Recap I

Lecture 40

- **Quantum Mechanics:**
  - Wave function $\Psi(x,y,z,t)$ } computational device; contains information about the particle
  - Probability Density function:

$$P(x,t) = |\Psi(x,t)|^2$$

$$P(x,t)\,dx = \left\{\begin{array}{l}\text{probability that particle will be found} \\ \text{between } x \text{ and } (x+dx) \text{ when position is} \\ \text{measured at time } t\end{array}\right\}$$

$$\int_a^b P(x,t)\,dx = \int_a^b |\Psi(x,t)|^2\,dx = \left\{\begin{array}{l}\text{probability that particle will} \\ \text{be found between } a \text{ and } b \\ \text{when position is measured at time } t\end{array}\right\}$$

$$\int_{-\infty}^{+\infty} |\Psi|^2\,dx = 1$$ } Normalization condition

Recap II

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

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

time independent Schrödinger equation for 1-D motion

mass of particle

potential energy

total mechanical energy of the particle

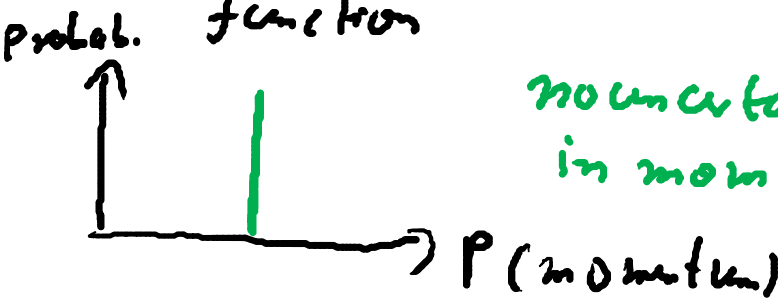
and $\boxed{\Psi(x,t) = \psi(x)\,e^{-i\omega t}}$

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

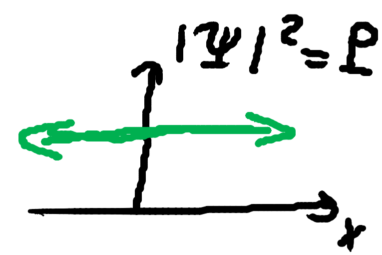
- Free particle with definite momentum moving along $+x$:

⇒ Solution of Schrödinger's equation : $\Psi(x,t) = A\,e^{i(kx-\omega t)}$

⇒ Probability density function : $P(x,t) = |\Psi|^2 = |A|^2 = \text{const}$

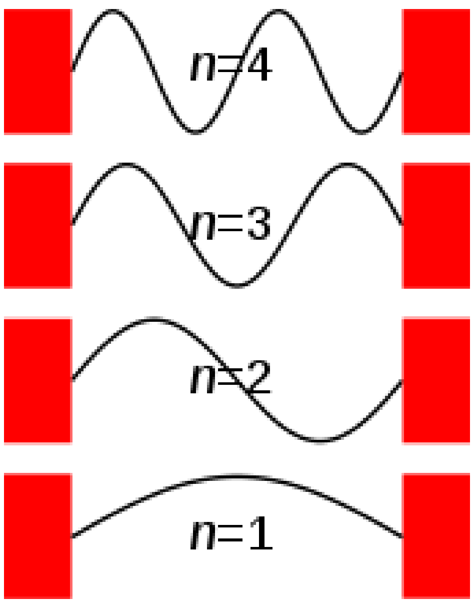


no uncertainty in momentum ⇒ infinitely great uncertainty in position



Today:

- **More quantum mechanics**
  - **Heisenberg's uncertainty principle**
  - **1-D infinite square well**
  - **Finite square well, tunneling…**



Heisenberg's Uncertainty Principle:

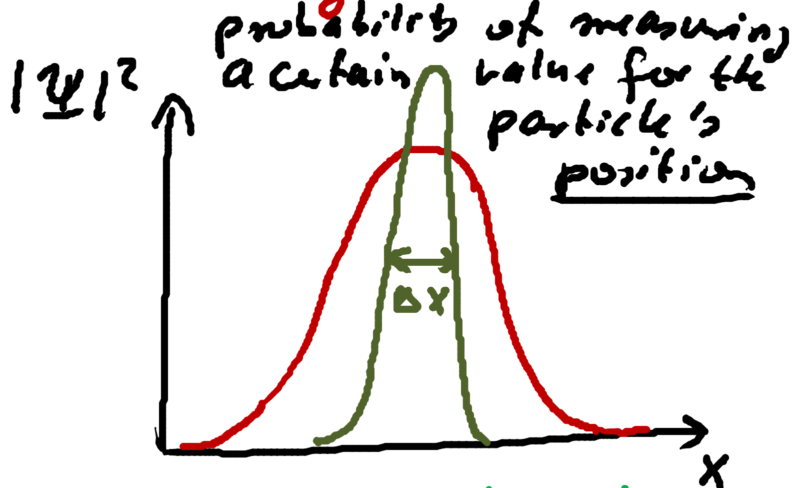
How then can a particle ever be localized?

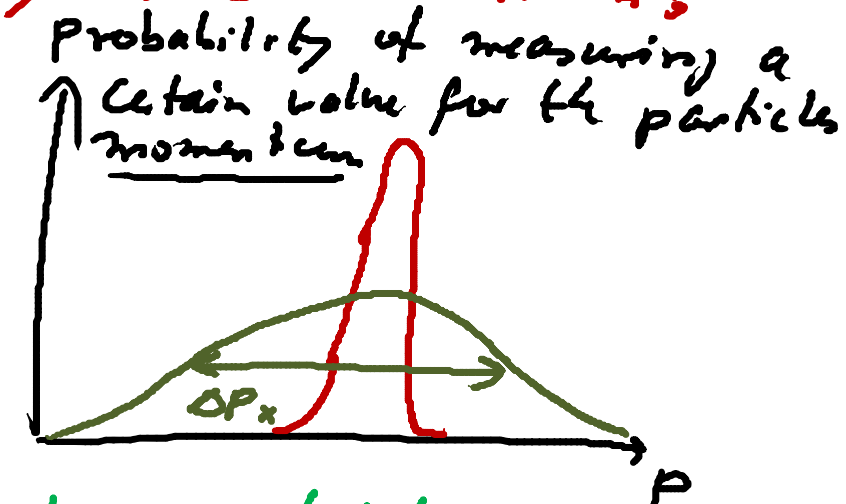
⇒ Need to add up wavefunctions with particle (de Broglie) wavelengths λ

⇒ get uncertainty in wavelength λ of particle

⇒ get uncertainty in momentum $p = h/\lambda$!

⇒ The more determined the position of a particle the larger the uncertainty is in its momentum!





⇒ small uncertainty Δx in position of particle

⇒ large uncertainty Δp_x in x-component of momentum!

Heisenberg's Uncertainty Principle:

$$\boxed{\Delta x \cdot \Delta p_x \geq \frac{h}{4\pi}}$$

always

uncert. in position

uncert. in momentum

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 $\Psi(x,t)$

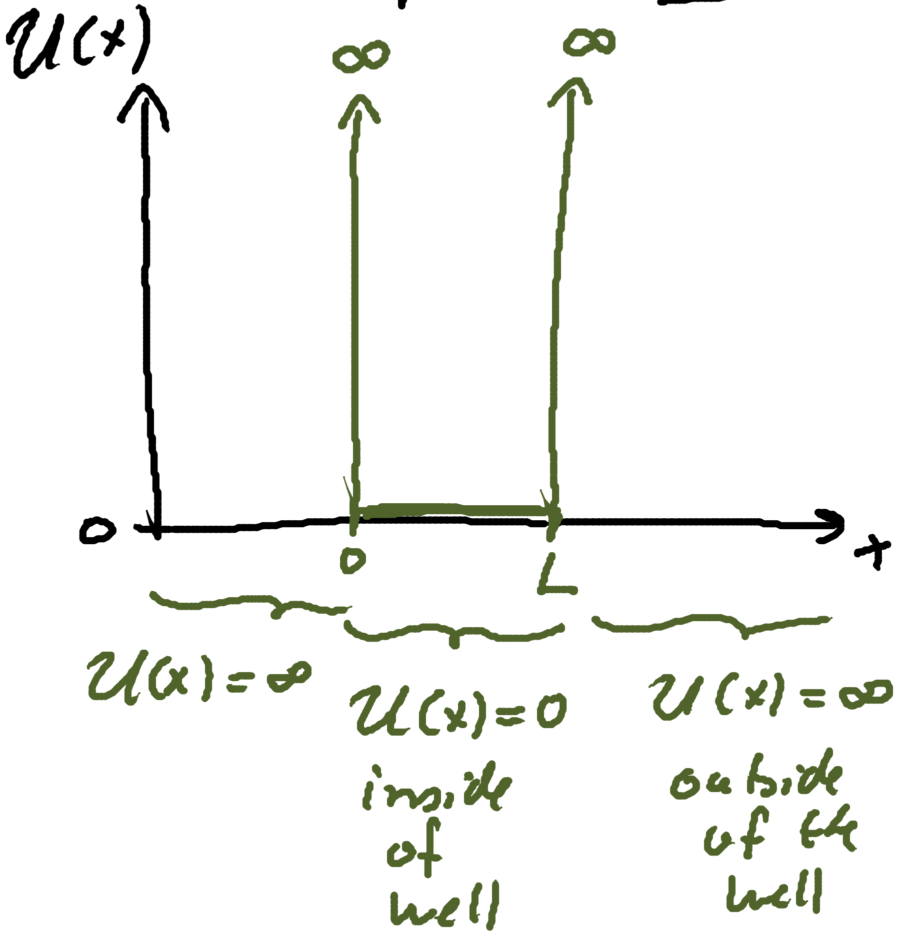
measure position on 500

$\Delta x \cdot \Delta p_x \geq h/4\pi$

always!

measure momentum on 500

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:
pobabability of finding particle = 0

$\Rightarrow \Psi(x) = 0$ for $x < 0$ and $x > L$

- Inside the well: $U(x) = 0$

$\Rightarrow$ Use Schrödinger's equation to find the wave function

$$-\frac{h^2}{8\pi^2 m}\frac{d^2\psi(x)}{dx^2} + \underbrace{0}_{} = E\,\psi(x)$$

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

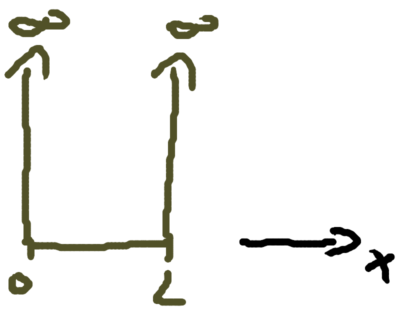
$\Rightarrow$ <u>general solution:</u>

$$\psi(x) = A \sin(kx) + B\cos(kx) \quad \text{with } k = \frac{\sqrt{8\pi^2 mE}}{h}$$

constants determined by <u>boundary conditions</u>

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

$\Rightarrow$ require: $\psi(x=0) = \psi(x=L) = 0$ at walls of ∞ well

$$\Rightarrow \psi(x=0) = A \sin(0) + B \cos(0) = B \stackrel{!}{=} 0$$

$$\Rightarrow \underline{B = 0}$$

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

$\Rightarrow$ need $kL = \pi$ or 2π or 3π ...

$\Rightarrow$ need $\underline{kL = n\pi}$ with $n = 1, 2, 3, \ldots$

$\Rightarrow$ Note: get distinct solution: $\boxed{k_n = \frac{n\pi}{L}}$ $n = 1, 2, 3 \ldots$

$\Rightarrow$ since $k = \frac{\sqrt{8\pi^2 m E}}{h}$

$$k = \frac{\sqrt{8\pi^2 m E}}{h} \stackrel{!}{=} \frac{n\pi}{L} \Rightarrow \boxed{E_n = \frac{h^2}{8 m L^2} n^2}$$

$n = 1, 2, 3 \ldots$

$\Rightarrow$ quantization of energy of particle confined in the well! (only certain energy values are allowed)

Note:

- $E_n = n^2 E_1$, $n = 1, 2, 3$
- $E_1 > 0$: "zero point energy"

  $\Rightarrow$ trapped particle can not have zero energy!
- Confined particle $\rightarrow$ get quantization of energy (recall atom)
- Example:

  $L = 1\,nm \Rightarrow E_1 \approx 0.5\,eV$ 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 $\psi_n(x) = A \sin(k_n x)$; $k_n = n\frac{\pi}{L}$

find constant A from normalization condition

$n = 1, 2, 3, \ldots$

require: $\int_{-\infty}^{+\infty} |\Psi|^2 dx = 1 = \int_0^L |A|^2 \sin^2(k_n x)\, dx = |A|^2 \frac{1}{2} L$

$\Rightarrow |A|^2 = \frac{2}{L}$ $\Rightarrow$ pick positive root:

$$A = \sqrt{\frac{2}{L}}$$ for all n

$\Rightarrow$ final result for particle in 1-D infinite deep well

- wave function : $\boxed{\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right)}$ $n = 1, 2, 3 \ldots$

for $0 \le x \le L$

(inside well)

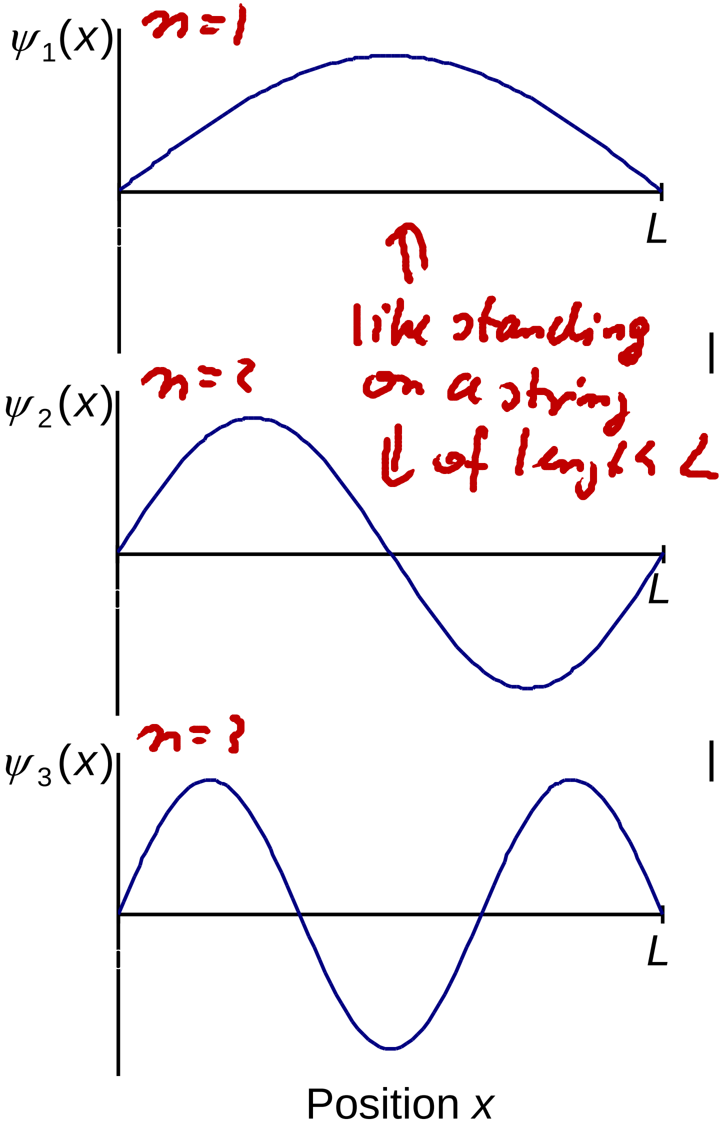
$\psi_n(x) = 0$ elsewhere (outside well)

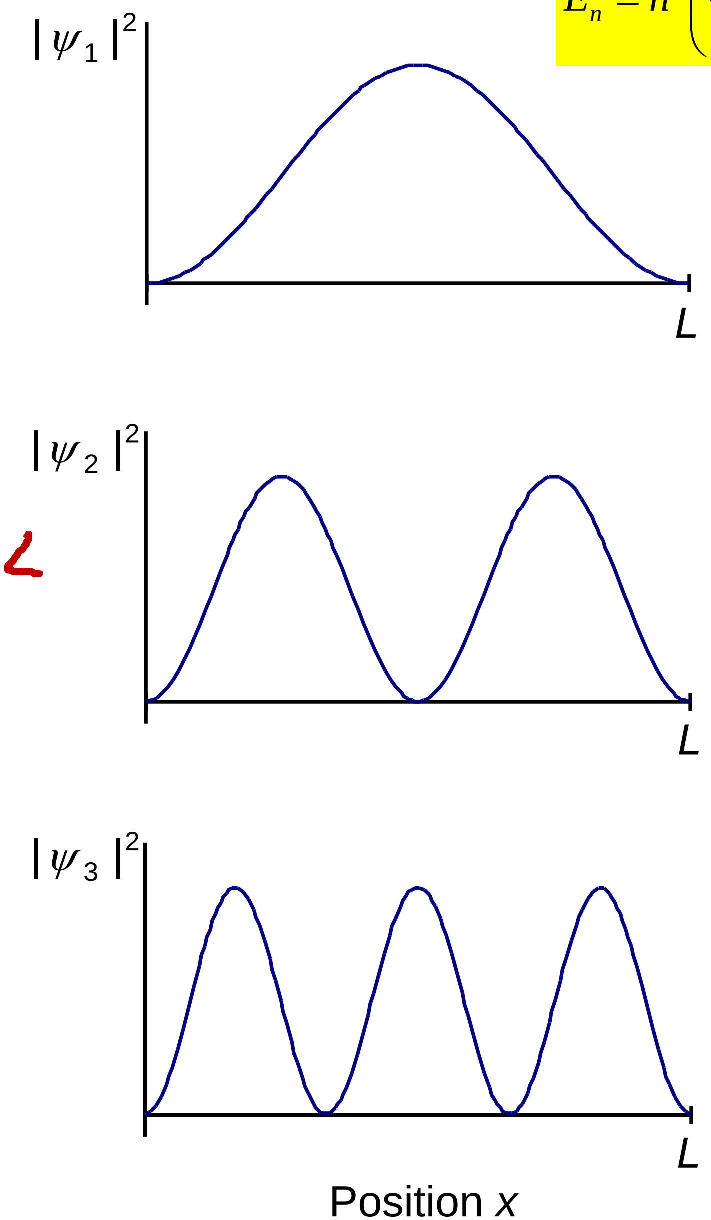
- with quantized energies : $\boxed{E_n = \frac{h^2}{8 m L^2} n^2 = E_1 n^2}$

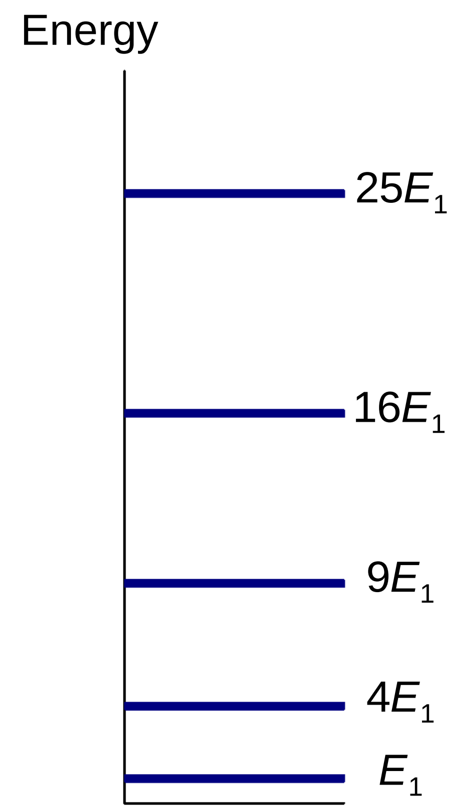
Infinite 1-D Square Well: Wave functions and Quantized Energy

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

$$E_n = n^2\left(\frac{h^2}{8mL^2}\right) = n^2 E_1, \; n = 1, 2, 3, \ldots.$$

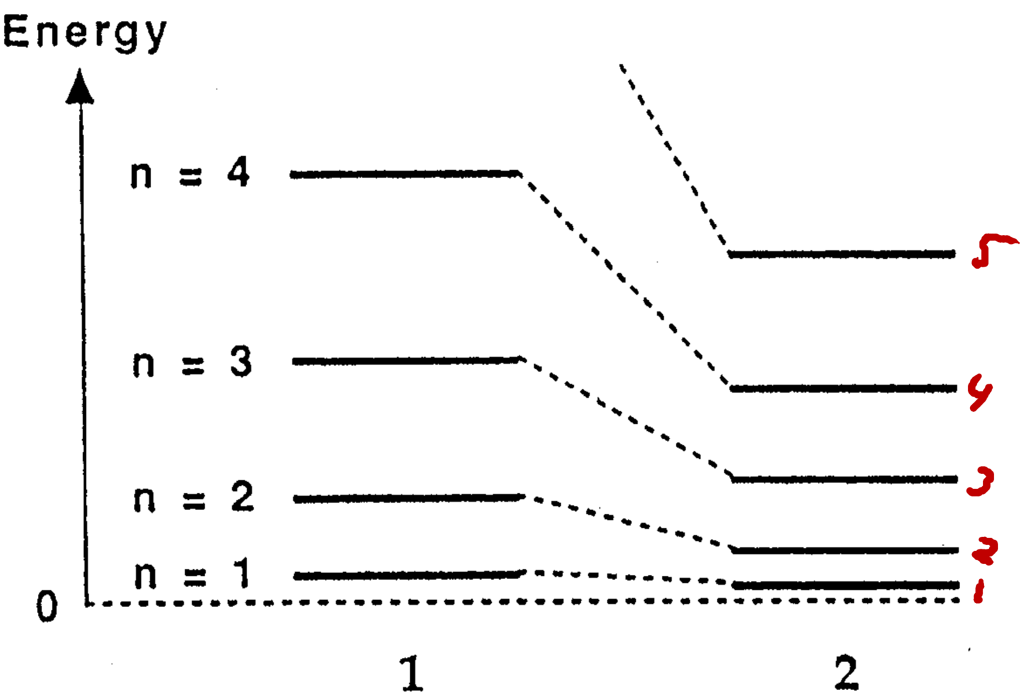






Electron (de Broglie Waves) in an Infinite 1-D Square Well

Which set of energy levels corresponds to the larger value of well size *L*?



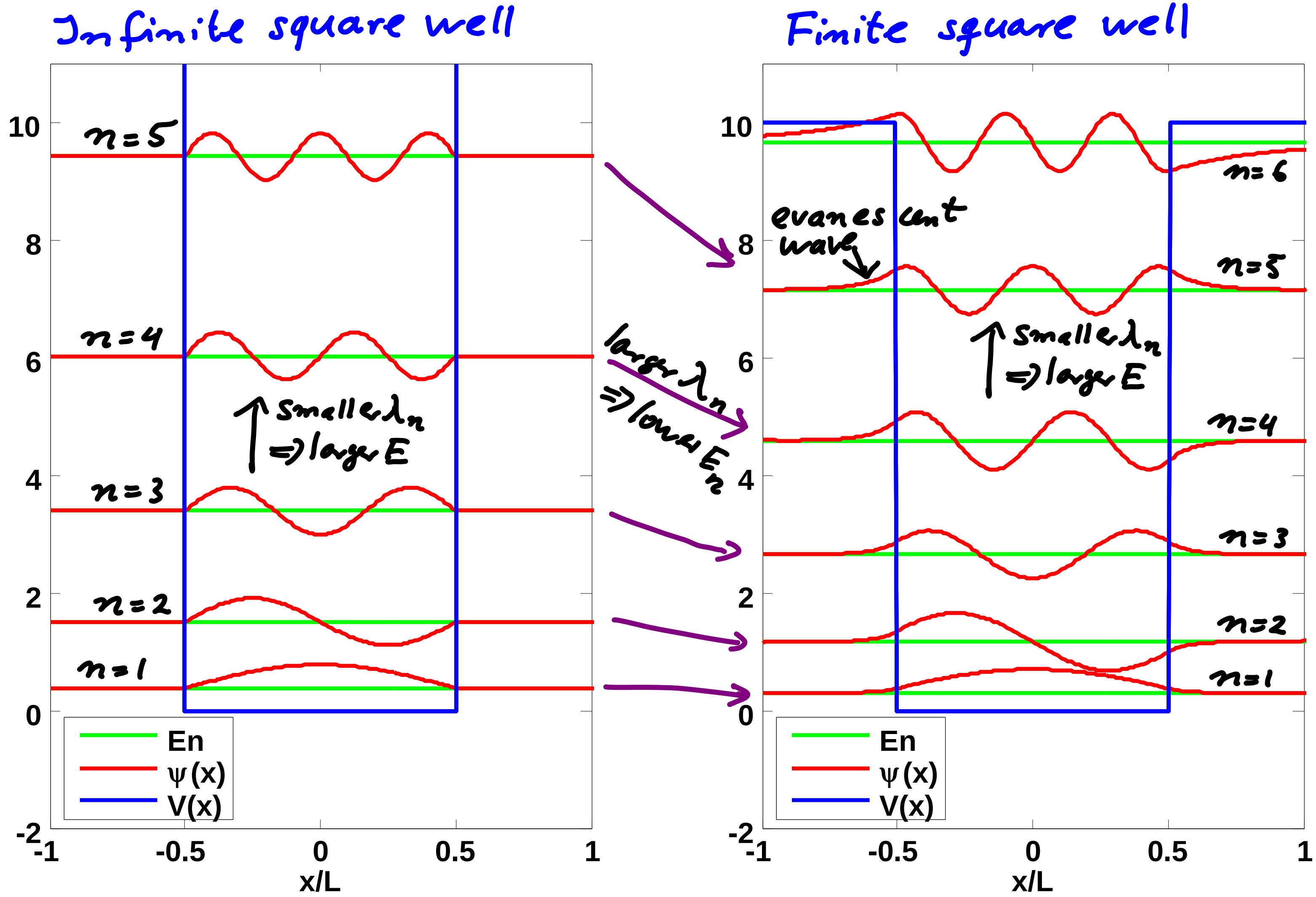
$E_n = \frac{h^2}{8mL^2} n^2 \propto \frac{1}{L^2}$

$\Rightarrow$ larger L gives lower E_n for a given n!
(larger $\lambda_n = \frac{2\pi}{k_n}$)

- **A.** **Set 1**
- **B.** **Set 2**
- **C.** **The spacing of energy levels does not depend on *L***

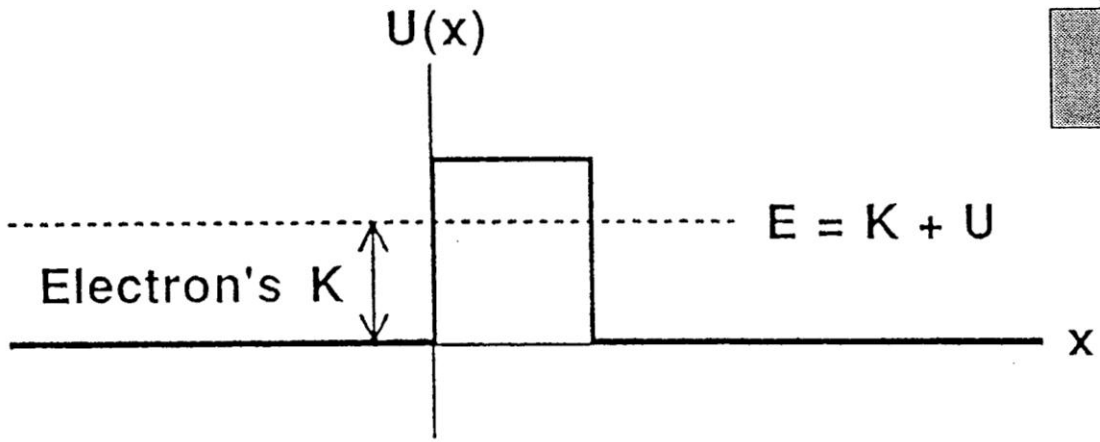
Finite 1-D square well:

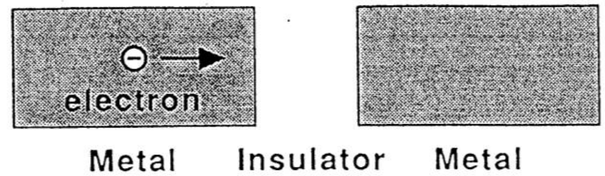
For an electron in a potential well of finite depth we must solve the time-independent Schrödinger equation with appropriate boundary conditions to get the wave functions.



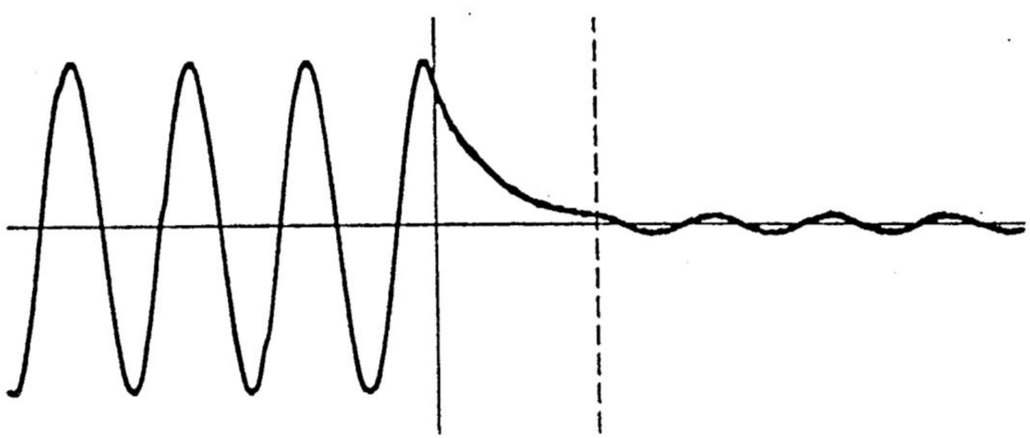
Quantum Tunneling

Electron's Potential Energy Barrier



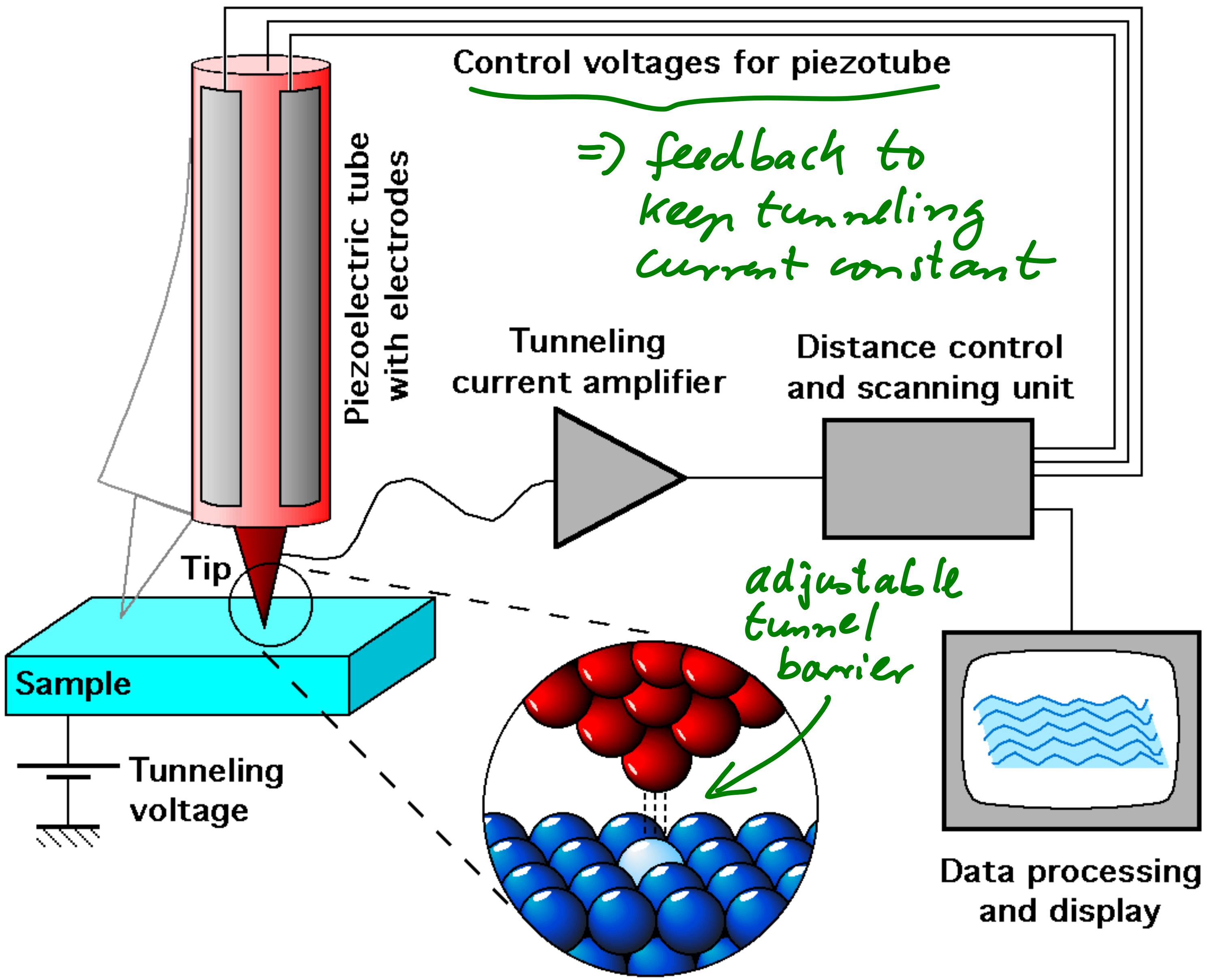


Electron's Wavefunction $\psi(x)$

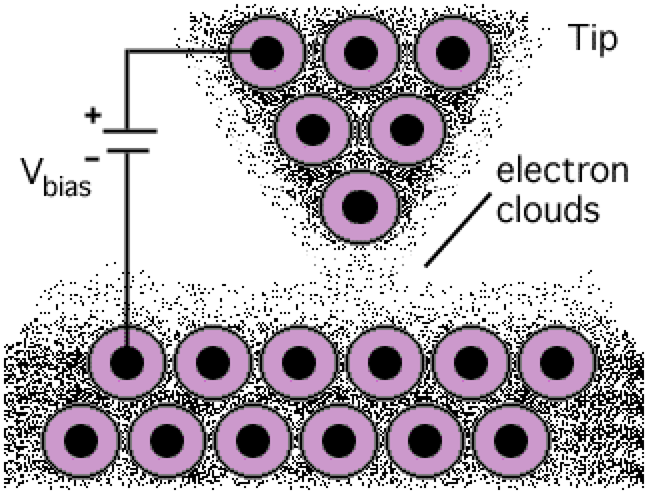


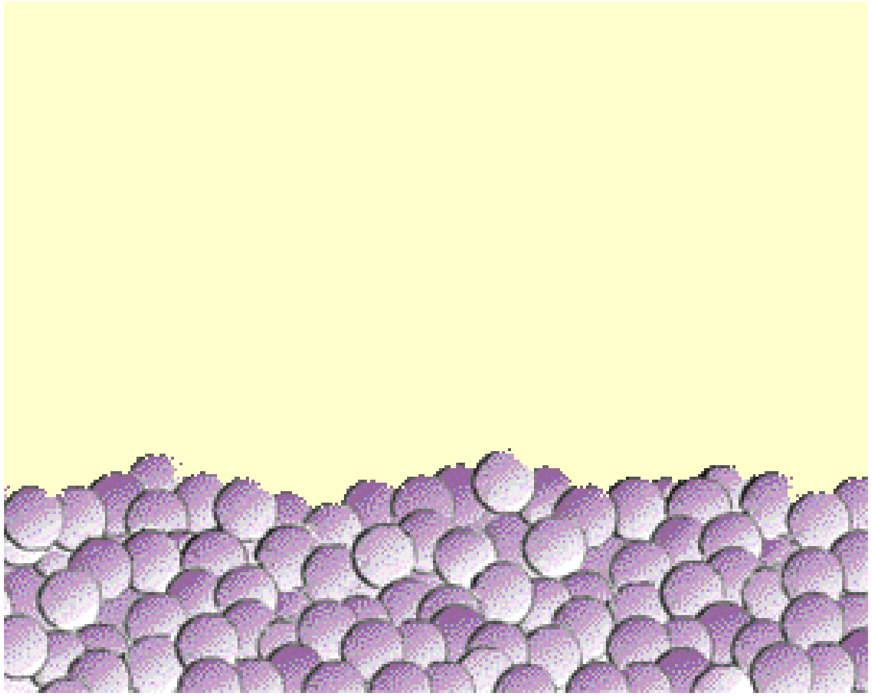
Particle can "tunnel" through a barrier that it classically could not surmount

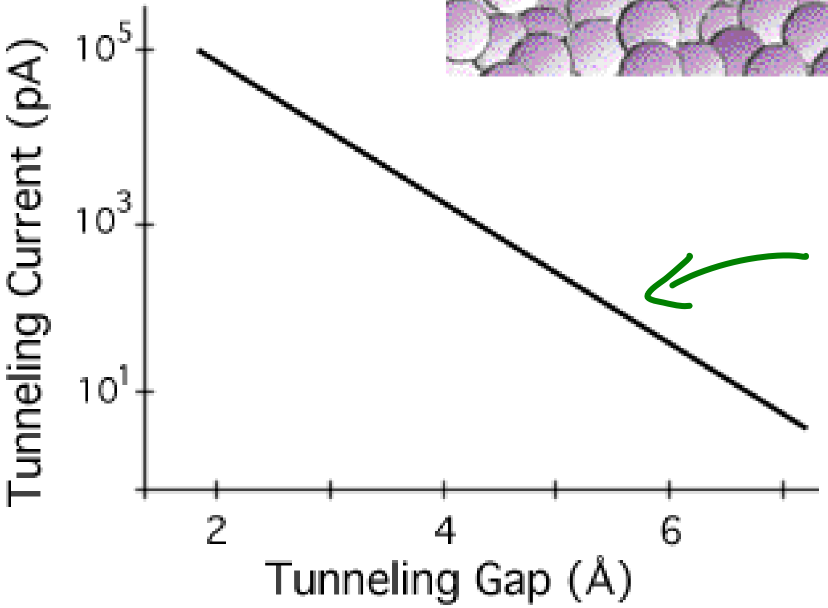
Example: Scanning Tunneling Microscope (STM)



Example: Scanning Tunneling Microscope (STM)







exponential dependence of current on distance

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 $S = \sqrt{s(s+1)}\frac{h}{2\pi}$, where **s** = 1/2 is the **spin quantum number** of an electron
  - Spin component along any axis can only have one the following two values:
  $$S_z = m_s \frac{h}{2\pi}$$
  with **spin magnetic quantum number** $\boldsymbol{m_s}$ = +½ or –½.

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 …).

$\Rightarrow$ **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 $m_s = +½$ and the other must have $m_s = -½$.**