Q: What's the difference between a quantum mechanic and an auto mechanic?

A: A quantum mechanic can get his car into the garage without opening the door!
Quantum Mechanics I
Physics 325

Emergence of Quantum Physics

SYLLABUS

1. The failure of classical mechanics
   Photoelectric effect, Einstein’s equation, electron diffraction and de Broglie relation.
   Compton scattering. Wave-particle duality, Uncertainty principle (Bohr microscope).

2. Steps towards wave mechanics
   Time-dependent and time-independent Schrödinger equations. The wave function and its interpretation.

3. One-dimensional time-independent problems

4. The formal basis of quantum mechanics
   The postulates of quantum mechanics — operators, observables, eigenvalues and eigenfunctions. Hermitian operators and the Expansion Postulate.

5. Angular momentum in quantum mechanics
   Operators, eigenvalues and eigenfunctions of \( \hat{l}_z \) and \( \hat{l}_z^2 \).
SYLLABUS (cont)

6. The hydrogen atom
   Separation of space and time parts of the 3D Schrödinger equation for a central field. The radial Schrödinger equation and its solution by series method. Degeneracy and spectroscopic notation.

7. Electron spin and total angular momentum

Photo-electric effect, Compton scattering
   Particle nature of light in quantum mechanics

\[ E = h\nu \]
\[ p = \frac{h}{\lambda} \]

Davison-Germer experiment, double-slit experiment
   Wave nature of matter in quantum mechanics

Wave-particle duality

Postulates:
   Operators, eigenvalues and eigenfunctions, expansions in complete sets, commutators, expectation values, time evolution

Time-dependent Schrödinger equation, Born interpretation

Time-independent Schrödinger equation

Quantum simple harmonic oscillator
   \[ E_n = (n + \frac{1}{2}) \hbar \omega_c \]

Hydrogenic atom

1D problems

Angular momentum operators \( L_z, L^2 \)

Angular solution \( \gamma_n^m (\theta, \phi) \)

Radial solution \( R_n, E = -\frac{1}{2} \frac{Z^2}{n^2} \)
Review of basic quantum physics

Quantum Mechanics developed to explain the failure of classical physics to describe properties of matter on atomic scale

- energy quantization → line spectra
- angular momentum quantization → fine structure
- quantum mechanical tunneling → nuclear $\alpha$ decay

Need of Quantum Mechanics

Materials are made of microscopic particles like molecules, atoms and electrons. In order to understand properties of materials, we need to understand the behaviors of the microscopic particles which cannot be described by the classical Newton’s mechanics. Physicists were forced to develop quantum mechanics.

Some Experiments that Defied Classical Physics

There are many experiments and observations started shaking the foundations of classical physics at the beginning the twentieth century. We will briefly review some of these critical experiments.
So, What Is It? A Misnomer…

It’s the mechanics of WAVES, instead of CLASSICAL particles.

Wave particle duality

- Light has wave-like properties (interference, diffraction, refraction) and particle-like properties (photo-electric effect, Compton effect)
- Particles show classical particle behaviour (scattering) and also have wave-like properties (double slit electron interference, neutron diffraction)
- A wave equation can be constructed which describes the state of a particle or system of particles (the Schroedinger equation)
Evidence for wave-particle duality
- Photoelectric effect
- Compton effect
- Electron diffraction
- Interference of matter-waves

Consequence: Heisenberg uncertainty principle

Wave behaving as particles: Blackbody radiation

A blackbody is an ideal object that absorbs any radiation (Electromagnetic waves). It emits radiation at different wavelengths. The intensity (power per unit area) of the radiation emitted between wavelengths $\lambda$ and $\lambda + d\lambda$ is defined as

$$dI = R(\lambda)d\lambda \quad (3.18)$$

where $R(\lambda)$ is called the radiancy. Physicists were interested in blackbodies because their radiancy vs. $\lambda$ depends on the temperature of the materials only.

Some observed facts:
- The total intensity obeys the Stefan’s law,

$$I = \int_0^\infty R(\lambda)d\lambda = \sigma T^4 \quad (3.19)$$

The constant $\sigma = 5.67 \times 10^{-8}$ W m$^{-2}$ K$^{-4}$, called the Stefan-Boltzmann constant.
- The radiancy maximizes at a certain wavelength $\lambda_{\text{max}}$, which depends on the temperature according to (Wien’s displacement law)

$$\lambda_{\text{max}} = \frac{2.898 \times 10^{-3} mK}{T} \quad (3.20)$$
The Rayleigh-Jeans and the Wien’s laws based on classical physics cannot explain the entire spectrum of blackbody radiation. Planck’s quantum theory: An electromagnetic wave with frequency $f$ exchanges energy with matter in a “quantum” given by

$$E = hf = h\omega$$

Here $h$ is Planck’s constant.

$$h = 6.6261 \times 10^{-34} \text{ J} \cdot \text{s} \quad \text{and} \quad h = \frac{1}{2\pi} = 1.05 \times 10^{-34} \text{ J} \cdot \text{s}$$

Light waves have well-defined energy like particles!

**PHOTOELECTRIC EFFECT**

When UV light is shone on a metal plate in a vacuum, it emits charged particles (Hertz 1887), which were later shown to be electrons by J.J. Thomson (1899).

Classical expectations

Electric field $E$ of light exerts force $F = eE$ on electrons. As intensity of light increases, force increases, so KE of ejected electrons should increase.

Electrons should be emitted whatever the frequency $\nu$ of the light, so long as $E$ is sufficiently large.

For very low intensities, expect a time lag between light exposure and emission, while electrons absorb enough energy to escape from material.
Wave behaving as particles: Photoelectric effect

In a photoelectric experiment, optical radiation impinges upon a metal and electrons are knocked out due to interaction of the light with the free electrons.

\[ KE_{\text{max}} = \frac{1}{2}mv_{\text{max}}^2 = eV_s \]

If the impinging light gives the electrons an energy \( E_{\text{em}} \), the electrons will emit from the metal with an energy \( E_{\text{em}} - \phi \). The maximum energy of the knocked out electrons is determined by the stopping voltage, \( V_s \).

Photoelectric Current/Voltage Graph

- The current increases with intensity, but reaches a saturation level for large \( \Delta V \)’s
- No current flows for voltages less than or equal to \(-\Delta V_s\), the stopping potential
  - The stopping potential is independent of the radiation intensity
Features Not Explained by Classical Physics/Wave Theory

- No electrons are emitted if the incident light frequency is below some cutoff frequency that is characteristic of the material being illuminated.
- The maximum kinetic energy of the photoelectrons is independent of the light intensity.
- The maximum kinetic energy of the photoelectrons increases with increasing light frequency.
- Electrons are emitted from the surface almost instantaneously, even at low intensities.

According to classical wave theory, we expect:
- \( KE_{\text{max}} \) should be proportional to the intensity of the impinging light wave.
- The electron emission should occur at any frequency as long as the intensity of the light is high enough.
- There should be a time interval between the switching on of the light and the emission of electrons, because \( E=I \times \text{area} \times t \).

Actual Observations:
- The \( KE_{\text{max}} \) is independent of the intensity!
- There is a threshold frequency below which no electron emissions regardless of intensity!!
- The initial electrons are emitted within a nanosecond or so – almost instantaneously!!!
Einstein’s quantum theory:

Light is regarded as made up of particles (photons) with energy

\[ E = hf = h\omega \]

Energy conservation says

\[ KE_{\text{max}} = hf - e\phi \]

Lowest frequency (threshold frequency) is

\[ f = \frac{e\phi}{h} \]

Experimental observations of photoelectric effect.

Einstein’s Explanation

- A tiny packet of light energy, called a photon, would be emitted when a quantized oscillator jumped from one energy level to the next lower one
  - Extended Planck’s idea of quantization to electromagnetic radiation
- The photon’s energy would be \( E = hf \)
- Each photon can give all its energy to an electron in the metal
- The maximum kinetic energy of the liberated photoelectron is
  \[ KE = hf - \Phi \]
- \( \Phi \) is called the work function of the metal
Explanation of Classical “Problems”

- The effect is not observed below a certain cutoff frequency since the photon energy must be greater than or equal to the work function.
  - Without this, electrons are not emitted, regardless of the intensity of the light.
- The maximum KE depends only on the frequency and the work function, not on the intensity.
- The maximum KE increases with increasing frequency.
- The effect is instantaneous since there is a one-to-one interaction between the photon and the electron.

Verification of Einstein’s Theory

- Experimental observations of a linear relationship between KE and frequency confirm Einstein’s theory.
  \[ f_c = \frac{\Phi}{h} \]
- The x-intercept is the cutoff frequency.
PHOTOELECTRIC EFFECT (cont)

The maximum KE of an emitted electron is then
\[ K_{\text{max}} = h \nu - W \]

**Actual results:**
- Maximum KE of ejected electrons is independent of intensity, but dependent on \( \nu \)
- For \( \nu < \nu_0 \) (i.e. for frequencies below a cut-off frequency) no electrons are emitted
- There is no time lag. However, rate of ejection of electrons depends on light intensity.

**Einstein’s interpretation (1905):**
- Light comes in packets of energy (photons)
  \[ E = h \nu \]
- An electron absorbs a single photon to leave the material

**Planck constant:** universal constant of nature
\[ h = 6.63 \times 10^{-34} \text{Js} \]

**Work function:** minimum energy needed for electron to escape from metal (depends on material, but usually 2-5eV)

Verified in detail through subsequent experiments by Millikan

Photoemission experiments today

Modern successor to original photoelectric effect experiments is ARPES (Angle-Resolved Photoemission Spectroscopy)

Emitted electrons give information on distribution of electrons within a material as a function of energy and momentum

February 2000

Physics World

Superconducting secrets

Superconducting secrets
SUMMARY OF PHOTON PROPERTIES

Relation between particle and wave properties of light

Energy and frequency \( E = h\nu \)

Also have relation between momentum and wavelength

Relativistic formula relating energy and momentum

\[ E^2 = p^2c^2 + m^2c^4 \]

For light \( E = pc \) and \( c = \lambda\nu \)

\[ p = \frac{h}{\lambda} = \frac{h\nu}{c} \]

Also commonly write these as

\[ E = \hbar\omega \quad p = \hbar k \quad \omega = 2\pi\nu \quad k = \frac{2\pi}{\lambda} \quad \hbar = \frac{h}{2\pi} \]

COMPTON SCATTERING

Compton (1923) measured intensity of scattered X-rays from solid target, as function of wavelength for different angles. He won the 1927 Nobel prize.

X-ray source

Collimator (selects angle)

Crystal (selects wavelength)

Target

Detector

Result: peak in scattered radiation shifts to longer wavelength than source. Amount depends on \( \theta \) (but not on the target material).

A.H. Compton, Phys. Rev. 22 409 (1923)
**COMPTON SCATTERING (cont)**

**Classical picture:** oscillating electromagnetic field causes oscillations in positions of charged particles, which re-radiate in all directions at *same frequency and wavelength* as incident radiation.

**Change in wavelength of scattered light is completely unexpected classically**

![Diagram showing incident light wave, electron, scattered electron, and scattered photon.]

Compton’s explanation: “billiard ball” collisions between particles of light (X-ray photons) and electrons in the material.

**Before**
- Incoming photon $p_{\nu}$
- Electron

**After**
- Scattered photon $p_{\nu'}$
- Scattered electron $p_e$

**Conservation of energy**

\[ h\nu + m_e c^2 = h\nu' + \left( p_e^2 c^2 + m_e^2 c^4 \right)^{1/2} \]

**Conservation of momentum**

\[ p_{\nu} = \frac{h}{\lambda} \hat{i} = p_{\nu'} + p_e \]

From this, Compton derived the change in wavelength:

\[ \lambda' - \lambda = \frac{h}{m_e c} \left( 1 - \cos \theta \right) \]

\[ = \frac{\lambda}{c} \left( 1 - \cos \theta \right) \geq 0 \]

\[ \lambda = \text{Compton wavelength} = \frac{h}{m_e c} = 2.4 \times 10^{-12} \text{ m} \]
Note that, at all angles there is also an unshifted peak. This comes from a collision between the X-ray photon and the nucleus of the atom

\[ \lambda' - \lambda = \frac{h}{m_Nc} (1 - \cos \theta) \sim 0 \]

since \( m_N \gg m_e \)

---

**WAVE-PARTICLE DUALITY OF LIGHT**

In 1924 Einstein wrote: “There are therefore now two theories of light, both indispensable, and ... without any logical connection.”

- Evidence for wave-nature of light
  - Diffraction and interference
- Evidence for particle-nature of light
  - Photoelectric effect
  - Compton effect

- Light exhibits diffraction and interference phenomena that are only explicable in terms of wave properties
- Light is always detected as packets (photons); if we look, we never observe half a photon
- Number of photons proportional to energy density (i.e. to square of electromagnetic field strength)
We have seen that light comes in discrete units (photons) with particle properties (energy and momentum) that are related to the wave-like properties of frequency and wavelength.

In 1923 Prince Louis de Broglie postulated that ordinary matter can have wave-like properties, with the wavelength $\lambda$ related to momentum $p$ in the same way as for light:

\[
\lambda = \frac{h}{p}
\]

Planck’s constant $h = 6.63 \times 10^{-34}$ Js

**de Broglie relation**

**de Broglie wavelength**

Predictation: We should see diffraction and interference of matter waves

**Estimate some de Broglie wavelengths**

- Wavelength of electron with 50eV kinetic energy
  
  \[
  K = \frac{p^2}{2m_e} = \frac{h^2}{2m_e\lambda^2} \Rightarrow \lambda = \frac{h}{\sqrt{2m_eK}} = 1.7 \times 10^{-10} \text{ m}
  \]

- Wavelength of Nitrogen molecule at room temperature
  
  \[
  \lambda = \frac{h}{\sqrt{3MkT}} = 2.8 \times 10^{-11} \text{ m}
  \]

- Wavelength of Rubidium(87) atom at 50nK
  
  \[
  \lambda = \frac{h}{\sqrt{3MkT}} = 1.2 \times 10^{-6} \text{ m}
  \]
If you are a wave, you interfere

Interference patterns

Wave Interactions

Constructive Interference

Destructive Interference
Interference out of slits

When is a particle like a wave?
Wavelength \cdot momentum = Planck
\[ \lambda \cdot p = h \]
\[ (h = 6.6 \times 10^{-34} \text{ J s}) \]

http://www.kfunigraz.ac.at/imawww/vqm/
**ELECTRON DIFFRACTION**

**The Davisson-Germer experiment (1927)**

The Davisson-Germer experiment: scattering a beam of electrons from a Ni crystal. Davisson got the 1937 Nobel prize.

At fixed accelerating voltage (fixed electron energy) find a pattern of sharp reflected beams from the crystal.

At fixed angle, find sharp peaks in intensity as a function of electron energy.

Davisson, C. J., "Are Electrons Waves?," Franklin Institute Journal 205, 597 (1928)

G.P. Thomson performed similar interference experiments with thin-film samples.

**ELECTRON DIFFRACTION (cont)**

Interpretation: similar to Bragg scattering of X-rays from crystals.

Path difference:

\[ a(\cos \theta_r - \cos \theta_i) \]

Constructive interference when

\[ a(\cos \theta_r - \cos \theta_i) = n\lambda \]

Electron scattering dominated by surface layers.

Note \( \theta_i \) and \( \theta_r \) not necessarily equal.

Note difference from usual “Bragg’s Law” geometry: the identical scattering planes are oriented perpendicular to the surface.
The electron has gone through both slits

Originally performed by Young (1801) to demonstrate the wave-nature of light. Has now been done with electrons, neutrons, He atoms among others.

For particles we expect two peaks, for waves an interference pattern
Soccer Balls Diffract

Neutrons, A Zeilinger et al. 1988 Reviews of Modern Physics 60 1067-1073


C_{60} molecules: M Arndt et al. 1999 Nature 401 680-682

Fringe visibility decreases as molecules are heated. L. Hackermüller et al. 2004 Nature 427 711-714

Interference patterns can not be explained classically - clear demonstration of matter waves

http://www.quantum.univie.ac.at/research/c60/
DOUBLE-SLIT EXPERIMENT WITH HELIUM ATOMS


Path difference: $d \sin \theta$

Constructive interference: $d \sin \theta = n\lambda$

Separation between maxima: $(proof\ following)$ $\Delta y = \frac{\lambda D}{d}$

Experiment: He atoms at 83K, with $d=8\mu m$ and $D=64cm$

Measured separation: $\Delta y = 8.2\mu m$

Predicted de Broglie wavelength:

\[
K = \frac{3kT}{2}, \quad \text{Mass} = 4m_u
\]

\[
\lambda = \frac{h}{\sqrt{3MKT}} = 1.03 \times 10^{-10}\ m
\]

Predicted separation: $\Delta y = 8.4 \pm 0.8\mu m$

Good agreement with experiment

FRINGE SPACING IN DOUBLE-SLIT EXPERIMENT

Maxima when: $d \sin \theta = n\lambda$

$D \gg d$ so use small angle approximation

$\theta \approx \frac{n\lambda}{d}$

$\Rightarrow \Delta \theta \approx \frac{\lambda}{d}$

Position on screen: $y = D \tan \theta \approx D \theta$

So separation between adjacent maxima:

$\Delta y \approx D \Delta \theta$

$\Rightarrow \Delta y = \frac{\lambda D}{d}$
DOUBLE-SLIT EXPERIMENT
INTERPRETATION

- The flux of particles arriving at the slits can be reduced so that only one particle arrives at a time. Interference fringes are still observed!
- Wave behaviour can be shown by a single atom.
- Each particle goes through both slits at once.
- A matter wave can interfere with itself. Hence matter-waves are distinct from H_2O molecules collectively giving rise to water waves.
- Wavelength of matter wave unconnected to any internal size of particle. Instead it is determined by the momentum.
- If we try to find out which slit the particle goes through the interference pattern vanishes!
  - We cannot see the wave/particle nature at the same time
  - If we know which path the particle takes, we lose the fringes.

The importance of the two-slit experiment has been memorably summarized by Richard Feynman: “…a phenomenon which is impossible, absolutely impossible, to explain in any classical way, and which has in it the heart of quantum mechanics. In reality it contains the only mystery.”

DOUBLE-SLIT EXPERIMENT
BIBLIOGRAPHY

Some key papers in the development of the double-slit experiment during the 20th century:

- Performed with a light source so faint that only one photon exists in the apparatus at any one time
- Performed with electrons
  - C Jönsson 1961 Zeitschrift für Physik 161 454-474,
    (translated 1974 American Journal of Physics 42 4-11)
- Performed with single electrons
  - A Tonomura et al. 1989 American Journal of Physics 57 117-120
- Performed with neutrons
  - A Zeilinger et al. 1988 Reviews of Modern Physics 60 1067-1073
- Performed with He atoms
- Performed with C60 molecules
  - M Arndt et al. 1999 Nature 401 680-682
- Performed with C70 molecules showing reduction in fringe visibility as temperature rises and the molecules “give away” their position by emitting photons
  - L. Hackermüller et al 2004 Nature 427 711-714
- Performed with Na Bose-Einstein Condensates
  - M R Andrews et al. 1997 Science 275 637-641

An excellent summary is available in Physics World (September 2002 issue, page 15) and at [http://physicsweb.org/](http://physicsweb.org/) (readers voted the double-slit experiment “the most beautiful in physics”).
A direct proof electron waves: The Davisson-Germer Experiment

Constructive interference of electrons scattered an array of surface atom at an angle $\phi$ is described by

$$dsin(\phi) = n\lambda \quad (3.32)$$

as found for X-ray!

Why surface atoms only?

HEISENBERG MICROSCOPE AND THE UNCERTAINTY PRINCIPLE

(also called the Bohr microscope, but the thought experiment is mainly due to Heisenberg).

The microscope is an imaginary device to measure the position ($y$) and momentum ($p$) of a particle.

Heisenberg

Resolving power of lens:

$$\Delta y \geq \frac{\lambda}{\theta}$$
HEISENBERG MICROSCOPE (cont)

Photons transfer momentum to the particle when they scatter.

Magnitude of $p$ is the same before and after the collision. Why?

Uncertainty in photon y-momentum
\[ -p \sin(\theta/2) \leq p_y \leq p \sin(\theta/2) \]

Small angle approximation
\[ \Delta p_y = 2p \sin(\theta/2) \approx p \theta \]

de Broglie relation gives $p = h/\lambda$ and so \[ \Delta p_y \approx \frac{h\theta}{\lambda} \]

From before \[ \Delta y \geq \frac{\lambda}{\theta} \] hence \[ \Delta p_y \Delta y \approx h \]

HEISENBERG UNCERTAINTY PRINCIPLE

Point for discussion

The thought experiment seems to imply that, while prior to experiment we have well defined values, it is the act of measurement which introduces the uncertainty by disturbing the particle’s position and momentum.

Nowadays it is more widely accepted that quantum uncertainty (lack of determinism) is intrinsic to the theory.
We will show formally (section 4)

\[
\Delta x \Delta p_x \geq \hbar / 2 \\
\Delta y \Delta p_y \geq \hbar / 2 \\
\Delta z \Delta p_z \geq \hbar / 2
\]

We cannot have simultaneous knowledge of ‘conjugate’ variables such as position and momenta.

Note, however, \( \Delta x \Delta p_y \geq 0 \) etc

Arbitrary precision is possible in principle for position in one direction and momentum in another.

There is a corresponding ‘spread’ in the emitted frequency.

An electron in \( n = 3 \) will spontaneously decay to a lower level after a lifetime of order \( \tau \sim 10^{-8} \) s

There is a corresponding ‘spread’ in the emitted frequency.
CONCLUSIONS

Light and matter exhibit wave-particle duality

Relation between wave and particle properties given by the de Broglie relations

\[ E = h\nu \quad p = \frac{h}{\lambda} \]

Evidence for particle properties of light
Photoelectric effect, Compton scattering

Evidence for wave properties of matter
Electron diffraction, interference of matter waves
(electrons, neutrons, He atoms, C60 molecules)

Heisenberg uncertainty principle limits simultaneous knowledge of conjugate variables

\[ \Delta x \Delta p_x \geq \frac{\hbar}{2} \]
\[ \Delta y \Delta p_y \geq \frac{\hbar}{2} \]
\[ \Delta z \Delta p_z \geq \frac{\hbar}{2} \]