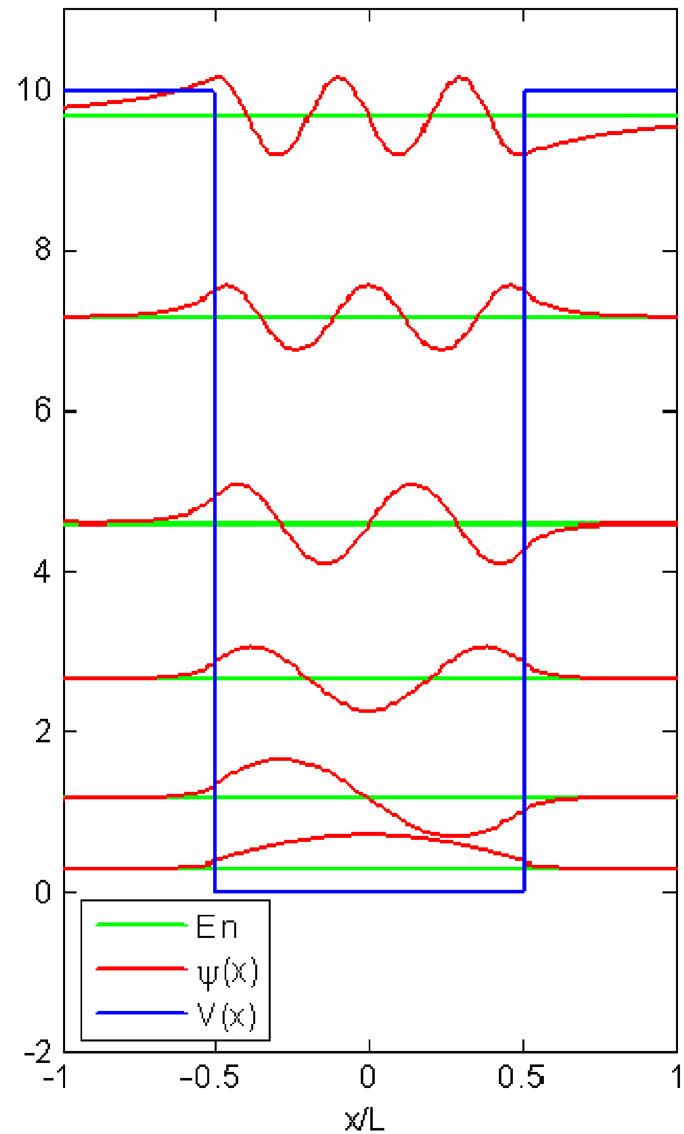
Lecture 15: 02/20/09

- The infinite square well
  - general solution

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



Recap

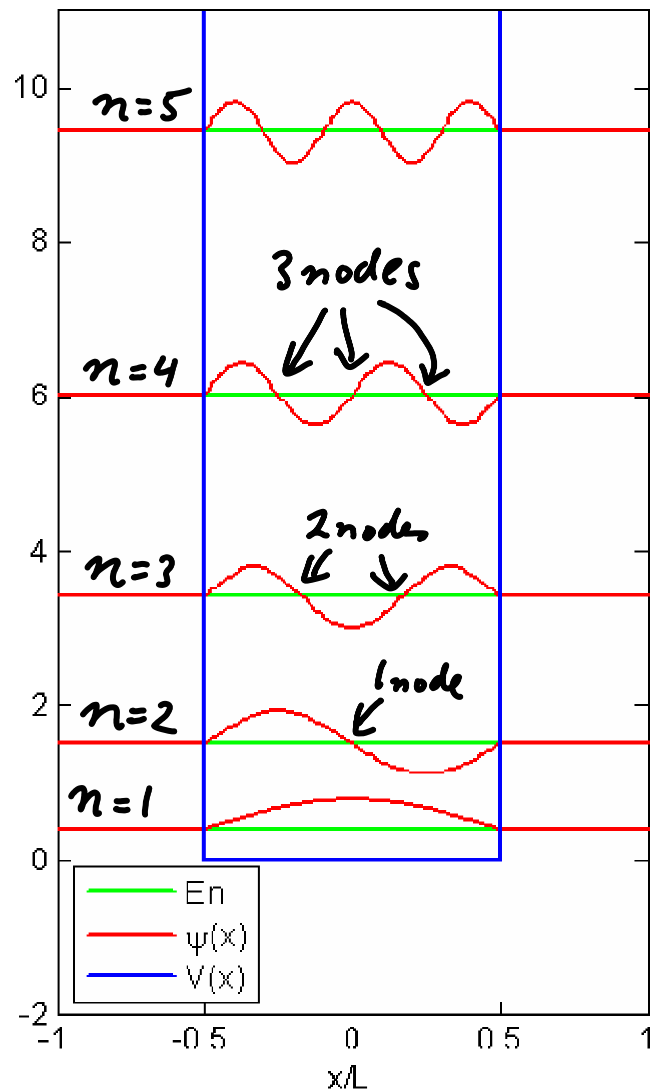
$II_{2,1}$ Infinite Square Well – Particle in a Box:

- Stationary states $\psi_n(x)$:

$$\Psi_n(x,t) = \underbrace{\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)}_{\psi_n(x)} e^{-i\frac{\hbar\pi^2}{2mL^2}n^2 t}$$

Quantized $E_n = \frac{\hbar^2\pi^2}{2mL^2}n^2 \qquad n = 1, 2, \ldots$

Quantization is result of boundary conditions at x=0 and x=L: $\psi(x)$ is continuous!



- Properties of stationary states:
  - alternately even and odd wrt. center of well
  - # of nodes = n-1
  - orthonormal:

$$\int_{-\infty}^{+\infty} \psi_m^*(x)\,\psi_n(x)\,dx = \delta_{mn}$$

- General solution of the time-dep. SE for infinite square well:

recall: general solution = linear combination of stationary states:

$$\Psi_n(x,t) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) e^{-i\left(\frac{n^2\pi^2\hbar}{2mL^2}\right)t}$$

$\Rightarrow$ general solution:

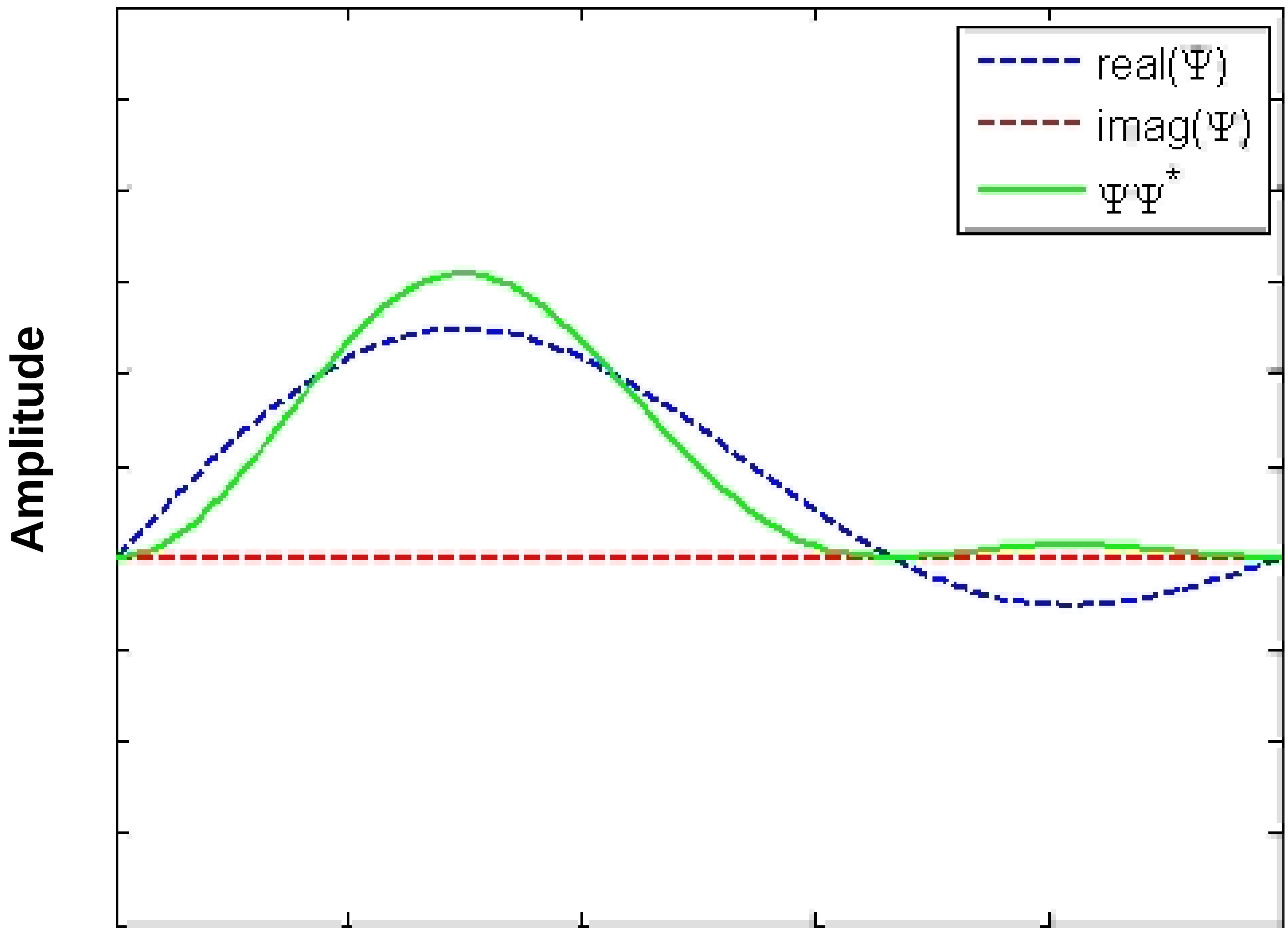
$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n}{L}x\right) e^{-i\left(\frac{n^2\pi^2\hbar}{2mL^2}\right)t}$$

add / drop $e^{-iE_n/\hbar\, t}$ factors

$$\Rightarrow \underbrace{\Psi(x,t=0)}_{\text{initial conditions (given)}} = \sum_{n=1}^{\infty} c_n \psi_n(x) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$$

need to find c_n's

Example: $\Psi(x,t=0) = \frac{1}{\sqrt{2}}\psi_1(x) + \frac{1}{\sqrt{2}}\psi_2(x)$



$\Rightarrow$ note: $|\Psi|^2$ (prob. density) is time dependent! (not a stat. state!)

$\Rightarrow$ if we know $\Psi(x, t=0)$ and stationary states $\psi_n(x)$, how can we find constants c_n?

look at: $\displaystyle\int_{-\infty}^{+\infty} \psi_n^*(x)\, \Psi(x, t=0)\, dx = \int_{-\infty}^{+\infty} \psi_n^*(x) \sum_{m=1}^{\infty} c_m \psi_m(x)\, dx$

$$= \sum_{m=1}^{\infty} c_m \int_{-\infty}^{+\infty} \psi_n^*(x)\, \psi_m(x)\, dx = \sum_{m=1}^{\infty} c_m \delta_{nm} = \underline{\underline{c_n}}$$

stat. states are ortogonal

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

$$= \int_0^L \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right) \Psi(x, t=0)\, dx \quad \Big\} \text{ for infinite square well}$$

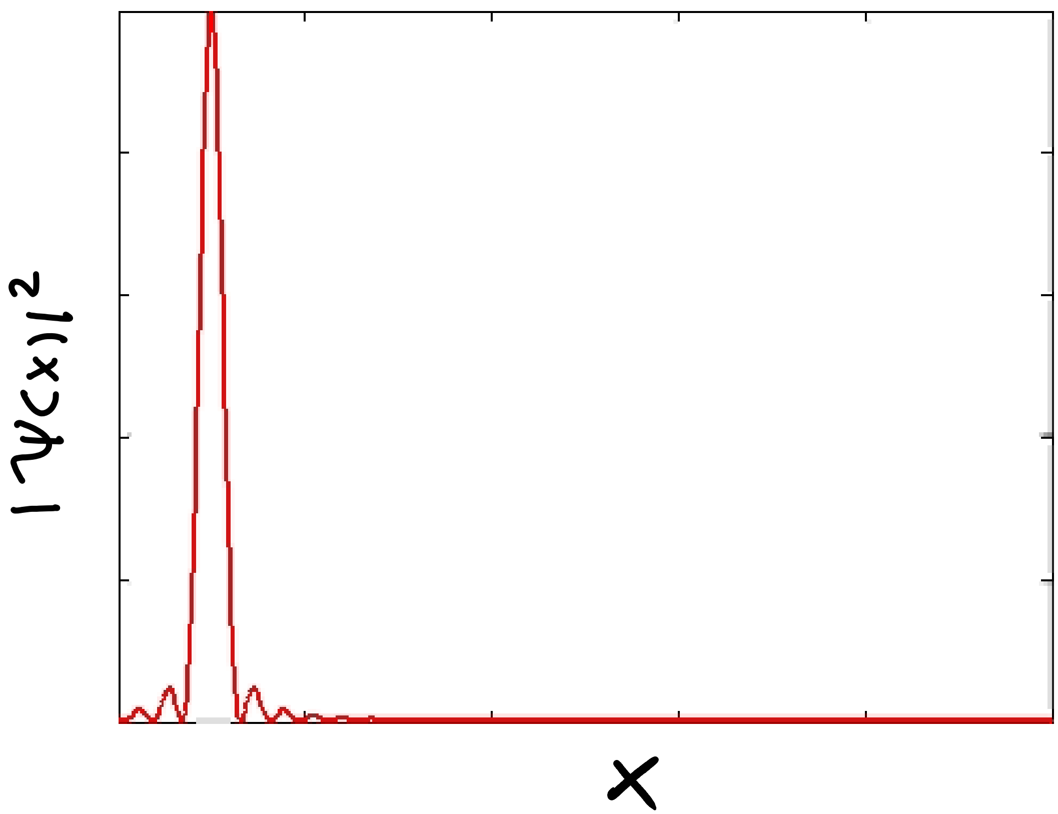
- General Solution of the time-dependent SE:

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

to find c_n:

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

Example:



A particle in an infinite square well is associated with the following initial wave function:

$$\Psi(x, t=0) = \frac{1}{\sqrt{2}} \psi_1(x) + \frac{1}{\sqrt{2}} \psi_2(x)$$

Which possible result(s) could a measurement of energy give?

A. Just E_1 or E_2

B. Something between E_1 and E_2

C. $(E_1+E_2)/2$

D. Any value

one only gets eigenvalues E_n's of given $\hat{H}$ if energy is measured

A particle in an infinite square well is associated with the following initial wave function:

$$\Psi(x, t=0) = \frac{1}{\sqrt{2}} \psi_1(x) + \frac{1}{\sqrt{2}} \psi_2(x)$$

What is the probability that a measurement of energy would give E_2 as result?

A. 0

B. $1/\sqrt{2}$

C. 1/2

D. 1

E. Something else

prob of measuring E_2

$= |c_2|^2 = \left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2}$

A particle in an infinite square well is associated with the following initial wave function:

$$\Psi(x, t=0) = \frac{1}{\sqrt{2}}\psi_1(x) + \frac{1}{\sqrt{2}}\psi_2(x) + 0\,\psi_3(x)$$

What is the probability that a measurement of energy would give E_3 as result?

- **A. 0**
- **B. $1/\sqrt{2}$**
- **C. 1/2**
- **D. 1**
- **E. Something else**

$$|c_3|^2 = 0$$

A particle in an infinite square well is associated with the following initial wave function:

$$\Psi(x, t=0) = \frac{1}{\sqrt{2}} \psi_1(x) + \frac{1}{\sqrt{2}} \psi_2(x)$$

What is the expectation value for the particle energy?

A. 0
B. E_1
C. E_2
D. $(E_1+E_2)/2$
E. Something else

$50\% \to E_1$

$50\% \to E_2$

$\Rightarrow$ average result for $E = \langle E \rangle$

$= 0.5\, E_1 + 0.5\, E_2$

$= \frac{E_1 + E_2}{2}$

$= |c_1|^2 E_1 + |c_2|^2 E_2$

- **What does c_n tell us?**

  - c_n: "amount of ψ_n in $\Psi(x,t)$"

  - $|c_n|^2$ = probability, that a measurement of the energy would yield the value E_n

    Note: only possible results are the E_n's!

  - Sum of probabilities $= \sum_{n=1}^{\infty} |c_n|^2 = 1$

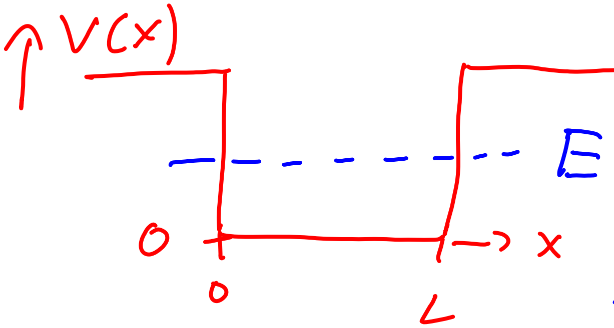
    (probability of measuring some value for energy $=1$)

  - Expectation value of the energy

$$\langle E \rangle = \langle H \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n$$

[proof → co-op? in section]

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



$$V(x) = \begin{cases} V_0, \text{ if } x<0 \\ 0, \text{ if } 0 \le x \le L \\ V_0, \text{ if } x>L \end{cases}$$

$\Rightarrow$ calculate bound particle states with $E<V_0$!

1) Solve piecewise in different segments where $V(x) = \text{const}$
2) join pieces to get final solution

- for $0 \le x \le L$: inside the well : $E > V(x) = 0$

$\Rightarrow$ as for infinite square well:

note sign

time-indep. S.E.: $$\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2}E\,\psi(x) = -k^2\psi(x)$$

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

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

find A, B later from boundary conditions at $x=0$ and $x=L$

- for $x<0$: outside the well: $E<V_0$
  - classically: partical will never be in this region
  - But in QM:

note sign!

time-indep. S.E: $$\frac{d^2\psi(x)}{dx^2} = \underbrace{\frac{2m}{\hbar^2}(V_0-E)}^{>0}\psi(x) = \alpha^2\psi(x)$$

general solution:

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

with $\alpha = \frac{\sqrt{2m(V_0-E)}}{\hbar} > 0$

But: $\psi(x) \xrightarrow[x\to-\infty]{} \infty \Rightarrow |\psi(x)|^2 \xrightarrow[x\to-\infty]{} \infty$ if $D \neq 0$

$\Rightarrow$ can not be normalized $\Rightarrow$ not physical

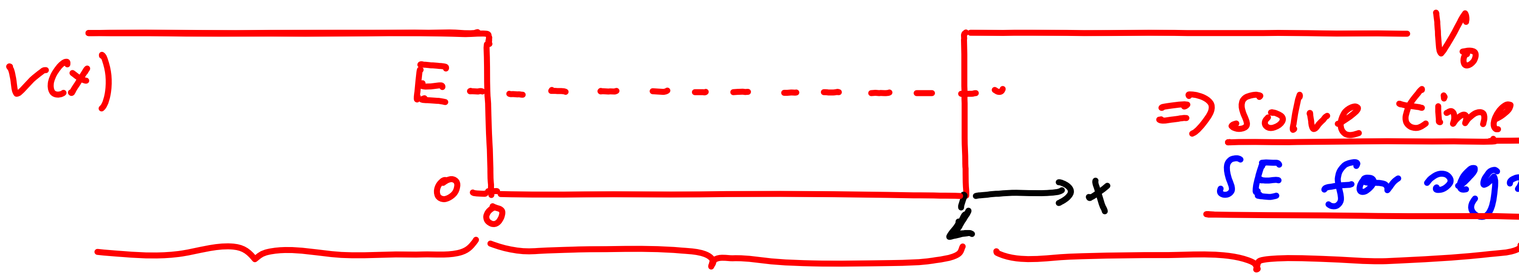
$\Rightarrow$ require $D=0$!

Note: the closer E to V_0, the slower the exponential decay!

$\Rightarrow$ $\psi(x) = C e^{\alpha x}$ is acceptable for $x<0$

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

Square Well of finite Depth:



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

$x < 0 \Rightarrow E < V_0$	$0 \le x \le L \Rightarrow E > V(x) = 0$	$x > 0 \Rightarrow E < V_0$
$\psi(x) = Ce^{\alpha x} + De^{-\alpha x}$	$\psi(x) = A\sin(kx) + B\cos(kx)$	$\psi(x) = Ce^{\alpha x} + De^{-\alpha x}$
require $\psi(x) \xrightarrow[x \to -\infty]{} 0$	$k = \dfrac{\sqrt{2mE}}{\hbar}$	require $\psi \xrightarrow[x \to +\infty]{} 0$
$\Rightarrow D = 0$		$\Rightarrow C = 0$
$\Rightarrow \psi(x) = Ce^{\alpha x}$		$\Rightarrow \psi(x) = De^{-\alpha x}$
$\alpha = \dfrac{\sqrt{2m(V_0 - E)}}{\hbar}$	decaying exponential solutions!	$\alpha = \dfrac{\sqrt{2m(V_0 - E)}}{\hbar}$

Note: 1) probability of finding particle outside well > 0

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