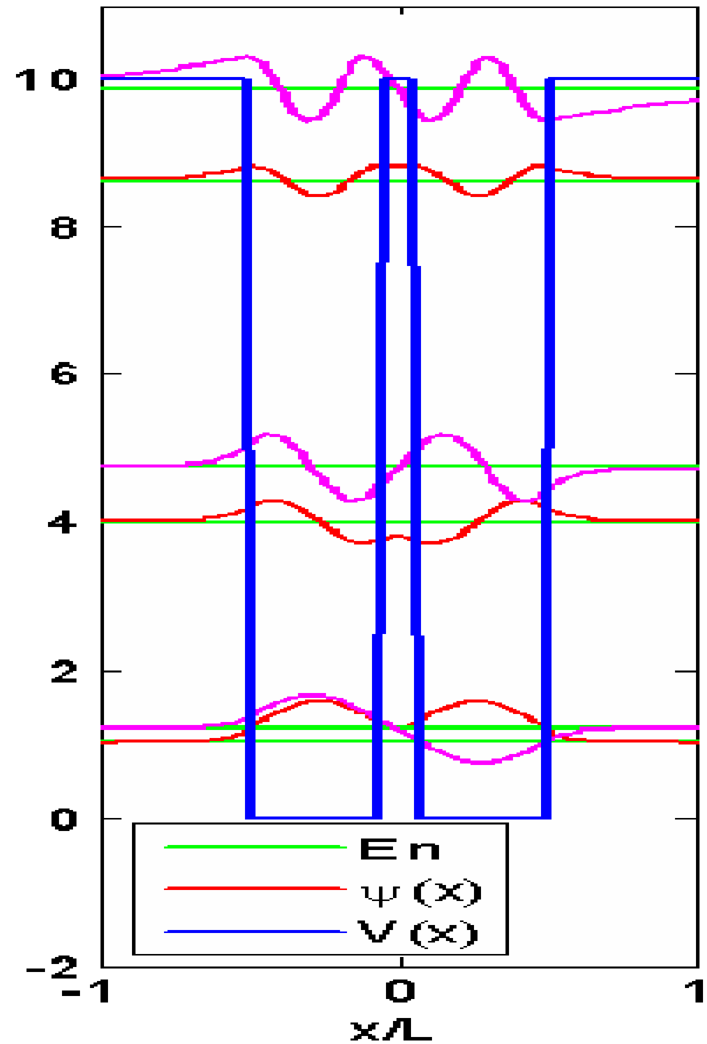
Lecture 16: 02/23/09

- Square well with finite depth
  - Boundary conditions
  - Evanescent waves

- Qualitative plots of bound-state wave functions



Recap

- **General Solution of the time-dependent SE:**

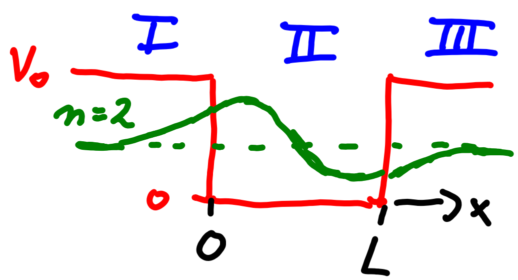
$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-i\frac{E_n}{\hbar}t} \Rightarrow \Psi(x,t=0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

to find c_n:

$$\boxed{c_n = \int_{-\infty}^{+\infty} \psi_n^*(x)\, \Psi(x,t=0)\, dx}$$

$|c_n|^2$ = probability that a measurement yields value E_n

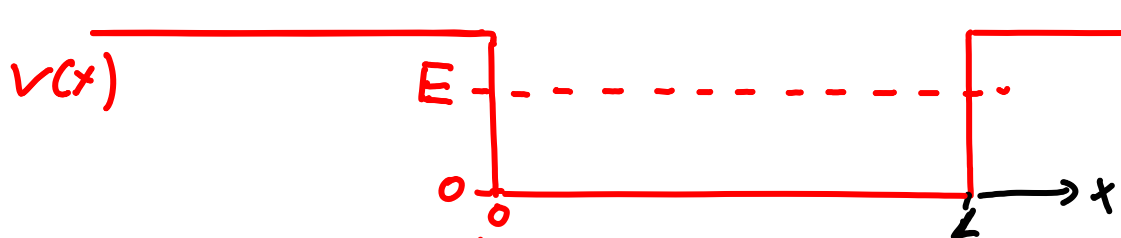
$II_{2,2}$ Square Well of Finite Depth:



1) Solve time-indep. SE for segments
2) Join pieces of $\psi(x)$

$\Rightarrow$ Need to have decaying exponential waves in region I, III

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



$\Rightarrow$ Solve time-indep. SE for segments!

$x < 0 \Rightarrow E < V_0$

$\psi(x) = C e^{\alpha x} + D e^{-\alpha x}$

require $\psi(x) \xrightarrow[x \to -\infty]{} 0$

$\Rightarrow D = 0$

$\Rightarrow \psi(x) = C e^{\alpha x}$

$\alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

$0 \leq x \leq L \Rightarrow E > V(x)$

$\psi(x) = A \sin(kx) + B \cos(kx)$

$k = \frac{\sqrt{2mE}}{\hbar}$

$x > 0 \Rightarrow E < V_0$

$\psi(x) = C e^{\alpha x} + D^{-\alpha x}$

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

$\Rightarrow C = 0$

$\Rightarrow \psi(x) = D e^{-\alpha x}$

$\alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

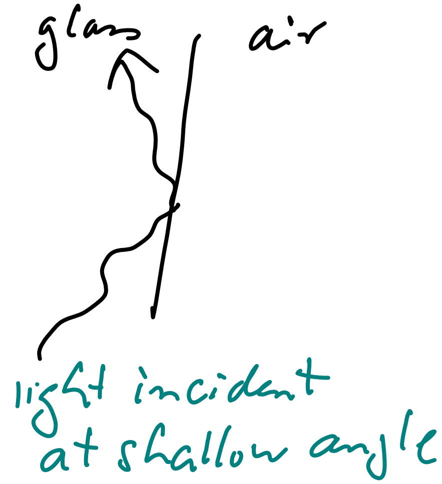
decaying exponential solutions!

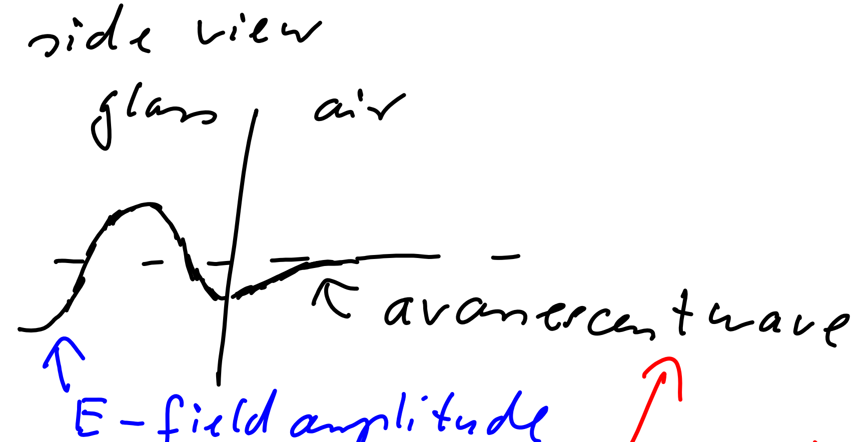
1) $\Rightarrow$ Probability of finding particle outside the well > 0!

2) How to join the pieces of $\psi(x)$ [i.e. find A, B, C, D]?

1) Probability of finding the particle outside the well > 0:

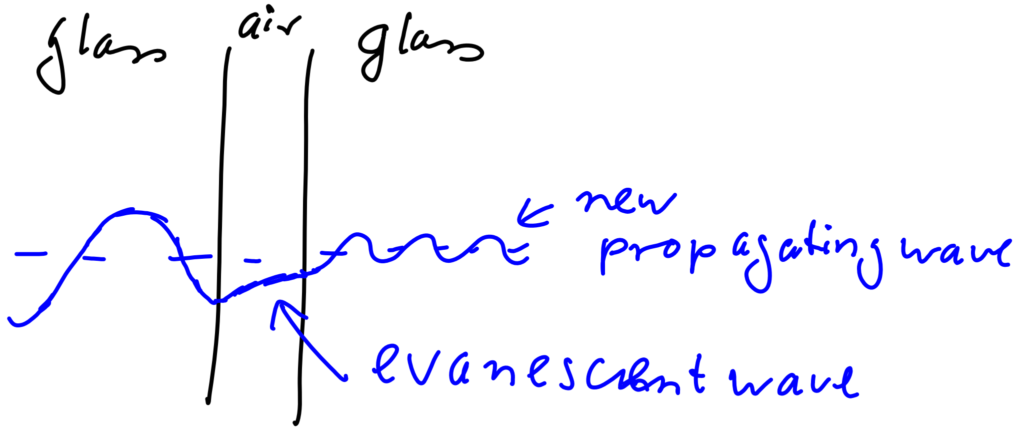
- recall: Evanescent waves
  - e.g. light in total internal reflection:





$E(x) \propto \underbrace{e^{-\alpha x}}\, e^{i\omega t}$

decaying exponential wave



light can propagate through thin air gap

⇒ particle waves can travel through thin potential wall

⇒ tunnel effect

2) How to join the pieces of $\psi(x)$ at boundaries $x=0, x=L$?

a) wave function must be normalizable

$$\Rightarrow \; |\psi(x)|^2 \longrightarrow 0 \quad \text{for } x \longrightarrow \pm\infty$$

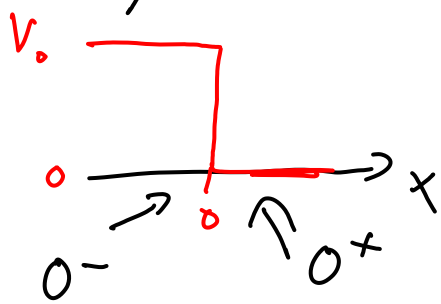
b) wave functions must be smooth

$\Rightarrow$ $\psi(x)$ and $\dfrac{d\psi(x)}{dx}$ must be continuous everywhere (also at boundaries!)

$\Rightarrow$ For <u>bound</u> particles, (a) and (b) together can be satisfied only for certain discrete particle energies!

$\Rightarrow$ quantization of energy!

Why? • consider one boundary



$\Rightarrow$ time-indep. S.E.: $\dfrac{d^2\psi}{dx^2} = -\dfrac{2m}{\hbar^2}\{E - V(x)\}\psi(x)$

$\Rightarrow$ jump in $V(x)$ requires jump in $\dfrac{d^2\psi}{dx^2}$

$\Rightarrow$ $\dfrac{d^2\psi(x)}{dx^2}$ is <u>not</u> continuous when $V(x)$ has steps

<u>But:</u> $\dfrac{d\psi}{dx}$ and $\psi(x)$ are still continuous:

Integrate S.E. $\displaystyle\int_{-d}^{+d}\frac{d^2\psi}{dx^2}\,dx = -\frac{2m}{\hbar^2}\int_{-d}^{+d}\underbrace{(E - V(x))\,\psi(x)\,dx}_{\text{if } V(x) \text{ is finite}} = \left.\frac{d\psi}{dx}\right|_{-d}^{+d}$

$\Rightarrow$ for $d \to 0$ $\quad \dfrac{d\psi}{dx}(0^+) - \dfrac{d\psi}{dx}(0^-) = 0$ ($\Leftarrow$ <u>not</u> for infinite square well!)

$\Rightarrow$ $\dfrac{d\psi}{dx}(0^+) = \dfrac{d\psi}{dx}(0^-)$ $\Rightarrow$ continuous at boundaries

$\Rightarrow$ $\psi(x)$ is also continuous!

$\Rightarrow$ for finite square well:

$\psi(x)$ and $\frac{d\psi}{dx}$ must be continuous everywhere (also at boundaries $x=0$, $x=L$: boundary conditions)

Note: 1) Need to have evanescent waves (i.e. $C, D \neq 0$)!

- Try without: $C=0$, $D=0 \Rightarrow \psi(0), \frac{d\psi}{dx}(0) = 0$

  inside well: $\psi = A\sin(kx) + B\cos(kx)$

  $\Rightarrow$ to make $\psi(x)$ continuous at $x=0 \Rightarrow B=0$

  $\Rightarrow$ to make $\frac{d\psi}{dx}$ continuous at $x=0 \Rightarrow A=0$

  $\Big\}$ $\psi(x) = 0$ for all x...

2) Boundary conditions can only be satisfied for certain energies of the particle (or $\psi(x)$ can not be normalized!)

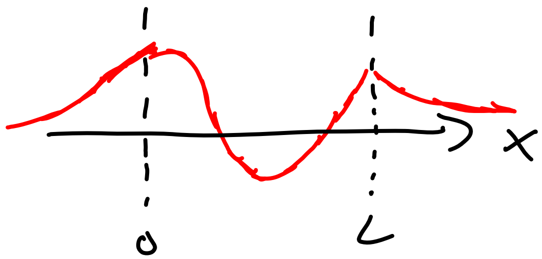
why?: have $\underline{\underline{4}}$ indep. parameter: $\frac{B}{A}, \frac{C}{A}, \frac{D}{A}$ (use A to normal. ψ) and k $\Leftrightarrow$ have $\underline{\underline{4}}$ boundary conditions (ψ, $\frac{d\psi}{dx}$ continuous at $x=0$ and $x=L$)

$\rightarrow$ only discrete energies (k-values) are allowed!

$\rightarrow$ this is a general property of bound states!

Examples: <u>If energy assumed is **wrong**, i.e. **not allowed:**</u>

1)

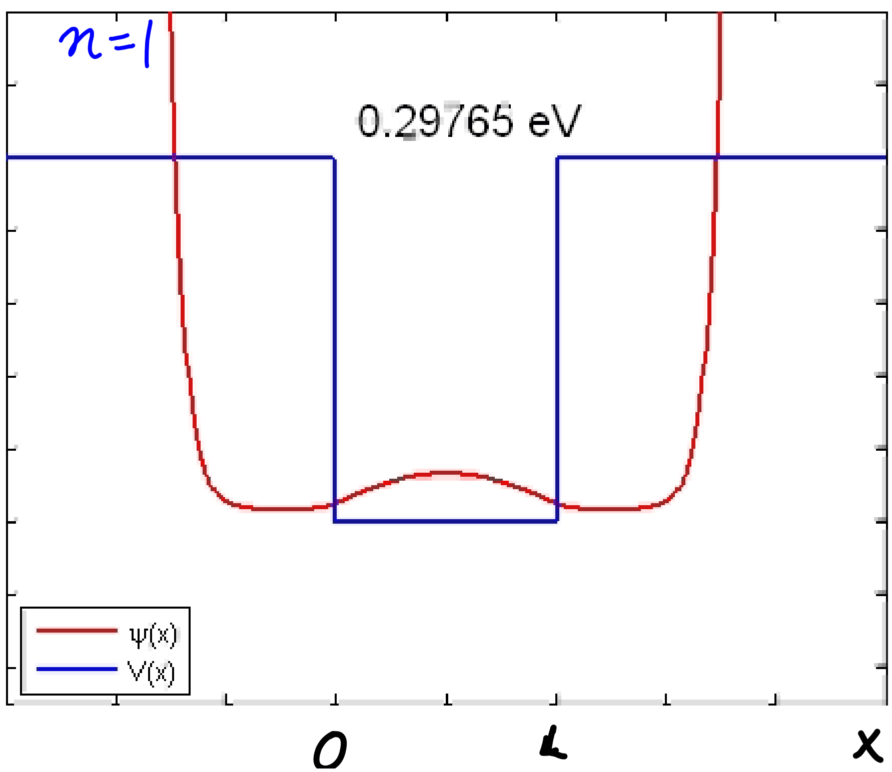


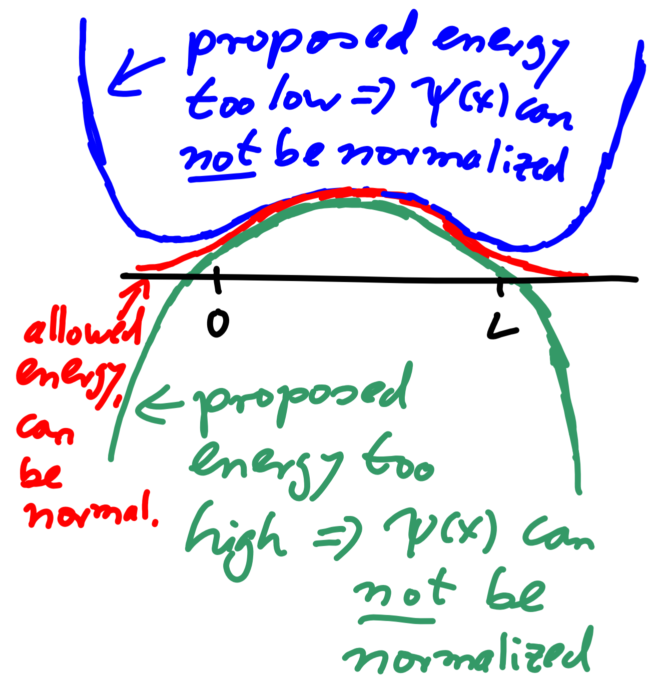
$\rightarrow \psi(x) \xrightarrow[x \to \pm\infty]{} 0$ but

can't join curves without dis-continuity in $d\psi/dx \Rightarrow$ energy not allowed

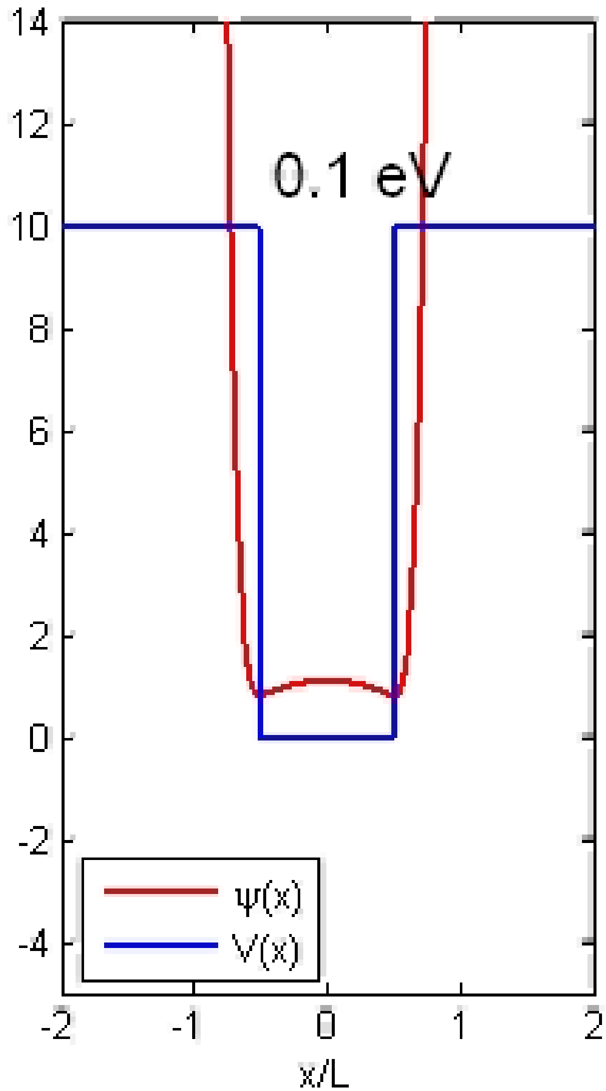
$\Rightarrow$ only at certain energies get right fractional numbers of wavelengths between 0 and L to join parts smoothly!

2)

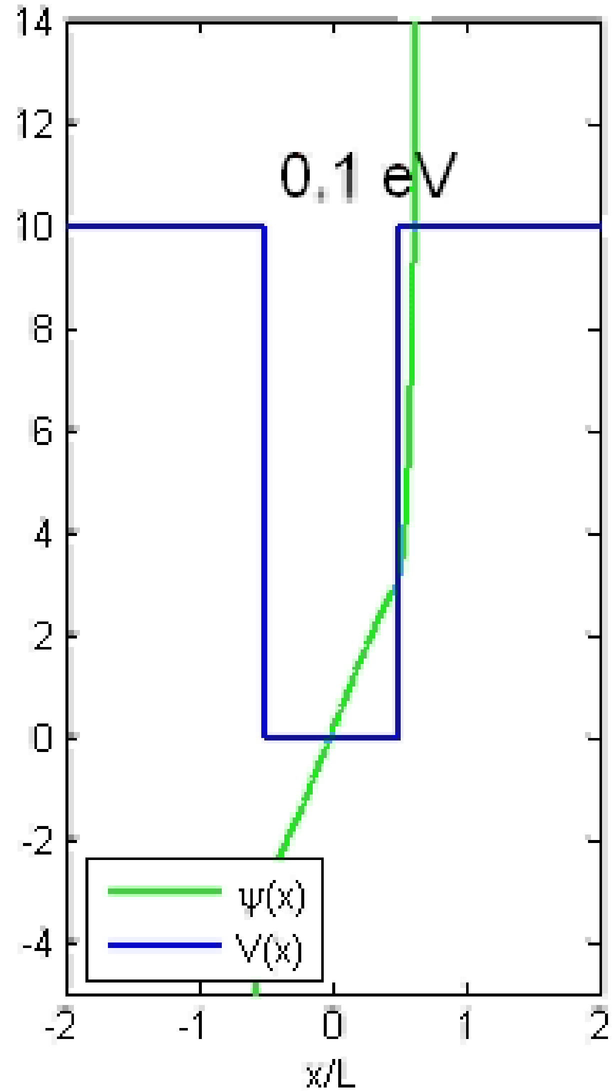




Even wave function



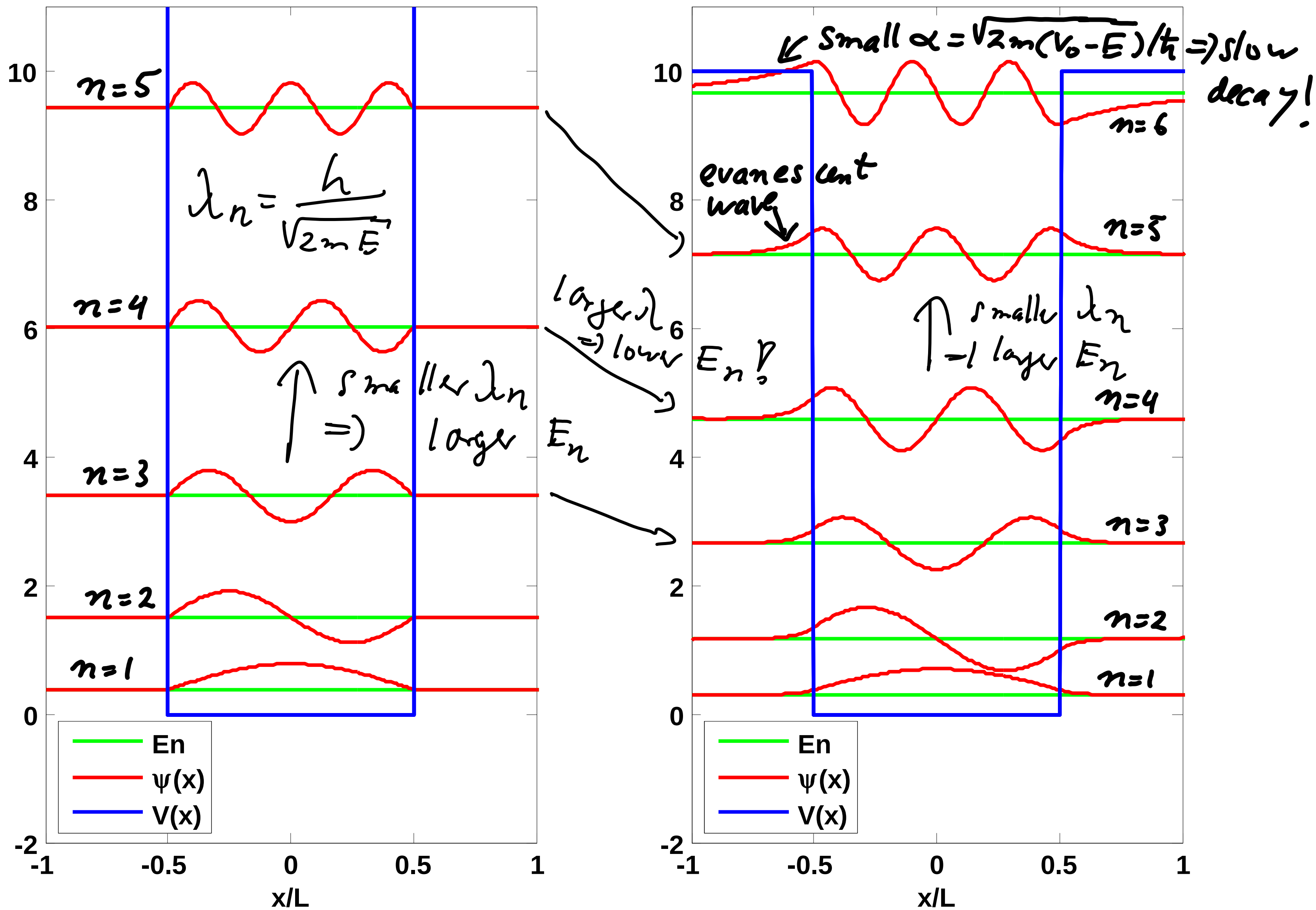
Odd wave function



⇒ For bound states: set of stationary states with discrete energy spectrum!

- **Solutions $\psi(x)$:**
  - # of nodes = $n-1$
  - still alternately even/odd solutions wrt. center of well

Infinite square well   Finite square well



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

given potential $V(x)$ $\Rightarrow$ goal: sketch solutions of stationary state $\psi(x)$ qualitatively, i.e. without solving S.E.

$\Rightarrow$ guidelines:

1) Curvature $\frac{d^2\psi}{dx^2}$

2) # of nodes (# of zero crossings) in stationary state wave functions

3) Amplitude of the wave function $\psi(x)$

4) Symmetry