0. INTRODUCTION

Quantum Mechanics (QM) is a radical generalisation of classical physics involving a new fundamental constant, *Planck's constant*,

$$\hbar = h/2\pi \approx 1.05\times10^{-34}\,\mathrm{Js}\,,$$

with dimensions $[\hbar] = \mathrm{M\,L^2T^{-1}} = [\text{position}]\times[\text{momentum}] = [\text{energy}]\times[\text{time}]$.

Profound new features of QM include:

• *Quantisation*. Physical quantities such as energy may be restricted to discrete sets of values, or may appear only in specific amounts, called *quanta*.

• *Inadequacy of classical wave and particle models*. The classical concepts of particle and wave are both inadequate to describe the behaviour predicted by quantum mechanics. Quantum objects may show either particle-like or wave-like behaviour in some circumstances, but neither model suffices in general.

• *Probability and uncertainty*. Predictions in QM are fundamentally *probabilistic*. In general, carrying out the same experiment many times will not produce the same result, although we can predict the possible outcomes and their probabilities. There are limits to what can be asked about a physical system, even in principle. A famous example is the *Heisenberg uncertainty relation* for position and momentum.

Despite these radical changes, classical physics must be recovered in the limit $\hbar \to 0$ (which may require careful interpretation).

The following sections (0.1, 0.2 and 0.3) provide some physical background and summarise key experimental evidence for these novel features of QM. These are discussed further in the printed lecture notes.

0.1 Light Quanta

An electromagnetic (EM) wave, e.g. light, consists of quanta called *photons*. Photons can be regarded as particles with energy, E, and momentum, p, related to frequency, ν or ω, and wavelength, λ, or wavenumber, k, according to

$$E = h\nu = \hbar\omega\,,$$
$$p = h/\lambda = \hbar k\,.$$

From the wave equation (satisfied by each EM field component)

$$c = \omega/k = \nu\lambda \qquad \text{or} \qquad E = cp$$

and so the relations above are consistent with photons being particles of rest mass zero, moving with the speed of light, c.

Compelling evidence for the existence of photons is provided by the *photoelectric effect*. Consider (Fig. 1) light or EM radiation (γ) of frequency ω incident on a metal surface. For certain metals and suitable frequencies this results in the emission of electrons (e^-) and their maximum kinetic energy K can be measured.

Experiments find that (i) the rate at which electrons are emitted is proportional to the intensity of the radiation (the 'brightness' of the source); (ii) K depends linearly on ω but *not* on the intensity; (iii) for $\omega < \omega_0$, some critical value, *no* electrons are emitted, irrespective of the intensity.

These results are extremely hard to understand in terms of classical EM waves. However, they follow naturally from the assumption that the wave consists of photons, each with energy $E = \hbar\omega$, and with the intensity of the radiation proportional to the number of photons incident per unit time. Suppose that an electron is emitted as a result of absorbing a single photon with sufficiently high energy. If W is the minimum energy needed to liberate an electron from the metal then

$$K = \hbar\omega - W$$

is the maximum kinetic energy of an emitted electron if $\omega > \omega_0$, where $\omega_0 = W/\hbar$, and no emission is possible if $\omega < \omega_0$ (Fig. 2). Furthermore, the rate at which electrons are emitted will be proportional to the rate at which incident photons arrive, and hence the intensity.

The energy-frequency relation for photons was introduced by Planck and used to derive the *black body spectrum*. This is the distribution of energy with frequency for EM radiation in thermal equilibrium, a fundamental result in thermodynamics of far-reaching importance (understanding the *cosmic microwave background*, for example). Einstein then applied the energy-frequency relation to explain the photoelectric effect. Further conclusive evidence for photons as particles, including the momentum-wavelength relation, came from subsequent experiments involving *Compton scattering*.

Consider a photon of wavelength λ colliding with an electron that is stationary in the laboratory frame. Let λ' be the wavelength of the photon after the collision and θ the angle through which it is deflected. Treating the photon as a massless relativistic particle, conservation of four-momentum implies

$$\lambda' - \lambda = \frac{h}{m_e c}(1 - \cos\theta)$$

This dependence of the change in wavelength (or decrease in energy) on the scattering angle θ can be verified experimentally (for X-rays or γ-rays, for instance).

0.2 The Bohr Model of the Atom

The *Rutherford model* of the atom was proposed to explain the results of scattering experiments (e.g. alpha particles scattered by gold foil). The key assumption is that most of the mass of the atom is concentrated in a compact, positively-charged *nucleus* (subsequently understood to consist of protons and neutrons), with light, negatively-charged electrons orbiting around it. The simplest case is the Hydrogen atom, in which a single electron with charge $-e$ and mass m_e orbits a nucleus consisting of a single proton with charge $+e$ and mass m_p. Since $m_p \gg m_e$ it is a good approximation to assume that the proton is stationary, at the origin, say. The electron and proton interact via Coulomb's Law: the potential energy of the electron and the force it experiences are

$$V(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}\,, \qquad \mathbf{F}(\mathbf{r}) = -\nabla V = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r^2}\,\hat{\mathbf{r}}\,.$$

The classical equations of motion for the electron imply that its angular momentum, $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, and its total energy,

$$E = \frac{1}{2}m_e v^2 - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}\,,$$

are constant. The orbits are therefore planar and they can be determined exactly. For any value of $E < 0$ there is a closed orbit and the electron is *bound* to the proton to form a Hydrogen atom. For orbits with $E > 0$ the electron eventually escapes to infinity: it is not bound to the proton.

Despite its success in accounting for Rutherford scattering, this model has a number of problems. The treatment is identical, mathematically, to planetary orbits governed by gravity (see Part IA Dynamics and Relativity, for example) but an important additional feature of electromagnetism has been left out. An accelerating charge radiates energy (carried away via EM fields) and this means that the electron would actually spiral inwards towards the proton: this is not a good model of a stable atom!

There is also experimental evidence for complex discrete structure within atoms. This comes from *line spectra*: bright emission lines (from a hot sample) or dark absorption lines (if radiation is passed through a cooler sample), both occurring at certain characteristic wavelengths or frequencies. This suggests that an atom can emit or absorb radiation only at these particular frequencies or wavelengths, which correspond to photons with particular energies.

The *Bohr model* restricts the classical orbits of the Rutherford model by postulating that the angular momentum of the electron obeys the *Bohr quantisation condition*:

$$L = n\hbar\,, \qquad n = 1, 2, \ldots\,,$$

with only these discrete values allowed. This might seem to be an unsatisfactory way to address the issue of stability, but it proves to be remarkably successful in reproducing the complex experimental data relating to line spectra.

Specialising to circular orbits (Fig. 4), for simplicity, we have

$$F = m_e v^2/r \qquad \text{and} \qquad L = m_e r v\,.$$

It is then straightforward to check that the quantisation condition leads to the following set of *Bohr orbits*:

$$r_n = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}\,n^2\,, \qquad v_n = \frac{e^2}{4\pi\epsilon_0\hbar}\frac{1}{n}\,, \qquad E_n = -\tfrac{1}{2}m_e\Big(\frac{e^2}{4\pi\epsilon_0\hbar}\Big)^2\frac{1}{n^2}\,, \qquad n = 1, 2, \ldots\,.$$

Note that the allowed energy levels are now discrete.

Suppose that an electron makes a transition between levels n and n' (with $n' > n$, say) accompanied by emission or absorption of a photon of frequency ω (Fig. 5). Then

$$\hbar\omega \;=\; E_{n'} - E_n \;=\; \tfrac{1}{2}m\Big(\frac{e^2}{4\pi\epsilon_0\hbar}\Big)^2\Big(\frac{1}{n^2} - \frac{1}{n'^2}\Big)\,.$$

This formula accounts for a vast amount of experimental data on spectral lines for Hydrogen. The Bohr model also provides an estimate for the *size* of the Hydrogen atom $r_1 \approx 5.29\times10^{-11}\,\mathrm{m}$, the *Bohr radius*. Despite these considerable successes, the origin of the Bohr quantisation condition seems obscure. A better explanation is needed.

0.3 Matter Waves

The relations used to associate particle properties (E and p) to waves can also be used to associate wave properties (ν or ω and λ or k) to particles. This applies not just to relativistic photons but also to non-relativistic particles, electrons for example, and λ is called the *de Broglie wavelength* of the particle. A strong hint that this might be important for a better understanding of the Bohr quantisation condition comes from observing that for a circular orbit

$$L = rp = n\hbar \qquad \Longleftrightarrow \qquad n\lambda = 2\pi r\,.$$

The Bohr condition therefore says that the circumference of the orbit is exactly an integral number of de Broglie wavelengths (e.g. $n = 3$ in Fig. 6).

It can also be verified experimentally that electrons do indeed exhibit wave-like behaviour, and a helpful idealisation is the *double slit experiment*, discussed in the printed lecture notes.

Some Constants and Units

- Planck's Constant: $\hbar = 1.05\times10^{-34}$ Js , or $h = 2\pi\hbar = 6.63\times10^{-34}$ Js
- Speed of light: $c = 3.00\times10^{8}$ ms^{-1} ; Wavelength of visible light (approx) 4×10^{-7}m to 7×10^{-7}m
- Unit of electric charge: $e = 1.60\times10^{-19}$ C ; Unit of energy: electron-volt, 1 eV $= 1.60\times10^{-19}$ J
- Fine structure constant: $\alpha = e^2/4\pi\epsilon_0\hbar c \approx 1/137$ (dimensionless)
- Electron mass: $m_e = 9.11\times10^{-31}$ kg ; Proton mass: $m_p = 1.67\times10^{-27}$ kg
- Bohr radius: $r_1 = 4\pi\epsilon_0\hbar^2/m_e e^2 = \hbar/m_e c\alpha = 5.29\times10^{-11}$ m

Wave Behaviour

We will refer to any real or complex valued function with periodicity in time and/or space as a *wave*. The following remarks summarise a few useful definitions and ideas.

- A function of time t obeying $f(t+T) = f(t)$ has *period* T, *frequency* $\nu = 1/T$, and *angular* or *circular frequency*

$$\omega = 2\pi\nu = 2\pi/T \ .$$

Familiar examples are $f(t) = \cos\omega t$, $\sin\omega t$ or $\exp\pm i\omega t$. It is also customary to refer to ω as the frequency, provided this leads to no confusion.

A function of position x (in one dimension) obeying $f(x+\lambda) = f(x)$ has *wavelength* λ and *wavenumber*

$$k = 2\pi/\lambda$$

Examples are $f(x) = \cos kx$, $\sin kx$ or $\exp\pm ikx$. The analogous functions of a position vector $\mathbf{x}$ with periodicity in three dimensions are $f(\mathbf{x}) = \exp i\mathbf{k}\cdot\mathbf{x}$ where $\mathbf{k}$ is the *wave vector*, and the wavelength is then $\lambda = 2\pi/|\mathbf{k}|$. We shall refer to such functions as *plane waves*.

- The wave equation in one dimension for a function $f(x,t)$ is

$$\frac{\partial^2 f}{\partial t^2} - c^2\frac{\partial^2 f}{\partial x^2} = 0$$

where c is some constant. This has solutions which are periodic in both position and time:

$$f_\pm(x,t) \ = \ A_\pm \exp(\ \pm ikx - i\omega t\ ) \qquad (*)$$

provided that the wavelength and frequency are related by

$$\omega = ck \qquad \text{or} \qquad \lambda\nu = c \ .$$

Such solutions represent waves which move or *propagate* with speed c to the right or left, according to the sign in $(*)$ (assuming ω, $k > 0$). The constant $A_\pm$ is the *amplitude* of the wave.

In electromagnetic (EM) waves, the field components obey the three dimensional wave equation, obtained by replacing $\partial^2/\partial x^2$ by ∇^2 above. This has solutions of an analogous form

$$f(\mathbf{x},t) \ = \ A\exp(\ i\mathbf{k}\cdot\mathbf{x} \ - \ i\omega t\ ) \qquad \text{with} \qquad \omega = c|\mathbf{k}| \ .$$

Such a wave propagates in the direction of $\mathbf{k}$, with speed c, now the speed of light.

- Other kinds of waves arise as solutions of other *governing equations* which may differ significantly from the standard wave equation. A function does not have to satisfy the standard wave equation in order to be usefully thought of as a wave! The *Schrödinger Equation* is one example of an alternative governing equation; it is the central equation in QM and we will study it in some depth. (In other physical applications, e.g. waves in real fluids, we should expect the wave equation to be modified by friction or dissipative terms.)

• Many different governing equations give rise to propagating solutions of the form $(*)$, provided the frequency is chosen to be a suitable function of the wavenumber, $\omega(k)$. Moreover, if the governing equation is *linear* in f, then any solutions f_1 and f_2 can be combined to give a new solution:

$$f = f_1 + f_2$$

This is the *Principle of Superposition* and it is responsible for much behaviour we tend to think of as *wave-like*.

• *Interference* or *diffraction* occurs when waves from different sources merge, or when parts of a wave recombine after passing around or through some obstacle. When a number of such waves are superposed, they may interfere *constructively*, increasing the size of the amplitude, or *destructively*, diminishing the amplitude. The result is an interference or diffraction pattern which depends on the sources or the obstacles.

When light is passed through a number of narrow slits, the resulting diffraction pattern provides conclusive evidence that light is a wave. Passing higher energy waves, such as X-rays, through matter gives a way of determining the crystalline arrangement of atoms from the resulting diffraction patterns.

A Few Historical Highlights

• 1801-03: Interference/diffraction experiments by Young show that light is a wave

• 1862-4: Maxwell identifies light as an EM (electromagnetic) wave

• 1897: Thompson discovers the electron, the first elementary particle

• 1900: Planck introduces the energy-frequency relation, with h as a new physical constant, and derives the *black body spectrum* (the distribution of energy with frequency for EM radiation in thermal equilibrium)

• 1905: Einstein imparts clearer physical meaning to photons, using them to explain the *photoelectric effect*, and other experimental results

• 1909: In a version of the double slit experiment, G.I. Taylor demonstrates that light produces a wave-like interference pattern on photographic film even when the light source is filtered so that only one photon at a time is recorded by the film.

• 1911: Based on scattering experiments, Rutherford proposes a model of the atom with most of its mass concentrated in a small, compact *nucleus*

• 1913: Bohr proposes an atomic model with electrons orbiting a nucleus and with quantisation of their angular momentum, using this to derive observed line spectra

• 1923: Compton scattering of X-rays on electrons confirms that photons are relativistic particles of zero rest mass

• 1923-24: de Broglie proposes *wave-particle duality* for matter, as for radiation

• 1925-30: The emergence of *Quantum Mechanics*, through work of Heisenberg, Born, Jordan, Dirac, Pauli, Schrödinger, and others

• 1927-28: Diffraction experiments of Davisson, Germer and Thompson confirm that electrons behave as waves as well as particles

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