Motivations for Quantum Mechanics

- Atomic spectra (emission spectra, absorption spectra, Balmer series, Rydberg relationship, Bohr’s semi-classical theory, Bohr-Sommerfeld theory)
- Photoelectric effect (emission from metals, work function, dependence on wavelength, dependence on intensity)

Motivations for Quantum Mechanics

- Rayleigh-Jeans radiation theory
- Calculation using classical oscillators in equilibrium with electromagnetic radiation
- Jeans corrected Rayleigh’s theory with an additional factor of 2 for polarization
- Theory predicted infinite intensity at infinite frequency—“ultraviolet catastrophe”

Major Steps in Formulating Quantum Mechanics

- Einstein proposed a theory of the photoelectric effect in which light energy was quantized as "photons" with energy $h\nu$, where h is a constant (6.6 x 10^{-34} J-s)and ν is the frequency of the radiation
- Planck proposed modification of Rayleigh calculation with oscillators with quantized in steps of $h\nu$. h is now called Planck's constant.

Major Steps in Formulating Quantum Mechanics

- deBroglie proposes that particles are characterized by a wavelength $\lambda = h/p$. Bohr quantization then results from a circular boundary condition
- Schroedinger proposes that all mechanics can be described in terms of a wave equation—a partial differential equation in space and time

Major Steps in Formulating Quantum Mechanics

- Simultaneously, Heisenberg formulates an equivalent theory of quantum mechanics based on operator-algebra and vector spaces

Schroedinger Equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+U(x)\Psi(x,t)=i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

$\hbar=\frac{h}{2\pi}$, $\Psi(x,t)$ is called the wave function

$$\mathrm{P(x,t)}=|\Psi(x,t)|^2=\Psi^*\Psi$$

$$\int_{all\ \ space}\Psi^*\Psi=1$$

Schroedinger Equation

- Premise of quantum mechanics is that all knowable information about a system is contained in the wave function
- Note that a particle wave function does not say where a particle is. It only gives the probability that a particle is at a specific location

Heisenberg Uncertainty Principle

- Schroedinger formulation of quantum mechanics implies the Heisenberg uncertainty principle
- Uncertainty principle exists for all waves
- A monochromatic wave is spatially diffuse
- A compact wave packet consists of many frequencies

Wave Function

- Since all knowable information is contained in the wave function, everything knowable can be determined by solving the Schroedinger equation for the wave function
- A general approach to solving PDE's if U depends on x alone is a separation of variables

$$\Psi(x,t) = \varphi(x)e^{-i\omega t}$$

Time-Independent SE

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+U(x)\Psi(x,t)=i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

$$\Psi(x,t)=\varphi(x)e^{-i\omega t}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x)e^{-i\omega t}}{\partial x^2}+U(x)\varphi(x)e^{-i\omega t}=(i\hbar)(-i\omega)\varphi(x)e^{-i\omega t}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x)}{\partial x^2}+U(x)\varphi(x)=\hbar\omega\varphi(x)=E\varphi(x)$$

$$H=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x),\ \ H\varphi(x)=E\varphi(x)$$

Time-Independent SE

- If the potential U(x,t) is a function of x alone (*i.e.*, time independent), then the solution of the SE (*i.e.*, the wave function) can be written as the product of

$$\varphi(x) \;\; and \;\; e^{-i\omega t}$$

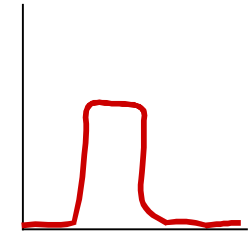
Time-Independent SE

- The spatial term $\psi(x)$ is a solution of a total differential equation known as the time-independent SE
- The time-independent SE can be written as shown on the next slide where H is an operator called the Hamiltonian
- The energies E are the eigenvalues of H

Time-Independent SE

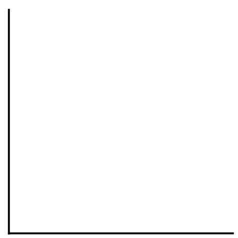
$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x), \quad H\varphi(x) = E\varphi(x)$$

Time-Independent SE

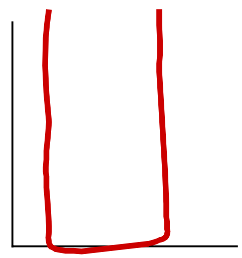


Barrier

- Solve the time-independent SE for various potential energy functions

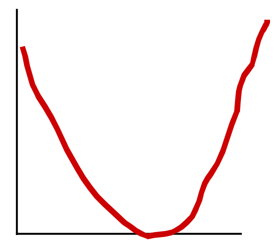


Free particle



Infinite Square Well

Finite Square Well



Harmonic Oscillator

Time-Independent SE

- Solution to time-independent SE in 3-dimensions uses Spherical Harmonics (generalization of Legendre Polynomials)
- Identical particles requires symmetric (anti-summetric) wave function depending on whether particles are bosons (fermions)