Lecture 4
Introduction to Quantum Mechanical Way of Thinking.

Today's Program

1. Brief history of quantum mechanics (QM).
2. Wavefunctions in QM (First postulate)
3. Schrodinger's Equation

Questions you should be able to answer by the end of today's lecture:

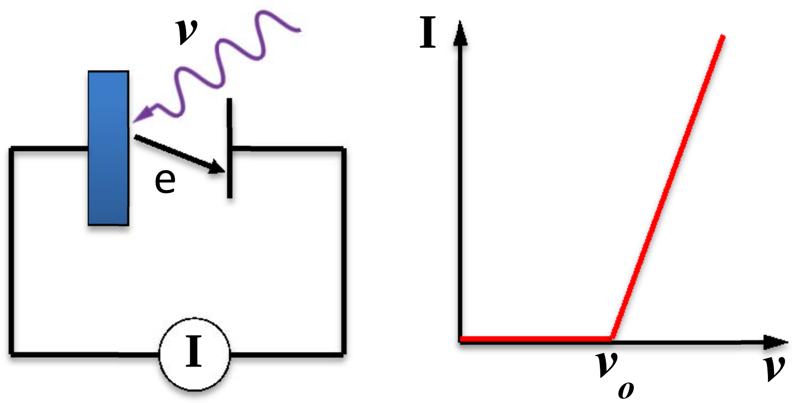
1. When do you observe wave-particle duality?
2. How to determine particle's wavelength if you know its momentum?
3. What does the wavefunction represent?
4. How does wavefunction evolve in time?

References for Today's lecture:

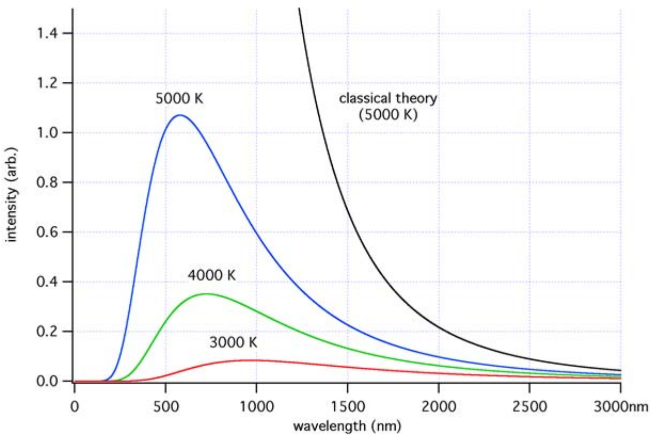
1. Introductory Applied Quantum and Statistical Mechanics, Hagelstein, Senturia, Orlando.
2. Introduction to Quantum Mechanics, Griffiths.

In the end of 19th century and beginning of the 20th century, scientists were convinced they understood physics. Only a "handful" of experiments remained unexplained. These experiments became a foundation for the new kind of physics, which we now know as Quantum Mechanics. Today a lot of devices (all electronics, all optics) surrounding us are fundamentally quantum mechanical in their design and principles of operation.

1887, Hertz: Photoelectric effect.
When illuminated with ultraviolet (UV) light metallic sample emitted electrons. However, the lower frequency (higher wavelength) light did not initiate electron emission even at higher incident light powers.



Black Body Spectrum: The physicists were puzzled by the radiation of a black body, as it could not be explained by the Maxwell's equations.



Blackbody curves for various temperatures and comparison with classical theory. (This image is in the public domain. Source: Wikimedia Commons.)

For **short wavelength** (high frequency) limit **Wien's law** provided an approximation:

$$P(\lambda,T)\sim\frac{1}{\lambda^5}e^{-\frac{const}{\lambda T}}$$

$$P(\nu,T)\sim\nu^3 e^{-\frac{const}{T}\cdot\nu}$$

For **long wavelength** (low frequency) **Rayleigh-Jeans** law provided another approximation:

$$P(\lambda, T) \sim Const \cdot \frac{T}{\lambda^4}$$

$$P(\nu, T) \sim Const \cdot T\nu^2$$

Which, if correct, would have resulted in rapid increase of power at short wavelength (high frequency) labeled as "***ultraviolet catastrophe***".

In 1900, Planck proposed a revolutionary idea: Electromagnetic energy is quantized!
There are portions or "quanta" of energy "photons" with energy:

$$E_{ph} = h\nu = \hbar\omega = \frac{2\pi c\hbar}{\lambda} = \frac{ch}{\lambda}, \quad \hbar = \frac{h}{2\pi} = \frac{6.63\times10^{-34} m^2 kg/s}{2\pi} \cong 1.06\times10^{-34} m^2 kg/s$$

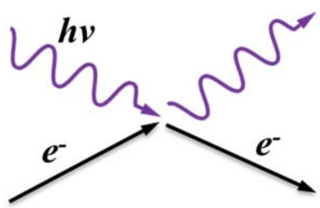
Here ***h*** is a Planck's constant.
Using the assumption of energy quantization Planck was able to derive Black Body spectrum:

$$B_\lambda(T) = \frac{2hc^2}{\lambda^5}\frac{1}{e^{hc/\lambda k_B T} - 1}$$

$$B_\nu(T) = \frac{2h\nu^3}{c^2}\frac{1}{e^{h\nu/k_B T} - 1}$$

Planck's hypothesis implied that electromagnetic waves were quantized and could be thought of as particles.

1923, Compton's scattering experiment.
Planck's assumption was further confirmed, when Compton observed that electrons could be deflected by electromagnetic radiation akin to elastic scattering:



This experiment established that ***photons have momentum.*** From relativistic mechanics and Maxwell's equations we can then find the relationship between the momentum and energy: $E = \sqrt{p^2c^2 + m_0^2c^4}; \quad m_0 = 0 \Rightarrow p = \frac{E}{c} = \frac{\hbar\omega}{c} = \hbar k$. Here ***k*** is a wavevector.

But if waves behave like particles, could it be that particles could behave like waves?

1925, Davisson and Germer: Diffraction of electrons on Ni lattice.
They found that electrons scattered through the Ni lattice form a diffraction pattern akin to electromagnetic waves scattered on the grating. **Electrons behaved like waves!** (Despite having a non-zero mass).

These experiments were unified by the De Broglie conjecture:
All particles are waves and all waves are particles.
The wavelength and momentum are related:

$$p = \hbar k = \hbar \frac{2\pi}{\lambda}$$

So if all particles are waves, then what are those waves? – Probability!
There is a certain probability of finding a particle at a certain point in space and time.

First Postulate of Quantum Mechanics:
Any quantum mechanical particle or a system in general can be described by a wavefunction wavefunction $\psi(x,t)$. (Depending on a system ψ may be in a vector form).The wavefunctions belong to a state space, which has the properties of a vector space.
The general properties of wavefunctions are:

(a) single valued

(b) square integrable

(c) nowhere infinite (at infinity as well as elsewhere)

(d) continuous

(e) piecewise continuous first derivative

We can think of wavefunctions as amplitudes of probability. Then the probability to find a particle at a time t_0 at a point $\vec{r_0}$ is: $P(\vec{r_0}, t_0) = |\psi(\vec{r_0}, t_0)|^2$
Since the particle has to be somewhere at all times, and the total probability cannot exceed 1:

$$P_{All\ space} = 1 = \int_{all\ space} |\psi(\vec{r}, t)| d^3r$$

Then we can find the particle average position: $\langle \vec{r} \rangle = \int_{all\ space} P(\vec{r}, t) \vec{r} d^3r = \int_{all\ space} |\psi(\vec{r}, t)|^2 \vec{r} d^3r$

Now let's consider the simplest wavefunction for a particle. In a free space such as vacuum with no external forces the particle can be approximated as a plane wave: $e^{ikx-i\omega t}$, where $k = \frac{p}{\hbar}$ is the wavevector. Since there are no external forces then the energy of a particle is $E = \frac{mv^2}{2} = \frac{p^2}{2m}$.
How does this wave propagate in time and space?

$$\frac{\partial}{\partial x} e^{ikx-i\omega t} = ike^{ikx-i\omega t}$$

$$\frac{\partial^2}{\partial x^2} e^{ikx-i\omega t} = -k^2 e^{ikx-i\omega t}$$

$$\frac{\partial^2}{\partial x^2} e^{ikx-i\omega t} = -\frac{p^2}{\hbar^2} e^{ikx-i\omega t}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} e^{ikx-i\omega t} = \underbrace{\frac{p^2}{2m}}_{E} e^{ikx-i\omega t}$$

$$\frac{\partial}{\partial t} e^{ikx-i\omega t} = -i\omega e^{ikx-i\omega t}$$

$$\frac{\partial}{\partial t} e^{ikx-i\omega t} = -i\frac{E}{\hbar} e^{ikx-i\omega t}$$

$$i\hbar\frac{\partial}{\partial t} e^{ikx-i\omega t} = Ee^{ikx-i\omega t}$$

This exercise results in a curious statement about the propagation of particle ~ plane wave in free space: $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}e^{ikx-i\omega t} = i\hbar\frac{\partial}{\partial t}e^{ikx-i\omega t}$

In general in the presence of forces in 3D space energy of a particle would be:

$E = \frac{\vec{p}^{\,2}}{2m} + V(x,t)$, which would yield a following equation for the particle described by a wavefunction $\psi(\vec{r},t)$:

$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) + V(x,t)\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)$ - This equation is known as Schrodinger's equation and is usually written in the form:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x,t)\right]\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)$$