

**PHYS20101**  
**Introduction to Quantum Mechanics**

**SUMMARY OF IMPORTANT CONCEPTS**

**The following is a summary originally prepared by A C Phillips, adapted by G D Lafferty, A J Bray and W R Flavell**

**QUANTUM WAVEFUNCTIONS**

- Particle and wave properties are described by a wavefunction  $\Psi$  which ebbs and flows in accordance with the time-dependent Schrödinger equation (TDSE),

$$\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

where  $\hat{H}$  is the ‘energy operator’, usually called the Hamiltonian operator.

- $|\Psi|^2$  is a probability density for position.

In one dimension,

$P(x,t)dx = |\Psi(x,t)|^2 dx =$  the probability of finding  
the particle at time  $t$  between  $x$  and  $x + dx$

- If you look everywhere, you will be certain to find the particle.  $\Psi$  is normalised at all times  $t$  such that, integrated over all space, the probability of finding the particle is unity.

In one dimension:

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = 1$$

## QUANTUM STATES

Wavefunctions represent the possible states of motion of real particles. They bear only a passing resemblance to the well-defined particle trajectories encountered in classical physics, and are called quantum states (QS).

- A QS provides precise predictions for the probabilities of the results of measurements.
- In the absence of measurements, a QS evolves deterministically in accordance with the time-dependent Schrödinger equation.
- Any linear superposition of solutions of the TDSE is also a solution. (This is not true of superpositions of solutions of the time-independent Schrödinger equation (TISE) unless they have the same energy, *i.e.* they are degenerate.)
- A QS is fragile. A measurement destroys it and replaces it by a new quantum state which is compatible with the outcome of the measurement.
- However, we still do not understand the link between the statistical nature of some of the predictions of quantum mechanics and the certainties we measure in the macroscopic world.

## QUANTUM EVOLUTION

- Time evolution is governed by the TDSE

$$\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t}.$$

- If the QS is a state of certain energy  $E$ , then

$$\Psi = \psi e^{-iEt/\hbar},$$

where  $\psi$  satisfies the TISE

$$\hat{H}\psi = E\psi,$$

and all observable properties are constant in time, Such a state is called a stationary state.

- If the QS is a state of uncertain energy with normalised wavefunction given by

$$\Psi = c_1\psi_1 e^{-iE_1t/\hbar} + c_2\psi_2 e^{-iE_2t/\hbar},$$

an energy measurement results in  $E_1$  with probability  $|c_1|^2$  or  $E_2$  with probability  $|c_2|^2$ , and observable properties oscillate with a period  $2\pi\hbar/|E_2 - E_1|$ .

Thus if the QS is a state of uncertain energy  $\Delta E$ , the timescale ( $\delta t$ ) for change of observable properties is of the order  $\delta t \cdot \Delta E \approx \hbar$ .

## QUANTUM MECHANICAL TUNNELLING

- If a quantum particle is subject to a confining potential  $V$ , there is a finite probability of finding the particle in classically forbidden regions (where  $E < V$ ) unless the confining potential is infinite.
- A particle may thus ‘tunnel’ through a thin barrier of thickness  $a$  with a tunnelling probability that depends upon  $e^{-2\beta a}$ , where  $\beta = \frac{\sqrt{2m(V - E)}}{\hbar}$ .

Hence the wavefunction decays exponentially in the classically forbidden barrier region.

## QUANTUM OBSERVABLES

A measurable quantity or observable,  $A$ , is represented in quantum mechanics by an operator  $\hat{A}$ .

In general, the outcome of a measurement of  $A$  is uncertain:

- For a system in the state  $\Psi(x,t)$ , the expectation value of  $A$  is

$$\langle A \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t) \hat{A} \Psi(x,t) dx$$

- The expectation value of  $A^2$  is

$$\langle A^2 \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t) \hat{A}^2 \Psi(x,t) dx$$

- The uncertainty in the outcome is

$$\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$$

Sometimes the outcome is certain:

- If the quantum state is an eigenstate of  $\hat{A}$ ,

$$\Psi = \psi_n \text{ where } \hat{A}\psi_n = A_n\psi_n,$$

the outcome is equal to the eigenvalue  $A_n$ .

## QUANTUM COMPATIBILITY

When are observables  $A$  and  $B$  compatible?

- Physically, if we can know both precisely at the same time.
- Mathematically, if the commutator  $[\hat{A}, \hat{B}]$  is zero, so that there exists a complete set of QS's with certain values for both  $A$  and  $B$ .

Examples

- Position and momentum are incompatible because

$$[\hat{x}, \hat{p}] = i\hbar$$

- The  $x$  and  $y$  components of angular momentum are incompatible because

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$

- The  $z$  component of angular momentum and its magnitude are compatible because

$$[\hat{L}^2, \hat{L}_z] = 0$$

## ANGULAR MOMENTUM IN QUANTUM MECHANICS

- Orbital angular momentum has uncertain direction. At best, the magnitude and only one component can be determined with certainty.
- For a particle moving in a central potential  $V(r, \theta, \phi) = V(r)$ , angular momentum is conserved.
- In such systems, the separable wavefunction  $\psi(r, \theta, \phi) = R(r)Y_{l, m_l}(\theta, \phi)$  is an eigenfunction of certain  $L^2$  and  $L_z$ , but uncertain  $L_x$  and  $L_y$ .
- The eigenvalues  $L^2$  and  $L_z$  are quantised:

$$L^2 = l(l+1)\hbar^2$$

$$L_z = m_l \hbar$$

where  $l = 0, 1, 2, \dots$  and, for a given  $l$ :

$$m_l = -l, -(l-1), \dots, 0, \dots, l-1, l$$

*i.e.*  $|m_l| \leq l$ ;  $m_l$  is an integer

$l$  is called the ‘orbital angular momentum quantum number’ (or just ‘orbital quantum number’).

$m_l$  is the ‘azimuthal angular momentum quantum number’ (or just ‘azimuthal quantum number’).

- The eigenfunctions have specific angular shape. For example,

$$Y_{1,1} = -\sqrt{\frac{3}{8\pi}} \sin\theta e^{+i\phi}, \quad Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos\theta, \quad Y_{1,-1} = \sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\phi}$$

## QUANTUM STATES IN A CENTRAL POTENTIAL

For a particle in a central potential:

- There exist eigenfunctions with certain  $E$ ,  $L^2$  and  $L_z$  of the form

$$\psi(r, \theta, \phi) = \frac{U(r)}{r} Y_{l, m_l}(\theta, \phi)$$

where the radial wavefunction  $R(r)$  is given by  $U(r)/r$ .

- For a system such as an atom, where the central potential is a Coulomb potential, the possible energies,  $E$ , for each value of the orbital angular momentum quantum number,  $l$ , are found by solving the radial TISE,

$$\left[ -\frac{\hbar^2}{2m_e} \frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2m_e r^2} - \frac{e^2}{4\pi\epsilon_0 r} \right] U(r) = EU(r),$$

where  $\frac{l(l+1)\hbar^2}{2m_e r^2}$  is the 'centrifugal potential',

subject to the boundary conditions  $U(r)=0$  at  $r=0$  and at  $r=\infty$ .

- The allowed energies of bound state solutions depend only on the value of the principal quantum number,  $n$ , as  $E_n \propto -1/n^2$ .  $n$  has values  $(l+1)$ ,  $(l+2)$ ,  $(l+3)$ ....., hence  $n=1, 2, 3, \dots, \infty$ . The maximum value of  $l$  is thus  $(n-1)$ .
- The complete wavefunctions for the hydrogen atom have the form

$$\psi_{n, l, m_l}(r, \theta, \phi) = \text{constant} \times r^l e^{-r/na_0} \sum_{k=0}^{n-l-1} (-1)^k c_k \left( \frac{r}{a_0} \right)^k \times P_{l, m_l}(\theta) \times e^{im_l \phi}$$

where  $P_{l, m_l}(\theta)$  are the associated Legendre polynomials

and the polynomials in  $r/a_0$  are known as the associated Laguerre polynomials.

The index  $n-l-1$  corresponds to the number of nodes in the radial part of the wavefunction.