Quiz 7

- Final Exam will emphasize later chapters
- Finals Review on Saturday 15 March, WLH2001
Operators $\rightarrow$ Information Extractors

$p$ or $\hat{p} = \frac{\hbar}{i} \frac{d}{dx}$

Momentum Operator

gives the value of average momentum in the following way:

$$<p> = \int_{-\infty}^{+\infty} \psi^*(x)p\psi(x)dx = \int_{-\infty}^{+\infty} \psi^*(x)\left(\frac{\hbar}{i}\right)d\frac{\psi}{dx}dx$$

Similarly:

$[K]$ or $\hat{K} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$ gives the value of average KE

$$<K> = \int_{-\infty}^{+\infty} \psi^*(x)[K]\psi(x)dx = \int_{-\infty}^{+\infty} \psi^*(x)\left(-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}\right)dx$$

Similarly

$$<U> = \int_{-\infty}^{+\infty} \psi^*(x)[U(x)]\psi(x)dx$$ plug in the $U(x)$ fn for that case

and

$$<E> = \int_{-\infty}^{+\infty} \psi^*(x)[K + U(x)]\psi(x)dx = \int_{-\infty}^{+\infty} \psi^*(x)\left(-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\right)dx$$

Hamiltonian Operator $[H] = [K] + [U]$

The Energy Operator $[E] = i\hbar\frac{\partial}{\partial t}$ informs you of the average energy
[H] & [E] Operators

• [H] is a function of x
• [E] is a function of t ……they are really different operators
• But they produce identical results when applied to any solution of the time-dependent Schrödinger Eq.

\[
[H] \Psi(x,t) = [E] \Psi(x,t)
\]

Think of S. Eq as an expression for Energy conservation for a Quantum system
Where do Operators come from? A touchy-feely answer

**Example:** $[p]$  The momentum Extractor (operator):

Consider as an example: Free Particle Wavefunction

$$\Psi(x,t) = Ae^{i(kx-\omega t)} ; \quad k = \frac{2\pi}{\lambda}, \quad \lambda = \frac{\hbar}{p} \Rightarrow k = \frac{p}{\hbar}$$

**Rewrite**

$$\Psi(x,t) = Ae^{i\left(\frac{p}{\hbar}x-\omega t\right)} ; \quad \frac{\partial\Psi(x,t)}{\partial x} = \frac{i}{\hbar} p Ae^{i\left(\frac{p}{\hbar}x-\omega t\right)} = \frac{i}{\hbar} p \Psi(x,t)$$

$$\Rightarrow \left[\frac{\hbar}{i} \frac{\partial}{\partial x}\right] \Psi(x,t) = p \Psi(x,t)$$

So it is not unreasonable to associate $[p]=\left[\frac{\hbar}{i} \frac{\partial}{\partial x}\right]$ with observable $p$.
Example: Average Momentum of particle in box

- Given the symmetry of the 1D box, we argued last time that \( <p> = 0 \) : now some inglorious math to prove it!
  - Be lazy, when you can get away with a symmetry argument to solve a problem, do it & avoid the evil integration & algebra…..but be sure!

\[
\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right) \quad \& \quad \psi^*_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right)
\]

\[
< p > = \int_{-\infty}^{\infty} \psi^*[p] \psi dx = \int_{-\infty}^{\infty} \psi^* \left[ \frac{\hbar}{i} \frac{d}{dx} \right] \psi dx
\]

\[
< p > = \frac{\hbar}{iL} \int_{-\infty}^{\infty} \sin\left(\frac{n\pi}{L} x\right) \cos\left(\frac{n\pi}{L} x\right) dx
\]

Since \( \int \sin ax \cos ax \, dx = \frac{1}{2a} \sin^2 ax \) …here \( a = \frac{n\pi}{L} \)

\[
\Rightarrow < p > = \frac{\hbar}{iL} \left[ \sin^2 \left(\frac{n\pi}{L} x\right) \right]_{x=L}^{x=0} = 0 \text{ since } \sin^2(0) = \sin^2(n\pi) = 0
\]

We knew THAT before doing any math!

Quiz 1: What is the \( <p> \) for the Quantum Oscillator in its symmetric ground state
Quiz 2: What is the \( <p> \) for the Quantum Oscillator in its asymmetric first excited state
But what about the $\langle KE \rangle$ of the Particle in Box?

$\langle p \rangle = 0$ so what about expectation value of $K = \frac{p^2}{2m}$?

$\langle K \rangle = 0$ because $\langle p \rangle = 0$; clearly not, since we showed $E = KE \neq 0$

Why? What gives?

Because $p_n = \pm \sqrt{2mE_n} = \pm \frac{n\pi \hbar}{L}$; "±" is the key!

AVERAGE $p = 0$, particle is moving back & forth

$\langle KE \rangle = \langle \frac{p^2}{2m} \rangle \neq 0$ not $\frac{\langle p \rangle^2}{2m}$!

Be careful when being "lazy"

Quiz: what about $\langle KE \rangle$ of a quantum Oscillator?

Does similar logic apply??
Recall when potential does not depend on time explicitly $U(x,t)$ = $U(x)$ only...we used separation of $x,t$ variables to simplify $\Psi(x,t) = \psi(x) \phi(t)$ & broke S. Eq. into two: one with $x$ only and another with $t$ only.

$$\Psi(x,t) = \psi(x)\phi(t)$$

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + U(x)\psi(x) \right) = E \psi(x)$$

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

How to put Humpty-Dumpty back together? E.g to say how to go from an expression of $\psi(x) \rightarrow \Psi(x,t)$ which describes time-evolution of the overall wave function.
Schrodinger Eqn: Stationary State Form

Since \( \frac{d}{dt} \left[ \ln f(t) \right] = \frac{1}{f(t)} \frac{df(t)}{dt} \)

\[
\ln \ i\hbar \frac{\partial \phi(t)}{\partial t} = E\phi(t) , \ \text{rewrite as} \quad \frac{1}{\phi(t)} \frac{\partial \phi(t)}{\partial t} = \frac{E}{i\hbar} = - \frac{iE}{\hbar}
\]

and integrate both sides w.r.t. time

\[
\int_{t=0}^{t=t} \frac{1}{\phi(t)} \frac{\partial \phi(t)}{\partial t} dt = \int_{0}^{t} - \frac{iE}{\hbar} dt \Rightarrow \int_{0}^{t} \frac{1}{\phi(t)} \frac{d\phi(t)}{dt} dt = - \frac{iE}{\hbar}
\]

\[\therefore \ln \phi(t) - \ln \phi(0) = - \frac{iE}{\hbar} t , \ \text{now exponentiate both sides} \]

\[\Rightarrow \phi(t) = \phi(0)e^{-\frac{iEt}{\hbar}} ; \ \phi(0) = \text{constant} = \text{initial condition} = 1 (\text{e.g}) \]

\[\Rightarrow \phi(t) = e^{-\frac{iEt}{\hbar}} & \ \text{Thus} \ \Psi(x,t) = \psi(x)e^{-\frac{iEt}{\hbar}} \ \text{where} \ E = \text{energy of system} \]
$P(x,t) = \Psi^* \Psi = \psi^*(x) e^{\frac{iE}{\hbar} t} \psi(x) e^{-\frac{iE}{\hbar} t} = \psi^*(x)\psi(x)e^{\frac{iE}{\hbar} t - \frac{iE}{\hbar} t} = |\psi(x)|^2$

In such cases, $P(x,t)$ is INDEPENDENT of time. These are called "stationary" states because Prob is independent of time.

Examples: Particle in a box (why?)
: Quantum Oscillator (why?)

Total energy of the system depends on the spatial orientation of the system: characteristic of the potential situation!
The Case of a Rusty “Twisted Pair” of Naked Wires & How Quantum Mechanics Saved ECE Majors!

- Twisted pair of Cu Wire (metal) in virgin form
- Does not stay that way for long in the atmosphere
  - Gets oxidized in dry air quickly Cu $\rightarrow$ Cu$_2$O
  - In wet air Cu $\rightarrow$ Cu(OH)$_2$ (the green stuff on wires)
- Oxides or Hydride are non-conducting ..so no current can flow across the junction between two metal wires
- No current means no circuits $\rightarrow$ no EE, no ECE !!
- All ECE majors must now switch to Chemistry instead & play with benzene !!! Bad news!
Consider George as a “free Particle/Wave” with Energy $E$ incident from Left.
Free particle are under no Force; have wavefunctions like

$$\Psi = A \ e^{i(kx - wt)} \ or \ B \ e^{i(-kx - wt)}$$
Tunneling Through A Potential Barrier

Classical & Quantum Pictures compared: When E > U & when E < U
Classically, an particle or a beam of particles incident from left encounters barrier:
- when E > U → Particle just goes over the barrier (gets transmitted)
- When E < U → particle is stuck in region I, gets entirely reflected, no transmission (T)

What happens in a Quantum Mechanical barrier? No region is inaccessible for particle since the wave function is (sometimes small) but finite....depends on length of the barrier as you shall see.
Beam Of Particles With E < U Incident On Barrier From Left

Region I

Incident Beam

Reflected Beam

Region III

Transmitted Beam

Description Of WaveFunctions in Various regions: Simple Ones first

In Region I: \( \Psi_1(x,t) = A e^{i(kx - \omega t)} + B e^{i(-kx - \omega t)} \) = incident + reflected Waves

with \( E = \hbar \omega = \frac{\hbar^2 k^2}{2m} \)

Define Reflection Coefficient: \( R = \frac{|B|^2}{|A|^2} = \frac{\text{fraction of incident wave intensity reflected back}}{\text{incident wave intensity}} \)

In Region III: \( \Psi_\text{III}(x,t) = F e^{i(kx - \omega t)} + Ge^{i(-kx - \omega t)} \) = transmitted

Note: \( Ge^{i(-kx - \omega t)} \) corresponds to wave incident from right!

This piece does not exist in the scattering picture we are thinking of now (G=0)

So \( \Psi_\text{III}(x,t) = F e^{i(kx - \omega t)} \) represents transmitted beam. Define \( T = \frac{|F|^2}{|A|^2} \)

Unitarity Condition \( \Rightarrow R + T = 1 \) (particle is either reflected or transmitted)