Lec 18: 10/07/2009

As the next example, let us estimate the ground state energy of the Hydrogen atom. This is a three-dimensional system with spherical symmetry:

$$H = \frac{P_x^2 + P_y^2 + P_z^2}{2m} - \frac{e^2}{R}, \quad R = (X^2 + Y^2 + Z^2)^{1/2}$$

The symmetry implies that in the ground state:

$$\langle P_x^2 \rangle = \langle P_y^2 \rangle = \langle P_z^2 \rangle, \quad \langle X^2 \rangle = \langle Y^2 \rangle = \langle Z^2 \rangle$$

For a positive definite operator Ω, in general we have $\langle \underbrace{\Omega \Omega^{-1}}_{I} \rangle \geq \langle \Omega \rangle \langle \Omega^{-1} \rangle$ and $\langle \Omega^2 \rangle^{1/2} \geq \langle \Omega \rangle$.

Hence:

$$\left\langle \frac{1}{(X^2+Y^2+Z^2)^{1/2}} \right\rangle \leq \frac{1}{\langle (X^2+Y^2+Z^2)^{1/2} \rangle} \geq \frac{1}{\langle X^2+Y^2+Z^2 \rangle^{1/2}}$$

Here we make approximations so that:

$$\left\langle \frac{1}{(X^2+Y^2+Z^2)^{1/2}} \right\rangle \simeq \frac{1}{\langle (X^2+Y^2+Z^2)^{1/2} \rangle} \simeq \frac{1}{\langle X^2+Y^2+Z^2 \rangle^{1/2}}$$

Using $\langle P_x^2 \rangle = \langle P_y^2 \rangle = \langle P_z^2 \rangle$ and $\langle X^2 \rangle = \langle Y^2 \rangle = \langle Z^2 \rangle$, we find:

$$\langle H\rangle = \frac{\langle P_x^2 + P_y^2 + P_z^2\rangle}{2m} - \frac{e^2}{\langle (X^2+Y^2+Z^2)^{1/2}\rangle} \simeq$$

$$\frac{3\langle P_x^2\rangle}{2m} - \frac{e^2}{\langle (3X^2)^{1/2}\rangle} = \frac{3\langle P_x^2\rangle}{2m} - \frac{e^2}{\sqrt{3}\langle X^2\rangle^{1/2}}$$

Again, because of the spherical symmetry, we have $\langle X\rangle = \langle Y\rangle = \langle Z\rangle = 0$ and $\langle P_x\rangle = \langle P_y\rangle = \langle P_z\rangle = 0$ for an energy eigenstate. Thus:

$\langle P_x^2\rangle = \Delta P_x^2$, $\langle X^2\rangle = \Delta X^2$

This results in:

$$\langle H\rangle \geq \frac{3\,\Delta P_x^2}{2m} - \frac{e^2}{\sqrt{3}\,\Delta X}$$

The Heisenberg uncertainty principle: $\Delta X \Delta P_x \geq \frac{\hbar}{2}$ then yields:

$$\langle H\rangle \geq \frac{3}{8}\frac{\hbar^2}{m\Delta X^2} - \frac{e^2}{\sqrt{3}\,\Delta X}$$

The right-hand side has a minimum for $\Delta X = \frac{3\sqrt{3}\,\hbar^2}{4me^2}$.

Therefore:

$$\langle H\rangle \geq \frac{-2me^4}{9\hbar^2}$$

The exact ground state energy (that we will find later) is:

$$E_g = \frac{-me^4}{2\hbar^2}$$

The lower bound on $\langle H\rangle$ that we just found is within a factor of two from E_g. This is pretty good considering the approximations that we made and the fact that the ground state wavefunction is not a Gaussian wavepacket in this case.

As the third example, lets find the ground state energy of the harmonic oscillator. In this case we have:

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2 \Rightarrow \langle H\rangle = \frac{\langle P^2\rangle}{2m} + \frac{1}{2}m\omega^2\langle X^2\rangle$$

The symmetry of this problem implies that

$\langle x \rangle = \langle p \rangle = 0$ in an energy eigenstate. Hence;

$$\langle H \rangle = \frac{\Delta p^2}{2m} + \frac{1}{2} m\omega^2 \Delta x^2$$

$$\Delta p \Delta x \geq \frac{\hbar}{2} \Rightarrow \langle H \rangle \geq \frac{\hbar^2}{8m\Delta x^2} + \frac{1}{2} m\omega^2 \Delta x^2$$

The right hand side is minimized for $\Delta x = \sqrt{\frac{\hbar}{2m\omega}}$.

Thus;

$$\langle H \rangle \geq \frac{\hbar\omega}{2}$$

Interestingly, the lower bound exactly matches the ground state energy in this case. This is not surprising as we know the wavefunction is a Gaussian wavepacket that minimizes the uncertainty.

Classical Limit:

The uncertainty principle involves intrinsic quantum mechanical uncertainties in the position and momentum. In a classical description, however, position and momentum can be known to arbitrary precision (in principle). In many cases classical language give a sufficiently good description of a system. So, the question is how to reconcile the uncertainty principle with a classical approximation.

The key point is that there is always an experimental uncertainty in a measurement that comes from limited accuracy of the apparatus involved. What we should do is to compare this uncertainty Δx_{exp} with the intrinsic uncertainty $\Delta x_{quantum}$ that obeys the uncertainty principle.

If $\Delta x_{exp} > \Delta x_{quantum}$, the latter is irrelevant. It can be considered as a "noise" that is overwhelmed by experimental uncertainties in the apparatus. Classical description will be adequate in this case.

On the other hand, if $\Delta X_{quantum} > \Delta X_{exp}$, then we have entered the realm of quantum mechanics. The intrinsic uncertainties are dominant in this case and we must use quantum mechanics for a correct description of the system.

Note that:

$$\Delta X_{quantum} \geq \frac{\hbar}{2\Delta p} \quad , \quad \Delta p \cancel{\leq} \langle p^2 \rangle^{\frac{1}{2}}$$

Thus:

$$\Delta X_{quantum} \geq \frac{\hbar}{2\langle p^2 \rangle^{\frac{1}{2}}} \Rightarrow \Delta X_{quantum} \sim \lambda_{de\ Broglie}$$

$$\lambda_{de\ Broglie} \simeq \frac{\hbar}{\langle p^2 \rangle^{\frac{1}{2}}}$$

As a rule of thumb, we compare ΔX_{exp} with $\lambda_{de\ Broglie}$. If $\Delta X_{exp} \gg \lambda_{de\ Broglie}$, we are in the classical limit. Otherwise, quantum mechanics must be taken into account.

For a particl of mass m and velocity dispersion $\langle v^2 \rangle^{\frac{1}{2}}$, we have;

$$\lambda_{\text{de Broglie}} \simeq \frac{\hbar}{m \langle v^2 \rangle^{\frac{1}{2}}}$$

For a fixed $\langle v^2 \rangle^{\frac{1}{2}}$, $\lambda_{\text{de Broglie}}$ increases as m gets smaller. Therefore quantum mechanics is more important for lighter particles (Hydrogen atom vs baseball).

Also, as the size of a system decreases, ΔX_{exp} gets smaller, and hence quantum effects become more important. This is why microscopic systems are described by quantum mechanics.