Lecture 2

Physics Classifications:

Classical and Quantum Mechanics

Reading:

Notes, and Brennan 1.1-1.2

Classifications in Physics

- Classical Mechanics
    - Assumes allowable energies are continuous values and all energies are allowed.
        - Newtonian Mechanics
            - Most popular formalism of classical mechanics
        - Hamiltonian Mechanics
            - Energy focused approach to classical mechanics
- Quantum mechanics
    - Involves the physical laws of nature that govern the movement of small particles.
    - Assumes allowable energies are discrete values and some energies are not allowed.

- Correspondence Principle states that quantum mechanics merges with classical mechanics as the energies involved increase (we will find this also means they merge as the distances increase). Thus, in the classical limit, classical and quantum mechanics predict the same results.

Comments about Quantum Mechanics

•Quantum mechanics involved the physical laws of nature that govern the movement of small particles.

•Quantum mechanics involves physics but also has philosophical and even "religious" implications.

> •Example 1: Since classical mechanics predicts a known outcome for any predetermined state, classical mechanics would predict the end result of the universe from a known origin without the possibility of deviation. However, Quantum Mechanics is less "deterministic" with the best known outcome being "probabilistic" but not absolutely predetermined. Such "predestination" or "non-predestination" debate has been the subject of great philosophers and theologians for hundreds of years. Early scientists were persecuted for heresy when they stated that outcomes in the physical world could be predicted based on "Laws of Nature" – if they only had quantum mechanics ...

> •Example 2: However, unlikely, quantum mechanics tells us that any "allowable event" can occur but maybe not in our lifetime. All the electrons in your device can suddenly end up is one small corner of the device instead of randomly exsisting throughout the device – highly unlikely but possible.

> •Another example: String theory...

Classical Newtonian Mechanics

• Sir Isaac Newton's (and other contributors) observations of the way things react in nature resulted in two linear equations (although the second is a linear 2nd order equation).

Momentum (Newton's 1st Law):

2.1)
$$p(t) = mv(t) = m\frac{dx(t)}{dt}$$

Force (Newton's 2nd Law):

2.2)
$$F(t) = ma = m\frac{d^2x(t)}{dt^2}$$

Newton's approach is momentum and force driven. Energy is an "afterthought" derived from the main Newtonian laws.

Work (Energy Increase):

2.3)
$$W(t) = \int_o^x F(x)dx$$

Classical Newtonian Mechanics

•Newtonian Energy can be broken up into Kinetic (energy of motion) and Potential (stored) Energy

Kinetic Energy (inserting 2.2 into 2.3):

2.4)
$$E_{Kinetic} = \int_0^x m \frac{d^2 x(t)}{dt^2} dx = m \int_0^x \frac{d}{dt}(v) dx = m \int_0^x v \left(\frac{d}{dx} v \right) dx$$

$$E_{Kinetic} = \frac{1}{2} m v^2 = \frac{p^2}{2m}$$

Potential Energy (negative of work performed as potential energy is "stored energy"):

2.5)
$$W(t) = -U(x) \quad \Rightarrow \quad F(x) = -\frac{d}{dx} U(x) \quad \longleftarrow \quad \text{"Energy Band Bending" exerts a force on a particle}$$

Total Energy:

2.6)
$$E_{Total} = E_{Kinetic} + E_{Potential} = \frac{p^2}{2m} + U(x)$$

Classical Newtonian Mechanics

•Newtonian Energy is derived from the state variables (given values that define an objects state of being) position, x(t), and momentum, p(t), in the presence of a force F.

$$E_{Total} = E_{Kinetic} + E_{Potential} = \frac{p^2}{2m} + U(x)$$

Classical Hamiltonian Mechanics

•Hamiltonian Mechanics is energy focused with the "Hamiltonian Function", H defined as the total energy of a system.

Hamiltonian Function :

2.7)

$$H = \frac{p^2}{2m} + U(x)$$

In the Hamiltonian approach, position and momentum are derived from the total energy and can be found by taking the partial derivatives of 2.7 noting that p is independent of x and U(x) is independent of p.

$$\frac{\partial H}{\partial x} = \frac{d}{dx} U(x)$$

$$\frac{\partial H}{\partial p} = \frac{p}{m}$$

Using 2.1), 2.2) and 2.5),

$$\boxed{\begin{array}{l} \dfrac{dp}{dt} = -\dfrac{\partial H}{\partial x} \\[2mm] \dfrac{dx}{dt} = \dfrac{\partial H}{\partial p} \end{array}}$$

$$\Rightarrow \left(-\frac{\partial H}{\partial x} = -\frac{dU(x)}{dx} = F(x) = m\left(\frac{d}{dt} v(t) \right) = \frac{dp}{dt} \right)$$

$$\Rightarrow \left(\frac{\partial H}{\partial p} = \frac{p}{m} = \frac{mv}{m} = \frac{dx}{dt} \right)$$
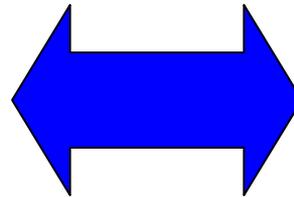
Classical Hamiltonian Mechanics

•Note that the linear and linear second order differential equations Newton used to define the state of a particle have been converted to two linear partial differential equations derived from the total energy of the particle. The Hamiltonian approach emphasizes the importance of the total energy in determining the state of a particle but both approaches contain the same information, only in different forms.

Newtonian Mechanics

$$p(t) = mv(t) = m\frac{dx(t)}{dt}$$

$$F(t) = ma = m\frac{d^2x(t)}{dt^2}$$

Hamiltonian Mechanics

$$\frac{dp}{dt} = -\frac{\partial H}{\partial x}$$

$$\frac{dx}{dt} = \frac{\partial H}{\partial p}$$

•Quantum mechanics is largely taken from the Hamiltonian approach while most students are most "comfortable" with the Newtonian approach. This discrepancy sometimes results in uncomfortable "translations" when discussing Quantum Mechanical predictions.

The Breakdown of Classical Mechanics

Both the Newtonian approach and the Hamiltonian approach assume a continuum of allowed energies and no "disallowed" energies. They also assume the article described by the previous equations is a simple particle. However, several observations refute this explanation of our universe.

- Quantization of Energy
    - Disallowed Energy values
- Slit Experiments
- Wavelength-Particle Duality
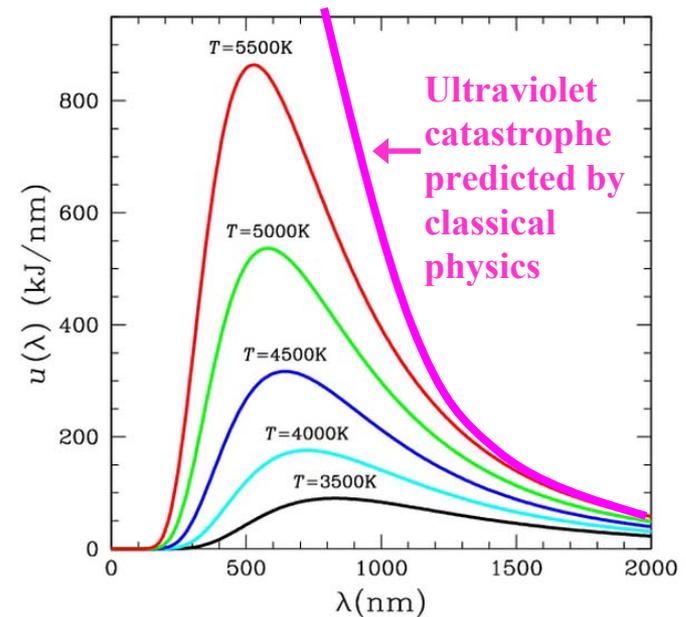- Photoelectric Effect
- Compton Effect (Homework?)

The Breakdown of Classical Mechanics

•**Quantization of Energy**:

Max Planck started the evolution toward modern Quantum Mechanics when he developed his model to describe "black body radiation" *. While the details are not presented here, Planck's model required the description of light as individual "oscillators" of a "quantized energy" and also predicted disallowed energy values. Classical mechanics had previously considered light to have a continuous allowable energy range.

Ultraviolet catastrophe predicted by classical physics

$$E = \hbar\omega, 2\hbar\omega, 3\hbar\omega, 4\hbar\omega, 5\hbar\omega, \ldots = \hbar c \frac{2\pi}{\lambda}, 2\hbar c \frac{2\pi}{\lambda}, 3\hbar c \frac{2\pi}{\lambda}, 4\hbar c \frac{2\pi}{\lambda}, 5\hbar c \frac{2\pi}{\lambda}, \ldots$$

but not

$$E = \frac{1}{2}\hbar\omega \quad \text{for example}$$

*Max Planck's published law of black-body radiation: "On the Law of Distribution of Energy in the Normal Spectrum". Annalen der Physik 4 (1901)

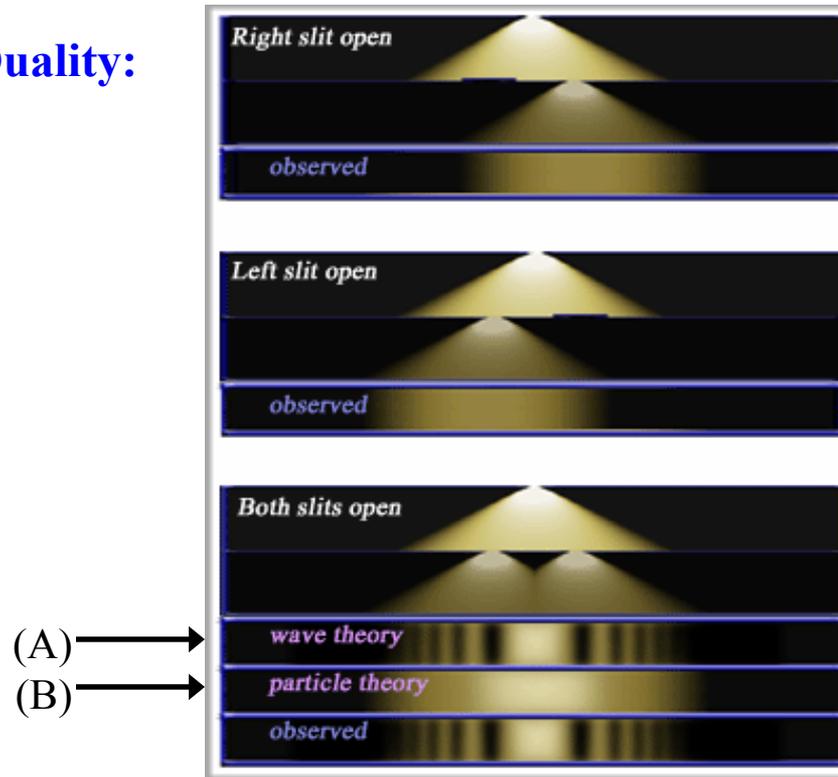# The Breakdown of Classical Mechanics

•**Quantization of Energy**:

Details*: "The observed spectrum of black-body radiation could not be explained by classical electromagnetism and statistical mechanics: these predicted infinite brightness at low wavelength (i.e. high frequencies), a prediction often called the ultraviolet catastrophe. This theoretical problem was solved by Max Planck, who had to assume that electromagnetic radiation could propagate only in discrete packets, or quanta. This idea was later used by Einstein to explain the photoelectric effect. These theoretical advances eventually resulted in the replacement of classical electromagnetism by quantum mechanics. Today, the quanta are called photons."

*Text from http//en.wikipedia.org (see for more details)

The Breakdown of Classical Mechanics

•**Wavelength-Particle Duality:**

(A)

(B)

The double-slit experiment involves sending light, electrons, atoms and even small molecules (all have been demonstrated) through a series of slits as shown above. The quantum particles interact to form interference patterns consistent with wavelike behavior. If the particles were merely particles, the intensities would add as in the slice marked (A). The observation is actually similar to the slice marked (B) indicating addition of amplitudes in and out of phase (i.e. constructive and destructive interference). This is taken as evidence of the "wave-particle duality" explained by quantum physics.

Thomas Young originally performed this experiment in ~1805 to prove that light was composed of waves. The extension to electrons and later atoms and molecules has shown that for multiple single electron events the results still hold true but each event carries a quanta of charge i.e. the electron charge is not fractional..

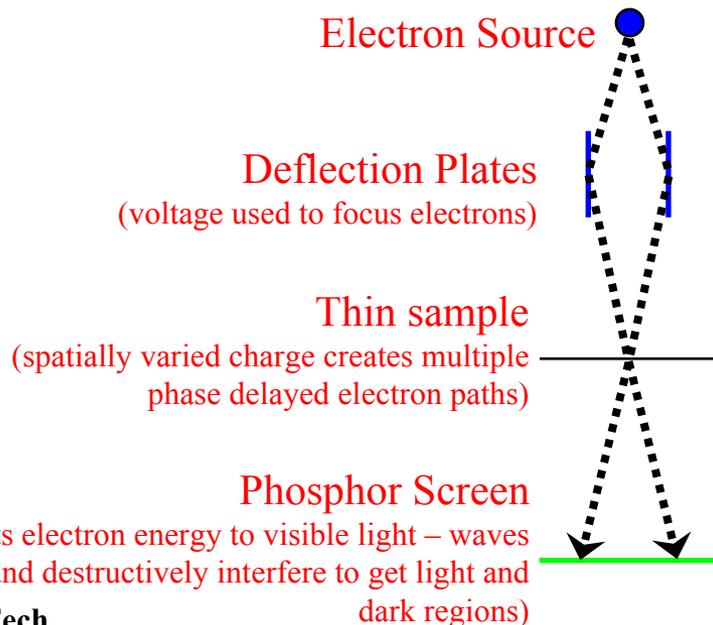*Figures from http//en.wikipedia.org (see for more details)

The Breakdown of Classical Mechanics

•**Wavelength-Particle Duality:**

•To fully understand the origin of the energy bandgap and effective mass concepts as well as future topics of energy states in quantum wells and tunneling currents, one must have at least a basic understanding of electron motion in free space and in the presence of other sources of electrostatic potential (atomic cores for example). This requires an understanding of the dual wave-particle nature of electrons and in turn quantum mechanics.

•Consider the electron microscope:

   •Electrons have a charge and thus can be focused ***like a particle***...
   •...but also have a phase and thus can interfere with each other destructively or constructively ***like a wave***

Electron Source

Deflection Plates
(voltage used to focus electrons)

Thin sample
(spatially varied charge creates multiple phase delayed electron paths)

Phosphor Screen
(converts electron energy to visible light – waves constructively and destructively interfere to get light and dark regions)

$$\upsilon = \frac{h}{m\lambda}$$

$$\upsilon = \frac{6.6 \times 10^{-34} Js}{9.1 \times 10^{-31} kg \times 10^{-11} meters} = 7.25 \times 10^7 m/s$$

$$KE = \frac{1}{2}m\upsilon^2 = qV$$

$$V = \frac{9.1 \times 10^{-31}(7.25 \times 10^7 m/s)^2}{2 \times 1.6 \times 10^{-19}C} = 15,000 \ V$$

15 KV gives sub atomic resolution!

The Breakdown of Classical Mechanics

- **Wavelength-Particle Duality:**

- What is the wavelength of macroscopic particles? Consider a bullet (1km/s 1 gram)?

$$1000 m/s = \frac{6.6 \times 10^{-34} Js}{1 \times 10^{-3} kg \times \lambda} \Rightarrow \lambda = 6.6 \times 10^{-34} m$$

- Though it acts as a wave, it's wavelength is too small to ever measure/observe.

- So an electron (or every particle) acts as a wave AND a particle simultaneously. How can we describe this?

Describe particles by a wave equation → Later...

- Other useful properties of "energy-particle waves":
$$E = hf = \left(\frac{h}{2\pi}\right)(2\pi f) = \hbar\omega = mc^2$$

Or the momentum of the photon is...

$$p = mc = \frac{hf}{c} = \frac{h}{\lambda} = \hbar\left(\frac{2\pi}{\lambda}\right) = \hbar k$$

$$p = \frac{h}{\lambda}$$ this is known as the de Broglie hypothesis

Where scalar, k, is known as the wave number. If momentum, **p** is expressed as a vector, **k** is known as the wave vector.

The Breakdown of Classical Mechanics

•**Wavelength-Particle Duality:**

The relationship de Broglie postulated, p=ℏk , where the wave number is k=2π/λ ,created a "bridge" between the classical concepts of momentum and wavelength.

Why do we use "k" or "**k**" instead of "p" or "**p**"?

Wave numbers (k=2π/λ), wave vectors and wavelengths of particles are independent of mass. Classically, **p**=m**v**. However, we will show that the "mass"* of an electron, for example, will change with crystalline direction allowing two parameters (m and v) to change the momentum. Thus, k is simpler to consider.

Classically, momentum, p=mv and kinetic energy is ½ (mv²) leading to

$$E_{Kinetic} = \frac{1}{2}mv^2 = \frac{1}{2}\frac{(mv)^2}{m} = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$
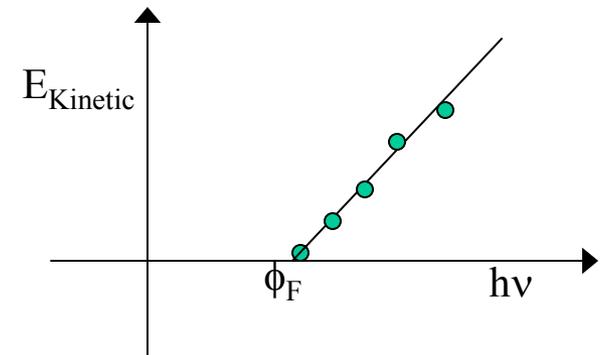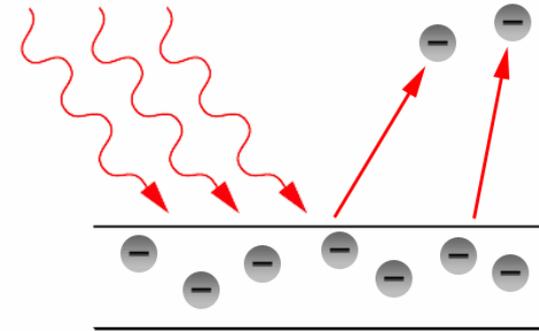
*actually the effective mass is what changes with crystalline direction.

The Breakdown of Classical Mechanics

•Photoelectric Effect:

The photoelectric effect is the emission of electrons from a material surface upon exposure to, and absorption of, electromagnetic radiation. The importance of this experiment comes from the fact that there exists a threshold energy, the material work function which is related to the atomic bond strengths, below which electrons can not be emitted. The previous belief was that an electron could collect and build up energy until it was released. If this were true then the number of emitted electrons would be proportional to the light intensity, even for light below the work function energy. Experiment showed it was not. However, when energy above the work function energy was used the kinetic energy of the emitted electron increased linearly with light frequency. This experiment was the foundation for state to state transitions and also showed that energy was not infinitely divisible but instead came in quantized units.

Albert Einstein explained this in 1905 in "On a Heuristic Viewpoint Concerning the Production and Transformation of Light". This paper proposed "light quanta" (later called "photons") and won Einstein the Nobel Prize of 1921.

$$h\upsilon = \qquad h\upsilon_o \quad + \qquad E_{Kinetic}$$

$$\uparrow \qquad\qquad \uparrow \qquad\qquad\qquad \uparrow$$

Incoming photon energy　Material Work Function, φ_F　Outgoing electron energy

Some figures from http//en.wikipedia.org (see for more details)

The Need for a New Approach: The Birth of Quantum Mechanics

To explain these and many other observations that Classical Mechanics failed to adequately explain, the Quantum Mechanical Fathers slowly pieced together theories that collectively have become what we now call Quantum Mechanics. This took decades to fully mature with many brilliant physicists never fully accepting Quantum Mechanics before their death. For example, Einstein* had legitimate problems with QM because it appeared to be in conflict with his theory of general relativity. Some modern day efforts, String theory** among others, are still attempting to reconcile these discrepancies.

*Einstein is often quoted as saying that "God does not play dice". While this quote is often taken out of context, there is little argument that Einstein worked in vain much of his later life toward the goal of unifying QM with General Relativity.

**For a terse overview of String Theory and this conflict, see "The elegant universe" by Brian Greene.