• The infinite square well
  - General solution

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

Infinite Square Well – Particle in a Box:

- **Stationary states** $\psi_n(x)$:
  $$\psi_n(x, t) = \psi_n(x) e^{-i \frac{\hbar^2 \pi^2}{2mL^2} n^2 t}$$
  
  **Quantized** $E_n = \frac{\hbar^2 \pi^2}{2mL^2} n^2$, $n = 1, 2, ...$

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-dependent SE for infinite square well:

Recall: general solution = linear combination of stationary states:

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

$$\Rightarrow \text{general solution:}$$

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

Add/drop $e^{-i\frac{En}{\hbar} t}$ factor

$$\Rightarrow \Psi(x,t=0) = \sum_{n=1}^{\infty} c_n \Psi_n(x) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{L}} \sin \left( \frac{n\pi}{L} x \right)$$

(initial conditions given)

Need to find $c_n$'s
Example: \( \psi(x, t=0) = \frac{1}{\sqrt{2}} \psi_1(x) + \frac{1}{\sqrt{2}} \psi_2(x) \)

\(=\) note: \( |\psi|^2 \) (prob. density) \( x \) time dependent! (not a stat. state!)
if we know \( \Psi(x, t=0) \) and stationary states \( \Psi_n(x) \), how can we find constants \( C_n \)?

\[
\text{look at: } \int_{-\infty}^{\infty} \Psi_n^*(x) \Psi(x, t=0) \, dx = \int_{-\infty}^{\infty} \Psi_n^*(x) \sum_{m=1}^{\infty} C_m \Psi_m(x) \, dx
\]

\[
= \sum_{m=1}^{\infty} C_m \int_{-\infty}^{\infty} \Psi_n^*(x) \Psi_n(x) \, dx = \sum_{m=1}^{\infty} C_m \delta_{nm} = C_n
\]

\( \text{all states are orthogonal} \)

\[
C_n = \int_{-\infty}^{\infty} \Psi_n^*(x) \Psi(x, t=0) \, dx
\]

\[
= \int_{0}^{\infty} \sqrt{\frac{2}{L}} \sin \left( \frac{n \pi}{L} x \right) \Psi(x, t=0) \, dx \text{ for infinite square well}
\]
General Solution of the Time-dependent SE:

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

to find \( c_n \):

\[ c_n = \int_{-\infty}^{\infty} \psi_n^*(x) \Psi(x,t=0) \, dx \]

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

\[ \text{one only get eigenvalues } E_n \text{ of given } \psi \]
\[ \text{if energy is measured} \]
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. \(\frac{1}{\sqrt{2}}\)  
C. \(\frac{1}{2}\)  
D. 1  
E. Something else

\[
\text{Prob of measuring } E_2 = |C_2|^2 = \left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2}
\]
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

\[
50\% \to E_1 \\
50\% \to E_2 \\
= \text{average result for } \langle \hat{E} \rangle \\
= 0.5 E_1 + 0.5 E_2 \\
= \frac{E_1 + E_2}{2} \\
= |C_1|^2 E_1 + |C_2|^2 E_2
\]
• What does $c_n$ tell us?
  
  - $c_n$: "amount of $\Psi_n$ 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
    
    $\langle E \rangle = \langle H \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n$
    
    $[\text{proof } \rightarrow \text{co-op) in section}]$
\( \text{II}_{2,2} \text{ Square Well of Finite Depth:} \)

\[
V(x) = \begin{cases} 
  V_0, & \text{if } x < 0 \\
  0, & \text{if } 0 \leq x \leq L \\
  V_0, & \text{if } x > L \end{cases}
\]

\( L = ) \) calculate bound particle states with \( E < V \).

1) Solve piecewise in different segments where \( V(x) = \text{const} \)

2) Join pieces to get final solution

\( \text{for } 0 \leq x \leq L : \text{inside the well: } E > V(x) = 0 \)

\( = ) \) as for infinite square well:

\( \text{time-independent: } \frac{d^2 \Psi(x)}{dx^2} = -\frac{2m}{\hbar^2} E \Psi(x) = -k^2 \Psi(x) \)

**General solution:** \( \Psi(x) = A \sin(kx) + B \cos(kx) \)

\( \text{with } k = \sqrt{\frac{2mE}{\hbar^2}} \)

\( \text{find } A, B \text{ later from boundary conditions at } x = 0 \text{ and } x = L \)
For $x < 0$: outside the well: $E < V_0$

- Classically: particle will never be in this region
- But in QM:

$$\frac{d^2 \psi(x)}{dx^2} = \frac{2m}{\hbar^2} (V_0 - E) \psi(x)$$

Time-independent SE: $\psi(x)$ > 0

General solution:

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

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

But:

$$\psi(x) \xrightarrow{x \to -\infty} \infty = \lim_{x \to -\infty} (\psi(x))^2 = \infty$$

- Can not be normalized = not physical
- 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 $x < 0$

- Probability of finding particle outside the well > 0
Square Well of Finite Depth:

\[ V(x) \]

\[ \begin{align*}
E & \quad \text{Solve time-indep. SE for segments} \\
0 & \leq x \leq \ell & E > V(x) = 0 \\
& \quad \text{for } x > 0 \Rightarrow E < V_0
\end{align*} \]

\[ \Psi(x) = C e^{\alpha x} + D e^{-\alpha x} \]

\[ \Psi(x) = A \sin(kx) + B \cos(kx) \]

\[ \Psi(x) = C e^{\alpha x} + D e^{-\alpha x} \]

\[ h = \sqrt{\frac{2mE}{\hbar}} \]

\[ k = \sqrt{\frac{2mE}{\hbar}} \]

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

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

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

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