Recap I

- **Quantum Mechanics**:
  - Wave function \( \psi (x, y, z, t) \)
  - Contains information about the particle

- **Probability Density function**:
  \[ P(x, t) = |\psi(x, t)|^2 \]
  \[ P(x, t) \, dx = \{ \text{probability that particle will be found between } x \text{ and } (x + dx) \text{ when position is measured at time } t \} \]
  \[ \int_a^b P(x, t) \, dx = \int_a^b |\psi(x, t)|^2 \, dx = \{ \text{probability that particle will be found between } a \text{ and } b \text{ when position is measured at time } t \} \]
  \[ \int_{-\infty}^{+\infty} |\psi|^2 \, dx = 1 \quad \{ \text{Normalization condition} \} \]
Recap II

- Wave function $\psi(x,t)$ is solution of the wave equation:

$$-\frac{\hbar^2}{8\pi^2m} \frac{d^2\psi}{dx^2} + U(x)\psi(x) = E\psi(x)$$

- Time independent Schrödinger equation for 1-D motion

- Mass of particle
- Potential energy
- Total mechanical energy of the particle

and $\psi(x,t) = \psi(x)e^{-i\omega t}$

⇒ for given $U(x)$, need to find solution $\psi(x)$

- Free particle with definite momentum moving along $+x$:

⇒ Solution of Schrödinger's equation:

$$\psi(x,t) = A e^{i(kx - \omega t)}$$

⇒ Probability density:

$$\rho(x,t) = |\psi|^2 = |A|^2 = \text{const}$$

⇒ Uncertainty in momentum infinitely great

⇒ Uncertainty in position $\sqrt{\int |\psi|^2 dx}$

$$\int |\psi|^2 dx = \rho$$
Today:

• More quantum mechanics

• Heisenberg’s uncertainty principle

• 1-D infinite square well

• Finite square well, tunneling…
Heisenberg's Uncertainty Principle:

How then can a particle ever be localized?

\[ \Rightarrow \text{Need to add up wave functions with particle (de Broglie) wavelengths } \lambda \]

\[ \Rightarrow \text{get uncertainty in wavelength } \lambda \text{ of particle} \]

\[ \Rightarrow \text{get uncertainty in momentum } p = h/\lambda \]

\[ \Rightarrow \text{The more determined the position of a particle, the larger the uncertainty is in its momentum!} \]

\[ \frac{1}{\sqrt{12}} \]

\[ \text{Probability of measuring a certain value for the particle's position} \]

\[ \text{Probability of measuring a certain value for the particle's momentum} \]

\[ \Rightarrow \text{small uncertainty } \Delta x \text{ in position of particle} \]

\[ \Rightarrow \text{large uncertainty } \Delta p_x \text{ in } x \text{-component of momentum!} \]
Heisenberg's Uncertainty Principle:

\[ \Delta x \cdot \Delta p_x \geq \frac{\hbar}{2\pi} \]

always

Note: This is not a measurement problem (i.e., a better measuring instrument would not help).

Example: Consider 1000 identical particles, all associated with an identical wave function \( \psi(x,t) \).

- Measure position on 500
- Measure momentum on 500

\[ \Delta x \cdot \Delta p_x \geq \frac{h}{4\pi} \]

always!
Example 2: "Particle confined in a Box"

Consider a particle of mass m confined (trapped) in an infinitely deep potential energy well.

- **Outside the well:** probability of finding particle = 0
  \[ \Psi(x) = 0 \text{ for } x < 0 \text{ and } x > L \]
- Inside the well: $U(x) = 0$

\[ -\frac{\hbar^2}{8\pi^2 m} \frac{d^2 \psi(x)}{dx^2} + 0 = E \psi(x) \]

Since $U(x) = 0$ inside the well

\[ \Rightarrow \text{general solution:} \]

\[ \psi(x) = A \sin(kx) + B \cos(kx) \quad \text{with} \quad k = \frac{\sqrt{8\pi^2 m E}}{\hbar} \]

\[ \text{constants determined by boundary conditions} \]
⇒ boundary conditions:

**Key idea:** Wave function $\Psi(x)$ needs to be a continuous function $\Rightarrow$ no jumps in $\Psi(x)$

outside well: $\Psi(x) = 0$

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

$⇒ x = 0$ ⇒ require: $\Psi(x=0) = \Psi(x=L) = 0$

at walls of a well

$⇒ \Psi(x=0) = A \sin(0) + B \cos(0) = B \neq 0$

$⇒ B = 0$

$⇒ \Psi(x) = A \sin(kx)$ inside the well
but also need: \( \Psi(x=L) = A \sin(kL) = 0 \)

\[\Rightarrow\text{ need } kL = \pi \text{ or } 2\pi \text{ or } 3\pi \ldots\]

\[\Rightarrow\text{ need } kL = \frac{n\pi}{L} \quad \text{with } n=1,2,3,\ldots\]

\[\Rightarrow \text{ Note: get distinct solution: } K_n = \frac{n\pi}{L} \quad n=1,2,3,\ldots\]

\[\Rightarrow \text{ since } k = \frac{\sqrt{8mE}}{h} \]

\[h = \frac{\sqrt{8mE}}{h} \quad \therefore \frac{n\pi}{L} = \frac{h^2}{8mL^2} n^2 \quad \Rightarrow E_n = \frac{h^2}{8mL^2} n^2\]

\[\Rightarrow \text{ quantization of energy of particle confined in the well? (only certain energy values are allowed)}\]

\(n=1,2,3,\ldots\)
Note:
- \( E_n = n^2 E_i \), \( n = 1, 2, 3 \)
- \( E_i > 0 : \) "zero point energy"
  \( \Rightarrow \) trapped particle cannot have zero energy!

- Confined particle \( \rightarrow \) get quantization of energy (recall atom)

- Example:
  \( L = 1 \text{nm} \implies E_i \approx 0.5 \text{eV} \) for an electron in a 1-D box
next: allowed wave function of particle in 1-D infinite well

outside well: \( \Psi_n(x, t) = 0 \)

inside well: \( \Psi(x, t) = \Psi_n(x) e^{-i \omega_n t} \)

with \( \Psi_n(x) = A \sin (K_n x) ; K_n = \frac{n \pi}{L} \)

find constant \( A \) from

normalization condition

\[
\int_{-\infty}^{\infty} |\Psi|^2 dx = 1 = \int_{-\frac{L}{2}}^{\frac{L}{2}} |A|^2 \sin^2 (K_n x) dx = |A|^2 \frac{1}{2} L
\]

\( \Rightarrow |A|^2 = \frac{2}{L} \)

pick positive root:

\( A = \sqrt{\frac{2}{L}} \) for all \( n \)
Final result for particle in 1-D infinite deep well

- Wave function: \( \Psi_n(x) = \sqrt{\frac{2}{L}} \sin \left( \frac{n\pi}{L} x \right) \) for \( n = 1, 2, 3, ... \)

- For \( 0 \leq x < L \)

- \( \Psi_n(x) = 0 \) elsewhere (outside well)

- With quantized energies:

\[
E_n = \frac{\hbar^2}{8mL^2} \quad n^2 = E, \quad n^2
\]
Infinite 1-D Square Well: Wave functions and Quantized Energy

\[ \psi_n(x) = A \sin \left( \frac{n \pi x}{L} \right), \text{ for } 0 \leq x \leq L. \]

\[ E_n = n^2 \left( \frac{\hbar^2}{8mL^2} \right) = n^2 E_1, \quad n = 1, 2, 3, \ldots \]

\[ \psi_1(x) \]

\[ \psi_2(x) \]

\[ \psi_3(x) \]

Position x

Energy

- \( E_1 \)
- \( 4E_1 \)
- \( 9E_1 \)
- \( 16E_1 \)
- \( 25E_1 \)
Electron (de Broglie Waves) in an Infinite 1-D Square Well

Which set of energy levels corresponds to the larger value of well size \( L \)?

\[
E_n = \frac{\hbar^2}{8mL^2} \, n^2 \propto \frac{1}{L^2}
\]

\( \Rightarrow \) large \( L \) give lower \( E_n \) for a given \( n \)?

C. The spacing of energy levels does not depend on \( L \)

A. Set 1

B. Set 2

C. The spacing of energy levels does not depend on \( L \)
Finite 1-D square well:

For an electron in a potential well of finite depth we must solve the time-independent Schrödinger equation with appropriate boundary conditions to get the wave functions.
Quantum Tunneling

Particle can “tunnel” through a barrier that it classically could not surmount.
Example: Scanning Tunneling Microscope (STM)

Control voltages for piezotube

= feedback to keep tunneling current constant

Piezoelectric tube with electrodes

Tunneling current amplifier

Distance control and scanning unit

Tip

Sample

Tunneling voltage

adjustable tunnel barrier

Data processing and display
Example: Scanning Tunneling Microscope (STM)

- Tip
- Electron clouds
- $V_{bias}$

Graph: exponential dependence of current on distance

- Tunneling Current (pA)
- Tunneling Gap (Å)
Spin

• Electrons (and many other particles) have an intrinsic property (like mass & charge) called spin angular momentum, \( \vec{S} \), (or just called spin).

• The component of \( \vec{S} \) measured along any axis is quantized.

• For electrons:
  • Have spin \( S = \sqrt{s(s+1)} \frac{\hbar}{2\pi} \), where \( s = 1/2 \) is the spin quantum number of an electron
  • Spin component along any axis can only have one of the following two values:
    \[ S_z = m_s \frac{\hbar}{2\pi} \]
    with spin magnetic quantum number \( m_s = +\frac{1}{2} \) or \( -\frac{1}{2} \).
The Pauli Exclusion Principle
(Wolfgang Pauli, 1925):

No two electrons confined to the same trap can have the same set of values for their quantum numbers \((n, m_s \ldots)\).

⇒ In a given trap, only two electrons, at most, can occupy a state with the same (single-particle) wave function (solution of the Schrödinger equation). One must have \(m_s = +\frac{1}{2}\) and the other must have \(m_s = -\frac{1}{2}\).