Advanced Quantum Theory

AN OUTLINE OF THE FUNDAMENTAL IDEAS

by

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Preface

Those who fall in love with practice without science are like a sailor who enters a ship without helm or compass, and who never can be certain whither he is going.

LEONARDO DA VINCI

In view of the fact that there is an abundance of excellent textbooks and monographs already on the market, it takes some special motivation of purpose, if not presumptuousness, to write yet another book on quantum theory. In the present case, the motivation was to fill a need of graduate students in theoretical physics that became apparent to me while teaching intermediate and advanced topics in quantum theory, during the last ten years or so, at universities in Europe, England, and the United States of America. I observed that there is dire need for a text which, although incomplete in many ways, is unified in style and presentation and could lead the student, in a gentle manner, from the realm of basic quantum mechanics (in which he already acquired a working knowledge) to the peaks of present-day research methods and concepts. While it is possible to cover every single step of this process by the appropriate chapter of one or more well-known textbooks, I came to feel that a single volume, concentrating on ideas and basic methods, would serve a legitimate purpose.

After this statement of purpose, I feel that the title of this book needs some explanation. It is not easy to define the vague epithet "advanced." Certainly I did not imply thereby a kind of "highbrow" treatment, nor did I mean to indicate that, after having worked through this book, the student will have become a person with advanced experience or knowledge. All I wanted to convey was that this book is meant to be used in the so-called advanced graduate courses on quantum theory, and should prepare the student for further studies in genuinely advanced *special topics*, such as relativistic quantum field theory, theory of elementary particles, or the many-body problem.

The other, less conspicuous, word in the title, viz., the use of the term quantum *theory* rather than quantum *mechanics*, serves to emphasize that the treatment was kept as general as possible, covering not only quantized systems with a mechanical analog but also any system of the micro-world. Special attention has been paid to *quantized fields*, although for very good reasons *relativistic* quantum field theory has been completely omitted. On the other hand, the rudiments of relativistic quantum *mechanics* have been included (Chapter 2 and Appendix 3), since I felt that a first acquaintance with the nonquantized Klein-Gordon and Dirac equations are both desirable and feasible at this stage of study.

In view of the detailed Table of Contents, it appears unnecessary to review here the contents of this treatise. The only remark I wish to make is that the four Appendices, although purely mathematical in nature and rather sketchy, form an essential part of the text. In particular, I felt it worthwhile to make Appendix 2 (on the elements of group theory) more extensive than is actually demanded for the understanding of the main text. It should also be pointed out that at the end of each chapter, the reader will find a brief résumé which serves to put the fragments of acquired knowledge into proper perspective.

Since the topics covered in advanced quantum theory courses vary considerably from school to school, it is clear that no unique choice of subject material could be made. For similar reasons, certain topics which are often treated in lower-level courses have also been included, because a somewhat more critical and systematic review of some superficially familiar subjects can be a great advantage to many students.

It is obviously impossible to cover this text in a one-year course. There are, however, two possible ways for using this book as a textbook. In some schools, the stage has been reached when *two* full years of intermediate and advanced quantum theory are offered, followed or paralleled by special, highly advanced topics. It is hoped that the number of such institutions is increasing. In the majority of universities, where there is time for only one year of study in this field, the lecturer will be able to select the appropriate topics of his own preference; this can be done in several different ways. Finally, some sections, such as those covering the elements of dispersion relation techniques (Chapter 3, Sections 3–4 and 3–5c; Chapter 4, Sections 4–4e and 4–4f) or those concerned with the rudiments of the many-body problem (Chapter 4, Section 4–6), can be used also as introductory material to highly specialized courses and can be given after the general advanced quantum theory sequence.

It is often said, and quite rightly, that the complete understanding of a subject cannot be achieved without applying it. Carrying this reasoning beyond its limits, one sometimes hears that "things are learned through their applications." In my opinion, this is an oversimplification of the complicated process of learning. Entering a new world, we must first get familiarized with the overall features of the landscape, draw a map, and learn about the riches of the country before we can start exploiting them. Likewise, I feel, many young would-be scientists are misled by a premature rush into applications before completing a systematic survey of the field and an adequate assimilation of the fundamental ideas and methodology. Physics, unlike agriculture, plumbing, or even engineering at its very best, is not merely a professional activity. In bygone days, physics was often referred to as "natural philosophy." Physics has been the product of the ever-searching, restlessly enquiring, wondering human mind, the outcome of a longing for understanding and appreciating the world we live in. It is this aspect of physics which, in this book, I tried to stress most. The young student of today is only too often bewildered by and lost in abundance of detail, and I feel that a review from well-chosen vantage points is badly needed for his real progress. Experience shows that a large majority of students greatly welcomes a thorough explanation of what is often called "the formalism," and they find that after having mastered this formalism, then and only then will they be able to individually work their way through the host of nontrivial applications of the formalism.

But there is a solid bridge between the formalism and applied research based on it. The arches of this bridge are spanned by exercises of varying degrees of difficulty, and it is for this reason that a sizable number of problems have been added to each chapter. These problems form an intrinsic and absolutely essential part of the text, and the student is seriously urged to solve as many problems as his time permits—and more. The problems are all straightforward and never go beyond the framework of this book; no extra reading or referencing is needed for their solution. In some cases, the problems contain ramifications of the text, extensions of topics dealt with in the corresponding chapter, and new theorems or methods.

Finally, I feel obliged to comment on the system of giving references, or rather, on the lack of systematic referencing. To do justice even to the most important contributions to quantum theory would have necessitated the addition of a volume of its own. I therefore restricted myself to give, at the end of each chapter, a rather short list of references, consisting of current textbooks, monographs, and reviews. These references serve only to advise the reader from which sources he could fill in gaps of his previous knowledge and where he could turn for further reading. Occasionally, when a proof was skipped or the discussion, out of necessity was brief, I included a reference in a footnote.

If a substantial fraction of users of this book feel that it helped them to overcome difficulties of understanding and enlarged their outlook, the purpose of this work will have been fulfilled. I would greatly appreciate any comments and rectifications, including even correction of misprints.

I am obliged to several colleagues and students of mine who helped me in clarifying my own ideas. I am also obliged to the U.S. Air Force Office of Scientific Research for continuing grants during the long period of writing this book and thus graciously tolerating a considerably reduced research output on my side. Foremost of all, whether or not it be commonplace to say, I am grateful to my wife, Cordula, for the understanding and patience that she demonstrated during the strained years of writing this book.

P.R.

Boston, Massachusetts
May 1964

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PART I

The Framework of Quantum Theory

CHAPTER 1

Description of Quantized Systems

Quantum theory is a self-contained physical discipline aiming at the appropriate formulation of the basic laws that govern the behavior of the microworld. It is concerned with the description of the properties and behavior of elementary particles, atomic nuclei, atoms, molecules, and possibly somewhat bigger atomic systems, such as crystals.

The phenomena of the macroworld, i.e., those of extended, massive bodies with a complicated structure, are the outcome of averages taken over an enormous number of basic microphenomena. Therefore, many properties of the microworld may be lost when we observe only the macroworld: the laws of macrophysics appear as approximations of the microscopic laws if applied to a very big number of individual processes. Thus, the laws of microphysics, i.e., quantum theory, must be based on a *set of axioms* (or postulates), which cannot be derived from the laws of the macroworld (i.e., from Newton's laws of motion and Maxwell's equations). Instead these axioms can be established and tested only by experiments which refer directly to microphenomena. These basic laws of the microworld have been discovered and developed, by trial and error, roughly speaking during the period from 1900–1930.

We assume that the reader is already familiar with the most important features and basic applications of quantum theory and has also achieved some versatility in performing quantum-mechanical calculations. Therefore, in this first chapter, we endeavor to present only a concise, but sufficiently deep, picture of the complete conceptual framework on which the theory is firmly based. We believe that the clearest understanding and most transparent view of this magnificent edifice is obtained by a more or less axiomatic presentation of the concepts and basic laws with which, in one form or another, the reader has already had some contact. We by no means claim that the "postulates" set forth below are (in the terminology of axiomatics) "nonreducible" or "complete," but we hope that they will facilitate a thorough understanding of the structure of quantum theory. For a more rigorous treatment, both mathematical and physical, the reader is referred to some of the classic books listed in the references.

The most appropriate mathematical language for the formulation of the framework of quantum theory is provided by that of *linear algebra.* The basic notions of this powerful mathematical discipline, including the fundamentals of Hilbert space theory, are summarized in Appendix 1. We emphatically recommend that the reader first study the appendix thoroughly before turning to the main body of the book. This preliminary mathematical study will certainly not be a waste of time, if, for no other reason, than that it will make the reader familiar with our notation and terminology.

1-1 PHYSICAL OBSERVABLES

Quantities of fundamental importance in any physical theory are the observables of the system, i.e., entities which, in principle at least, can be measured on the system by a suitable and reproducible device. Our first postulate sets, so to speak, the tone of the quantum-mechanical language and states that:

> **Postulate I.** *All observable physical quantities correspond to Hermitian operators. The only measurable values of a physical observable are the various eigenvalues of the corresponding operator.*

In order to understand the contents of this axiom, we recall that in classical (macroscopic) physics the physical observables of a system correspond to *functions* of some basic variables. The measured values of an observable in classical physics are the numerical values taken on by the corresponding function. In contrast, in quantum theory, the observables are associated with operators which act on the state of the system. [The state of a quantum-mechanical system will be introduced and specified by Postulates III(a) and III(b) below.] Thus the concept of an observable is more closely related to the process of measurement in quantum mechanics than it is in classical physics. We shall elaborate on this later.

It is necessary that an operator be Hermitian in order for it to correspond to a physical observable. Only this property ensures that all its eigenvalues are real, as indeed they must be if, according to the second part of Postulate I, we wish to identify the eigenvalues with the possible measured values. (All physical measurements yield real numbers.) Furthermore, it will be necessary to restrict ourselves to *bounded* Hermitian operators which have a *complete set* of eigenstates. (Concerning the completeness concept, see Section A1-3, in particular p. 653.) In the following we shall always assume that the operators corresponding to physical observables satisfy these criteria.*

Postulate I already contains the most remarkable feature of quantum physics, namely that, in general, an observable physical quantity may not attain arbitrary values. Because of the association of observed values with the eigenvalues of an operator, only a certain "spectrum" of measurable values is allowed to occur.

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* On the other hand, not every bounded Hermitian operator represents a physical observable. This will be discussed in Section 1-4b in connection with superselection principles.

In fact the eigenvalue spectrum of an operator is, in general, not continuous, or at least the spectrum contains a discrete part. Thus Postulate I expresses the experimental fact of *quantum levels*.

The question now arises as to how one can find the operator which corresponds to a certain physical observable. This problem is settled by Postulates II(a) and II(b).

Postulate II(a). *Any classical physical quantity must be considered to be constructed from pairs of canonically conjugate variables. The corresponding quantum-mechanical operator is then obtained by replacing the classical canonical variables by their corresponding quantum-mechanical operators.**†

It is important to set out precisely what is meant by canonically conjugate variables. As is well known, classical physics can be formulated in terms of a variational principle. If we restrict ourselves, for simplicity, to mechanical mass-point systems,‡ we denote the generalized coordinates (degrees of freedom) by q_i $(i = 1, 2, \ldots, N)$. Then we define a Lagrangian $L = L(q_i, \dot{q}_i, t)$ and an action integral

$$W = \int_{t_1}^{t_2} L(q_i, \dot{q}_i, t)\, dt \tag{1–1}$$

such that the variational problem

$$\delta_{q_i} W = 0 \tag{1–2}$$

with respect to the q_i and with the boundary conditions $\delta q_i = 0$ for t_1 and t_2 yields the equations of motion (see Fig. 1–1a). It is known that the solution of this problem is given by the Euler-Lagrange equations as

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = 0. \tag{1–3}$$

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* If for the description of the system we also need variables that have no classical counterpart (such as spin or isobaric spin) then, of course, Postulate II(a) is useless. In these cases, we must rely on *ad hoc* methods or utilize symmetry properties and conservation rules to find the representing operator. Specific examples set forth in later chapters will illuminate this point.

† In some cases, when obtaining the quantum analog of a classical observable by means of replacing the classical canonical variables with their corresponding operators, special care has to be exercised to ensure that the resulting operator be Hermitian. For example, a term of the form pq is not Hermitian, because p and q do not commute. In such cases, the classical expression must first be properly symmetrized in the canonical variables. In the given example, instead of pq, we must write the expression $1/2(pq + qp)$, which in *classical* theory is identical to pq. Therefore, when considering p and q as operators, we now have a Hermitian term, irrespective of the commutation properties of p and q.

‡ Concerning fields, i.e., systems with infinite many degrees of freedom, cf. Section 1–7, in particular 1–7e.

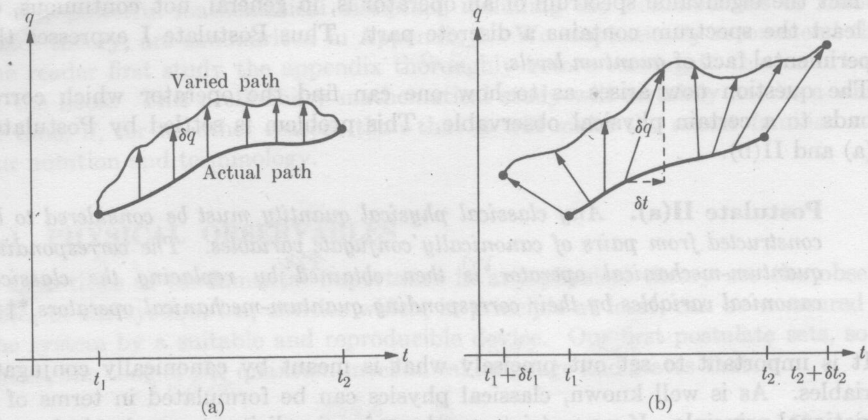

FIGURE 1–1

Now we want to perform a more general variation. Besides q_i, we shall also vary the time t, as well as the endpoints, t_1 and t_2, of the "path." In other words, we perform the transformations (see Fig. 1–1b)

$$q_i(t) \to q_i'(t) = q_i(t) + \delta q_i, \qquad t \to t' = t + \delta t,$$

with arbitrary and independent δq_i and δt, and we define

$$\delta W \equiv \int_{t_1+\delta t_1}^{t_2+\delta t_2} L(q_i + \delta q_i, \dot{q}_i + \delta\dot{q}_i, t + \delta t)\, d(t + \delta t) - \int_{t_1}^{t_2} L(q_i, \dot{q}_i, t)\, dt.$$

Then, as one can easily verify, retaining only terms up to the first order, this general variation of W comes out to be

$$\delta W = \int_{t_1}^{t_2} \sum_{i=1}^{N} \left(\frac{\partial L}{\partial q_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i}\right) \delta q_i\, dt + \left[\sum_{i=1}^{N} p_i\, \not{\delta} q_i - H\, \delta t\right]_{t_1}^{t_2}. \tag{1–4}$$

Here we have used the notation $\not{\delta} q_i$ for the *complete* change of the coordinates in the endpoints, that is,

$$\not{\delta} q_i \equiv q_i'(t + \delta t) - q_i(t) = q_i'(t) - q_i(t) + \dot{q}_i\, \delta t = \delta q_i + \dot{q}_i\, \delta t. \tag{1–5}$$

Further, for brevity, we have *defined*

$$p_i \equiv \frac{\partial L}{\partial \dot{q}_i}, \tag{1–5a}$$

$$H \equiv \sum_{i=1}^{N} p_i \dot{q}_i - L. \tag{1–5b}$$

The first term in (1–4) vanishes due to the equations of motion (1–3), so that

$$\delta W = \left[\sum_{i=1}^{N} p_i \, \delta q_i - H \, \delta t\right]_{t_1}^{t_2}. \tag{1–6}$$

We now use this general variation of the action integral to *define* the canonically conjugate pairs of variables. We agree to call the coefficient in (1–6) of the variation of any variable the canonically conjugate variable. Thus the canonically conjugate variable associated with the generalized coordinate q_i is p_i (defined by 1–5a) and the canonical conjugate variable to the time t is the function $-H$ (defined by 1–5b). Here H is called the Hamiltonian.

One can easily find that if the mechanical system is conservative and if we choose $q_i = x_i$, where the x_i's denote ordinary Cartesian coordinates, then

$$p_i = m\dot{x}_i, \qquad H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + V(x_i),$$

where m is the mass and V the potential energy. However if we use appropriate angle variables for generalized coordinates, then their corresponding canonical conjugates are found to be the components of angular momentum.

The above definition of canonically conjugate variables is extremely useful when we have to deal with systems which have awkward generalized coordinates. Even more important is the fact that this variational method of introducing canonically conjugate variables can very easily be extended to cover systems with infinitely many degrees of freedom, i.e., physical *fields*. In Section 1–7 we shall have occasion to see in detail how the canonical theory works for quantized fields; but, of course, all the material which will be discussed presently is equally valid for point-mechanical systems and fields.

Once the appropriate canonically conjugate pairs of variables have been introduced, then the equations of motion may be recast into the form of Hamilton's equations,

$$\dot{q}_k = \frac{\partial H}{\partial p_k}, \quad \dot{p}_k = -\frac{\partial H}{\partial q_k}. \tag{1–7}$$

The simplest way to derive these equations is first to write formally

$$\delta H = \sum_{i=1}^{N} \left(\frac{\partial H}{\partial q_i}\,\delta q_i + \frac{\partial H}{\partial p_i}\,\delta p_i\right),$$

and then, using the definition (1–5b) and utilizing the equations of motion (1–3), to compute explicitly δH; and finally, to identify the coefficients of δq_i and δp_i respectively.

For further applications, we now point out an interesting property of the general variation δW of the action integral. If we set

$$F(t) \equiv \sum_{i=1}^{N} p_i \, \delta q_i - H \, \delta t, \tag{1–8}$$