Classical Limits

We want to explore the "classical limits" of Quantum Mechanics (when and it what sense does a QM system resemble classical counterparts). In particular, we want to discuss when and how QM systems exhibit "particle-like" properties, "wave-like" properties, and "fluid-like" properties.

Point-like particle properties – the role of expectation values for position

Let's revisit the normalized Gaussian wave package;

$$\Psi(x,t=0)=\sqrt{\frac{1}{\sqrt{2\pi}\sigma}}e^{ip_0x/\hbar}e^{-x^2/4\sigma^2} \qquad \sigma: some\ length\ scale$$

In which a particle moves in x direction with a velocity v, p_0=mv, x(t)=vt

$$\langle X\rangle_{t=0}=0$$

What is time dependence of this observable variable? Of course,

$$\frac{d}{dt}\langle X\rangle=\frac{1}{i\hbar}\langle[X,H]\rangle$$

We know the Hamiltonian which is free Hamiltonian in this case. $H=\frac{P^2}{2m}$

$$\langle[X,H]\rangle=\frac{1}{2m}\langle[X,P^2]\rangle$$

$$[X,P^2]=P[X,P]+[X,P]P=Pi\hbar\mathbb{1}+i\hbar\mathbb{1}P=2i\hbar P$$

$$\frac{d}{dt}\langle X\rangle=\frac{1}{i\hbar}\langle[X,H]\rangle=\frac{1}{i\hbar}\cdot\frac{1}{2m}\cdot 2i\hbar\langle P\rangle=\frac{\langle P\rangle}{m}$$

This is the direct analogue of classical mechanics.

By the Fourier transformation the wave function becomes

$$\widetilde{\Psi}(p,t=0)=\sqrt{\frac{1}{\sqrt{2\pi}\frac{\hbar}{2\sigma}}}e^{-\frac{(p-p_0)^2}{4}\left(\frac{\hbar}{2\sigma}\right)^2}$$

$$\langle P\rangle_{t=0}=p_0$$

Now what is the time dependence of the momentum?

$$\frac{d}{dt}\langle P\rangle = \frac{1}{i\hbar}\langle [P,H]\rangle = 0$$

Therefore P does not change

$$\langle P\rangle_{t=0} = p_0 = \langle P\rangle(t)$$

$$\langle X\rangle(t) = \frac{\langle P\rangle}{m}(t)$$

Then, where is the quantum aspect? Instead of just x and p we are talking about <x> and <p>. There is uncertainty associated with them.

$$\langle X^2\rangle_{t=0} = (\Delta X)^2 = \sigma^2$$

$$\langle P^2\rangle = {p_0}^2 + \left(\frac{\hbar}{2\sigma}\right)^2$$

$$(\Delta P)^2 = \langle P^2\rangle - \langle P\rangle^2 = \left(\frac{\hbar}{2\sigma}\right)^2$$

Does this affect anything in every day life in a visible manner?

$$\hbar \cong \frac{10^{-34} kg\cdot m^2}{s} = 197.33\ eVnm/c = 197.33\ MeVfm/c = \ 2\Delta X\cdot\Delta v\cdot m$$

Considering a tiny mass, 10^{-9} kg

$$\Delta X\cdot\Delta v = 10^{-25}\ m\cdot m/s$$

How well could anyone localize (position) this mass, realistically? Making an extreme assumption: $\Delta x=10^{-9}$m => $\Delta v=10^{-16}$ m/s

Can any experiment measure the velocity in this precision? No way!

In general, Δx is not constant.

$$(\Delta X)^2(t) = \sigma^2 + \Delta v^2 t^2$$

However, even this tiny mass (10^{-9} kg) is still humongous compared to the atomic scale With the example above, it would take 3 months before the velocity uncertainty increases the position uncertainty significantly (by 40%). For an electron located within 1 nm, though, the velocity uncertainty would be so large that it would “smear out” in an instance.

However, in experiments at JLab even the scattered electrons are treated as classical particles and the flight paths are measured! How can the path of the quantum particle be measured? It’s possible under this condition:

$$p \cong 1000\ MeV/c$$

$$\Delta p \cong 0.1\ MeV/c$$

$$\Delta x \cong 2000\ fm = 2\ pm = 0.002\ nm$$

The location within .002 nm error is good enough to say where the electron went through. Practically Δx≈10 μm is good.

In addition to the well-known Heisenberg uncertainty relationship above, one can also formulate a more "subjective" relationship between the accuracy in which the energy of a system is known, and time.

$$\Delta E \Delta T \geq \frac{\hbar}{2}$$

$$\Delta E = \sqrt{\langle H^2 \rangle - \langle H \rangle^2}$$

But what is ΔT (T is NOT an operator)? Here's one way to interpret, again with the example of the Gaussian wave packet:

Let's say we define *T* as the time how long the wave takes to move some distance *L*. Then *T* = *L*/*v* where *L* is the distance and *v* is velocity. There is uncertainty in this time since you don't know the exact location of the wave. Therefore,

$$\Delta T = \frac{\sigma}{v}$$

What is ΔE? First, what's <E>?

$$\langle E \rangle = \langle \frac{P^2}{2m} \rangle = \frac{{p_0}^2}{2m} + \left(\frac{\hbar}{2\sigma}\right)^2$$

NOTE: The average energy is (slightly) higher than the classical energy, so although position and momentum for the Gaussian wave package are following classical trajectories, the agreement is not perfect.

$$\langle E^2 \rangle - \langle E \rangle^2 = \left(\frac{1}{2m}\right)^2 \left[4{p_0}^2 + 2\left(\frac{\hbar}{2\sigma}\right)^2\right]\left(\frac{\hbar}{2\sigma}\right)^2$$

$$\Delta E \approx v \cdot \Delta P$$

$$\Delta E \Delta T = v \cdot \Delta P \frac{\sigma}{v} = \Delta P \sigma = \frac{\hbar}{2}$$

The reason the motion of the Gaussian wave packet comes out close to classical mechanics is because;

$$\frac{d}{dt}\langle P\rangle = \frac{1}{i\hbar}\langle [P,H]\rangle = 0$$

so the average position and the average momentum follow the classical Hamilton equations of motion.

But the r.h.s. is not necessarily always 0. In general, it would be

$$\frac{d}{dt}\langle P\rangle = \frac{1}{i\hbar}\langle [P,H]\rangle = -\langle\frac{\partial V}{\partial x}\rangle \quad \text{where V is a potential that can be written as a power series in X.}$$

This seems to agree with the result in classical mechanics, where $\frac{dP}{dt} = -\frac{\partial V}{\partial x}$. However, the derivative would have to be evaluated at the average <*X*> to make the parallel exact. In other words, instead of taking the average of the derivative, one would have to take the derivative at the average *x*. This difference makes for an important difference between quantum mechanics and classical mechanics, although it only exists if the third derivative of the potential is non-zero (in other words, if the 1st derivative of the force varies appreciably over the range of spatial uncertainty, Δx – see Shankar.). Therefore, one expects that the "motion" of the expectation value <*x*> in a Harmonic Oscillator potential is exactly like that in the classical case – sinusoidal oscillation with frequency ω, while the classical approximation is probably less good for a particle in a box or in a Coulomb potential (where the force does not depend linearly on position). The problem is that the wave function "samples" the potential "everywhere" at once, while classically, only the potential and its derivative at the exact position of the particle matter. Let's look at this more in detail:

a) The Harmonic Oscillator: We already showed that IF the HO is in a superposition of adjacent eigenstates, the motion is indeed exactly a sinusoidal oscillation, $\langle X\rangle(t) \sim \frac{A}{2}\cos\omega t$, with the right frequency (see HW#8 last semester). Note two interesting aspects: i) If the HO is in an eigenstate of the Hamiltonian, it doesn't "move" at all (<*x*> = 0 at all times). This goes with the fact that oscillations can be used to measure time, but if the energy uncertainty is infinitely small (eigenstate), then the time uncertainty must be infinitely large (see above). ii) Vice versa, because a superposition of eigenstates does not have a well-defined energy, time can be measured. However, the **amplitude** of the motion does not agree with the classical expectation, even if we use the average energy. This is due to the fact that the QM energy always has an additional term (again, see above) which is due to the "zero-point" energy simply required by the Heisenberg uncertainty principle.

b) Hydrogen atom

Again, for a single eigenstate of the Hamiltonian, nothing depends on time. However, if the angular momentum *l* becomes large, the "orbits" predicted by quantum mechanics approach those of classical mechanics (circular orbits of radius r). Specifically, if we choose

$$m = l$$

$$Y_l^l \sim (\sin\theta)^l e^{il\varphi}$$

we see that the electron is moving in a plane (Y_l^l is only significantly non-zero around $\theta = \pi/2$ for large *l*).

The radial part? Let's choose the minimal value for the main quantum number *n*,

$$n \geq l + 1$$

$$\frac{1}{r} L(2\rho) \rho^l e^{-\rho}$$

If *l* = *n*-1 , L becomes a constant.

$$\Psi = \frac{c}{r} \rho^l e^{-\rho} Y_l^l$$

Probability of being between r and r+dr is

$$dP(r, r+dr) = 2\pi r^2 dr \int |\Psi|^2 d\cos\theta \sim \rho^{2l} e^{-2\rho} dr \int Y_l^{l2} d\cos\theta$$

This probability peaks around $\rho = \kappa r = l$.

$$\Rightarrow r = \frac{l \cdot \hbar}{\sqrt{2m|E|}}, \qquad l \cdot \hbar = l_z$$

This is the exact classical answer of the orbit in Coulomb field (to be shown in HW Problem Set 5).

Meanwhile, if you had a "classical" electron circling the nucleus with angular momentum l_z and energy *E*, it would look like and oscillating dipole with frequency ω , with $\omega = \frac{l_z}{mr^2}$. Of course, such an orbit would loose energy through dipole radiation of the same frequency and decay instantly. Meanwhile, quantum mechanics tells us that each orbit by itself does **not** radiate, but if we have a transition between two energy levels, the emitted radiation will have a frequency of $\omega = \delta E / \hbar$, with

$$\delta E = Ry \left(\frac{1}{n^2} - \frac{1}{m^2} \right)$$

In particular, it turns out that the frequency of the radiation emitted in a transition

$$n \to n - 1$$

has the same value as the classical expectation if *n* becomes very large (again, to be shown by you in the next HW problem).

Wavelike Properties

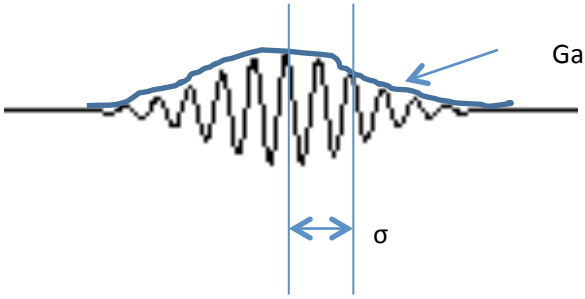
Back again to the Gaussian Wave packet:

How does the wave function look like?

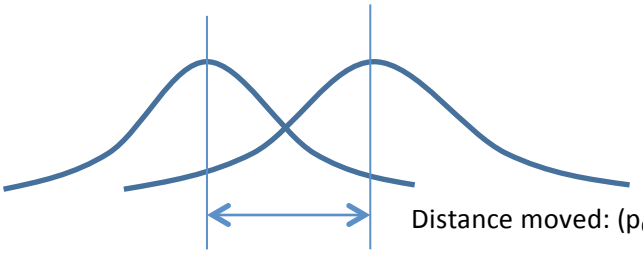
$$p_0 \gg \Delta p = \frac{\hbar}{2\sigma}$$

$$\lambda = \frac{2\pi\hbar}{p_0}$$

Because σ is much larger than λ



(picture from http://www.jick.net/~jess/hr/skept/GWP/packet1.gif)



Is the wave phase velocity equal to v? No. Look at the wave function. We can approximately write (see below)

$$\Psi(x,t) = \sqrt{\frac{1}{\sqrt{2\pi}\sigma}} e^{ip_0 x/\hbar} e^{-x^2/4\sigma^2} e^{-iEt/\hbar}$$

$$k = \frac{p_0}{\hbar}, \quad \omega = \frac{E}{\hbar}, \quad \nu = \frac{E}{2\pi\hbar}$$

$$c_{ph} = \frac{E}{p_0}$$

What's E? E=P_0^2/2m. E is not well defined here. But let's say for now.

$$c_{ph} = \frac{E}{p_0} \sim \frac{\frac{{p_0}^2}{2m}}{p_0} = \frac{p_0}{2m} = \frac{1}{2}v$$

Quantum mechanical wave behaves like ones in highly dispersive media.

The envelope moves v but the small waves in the envelope move half of v.

$$\frac{p_0}{m} = v_{group} = \frac{\partial \omega}{\partial k}$$

Fluid-like Properties

We already introduced the (probability) density $\rho(\vec{r}) = |\psi(\vec{r})|^2$ and the (probability) current density

$$\vec{j}(\vec{r}) = \frac{\hbar}{2mi}\left(\psi^*(\vec{r})\vec{\nabla}\psi(\vec{r}) - \psi(\vec{r})\vec{\nabla}\psi^*(\vec{r})\right) = \frac{1}{2m}\left[\langle\psi|\vec{r}\rangle\langle\vec{r}|\vec{\mathbf{P}}|\psi\rangle + \left(\langle\psi|\vec{r}\rangle\langle\vec{r}|\vec{\mathbf{P}}|\psi\rangle\right)^*\right] = \frac{1}{m}\mathbf{Re}\left(\langle\psi|\vec{r}\rangle\langle\vec{r}|\vec{\mathbf{P}}|\psi\rangle\right)$$

We can interpret the last term as the product of the density at point $\vec{r}$, multiplied with the average velocity $\vec{v} = \frac{\vec{p}}{m}$ at that point. In other words, the probability density and current are equivalent to the mass density and current density of a fluid (like a gas). The continuity equation (which we know holds for the QM probability density and current, because of Schrödinger's equation) then guarantees that this flow of the "equivalent fluid" does not violate mass conservation. More details will follow next lecture.