QUANTUM MECHANICS

Fayyazuddin

Riazuddin

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Fayyazuddin
King Abdulaziz University

Riazuddin
King Fahd University of Petroleum and Minerals

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PREFACE

Quantum Mechanics was discovered in 1920's to explain the stability of atom. It is undoubtedly one of the greatest achievements in theoretical physics in the century. It is the basic theory for atomic and subatomic phenomena.

The concepts of quantum theory are radically different from the classical theory, which describes the everyday phenomena successfully. The quantum mechanical concepts are described in mathematical language. This is the approach we have followed in this book. We, however, do not assume any advanced knowledge of mathematics. The knowledge of differential and integral calculus and familiarity with matrices are sufficient to understand this book. The mathematics needed beyond this is developed in the text.

We have tried to keep the presentation well motivated and to provide sufficient details in order to facilitate the understanding of the subject. Our emphasis is on the basic theory rather than on specific applications in atomic, molecular, solid state and nuclear physics.

The book could be divided into 3 semester courses. Chapters 1–7, Chapter 8 (Secs. 1–7) and Chapter 12 (Secs. 1–2) could form one semester undergraduate course. Chapter 8 (Secs. 8–13), Chapter 9, Chapter 10 (Secs. 1–3), Chapter 11 (Secs. 1–5), Chapter 12 (Sec. 4), Chapters 13 and 14 should be suitable for the second semester undergraduate course. The rest of the sections and chapters could form one semester graduate course.

This book is based on course of lectures which we have given at the Punjab University, Lahore, The Quaid-I-Azam University, Islamabad, The King Fahd University of Petroleum and Minerals, Dhahran(R), The King Saud University, Riyadh(F) and the Ummal-Qura University, Makkah Al-Mukarramah(F) at various times. In fact we have been encouraged by our students to write these lectures in a book form. We would like to express our thanks to them and acknowledge the respective universities for their support.

In particular we are grateful to our former students Dr. M. M. Ilyas and especially Dr. Sajjad Mahmood for help in preparing this book for publication. We are grateful to our colleagues Dr. Fahim Hussain and Dr. Pervais Hoodbhouy for reading the first draft of the manuscript and for some useful suggestions.

We also wish to express our thanks to Mr. Shbahat Ullah Khan for typing the first draft of the manuscript.

We were first introduced to this subject by Prof. Abdus Salam. We would like to take this opportunity to express our deep sense of gratitude to him for the encouragement throughout our careers.

Fayyazuddin
Riazuddin

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Chapter 1

BREAKDOWN OF CLASSICAL CONCEPTS

1.1 Introduction

Quantum mechanics is the theory which describes phenomena on the atomic and molecular scale. An event in this domain is not visible to the human eye. The concepts of classical physics which have been developed to describe phenomena on the macroscopic scale may not be applicable for processes on the microscopic scale of dimensions 10^{-6} to 10^{-13} cm. There are, however, some macroscopic quantum systems, e.g. superfluids, superconductors, transistors and main sequence stars.

We first outline the concepts of classical theory and then describe how, for the microphysical world, the necessity for departure from classical physics is clearly shown by experimental results.

In classical physics, matter is treated in terms of particles of definite mass, and radiation is described as wave motion. The two great disciplines of classical physics are Newtonian Mechanics and Maxwell's theory. The former describes the motion of material particles according to Newton's Laws. Classical mechanics successfully describes the electrically neutral macroscopic systems. Energy E and momentum $\mathbf{p}$ of a particle are two important dynamical variables.

The electric and magnetic phenomena are described in terms of electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$ which satisfy Maxwell's equations

$$\operatorname{div}\mathbf{E} = 4\pi\rho \tag{1.1a}$$

$$\operatorname{curl}\mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} \tag{1.1b}$$

$$\operatorname{curl}\mathbf{B} = \frac{4\pi}{c}\mathbf{j} + \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t} \tag{1.1c}$$

$$\operatorname{div}\mathbf{B} = 0 .$$

Here ρ is the charge density and $\mathbf{j}$ is the electric current and they satisfy the continuity equation

$$\frac{\partial \rho}{\partial t} + \operatorname{div}\mathbf{j} = 0 . \tag{1.2}$$

In free space, $\mathbf{E}$ and $\mathbf{B}$ satisfy the wave equation

$$\left(\frac{1}{c}\frac{\partial^2}{\partial t^2} - \nabla^2\right)\mathbf{E}, \mathbf{B} = 0 . \tag{1.3}$$

A solution of this equation shows that $\mathbf{E}$ and $\mathbf{B}$ propagate through space as waves with speed c. For appropriate frequencies, these waves should be identified with visible light. The whole spectrum of radiation from extremely long wave length region of radio waves, through visible range, to extremely small wave length region of X-rays and γ-rays is described in terms of electromagnetic waves as given by Maxwell's theory.

1.2 Wave Packet

As we have seen, electromagnetic radiation is regarded as consisting of waves which propagate through space with velocity c. A typical wave in x-direction is expressed as:

$$\begin{aligned} \psi(x,t) &= Ae^{i(\frac{2\pi}{\lambda}x - 2\pi\nu t)} \\ \lambda &: \text{ wave length} \\ \tau &= 1/\nu : \text{periodic time } (\nu \text{ frequency}) \\ k &= \frac{2\pi}{\lambda} : \text{wave number} \\ \omega &= 2\pi\nu : \text{angular frequency} . \end{aligned} \tag{1.4}$$

k can be regarded as vector. A wave in 3 dimensions can be written as

$$\psi(\mathbf{r},t) = Ae^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)} . \tag{1.5}$$

We define a phase $\theta \equiv \mathbf{k} \cdot \mathbf{r} - \omega t$. A surface of constant phase is called a wave front. The velocity with which this surface moves is called the phase velocity. To calculate the phase velocity we note that θ is constant on this surface:

$$\frac{d\theta}{dt} = 0$$

or

$$\mathbf{k} \cdot \frac{d\mathbf{r}}{dt} - \omega = 0 \, .$$

This gives the phase velocity $[\mathbf{k} = |\mathbf{k}|\mathbf{n}]$

$$\mathbf{n} \cdot \mathbf{u} = \frac{\omega}{|\mathbf{k}|} = \nu\lambda \, . \tag{1.6}$$

We cannot send a signal in the form of a monochromatic wave. However, what we do, in practise, is to send a signal in the form of a wave packet or group of waves. The only velocity which can be experimentally measured is the group velocity which we define below. The wave packet can be generated by superposition of a number of simple harmonic waves with wave numbers centered round the mean wave number. Consider first the superposition of two waves

$$\begin{aligned}
\psi_1 &= Ae^{i(kx-\omega t)} \\
\psi_2 &= Ae^{i[(k+\Delta k)x-(\omega+\Delta\omega)t]} \\
\psi &= \psi_1 + \psi_2 \\
&= A\exp\left[i\left(\frac{2k+\Delta k}{2}x - \frac{2\omega+\Delta\omega}{2}\right)t\right] \\
&\qquad \times \exp\left[i\left(\frac{1}{2}\Delta kx - \frac{1}{2}\Delta\omega t\right)\right] + \exp\left[-i\left(\frac{1}{2}\Delta kx - \frac{1}{2}\Delta\omega t\right)\right] \\
&= A\underbrace{e^{i(kx-\omega t)}}_{\text{carrier wave}}\underbrace{2\cos\left(\frac{1}{2}(\Delta k)x - \frac{1}{2}(\Delta\omega)t\right)}_{\text{modulation}} ,
\end{aligned} \tag{1.7}$$

where we have put

$$\begin{aligned}
2k + \Delta k &\approx 2k \\
2\omega + \Delta\omega &\approx 2\omega \, .
\end{aligned}$$

The phase velocity as before is given by

$$u = \frac{\omega}{k} = \nu\lambda .$$

On the other hand, the maximum of the amplitude moves with velocity

$$v_g = \frac{\Delta\omega}{\Delta k} = \frac{\Delta\nu}{\Delta(1/\lambda)} . \tag{1.8}$$

This is the group velocity.

The wave length of modulation is given by

$$\lambda_m = \frac{2\pi}{\frac{1}{2}\Delta k} = \frac{4\pi}{\Delta k} . \tag{1.9}$$

The plot of Eq. (1.7) is shown in Fig. 1.1.

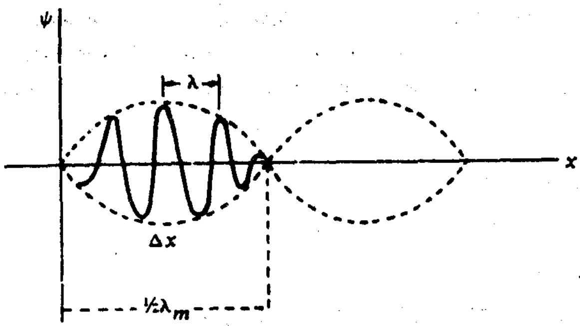

Fig. 1.1. The superposition of two simple harmonic waves of slightly different frequencies and wave numbers.

The width of the wave packet is evidently given by (half the wave length of the modulation)

$$\Delta x = \frac{1}{2}\lambda_m = \frac{2\pi}{\Delta k}$$

or

$$\Delta k \Delta x = 2\pi$$

or

$$\Delta k \Delta x > 1 . \tag{1.10}$$

In general, we can represent a wave packet (which is a superposition of monochromatic waves with wave numbers centered around the mean value k_0) as:

$$\psi(x,t) = \int_{-\infty}^{\infty} A(k)e^{i(kx-\omega(k)t)}dk \tag{1.11a}$$

$$\psi(x,0) = \int_{-\infty}^{\infty} A(k)e^{ikx}dk \tag{1.11b}$$

$$A(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \psi(x)e^{-ikx}dx\,. \tag{1.11c}$$

The wave packet is localised within a distance Δx and has a spread Δk in wave number as shown in Fig. 1.2. It can be shown by Fourier analysis that Δx and Δk are such that

$$\Delta x \Delta k \gtrsim 1\,.$$

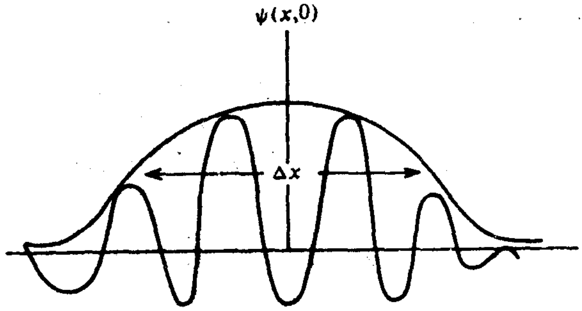

Fig. 1.2a. A wave packet pictured at $t = 0$.

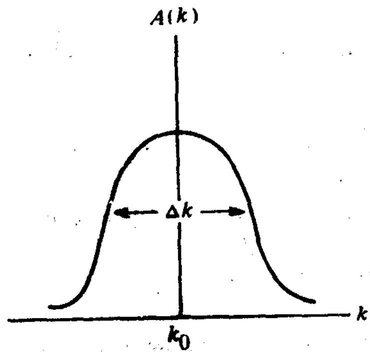

Fig. 1.2b. Picture of $A(k)$.

Since ω is a function of k, i.e.

$$\omega = \omega(k) \, , \tag{1.12}$$

in general there will be dispersion in the wave, the wave packet spreading out as it moves along. The range over which $A(k)$ is appreciably different from zero is

$$k_0 - \frac{1}{2}\Delta k \leq k \leq k_0 + \frac{1}{2}\Delta k \, . \tag{1.13}$$

To reduce the dispersion, we take

$$\Delta k \ll k_0 \, ,$$

and expand Eq. (1.12) around k_0:

$$\omega(k) = \omega(k_0) + \left(\frac{\partial \omega}{\partial k}\right)_{k_0} (k - k_0) + \dots \, . \tag{1.14}$$

Now let us rewrite Eq. (1.11b) in the following way

$$\begin{aligned} \psi(x,0) &= \int_{-\infty}^{\infty} A(k) e^{ik_0 x + i(k-k_0)x} dk \\ &= e^{ik_0 x} \int_{-\infty}^{\infty} A(k) e^{i(k-k_0)x} dk \end{aligned} \tag{1.15}$$

or

$$\psi(x) = e^{ik_0 x} X(x) \, , \tag{1.16}$$

where

$$X(x) = \int_{-\infty}^{\infty} A(k) e^{i(k-k_0)x} dk \tag{1.17}$$

is appreciably different from zero only in the range Δx. Now using Eq. (1.14) in Eq. (1.11a)

$$\begin{aligned} \psi(x,t) &\approx \int_{-\infty}^{\infty} A(k) e^{ik_0 x + i(k-k_0)x} e^{-i(\omega_0 t + v_g (k-k_0) t)} dk \\ &= e^{i(k_0 x - \omega_0 t)} \int_{-\infty}^{\infty} A(k) e^{i(k-k_0)(x - v_g t)} dk \\ &= e^{i(k_0 x - \omega_0 t)} X(x - v_g t) \, . \end{aligned} \tag{1.18}$$

The wave packet is composed of two factors: the first factor represents a wave of frequency $\omega_0/2\pi$ and wave length $2\pi/k_0$; the last factor describes