

### 1 MOTIVATION

At the turn of the 20<sup>th</sup> century a number of landmark experiments revealed the limitations of classical physics. In order to explain these experiments a new framework was needed: Quantum Mechanics. **The photoelectric effect**, i.e. the emission of electrons from a material as light is shone onto it, was explained by Einstein in 1905 in terms of particles of light (photons) hitting the electrons and transferring energy to them. This contradicts the classical, wave-like picture of light (Maxwell). The energy  $E$  of such particles of light is related to their frequency  $\nu$  by the Planck-Einstein relation:

$$E = h\nu. \quad (1)$$

where  $h \approx 6.626 \times 10^{-34}$  Js is known as **Planck's constant**. This relation had actually been already suggested by Planck, who showed that the energy of the radiation emitted by a black body is quantized, with energy levels given by multiples of  $h\nu$ . It was also shown that photons carry a definite momentum (see **Compton effect**).

These discoveries led de Broglie to suggest that particles can display wave properties; the prominent example is the double-slit experiment, in which electrons are observed to interfere in a wave-like manner. The wavelength ( $\lambda$ ) of such matter-waves is given by the de Broglie relationship:

$$\lambda = \frac{h}{p} \quad (2)$$

where  $p$  is the particle's momentum. This idea opened the way to modern applications including **electron microscopy**.

The combined outcome of these experiments lead to the idea of a **wave-particle duality**, i.e. that objects can exhibit both wave- and particle-like properties, a fundamental pillar of Quantum Mechanics.

### 2 INTRODUCTION TO THE SCHRÖDINGER EQUATION

The Schrödinger equation is the most important equation in Quantum Mechanics. It encodes the full information about a given quantum mechanical system, and it contains all of the physical features described above. Schrödinger wanted to describe particles by an equation whose solution would be a wave. A standard form for writing a plane wave is, in complex notation,

$$\psi(x, t) = e^{i(kx - \omega t)}. \quad (3)$$

In terms of the **wavenumber**  $k \equiv 2\pi/\lambda$  and the angular frequency  $\omega \equiv 2\pi\nu$ . Using the relations in Section 1, we can express  $\omega$  and  $k$  in terms of the energy and momentum of the particle:

$$\psi(x, t) = e^{\frac{i}{\hbar}(px - Et)}. \quad (4)$$

where we defined the **reduced Planck constant**  $\hbar \equiv h/2\pi$ . The classical energy of a free particle is

$$E = \frac{p^2}{2m}. \quad (5)$$

We can reproduce this result from our wave solution [see *problem set 1*] if we postulate an equation of the form:

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) \quad (6)$$

The differential operator  $i\hbar \partial/\partial t$  returns the energy  $E$  by 'operating' on  $\psi(x, t)$ , whereas  $-\hbar^2 \partial^2/\partial x^2$  returns the momentum. This is the first instance of **operators** we encounter in Quantum Mechanics. They are used extensively, and we'll learn more about them in the third lecture.

For a particle in a potential  $V$ , the energy is given by:

$$E = \frac{p^2}{2m} + V \quad (7)$$

Incorporating this additional term in our wave equation gives the full **time-dependent Schrödinger equation**,

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + V\psi(x, t) \quad (8)$$

### 3 WAVEFUNCTIONS

Solutions  $\psi(x, t)$  to the Schrödinger equation (or linear combinations thereof) are known as **wavefunctions**. Wavefunctions are complex-valued objects which encode the full information of a given quantum system, but they don't have a direct physical interpretation on their own. However, their modulus squared can be interpreted as a probability density, such that the probability of finding a particle between two points  $A$  and  $B$  is given by:

$$\int_A^B |\psi(x, t)|^2 dx. \quad (9)$$

More generally, physical observables can be extracted from the wavefunction by the action of **operators** on it. We have seen two examples of these objects, the position and momentum operators, when introducing the Schrödinger equation. Operators are conventionally indicated by a hat, e.g.  $\hat{O}$ . The expectation value of a given operator  $\hat{O}$  is computed as:

$$\langle \hat{O} \rangle = \int \psi(x, t)^* \hat{O} \psi(x, t) dx. \quad (10)$$

Operators corresponding to physical observables must have real expectation values.

### 4 THE UNCERTAINTY PRINCIPLE

Free particles are described by plane waves, which, through the de Broglie relation Eq. (2), are characterised by a well-defined momentum. However, plane waves are spread out over all space. Localised solutions to the Schrödinger equation can be constructed

by **superposing** (i.e. combining) plane waves with different wavelengths. By the de Broglie relation, the fact that such wavefunctions contain plane waves having many wavelengths means that they don't have a well-defined momentum but, rather, they contain a spread of momentum values. The extreme case is a wavefunction fully localized at one point in space, described by a delta function  $\delta(x)$ . This function can be constructed by superposing plane waves with all wavelengths, and thus is characterized by a uniform distribution of momenta. Physical solutions of the Schrödinger equation lie between the two extremes of the plane wave and the delta function and thus have finite width in position space as well as finite spread of momentum values. Position and momentum distributions are related by a mathematical operation known as the **Fourier Transform**. This is illustrated in Figure 1 by showing the distributions of position and momentum values for three different Gaussian wavefunctions, characterized by different standard deviations  $\sigma$ .

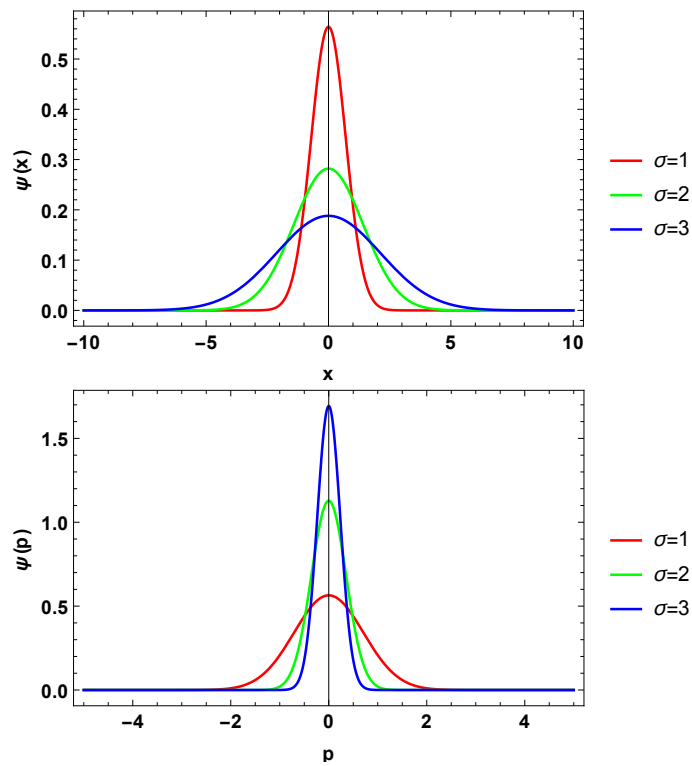


Figure 1: Illustration of the uncertainty principle in position (top) and momentum (bottom) space.  $\psi(p)$  is the momentum-space representation of the wavefunction; it is computed by Fourier-transforming  $\psi(x)$  and its modulus squared has an analogue interpretation as a probability density for momentum.

We notice that the distribution of momentum values becomes broader as the wavefunction becomes more and more localised. This is a general feature in Quantum Mechanics which is captured by the Heisenberg uncertainty principle:

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \quad (11)$$

Where  $\Delta x$  is the uncertainty in position which can be interpreted as the width in the position distribution, and similarly for momentum.

## APPENDIX

### A: The photoelectric effect

Electrons are emitted when certain materials are illuminated by light. However, the properties of this current are at odds with a classical, wave-like picture of light: the number of emitted electrons is proportional to the intensity of the light, but their maximum individual energy is actually proportional to its frequency; furthermore, there is no emission of electrons below a certain frequency of the light. This was explained by Einstein who postulated that light is made of discrete quanta (**photons**), which carry definite energy and momentum. For light of frequency  $\nu$  the energy of a photon is given by:

$$E = h\nu. \quad (12)$$

The emission can only happen if the energy of the incoming photon overcomes the minimum binding energy felt by an electron, known as the work function  $W$ . This gives rise to an energy and frequency threshold under which no electrons will be emitted. This behaviour is captured by Einstein's formula:

$$E_{kin} = (h\nu - W), \quad (13)$$

where  $E_{kin}$  is the maximum kinetic energy of the outgoing electrons, which has to be positive and thus determines the threshold frequency  $\nu_t = W/h$ .

### B: Recommended Links

- A java applet which illustrates many of the above ideas including the uncertainty principle, wavefunctions and much more:

<http://www.falstad.com/qm1d/>