the derivation of the canonical commutation relations, and the generalised uncertainty relations. The main emphasis in these sections is on the basic mathematical framework, and therefore I have adopted a pragmatic, rather instrumentalist view of quantum theory that leaves open the question of what other types of interpretation are possible.

The interpretation of quantum theory is addressed in Chapter 8 where we turn to conceptual matters in a more formal way. The material is organised around four major topics: the meaning of probability, the role of measurement, reduction of the state vector, and quantum entanglement. These issues are of fundamental importance in any attempt to find a more realist interpretation of quantum theory: a key issue for anyone who, like myself, is interested in quantum cosmology. This challenge of realism is studied directly in the final chapter that deals with the status of 'properties' in quantum theory. The main topics discussed are the Kochen–Specker theorem, a short introduction to quantum logic, and the Bell inequalities.

The book concludes with a number of worked problems aimed at developing facility in the type of mathematical manipulations that are essential for any theoretical physicist who wants to use the vector space approach to quantum theory. Several worked problems are also included in the text proper as an aid to understanding various pieces of general formalism.

A quick note on references. The rather short bibliography reflects the origin of the book as lecture notes for an undergraduate course. For this reason, I have concentrated on citing papers and books that should be accessible to an advanced physics undergraduate and which, if dipped into, will genuinely enhance his or her understanding without needing a lifetime of study devoted to the task. As emphasised in the Preface, this is intended to be a short textbook for undergraduates—it is not meant to be a definitive review of modern quantum theory!

1.2 A Summary of Wave Mechanics

It is useful to begin by summarising some of the basic formalism of elementary wave mechanics. This will be presented, with the minimum of comment, in the form of four rules that will be generalised in Chapter 5 to apply to arbitrary quantum systems. For simplicity, I shall present the ideas for motion in one dimension; the extension to three dimensions is straightforward and involves no new principles. In writing these rules we recall the following:

- A number a is an *eigenvalue* of a differential operator $\hat{A}$ if it satisfies the differential equation

$$\hat{A}u(x) = au(x) \tag{1.1}$$

  plus appropriate boundary conditions on the function $u(x)$ (for example, that it be square-integrable[3]). The function $u(x)$ is said to be an *eigenfunction* of $\hat{A}$ associated with the eigenvalue a.

- A *self-adjoint* (or *hermitian*) operator $\hat{A}$ is one for which[4]

$$\int_{-\infty}^{\infty} (\hat{A}\psi)^*(x)\phi(x)\,dx = \int_{-\infty}^{\infty} \psi^*(x)(\hat{A}\phi)(x)\,dx \tag{1.2}$$

  for all square-integrable wave functions ψ and ϕ.

With this in mind, the four rules are as follows.

Rule 1. The quantum state of a point particle moving in one dimension is represented by a complex-valued wave function $\psi(x)$ that can be normalised to one:

$$\int_{-\infty}^{\infty} |\psi(x)|^2\,dx = 1. \tag{1.3}$$

A crucial idea in quantum theory is that any pair of wave functions ψ_1 and ψ_2 can be *superimposed* with arbitrary complex coefficients α_1 and α_2 to give a new wave function $\alpha_1\psi_1(x) + \alpha_2\psi_2(x)$ (provided that α_1 and α_2 are chosen such that this new function is normalised to one).

Rule 2. Any physical quantity that can be measured (*i.e.*, an observable) is represented by a linear differential operator that acts on the wave functions, and is self-adjoint.

[3]A function ψ is *square-integrable* if $\int_{-\infty}^{\infty} |\psi(x)|^2\,dx < \infty$.

[4]The symbol * denotes the complex conjugate.

Rule 3. (i) The only possible result of measuring an observable A is one of the eigenvalues of the self-adjoint operator $\widehat{A}$ that represents it.

(ii) Assume for simplicity that there is no degeneracy (*i.e.,* any two eigenfunctions of $\widehat{A}$ with the same eigenvalue are proportional to each other) and that $\widehat{A}$ has only a discrete set of eigenvalues $a_1, a_2, \ldots$, with corresponding eigenfunctions $u_1, u_2, \ldots$. Then, if the quantum state is $\psi(x)$, the probability that a measurement of A will yield a particular eigenvalue a_n is

$$\boxed{\mathrm{Prob}(A = a_n; \psi) = |\psi_n|^2} \tag{1.4}$$

where the complex numbers ψ_n are the coefficients in the expansion

$$\psi(x) = \sum_{n=1}^{\infty} \psi_n u_n(x) \tag{1.5}$$

of the wave function $\psi(x)$ as a linear combination of the (normalised) eigenfunctions of $\widehat{A}$.

Rule 4. The state function evolves in time according to the time-dependent Schrödinger equation

$$\boxed{i\hbar \frac{\partial \psi(x,t)}{\partial t} = \widehat{H}\psi(x,t)} \tag{1.6}$$

where the Hamiltonian operator $\widehat{H}$ is obtained from the classical energy expression

$$H = \frac{p^2}{2m} + V(x) \tag{1.7}$$

by replacing the momentum p and position x by their corresponding operators $\widehat{p}$ and $\widehat{x}$.

Comments

1. The eigenvalues and eigenfunctions of a self-adjoint operator have three crucial mathematical properties that are central to their use in quantum theory:

- The eigenvalues are *real* numbers (as they should be if they are to correspond to the results of measurements).
- The eigenfunctions form a *complete* set, *i.e.,* any wave function can be expanded uniquely as in Eq. (1.5).
- The normalised eigenfunctions satisfy the *orthogonality* condition

  $$\int_{-\infty}^{\infty} u_m^*(x) u_n(x)\, dx = \delta_{mn} \tag{1.8}$$

  where δ_{mn} is the Kronecker delta, defined to equal 1 if $m = n$, and 0 otherwise.

  One consequence is that the expansion coefficients ψ_n in Eq. (1.5) can be calculated explicitly from the wave function $\psi(x)$ as

  $$\psi_n = \int_{-\infty}^{\infty} u_n^*(x) \psi(x)\, dx. \tag{1.9}$$

  In particular, this shows that the expansion coefficients are *unique*.

It can be shown from these results that, for any pair of wave functions ψ and ϕ,

$$\int_{-\infty}^{\infty} \psi^*(x) \phi(x)\, dx = \sum_{n=1}^{\infty} \psi_n^* \phi_n \tag{1.10}$$

and hence, in particular,

$$\int_{-\infty}^{\infty} |\psi(x)|^2\, dx = \sum_{n=1}^{\infty} |\psi_n|^2. \tag{1.11}$$

Thus, if ψ is normalised as in Eq. (1.3), we see that

$$\boxed{\sum_{n=1}^{\infty} \mathrm{Prob}(A = a_n; \psi) = 1} \tag{1.12}$$

which is necessary for the probability interpretation to be consistent (the probability that *some* result is obtained for any measurement must be one).

2. The basic interpretative Rule 3 implies that the long term average value of the results of repeated measurements of an observable A is

$$\langle A\rangle_\psi = \int_{-\infty}^{\infty} \psi^*(x)(\widehat{A}\psi)(x)\,dx. \tag{1.13}$$

3. As they stand, the rules above are incomplete since they give no information on how to construct the actual operator that represents any specific observable for a given physical system. This is usually done by invoking the 'substitution rule' which says that the operator that represents the classical observable $A(x,p)$ is $A(\widehat{x},\widehat{p})$ (an ambiguous expression, as we shall see later). This has been invoked already in Rule 4 by requiring the quantum Hamiltonian operator to be given by operator substitution in Eq. (1.7).

However, the theoretical structure is still incomplete since no specification has been given of the operators $\widehat{x}$ and $\widehat{p}$. This is part of the far more general question of what it means to construct the 'quantum analogue' of any given classical system. In the context of elementary wave mechanics, this gap is filled by postulating the operators that represent position and momentum to be

$$(\widehat{x}\psi)(x) = x\psi(x) \tag{1.14}$$

$$(\widehat{p}\psi)(x) = -i\hbar\frac{d\psi}{dx}(x) \tag{1.15}$$

which satisfy the famous 'canonical commutation relation'

$$[\,\widehat{x},\widehat{p}\,] = i\hbar. \tag{1.16}$$

4. Angular momentum plays an important role in many different areas of quantum theory, and is treated in wave mechanics using the operators defined above. Specifically, the components of angular momentum in classical physics are $L_x = yp_z - zp_y$, $L_y = zp_x - xp_z$ and $L_z = xp_y - yp_x$, and it is assumed that the corresponding quantum operators are formed using the substitution rule, so that $\widehat{L}_x = \widehat{y}\widehat{p}_z - \widehat{z}\widehat{p}_y$, $\widehat{L}_y = \widehat{z}\widehat{p}_x - \widehat{x}\widehat{p}_z$ and $\widehat{L}_z = \widehat{x}\widehat{p}_y - \widehat{y}\widehat{p}_x$.

It is straightforward to show from Eq. (1.16) that the angular momentum operators have the commutation relations

$$[\,\widehat{L}_x,\widehat{L}_y\,] = i\hbar\widehat{L}_z \tag{1.17}$$

$$[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x \tag{1.18}$$
$$[\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y \tag{1.19}$$

which, in turn, imply that

$$[\hat{L}\cdot\hat{L}, \hat{L}_x] = [\hat{L}\cdot\hat{L}, \hat{L}_y] = [\hat{L}\cdot\hat{L}, \hat{L}_z] = 0, \tag{1.20}$$

where the total angular-momentum operator $\hat{L}\cdot\hat{L}$ is defined as the sum $\hat{L}_x\hat{L}_x + \hat{L}_y\hat{L}_y + \hat{L}_z\hat{L}_z$. The vanishing commutators of Eq. (1.20) mean that simultaneous eigenfunctions exist of $\hat{L}\cdot\hat{L}$ and any one[5] of $\hat{L}_x$, $\hat{L}_y$ or $\hat{L}_z$. For various psychological reasons, the usual choice is $\hat{L}_z$, with the z-axis being drawn pointing upwards.

One of the less gripping tasks in a course on wave-mechanics is to compute the explicit form of these simultaneous eigenfunctions, and to find their associated eigenvalues. The well-known result is that the eigenvalues of $\hat{L}\cdot\hat{L}$ have the form $\ell(\ell+1)\hbar^2$, where ℓ is an integer with $\ell \geq 0$. For any given value of ℓ, the associated eigenvalues of $\hat{L}_z$ are of the form $m\hbar$, where the integer m ranges from $-\ell$ to $+\ell$ in steps of 1. The corresponding simultaneous eigenfunctions u_{lm} are the famous *associated Legendre polynomials*.

1.3 Beyond Introductory Wave Mechanics

The rules and postulates of wave mechanics have been used widely, and with considerable empirical success. However, a number of subtle and important issues wait to be uncovered. For example:

- What is the precise meaning of 'probability' as it arises in the context of quantum theory? And why does 'measurement' play such a prominent role? Can a measurement be regarded as just another type of physical interaction, or does it need to be considered as a fundamental concept in the very foundations of the theory? If the latter is true, how can this be reconciled with the fact that real measuring devices are composed of atoms, which certainly need to be described in quantum-mechanical terms?

[5]It is only *one* of the operators $\hat{L}_x$, $\hat{L}_y$ or $\hat{L}_z$ since a simultaneous eigenfunction of, for example, the pair of operators $\hat{L}\cdot\hat{L}$ and $\hat{L}_z$ will generally *not* be a simultaneous eigenfunction of the pair $\hat{L}\cdot\hat{L}$ and $\hat{L}_x$, or the pair $\hat{L}\cdot\hat{L}$ and $\hat{L}_y$.