Chapter 6. Commuting and Noncommuting Operators

Order of operations might be important in QM!

Two operators commute if the commutator is zero

$$[\hat{\Omega}_1, \hat{\Omega}_2] = \hat{\Omega}_1\hat{\Omega}_2 - \hat{\Omega}_2\hat{\Omega}_1 = 0$$

$\hat{p}$ and $\hat{T}$ commute:

$$\left[\hat{p}, \frac{\hat{p}^2}{2m}\right] f(x) = \hat{p}\frac{\hat{p}^2}{2m} f(x) - \frac{\hat{p}^2}{2m}\hat{p}f(x) = \left[\frac{\hat{p}^3}{2m} - \frac{\hat{p}^3}{2m}\right] f(x) = 0$$

where f is an arbitrary function.

However, $\hat{x}$ and $\hat{p}$ do not commute:

$$\hat{x}\hat{p}f(x) = \frac{\hbar}{i} x \frac{df(x)}{dx}$$

$$\hat{p}\hat{x}f(x) = \frac{\hbar}{i}\left[f(x) + x\frac{df(x)}{dx}\right]$$

$$[\hat{x}, \hat{p}] f(x) = \frac{\hbar}{i} x \frac{df(x)}{dx} - \frac{\hbar}{i}\left[x\frac{df(x)}{dx} + f(x)\right] = i\hbar f(x)$$

$$[\hat{x}, \hat{p}] = i\hbar \neq 0$$

Position and momentum are a pair of complementary variables.

$$\Delta O_1 \Delta O_2 \geq \frac{1}{2}\left|\int \Psi^*(x)[\hat{O}_1, \hat{O}_2]\Psi(x)dx\right|$$

Indeed

$$\Delta p \Delta T \geq \frac{1}{2}\left|\int \Psi^*(x)[\hat{p}, \hat{H}]\Psi(x)dx\right| = 0$$

and

$$\Delta x \Delta p \geq \frac{1}{2}\left|\int \Psi^*(x)[\hat{x}, \hat{p}]\Psi(x)dx\right| = \frac{\hbar}{2}$$

Uncertainty principle (1925, Heisenberg)

The wave-particle duality causes problems in measurement.

This is because if an electron is to be located with uncertainty of Δx, the light used to detect the electron has to have a wavelength that is comparable to Δx, which will lead to a very large momentum according to de Broglie, $p=h/\lambda$. A portion of this large momentum will be transferred to the electron when they interact, causing a large uncertainty in the momentum (Δp) of the electron.

It is impossible to specify simultaneously, with arbitrary precision, both the momentum and position of a particle:

$$\Delta p \, \Delta x \geq \hbar/2$$

Similarly:

$$\Delta E \, \Delta t \geq \hbar/2$$

For plane wave $\Psi = Ae^{-ikx}$, its momentum is precisely known: $p = k\hbar$. The probability for finding the particle in a particular position is

$$P(x) = \Psi^*\Psi = |A|^2 e^{ikx}e^{-ikx} = |A|^2$$

Since it is independent of *x*, the probability is equal everywhere, position completely uncertain!

In particle in a box,

$$\Delta x = L$$
$$\Delta p = \frac{\hbar}{2\Delta x} = \frac{\hbar}{2L}$$

$$\frac{(\Delta p)^2}{2m} = \frac{\hbar^2}{8mL^2} \propto E_1$$

ZPE, a quantum effect, is due to restriction of motion.

Example: Calc. the position uncertainty of a 1.0 kg particle with a speed uncertainty of 10^{-6} m/s. What if the mass is 1.0×10^{-31} kg?

$$\Delta x = \hbar/(2\Delta p) = \hbar/(2m\Delta \upsilon)$$
$$= 1.05\times10^{-34}\ Js/(2\times1.0\ kg\times1.0\times10^{-6}\ m/s)$$
$$= 5.25\times10^{-29}\ m$$

However, for a particle with the electronic size

$$\Delta x = 525\ m$$