INTRODUCTORY QUANTUM MECHANICS

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PREFACE

This work has emerged from an undergraduate course in quantum mechanics which I have taught for the past number of years. The material divides naturally into two major components. In Part I, Chapters 1 to 8, fundamental concepts are developed and these are applied to problems predominantly in one dimension. In Part II, Chapters 9 to 14, further development of the theory is pursued together with applications to problems in three dimensions.

Part I begins with a review of elements of classical mechanics which are important to a firm understanding of quantum mechanics. The second chapter continues with a historical review of the early experiments and theories of quantum mechanics. The postulates of quantum mechanics are presented in Chapter 3 together with development of mathematical notions contained in the statements of these postulates. The time-dependent Schrödinger equation emerges in this chapter.

Solutions to the elementary problems of a free particle and that of a particle in a one-dimensional box are employed in Chapter 4 in the descriptions of Hilbert space and Hermitian operators. These abstract mathematical notions are described in geometrical language which I have found in most instances to be easily understood by students.

The cornerstone of this introductory material is the superposition principle, described in Chapter 5. In this principle the student comes to grips with the inherent dissimilarity between classical and quantum mechanics. Commutation relations and their relation to the uncertainty principle are also described, as well as the concept of a complete set of commuting observables. Quantum conservation principles are presented in Chapter 6.

Applications to important problems in one dimension are given in Chapters 7 and 8. Creation and annihilation operators are introduced in algebraic construction of the eigenstates of a harmonic oscillator. Transmission and reflection coefficients are obtained for one-dimensional barrier problems. Chapter 8 is devoted primarily to the problem of a particle in a periodic potential. The band structure of the energy spectrum for this configuration is obtained and related to the theory of electrical conduction in solids.

Part II begins with a quantum mechanical description of angular momentum.

Fundamental commutator relations between the Cartesian components of angular momentum serve to generate eigenvalues. These commutator relations further indicate compatibility between the square of total angular momentum and only one of its Cartesian components. It is through these commutator relations that a distinction between spin and orbital angular momentum emerges. Properties of angular momentum developed in this chapter are reemployed throughout the text.

In Chapter 10 the Schrödinger equation for a particle moving in three dimensions is analyzed and applied to the examples of a free particle, a charged particle in a magnetic field, and the hydrogen atom.

In Chapter 11 the theory of representations and elements of matrix mechanics are developed for the purpose of obtaining a more complete description of spin angular momentum. A host of problems involving a spinning electron in a magnetic field are presented. The theory of the density matrix is developed and applied to a beam of spinning electrons.

In Chapter 12 preceding formalisms are employed in conjunction with the Pauli principle, in the analysis of some basic problems in atomic and molecular physics. Also included in this chapter are brief descriptions of the quantum models for superconductivity and superfluidity.

Perturbation theory is developed in Chapter 13. Among the many applications included is that of the problem of a particle in a periodic potential, considered previously in Chapter 8. Harmonic perturbation theory is applied in Einstein's derivation of the Planck radiation formula and the theory of the laser. The text concludes with a brief chapter devoted to an elementary description of the quantum theory of scattering.

Problems abound throughout the text, and many of them include solutions. Figures are also plentiful and hopefully lend to the instructional quality of the writing. A small introductory paragraph precedes each chapter and serves to knit the material together. A list of symbols appears before the appendixes.

Interspersed throughout the text, especially in the problems, one finds concepts from other disciplines with which the student is assumed to have some familiarity. These include, for example: dynamics, thermodynamics, elementary relativity, and electrodynamics. This policy follows the spirit of one of my cherished late professors, Hartmut Kalman: "Physics is not a sausage that one cuts into little pieces."

I trust that a mastery of the concepts and their applications as presented in this work will form a solid foundation on which to build a more complete study of quantum mechanics.

Many individuals have been helpful in the preparation of this text. I remain indebted to these kind, patient, and well-informed colleagues: D. Heffernan, M. Guillen, E. Dorchak, D. Faulconer, G. Lasher, I. Nebenzahl, M. Nelkin, T. Fine,

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During visits at the Université Libre de Bruxelles and later at the Université de Paris XI–Centre d'Orsay, I was able to work on material related to this text. I am extremely grateful to Professor I. Prigogine and Professor J. L. Delcroix for the intellectual freedom accorded me during these occasions.

R. L. LIBOFF

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"By nature I am peacefully inclined and reject all doubtful adventures. But a theoretical interpretation had to be found at any cost, no matter how high. . . . I was ready to sacrifice every one of my previous convictions about physical laws."

Max Planck
commenting on
his derivation of
the radiation law

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Appendixes

PART I

ELEMENTARY PRINCIPLES AND APPLICATIONS TO PROBLEMS IN ONE DIMENSION

CHAPTER 1

REVIEW OF CONCEPTS OF CLASSICAL MECHANICS

This is a preparatory chapter in which we review fundamental concepts of classical mechanics important to the development and understanding of quantum mechanics. Hamilton's equations are introduced and the relevance of cyclic coordinates and constants of the motion is noted. In discussing the state of a system, we briefly encounter our first distinction between classical and quantum descriptions. The notions of forbidden domains and turning points relevant to classical motion, which find application in quantum mechanics as well, are also described. The experimental motivation and historical background of quantum mechanics are described in Chapter 2.

1.1 GENERALIZED OR "GOOD" COORDINATES

Our discussion begins with the concept of *generalized* or *good* coordinates.

A bead (idealized to a point particle) constrained to move on a straight rigid wire has *one degree of freedom* (Fig. 1.1). This means that only one variable (or parameter) is needed to uniquely specify the location of the bead in space. For the problem under discussion, the variable may be displacement from an arbitrary but specified origin along the wire.

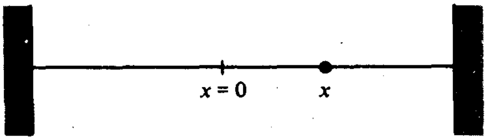

FIGURE 1.1 A bead constrained to move on a straight wire has one degree of freedom.

A particle constrained to move on a flat plane has two degrees of freedom. Two independent variables suffice to uniquely determine the location of the particle in space. With respect to an arbitrary, but specified origin in the plane, such variables might be the Cartesian coordinates (x, y) or the polar coordinates (r, θ) of the particle (Fig. 1.2).

Two beads constrained to move on the same straight rigid wire have two degrees of freedom. A set of appropriate coördinates are the displacements of the individual particles (x_1, x_2) (Fig. 1.3).

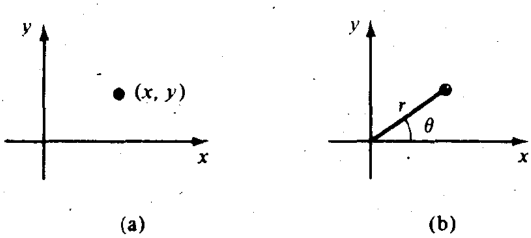

FIGURE 1.2 A particle constrained to move in a plane has two degrees of freedom. Examples of coordinates are (x, y) or (r, θ).

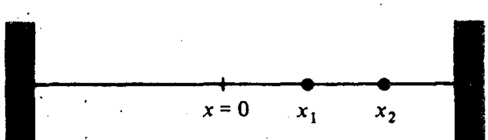

FIGURE 1.3 Two beads on a wire have two degrees of freedom. The coordinates x_1 and x_2 denote displacements of particles 1 and 2, respectively.

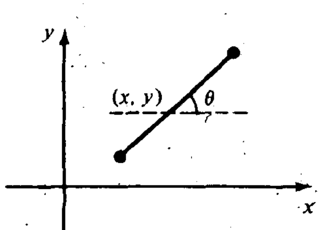

FIGURE 1.4 A rigid dumbbell in a plane has three degrees of freedom. A good set of coordinates are: (x, y), the location of the center, and θ, the inclination of the rod with the horizontal.

A rigid rod (or dumbbell) constrained to move in a plane has three degrees of freedom. Appropriate coordinates are: the location of its center (x, y) and the angular displacement of the rod from the horizontal, θ (Fig. 1.4).

Independent coordinates that serve to uniquely determine the orientation and location of a system in physical space are called *generalized* or *canonical* or *good* coordinates. *A system with N generalized coordinates has N degrees of freedom.* The orientation and location of a system with, say, three degrees of freedom are not specified until all three generalized coordinates are specified. The fact that *good* coordinates may be specified independently of one another means that given the values of all but one of the coordinates, the last coordinate remains arbitrary. Having specified (x, y) for a point particle in 3-space, one is still free to choose z independently of the assigned values of x and y.

PROBLEMS

1.1 For each of the following systems, specify the number of degrees of freedom and a set of good coordinates.

(a) A bead constrained to move on a closed circular hoop that is fixed in space.
(b) A bead constrained to move on a helix of constant pitch and constant radius.
(c) A particle on a right circular cylinder.
(d) A pair of scissors on a plane.
(e) A rigid rod in 3-space.
(f) A rigid cross in 3-space.
(g) A linear spring in 3-space.
(h) Any rigid body with one point fixed.
(i) A hydrogen atom.
(j) A lithium atom.
(k) A compound pendulum (two pendulums attached end to end).

1.2 Show that a particle constrained to move on a curve of any shape has one degree of freedom.

Answer

A curve is a one-dimensional locus and may be generated by the parameterized equations

$$x = x(\eta), \qquad y = y(\eta), \qquad z = z(\eta)$$

Once the independent variable η (e.g., length along the curve) is given, x, y, and z are specified.

1.3 Show that a particle constrained to move on a surface of arbitrary shape has two degrees of freedom.

Answer

A surface is a two-dimensional locus. It is generated by the equation

$$u(x, y, z) = 0$$