Week 2

The Schrödinger Equation

2.1 Particle-Wave Duality and Uncertainty Relations

• Particle-wave duality (de Brogelie's original formulation):

$$\lambda \nu = c$$
 $E = h \nu$ $p = \frac{h}{\lambda}$

• Angular frequency: The quantity $\omega = 2\pi r$.

• Wavenumber: The quantity $k = 2\pi/\lambda$.

• We can create a symmetrical formulation of the de Broglie relation using these new quantities:

$$E = \hbar \omega \qquad \qquad p = \hbar k$$

• What is the wave that we might associate with a de Broglie particle?

$$\Psi(x) = Ae^{ikx - i\omega t}$$

• Probability:

- Classically, such a wave might be associated with EM radiation hitting a surface with intensity $I = |\Psi(x)|^2 = \Psi(x)\Psi^*(x)$.
- As soon as we associate a particle (photon) with the wave, the intensity may be re-interpreted as the number of particles reaching the surface or the probability of a particle being at the surface.
- Thus, the probability of finding a particle at the surface becomes $|\Psi(x)|^2$, as well.
- Following de Broglie, we also associate waves with particles such as electrons.
 - With the association of light as a particle, the particle wave duality leads to the appearance of probability.
- What is the probability of finding the particle at the origin?

$$Pr = \left| Ae^{ik \cdot 0} \right|^2$$
$$= |A|^2$$

- Since the probability is not dependent on position, it is the same everywhere.
- We also run into issues **normalizing** this unbounded wavefunction.

- We know this particle's momentum exactly, but we know nothing about its position.
- **Normalizing** (a wavefunction): Guaranteeing that the integral for the entire wavefunction is equal to 1.
- Free particle: A particle that does not have constraints on where it is more likely to be.
- Heisenberg's uncertainty relations are formalized in terms of matrix mechanics.
 - We can Fourier transform the wave function of particle to convert it from a function of position to a function of momentum.
 - The Fourier transform will yield one spike at $\hbar k$ and will be 0 everywhere else just like the Dirac delta function.
 - Thus,

$$\Psi(p) = \delta(p - \hbar k)$$

• Consider a Gaussian wave packet at p = 0. Then

$$\phi(p) = C e^{-\frac{p^2}{2(\Delta p)^2}}$$

- $-\Delta p$ is the standard deviation of the Gaussian/width of the distribution. It is a constant such that the probability drops to 1/e of its maximum at p=0.
- With the Fourier Transform of $\Psi(p)$, we obtain

$$\Psi(x) = De^{-\frac{(\Delta p)^2 x^2}{2\hbar^2}}$$

- Thus, a Gaussian quantum function produces a Gaussian position function via an FT as well, i.e.,

$$\Psi(x) = De^{-\frac{x^2}{2(\Delta x)^2}}$$

• Now if we set the last two equations equal to each other, we get

$$\frac{(\Delta p)^2}{2\hbar^2} = \frac{1}{2(\Delta x)^2}$$
$$(\Delta p)^2 (\Delta x)^2 = \hbar^2$$
$$\Delta p \Delta x = \hbar = \frac{h}{2\pi}$$

- This implies that the spread of the Gaussian in momentum times the spread of the Gaussian in position is a constant.
- If we make one Gaussian wave packet more specific, the other gets more spread out, and vice versa.
- Note that the above equality does satisfy the Heisenberg uncertainty principle, but it is not it itself.