

## Quantum Mechanics

Book: *Introduction to Quantum Mechanics*, Liboff

2<sup>nd</sup>: Griffith's

3<sup>rd</sup>: Schaum's Outline

## Classical Quantum Mechanics

We start with a review of classical mechanics: predicting the dynamic variables that characterize the state of a system.

1. Define Position
2. Energy (E), Momentum (p), Angular Momentum (L), Hamiltonian (H)

Position:  $[x(t), y(t), z(t)]$

Energy:  $E = KE + PE = \frac{m}{2}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) + V(x, y, z)$

Classical force:  $\vec{F} = -\vec{\nabla}V$

Classical gravitational potential:  $V = mgz$

Momentum Term

Linear:  $\vec{p} = m\vec{v}$       Force:  $\frac{d\vec{p}}{dt} = \vec{F}$

Angular:  $\vec{L} = \vec{r} \times \vec{p}$       Torque:  $\frac{d\vec{L}}{dt} = \vec{N} = \vec{r} \times \vec{F}$

Recall BAC-CAB rule for finding components of angular momentum:

$$\vec{L} = \begin{vmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} = (yp_z - zp_y)\mathbf{e}_x + (zp_x - xp_z)\mathbf{e}_y + (xp_y - yp_x)\mathbf{e}_z$$

**One Particle Hamiltonian**

Hamiltonian Mechanics = Newtonian Mechanics

$$(x, y, z, \dot{x}, \dot{y}, \dot{z}) \rightarrow (x, y, z, p_x, p_y, p_z)$$

$$E = \frac{m}{2}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) + mgz$$

$$H = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + mgz$$

How the particle moves in the system:

$$\frac{\partial H}{\partial x} = -\dot{p}_x \qquad \frac{\partial H}{\partial p_x} = \dot{x}$$

$$\frac{\partial H}{\partial y} = -\dot{p}_y \qquad \frac{\partial H}{\partial p_y} = \dot{y}$$

$$\frac{\partial H}{\partial z} = -\dot{p}_z \qquad \frac{\partial H}{\partial p_z} = \dot{z}$$

**Many Particles:**

$$(q_1, q_2, q_3, \dots, q_n, p_1, p_2, p_3, \dots, p_n)$$

$$\frac{\partial H}{\partial q_l} = -\dot{p}_l \qquad \frac{\partial H}{\partial p_l} = \dot{q}_l$$

### H, L, and E in Spherical Coordinates

Expressions for energy, the Hamiltonian, and angular momentum were given in spherical coordinates, and it was suggested that students work out the steps to show these relations. This material is also in Section 1.2 Liboff.

$$r \rightarrow p_r = m\dot{r}$$

$$\theta \rightarrow p_\theta = mr^2\dot{\theta} \quad (\text{this corresponds to angular momentum})$$

$$\phi \rightarrow p_\phi = m(r \sin \theta)^2 \dot{\phi}$$

$$E = \frac{m}{2} (\dot{r}^2 + r^2 \dot{\theta}^2 + (r \sin \theta)^2 \dot{\phi}^2) + mg(r \cos \theta)$$

so

$$H = \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + \frac{p_\phi^2}{2m(r \sin \theta)^2}$$

$$x = r \cos \phi \sin \theta$$

$$y = r \sin \phi \sin \theta$$

$$z = r \cos \theta$$

$$\dot{x} = \dot{r}(\cos \phi \sin \theta) + r(-\sin \phi)\dot{\phi} \sin \theta + r \cos \phi \cos \theta \dot{\theta}$$

$$\dot{y} = \dot{r}(\sin \phi \sin \theta) + r(\cos \phi)\dot{\phi} \sin \theta + r \sin \phi \cos \theta \dot{\theta}$$

$$\dot{z} = \dot{r}(\cos \theta) + r(-\sin \theta)\dot{\theta}$$

$$\dot{x}^2 = \dot{r}^2 \cos^2 \phi \sin^2 \theta - 2r\dot{r} \cos \phi \sin \phi \dot{\phi} \sin^2 \theta + 2r\dot{r} \cos^2 \phi \sin \theta \cos \theta \dot{\theta}$$

$$+ r^2 \sin^2 \phi \dot{\phi}^2 \sin^2 \theta - 2r \sin \phi \dot{\phi} \sin \theta r \cos \phi \cos \theta \dot{\theta} + r^2 \cos^2 \phi \cos^2 \theta \dot{\theta}^2$$

$$\dot{y}^2 = \dot{r}^2 \sin^2 \phi \sin^2 \theta + 2r\dot{r} \cos \phi \sin \phi \dot{\phi} \sin^2 \theta + 2r\dot{r} \sin^2 \phi \sin \theta \cos \theta \dot{\theta}$$

$$+ r^2 \cos^2 \phi \dot{\phi}^2 \sin^2 \theta + 2r \sin \phi \dot{\phi} \sin \theta r \cos \phi \cos \theta \dot{\theta} + r^2 \sin^2 \phi \cos^2 \theta \dot{\theta}^2$$

$$\dot{z}^2 = \dot{r}^2 \sin^2 \theta - 2r\dot{r} \sin \theta \dot{\theta} + r^2 \sin^2 \theta \dot{\theta}^2$$

$$E = \frac{m}{2} (\dot{r}^2 + r^2 \dot{\theta}^2 + r^2 \dot{\phi}^2 \sin^2 \theta) + mgr \cos \theta$$

**H, L, and E in Cylindrical Coordinates**

Energy was expressed in cylindrical coordinates, and it was suggested that students work out the steps to show these relations and express momentum and the Hamiltonian in cylindrical coordinates. This material is also in Section 1.2 Liboff.

$$x = \rho \cos \phi$$

$$\dot{x} = \dot{\rho} \cos \phi + \rho(-\sin \phi)\dot{\phi}$$

$$y = \rho \sin \phi$$

$$\dot{y} = \dot{\rho} \sin \phi + \rho(\cos \phi)\dot{\phi}$$

$$\dot{x}^2 = \dot{\rho}^2 \cos^2 \phi - 2\rho\dot{\rho}\dot{\phi} \sin \phi \cos \phi + \rho^2 \dot{\phi}^2 \sin^2 \phi$$

$$\dot{y}^2 = \dot{\rho}^2 \sin^2 \phi + 2\rho\dot{\rho}\dot{\phi} \sin \phi \cos \phi + \rho^2 \dot{\phi}^2 \cos^2 \phi$$

$$E = \frac{m}{2}(\dot{\rho}^2 + \rho^2 \dot{\phi}^2 + \dot{z}^2) + mgz$$

## Quantum Mechanics vs. Classical Mechanics

Material in Section 1.4 was discussed. In classical mechanics, you know the values of all dynamic variable simultaneously. The state of the system of one particle in classical mechanics:

$$P(x, y, z, p_x, p_y, p_z)$$

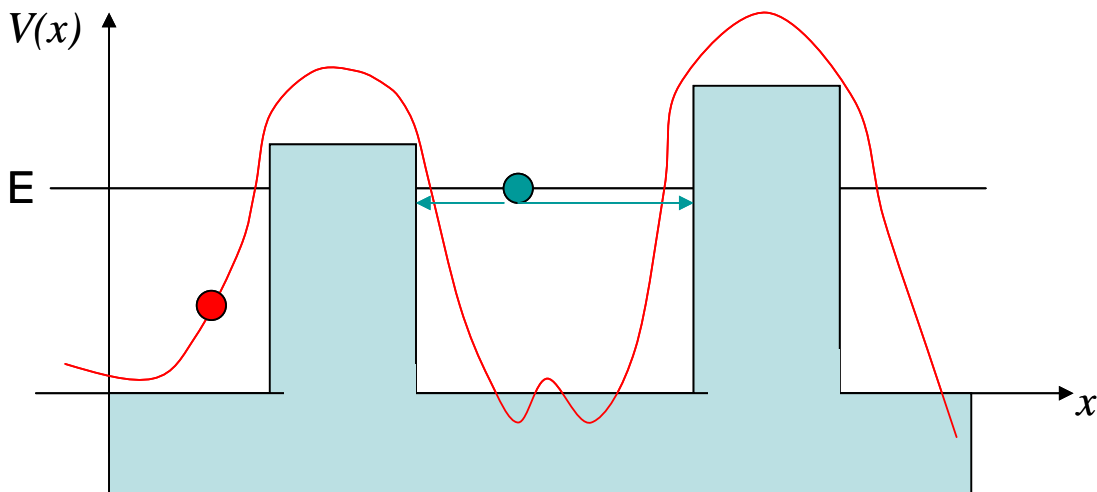
In quantum mechanics, such simultaneous specifications can't be made. If you know the position, then you don't know the momentum. Examples of quantum mechanics state of system of one particle:

$$P(E, \vec{p})$$

$$P(L^2, L_z, E)$$

$$P(L_1^2, L_2^2, L_z^2)$$

Consider a particle trapped in a potential well with energy  $E = V(x) + \frac{1}{2}mv^2$ . In classical mechanics (blue), the particle is confined to move only in the well because of the energy barrier. In quantum mechanics (red), it is possible for the particle to tunnel into forbidden regions.



## Dates

The historical development of quantum mechanics was briefly discussed.  
This material is also in Section 2.1

1901 Planck Blackbody radiator

1905 Einstein Photoelectric effect

1911 Rutherford Model of the Atom

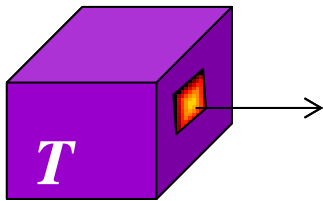
1913 Bohr Quantum Theory of Spectra of an Atom

...

1925 de Broglie Matter Wave

## Blackbody Radiation

Cavity held at constant Temp.



Cavity is held at constant temperature T.

By using the relation  $h\nu$  to define the energy of an electromagnetic wave, Planck expressed the energy per unit  $d\nu$ , or energy per unit  $d\lambda$ , that matches experimental data. A quantum of electromagnetic wave is called a photon.

The total energy per unit volume in the radiation field in the cavity is :

$$U = \int_{-\infty}^{\infty} u(\nu) d\nu$$

The energy per unit  $d\nu$  :

$$u(\nu) = \frac{8\pi h \nu^3}{c^3} \frac{1}{e^{h\nu/k_B T} - 1}$$

where

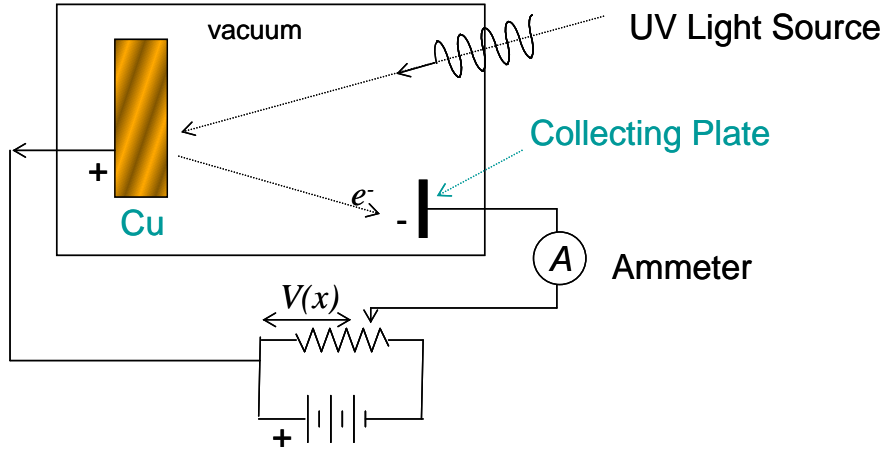
$h$  = Planck Constant =  $6.626 \times 10^{-27}$  erg - s

$k_B$  = Boltzman Constant

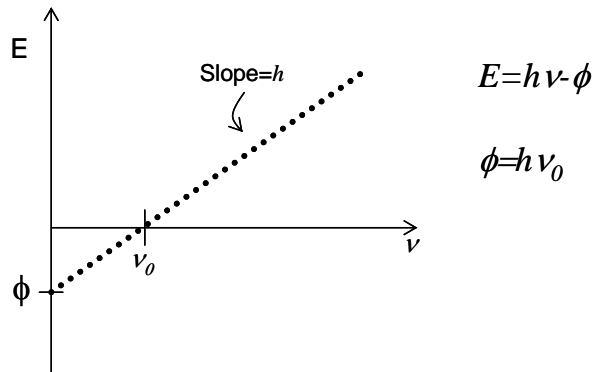
$T$  = Temperature

### Photoelectric Effect

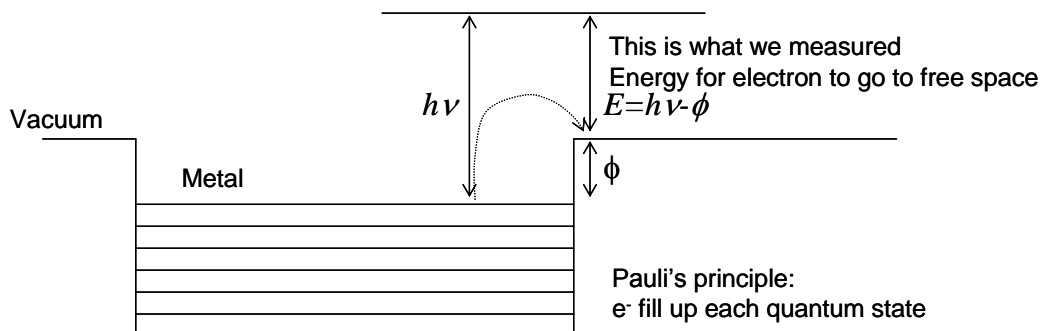
Einstein used Planck's photon concept to explain the photoelectric effect.



The energy of the emitted electrons (from the Copper plate) is a function of the frequency of light from the light source. The photoelectric experiment can be used to measure Planck's constant directly.



Model the energy distribution of electrons in a metal (the copper). Electrons distribute themselves according to the Pauli principle and filling lowest energy states first.



**Bohr's Atom**

For any kind of atom, the spectrum of emission lines is observed. Bohr used the quantum relation:

$$\oint p_{\theta} d\theta = nh$$

to develop the energy levels of the atom.

Only consider the electron with  $m_e \ll M_p$

$$E = \frac{1}{2}mv^2 - \frac{e^2}{r}$$

$$\frac{mv^2}{r} = \frac{e^2}{r} = \frac{p_{\theta}^2}{mr^3}$$

$$E = \frac{p_{\theta}^2}{2mr^2} - \frac{e^2}{r}$$

$$2\pi p_{\theta} = nh$$

$$n = 1, 2, 3, \dots$$

$$r_n = \frac{n^2 \hbar^2}{me^2}$$

$$E = \frac{-R}{n^2}$$

$$R = \frac{me^4}{2\hbar^2} = 13.6eV$$

Ground state = -13.6 eV. Bohr radius  $a_0 \sim 0.5\text{\AA}$  is:

$$a_0 = \frac{\hbar^2}{me^2} = 5.29 \times 10^{-9} \text{ cm}$$



**Relationship of Light and Matter**

De Broglie hypothesis is that matter has a wavelike property and a particle-like property.

Equations of Light:

$$E = \hbar\omega = h\nu$$

$$p = \hbar k$$

$$\omega = ck$$

Equations of Matter:

$$E = \frac{p^2}{2m}$$

$$\lambda = \frac{h}{p}$$

$$p = \hbar k$$

Duality:

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

$$\lambda = h\nu$$

$$\omega = 2\pi\nu$$

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

☼ Homework: 1.5, 1.7, 1.8, 1.21, 2.23