

**CHEM 322 Notes**  
**Chapter 11 – Quantum Theory: Introduction and Principles**

- I. Classical Mechanics vs. Quantum Mechanics
- a. **Classical Mechanics** – the laws introduced in the seventeenth century by Sir Isaac Newton, which was successful at explaining the motion of the normal macroscopic world.
  - b. In classical mechanics, there are no constraints on:
    - i. The energy that something may have
    - ii. How fast something may go, etc.
  - c. Classical mechanics:
    - i. Predicts a precise trajectory for particles, with precisely specified locations and momenta at each instant.
    - ii. Allows the translational, rotational, and vibrational modes of motion to be excited to any energy simply by controlling the forces that are applied.
  - d. During the last-half of the nineteenth century, various experiments were conducted on atomic and molecular systems which showed a limitation in the understanding of classical mechanics. As a result, a new mechanics, **quantum mechanics**, was developed to explain these puzzling observations.
  - e. In quantum mechanics, atomic and molecular systems can have only specific “**quantized**” energies.

II. Brief Review of Classical Mechanics

- a. **Kinetic Energy** – energy of motion.

$$T = \frac{1}{2}mv^2 \quad (1)$$

where  $m$  is the mass of the particle and  $v$  is the particle's velocity. However, linear momentum ( $p$ ) is defined as:

$$p = mv \quad (2)$$

and the kinetic energy of a particle may be expressed as:

$$T = \frac{p^2}{2m} \quad (3)$$

- b. **Potential Energy** – the amount of energy stored to do work. There are many types of potential energy, such as:

- i. For a spring (or harmonic oscillator):

$$V(x) = \frac{1}{2}kx^2 \quad (\text{Hook's Law}) \quad (4)$$

where  $k$  is the “spring constant” or force constant and  $x$  is the displacement.

- ii. Electrostatic Potential:

$$V(x) = -\frac{q_1q_2}{r} \quad (5)$$

where  $q$  is the charge of the particles and  $r$  is the separation between the particles.

- c. The **total energy** (E) is the sum of the kinetic and potential energy of the system.

$$E = T + V \quad (6)$$

$$E = \frac{1}{2}mv^2 + V(x) \quad (7)$$

$$E = \frac{p^2}{2m} + V(x) \quad (8)$$

- d. The simplest case is when  $V=0$  which is for a particle in a vacuum with no gravity. Then:

$$E = T = \frac{1}{2}mv^2 \quad (9)$$

- e. Since

$$v = \frac{dx}{dt} = \dot{x} = \left(\frac{2E}{m}\right)^{\frac{1}{2}} \quad (10)$$

This equation is a “differential equation” with solutions for x:

$$x(t) = x(0) + \left(\frac{2E}{m}\right)^{\frac{1}{2}} t \quad (11)$$

or

$$x(t) = x(0) + \frac{p}{m} t \quad (12)$$

where  $x(0)$  is the position at  $t = 0$ . **Meaning:** If you know the initial position  $x(0)$  and the momentum  $p = p(0) = p(t)$ , then you can calculate the position of the particle at any time.

- f. Consider Newton’s Second Law of Motion:

$$F = ma \quad (13)$$

$$F = m \frac{d^2x}{dt^2} = m\ddot{x} \quad (14)$$

where  $m$  is the mass of the particle and  $a$  is the particle’s acceleration. Since

$$p = mv = m \frac{dx}{dt} = m\dot{x}, \quad (15)$$

then,

$$\dot{p} = \frac{dp}{dt} = m\ddot{x} \quad (16)$$

and it follows that:

$$F = \dot{p} \quad (17)$$

**Meaning:** If a constant force  $F$  acts on a particle, we can always calculate its momentum ( $p$ ) and thus its position.