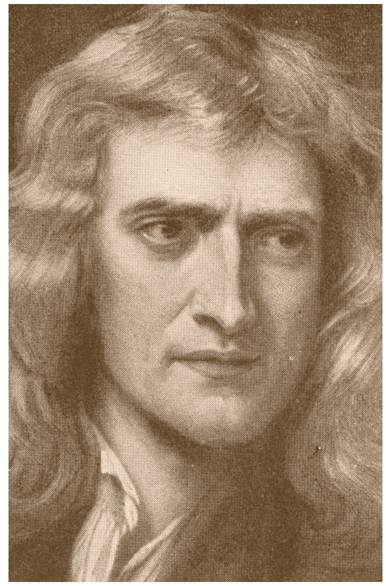
 $\approx$  ?

Lecture 13: The classical limit

Phy851/fall 2009

Wavepacket Evolution

- For a wavepacket in free space, we have already seen that

$$\langle x \rangle = x_0 + \frac{p_0}{M} t$$

$$\langle p \rangle = p_0$$

  - So that the center of the wavepacket obeys Newton's Second Law (with no force):

$$\frac{d}{dt}\langle x \rangle = \frac{\langle p \rangle}{m}$$

$$\frac{d}{dt}\langle p \rangle = 0$$

- Assuming that:
  - The wavepacket is very narrow
  - spreading is negligible on the relevant time-scale
- Would Classical Mechanics provide a quantitatively accurate description of the wavepacket evolution?
  - How narrow is narrow enough?

- What happens when we add a potential, $V(x)$?
  - Will we find that the wavepacket obeys Newton's Second Law of Motion?

Equation of motion for expectation value

- How do we find equations of motion for expectation values of observables?
  - Consider a system described by an arbitrary Hamiltonian, *H*
  - Let *A* be an observable for the system
  - Question: what is:

$$\frac{d}{dt}\langle A\rangle \quad ?$$

- Answer:

$$\frac{d}{dt}\langle A\rangle = \frac{d}{dt}\langle\psi(t)|A|\psi(t)\rangle$$

$$= \left(\frac{d}{dt}\langle\psi(t)|\right)A|\psi(t)\rangle + \langle\psi(t)|\left(\frac{\partial A}{\partial t}\right)|\psi(t)\rangle + \langle\psi(t)|A\left(\frac{d}{dt}|\psi(t)\rangle\right)$$

$$= \frac{i}{\hbar}\langle\psi(t)|HA|\psi(t)\rangle - \frac{i}{\hbar}\langle\psi(t)|AH|\psi(t)\rangle + \left\langle\frac{\partial A}{\partial t}\right\rangle$$

$$\boxed{\frac{d}{dt}\langle A\rangle = -\frac{i}{\hbar}\langle[A,H]\rangle + \left\langle\frac{\partial A}{\partial t}\right\rangle}$$

Example 1: A free particle

- Assuming that $\dfrac{\partial A}{\partial t} = 0$
- The basic equation of motion is:

$$\frac{d}{dt}\langle A\rangle = -\frac{i}{\hbar}\langle [A,H]\rangle$$

- For a free particle, we have: $H = \dfrac{P^2}{2M}$

$$\begin{aligned}
[X,H] &= \frac{1}{2M}[X,P^2] \\
&= \frac{1}{2M}\left(XP^2 - P^2X\right) \\
&= \frac{1}{2M}\left(XP^2 - PXP + PXP - P^2X\right) \\
&= \frac{1}{2M}\left([X,P]P + P[X,P]\right) \\
&= i\hbar\frac{P}{M}
\end{aligned}$$

$$[H,P] = 0$$

Very common trick in QM to become familiar with

$$\frac{d}{dt}\langle X\rangle = -\frac{i}{\hbar}\left\langle i\hbar\frac{P}{m}\right\rangle = \frac{\langle P\rangle}{m}$$

$$\frac{d}{dt}\langle P\rangle = 0$$

Adding the Potential

- Let $$H = \frac{P^2}{2M} + V(X)$$

$$\left[X,H\right] = \frac{1}{2M}\left[X,P^2\right] + \underset{=0}{\left[X,V(X)\right]}$$

$$= \frac{1}{2M}\left[X,P^2\right]$$

$$= i\hbar \frac{P}{M}$$

$$\left[H,P\right] = \frac{1}{2M}\underset{=0}{\left[P^2,P\right]} + \left[V(X),P\right]$$

$$= -\left[P,V(X)\right]$$

- How do we handle this commutator?

One possible approach

- We want an expression for: $\left[P, V(X)\right]$
- We can instead evaluate: $\left\langle x \middle| \left[P, V(X)\right] \middle| \psi \right\rangle$

Theorem: If $\langle x|A|\psi\rangle = \langle x|B|\psi\rangle$ is true for any x and $|\psi\rangle$, then it follows that $A=B$.

- Will need to make use of

$$\left\langle x \middle| P \middle| \psi \right\rangle = -i\hbar \frac{d}{dx} \left\langle x \middle| \psi \right\rangle$$

You should think of this as the defining equation for how to handle P in x-basis

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$$\left\langle x \middle| \left[P, V(X)\right] \middle| \psi \right\rangle = \left\langle x \middle| P V(X) \middle| \psi \right\rangle - \left\langle x \middle| V(X) P \middle| \psi \right\rangle$$

$$= -i\hbar \left\langle x \middle| V'(X) \middle| \psi \right\rangle$$

You will derive this in the HW

– Where $V'(x) = \frac{d}{dx} V(x)$

- Thus we have:

$$\left[P, V(X)\right] = -i\hbar V'(X)$$

Equations of motion for $\langle X\rangle$ and $\langle P\rangle$

- As long as: $$H = \frac{P^2}{2M} + V(X)$$

- The we will have: $$\frac{d}{dt}\langle X\rangle = \frac{\langle P\rangle}{m}$$

  – Not just true for a wavepacket

- For the momentum we have:

$$\frac{d}{dt}\langle P\rangle = -\frac{i}{\hbar}\langle [P, V(X)]\rangle$$

$$= -\frac{i}{\hbar}\langle -i\hbar V'(X)\rangle$$

$$= -\langle V'(X)\rangle$$

$$= \langle F(X)\rangle$$

F(X) is the Force operator

$$F(x) = -\frac{d}{dx}V(x)$$

- The QM form of the Second Law is Thus:

$$M\frac{d^2}{dt^2}\langle X\rangle = \langle F(X)\rangle$$

Difference between classical and QM forms of the 2nd Law of Motion

- Classical: $$M\frac{d^2}{dt^2}x = F(x)$$

- Quantum: $$M\frac{d^2}{dt^2}\langle X\rangle = \langle F(X)\rangle$$

- Classical Mechanics would be an accurate description of the motion of the center of a wavepacket, defined as $x(t) = \langle X\rangle$, if:

$$\langle F(X)\rangle \approx F\left(\langle X\rangle\right)$$

- So that $$M\frac{d^2}{dt^2}\langle X\rangle = F(\langle X\rangle)$$

- This condition is satisfied in the limit as the width of the wavepacket goes to zero

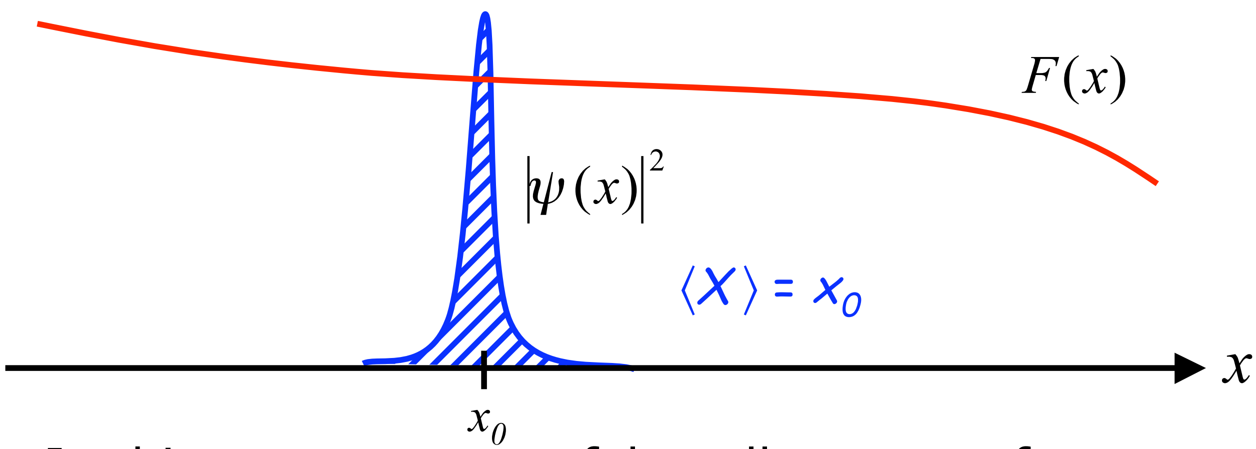
- ALWAYS TRUE for a constant (e.g. gravity) or linear force (harmonic oscillator potential), regardless of the shape of the wavefunction

Narrow wavepacket

- The expectation value of the Force is:

$$\langle F(X) \rangle = \int dx\, F(x) |\psi(x)|^2$$

- Let us assume that the force $F(x)$ does not change much over the length scale σ



- In this case we can safely pull $F(x)$ out of integral:

$$\langle F(X) \rangle \approx F(x_0) \int dx\, |\psi(x)|^2$$

$$\approx F(x_0)$$

$$\approx F(\langle X \rangle)$$

- So CM is a valid description if the wavepacket is narrow enough

A More Precise Formulation

$$\langle F(X) \rangle = \int dx\, F(x) |\psi(x)|^2$$

- Expand $F(x)$ around $x = \langle X \rangle$:

$$F(X) = F(\langle X \rangle) + F'(\langle X \rangle)(X - \langle X \rangle) + F''(\langle X \rangle)\frac{(X - \langle X \rangle)^2}{2} + \ldots$$

- Then take the expectation value:

$$\langle F(X) \rangle = F(\langle X \rangle)\langle I \rangle + F'(\langle X \rangle)\langle X - \langle X \rangle \rangle + F''(\langle X \rangle)\frac{\left\langle \left(X - \rangle X \langle\right)^2 \right\rangle}{2} + \ldots$$

$$\langle I \rangle = 1$$

$$\langle X - \langle X \rangle \rangle = \langle X \rangle - \langle X \rangle = 0$$

$$\begin{aligned}\left\langle (X - \langle X \rangle)^2 \right\rangle &= \left\langle X^2 - 2X\langle X \rangle + \langle X \rangle^2 \right\rangle \\ &= \left\langle X^2 \right\rangle - \langle X \rangle^2 \\ &:= (\Delta X)^2\end{aligned}$$

This is known as the Quantum Mechanical Variance. We will study it more formally later.

- We have:

$$\langle F(X)\rangle = F(\langle X\rangle) + F''(\langle X\rangle)\frac{(\Delta X)^2}{2} + \dots$$

- For CM to be a good approximation, it is therefore necessary that:

$$\left|F(\langle X\rangle)\right| >> \left|F''(\langle X\rangle)\right|\frac{(\Delta X)^2}{2}$$

  - The width of the wavepacket squared times the curvature of the force should be small compared to the force itself

- CAUTION: Even if the width of the wavepacket is small enough at one instant to satisfy this inequality, we also need to consider the rate of spreading

Example 1: Baseball

- Lets consider a baseball accelerating under the force of gravity:
  - $m = 1$ kg
  - let $\Delta X = 10^{-10}$ m
    - Will then be stable for 30 million years
  - The force is: $$F(X) = -\frac{GMm}{X^2}$$

$$F'(X) = \frac{2GMm}{X^3}$$

$$F''(X) = -\frac{6GMm}{X^4}$$

- Requirement for CM validity is:

$$\left|F\left(\langle X\rangle\right)\right| >> \left|F''\left(\langle X\rangle\right)\right|\left(\Delta X\right)^2$$

$$\frac{GMm}{\langle X\rangle^2} >> \frac{6GMm}{\langle X\rangle^4}\left(\Delta X\right)^2$$

$$\langle X\rangle^2 >> 6\left(\Delta X\right)^2$$

- Since $X \approx R_e = 6\_10^{7}$ m this gives $10^{15} >> 10^{-14}$

- So CM should work pretty well for a baseball

Example 2: Hydrogen atom

- Consider the very similar problem of an electron orbiting a proton:
  - Use ground state parameters

$$F(\langle x \rangle) = -\frac{e^2}{4\pi\varepsilon_0 \langle x \rangle^2}$$

$$F''(\langle X \rangle) = \frac{6F(\langle X \rangle)}{\langle X \rangle^4}$$

- Thus applicability of classical mechanics requires:

$$\langle X \rangle^2 >> 6(\Delta X)^2$$

- In the ground state we have: $\langle X \rangle \to 0$

$$\Delta X \sim a_0 = 10^{-10}\ \text{m}$$

- Which gives $0 >> 10^{-20}$
  - So CM will *not* be valid for an electron in the hydrogen ground state
- Highly excited `wavepacket' states can be described classically → Rydberg States
  - Because $\langle X \rangle$ can get extremely large

Rydberg States in Hydrogen

- The coulomb potential is