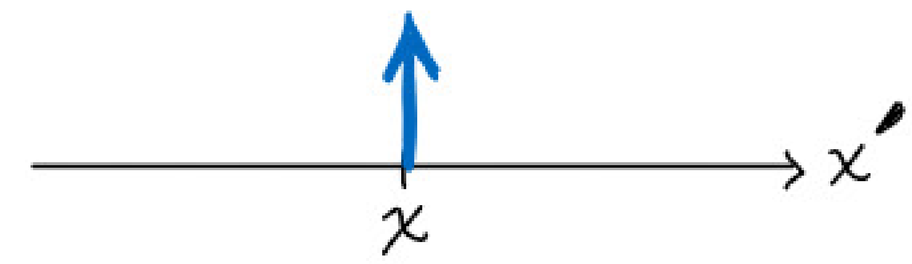
Uncertainty, Fourier Transforms, and Wave Mechanics as an Eigenvalue Problem (Quantum Part 1...)

① Uncertainty and Fourier Transforms: Space of $\mathbb{C}$-valued Functions on the Entire Real Line

- Position Eigenket $\hat{X}|x\rangle = x|x\rangle$
  - Completely localized in position $\langle x'|x\rangle = \delta(x'-x)$



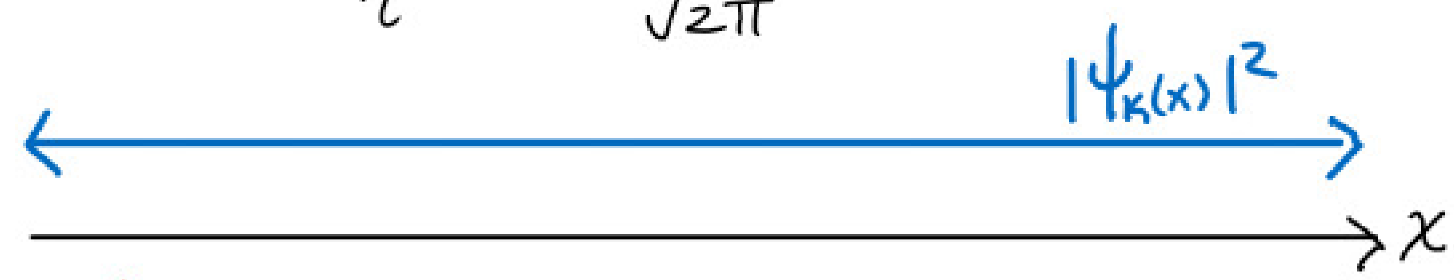
  - Composed of ALL POSSIBLE plane waves, i.e. Wavenumber Eigenkets

$$\langle k|x\rangle = \langle x|k\rangle^* = \frac{1}{\sqrt{2\pi}}e^{-ikx} \Rightarrow \quad |x\rangle = \hat{\mathbb{I}}|x\rangle = \int_{-\infty}^{\infty} dk\, |k\rangle\langle k|x\rangle$$

$\therefore$ Wavenumber of $|x\rangle$ is "ill-defined":
$|x\rangle$ is a superposition (lin. combo) of ALL $\{|k\rangle\}$

$$= \int_{-\infty}^{\infty} dk\, |k\rangle\, e^{-ikx}$$

- Wavenumber Eigenket $\hat{K}|k\rangle = k|k\rangle$
  - Completely localized in k-space: $\langle k'|k\rangle = \delta(k'-k)$
  - Completely delocalized in position: $\langle x|k\rangle \equiv \psi_k(x) = \frac{e^{ikx}}{\sqrt{2\pi}}$



$\Rightarrow$ These are two extremes of a general "Uncertainty" Principle for Fourier XFMs:

Uncertainty Principle: (1st Version)

- Let $\langle x|f\rangle = f(x)$; $\langle k|f\rangle = \int_{-\infty}^{\infty} dx\, \langle k|x\rangle\langle x|f\rangle = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-ikx} f(x) \equiv \tilde{f}(k)$ "Fourier XFM of $f(x)$"
- The more "localized" $f(x)$ is in position,
  the more "delocalized" (spread out) $\tilde{f}(k)$ is in wavenumber

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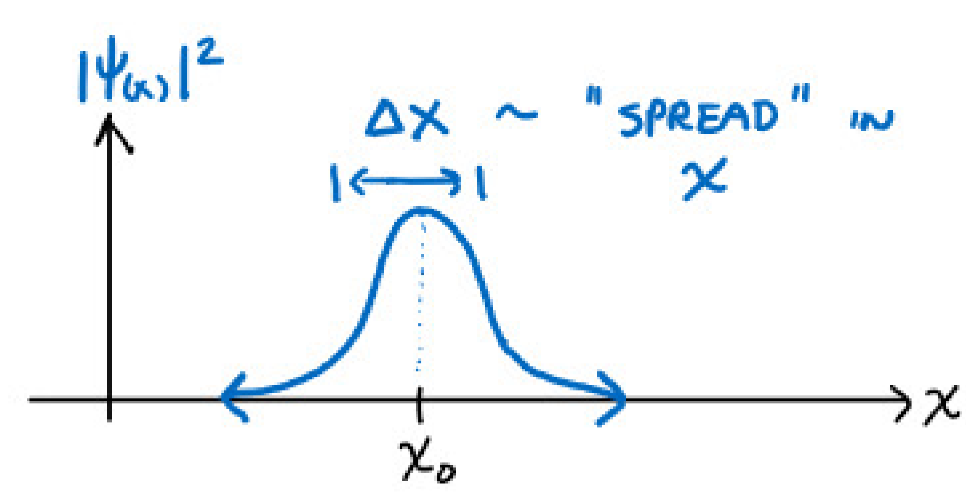
Example: Fourier Transform of a Gaussian



$$\psi(x) = \langle x|\psi\rangle \equiv \frac{1}{(\pi\Delta^2)^{1/4}} e^{ik_0 x} e^{-\frac{(x-x_0)^2}{2\Delta^2}} \; ; \quad |\psi(x)|^2 = \frac{1}{(\pi\Delta^2)^{1/2}} e^{-\frac{(x-x_0)^2}{\Delta^2}}$$

- Normalized: $\langle\psi|\psi\rangle = \int_{-\infty}^{\infty} dx\, |\psi(x)|^2 = \int_{-\infty}^{\infty} \frac{dx}{\Delta\sqrt{\pi}} e^{-\frac{(x-x_0)^2}{\Delta^2}} = \int_{-\infty}^{\infty} \frac{dy}{\sqrt{\pi}} e^{-y^2} = 1$ $\Leftarrow$ Homework!

  $y \equiv \frac{(x-x_0)}{\Delta}$; $dy = \frac{dx}{\Delta}$

- Avg. Position:

$$\langle\psi|\hat{X}|\psi\rangle \equiv \langle\hat{X}\rangle = \int_{-\infty}^{\infty} \frac{dx}{\Delta\sqrt{\pi}}\, x\, e^{-\frac{(x-x_0)^2}{\Delta^2}} = \int_{-\infty}^{\infty} \frac{dy}{\sqrt{\pi}} (\cancel{\Delta y} + x_0)\, e^{-y^2} = x_0 \; ✓$$

Odd function in y

$y \equiv \frac{(x-x_0)}{\Delta}$

- $\underline{\text{Variance in Position} \equiv (\Delta X)^2}$

$$(\Delta X)^2 \equiv \langle \underbrace{(\hat{X} - \langle \hat{X} \rangle)^2}_{\substack{\text{squared spread} \\ \text{of the state } |\psi\rangle}} \rangle = \langle \hat{X}^2 - \langle \hat{X} \rangle^2 \rangle = \langle \psi | \hat{X}^2 | \psi \rangle - x_0^2 \, ;$$

$$\langle \psi | \hat{X}^2 | \psi \rangle = \int_{-\infty}^{\infty} \frac{dx}{\Delta \sqrt{\pi}} (x + x_0)^2 \, e^{-\frac{x^2}{\Delta^2}}$$

$$(x + x_0)^2 = (x^2 + \cancel{2 x x_0} + \cancel{x_0^2})$$

ODD

CANCELS WITH

$$\Rightarrow (\Delta x)^2 = \Delta^2 \int_{-\infty}^{\infty} \frac{dy}{\sqrt{\pi}} y^2 e^{-y^2} = \frac{\Delta^2}{2} \quad \text{(HOMEWORK)}$$

$\therefore$ $\Delta X = \frac{\Delta}{\sqrt{2}}$ FOR THE SQUARE-NORMALIZED GAUSSIAN STATE $|\psi\rangle$

$\Delta X \equiv \sqrt{\langle \psi | \hat{X}^2 - \langle \hat{X} \rangle^2 | \psi \rangle}$ UNCERTAINTY IN POSITION DEFINED FOR ANY STATE (SQUARE-NORMALIZED) $|\psi\rangle$, SQUARE ROOT OF THE VARIANCE

- $\underline{\text{Fourier Transform of Gaussian "Wavepacket" } \psi(x)}$

$$\langle k | \psi \rangle \equiv \tilde{\psi}(k) = \int_{-\infty}^{\infty} dx \, \frac{e^{-ikx}}{\sqrt{2\pi}} \, \frac{1}{(\pi \Delta^2)^{1/4}} \, e^{i k_0 x} \, e^{-\frac{(x - x_0)^2}{2\Delta^2}} = \frac{\Delta \, e^{i(k_0 - k) x_0}}{\sqrt{2\pi} (\pi \Delta^2)^{1/4}} \int_{-\infty}^{\infty} dy \, e^{i(k_0 - k)\Delta y} \, e^{-\frac{y^2}{2}}$$

$y \equiv \frac{x - x_0}{\Delta}$; $x = \Delta y + x_0$

TRICK: COMPLETING THE SQUARE

CONSIDER
$$\int_{-\infty}^{\infty} dx \, e^{-\frac{\alpha x^2}{2} + \beta x} = \int_{-\infty}^{\infty} dx \, e^{-\frac{\alpha}{2}\left[x^2 - 2x\left(\frac{\beta}{\alpha}\right) + \left(\frac{\beta}{\alpha}\right)^2\right] + \frac{\alpha}{2}\left(\frac{\beta}{\alpha}\right)^2} = \int_{-\infty}^{\infty} dx \, e^{-\frac{\alpha x^2}{2} + \frac{\beta^2}{2\alpha}} = e^{\frac{\beta^2}{2\alpha}} \left[\int_{-\infty}^{\infty} dx \, e^{-\frac{\alpha x^2}{2}} = \sqrt{\frac{2\pi}{\alpha}} \right]$$

HERE:
$$\int_{-\infty}^{\infty} dy \, e^{-\frac{y^2}{2} + (k_0 - k)\Delta i y} = \sqrt{2\pi} \, e^{\frac{\beta^2}{2\alpha}} = \sqrt{2\pi} \, e^{-\frac{1}{2}\Delta^2 (k - k_0)^2}$$

$\Rightarrow \alpha = 1$; $\beta = i\Delta(k_0 - k)$ • COMPLETING THE SQUARE WORKS EVEN FOR COMPLEX β, SO LONG AS $\alpha > 0$ (INTEGRAL CONVERGES)

$$\therefore \quad \boxed{\tilde{\psi}(k) = \frac{\sqrt{\Delta}}{\pi^{1/4}} \, e^{i(k_0 - k)x_0} \, e^{-\frac{\Delta^2}{2}(k - k_0)^2}}$$

NOTE: $|\tilde{\psi}(k)|^2$ TAKES SAME FORM (GAUSSIAN!) AS $|\psi(x)|^2$, WITH
- $x \to k$, $x_0 \to k_0$
- $\Delta \to 1/\Delta$

- AVG. WAVENUMBER: $\langle \psi | \hat{k} | \psi \rangle \equiv \langle \hat{k} \rangle = k_0$
- VARIANCE: $(\Delta k)^2 \equiv \langle \psi | \hat{k}^2 - \langle \hat{k} \rangle^2 | \psi \rangle = \frac{1}{2\Delta^2}$
- UNCERTAINTY IN WAVENUMBER: $\Delta k = \frac{1}{\sqrt{2}\Delta}$ FOR GAUSSIAN PACKET • WIDTH $\Delta k \propto \frac{1}{\Delta X}$ [AND UNITS WORK OUT, OF COURSE]

$\Rightarrow$ SMALLER ΔX, LARGER ΔK (AND VICE-VERSA!)

$\Rightarrow$ FOR SQUARE-NORMALIZED GAUSSIAN $|\psi\rangle$, $(\Delta X)(\Delta k) = \frac{1}{2}$

CLAIM: THIS IS A MINIMUM BOUND (NOT PROVEN HERE)

UNCERTAINTY PRINCIPLE FOR FOURIER TRANSFORMS:

$$\Delta X \cdot \Delta k \geq \frac{1}{2}$$

Uncertainty for Time-Frequency Fourier Transforms

Although we will not view time as a continuous Hilbert space in Quantum Mechanics, it is obvious that we can define an analogous Fourier Trans. Pair for

[For practical reasons, easier to view time t as a parameter, not a ket $|t\rangle$, in Quantum Physics]

Time t and Frequency ω:

$$\tilde{f}(\omega) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt \; e^{i\omega t} \; f(t)$$

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega \; e^{-i\omega t} \; \tilde{f}(\omega)$$

Since these are mathematically identical to x-k Fourier transforms, there is an analogous uncertainty statement:

$$\Delta t \, \Delta \omega \geq 1/2$$

- A signal localized in time has broad freq. content
- A signal with a narrow freq. range is "delocalized" in time

$\Rightarrow$ Familiar to any engineer who studies signals

Finally, some Quantum Physics: Postulates (1st pass...)

First, a quick reminder from Early Quantum Theory: Planck's Blackbody Theory

Key Idea: Light (E+M radiation) consists of (massless) particles called photons

- Energy of a single photon for a monochromatic light beam with freq ω:

$$E = \hbar\omega = h\nu,$$

Units of energy $\equiv [E]$ — Units of inverse time $\frac{1}{[t]}$

- ν = frequency in inverse seconds (Hz)
- $\omega = 2\pi\nu$ "radian freq." (usually used in Physics)
- $\hbar = \frac{h}{2\pi}$ Planck's constant

$\therefore \; [\hbar] = [E][t] = 1.055 \cdot 10^{-34}$ Joule $\cdot$ sec

$= 6.582 \cdot 10^{-16}$ eV $\cdot$ sec

- $\hbar$: Fund. constant with units of energy $\times$ time
- suggests Energy-Time uncertainty principle for quantum systems:

$$\Delta E \, \Delta t \geq \frac{\hbar}{2}$$

- A quantum state with well-defined energy must live for a very long time!

Postulates of Quantum Mechanics (1st Pass...)

① The state of a quantum system (particle, qubit, collection thereof...) is represented by a state $|\psi\rangle$ in a Lin. Vector Space

② Physical Observables such as position, momentum, angular momentum, etc. are associated to Hermitian Operators

ex: Position $\hat{X} = \hat{X}^{\dagger}$

③ Quantum Mechanics predicts the probability that an observable $\hat{\Omega} = \hat{\Omega}^{\dagger}$ gives a measured value ω_i assoc. to E'vector $|\omega_i\rangle$:

$$\hat{\Omega}|\omega_i\rangle = \omega_i|\omega_i\rangle$$

For an "Ideal Measurement," assuming $\langle\psi|\psi\rangle = 1$, the probability of measuring value ω_i is given by $|\langle\omega_i|\psi\rangle|^2$

- Outcome of any particular measurement is random! $\Rightarrow$ cannot be predicted, even in principle!

- Distribution of outcomes is precisely predicted:

Prob. to obs. value ω_i for obs. $\hat{\Omega}$: $\equiv P_{\omega_i} = |\langle\omega_i|\psi\rangle|^2$

RECALL ENERGY-TIME UNCERTAINTY: $\Delta E \, \Delta t \geq \hbar/2$

(4.) FOR AN ISOLATED QUANTUM SYSTEM [NO INTERACTION WITH ENVIRONMENT ; NO OUTSIDE TIME-DEPT. FORCING]

THERE EXISTS A SPECIAL ENERGY EIGENBASIS $\{|E\rangle\}$
WHERE STATE $|E\rangle$

- HAS SHARP (WELL-DEFINED) ENERGY E
- HAS OBSERVABLE PROPERTIES (PROBABILITIES) THAT DO NOT DEPEND ON TIME.

THESE STATES SATISFY THE EIGENSTATE EQUATION

$$\hat{H}|E\rangle = E|E\rangle; \quad \hat{H} \equiv \text{"HAMILTONIAN" OF THE SYSTEM}$$

THE HAMILTONIAN IS SIMPLY THE OPERATOR THAT MEASURES THE TOTAL ENERGY IN THE SYSTEM, AS YOU WILL LEARN IN PHYS 301 *

(*) ACTUALLY, IN CLASSICAL MECH., THERE ARE SPECIAL SITUATIONS WHERE THE HAMILTONIAN IS <u>NOT</u> EQUIV. TO THE TOTAL ENERGY. BUT THESE INVOLVE TIME-DEPT. EXTERNAL DRIVING OR "FICTITIOUS" FORCES IN NON-INERTIAL REF. FRAMES. BY ASSUMPTION WE EXCLUDED EXT. t-DEPT. FORCES IN POSTULATE (4), AND WE WON'T DEAL WITH NON-INERTIAL FRAMES IN THIS CLASS

<u>QUANTUM MECH. OF A PARTICLE IN ONE SPATIAL DIM.</u>, i.e. $|\psi\rangle$ BELONGS TO THE HILBERT SPACE OF FUNCTIONS ON THE REAL LINE

$\langle x|\psi\rangle = \psi(x)$: "wave function" of particle

<u>OPERATORS:</u>

(1) POSITION: $\hat{X}|x\rangle = x|x\rangle$ (2) MOMENTUM: $\hat{P}|p\rangle = p|p\rangle$

MOMENTUM : MASS $\times \dfrac{\text{LENGTH}}{\text{TIME}}$; ENERGY : MASS $\times \left(\dfrac{\text{LENGTH}}{\text{TIME}}\right)^2$

$\therefore$ MOMENTUM : ENERGY $\times \left(\dfrac{\text{TIME}}{\text{LENGTH}}\right) = (\text{ENERGY} \times \text{TIME})\left(\dfrac{1}{\text{LENGTH}}\right)$

QUANTUM: IDENTIFY $\hat{P} \equiv \hbar \hat{K}$, $\hbar \times$ WAVENUMBER OP.!

- $\hat{P}$: (Energy·Time) $\frac{1}{\text{Length}}$
- $\hat{K}$: $\frac{1}{\text{LENGTH}}$
- $\hbar$: ENERGY × TIME

$\Rightarrow$ IMPLIES THE FAMOUS HEISENBERG UNCERTAINTY RELATION:
(POSITION – MOMENTUM)

$$\Delta X \, \Delta P \geq \hbar/2 \quad ; \quad \begin{aligned} \Delta x &\equiv \sqrt{\langle\psi|\hat{X}^2 - \langle\hat{X}\rangle^2|\psi\rangle} \\ \Delta P &\equiv \hbar\sqrt{\langle\psi|\hat{K}^2 - \langle\hat{K}\rangle^2|\psi\rangle} \end{aligned}$$

$\Rightarrow$ FOR A QUANTUM PARTICLE IN 1D, POSITION AND MOMENTUM CANNOT BOTH BE SIMULTANEOUSLY DETERMINED PRECISELY!

THIS IS ALSO APPARENT FROM THE "CANONICAL" COMMUTATION RELATIONS:

LEC. $\frac{8}{\text{''''}}$, P. 1: $[\hat{X}, \hat{K}] = i\,\hat{\mathbb{I}}$ $\quad\therefore\quad$ $[\hat{X}, \hat{P}] = i\hbar\,\hat{\mathbb{I}}$

$\Rightarrow$ $\hat{X}$ AND $\hat{P}$ ARE BOTH HERMITIAN OP.S = OBSERVABLES

BUT: THEY CANNOT BE SIMULTANEOUSLY DIAGONALIZED (THEOREM 12, LEC. $\frac{5}{\text{''''}}$, P. 2)

MOMENTUM OP.: SUMMARY

REFER TO THE "SUMMARY ON HERM. OP.S ON HILBERT SPACE POSITION, WAVENUMBER" NOTE

- RESOLUTION OF THE IDENTITY

$$\langle x|\hat{\mathbb{I}}|x'\rangle = \int_{-\infty}^{\infty} dK \, \frac{1}{2\pi} e^{iK(x-x')} = \int_{-\infty}^{\infty} dP \, \frac{1}{2\pi\hbar} e^{i\frac{P(x-x')}{\hbar}} = \langle x| \int_{-\infty}^{\infty} dp \, |p\rangle\langle p| x'\rangle$$

- EIGENSTATES: $\hat{P}|p\rangle = p|p\rangle$

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{p\cdot x}{\hbar}}$$

- MATRIX ELEMENTS
  - $|x\rangle$ BASIS: $\langle x|\hat{P}|x'\rangle = -i\hbar\frac{d}{dx}\delta(x-x') = \delta(x-x')\left[-i\hbar\frac{d}{dx'}\right]$
  - $|p\rangle$ BASIS: $\langle p|\hat{P}|p'\rangle = p\,\delta(p-p')$

- EFFECT ON GENERIC STATE $|\psi\rangle$:
  - $|x\rangle$ BASIS: $\langle x|\hat{P}|\psi\rangle = \int_{-\infty}^{\infty} dx' \langle x|\hat{P}|x'\rangle\langle x'|\psi\rangle = -i\hbar\frac{d\psi}{dx}$
  - $|p\rangle$ BASIS: $\langle p|\hat{P}|\psi\rangle = \int_{-\infty}^{\infty} dp' \langle p|\hat{P}|p'\rangle \underbrace{\langle p'|\psi\rangle}_{\equiv \tilde{\psi}(p')} = p\,\tilde{\psi}(p)$

The Time-Indept. Schrödinger Eqn as an Energy Eigenvalue Problem

$\hat{H}|E\rangle = E|E\rangle$. What is the "Hamiltonian" $\hat{H}$ for a non-relativistic particle in 1D?

$$\hat{H} = \text{Total Energy} = (\text{Kinetic}) + (\text{Potential})$$

Classical Mech: $H = E = \frac{p^2}{2m} + V(x)$, $V(x)$ is the potential energy (due, e.g., to a static electric field)

Quantum: Replace with assoc. operator

$$\hat{H} = \frac{\hat{P}^2}{2m} + \hat{V}(\hat{X})$$

a function of $\hat{X}$ ⇒ Lec. 6

$$\therefore \quad \hat{H}|E\rangle = \left(\frac{\hat{P}^2}{2m} + \hat{V}(\hat{X})\right)|E\rangle = E|E\rangle$$

Project into position basis: $\langle x|E\rangle \equiv \psi_E(x)$ "wave function"

$$\Rightarrow \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi_E(x) = E\,\psi_E(x)$$

∴ Time-Indept. Schrödinger Eqn. in Wave Mechanics = Energy Eigenvalue Problem in the Position Basis!

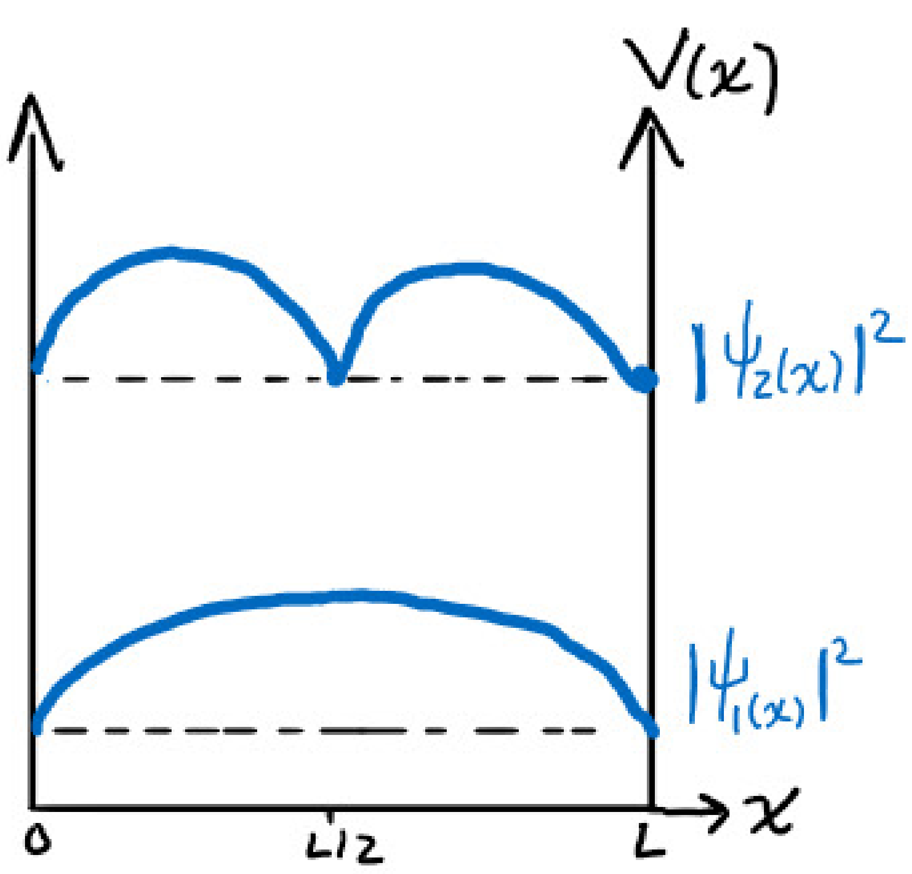
Can now revisit Phys 202 problems

① Infinite Square Well: $V = 0$, $0 \leq x \leq L$; $V = \infty$ else $\Rightarrow \psi_E(0) = \psi_E(L) = 0$.

$$-\frac{d^2}{dx^2}\psi_E = \frac{2mE}{\hbar^2}\psi_E \equiv k^2\psi_E$$

Same as the homog. string with Dirichlet B.C.! (Lec. 1)

$$\therefore \quad k_n = \frac{n\pi}{L} \; ; \quad E_n = \frac{\hbar^2}{2m}k_n^2 = \left(\frac{\hbar^2}{2m}\right)\left(\frac{n\pi}{L}\right)^2$$



Wave Functions:

$$\psi_E(x) = \sqrt{\frac{2}{L}}\,\sin(k_n x)$$

Interpretation:

$$|\psi_E(x)|^2 = \frac{2}{L}\sin^2(k_n x) =$$ Probability density to find particle with energy E at position x