Physics 491

Lecture #11: Put Mechanics in Quantum Mechanics

Quantum Dynamics and Ehrenfest's Theorem

We have seen that if the observable $\hat{A}$ represents a conserved quantity, then $\frac{d\langle\hat{A}\rangle}{dt} = 0$. What can we say in general?

Consider a general observable $\hat{A}(t)$. Note: Here we have allowed $\hat{A}$ to have some explicit time dependence (i.e. due to a time dependent forcing)

$$\langle\hat{A}\rangle_t = \int dx\, \psi^*_{(x,t)}\, \hat{A}(t)\, \psi_{(x,t)}$$

($\psi^*_{(x,t)}$: time dependent state; $\hat{A}(t)$: time dependent observable)

$$\Rightarrow \frac{d}{dt}\langle\hat{A}\rangle_t = \int dx \left(\frac{\partial\psi}{\partial t}\right)^* \hat{A}\,\psi + \int dx\, \psi^* \frac{\partial\hat{A}}{\partial t}\,\psi + \int dx\, \psi^* \hat{A} \frac{\partial\psi}{\partial t}$$

Now we can use the T.D.S.E. $\frac{\partial}{\partial t}\psi_{(x,t)} = \frac{-i}{\hbar}\hat{H}\psi$

$$\Rightarrow \frac{d}{dt}\langle\hat{A}\rangle_t = \int dt \left(\tfrac{-i}{\hbar}\hat{H}\psi\right)^* \hat{A}\,\psi + \int dx\, \psi^* \left(\frac{\partial A}{\partial t}\right)\psi + \int dt\, \psi^* \hat{A} \left(\tfrac{-i}{\hbar}\hat{H}\psi\right)$$

$$\Rightarrow \frac{d}{dt}\langle \hat{A} \rangle_t = \frac{-i}{\hbar} \int d\tau\, \psi^* \underbrace{(\hat{A}\hat{H} - \hat{H}\hat{A})}_{[\hat{A},\hat{H}]} \psi + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle_t$$

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

Note: If $[\hat{A},\hat{H}] = 0$ (and $\hat{A}$ is not explicitly time dependent)

$$\frac{d}{dt}\langle \hat{A} \rangle_t = 0 \Rightarrow \text{Conserved}$$

Note: For problems without an explicit time dependence $\frac{d}{dt}\langle \hat{H} \rangle_t = 0$

Since $[\hat{H},\hat{H}] = 0 \Rightarrow$ energy is conserved

This semester we will deal with only problems without an explicit time dependent force so all observables have no explicit time dependence. We will return to time dependent perturbations next semester.

Thus, without explicit time dependence

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

Consider 1D problems with Hamiltonian

$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m}}_{\equiv \hat{T}\ \text{(kinetic energy}} + \underbrace{V(\hat{x})}_{\leftarrow \text{potential energy}}$$

$$\Rightarrow \frac{d}{dt}\langle \hat{x} \rangle = \frac{-i}{\hbar}\langle [\hat{x}, \hat{H}] \rangle = \frac{-i}{\hbar}\left(\langle [\hat{x}, \hat{T}] \rangle + \langle [\hat{x}, \hat{V}] \rangle \right)$$

Aside: $[\hat{x}, V(\hat{x})] = 0$ (Any operator commutes with functions of itself)

$$[\hat{x}, \hat{T}] = \left[\hat{x}, \frac{\hat{p}^2}{2m}\right] = \frac{1}{2m}[\hat{x}, \hat{p}^2] = \frac{1}{2m}\left(\hat{p}[\hat{x}, \hat{p}] + [\hat{x}, \hat{p}]\hat{p}\right)$$

$$= \frac{i\hbar}{m}\hat{p}$$

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

This is exactly the equation of motion for the classical variables (x_{cl}, p_{cl}): $\frac{dx_{cl}}{dt} = \frac{p_{cl}}{m}$

Consider $\frac{d}{dt}\langle \hat{p} \rangle = \frac{-i}{\hbar}\langle [\hat{p}, \hat{H}] \rangle = \frac{-i}{\hbar}\left(\langle [\hat{p}, \hat{T}] \rangle + \langle [\hat{p}, \hat{V}] \rangle \right)$

Aside: $[\hat{p}, \hat{T}] = \left[\hat{p}, \frac{\hat{p}^2}{2m}\right] = 0$

$$[\hat{p}, V(\hat{x})] = \frac{\hbar}{i}\left.\frac{\partial V}{\partial x}\right|_{x=\hat{x}}$$ (see P.S. #4)

$$\therefore \boxed{\frac{d}{dt}\langle \hat{p} \rangle_t = - \left\langle \frac{\partial V}{\partial x} \Big|_{x=\hat{x}} \right\rangle_t}$$

If we combine the two first order eqns for $\langle \hat{x} \rangle$ and $\langle \hat{p} \rangle$

$$\Rightarrow \frac{d}{dt}\langle \hat{p} \rangle_t = \boxed{m \frac{d^2}{dt^2}\langle \hat{x} \rangle_t = - \left\langle \frac{\partial V}{\partial x} \Big|_{x=\hat{x}} \right\rangle_t}$$

This looks like Newton's Law for classical trajectories $F_{cl} = m a_{cl}$ where $\begin{cases} F_{cl} = -\frac{\partial V}{\partial x}(x_{cl}) \\ a_{cl} = \frac{d^2 x_{cl}}{dt^2} \end{cases}$

Thus, we are led to Ehrenfest's "theorem"

The quantum expectation values follow the classical trajectories (or at least it looks that way)

In fact Ehrenfest's theorem is <u>not</u> true in general. If were we would never see quantum phenomena such as interference or tunnelling.

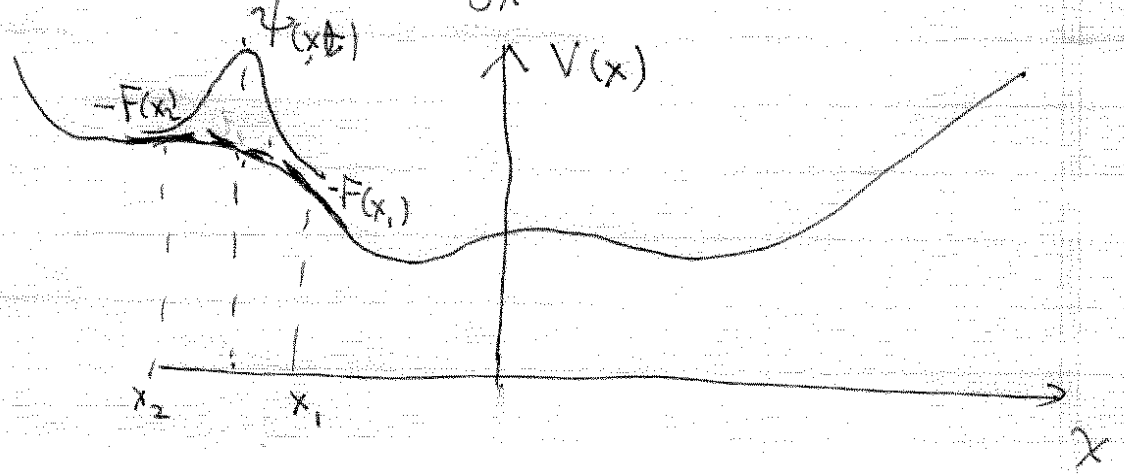
(Next page)

The subtle point is that in general

$$\left\langle \left.\frac{\partial V}{\partial x}\right|_{x=\hat{x}} \right\rangle_t \neq \left.\frac{\partial V}{\partial x}\right|_{x=\langle \hat{x} \rangle_t \to x_{ce}}$$

This equality is required for Ehrenfest's theorem to be true

Pictorally we can understand this as follows. Consider motion in a 1D potential $V(x)$, with force $F(x) = -\frac{\partial V}{\partial x}$



Shown above is a wave packet centered at $x_{ce} = \langle \hat{x} \rangle$. The force at x_{ce} $F(x_{ce}) = -\frac{\partial V}{\partial x} = \left.\frac{\partial V}{\partial x}\right|_{x=\langle \hat{x} \rangle}$.

However, the wave packet has a finite extent. Thus, generally, the force at different x is different. These different trajectories interfere.

Thus, Ehrenfest's theorem holds only approximately since the force can be a nonlinear function of position. Unless the packet is very localized

$\Rightarrow \Delta x \ll$ Scale of change in $F(x)$

This is the classical limit

Review: General features of classical motion in 1D

Let us look at the Classical Hamiltonian

$$H = \frac{p^2}{2m} + V(x) = E \quad \text{energy}$$

the motion is along trajectories $x(t)$, $p(t)$

where $\frac{dx}{dt} = \frac{p}{m}$ $\qquad$ $\frac{dp}{dt} = -\frac{\partial V}{\partial x}$

Momentum and position are constrained by conservation of energy $\Rightarrow$ at any time

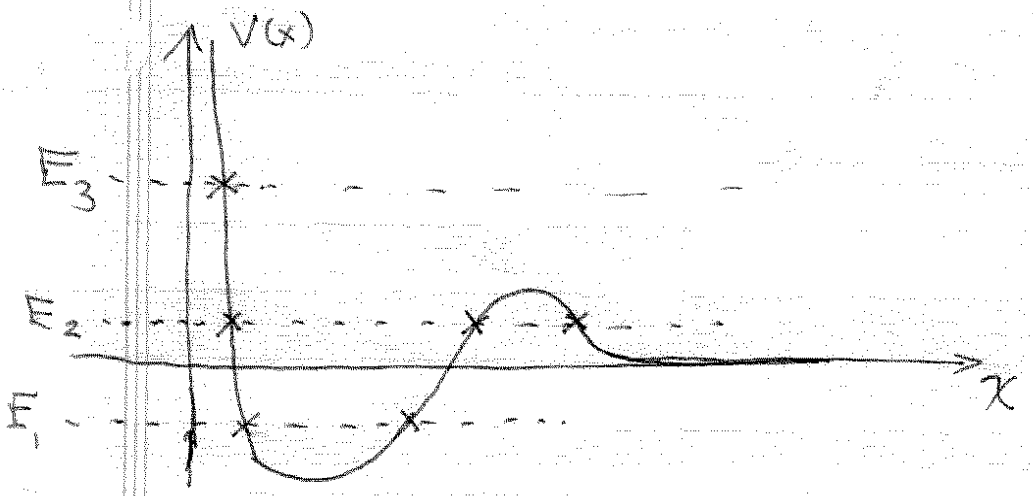
$$\frac{p^2(t)}{2m} + V(x(t)) = E$$

$$\Rightarrow \quad p(t) = \pm \sqrt{2m\,(E - V(x(t)))}$$

Often we look at this independent of time

$$p = \pm \sqrt{2m\,(E - V(x))} \quad \text{must be real}$$

Classifying trajectories : Use $V(x)$



Shown above is a generic potential energy $V(x)$. Remember, the zero of potential is arbitrary. Here I have chosen it so that $V \to 0$ as $x \to \infty$. On top of the curve three different energies are drawn. Important points are shown as crosses when $E = V(x)$. These are the turning points of a trajectory. Since $p(x) = 0 \Rightarrow$ Particle stops.

Classical trajectories are divided into two classes.

- Bound motion: between two turning points
  $\Rightarrow$ Particle oscillates

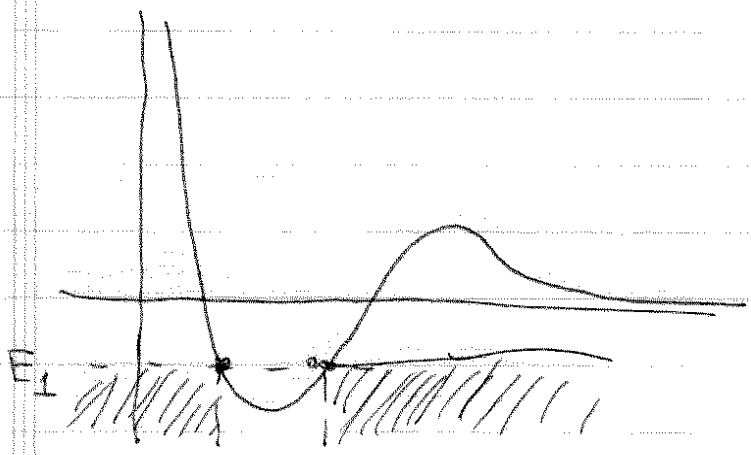
- Scattering motion:
  $\Rightarrow$ Particle moves freely, bouncing off no more than one turning point.

For a given energy, the regions of allowed motion are those for which

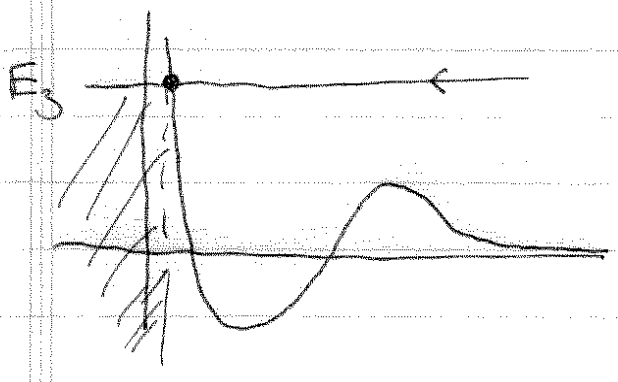
$$E > V(x) \quad : \quad \text{Classically allowed}$$

Since kinetic energy is always positive

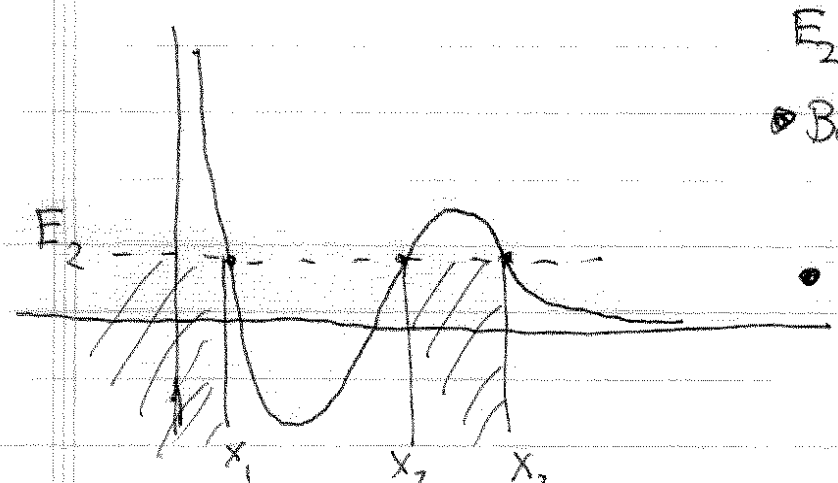
For the potential drawn on the previous page:



$E_1 \Rightarrow$ Bound motion between turning points. The classically forbidden region is shaded



$E_3 \Rightarrow$ Scattering motion. A particle coming from right will bounce off potential as move to $+\infty$



E_2: Two degenerate trajectories

- Bound motion between x_1 and x_2
- Scattering from x_3

Quantum Description: In Q.M. we describe the state by a wave function $\psi(x,t)$ satisfying $\frac{\partial \psi}{\partial t} = \frac{-i}{\hbar}\hat{H}\psi$ where $\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}$

Because any state can be decomposed into a complete set of stationary states (energy eigenfunctions) we concentrate on solution to the T.I.S.E.

$$\hat{H}\,u_E(x) = E\,u_E(x)$$

$$\Rightarrow \boxed{\frac{-\hbar^2}{2m}\frac{d^2u_E}{dx^2} + V(x)\,u_E = E\,u_E}$$

The solution to this diff'l eqn is subject to the following conditions:

(i) $u_E(x)$ is continuous so derivatives are well defines

(ii) If $V(x)$ is non-singular (does not go to infinity anywhere) $\frac{du_E}{dx}$ is continuous

For the follow few lectures we will seek solutions to this Eq. and contrast its features with the classical description.