

Lecture #1: Quantum Mechanics – Historical Background

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TEXTBOOK: Quantum Chemistry, 2nd Edition, D. McQuarrie, University Science (2007)

GRADING:	<u>Points</u>
3 Thursday evening 1 hour exams (7:30 – 8:30 PM) tentatively October 3, 24, and November 21 One Lecture cancelled for each exam	300 (100 each)
~9 problem sets	100
~ 35 “clicker” outcomes, one in every class	50
3-Hour Final Exam during Exam Week (December 16-20)	200
TOTAL	<hr/> 650

The Lecture schedule is tentative. The Lecture Notes will be posted on the course website, usually several days before the class. Revisions, usually printed in red, will be posted usually the day after the class.

Lecture Notes are pseudo-text. Everything in them is exam-relevant.

Let's begin:

Chalk demonstration.

Trajectory $x(t)$, $p(t)$: can predict end-point x_{end} , p_{end} , t_{end} , after observation of short segment of trajectory at early t .

Decrease mass of thrower, chalk, and target by 100× without modifying observers. What happens?

Decrease by factor of 10^{20} . What happens? How sure are you?

Quantum Mechanics is a theory that describes unexpected phenomena in the microscopic world without requiring any change of our understanding of the macroscopic world.

Quantum Mechanics is based on a theory of (in principle) measurement without knowledge being allowed of what goes on between measurements. Everything you can know must be the result of a (possible) measurement.

Key ideas of Quantum Mechanics to be seen in first few lectures

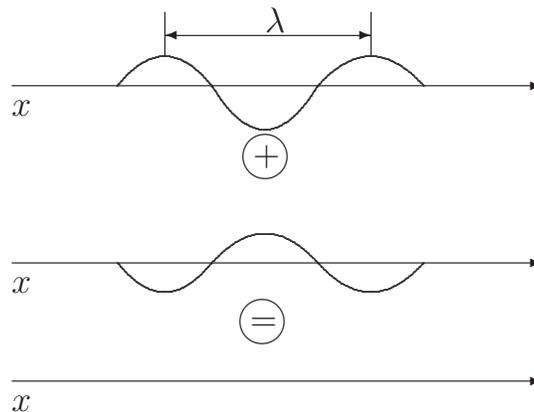
- * lack of determinism: probabilistic
- * wave-particle duality for both light and matter
- * energy quantization and line spectra — some of this should really bother you

TODAY: Light is both wave and particle.

What are the familiar properties of light that make us believe that light is wave-like (as opposed to particle-like)?

- * refraction, prism and lens
- * diffraction; grating and pinhole
- * two-slit experiment

Many wave phenomena involve *interference effects*. Add two waves (amplitude vs. spatial coordinate):



The result is *perfect destructive interference*

Waves have + and – amplitudes.

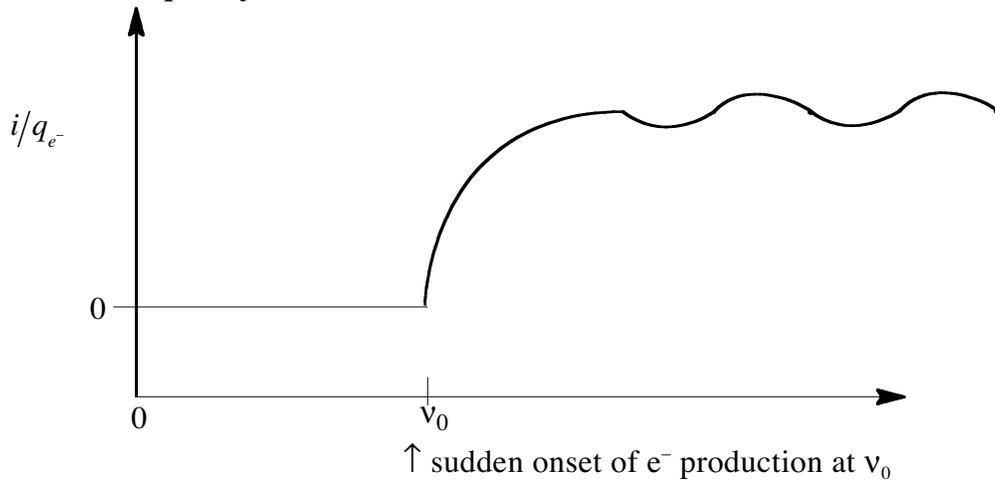
Destructive and Constructive Interference.

What's nu?

$$\nu = \frac{c}{\lambda}$$

frequency (s^{-1})
speed of light in vacuum (cm/s)
wavelength (cm)

Return to this in next lecture on wave characteristics of matter

2. e^-/sec vs. **frequency** at constant I

“work function” of metal (energy required to remove
one electron from the bulk)

$\nu_0 \equiv \phi/h$ ← arbitrary constant

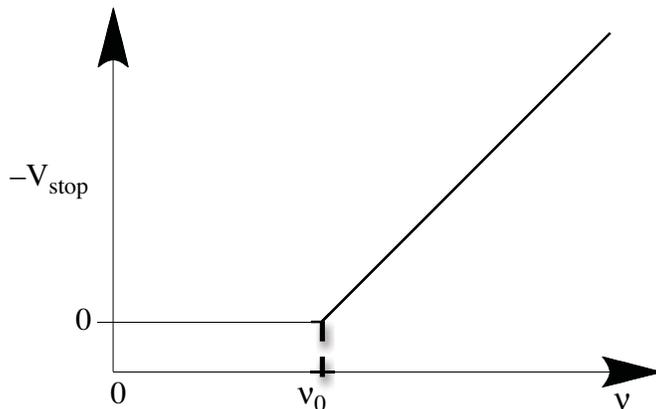
onset

3. **KE** of ejected e^- vs. ν at constant I. Measure by asking how high a potential energy hill can the ejected e^- *just barely* climb?

$$E_{\text{stop}} = q_{e^-} V_{\text{stop}} > 0 \quad (q_{e^-} < 0, V_{\text{stop}} < 0)$$

e^- must climb hill of height $q_{e^-} V_{\text{stop}}$.

This is the energy required to cancel the KE of the ejected e^- vs. the frequency of the incident light.



- * straight line with positive slope
- * onset at ν_0 , slope independent of I
- * slope independent of which metal

Experimental results are described by the following equation:

Planck's constant. Same for every metal!

$$E_{\text{stop}}(\nu) = q_{e^-} V_{\text{stop}}(\nu) = h(\nu - \nu_0) = h\nu - \phi$$

work function of metal
(Different for each metal)

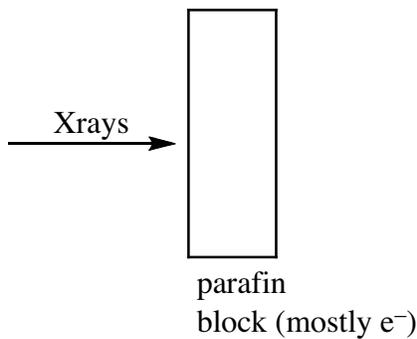
Planck's constant is directly measured by slope of E_{stop} vs. ν .

Leads us to think of light as composed of discrete packets of energy called "photons".

Energy of photon is $E = h\nu$. Is this the only sensible explanation of all of the experimental observations?

Another property of photons:

Compton Scattering 1923



Observe angular distribution of scattered X-ray radiation as well as that of the e^- ejected from the parafin target.

This experiment provides evidence that light acts as a billiard-like particle with definite *kinetic energy* (a scalar quantity), T , and *momentum* (a vector quantity), p . The scattering is explained by conservation of KE and p .

We start with the idea, established by the previously discussed photoelectric effect, that light consists of photons with kinetic energy KE.

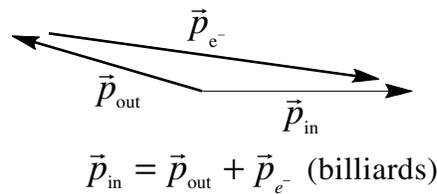
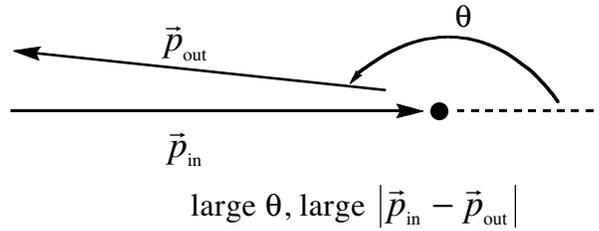
$$KE = E(\nu) = h\nu$$

Hypothesize that photons also have momentum:

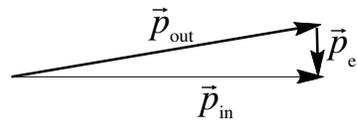
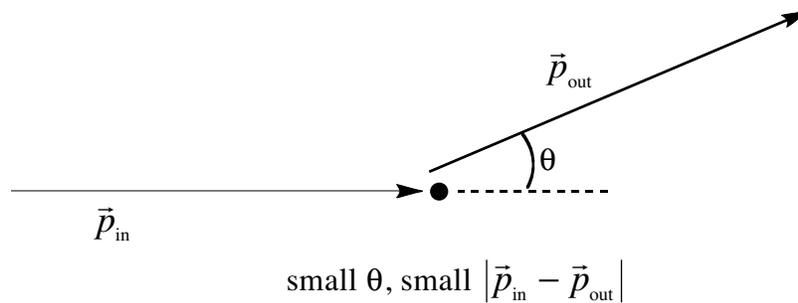
$$p = E/c = \frac{h\nu}{c} = \frac{h}{\lambda} \quad (E/c \text{ has units of momentum})$$

Use conservation of E and p to predict features of the scattering that could only be explained by the particle nature of light.

Back
Scatter
of photon



Forward
Scatter



Since photon transfers some of its energy to e^- , the scattered photon will have less energy (longer λ) than the incident photon. Can show that

$$\lambda_{\text{out}} - \lambda_{\text{in}} \equiv \Delta\lambda = \frac{2h}{m_e c} \sin^2 \theta/2 \geq 0 \quad \text{red shift}$$

The wavelength shift depends on the direction of the scattered photon.

$$\theta = 0 \text{ (forward)} \quad \Delta\lambda = 0$$

$$\theta = \pi \text{ (backward)} \quad \Delta\lambda = \frac{2h}{m_e c}$$

$$\frac{h}{m_e c} = 0.0243 \text{ \AA}$$

Compton λ of e^-

Scattered light at $\theta \neq 0$ is always red-shifted.

Dependence of $\Delta\lambda$ on θ is independent of λ_{in} .

Experimental Verification: Use X-ray region (short λ) so that $\frac{\Delta \lambda}{\lambda}$ is large enough to measure accurately.

Light passes all tests for *both* particle-like and wave-like character.

NON-LECTURE

Derive Compton formula for $\theta = \pi$

$$\Delta \lambda = \frac{2h}{m_e c}$$

Conservation of \vec{p}

$$\vec{p}_{\text{in}} = \vec{p}_{\text{out}} + \vec{p}_{e^-}$$

$$\text{for photon } |p| = E/c = \frac{h\nu}{c} = \frac{h}{\lambda}$$

back scattering

$$\vec{p}_{\text{out}} = -\frac{h}{\lambda_{\text{out}}} \hat{z} \quad \leftarrow \text{unit vector pointing in } +z \text{ direction}$$

$$\vec{p}_{\text{in}} = \frac{h}{\lambda_{\text{in}}} \hat{z}$$

Momentum removed from photon is transferred to the electron.

Conservation of p: $h \left(\frac{1}{\lambda_{\text{in}}} + \frac{1}{\lambda_{\text{out}}} \right) = p_{e^-} \approx h \frac{2}{\bar{\lambda}}$ (It is not necessary to make this approximation)

$$\bar{\lambda} \equiv \frac{\lambda_{\text{in}} + \lambda_{\text{out}}}{2}$$

Conservation of E:

$$\begin{aligned}
 h\nu_{in} &= h\nu_{out} + p_{e^-}^2 / 2m_e \\
 h \frac{c}{\lambda_{in}} &= h \frac{c}{\lambda_{out}} + p_{e^-}^2 / 2m_e \\
 \frac{1}{\lambda_{in}} - \frac{1}{\lambda_{out}} &= \frac{p_{e^-}^2}{2hcm_e} \\
 \frac{\lambda_{out} - \lambda_{in}}{\lambda_{in}\lambda_{out}} &= \frac{p_{e^-}^2}{2hcm_e}
 \end{aligned}$$

insert conservation of p result

$$\frac{\lambda_{out} - \lambda_{in}}{\lambda^2} = \frac{\left[h \left(\frac{2}{\lambda} \right) \right]^2}{2hm_e c}$$

$$\lambda_{out} - \lambda_{in} = \frac{4h^2}{2hm_e c} = \frac{2h}{m_e c} \quad (\text{red shift})$$

$$\boxed{\Delta \lambda = \frac{2h}{m_e c} \quad \text{for } \theta = \pi}$$

A beautiful demonstration of Compton scattering is an e^- , photon *coincidence experiment*.

Cross and Ramsey, *Phys. Rev.* **80**, 929 (1950).

Measure scattered the single photon and the single scattered e^- that result from a single event.

The scattering angles are consistent with E,p conservation laws.

END OF NON-LECTURE

Today: we saw two kinds of evidence for why *light* acts as a *particle*.

- * photoelectric effect: light comes in discrete packets with $E = h\nu$
- * Compton scattering: light packet has definite momentum.

NEXT LECTURE: evidence for wave nature of e^-

1. Rutherford planetary atom — a lot of empty space. Why no radiative collapse of e^- in circular orbit?
2. Diffraction of X-ray and e^- by metal foil
3. Bohr model
 - * Bohr assumed that angular momentum is quantized
 - * de Broglie showed that there are integer number of e^- wavelengths around a Bohr orbit.

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5.61 Physical Chemistry
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