}$$

$$\Rightarrow F(x) \approx -c\,(x - A_A) \; : \text{Hooke's law}$$

$\Rightarrow$ resulting potential energy:

$$V(x) = -\int F(x)\,dx = \frac{1}{2} c\,(x - x_A)^2$$

take $x_A = 0$ to take advantage of symmetry

$$\Rightarrow \underline{\underline{V(x)}} = \frac{1}{2} c x^2 = \frac{1}{2} m \omega^2 x^2$$

classical ω

⟹ Find bound state wave functions ψ_n and associated allowed energies E_n for $V = \frac{1}{2} m\omega^2 x^2$

- time independent Schrödinger equation:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + \frac{1}{2} m\omega^2 x^2 \psi(x) = E\,\psi(x)$$

- introduce dimensionless variables:

$$x_i \rightarrow \xi \equiv \sqrt{\frac{m\omega}{\hbar}}\; x$$

and energy in units of $\frac{1}{2}\hbar\omega$

$$\mathcal{K} \equiv \frac{E}{\frac{1}{2}\hbar\omega} \Leftrightarrow E = \frac{1}{2}\hbar\omega\mathcal{K}$$

⟹ time-indep. S.E. for simple harmonic oscill. pot.

$$\frac{d^2\psi(\xi)}{d\xi^2} = (\xi^2 - \mathcal{K})\,\psi(\xi)$$