Factorization Condition For Wave Function Leads to:

\[-\hbar^2 \frac{\partial^2 \Psi(x)}{2m \partial^2 x} + U(x) \Psi(x) = E \, \Psi(x)\]

\[i\hbar \frac{\partial \phi(t)}{\partial t} = E \phi(t)\]

What is the Constant E? How to Interpret it?

Back to a Free particle:

\[\Psi(x,t) = A e^{ikx} e^{-i\omega t}, \, \Psi(x) = A e^{ikx}\]

\[U(x,t) = 0\]

Plug it into the Time Independent Schrödinger Equation (TISE) ⇒

\[-\hbar^2 \frac{d^2 (Ae^{ikx})}{2m dx^2} + 0 = E \, Ae^{ikx} \Rightarrow E = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m} = \text{(NR Energy)}\]

Stationary states of the free particle: \[\Psi(x,t) = \psi(x)e^{-i\omega t}\]

\[\Rightarrow |\Psi(x,t)|^2 = |
\psi(x)|^2\]

Probability is static in time t, character of wave function depends on \(\psi(x)\)
A More Interesting Potential: Particle In a Box (like an atom)

Classical Picture:
- Particle dances back and forth
- Constant speed, const KE
- Average $\langle P \rangle = 0$
- No restriction on energy value
  - $E = K + U = K + 0 = P^2/2m$
- Particle can not exist outside box
  - Can’t get out because needs to borrow infinite energy to overcome potential of wall

Write the Form of Potential: Infinite Wall

$U(x,t) = \infty$; $x \leq 0$, $x \geq L$

$U(x,t) = 0$; $0 > X > L$

What happens when the joker is subatomic in size??
(a) Electron placed between 2 set of electrodes C & grids G experiences no force in the region between grids, which are held at Ground Potential. However in the regions between each C & G is a repelling electric field whose strength depends on the magnitude of V.

(b) If V is small, then electron’s potential energy vs x has low sloping “walls”.

(c) If V is large, the “walls” become very high & steep becoming infinitely high for $V \rightarrow \infty$.

(d) The Straight infinite walls are an approximation of such a situation.
\[ \Psi(x) \text{ for Particle Inside 1D Box with Infinite Potential Walls} \]

Inside the box, no force \( \Rightarrow U=0 \) or constant (same thing)

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

\[ \Rightarrow \frac{d^2\psi(x)}{dx^2} = -k^2\psi(x) ; \quad k^2 = \frac{2mE}{\hbar^2} \]

or \[ \frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \] \( \Leftarrow \) figure out what \( \psi(x) \) solves this diff eq.

In General the solution is \( \psi(x) = A \sin kx + B \cos kx \) (A,B are constants)

Need to figure out values of A, B : How to do that?

Apply BOUNDARY Conditions on the Physical Wavefunction

We said \( \psi(x) \) must be continuous everywhere

So match the wavefunction just outside box to the wavefunction value just inside the box

\( \Rightarrow \) At \( x = 0 \) \( \Rightarrow \psi(x = 0) = 0 \) & At \( x = L \) \( \Rightarrow \psi(x = L) = 0 \)

\( \therefore \quad \psi(x = 0) = B = 0 \) (Continuity condition at \( x =0 \))

& \( \psi(x = L) = 0 \) \( \Rightarrow \) A Sin \( kL = 0 \) (Continuity condition at \( x =L \))

\( \Rightarrow kL = n\pi \Rightarrow k = \frac{n\pi}{L}, n = 1, 2, 3, \ldots \infty \)

So what does this say about Energy \( E \) ?:

\[ E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \] Quantized (not Continuous)!
Quantized Energy levels of Particle in a Box

\[ E_n = n^2 E_1 \]

\[ E_1 = \frac{\pi^2 \hbar^2}{2mL^2} \]
What About the Wave Function Normalization?

The particle's Energy and Wavefunction are determined by a number \( n \).

We will call \( n \rightarrow \) Quantum Number, just like in Bohr's Hydrogen atom.

What about the wave functions corresponding to each of these energy states?

\[
\psi_n = A \sin(kx) = A \sin\left(\frac{n\pi x}{L}\right) \quad \text{for} \quad 0 < x < L
\]
\[
= 0 \quad \text{for} \quad x \geq 0, \ x \geq L
\]

Normalized Condition:

\[
1 = \int_0^L \psi_n^* \psi_n \, dx = A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) \quad \text{Use} \ 2\sin^2\theta = 1 - 2\cos2\theta
\]

\[
1 = \frac{A^2}{2} \int_0^L \left(1 - \cos\left(\frac{2n\pi x}{L}\right)\right) \quad \text{and since} \ \int \cos \theta = \sin \theta
\]

\[
1 = \frac{A^2}{2} L \quad \Rightarrow A = \sqrt{\frac{2}{L}}
\]

So \( \psi_n = \sqrt{\frac{2}{L}} \sin(kx) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \) ...What does this look like?
Wave Functions: Shapes Depend on Quantum # n

Probability $P(x)$: Where the particle likely to be

Zero Prob
Where in The World is Carmen San Diego?

- We can only guess the probability of finding the particle somewhere in x
  - For n=1 (ground state) particle most likely at x = L/2
  - For n=2 (first excited state) particle most likely at L/4, 3L/4
- Prob. Vanishes at x = L/2 & L
  - How does the particle get from just before x=L/2 to just after?
    » QUIT thinking this way, particles don’t have trajectories
    » Just probabilities of being somewhere

Classically, where is the particle most Likely to be: Equal prob of being anywhere inside the Box
NOT SO says Quantum Mechanics!
Remember Sesame Street?

This particle in the Box is
Brought to you by the letter

n
Its the Big Boss
Quantum Number
Consider \( n = 1 \) state of the particle

Ask: What is \( P \left( \frac{L}{4} \leq x \leq \frac{3L}{4} \right) \)?

\[
P = \int_{\frac{L}{4}}^{\frac{3L}{4}} \left| \psi_1 \right|^2 \, dx = \frac{2}{L} \int_{\frac{L}{4}}^{\frac{3L}{4}} \sin^2 \left( \frac{\pi x}{L} \right) \, dx = \left( \frac{2}{L} \right) \cdot \frac{1}{2} \int_{\frac{L}{4}}^{\frac{3L}{4}} \left( 1 - \cos \left( \frac{2\pi x}{L} \right) \right) \, dx
\]

\[
P = \frac{1}{L} \left[ \frac{L}{2} - \right] \left[ \frac{L}{2\pi} \sin \left( \frac{2\pi}{L} \right) \right]^{3L/4} = \frac{1}{2} - \frac{1}{2\pi} \left( \sin \left( \frac{2\pi}{L} \cdot \frac{3L}{4} \right) - \sin \left( \frac{2\pi}{L} \cdot \frac{L}{4} \right) \right)
\]

\[
P = \frac{1}{2} - \frac{1}{2\pi} (-1 - 1) = 0.818 \Rightarrow 81.8\%
\]

Classically \( \Rightarrow 50\% \) (equal prob over half the box size)

\( \Rightarrow \) Substantial difference between Classical & Quantum predictions
When The Classical & Quantum Pictures Merge: $n \to \infty$

But one issue is irreconcilable:

Quantum Mechanically the particle cannot have $E = 0$

This is a consequence of the Uncertainty Principle

The particle moves around with KE inversely proportional to the Length Of the 1D Box
Finite Potential Barrier

- There are no Infinite Potentials in the real world
  - Imagine the cost of a battery with infinite potential difference
    - Will cost infinite $ sum + not available at Radio Shack
- Imagine a realistic potential: Large $U$ compared to KE but not infinite

Classical Picture: A bound particle (no escape) in $0 < x < L$
Quantum Mechanical Picture: Use $\Delta E \cdot \Delta t \leq \hbar/2\pi$
Particle can leak out of the Box of finite potential $P(|x| > L) \neq 0$
Finite Potential Well

Schroedinger Eq:

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

\[\Rightarrow \quad \frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2}(U - E)\psi(x)\]

\[= \alpha^2\psi(x); \quad \alpha = \sqrt{\frac{2m(U-E)}{\hbar^2}}\]

\[\Rightarrow \text{General Solutions: } \psi(x) = Ae^{\alpha x} + Be^{-\alpha x}\]

Require finiteness of \(\psi(x)\)

\[\Rightarrow \psi(x) = Ae^{\alpha x} \quad \text{.....} x<0 \quad \text{(region I)}\]

\[\psi(x) = Ae^{-\alpha x} \quad \text{.....} x>L \quad \text{(region III)}\]

Again, coefficients A & B come from matching conditions at the edge of the walls (x =0, L)

But note that wave fn at \(\psi(x)\) at (x =0, L) \(\neq 0\)!! (why?)

Further require Continuity of \(\psi(x)\) and \(\frac{d\psi(x)}{dx}\)

These lead to rather different wave functions
Finite Potential Well: Particle can burrow outside box
Particle can be outside the box but only for a time $\Delta t \approx \frac{h}{\Delta E}$

$\Delta E = $ Energy particle needs to borrow to Get outside $\Delta E = U - E + KE$

The Cinderella act (of violating E Conservation) cant last very long

Particle must hurry back (cant be caught with its hand inside the cookie-jar)

Penetration Length $\delta = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(U-E)}}$

If $U \gg E \Rightarrow$ Tiny penetration

If $U \to \infty \Rightarrow \delta \to 0$
Finite Potential Well: Particle can Burrow Outside Box

Penetration Length \( \delta = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(U - E)}} \)

If \( U \gg E \) \( \Rightarrow \) Tiny penetration

If \( U \rightarrow \infty \) \( \Rightarrow \) \( \delta \rightarrow 0 \)

\( E_n = \frac{n^2 \pi^2 \hbar^2}{2m(L + 2\delta)^2}, n = 1, 2, 3, 4... \)

When \( E = U \) then solutions blow up

\( \Rightarrow \) Limits to number of bound states (\( E_n < U \))

When \( E > U \), particle is not bound and can get either reflected or transmitted across the potential "barrier"
Particle of mass \( m \) within a potential \( U(x) \)

\[
\ddot{F}(x) = - \frac{dU(x)}{dx}
\]

\[
\ddot{F}(x=a) = - \frac{dU(x)}{dx} \bigg|_{x=a} = 0,
\]

\[
\ddot{F}(x=b) = 0, \quad \ddot{F}(x=c) = 0 \quad \text{... But...}
\]

Look at the Curvature:

\[
\frac{d^2U}{dx^2} > 0 \quad \text{(stable)}, \quad \frac{d^2U}{dx^2} < 0 \quad \text{(unstable)}
\]

Stable Equilibrium: General Form:

\[
U(x) = U(a) + \frac{1}{2} k(x-a)^2
\]

Rescale \( \Rightarrow U(x) = \frac{1}{2} k(x-a)^2 \)

Motion of a Classical Oscillator (ideal)

Ball originally displaced from its equilibrium position, motion confined between \( x=0 \) & \( x=A \)

\[
U(x) = \frac{1}{2} kx^2 = \frac{1}{2} m\omega^2 x^2; \quad \omega = \sqrt{\frac{k}{m}} = \text{Ang. Freq}
\]

\[
E = \frac{1}{2} kA^2 \quad \Rightarrow \text{Changing } A \text{ changes } E
\]

\( E \) can take any value & \( \text{if } A \rightarrow 0, \ E \rightarrow 0 \)

Max. KE at \( x = 0 \), KE = 0 at \( x = \pm A \)
Find the Ground state Wave Function $\psi(x)$

Find the Ground state Energy $E$ when $U(x) = \frac{1}{2} m \omega^2 x^2$

Time Dependent Schrodinger Eqn:

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \psi(x) = E \psi(x)$$

$$\Rightarrow \frac{d^2 \psi(x)}{dx^2} = \frac{2m}{\hbar^2} \left( E - \frac{1}{2} m \omega^2 x^2 \right) \psi(x) = 0$$

What $\psi(x)$ solves this?

Two guesses about the simplest Wavefunction:

1. $\psi(x)$ should be symmetric about $x$
2. $\psi(x) \to 0$ as $x \to \infty$

$\psi(x)$ should be continuous & $\frac{d \psi(x)}{dx}$ = continuous

My guess: $\psi(x) = C_0 e^{-\alpha x^2}$; Need to find $C_0$ & $\alpha$:

What does this wavefunction & PDF look like?
Quantum Picture: Harmonic Oscillator

\[ \psi(x) = C_0 e^{-\alpha x^2} \]

\[ P(x) = C_0^2 e^{-2\alpha x^2} \]

How to Get \( C_0 \) & \( \alpha \) ?? …Try plugging in the Wavefunction into Time-Independent Schr. Eqn.