FOUNDATIONS OF QUANTUM MECHANICS

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PREFACE

This book is an advanced text on elementary quantum mechanics.

By "elementary" I designate here the subject matter of nonrelativistic quantum mechanics for the simplest physical systems. With the word "advanced" I refer to the use of modern mathematical tools and the careful study of difficult questions concerning the physical interpretation of quantum mechanics.

These questions of interpretation have been a source of difficulties from the beginning of the theory in the late twenties to the present day. They have been the subject of numerous controversies and they continue to worry contemporary thoughtful students of the subject.

In spite of these difficulties, quantum mechanics is indispensable for most modern research in physics. For this reason every physicist worth his salt must know how to use at least the language of quantum mechanics. For many forms of communication, knowledge of the approved usage of the language may be quite sufficient. A deeper understanding of the meaning is then not absolutely indispensable.

The pragmatic tendency of modern research has often obscured the difference between *knowing the usage of a language* and *understanding the meaning of its concepts.* There are many students everywhere who pass their examinations in quantum mechanics with top grades without really understanding what it all means. Often it is even worse than that. Instead of learning quantum mechanics in parrot-like fashion, they may learn in this fashion only particular approximation techniques (such as perturbation theory, Feynman diagrams or dispersion relations), which then lead them to believe that these useful techniques are identical with the conceptual basis of the theory. This tendency appears in scores of textbooks and is encouraged by some prominent physicists.

This text, on the contrary, is not concerned with applications or approximations, but with the conceptual foundations of quantum mechanics. It is restricted to the general aspects of the nonrelativistic theory. Other fundamental topics such as scattering theory, quantum statistics and relativistic quantum mechanics will be reserved for subsequent publications.

When I wrote this book I had three categories of readers in mind: the student of physics who has already acquired a first knowledge of quantum mechanics, the experienced physicist who is in search of a deeper understanding, and the mathematician who is interested in the mathematical problems of quantum mechanics.

The book consists of three parts. Part 1, called Mathematical Foundations, contains in four chapters a sundry collection of mathematical results, not usually found in the arsenal of a physicist but indispensable for understanding the rest of the book. I have taken special care to explain, motivate, and define the basic concepts and to state the important theorems. The theorems are rarely proved, however. Most of the concepts are from functional analysis and algebra. For a physicist this part may be useful as a short introduction to certain mathematical results which are applicable in many other domains of physics. The mathematician will find nothing new here, and after a glance at the notation can proceed to Chapter 5.

In Part 2, called Physical Foundations, I present in an axiomatic form the basic notions of general quantum mechanics, together with a detailed analysis of the deep epistemological problems connected with them.

The central theme here is the lattice of propositions, an empirically determined algebraic structure which characterizes the intrinsic physical properties of a quantum system.

Part 3 is devoted to the quantum mechanics of elementary particles. The important new notion which is introduced here is localizability, together with homogeneity and isotropy of the physical space. In this part the reader will finally find the link with the conventional presentation of quantum mechanics. And it is here also that he encounters Planck's constant, which fixes the scale of the quantum features.

Of previous publications those of von Neumann have most strongly influenced the work presented here. There is also considerable overlap with the book by G. Ludwig and with lecture notes by G. Mackey. In addition to material available in these and other references, it also contains the results of recent research on the foundations of quantum mechanics carried out in Geneva over the past seven years.

The presentation uses a more modern mathematical language than is customary in textbooks of quantum mechanics. There are essentially three reasons for this:

First of all, I believe that mathematics itself can profit by maintaining its relations with the development of physical ideas. In the past, mathematics has always renewed itself in contact with nature, and without such contacts it is doomed to become pure symbolism of ever-increasing abstraction.

Second, physical ideas can be expressed much more forcefully and clearly if they are presented in the appropriate language. The use of such a language will enable us to distinguish more easily the difficulties which we

might call syntactical from those of interpretation. Contrary to a widespread belief, mathematical rigor, appropriately applied, does not necessarily introduce complications. In physics it means that we replace a traditional and often antiquated language by a precise but necessarily abstract mathematical language, with the result that many physically important notions formerly shrouded in a fog of words become crystal clear and of surprising simplicity.

Third, in all properly formulated physical ideas there is an economy of thought which is beautiful to contemplate. I have always been convinced that this esthetic aspect of a well-expressed physical theory is just as indispensable as its agreement with experience. Only beauty can lead to that "passionate sympathetic contemplation" of the marvels of the physical world which the ancient Greeks expressed with the orphic word "theory."

About 350 problems appear throughout the book. Most of them are short exercises designed to reinforce the notions introduced in the text. Others are more or less obvious supplements of the text. There are also some deeper problems indicated by an asterisk. The latter kind are all supplied with a reference or a hint.

There remains the pleasant task of remembering here the many colleagues, collaborators, and students who in one way or another have helped to shape the content and the form of this book.

My first attempts to rethink quantum mechanics were very much stimulated by Prof. D. Finkelstein of Yeshiva University and Prof. D. Speiser of the University of Louvain. It was during the year 1958, when all three of us were spending a very stimulating year at CERN, that we began examining the question of possible generalizations of quantum mechanics. Many of the ideas conceived during this time were subsequently elaborated in publications of my students at the University of Geneva. I should mention here especially the work of G. Emch, M. Guenin, J. P. Marchand, B. Misra, and C. Piron.

In the early stages I profited much from various discussions and correspondence with Professor G. Mackey. Many colleagues have read and criticized different portions of the manuscript. I mention here especially Dr. R. Hagedorn of CERN, whose severe criticism of the pedagogical aspects of the first four chapters has been most valuable. With Dr. J. Bell of CERN, I debated especially the sections on hidden variables and the measuring process. The chapter on the measuring process has also been influenced by correspondence with Prof. E. Wigner of Princeton and with Prof. L. Rosenfeld of Copenhagen. Several other sections were improved by criticism from Prof. R. Ascoli of Palermo, Prof. F. Rohrlich of Syracuse, New York, Prof. dell'Antonio of Naples, and Dr. G. Baron of Rye, New York. Prof. C. F. v. Weizsäcker of Hamburg read and commented on the philosophical section of Chapter 5. Professor G. Mackey read critically

the entire manuscript and suggested many improvements. Dr. C. Piron and Mr. A. Salah read the proofs, and I am much indebted to them for their conscientious and patient collaboration. To all of them, and many others too numerous to mention, I wish to express here my thanks.

The major portion of the book was written while I had the privilege of holding an invited professorship at the University of California in Los Angeles, during the winter semester of 1964. May Professors D. Saxon and R. Finkelstein find here my deeply felt gratitude for making this sojourn, and thereby this book, possible. The University of Geneva contributed its share by granting a leave of absence which liberated me from teaching duties for three months.

I have also enjoyed the active support of CERN, which, by according me the status of visiting scientist, has greatly facilitated my access to its excellent research facilities and contact with numerous other physicists interested in the matters treated in this book.

It is unavoidable that my interpretation of controversial questions is not shared by all of my correspondents. Of course, I alone am responsible for the answers to such questions which appear in this book.

Mrs. Dorothy Pederson of Los Angeles and Mlle. Frances Prost of Geneva gave generously of their competent services in typing a difficult manuscript. May they, too, as well as their collaborators, find here my expression of gratitude.

Geneva, Switzerland J. M. J.
August 1966

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PART 1

Mathematical Foundations

CHAPTER 1

MEASURE AND INTEGRAL

Therefore there is no perfect measure of continuous quantity except by means of indivisible continuous quantity, for example by means of a point, and no quantity can be perfectly measured unless it is known how many individual points it contains. And since these are infinite, therefore their number cannot be known by a creature but by God alone, who disposes everything in number, weight, and measure.

ROBERT GROSSETESTE,
13th century A.D.

The purpose of this chapter is to acquaint the reader with the modern theory of integration. Section 1-1 contains some basic notions of set theory together with a list of terms and formulas. In Section 1-2 we present the notion of measure space and some properties of measures. We define measures on σ-rings of a class of measurable sets, but we pay no attention to the maximal extensions of such measures. The following section (1-3) introduces the measurable and integrable functions and defines the notion of integral. Section 1-4 introduces the theorem of Radon-Nikodym by way of a trivial example. The last section (1-5) on function spaces forms the bridge to the general theory of Hilbert space to be presented in Chapter 2.

1-1. SOME NOTIONS AND NOTATIONS FROM SET THEORY

A collection of objects taken as a whole is called a *set*. The objects which make up a set are called the *elements* of the set. We denote sets by capital letters, for instance $A, B, \ldots, S$; and the elements by small letters, for instance $a, b, \ldots, x$. If the element x is contained in the set S we write $x \in S$; if it is not contained in the set S we write $x \notin S$. If every element of a set A is contained in B we write $A \subset B$ or $B \supset A$, and we say A is a *subset* of B.

If $A \subset B$ and $B \subset A$, then we say the two sets are *equal* and we write $A = B$.

The set $A \cup B$ denotes the set of elements which are either in A or in B or in both. It will be called the *union* of A and B.

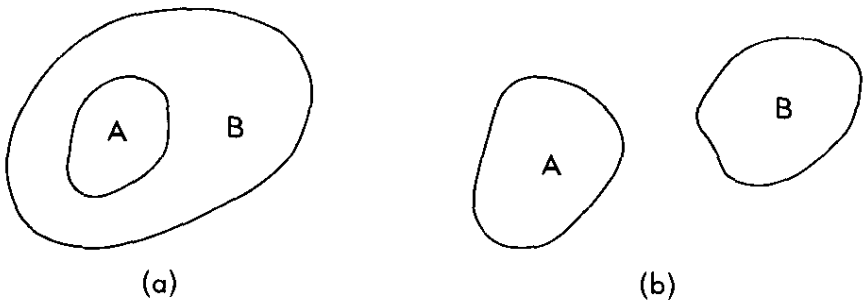

Fig. 1–1 Relations between point sets: (a) $A \subset B$ (A subset of B); (b) $A \cap B = \emptyset$ (disjoint sets).

The set $A \cap B$ denotes the set of elements which are in A as well as in B. It is called the *intersection* of A and B.

If A is a subset of a set S, we define by A' (with respect to S) the set of all elements which are in S but *not* in A. The set $A \cap B' = A - B$ is called the *difference* of A and B, or the *relative complement* of B in A.

A subset of a general set S can be defined by a certain property $\pi(x)$. The set A of all elements which have property $\pi(x)$ is written

$$A = \{x : \pi(x)\}.$$

It means: A is the set of all elements which satisfy property $\pi(x)$. Thus for instance the operation $A \cup B$ can be defined by

$$A \cup B = \{x : x \in A \text{ and/or } x \in B\}.$$

Similarly we write

$$A \cap B = \{x : x \in A \text{ and } x \in B\}.$$

If there exists no element which has property $\pi(x)$, then the set $\emptyset = \{x : \pi(x)\}$ defines the *empty set*. We have always, for any set $A \subset S$:

$$\emptyset \subset A, \qquad \emptyset \cup A = A, \qquad \emptyset \cap A = \emptyset, \qquad \emptyset' = S.$$

If two sets A and B are such that $A \cap B = \emptyset$, they are called *disjoint*.

All these notions can be easily illustrated and remembered by using point sets in a plane (see Figs. 1–1 and 1–2).

We shall now go a step further and consider collections of subsets of a set. We speak then of a *class* of subsets. Of particular interest are classes which are closed with respect to certain operations defined above.

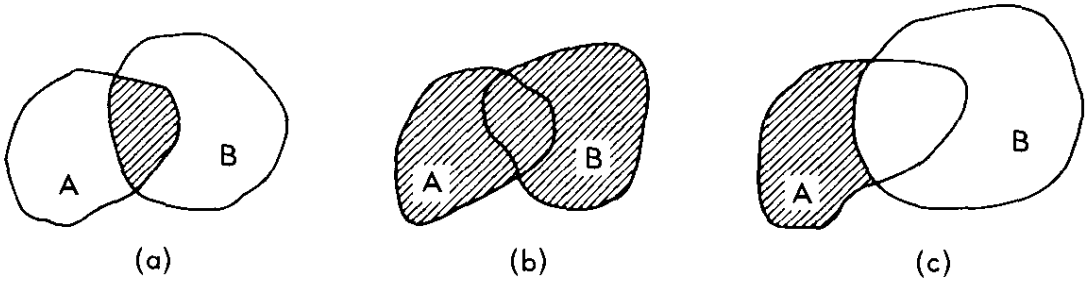

Fig. 1–2 Intersection-, union-, and difference-sets: (a) $A \cap B$; (b) $A \cup B$; (c) A B $A \cap B'$ (for S the entire plane).

The most useful notion is that of a ring. A nonempty class of subsets is called a *ring* $\mathscr{R}$ if, for $A \in \mathscr{R}$ and $B \in \mathscr{R}$, it follows that $A \cup B \in \mathscr{R}$ and $A - B \in \mathscr{R}$. Examples of rings are easily constructed. One of the simplest possible is the ring consisting of an arbitrary subset $A \subset S$, together with the sets $\emptyset$, A' and S.

Since $A - A = \emptyset$, every ring contains the empty set. One proves by mathematical induction that if $A_1, A_2, \ldots, A_n$ is a finite collection of subsets in $\mathscr{R}$, then

$$\bigcup_{i=1}^{n} A_i \in \mathscr{R} \qquad \text{and} \qquad \bigcap_{i=1}^{n} A_i \in \mathscr{R}.$$

Here we have introduced the easily understandable notation

$$\bigcup_{i=1}^{n} A_i \equiv A_1 \cup A_2 \cup \cdots \cup A_n$$

and

$$\bigcap_{i=1}^{n} A_i \equiv A_1 \cap A_2 \cap \cdots \cap A_n.$$

A *σ-ring* is a ring with the additional property that, for every countable sequence A_i $(i = 1, 2, \ldots)$ of sets contained in $\mathscr{R}$, we have

$$\bigcup_{i=1}^{\infty} A_i \in \mathscr{R}.$$

A ring is called an *algebra* (or Boolean algebra) if it contains S, or equivalently if $A \in \mathscr{R}$ implies $A' \in \mathscr{R}$.

The primary purpose for introducing the notions of ring, σ-ring, and algebra of sets is to obtain sufficiently large classes of sets to be useful for a theory of integration. On the other hand, for the construction of a measure, the class of sets must be restricted so that an explicit construction of a measure is possible. This class must contain certain simple sets and for this reason we want to construct σ-rings of sets generated by a certain class of subsets. How this is done is now to be explained.

If $\mathscr{E}$ is any class of sets, we may define a unique ring called the *ring generated by* $\mathscr{E}$, denoted by $\mathscr{R}(\mathscr{E})$. It is defined as follows: Denote by $\mathscr{R}_i$ ($i \in I$ = some index set) the family of all the rings which contain the class $\mathscr{E}$. The intersection of all $\mathscr{R}_i$ is again a ring (Problem 9) and it defines the ring generated by $\mathscr{E}$:

$$\mathscr{R}(\mathscr{E}) = \bigcap_{i} \mathscr{R}_i.$$

It is clearly the smallest ring which contains the class $\mathscr{E}$ of sets. Furthermore it is unique. The same procedure can be used for σ-rings.

We are now prepared for the most important notion of this section, the Borel set.

Let S be the real line $S = \{x : -\infty < x < +\infty\}$.

For $\mathscr{E}$ we choose the set of all bounded semiclosed intervals of the form

$$[a, b) \equiv \{x : a \leq x < b\}.$$

The *Borel sets* on the real line are the sets contained in the σ-ring $\mathscr{R}(\mathscr{E})$ generated by this class $\mathscr{E}$.

The choice of semiclosed intervals as starting sets might be somewhat surprising, but there is a technical reason for this. The finite unions of semiopen intervals are a ring (Problem 7), while this is not so for closed or open intervals. It is, however, *a posteriori* possible to show that the σ-ring generated by the open or the closed interval is also the class of Borel sets. These properties are not difficult to prove, but they require certain technical devices which transcend the purpose of this book ([1], §15). We shall therefore state them without proof:

1) The class of all Borel sets is the σ-ring generated by all open or all closed sets.
2) The entire set S is a Borel set. The σ-ring of Borel sets is thus an algebra.
3) Every countable set is a Borel set.

The first of these properties permits an extension of the notion of Borel sets to certain topological spaces. For instance, in a locally compact Hausdorff space one defines the Borel sets as the σ-ring generated by all closed subsets [1, Chapter 10].

With this general notion one can define Borel sets, for instance, on an n-dimensional Euclidean space, on a finite-dimensional manifold, such as a circle, a torus, or a sphere, and on many other much more complicated spaces. In many applications which we shall use we have to deal with the Borel sets for an arbitrary closed subset of the real line.

PROBLEMS

1. $(A')' = A$ for all sets A. [*Note*: In order to prove equality of two sets A and B, one must prove separately $A \subset B$ and $B \subset A$.]
2. $A \subset B$ implies $B' \subset A'$.
3. A and B are disjoint if and only if $A \subset B'$, or equivalently $B \subset A'$.
4. $(A \cap B)' = A' \cup B'$.
5. $(A - B)' = A' \cup B$.
6. The class of all subsets of a set S is a ring.
7. Let $S = \{x : -\infty < x < +\infty\}$; then the class of all subsets of S of the form

$$\bigcup_{i=1}^{n} \{x : a_i \leq x < b_i\}$$

is a ring.

8. If a ring $\mathscr{R}$ of subsets of S contains S, then $A \in \mathscr{R}$ implies $A' \in \mathscr{R}$, and vice versa.
9. The intersection of any family of rings (σ-rings) $\mathscr{R}_\iota$ is a ring (σ-ring).

1-2. THE MEASURE SPACE

A *measure space* is a set of elements S, together with a σ-ring M of subsets of S and a nonnegative function $\mu(A)$, defined on all subsets of the class M, which satisfies certain properties to be enumerated below.

The subsets of the σ-ring M are called the *measurable* sets. We denote the measure space by (S, M, μ). Sometimes the explicit reference to the measurable sets and the measure μ is suppressed, and we then simply refer to S as a measure space. Because M is a ring, $\emptyset \in M$ and so the null set is always measurable. It is always possible to arrange that $S \in M$, too, so that M is an algebra.

The conditions to be satisfied by the set-function $\mu(A)$ for $A \in M$ are as follows:

1) $0 \leq \mu(A) < \infty$;

2) $\mu(\emptyset) = 0$;

3) For any disjoint sequence of sets $A_i \in M$ $(i = 1, 2, \ldots)$,

$$\mu\left(\bigcup_{i=1}^{\infty} A_i\right) = \sum_{i=1}^{\infty} \mu(A_i).$$

Property 1 may be relaxed to include infinite measures. Then we can only require $0 \leq \mu(A) \leq \infty$. (Most applications, however, will be for finite measures.) A set function which satisfies property (3) is called *σ-additive*.

The sets $A \in M$ with $\mu(A) = 0$ are called the *sets of measure zero*. A property which is true for all $x \in S$ except on a set of measure zero is said to be true "almost everywhere" (abbreviated a.e.).

Naturally the question arises whether any measures exist and what their properties are. Instead of entering into these rather difficult questions, we shall explicitly exhibit two types of measures which we shall use constantly: the Lebesgue measure and the Lebesgue-Stieltjes measure.

For the *Lebesgue measure*, the σ-ring of measurable sets consists of the Borel sets on the real line. On the half-open intervals $[a, b)$, with $a \leq b$, we define

$$\mu\{[a, b)\} = b - a.$$

In the theory of measure, one proves that this set function on the half-open intervals has a unique extension to the Borel sets such that it satisfies conditions (1), (2), and (3). This extension will be called the *Lebesgue measure* on the real line. (Actually the measure can be further extended to the class of Lebesgue measurable sets, but we shall not need this extension explicitly.)

The *Lebesgue-Stieltjes measure* is a generalization of the Lebesgue measure obtained in the following way: Let $\rho(\lambda)$ be a real valued, non-decreasing function, defined for $-\infty \leq \lambda \leq +\infty$, and such that

$$\rho(\lambda + 0) = \lim_{\varepsilon \to +0} \rho(\lambda + \varepsilon) = \rho(\lambda).$$

For any semiopen interval $[a, b)$, $(a \leq b)$, we define

$$\mu\{[a, b)\} = \rho(b) - \rho(a).$$

The unique extension of this set function to the Borel sets on the real line is called the Lebesgue-Stieltjes measure on the real line.

For $\rho(\lambda) = \lambda$ this measure reduces to the Lebesgue measure. The greater generality of the Lebesgue-Stieltjes measure is especially convenient for discrete measures.

We obtain a *discrete measure* by letting $\rho(\lambda)$ be constant except for a countable number of discontinuities λ_k, where

$$\rho(\lambda_k) = \rho(\lambda_k - 0) + \rho_k.$$

The measure is then said to be concentrated at the points λ_k with the weights ρ_k.

We say two measures μ_1 and μ_2 are *comparable* if they are defined on the same σ-ring of measurable sets. Thus all measures on the Borel sets are comparable.

In the following we shall examine the relation between different comparable measures. The main point is the observation that comparable measures can be partially ordered. In the following we shall assume all measures to be comparable without repeating it.

A measure μ_1 is said to be *inferior* to a measure μ_2 if all sets of μ_2-measure zero are also of μ_1-measure zero. μ_1 is also called *absolutely continuous* with respect to μ_2. We use the notation $\mu_1 \prec \mu_2$. Thus $\mu_1 \prec \mu_2$ if and only if $\mu_2(A) = 0$ implies $\mu_1(A) = 0$. Two measures μ_1, μ_2 are said to be *equivalent* if both

$$\mu_1 \prec \mu_2 \qquad \text{and} \qquad \mu_2 \prec \mu_1.$$

The two measures have then the same null sets. We write for this relation $\mu_1 \sim \mu_2$ and we note that it is an equivalence relation (Problem 2).

Two measures μ_1 and μ_2 are said to be mutually singular if there exist two disjoint sets A and B such that $A \cup B = S$ and such that, for every measurable set $X \subset S$,

$$\mu_1(A \cap X) = \mu_2(B \cap X) = 0.$$

Examples of mutually singular measures are easily constructed (Problem 8).

If a measure μ is absolutely continuous with respect to Lebesgue measure, it is simply called absolutely continuous.

PROBLEMS

1. Let μ be a discrete Lebesgue-Stieltjes measure. For every Borel set A, $\mu(A) = \sum_{k_i} \rho_{k_i}$ where the sum extends over all $\lambda_{k_i} \in A$.
2. The relation $\sim$ is an equivalence relation; this means it is reflexive, symmetrical, and transitive:
   (a) $\mu \sim \mu$;
   (b) $\mu_1 \sim \mu_2$ implies $\mu_2 \sim \mu_1$;
   (c) $\mu_1 \sim \mu_2$ and $\mu_2 \sim \mu_3$ implies $\mu_1 \sim \mu_3$.
3. Two discrete measures μ_1 and μ_2 on the real line are equivalent if and only if they are concentrated in the same points and their respective weights are nonzero.
4. Every Lebesgue-Stieltjes measure on the real line can be decomposed uniquely into a discrete part and a continuous part, corresponding to the decomposition of the nondecreasing function $\rho(\lambda) = \rho_d(\lambda) + \rho_c(\lambda)$ into a discrete and a continuous function. The discrete part $\rho_d(\lambda)$ is constant except on a finite or countably infinite set of points where $\rho_d(\lambda)$ is discontinuous.

*5. Every continuous nondecreasing function $\rho_c(\lambda)$ can be decomposed into an absolutely continuous and a singular function $\rho_c(\lambda) = \rho_a(\lambda) + \rho_s(\lambda)$. The function $\rho_s(\lambda)$ is singular in the sense that its derivative $\rho_s'(\lambda)$ exists almost everywhere and is equal to zero, yet $\rho_s(\lambda)$ is continuous and nondecreasing ([2], Section 25).

*6. ***Theorem*** (Lebesgue). *A finite nondecreasing function* $\rho(\lambda)$ (*or, more generally, a function of bounded variation*) *possesses a finite derivative* a.e. ([2], Section 4).

*7. ***Theorem*** (Lebesgue). *The necessary and sufficient condition that a finite, continuous and nondecreasing function is equal to the integral of its derivative is that it is absolutely continuous* ([2], Section 25).

8. Let μ_1 be a discrete measure concentrated at the points $\lambda_i^{(1)}$ and μ_2 another discrete measure concentrated at the points $\lambda_k^{(2)}$. Then the two measures are singular with respect to one another if and only if $\lambda_i^{(1)} \neq \lambda_k^{(2)}$ for all pairs of indices i and k.

1-3. MEASURABLE AND INTEGRABLE FUNCTIONS

The theory of measure spaces permits a definition of the integral of functions which is much more general than the so-called Riemann integral usually introduced in elementary calculus. This more general type of integral, to be defined now, is absolutely indispensable for the definition of Hilbert space and other function spaces used constantly in quantum mechanics.

We start with the definition of a function. A function f is a correspondence between the elements of a set D_f, called the *domain* of f, and a set Δ_f, called the *range* of f, such that to every $x \in D_f$ there corresponds exactly one element $f(x) \in \Delta_f$. The elements of D_f are called the *argument* of the function.

We remark especially that we define here what is sometimes called a *single-valued* function. It is possible (and, for a systematic exposition, advisable) to treat multivalued functions by reducing them to single-valued ones. In analytic function theory this procedure leads in a natural manner to the theory of Riemann surfaces.

We emphasize, too, that a function has three determining elements: A domain, a range, and a rule of correspondence $x \to f(x)$. It will sometimes be necessary to distinguish two functions which have different domains, although in a common part of these domains the value of the two functions may agree.

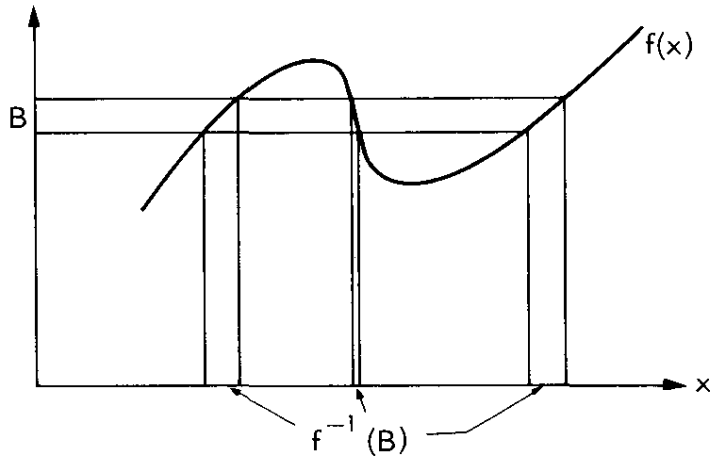

Fig. 1–3 The inverse image† of a function $f(x)$.

The sets D_f and Δ_f may be quite general sets—for instance, subsets of real or complex numbers. In that case we obtain real or complex functions. But more often they will consist of points in a topological space, functions in a function space, or even subsets of sets. In the latter case we speak also of *set functions*.

An example of a set function of great importance is the following:

Let B be a subset of the range Δ_f; we define the *inverse image* $f^{-1}(B)$ (see Fig. 1–3) by setting

$$f^{-1}(B) = \{x : f(x) \in B\}.$$

If the correspondence f between D_f and Δ_f is one-to-one, we can define the *inverse function*, also denoted by f^{-1} but with arguments $y \in \Delta_f$. The inverse function $f^{-1}(y)$ has domain $D_{f^{-1}} = \Delta_f$, range $\Delta_{f^{-1}} = D_f$, and satisfies

$$f^{-1}(f(x)) = x \qquad \text{for all } x \in D_f$$

and

$$f(f^{-1}(y)) = y \qquad \text{for all } y \in \Delta_f.$$

† Note that the inverse image is not the inverse function. As a function it is defined on the subsets of Δ_f, and its values are subsets of D_f.

Although, strictly speaking, these two identity functions should be distinguished (since in one case the domain is D_f, in the other Δ_f), they are usually considered identical, an assumption which is entirely correct only if $D_f = \Delta_f$.

For the rest of this section we shall consider real-valued functions over a measure space. Δ_f is then a subset of the real line $\mathscr{R}$.

Let (S, M, μ) be a measure space and f a real-valued function with domain $D_f = S$. We call the function f *measurable* on S if for every Borel set B on the real line, the set $f^{-1}(B)$ is measurable.

The simplest examples of measurable functions are obtained from the set functions $\chi_A(x)$ defined by

$$\chi_A(x) = \begin{cases} 1 & \text{for } x \in A, \\ 0 & \text{for } x \notin A. \end{cases}$$

A set function is measurable if and only if the set A is measurable. Indeed we find immediately that

$$\chi_A^{-1}(B) = \begin{cases} A & \text{if } 1 \in B, \\ \emptyset & \text{if } 1 \notin B, \end{cases}$$

so that $\chi_A(x)$ is measurable if $A \in M$.

There is a resemblance between measurable functions in a measure space and continuous functions in a topological space S. A topological space is defined by the class of all open subsets of S. A function $f(x)$ from S onto $\Delta_f \in \mathscr{R}$ is then said to be continuous if the inverse image $f^{-1}(B)$ of any open set is an open set in S. One obtains the more general class of measurable functions by replacing the word "open" by "measurable," in the above definition of continuous function. The class is more general because (at least in all the measure spaces which we consider) the open sets are measurable sets. One of the most important problems in measure theory is to identify the class of measurable functions over a measure space. An efficient way of doing this is to construct the measurable functions from certain simple functions by the operations of sums, products, and the passage to the limit. In what follows we shall describe this process, without giving proofs.

First, one observes that if two functions f and g are measurable, then the functions

$$f + g \qquad \text{and} \qquad fg,$$

defined by

$$(f + g)(x) = f(x) + g(x),$$
$$fg(x) = f(x)g(x),$$

are also measurable. From this it follows that the so-called *simple functions* defined by

$$f(x) = \sum_{i=1}^{n} \alpha_i \chi_{A_i}(x),$$

with α_i real constants and $A_i \in M$, are also measurable. We define the *integral* of a simple function as

$$\int f \, d\mu = \sum_{i=1}^{n} \alpha_i \mu(A_i).$$

It is a finite number since the $\mu(A_i)$ are all finite (we admit only finite measures).

Next we consider sequences of functions $f_n(x)$ $(n = 1, 2, \ldots)$. We define *convergence in the measure* of such a sequence to a limit function f if, for every $\varepsilon > 0$,

$$\lim_{n \to \infty} \mu(\{x : |f_n(x) - f(x)| \geq \varepsilon\}) = 0.$$

The notion of measurability is more general than that of integrability, the latter being restricted by the condition that there exist a finite-valued integral. Since simple functions are not only measurable but also integrable, we can define the integrable functions as follows: A finite-valued function f on a measure space (S, M, μ) is *integrable* if there exists a sequence of simple functions f_n such that f_n tends to f in the measure. It follows then that the numbers $I_n = \int f_n \, d\mu$ tend to a limit which defines the integral of f:

$$\int f \, d\mu = \lim_{n \to \infty} \int f_n \, d\mu.$$

Various theorems then permit the usual operations with integrals. For instance, if f_1 and f_2 are integrable, so are $(f_1 + f_2)$ and $f_1 f_2$, and

$$\int (f_1 + f_2) \, d\mu = \int f_1 \, d\mu + \int f_2 \, d\mu.$$

Furthermore, if f is integrable, so is $|f|$, and

$$\int f \, d\mu \leq \int |f| \, d\mu.$$

The integral defined here corresponds to what in the elementary integration theory is called the *definite integral.* There is also a concept which generalizes the usual notion of the *indefinite integral.* In the usual definition, the indefinite integral depends on the lower and upper limit of the integration variable. It is thus an interval function.

More generally we may define a set function $\nu(A)$ for all $A \in M$ by setting

$$\nu(A) = \int \chi_A f \, d\mu \equiv \int_A f \, d\mu.$$

If the integrable function f is positive, the set function $\nu(A)$ is a new measure defined on the σ-ring M. It is easy to verify that the two measures ν and μ are equivalent. (The converse of this is an important theorem which we shall discuss in the next section.)

If the measure space S is the real line, M are the Borel sets, and μ the Lebesgue measure, then the integral is called the Lebesgue integral. We write for it

$$\int f(x)\,dx.$$

Some slight modifications are necessary in some of the definitions and theorems quoted above, since Lebesgue measure is not a finite measure.

Similarly we obtain the Lebesgue-Stieltjes integral if we define the measure corresponding to some nondecreasing function $\mu(x)$. We write for this integral

$$\int_{-\infty}^{+\infty} f\,d\mu(x).$$

The notion of measurable and integrable functions is easily extended to complex-valued functions by defining such a function as integrable if both real and imaginary parts are integrable. The integral of the function $f = f_1 + if_2$ is then defined by

$$\int f\,d\mu \equiv \int f_1\,d\mu + i\int f_2\,d\mu.$$

PROBLEMS

1. A continuous function is measurable.
2. There exist measurable functions which are not continuous.
3. A function has an inverse if and only if $f(x_1) = f(x_2)$ implies $x_1 = x_2$.
4. If two real-valued functions f and g are integrable, then cf, for a constant c, is integrable and $(f + g)$ is integrable.
5. If f is integrable, then the positive and negative parts of f defined by

$$f_+ = \tfrac{1}{2}(|f| + f) \qquad \text{and} \qquad f_- = \tfrac{1}{2}(|f| - f)$$

   are also integrable.
6. If the real-valued function f is integrable, then the indefinite integral of f defines a finite measure on the class of all measurable sets.
7. The measure of Problem 6 is absolutely continuous with respect to the measure which is used for the definition of the integral.

1-4. THE THEOREM OF RADON-NIKODYM

In this section we shall consider the relations between comparable measures on a fixed measure space. This relation is of the greatest importance in the applications of measure theory. We shall neither give the most general form of the theorem nor prove it; but we shall illustrate it with an example which renders it sufficiently plausible.

Let us begin with the example: Let S consist of all the integers, $S = 1, 2, \ldots, n, \ldots$, and let ρ_n be a set of positive numbers such that

$$\sum_{n=1}^{\infty} \rho_n < \infty.$$

The σ-ring of measurable sets consists of all the subsets of S, and the measure $\mu(A)$ is defined by

$$\mu(A) = \sum_{i \in A} \rho_i.$$

Let σ_n be another sequence of nonnegative numbers such that

$$\sum_{n=1}^{\infty} \sigma_n < \infty$$

and define another measure

$$\nu(A) = \sum_{i \in A} \sigma_i.$$

The only set of μ-measure zero is the null set $\emptyset$, which is of course also of ν-measure zero. Thus ν is absolutely continuous with respect to μ: $\nu \prec \mu$. We shall define the function $f(n)$ by setting $f(n) = \sigma_n/\rho_n$; then we find that

$$\nu(A) = \sum_{i \in A} f(i)\rho_i = \int f \, d\mu.$$

Thus we have established, in this particular case, that if $\nu \prec \mu$, there exists a nonnegative measurable function f on S such that for every measurable set A we have

$$\nu(A) = \int_A f \, d\mu.$$

In the special case which we have discussed, the function f is not only measurable but also integrable; but this is the case if and only if the measure ν is *finite*, as one can easily verify. The generalization of this property to any measure is the content of the following theorem.

> ***Theorem*** (Radon-Nikodym): *The necessary and sufficient condition that the measure on the real line S be absolutely continuous with respect to the measure ν is that there exists a* (a.e.) *uniquely determined bounded non-*

negative measurable function $f(x)$ with domain S such that

$$\nu(A) = \int_A f\,d\mu \qquad \text{for every } A \in M.$$

If, furthermore, the two measures ν and μ are equivalent, then the function f is positive a.e., *and*

$$\mu(A) = \int_A \frac{1}{f}\,d\nu.$$

If both measures are finite then both f and $1/f$ are integrable.

The function f is called the Radon-Nikodym derivative and it is often written as $f = d\nu/d\mu$. The notation underlines the analogy of this concept with the ordinary derivative of a nondecreasing function. The analogy is further enhanced by considering the Lebesgue-Stieltjes measure on the real line determined by a nondecreasing function $\rho(x)$. If $\sigma(x)$ is another measure of this kind, then the function f of the Radon-Nikodym theorem is given by

$$f(x) = \frac{d\rho}{d\sigma}.$$

If $\sigma(x) = x$, the measure induced by it is the Lebesgue measure, and we may write $f(x) = d\rho/dx$. In this case the function $f(x)$ coincides (a.e.) with the usual derivative of $\rho(x)$.

PROBLEMS

1. Let $S = \{1, 2, \ldots, n, \ldots\}$ and $\mu(n) = \rho_n > 0$. The σ-ring generated by the sets $\{n\}$, with $(n = 1, 2, \ldots)$, consists of all the subsets of S, and the measure μ on the sets $\{n\}$ has a unique extension to this ring given by

$$\mu(A) = \sum_{i \in A} \rho_i.$$

2. If ν is another measure on the measure space of Problem 1, then there exists a positive function $f(n)$, with $n = 1, 2, \ldots$, such that

$$\nu(A) = \int_A f\,d\mu,$$

and another positive function $g(n)$ such that

$$\mu(A) = \int_A g\,d\nu.$$

Furthermore, $f(n) = 1/g(n)$. If μ and ν are finite measures, both functions f and g are integrable.

3. If μ_1, μ_2, μ_3 are three measures such that $\mu_1 \prec \mu_2 \prec \mu_3$, then

$$\frac{d\mu_1}{d\mu_2} \cdot \frac{d\mu_2}{d\mu_3} = \frac{d\mu_1}{d\mu_3}.$$

1-5. FUNCTION SPACES

We consider the set of all complex, integrable functions on a measure space (S, M, μ), and denote it by L^1. If $f \in L^1$ then any scalar multiple cf is also in L^1. Likewise, if f_1 and $f_2 \in L^1$ then $f_1 + f_2 \in L^1$. The functions of the class L^1 are thus a *linear manifold.*

For any $f \in L^1$ we define the *norm* as

$$\|f\| = \int |f|\, d\mu < \infty,$$

and for any pair $f, g \in L^1$ we define a *distance function* $\rho(f, g)$ by setting

$$\rho(f, g) = \|f - g\|.$$

Two functions f and g for which $\rho(f, g) = 0$ are equal except possibly on a set of measure zero. Two such functions are said to be equivalent. The classes of equivalent functions form a *metric space*, with the metric defined by the distance functions $\rho(f, g)$.

An important property of the space L^1 is its completeness. A space is said to be *complete* if every fundamental sequence f_n has a limit. This means that for every sequence f_n with the property $\|f_n - f_m\| \to 0$ as $n, m \to \infty$, there exists an integrable function f such that

$$\|f_n - f\| \to 0 \qquad \text{for} \qquad n \to \infty.$$

Of more importance in quantum mechanics is the space $L^2(S, M, \mu) \equiv L^2$, which consists of all those measurable functions on S which are square-integrable. Thus $f \in L^2$ if

$$\|f\|^2 \equiv \int |f|^2\, d\mu < \infty.$$

Just as in L^1, we can define a distance function $\rho(f, g) = \|f - g\|$.

A more general concept is the *scalar product* (f, g) defined for any pair of functions f and g in L^2. It is defined by the formula

$$(f, g) = \int f^* g\, d\mu$$

where f^* is the complex conjugate of f. With this definition we have

$$\|f\|^2 = (f, f).$$

The space L^2 is also complete. Thus if f_n is a fundamental sequence, there exists a function f such that $\|f_n - f\| \to 0$. The space L^2 is the basic mathematical object for quantum mechanics and we shall devote the next three chapters to its study.

PROBLEMS

1. The space of all sequences $\{x_n\}$ of complex numbers satisfying the condition
$$\sum_{n=1}^{\infty} |x_n| < \infty$$
is an L^1-space.
2. The space of all sequences $\{x_n\}$ of complex numbers satisfying the condition
$$\sum_{n=1}^{\infty} |x_n|^2 < \infty$$
is an L^2-space.
3. Every element in L^1 of Problem 1 is contained in L^2 and there exist elements in L^2 which are not in L^1, so that $L^1 \subset L^2$.
4. In general neither $L^1 \subset L^2$ nor $L^2 \subset L^1$ is true.

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CHAPTER 2

THE AXIOMS OF HILBERT SPACE

I think we may safely say that the studies preliminary to the construction of a great theory should be at least as deliberate and thorough as those that are preliminary to the building of a dwelling-house.

CHARLES S. PIERCE

In this chapter we introduce the basic properties of Hilbert space in axiomatic form. The axioms are given in four groups in Section 2-1. The comments on the axioms in Section 2-2 introduce such basic material as linear manifolds, dimension, Schwartz's and Minkowski's inequalities, strong and weak convergence, and orthonormal systems. In Section 2-3 we discuss various realizations of the abstract Hilbert space. We devote the whole of Section 2-4 to the important distinction between manifolds and subspaces. We also discuss the decomposition theorem with respect to a subspace. In a final section (2-5) we introduce the notion of the lattice of subspaces, a notion which will play a fundamental role throughout this book.

2-1. THE AXIOMS OF HILBERT SPACE

The abstract Hilbert space $\mathscr{H}$ is a collection of objects called *vectors*, denoted by $f, g, \ldots$, which satisfy certain axioms to be enumerated below.

The axioms fall into four groups, each of which refers to a different structure property of Hilbert space. Group 1 expresses the fact that $\mathscr{H}$ is a linear *vector space* over the field of complex numbers. Group 2 defines the *scalar product* and the metric. Group 3 expresses *separability*, and group 4, *completeness*, of the space.

1. $\mathscr{H}$ is a linear vector space with complex coefficients. This means that to every pair of elements $f, g \in \mathscr{H}$ there is associated a third $(f + g) \in \mathscr{H}$. Furthermore to every element and every complex number λ there corresponds

another element $\lambda f \in \mathscr{H}$. The following rules are postulated:

$$f + g = g + f;$$

$$(f + g) + h = f + (g + h);$$

$$\lambda(f + g) = \lambda f + \lambda g;$$

$$(\lambda + \mu)f = \lambda f + \mu f;$$

$$\lambda(\mu f) = (\lambda\mu)f;$$

$$1 \cdot f = f.$$

There exists a unique zero vector $\boldsymbol{\theta}$ such that for all f

$$\boldsymbol{\theta} + f = f.$$

$$0 \cdot f = \boldsymbol{\theta}.$$

2. There exists a strictly positive scalar product in $\mathscr{H}$. The scalar product (f, g) is a function of pairs of elements $f, g \in \mathscr{H}$ with complex values and satisfying the following conditions:

$$(f, g) = (g, f)^*;$$

$$(f, g + h) = (f, g) + (f, h);$$

$$(f, \lambda g) = \lambda(f, g) \qquad \text{for all complex } \lambda;$$

$$\|f\|^2 \equiv (f, f) > 0 \qquad \text{unless } f = \boldsymbol{\theta}.$$

3. The space $\mathscr{H}$ is separable. This means that there exists a sequence $f_n \in \mathscr{H}$ $(n = 1, 2, \ldots)$ with the property that it is *dense* in $\mathscr{H}$ in the following sense: For any $f \in \mathscr{H}$ and any $\varepsilon > 0$, there exists at least one element f_n of the sequence such that

$$\|f - f_n\| < \varepsilon.$$

4. The space $\mathscr{H}$ is complete. Any sequence f_n with the property

$$\lim_{n,m \to \infty} \|f_n - f_m\| = 0$$

defines a unique limit $f \in \mathscr{H}$ such that

$$\lim_{n \to \infty} \|f - f_n\| = 0.$$

2-2. COMMENTS ON THE AXIOMS

The axioms of groups 1 and 2 describe the Hilbert space as a linear vector space with scalar product. The special choice of the complex numbers for the field of the coefficients will be justified later from a physical point of

view. Here we remark that one can define Hilbert spaces over the reals and the quaternions (or any other field), and they share many of the properties which one finds for the Hilbert space with complex numbers.

In the axioms of group 2 we require *positive definiteness* of the scalar product. There is no difficulty in defining spaces with indefinite scalar products. We shall, however, need only the *definite* scalar product. This too will be justified from a physical point of view.

Axioms 3 and 4 are restrictions on the size of the space in opposite directions. Here one should say that axiom 4 is in some sense superfluous since it can always be fulfilled by a standard procedure, called the *completion of the space*. It is the same kind of procedure used in the construction of the real numbers from a dense subset such as the rational numbers. It is the axiom which permits the notion of continuity in Hilbert space.

Axiom 3, on the other hand, is an important restriction on the *size* of the space. If it is omitted, one obtains nonseparable spaces. These will not be used in this book since their physical meaning is not yet understood, although many of the properties of separable spaces can be transferred to the nonseparable ones.

The reader may have noticed the absence of a *dimension axiom*. This axiom was omitted intentionally, since it is convenient to have a definition which is valid for finite- as well as for infinite-dimensional spaces.

In order to define the notion of the dimension, one needs the notion of linear independence. A finite or infinite sequence of vectors f_n is called *linearly independent* if a relation such as $\sum \lambda_n f_n = \mathbf{0}$ implies $\lambda_n = 0$ for all n. If this is not the case we shall call the sequence *linearly dependent*.

The maximal number of linearly independent vectors in $\mathscr{H}$ is called the *dimension* of $\mathscr{H}$. Thus we say $\mathscr{H}$ has the dimension $n = 1, 2, \ldots$, if there exists a set of n linearly independent elements in $\mathscr{H}$ but every set of $(n + 1)$ vectors is linearly dependent. If $n = \infty$, then we obtain what is usually called the Hilbert space.

An important question concerns the independence of the axioms. If the dimension $n < \infty$, then Axioms 3 and 4 are consequences of the others, but not for $n = \infty$.

If $\{f_\nu\}$ is a linearly independent sequence, then the set of all elements of the form

$$f = \sum_\nu \lambda_\nu f_\nu$$

is an example of a *linear manifold*. The elements of a linear manifold satisfy the axioms in groups 1 and 2 but *not* necessarily Axioms 3 and 4. The number n of elements in the set $\{f_\nu\}$ is called the *dimension* of the linear manifold. A formal definition and a more systematic discussion of linear manifolds will be given in Section 2-4.

If S is an arbitrary set of vectors in $\mathscr{H}$, we may consider the smallest linear manifold containing S. Such a linear manifold always exists and is unique. We call this the linear manifold *spanned* by S.

The positive definiteness of the scalar product implies the important inequality of Schwartz:

$$|(f, g)| \leq \|f\| \, \|g\|.$$

The proof of this is obtained immediately from the remark that the quantity $\|f + \alpha g\|^2$ is nonnegative for all complex numbers α, and for $\|g\| \neq 0$ its minimum is equal to†

$$\|f\|^2 - \frac{|(f, g)|^2}{\|g\|^2}.$$

One also sees from this proof that the equality sign holds if and only if f and g are linearly dependent.

An easy corollary is Minkowski's inequality (also called the triangle inequality):

$$\|f + g\| \leq \|f\| + \|g\|.$$

Hilbert space is not only a vector space but also a topological space. This means we have a notion of convergence (or equivalently the notion of open subsets). In order to define convergence we may use either the norm or the scalar product. When using the norm, we say a sequence f_n converges in the norm to f if

$$\lim_{n \to \infty} \|f_n - f\| = 0.$$

In this case we speak of *strong convergence.*

If we use the scalar product we may define a *weak convergence* as follows: The sequence f_n converges weakly towards f if, for every g,

$$\lim_{n \to \infty} (f_n, g) = (f, g).$$

The two kinds of convergence coalesce in finite dimensions, but not in infinite dimensions. A sequence which converges weakly toward a limit need not converge strongly toward anything (Problem 10).

Two vectors f and g with $(f, g) = 0$ are called *orthogonal.* A sequence of vectors $\{\varphi_\nu\}$ are called *orthonormal* if they satisfy

$$(\varphi_\mu, \varphi_\nu) = \delta_{\mu\nu}.$$

(We shall always denote vectors of norm 1 with Greek letters.)

† Cf. Problem 7.

For any vector f and any orthonormal sequence, Bessel's inequality (Problem 11) is valid for any f:

$$\sum_{\nu=1}^{\infty} |(\varphi_\nu, f)|^2 \leq \|f\|^2.$$

The orthonormal system $\{\varphi_\nu\}$ is called *complete* if Bessel's inequality is in fact an equality for any f. In that case one finds (Problem 11) that the partial sums $f_n \equiv \sum_{\nu=1}^{n} (\varphi_\nu, f)\varphi_\nu$ converge strongly towards f, so that one may write

$$f = \sum_{\nu=1}^{\infty} (\varphi_\nu, f)\varphi_\nu.$$

Such a system φ_ν is called a *coordinate system.* The existence of coordinate systems is an important consequence of separability (Axiom 3).

PROBLEMS

1. The complex numbers are a Hilbert space of dimension 1.
2. The set of all square matrices A of n rows and columns ($n < \infty$) makes up a Hilbert space of dimension n^2, if the scalar product is defined by $(A, B) = \mathrm{Tr}\, A^*B$, where Tr denotes the trace (sum of diagonal matrix elements).
3. In any Hilbert space one has the "law of the parallelogram":

$$\|f + g\|^2 + \|f - g\|^2 = 2\|f\|^2 + 2\|g\|^2.$$

*4. (Jordan and von Neumann [4].) A normed vector space permits the definition of a scalar product such that $(f, f) = \|f\|^2$ if and only if the norm satisfies the parallelogram law.

5. The vectors of a linear manifold satisfy the axioms in groups 1 and 2.
6. The intersection of any family $\mathcal{M}_i$ ($i \in I$) of linear manifolds is again a linear manifold.
7. For $g \neq 0$ the minimum value of $\|f + \alpha g\|^2$ as α runs through the complex numbers is

$$\|f\|^2 - \frac{|(f, g)|^2}{\|g\|^2}.$$

*8. (Generalization of the inequality of Schwartz.) Let $\{f_\nu,\}$ with $\nu = 1, \ldots, n$, be a finite set of vectors; then the determinant of Gram Det $(f_\nu, f_\mu) \geq 0$. Moreover, the equality sign holds if and only if the f_ν are linearly dependent.

9. Minkowski's inequality $\|f + g\| \leq \|f\| + \|g\|$ is a consequence of Schwartz's inequality.
10. Any infinite orthonormal sequence of vectors φ_n converges weakly to zero. No such sequence can converge strongly to a limit.
11. For any orthonormal system $\{\varphi_\nu\}$ one has the inequality

$$0 \leq \|f - \sum_{\nu} (\varphi_\nu, f)\varphi_\nu\|^2 = \|f\|^2 - \sum_{\nu} |(\varphi_\nu, f)|^2.$$

2-3. REALIZATIONS OF HILBERT SPACE

The axiomatic which we have described in the preceding two sections constitutes a definition of *abstract* Hilbert space. The abstract space is a most convenient notion when we wish to study very general properties which are not related to any particular realization of the space in terms of other mathematical objects. However, this is not the way Hilbert space appears in physics. In concrete physical problems involving quantum mechanics, Hilbert space appears always in a particular realization, for instance, as a function space or as a space of sequences of numbers.

Many realizations of Hilbert space are possible. Such realizations are also useful from a purely mathematical point of view, since they demonstrate that the axioms of Section 2-1 are consistent. We shall discuss only the infinite dimensional space here, since the finite dimensional case is already understood.

The first of these realizations is the space ℓ^2. It consists of all infinite sequences of complex numbers $f = \{x_n\}$ with the property

$$\sum_{n=1}^{\infty} |x_n|^2 < \infty.$$

If λ is a complex number, we define $\lambda f = \{\lambda x_n\}$, and if $g = \{y_n\}$ is another sequence with $\sum_{n=1}^{\infty} |y_n|^2 < \infty$, then we define

$$f + g = \{x_n + y_n\} \qquad \text{and} \qquad (f, g) = \sum_{n=1}^{\infty} x_n^* y_n.$$

One easily verifies the axioms of groups 1 and 2, but the proofs of the completeness and separability theorems require certain technical devices.

A second realization of Hilbert space is the function space $L^2(S, M, \mu)$ introduced at the end of Chapter 1. The elements of this space are classes of equivalent functions in $L^2(S, M, \mu)$, where two functions f and g are declared equivalent if

$$\int |f - g|^2 \, d\mu = 0.$$

The functions f and g are then equal a.e. with respect to the measure μ. If $f = \{f(x)\}$, $(x \in S)$, is a vector of this space, then we define $\lambda f = \{\lambda f(x)\}$. If $g = \{g(x)\}$ is another vector of this space, then we define

$$f + g = \{f(x) + g(x)\} \qquad \text{and} \qquad (f, g) = \int f^* g \, d\mu.$$

That with these operations we obtain a Hilbert space is a nontrivial assertion. Axioms 1 and 2 are easy enough to verify (Problem 3), but Axioms 3 and 4 are deep theorems [1].

If the measure μ is discrete and concentrated at an infinite number of points, we obtain a slight generalization of the space ℓ^2, consisting of all sequences $\{x_n\}$ subject to the condition that

$$\sum_{n=1}^{\infty} \rho_n |x_n|^2 < \infty,$$

for a fixed sequence of positive numbers ρ_n. If we choose for these numbers $\rho_n = 1$ we again obtain the space ℓ^2.

From the abstract point of view, all these different realizations represent the same abstract Hilbert space. This abstract space is completely determined by the axioms. Thus if we have two different realizations, then there exists a one-to-one mapping of one onto the other which preserves the Hilbert-space structure. Two realizations which stand in this relation to one another are said to be isomorphic. Two Hilbert spaces of the same dimensions are always isomorphic.

PROBLEMS

1. The space ℓ^2 is a linear vector space which satisfies the axioms of groups 1 and 2.

*2. The space ℓ^2 is separable and complete.

3. The function space $L^2(S, M, \mu)$ satisfies axioms 1 and 2 if scalar multiplication addition and scalar product are defined by

$$\lambda f = \{\lambda f(x)\},$$
$$f + g = \{f(x) + g(x)\},$$
$$(f, g) = \int f^* g \, d\mu.$$

2-4. LINEAR MANIFOLDS AND SUBSPACES

We shall now discuss with greater care a notion already introduced in Section 2-2, the linear manifold.

A subset $\mathcal{M}$ of a Hilbert space $\mathcal{H}$ is called a *linear manifold* if $f \in \mathcal{M}$ implies that $\lambda f \in \mathcal{M}$ and if $f \in \mathcal{M}$ and $g \in \mathcal{M}$ imply that $(f + g) \in \mathcal{M}$. We say the set $\mathcal{M}$ is stable with respect to multiplication with scalars and vector addition.

A linear manifold automatically satisfies axioms 1, 2, and 3. The first two are just the definition of linear manifold, and the third is a consequence of a theorem in topology which says that the subset of a separable set is also separable. But what about axiom 4?

Let us examine this question by means of an example. Consider the space ℓ^2. It is easy to verify (Problem 1) that all sequences with only a finite

number of components $\neq 0$ are a linear manifold in ℓ^2, which is not complete (Problem 2).

A vector $f \in \mathscr{H}$ is a limit vector of $\mathscr{M}$ if there exists a sequence of $f_n \in \mathscr{M}$ such that $f_n \to f$. If every limit vector of $\mathscr{M}$ belongs to $\mathscr{M}$, we call $\mathscr{M}$ a *closed linear manifold* M, or a *subspace*. A subspace is a Hilbert space. Every linear manifold $\mathscr{M}$ can be closed by adding to it all the limit vectors; if we want to express this process we denote it by $M = \bar{\mathscr{M}}$ and call it the *closure* of $\mathscr{M}$. The closure of $\mathscr{M}$ is thus the smallest subspace which contains $\mathscr{M}$.

If $\mathscr{S}$ is a set of vectors, we denote by $\mathscr{S}^\perp$ the set of all vectors orthogonal to all vectors of $\mathscr{S}$. Thus

$$\mathscr{S}^\perp = \{f : (f, g) = 0 \text{ for all } g \in \mathscr{S}\}.$$

It is easy to verify that $\mathscr{S}^\perp$ is a subspace (Problem 4). Furthermore, if $\mathscr{S}_1$ and $\mathscr{S}_2$ are two subsets of $\mathscr{H}$ such that $\mathscr{S}_1 \subset \mathscr{S}_2$, then $\mathscr{S}_2^\perp \subseteq \mathscr{S}_1^\perp$. Since $\mathscr{M} \subseteq M \equiv \bar{\mathscr{M}}$ it follows that $M^\perp \subseteq \mathscr{M}^\perp$ and therefore (Problem 8)

$$\mathscr{M}^{\perp\perp} \subseteq M^{\perp\perp} = M.$$

But M is the smallest subspace containing $\mathscr{M}$, and so we must have $\mathscr{M}^{\perp\perp} = M$. For every infinite dimensional subspace M there are infinitely many different linear manifolds which are dense in $\mathscr{M}$. (For physical applications the subspaces are more important than the linear manifolds.)

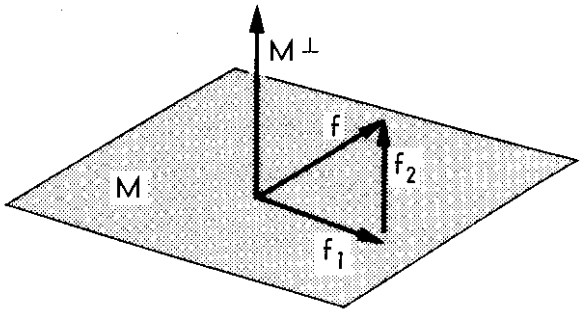

Fig. 2–1 Geometrical interpretation of the decomposition of a vector with respect to a subspace.

A very important property is the decomposition of vector f with respect to a subspace M: To every subspace M there belongs a unique decomposition $f = f_1 + f_2$ such that $f_1 \in M$ and $f_2 \in M^\perp$. The geometrical content of this theorem can be seen at a glance from Fig. 2–1.

These considerations can be generalized to more than one subspace. Suppose that $\{M_\nu\}$ is a sequence of mutually orthogonal subspaces such that $\{M_\nu\}^\perp = \mathbf{0}$. We say then that the M_ν span the entire space. We can then decompose every vector f in a unique manner as a sum

$$f = \sum_{\nu=1}^{\infty} f_\nu \qquad \text{with} \qquad f_\nu \in M_\nu.$$

This infinite sum is to be interpreted in the sense of strong convergence,

$$\left\| f - \sum_{\nu=1}^{n} f_\nu \right\| \to 0 \qquad \text{for} \qquad n \to \infty.$$

We say that the space $\mathscr{H}$ is represented as a direct sum of orthogonal subspaces M_ν, and we write

$$\mathscr{H} = M_1 \oplus M_2 \oplus \cdots \equiv \bigoplus_{\nu=1}^{\infty} M_\nu.$$

PROBLEMS

1. The set of all sequences $\{x_n\} \in \ell^2$ with only a finite number of $x_n \neq 0$, is a linear manifold $\mathscr{M}$ in ℓ^2 which is dense in ℓ^2.
2. The sequence $f_n = \{x_\nu^{(n)}\}$ defined by

$$x_\nu^{(n)} = \begin{cases} 1 & \nu \leq n \\ \dfrac{1}{\nu} & \\ 0 & \nu > n \end{cases}$$

   is a Cauchy sequence and therefore defines a limit f. All $f_n \in \mathscr{M}$ but $f \notin \mathscr{M}$. Thus $\mathscr{M} \subset \ell^2$.
3. The intersection of two subspaces is again a subspace.
4. The set $\mathscr{S}^\perp = \{f : (f, g) = 0 \text{ for all } g \in \mathscr{S}\}$ is a subspace.
5. If M and $M^\perp$ are two orthogonal subspaces, then the vectors f of the form $f = f_1 + f_2, f_1 \in M, f_2 \in M^\perp$, are a subspace.
6. The subspace of Problem 5 is the entire space.
7. If $f \in M$ and $f \in M^\perp$, then $f = \mathbf{0}$.
8. If M is a subspace then $M^{\perp\perp} = M$.

2-5. THE LATTICE OF SUBSPACES

While the preceding sections represent basic material of the theory of Hilbert space, the topic of this section is selected primarily with a view to the physical interpretation.

Let M and N be two subspaces. Their set-theoretic intersection $M \cap N$ is also a subspace. It is the largest subspace contained both in M and N. In a similar way we may define the smallest subspace containing both M and N, and we denote it by $M \cup N$.

The two operations $\cap$ and $\cup$ have properties similar to the set-theoretic intersections and unions introduced in Chapter 1, but there are some important differences which we shall now examine.

It is convenient to introduce sets of subspaces which are closed with respect to these two operations, intersection ($\cap$) and union ($\cup$). Such a system is an example of a *lattice*, and we denote it by $\mathscr{L}$.

If we require in addition that $\mathscr{L}$ be closed even with respect to a countably infinite number of intersections and unions, and, furthermore, that with M there is also $M^\perp$ in $\mathscr{L}$, then we obtain a complete, orthocomplemented lattice. Since $M \cap M^\perp = \mathbf{0}$ and $\mathbf{0}^\perp = \mathscr{H}$, such a lattice always contains $\mathbf{0}$ and $\mathscr{H}$. A formal definition and detailed discussion of this notion will be presented in Section 5-3.

If M_i ($i \in I$, some index set) is a family of subspaces, we denote the union and intersection of these subspaces by

$$\bigcup_i M_i = M_1 \cup M_2 \cup \cdots \qquad \text{and} \qquad \bigcap_i M_i = M_1 \cap M_2 \cap \cdots$$

The difference between this and the lattice of subsets of a set comes to light when we consider mixed operations involving unions and intersections in one and the same formula.

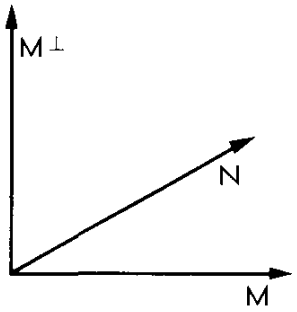

Fig. 2–2 Three subspaces of a two-dimensional space which do not satisfy the distributive law.

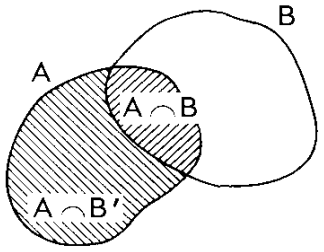

Fig. 2–3 Illustration of the relation $(A \cap B) \cup (A \cap B') = A$.

Let us examine this in a very special case which displays the characteristic features of the general situation. We take a two-dimensional Hilbert space $\mathscr{H}$ and choose two one-dimensional subspaces, M and $M^\perp$, for instance. Let N be any one-dimensional subspace $\neq M$ and $\neq M^\perp$; then we have (see Fig. 2–2)

$$N \cap (M \cup M^\perp) = N \cap \mathscr{H} = N,$$

but

$$N \cap M = \mathbf{0} = N \cap M^\perp.$$

We see therefore that the operations $\cup$ and $\cap$ do not always satisfy the distributive law as they do in the case for sets (Problem 3).

It is of great importance to have a criterion which tells under what conditions subspaces satisfy the distributive law. It is easy to see that for any pair of sets A and B we have an identity (Fig. 2–3):

$$(A \cap B) \cup (A \cap B') = A$$

which can be obtained immediately from the distributive law.

In the lattice of subspaces, the operation corresponding to the complement A' is the orthocomplement $M^\perp$. Thus we arrive at the following definition: Two subspaces M and N of a Hilbert space are called *compatible* if

$$(M \cap N) \cup (M \cap N^\perp) = M. \tag{2-1}$$

This defining property seems to be unsymmetrical. Actually it is not hard to show that the relation is, however, a symmetrical one (Problem 6), so that Eq. (2-1) implies also

$$(N \cap M) \cup (N \cap M^\perp) = N. \tag{2-2}$$

We shall introduce the notation $M \leftrightarrow N$ to designate two subspaces which satisfy either (and hence both) the relations (2-1) and (2-2).

There is another possibility of expressing the relation of compatibility. It is obtained by introducing the notion of disjoint subspaces. We say two subspaces M and N are *disjoint* if $M \subset N^\perp$. It follows then that $N \subset M^\perp$, so that the relation of disjointness is symmetrical. We shall write for it $M \perp N$.

Two subspaces M and N are compatible if there exist three mutually disjoint subspaces M_1, N_1, and K, such that

$$M = M_1 \cup K \qquad \text{and} \qquad N = N_1 \cup K.$$

It follows then that $K = M \cap N$ and $M_1 = M \cap K^\perp$, $N_1 = N \cap K^\perp$.

The following theorem finally gives the connection between compatibility and the distributive law:

Three subspaces L, M, and N which are pairwise compatible satisfy the distributive law

$$L \cap (M \cup N) = (L \cap M) \cup (L \cap N),$$

$$L \cup (M \cap N) = (L \cup M) \cap (L \cup N).$$

PROBLEMS

1. $M \cup N = (M^\perp \cap N^\perp)^\perp$.
2. The operations of intersection and union of subspaces are associative:

$$(M_1 \cap M_2) \cap M_3 = M_1 \cap (M_2 \cap M_3),$$
$$(M_1 \cup M_2) \cup M_3 = M_1 \cup (M_2 \cup M_3).$$

3. If A, B, and C are three subsets of a set, then one always has

$$A \cap (B \cup C) \supseteq (A \cap B) \cup (A \cap C)$$

and

$$A \cup (B \cap C) \subseteq (A \cup B) \cap (A \cup C).$$

4. If $M \subset N$ then $M \cup N = N$, and vice versa.
5. $M \leftrightarrow N$ implies

$$M \cup (N \cap M^{\perp}) = M \cup N = N \cup (M \cap N^{\perp}).$$

6. The relation $M \leftrightarrow N$ is symmetric.

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CHAPTER 3

LINEAR FUNCTIONALS AND LINEAR OPERATORS

Simplicio: "*Concerning natural things we need not always seek the necessity of mathematical demonstrations.*"
Sagredo: "*Of course, when you cannot reach it. But if you can, why not?*"

GALILEO GALILEI, Dialogue on the Two Major Systems of the World

The two notions of linear functionals and linear operators are closely related and are treated in this chapter side by side. Sections 3-1 and 3-3 correspond to each other in this sense, and Section 3-2 on sesquilinear functionals is the link between the two. The central theorem here is the theorem of Riesz, which shows that linear functionals are scalar products. In Section 3-4 we collect a number of useful properties on projections, and introduce the notion of spectral measure. In Section 3-5 we expose enough of the difficulties which one encounters with unbounded operators to warn the unwary of the pitfalls. Our tactics will be to avoid if possible the unbounded operators, and, if that cannot be done, to subject them to such severe conditions of propriety that they cannot cause trouble. In the applications we shall be dealing mostly with symmetrical (Hermitian) operators; and here the reader should retain the important distinction between "symmetrical" and "self-adjoint."

3-1. BOUNDED LINEAR FUNCTIONALS

A bounded linear functional $\phi(f)$ on a Hilbert space is a function with domain $\mathscr{H}$, which has for its range the complex numbers C, and which satisfies the following conditions:

$$\phi(f + g) = \phi(f) + \phi(g) \qquad \text{for all } f, g \in \mathscr{H}$$

$$\phi(\lambda f) = \lambda\phi(f); \qquad \text{and all } \lambda \in C;$$

$$|\phi(f)| < M \|f\| \qquad (M < \infty).$$

The greatest lower bound of the numbers M which satisfy the last inequality is called the norm $\|\phi\|$ of the functional $\phi(f)$.

The simplest example of a functional is the scalar product of f with a fixed vector g,

$$\phi(f) = (g, f). \tag{3-1}$$

One verifies without difficulty that the norm of this functional is $\|\phi\| = \|g\|$ (Problem 1).

The bounded linear functionals form a linear vector space if one defines addition of $\phi_1(f)$ and $\phi_2(f)$ by $(\phi_1(f) + \phi_2(f))$, and multiplication of $\phi(f)$ with a scalar λ by $\lambda\phi(f)$. They are also a normed vector space with the norm defined by $\|\phi\|$.

We shall now show that the linear functionals also constitute a Hilbert space; that is, there exists a scalar product in this space. First we verify that $\phi(f)$ is a continuous function with respect to the strong topology in $\mathscr{H}$. To see this, let $f_n \to f$, so that $\|f_n - f\| \to 0$ as $n \to \infty$. Then

$$|\phi(f_n) - \phi(f)| = |\phi(f_n - f)| \leq \|\phi\| \, \|f_n - f\|,$$

and the left side tends to zero with the right.

We can now prove the following theorem.

Theorem (Riesz): *Every bounded linear functional ϕ in a Hilbert space $\mathscr{H}$ is of the form $\phi(f) = (g, f)$ with g some fixed vector in $\mathscr{H}$.*

Proof: Let $\{\varphi_n\}$ be a complete orthonormal system in $\mathscr{H}$, and let $f = \sum_n x_n\varphi_n$. Since $\phi(f)$ is continuous we have

$$\phi(f) = \sum_{n=1}^{\infty} x_n\phi(\varphi_n).$$

We then define

$$g \equiv \sum_{n=1}^{\infty} \phi^*(\varphi_n)\varphi_n,$$

and find

$$(g,f) = \sum_{n=1}^{\infty} \phi(\varphi_n)x_n = \phi(f). \qquad \text{Q.E.D.}$$

With the theorem of Riesz we have no difficulty defining a scalar product for linear functionals as follows, by setting

$$(\phi_1, \phi_2) = (g_2, g_1)$$

where $\phi_1(f) = (g_1, f)$ and $\phi_2(f) = (g_2, f)$.

The linear functionals are thus a linear manifold with a scalar product (also called a pre-Hilbert space). Its closure in the norm is a Hilbert space called the *dual space* $\hat{\mathscr{H}}$ of $\mathscr{H}$. There exists a natural mapping of the linear functionals $\phi \in \hat{\mathscr{H}}$ onto the vectors of $\mathscr{H}$ by assigning to the linear functional $\phi(f) = (g, f)$ the vector $g \in \mathscr{H}$. If $\phi \to g$ in this mapping, then $\lambda\phi \to \lambda^* g$; and if $\phi_1 \to g_1$ and $\phi_2 \to g_2$, then $(\phi_1 + \phi_2) \to (g_1 + g_2)$. Such a mapping is called antilinear.

If in the linear functional $\phi(f) = (g, f)$ we keep the vector f fixed and let g vary over the space $\mathscr{H}$, then we obtain a *conjugate linear functional* $\Psi(g) = (g, f)$. If $\Psi(g)$ is conjugate linear, then $\Psi^*(g)$ (the complex conjugate of Ψ) is a linear functional.

It follows from the foregoing that the bounded linear functionals of $\mathscr{H}$ are again a Hilbert space $\hat{\mathscr{H}}$, and that there exists a natural norm preserving linear mapping of $\hat{\mathscr{H}}$ onto $\mathscr{H}$. We can thus identify $\hat{\mathscr{H}}$ with $\mathscr{H}$.

This duality property of Hilbert space is exploited by Dirac in his notation of the *bra* and *ket* vectors [1, p. 18]. In fact, a ket $|f\rangle$ is a vector $f \in \mathscr{H}$, and a bra $\langle g|$ is a linear functional over $\mathscr{H}$ which for f takes on the value $\langle g|f\rangle = (g, f)$.

PROBLEMS

1. The norm of the bounded linear functional $\phi(f) = (g, f)$ for some fixed vector g is equal to $\|g\|$.
2. The norm of a bounded linear functional satisfies the parallelogram law:

$$\|\phi_1 + \phi_2\|^2 + \|\phi_1 - \phi_2\|^2 = 2\,\|\phi_1\|^2 + 2\,\|\phi_2\|^2$$

   (use the Riesz theorem).
3. A bounded linear functional is determined everywhere by its values on a subset $S \subset \mathscr{H}$ which spans $\mathscr{H}$.
4. A bounded linear functional is strongly and weakly continuous.

3-2. SESQUILINEAR FUNCTIONALS AND QUADRATIC FORMS

A sesquilinear functional is a complex-valued function $\phi(f, g)$ of two variable vectors f and $g \in \mathscr{H}$. Thus the domain of such a functional is the topological product $\mathscr{H} \times \mathscr{H}$ of the Hilbert space with itself consisting of all pairs of vectors, and the range is the complex numbers.

We shall restrict our discussion in this subsection to bounded sesquilinear functionals which we define by the requirements:

For fixed f the functional $\phi(f, g)$ is a bounded linear functional of g.

For fixed g the functional $\phi(f, g)$ is a bounded conjugate linear functional of f.

If, in addition to these properties, $\phi(f, g) = \phi^*(g, f)$, then the functional ϕ is called *symmetrical.*

Every sesquilinear functional defines a certain *quadratic form* $\hat{\phi}(f) \equiv \phi(f, f)$. Conversely, every such quadratic form defines uniquely a sesquilinear

functional by the formula (Problem 1):

$$4\phi(f, g) \equiv \hat{\phi}(f + g) - \hat{\phi}(f - g) + i\hat{\phi}(f - ig) - i\hat{\phi}(f + ig).$$

The process expressed in this equation is known as *polarization.*

This last result shows that a sesquilinear functional $\phi(f, g)$ is in fact completely determined by its values on the diagonal $\phi(f, f)$, that is, by its associated quadratic form $\hat{\phi}(f)$. It follows from this remark that a sesquilinear functional is *symmetrical* if and only if its associated quadratic form is real.

A sesquilinear functional $\phi(f, g)$ is called *positive* if its associated quadratic form takes only positive values: $\hat{\phi}(f) \geq 0$. It is called *strictly positive* if $\hat{\phi}(f) = 0$ implies $f = \mathbf{0}$.

An example of a strictly positive sesquilinear functional is the scalar product $\phi(f, g) = (f, g)$.

If $\phi(f, g)$ is a sesquilinear functional, then for every fixed f this is a linear functional of g. Thus by Riesz' theorem we can associate an f' with every f by the formula

$$\phi(f, g) = (f', g) \qquad \text{for all } g \in \mathscr{H}.$$

The correspondence $f \to f'$ has the following properties: $\lambda f \to \lambda f'$ and $(f_1 + f_2)' = f_1' + f_2'$ (Problem 3). Such a correspondence is called a linear operator. We shall devote the next section to the study of such operators.

PROBLEMS

1. If $\hat{\phi}(f) \equiv \phi(f, f)$ for some sesquilinear functional ϕ, then
$$4\phi(f, g) = \hat{\phi}(f + g) - \hat{\phi}(f - g) + i\hat{\phi}(f - ig) - i\hat{\phi}(f + ig).$$
2. A sesquilinear functional is symmetrical if and only if its associated quadratic form is real.
3. The correspondence $f \to f'$ established by the equation
$$\phi(f, g) = (f', g) \qquad \text{for all } g \in \mathscr{H}$$
has the properties
$$(\lambda f)' = \lambda f', \qquad (f_1 + f_2)' = f_1' + f_2'.$$

3-3. BOUNDED LINEAR OPERATORS

A bounded linear operator T is a function with a linear manifold D_T as domain and a subset Δ_T in $\mathscr{H}$ as range, and such that

$$T(f + g) = Tf + Tg \qquad \text{for all } f, g \in D_T;$$

$$T(\lambda f) = \lambda Tf \qquad \text{for all } f \in D_T \text{ and all complex } \lambda;$$

$$\|Tf\| \leq M \|f\| \qquad \text{for } 0 \leq M < \infty.$$

It follows immediately from this definition that the range is also a linear manifold. The greatest lower bound of the numbers M which satisfy the last inequality is called the *norm* of the operator T and is denoted by $\|T\|$. If there does not exist such an $M < \infty$, then the operator is said to be *unbounded*. In this section we shall discuss only bounded operators.

If $f_1 \neq f_2$ implies $Tf_1 \neq Tf_2$, then there exists another linear operator T^{-1}, called the *inverse* of T, with domain $D_{T^{-1}} = \Delta_T$ and range $\Delta_{T^{-1}} = D_T$. It has the property

$$T^{-1}Tf = f \qquad \text{for all } f \in D_T,$$

$$TT^{-1}g = g \qquad \text{for all } g \in \Delta_T.$$

An operator is said to be *continuous* at $f \in D_T$ if $f_n \in D_T$ and $f_n \to f$ implies $Tf_n \to Tf$. Every bounded operator is continuous everywhere. Conversely, every linear operator which is continuous at one point is continuous everywhere and bounded. Continuity and boundedness are thus interchangeable concepts for linear operators. (See Problems 2 and 3.)

If T_1 is a bounded linear operator defined on $D_{T_1} \supset D_T$ and agreeing with T on D_T, then we say T_1 is an *extension* of T, and we write $T_1 \supset T$ (or $T \subset T_1$).

If $f_n \in D_T$ is a Cauchy sequence and $f_n \to f$, then if $f \notin D_T$ we define

$$Tf = \lim_{n \to \infty} Tf_n.$$

This limit always exists, because with f_n, Tf_n is also a Cauchy sequence:

$$\|Tf_n - Tf_m\| \leq \|T\| \, \|f_n - f_m\|.$$

With this assignment we obtain an extension of the linear operator from D_T to the closure $\bar{D}_T$ (Problem 4). For this reason we can always assume that a bounded linear operator is defined on a subspace; in particular, if D_T is dense in $\mathscr{H}$, this is the entire space. The domain can even be extended to all of $\mathscr{H}$ if D_T is not dense in $\mathscr{H}$. We first extend T to $\bar{D}_T$ by continuity. Then we *define* T on $D_T^{\perp}$ as an arbitrary bounded linear operator; for instance, $Tf = 0$ for $f \in D_T^{\perp}$. On a general $f \in \mathscr{H}$, the extended operator is then defined by linearity; it has the same norm as the original operator. When nothing specific is said about the domain of a bounded operator T, we shall always assume that we are dealing with this maximal extension.

This remark is especially useful if we want to define the sum and the product of linear operators. For instance, let T_1 and T_2 be two operators; then the *sum* of these two operators is defined by the formula:

$$(T_1 + T_2)(f) = T_1 f + T_2 f.$$

Similarly we define the *product* T_1T_2 by setting

$$T_1T_2(f) = T_1(T_2f).$$

We can also define a *multiplication with scalars* by

$$(\lambda T)(f) = \lambda(Tf),$$

and it is easily seen that if T_1, T_2, and T are bounded operators, their sum, product, and scalar multiples are also (Problem 5).

Every bounded linear operator defines a sesquilinear functional ϕ as follows:

$$\phi(f, g) \equiv (f, Tg).$$

At the end of the preceding section we have shown that the converse of this is also true. Actually, every such functional defines not one but two bounded linear operators T and T^* by the formula

$$\phi(f, g) = (T^*f, g) = (f, Tg).$$

The two operators T and T^* are said to be *adjoint* to one another. One easily verifies the following properties:

$$(T_1T_2)^* = T_2^*T_1^*;$$

$$(\lambda T)^* = \lambda^*T^* \qquad (\lambda^* = \text{complex conjugate } \lambda);$$

$$(T_1 + T_2)^* = T_1^* + T_2^*;$$

$$(T^*)^* = T.$$

An operator T for which $T^* = T$ is called *self-adjoint* or symmetrical. From the definition of the adjoint operator one easily verifies that $\|T^*\| = \|T\|$ (Problem 6).

We describe a few examples of bounded linear operators.

1) The *identity operator* I: This is the operator which does nothing to the vectors so that $If = f$, for all $f \in \mathscr{H}$.

2) The *projection operators* E, defined everywhere, are characterized by the property $E^*E = E$.

   Every projection operator determines a subspace which is its range; and conversely, every subspace M determines a unique projection E with range M (Problem 7).

   If $f = f_1 + f_2$ with $f_1 \in M$ and $f_2 \in M^\perp$, then the projection E with range M is defined by the equation

$$Ef = f_1.$$

3) The *partial isometries* Ω are linear operators with the property: $\Omega^*\Omega = E$ is a projection. It is easy to verify that $F = \Omega\Omega^*$ is then also a projection (Problem 8). E and F are called *right-* and *left*-projections respectively.

4) The *unitary operators* are a special class of isometries, namely those for which both E and F are unit operators. Thus U is unitary if

$$U^*U = UU^* = I.$$

The prototype of an isometry which is not unitary is the *shift-operator* defined as follows: Let $\{\varphi_n\}$ $(n = 1, 2, \ldots)$ be a complete orthonormal system, and define the operator Ω on all φ_n by

$$\Omega\varphi_n = \varphi_{n+1}.$$

One easily finds then that Ω^* satisfies

$$\Omega^*\varphi_{n+1} = \varphi_n \qquad \text{and} \qquad \Omega^*\varphi_1 = \boldsymbol{\theta}.$$

For all other f we define

$$\Omega f = \sum_{n=1}^{\infty} x_n \Omega\varphi_n \qquad \text{if} \quad f = \sum_{n=1}^{\infty} x_n\varphi_n.$$

From these definitions it follows that

$$\Omega^*\Omega\varphi_n = \varphi_n \qquad (n = 1, 2, \ldots).$$

Thus $\Omega^*\Omega = I$. Furthermore,

$$\Omega\Omega^*\varphi_n = \varphi_n \quad \text{with } n = 2, 3, \ldots, \qquad \text{and} \qquad \Omega\Omega^*\varphi_1 = \boldsymbol{\theta}.$$

Thus we have verified that $\Omega\Omega^*$ is a projection on the orthogonal complement of φ_1.

Another example of an isometry is the continuous shift operator defined as follows: Let $\mathscr{H} = L^2(0, \infty)$, so that $f = \{f(x)\}$ when $0 \leq x < \infty$. If we set $f(x) = 0$ for $x < 0$, we can define an operator Ω by setting

$$(\Omega f)(x) = f(x - a), \qquad (\Omega^* f)(x) = f(x + a).$$

With this definition we find

$$(\Omega^*\Omega f)(x) = f(x),$$

$$(\Omega\Omega^* f)(x) = \begin{cases} f(x) & \text{for } x \geq a, \\ 0 & \text{for } x < a. \end{cases}$$

Thus we have verified that Ω is an isometry.

Examples of bounded self-adjoint linear operators are obtained easily as follows: Let $\{\varphi_n\}$ be a complete orthonormal system; define $A\varphi_n = \lambda_n\varphi_n$ (λ_n real) and extend by linearity to the entire space.

The sesquilinear functional associated with a self-adjoint operator is symmetrical (cf. Section 3-2), and every such functional defines a self-adjoint operator (Problem 10). We shall call a self-adjoint operator a *positive* operator if its associated quadratic form is positive.

PROBLEMS

1. The correspondence $f \to (\varphi, f)\varphi$ for some fixed normalized φ is a bounded linear operator with bound 1.
2. If a linear operator is continuous at one point, it is continuous everywhere.
3. A linear operator is continuous if and only if it is bounded.
4. Every bounded linear operator T with domain D_T admits a unique extension T_1 to the closure $\overline{D}_T$ without changing the norm, so that
$$D_{T_1} = \overline{D}_T \qquad \text{and} \qquad \|T_1\| = \|T\|.$$
5. If T_1 and T_2 are bounded linear operators, then $(T_1 + T_2)$ and T_1T_2 are, too. Furthermore, the bounds satisfy the inequalities
$$\|T_1 + T_2\| \leq \|T_1\| + \|T_2\|, \qquad \text{and} \qquad \|T_1T_2\| \leq \|T_1\|\,\|T_2\|.$$
6. $\|T^*\| = \|T\|$.
7. Every projection operator defines a unique subspace which is its range, and vice versa.
8. If Ω is a linear operator such that $\Omega^*\Omega = E$ is a projection, then $\Omega\Omega^* = F$ is also a projection.
9. In a finite-dimensional space, every isometry with right projection $E = I$ is unitary (that is, its left projection is also I).
10. A bounded self-adjoint operator defines a symmetrical sesquilinear functional, and vice versa.

3-4. PROJECTIONS

A linear operator E defined on all of $\mathscr{H}$ and satisfying the relation $EE^* = E$ is called a *projection*. It follows immediately from this relation that $E = E^*$ and consequently $E^2 = E$. Projections are thus self-adjoint and *idempotent*. The range Δ_E of a projection is a subspace, and to every subspace there corresponds a unique projection. We have therefore a one-to-one correspondence of projections to subspaces which permits us to replace one by the other.

It follows from this remark that the entire lattice structure of subspaces can be transferred to projections. They are, as are the subspaces, a partially ordered system. For instance, we say that $E_1 \leq E_2$ if for the corresponding subspaces M_1 and M_2 we have $M_1 \subseteq M_2$. It is easy to show that $E_1 \leq E_2$ if and only if $E_1E_2 = E_1$ (Problem 1).

If E is a projection with range M, then $(I - E)$ is the projection with range $M^\perp$. These remarks show that certain relations in the lattice of subspaces can be easily expressed in terms of *algebraic* operations on corresponding projections.

It is natural to ask the question how the operations of union and intersection of subspaces are expressed algebraically in terms of the corresponding projections: Let M_1 and M_2 be two subspaces, and E_1 and E_2 the projections with ranges M_1 and M_2 respectively. We have defined the intersection $M_1 \cap M_2$ as the subspace consisting of all the vectors common to M_1 and M_2. The projection F with range $N = M_1 \cap M_2$ must be a function of the projections E_1 and E_2. We shall denote it by $F = E_1 \cap E_2$, and it is by definition the largest projection contained in E_1 and in E_2. What is this function?

Our first impulse might be to suggest the answer $F = E_1E_2$. But this cannot be generally right, since F is a projection only if E_1 and E_2 commute (Problem 2). In that case the answer is correct, and $F \equiv E_1 \cap E_2 = E_1E_2$ (Problem 3).

If E_1 and E_2 do not commute, then the problem of finding $E_1 \cap E_2$ as a function of E_1 and E_2 is more difficult. We give here the result and shall be content with an illustration of the result in a special case.

Let us consider the situation of Fig. 3–1. The two projections E_1 and E_2 are represented by two (nonorthogonal) one-dimensional subspaces. The vectors $f_n = (E_1E_2)^n f$ are seen to converge to zero, illustrating that for this special case

$$E_1 \cap E_2 = \lim_{n \to \infty} (E_1E_2)^n = 0.$$

The general formula valid for any two projections is

$$E_1 \cap E_2 = \lim_{n \to \infty} (E_1E_2)^n. \qquad (3\text{–}2)$$

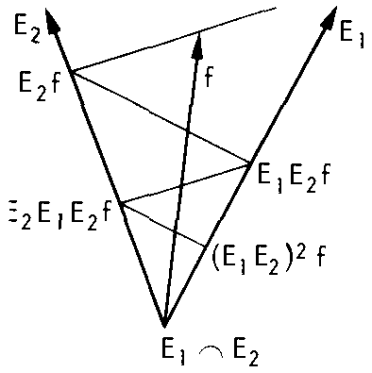

Fig. 3–1 Illustration of the formula

$$E_1 \cap E_2 = \lim_{n \to \infty} (E_1E_2)^n.$$

If E_1 and E_2 commute, then $(E_1E_2)^n = E_1E_2$, and we find, as before, that $E_1 \cap E_2 = E_1E_2$. It follows then that $E_1 \cup E_2 = E_1 + E_2 - E_1E_2$ (Problem 3).

Of special importance in quantum mechanics are families of commuting projections which are closed with respect to countable unions and intersections. If $\mathscr{L}$ is such a family and $E_n \in \mathscr{L}$ a sequence of projections in $\mathscr{L}$, then $\bigcup_n E_n$ and $\bigcap_n E_n$ are again in $\mathscr{L}$. Furthermore, with $E \in \mathscr{L}$, also $(I - E) \in \mathscr{L}$. If $\mathscr{L}$ contains also 0 and I, we obtain a Boolean algebra.

A canonical way of constructing such Boolean algebras of projections is the following:

Let $\mathscr{H} = L^2(S, M, \mu)$ and $\Delta \in M$ an arbitrary measurable set. To any such set one can associate a projection $E(\Delta)$ by defining, for any $f(x) \in L^2(S, M, \mu)$, $(x \in S)$, the operator $E(\Delta)$:

$$(E(\Delta)f)(x) = \chi_\Delta(x) f(x), \qquad (3\text{–}3)$$

where $\chi_\Delta(x)$ is the characteristic function of the set Δ; that is, the function defined by

$$\chi_\Delta(x) = \begin{cases} 1 & \text{for } x \in \Delta, \\ 0 & \text{for } x \notin \Delta. \end{cases}$$

Because the class M of measurable sets is σ-additive, the projections $E(\Delta)$ are σ-additive, too. That is, if Δ_n is any sequence of disjoint sets, then

$$\text{(a)} \qquad \sum_{n=1}^{\infty} E(\Delta_n) = E\left(\bigcup_{n=1}^{\infty} \Delta_n\right).$$

Furthermore, for any two sets Δ_1, Δ_2, we have

$$\text{(b)} \qquad \begin{aligned} E(\Delta_1) \cap E(\Delta_2) &= E(\Delta_1 \cap \Delta_2), \\ E(\Delta_1) \cup E(\Delta_2) &= E(\Delta_1 \cup \Delta_2); \end{aligned}$$

and finally,

$$\text{(c)} \qquad \begin{aligned} E(\emptyset) &= 0, \\ E(S) &= I. \end{aligned}$$

Such a map from the class of sets M to a Boolean algebra of projections which satisfies the relations (a), (b), and (c) is called a *spectral measure* over the measure space (S, M, μ). This fundamental notion will be used constantly in the following discussion.

The canonical spectral measure defined by the special property (3–3) is, of course, especially simple to realize. The spectral measure is obviously a generalization of a numerical measure. Instead of assigning a number to the sets, the spectral measure assigns projections in a Hilbert space. From any spectral measure, one can easily obtain a large number of numerical measures. It suffices to define for an arbitrary vector f

$$\mu_f(\Delta) = (f, E(\Delta)f).$$

This definition of measures depending on vectors f will be of great importance later on.

PROBLEMS

1. If E_1 and E_2 are two projections, and Δ_{E_1} and Δ_{E_2} their corresponding ranges, then $\Delta_{E_1} \subseteq \Delta_{E_2}$ if and only if $E_1E_2 = E_1$.
2. If E_1 and E_2 are projections, then $F = E_1E_2$ is one if and only if $E_1E_2 = E_2E_1$.
3. If $E_1E_2 = E_2E_1$, then $E_1 \cap E_2 = E_1E_2$ and $E_1 \cup E_2 = E_1 + E_2 - E_1E_2$.
4. Three commuting projections E_1, E_2, and E_3 satisfy the distributive law,

$$E_1 \cap (E_2 \cup E_3) \quad (E_1 \cap E_2) \cup (E_1 \cap E_3),$$

$$E_1 \cup (E_2 \cap E_3) \quad (E_1 \cup E_2) \cap (E_1 \cup E_3).$$

3-5. UNBOUNDED OPERATORS

We cannot avoid discussing the unbounded operators since they are constantly used in quantum mechanics. We do it here primarily to acquaint the reader with the mathematical complications which one encounters with unbounded operators. (For a more complete discussion, see reference 2.)

An unbounded linear operator is such that $\|Tf\|/\|f\|$ exceeds all finite bounds. For such operators one can always find an f such that for any finite M we have

$$\|Tf\| > M\,\|f\|.$$

Such operators exist only in the infinite-dimensional Hilbert space. In the finite-dimensional case every linear operator is bounded (Problem 1).

An example of an unbounded operator is easily constructed, for instance as follows: Let $\{\varphi_n\}$ be a complete orthonormal system and define $A\varphi_n = n\varphi_n$. The domain D_A of this operator consists of all linear combinations

$$f = \sum_{n=1}^{\infty} x_n\varphi_n \qquad \text{such that} \qquad \sum_{n=1}^{\infty} n^2\,|x_n|^2 < \infty.$$

This is a dense linear manifold $\subset \mathscr{H}$. The operator is unbounded because $\|A\varphi_n\| = n$; thus for n sufficiently large this norm exceeds any finite quantity. It is easy to verify that this operator cannot be continuous. Consider, for instance, the sequence of vectors $f_n = (1/n)\varphi_n$. We obtain $Af_n = \varphi_n$, and this does not tend to zero, although f_n does. Thus A is not continuous. We also observe that A is not defined everywhere in $\mathscr{H}$ since the vector f with components $x_n = 1/n$ is not contained in D_A.

These properties are, in a certain sense, to be made precise now, also characteristic, for the unbounded operators. In order to explain this in more detail we need a new concept which replaces that of continuity in the unbounded case.

A linear operator T is called *closed* if, for every sequence of vectors f_n in the domain D_T of T, the relations

$$f_n \to f \qquad \text{and} \qquad Tf_n \to g$$

imply that $f \in D_T$ and that $Tf = g$. Superficially this definition seems to be like the definition of continuity. But there is an important difference: For the definition of continuity, f is assumed to be in D_T and $Tf_n \to Tf$ is asserted, while for a closed operator, f is *asserted* to be in D_T under the assumption that Tf_n converges.

Since the domain of a continuous operator is always closed (cf. Section 3-3), a continuous operator is always closed, but there are closed operators which are not continuous.

An operator which is not closed may be extended to a closed one. We shall not examine under what conditions such an extension is possible. Suffice

it to remark here that all the unbounded operators which we need to consider do admit closures. If the closure is possible it is unique.

For closed unbounded operators one can prove that they cannot be defined in the entire space. We have the following theorem :

Theorem: *Every closed linear transformation on $\mathscr{H}$ is necessarily bounded* [3].

Let us now examine the definition of the adjoint transformation. This is a little more delicate, since D_T is not the entire space. We can and will, however, assume in the following discussion that D_T is dense in $\mathscr{H}$. This is not a severe restriction. Let us consider the expression $\Phi(g) = (f, Tg)$ for a fixed f. If there exists a vector f^* with the property

$$(f, Tg) = (f^*, g) \qquad \text{for all } g \in D_T,$$

then we say $f \in D_{T^*}$ and we *define* the operator T^* by setting $T^*f = f^*$. The operator T is called *symmetrical* (or Hermitian) if $T^* \supseteq T$; we have called an operator *self-adjoint* if $T^* = T$. Such an operator is thus always symmetrical.

In general we have the following situation for symmetrical operators T:

$$T \subseteq T^{**} \subseteq T^*,$$

and we may distinguish the following cases :

1) $T = T^{**}$ but $T^{**} \subset T^*$. The operator T is closed but not self-adjoint.
2) $T \subset T^{**} = T^*$. The operator T is not closed but its smallest closed extension T^{**} is self-adjoint (Problem 7). It is then called *essentially self-adjoint*.
3) $T \subset T^{**} \subset T^*$. The operator T is neither closed nor essentially self-adjoint.
4) $T = T^{**} = T^*$. The operator T is self-adjoint and hence closed.

A closed symmetrical operator, if it is not self-adjoint, may admit further symmetrical extensions. If there are no further extensions possible, then the symmetrical operator is called *maximal*. If there exists a maximal and self-adjoint extension, then the extended operator is called hypermaximal (see von Neumann [4]).

Von Neumann has given a complete characterization of symmetrical operators and their various extensions. In quantum mechanics the only symmetrical operators which have any useful physical interpretation are the essentially self-adjoint operators, in which we shall therefore be particularly interested.

The restriction in the domain of unbounded operators poses a great difficulty in the formation of sums and products of operators. Consider, for instance, the operators T_1 and T_2 with their respective domains D_1 and D_2.

The operator $T_1 + T_2$ is then definable only in the intersection $D_1 \cap D_2$, and there it is given by

$$(T_1 + T_2)f = T_1 f + T_2 f.$$

Similarly, for the definition of a product operator $T_1 T_2$, we need the conditions $f \in D_2$ and $T_2 f \in D_1$. Then we can define

$$(T_1 T_2)f = T_1(T_2 f).$$

The intersection of two domains is of course again a linear manifold, but it need not be dense. In fact it can be $\mathbf{0}$, even if both D_1 and D_2 are dense. It is seen from these remarks that the definition of sums and products of unbounded operators is already quite complicated for merely two operators.

There are two situations when a simplification is possible. The first occurs when there exists a common dense domain for two operators which is also invariant under the operations. The restriction of the operators to this dense domain permits the definition of unrestricted sums and products, and hence the formation of any algebraic expression.

The other simplification occurs when one of the two operators is bounded. Let T be an unbounded, and B any bounded operator; then $(T + B)$ and BT are defined in D_T. On the other hand, TB is defined only on the elements f for which $Bf \in D_T$.

This leads us to the definition: A bounded operator B commutes with the (unbounded) operator T if TB is an extension of BT,

$$BT \subseteq TB.$$

In particular, if B is a projection E, then $ET \subseteq TE$ implies $ETE = TE = ET$. A projection E which stands with an operator T in this relation is said to *reduce* T.

If the projection E reduces T, then $F = (I - E)$ also reduces T. We can then decompose the operator into two: $T = T^E + T^F$, where $T^E = TE$, $T^F = TF$ are called the reductions of T to the subspaces $M = E\mathscr{H}$ and $N = F\mathscr{H}$ respectively. T^E operates only in M and T^F only in N.

3-6. EXAMPLES OF OPERATORS

1. The position operator Q. The position operator Q is defined in a subset D_Q of the space $L^2(-\infty, +\infty)$ consisting of all Lebesgue square-integrable functions $\psi(x)$ by setting

$$(Q\psi)(x) = x\psi(x).$$

The subset D_Q is defined by

$$D_Q = \left\{\psi(x) : \int_{-\infty}^{+\infty} x^2 |\psi(x)|^2 \, dx < \infty\right\}.$$

The operator Q is symmetrical, since for every $\varphi \in D_Q$ and every $\psi \in D_Q$, we have

$$(\psi, Q\varphi) = \int_{-\infty}^{+\infty} x\psi^*(x)\varphi(x)\,dx = (Q\psi, \varphi).$$

This equation shows that for all such ψ, $Q^*\psi$ is defined and, in fact, $Q^*\psi = Q\psi$. Thus $D_Q \subseteq D_{Q^*}$ and $Q \subseteq Q^*$.

We shall now show that, for this domain D_Q, the operator Q is also self-adjoint. To see this, we verify that in fact $D_{Q^*} \subseteq D_Q$ so that $Q = Q^*$. Thus let $\psi \in D_{Q^*}$ and define $\psi_1 = Q^*\psi$; then

$$(\psi, Q\varphi) = (\psi_1, \varphi) \qquad \text{for all } \varphi \in D_Q.$$

Thus

$$\int_{-\infty}^{+\infty} (x\psi^*(x) - \psi_1(x))\varphi(x)\,dx = 0 \qquad \text{for all } \{\varphi(x)\} \in D_Q.$$

Since D_Q is dense in $\mathscr{H}$ we must have, a.e.,

$$x\psi(x) = \psi_1(x).$$

Therefore $\psi \in D_Q$ and $\psi_1 = Q\psi$.

2. The momentum operator. The operator P is defined on the subset D_P which consists of all absolutely continuous functions $\psi(x)$ which are differentiable a.e., and for which $(d\psi/dx) \in L^2(-\infty, +\infty)$. On this the set operator P is defined by

$$(P\psi)(x) = -i\,\frac{d\psi(x)}{dx}.$$

One can show that this operator, too, is self-adjoint [2, Chapter IV].

There exists, furthermore, a common dense domain D which is invariant under the operations Q and P, and on which both operators are defined. For any $\varphi \in D$ one finds (Problem 8)

$$(QP - PQ)\varphi = i\varphi. \tag{3–4}$$

We see that the operator $QP - PQ$ is bounded on the dense domain D, and therefore admits a unique extension to the entire space; so we may write the operator equation

$$QP - PQ \subset iI. \tag{3–5}$$

We shall call this the *canonical commutation rule*. It plays a fundamental role in quantum mechanics.

It is usually (incorrectly) written $QP - PQ = iI$, which disregards the fact that the left-hand side is defined only on a dense domain.

3. The creation and annihilation operators A^* and A. Let φ_n $(n = 0, 1, \ldots)$ be a complete orthonormal system in an abstract Hilbert space $\mathscr{H}$. Define

$$A\varphi_n = \sqrt{n}\varphi_{n-1} \qquad (n = 1, 2, \ldots),$$

$$A^*\varphi_n = \sqrt{n+1}\varphi_{n+1} \qquad (n = 0, 1, 2, \ldots),$$

$$A\varphi_0 = 0.$$

By linearity we can extend the definition of A and A^* to all linear combinations

$$f = \sum_{n=0}^{\infty} x_n\varphi_n \qquad \text{for which} \qquad \sum_{n=0}^{\infty} |x_n|^2 n < \infty.$$

On such f we define

$$Af = \sum_{n=0}^{\infty} x_n A\varphi_n = \sum_{n=1}^{\infty} x_n\sqrt{n}\varphi_{n-1}$$

and

$$A^*f = \sum_{n=0}^{\infty} x_n A^*\varphi_n = \sum_{n=0}^{\infty} x_n\sqrt{n+1}\varphi_{n+1}.$$

The two operators A and A^* are then the adjoint of one another, and $D_A = D = D_{A^*}$, so that the * has the usual significance of the adjoint for unbounded operators. There is a simple relation between the operators A, A^* on the one hand and Q, P on the other (Problem 9).

PROBLEMS

1. In a finite-dimensional Hilbert space, every linear operator is bounded.
2. The set of elements f with the property that, for some unbounded operator T with dense domain, there exists a vector f^* such that

$$(f, Tg) = (f^*, g) \qquad \text{for all } g \in D_T,$$

   is a linear manifold D_{T^*}.
3. If D_T is dense, then the vector f^* of Problem 2 is unique.
4. The operator T^* is always closed.
5. Every symmetrical operator T admits a closed symmetrical extension, namely T^{**}.
6. If E reduces the operator T, then F $(I$ $E)$ also reduces T.
7. If the symmetrical operator A has the property A^{**} A^*, then its smallest closed symmetrical extension A A^{**} is self-adjoint.

8. The functions

$$\varphi_n(x) = \frac{1}{\sqrt{\sqrt{\pi}\, 2^n n!}} e^{-x^2/2} H_n(x) \qquad (n = 0, 1, \ldots),$$

where $H_n(x)$ are the polynomials of Hermite [5, p. 62], are a complete orthonormal system in $L^2(-\infty, +\infty)$; and the finite linear combinations of the $\varphi_n(x)$ are a dense linear manifold D which is invariant under P and Q, and on which both P and Q are defined. For every $\varphi \in D$ one verifies

$$(QP - PQ)\varphi = i\varphi.$$

9. The operators

$$A = \frac{1}{\sqrt{2}}(Q + iP) \qquad \text{and} \qquad A^* = \frac{1}{\sqrt{2}}(Q - iP)$$

are adjoints of each other on the domain

$$D = \left\{ f : \sum_{n=0}^{\infty} |(f, \varphi_n)|^2 \, n < \infty \right\},$$

and they satisfy

$$A\varphi_n = \sqrt{n}\varphi_{n-1} \qquad (n = 1, 2, \ldots),$$

$$A\varphi_0 = 0,$$

$$A^*\varphi_n = \sqrt{n+1}\varphi_{n+1} \qquad (n = 0, 1, 2, \ldots).$$

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CHAPTER 4

SPECTRAL THEOREM AND SPECTRAL REPRESENTATION

Unless the vessel's pure, all you pour in turns sour.

HORACE

In this chapter we are concerned primarily with those aspects of self-adjoint linear operators which have to do with their realizations in a function space. Most of the practical calculations in the applications are done by means of such realizations. There is a canonical realization which we call the spectral representation. It uses for its Hilbert space a certain function space over the spectrum of the operator.

In order to formulate the spectral representation, we need several basic concepts and theorems which we introduce in an informal manner in Section 4-1, in the context of finite-dimensional spaces. There we present the notions of spectrum, spectral measure, simple spectrum, and spectral representation unencumbered by technical details of topology and measure theory.

In Section 4-2, we give the definition of the spectrum of a self-adjoint operator in terms of the domain of the resolvent operator. The central theorem of this chapter, the spectral theorem, is stated without proof in Section 4-3. It establishes a unique correspondence between spectral measures and self-adjoint operators, and it is an indispensable tool in the establishment of a functional calculus as explained in the following section (4-4). In Section 4-5, we prepare the ground for the spectral representation by studying some properties of the spectral density functions. This clarifies the role of the cyclic vector and leads to two equivalent definitions of the simple spectrum of an operator.

Section 4-6 gives a formulation of the spectral representation. The case of one operator is explained in sufficient detail to complete the existence proof without too much trouble, and to make the subsequent generalization to a countable family of operators at least plausible. In the final section (4-7), we sketch the method of eigenfunction expansion which, if available, gives a convenient method for calculating the spectral representation.

4-1. SELF-ADJOINT OPERATORS IN FINITE-DIMENSIONAL SPACES

In this section $\mathscr{H}$ will be a finite-dimensional Hilbert space, and we denote its dimension by $n < \infty$. We shall briefly recapitulate the principal properties of the self-adjoint linear operators A in $\mathscr{H}$. Since $n < \infty$,

$$D_A = \Delta_A = \mathscr{H}.$$

The equation $f' = Af$, which associates with every $f \in \mathscr{H}$ another $f' \in \mathscr{H}$, can always be realized as a finite linear system of equations by introducing a complete orthonormal system $\{\varphi_r\}$ with $r = 1, \ldots, n$, and $(\varphi_r, \varphi_s) = \delta_{rs}$. If

$$f = \sum_{r=1}^{n} x_r \varphi_r \qquad \text{and} \qquad f' = \sum_{r=1}^{n} x_r' \varphi_r,$$

then

$$x_r' = \sum_{s=1}^{n} A_{rs} x_s,$$

where

$$A_{rs} = (\varphi_r, A\varphi_s) = A_{sr}^* \qquad (r, s = 1, \ldots, n).$$

The structure of the operator is revealed by referring it to a particular coordinate system, consisting of *eigenvectors*. They are the nontrivial solutions of the equations

$$A\psi_r = \lambda_r \psi_r \qquad (r = 1, \ldots, n).$$

One can show that there always exist n nontrivial solutions of this equation where the numbers λ_r, *the eigenvalues*, are the solutions of the *secular equation*

$$|A_{rs} - \lambda \delta_{rs}| = 0.$$

The determinant of the left-hand side of this equation is a polynomial in λ and it has, according to the fundamental theorem of algebra, exactly n solutions; since A_{rs} is Hermitian, they are all real. These solutions are called the spectrum of the operator A. Some of these solutions may coincide; they must then be counted with their proper multiplicity. In the special case in which the roots are all simple (that is, of multiplicity 1), we shall call the eigenvalues *nondegenerate* and the spectrum *simple*.

The following facts are easily verified: If $\lambda_r \neq \lambda_s$, then the corresponding eigenvectors ψ_r and ψ_s are orthogonal: $(\psi_r, \psi_s) = 0$. Furthermore, if the eigenvalue λ_r has multiplicity $\alpha(r)$, then there exist $\alpha(r)$ linearly independent eigenvectors ψ_r with this eigenvalue (Problems 1 and 2). The eigenvectors which belong to λ_r are then an $\alpha(r)$-dimensional subspace of $\mathscr{H}$.

From the preceding remarks it follows that there always exists a coordinate system in $\mathscr{H}$ consisting of eigenvectors ψ_r $(r = 1, 2, \ldots, n)$. If the λ_r are all nondegenerate, the ψ_r are already orthogonal and complete. If they

are degenerate we can choose them to be so in many different ways. In this coordinate system the operator A appears in a particularly simple form: If $f = \sum_{r=1}^{n} x_r \psi_r$, then $f' = Af = \sum_{r=1}^{n} x'_r \psi_r$ with $x'_r = \lambda_r x_r$. This is the *spectral representation* of A.

For the sake of later generalizations of this important result, we shall formulate it as follows.

We have really two different spaces: $\mathscr{H}$ and ℓ_n^2. The latter consists of all sequences of n complex numbers $\{x_r\}$ with $r = 1, 2, \ldots, n$. By the formula $x_r = (\psi_r, f)$ we establish a one-to-one correspondence Ω between vectors f in the abstract space $\mathscr{H}$ and sequences $\{x_r\}$ in ℓ_n^2. This correspondence is isometric if the norm of sequences $\{x_r\}$ is defined by

$$\|\{x_r\}\|^2 = \sum_{r=1}^{n} |x_r|^2$$

(Problem 4). Isometric means that if $\{x_r\} = \Omega f$, then

$$\sum_{r=1}^{n} |x_r|^2 = \|f\|^2.$$

Two Hilbert spaces which are the linear isometric image of each other are identical in their abstract structure.

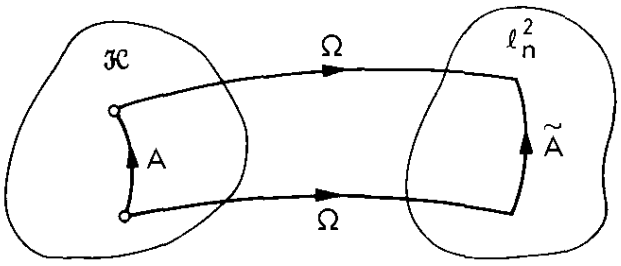

Fig. 4–1 Illustrating the equation $\tilde{A} = \Omega A \Omega^{-1}$.

The operator A defined in $\mathscr{H}$ may be considered an operator in ℓ_n^2 via the isometric image Ω of $\mathscr{H}$ onto ℓ_n^2. We shall denote it by $\tilde{A}$. Thus $\tilde{A} = \Omega A \Omega^{-1}$, and (cf. Fig. 4–1)

$$\tilde{A}\{x_r\} = \{\lambda_r x_r\}. \tag{4–1}$$

Every self-adjoint operator permits a spectral representation in finite-dimensional spaces. We are interested in the generalization of this result to the infinite-dimensional Hilbert space. In order to formulate the spectral representation in Hilbert space, it is necessary to introduce some new concepts which will permit an alternative but equivalent formulation of the above result. The main difficulty which we must negotiate is connected with the use of the coordinate system $\{\psi_r\}$. In Hilbert space a complete system of eigenvectors does not necessarily exist. It is thus necessary to seek a formulation which does not use such a system.

Let us begin by an alternative definition of the spectrum Λ of the operator A. We have seen that Λ is the set of numbers λ for which the equation $(A - \lambda \cdot I)\psi = \mathbf{0}$ has nontrivial solutions. In other words, if $\lambda \notin \Lambda$, then

this equation has only the trivial solution $\psi = \mathbf{0}$. A linear operator which has this property admits an inverse, which is again a linear operator. This means the operator

$$R_\lambda = (A - \lambda \cdot I)^{-1} \tag{4–2}$$

exists for $\lambda \notin \Lambda$. The operator R_λ is called the *resolvent operator.*

If (still in finite-dimensional spaces) $\lambda_r \in \Lambda$, then the set of ψ for which $(A - \lambda_r I)\psi = \mathbf{0}$ spans a finite-dimensional subspace M_r. Let P_r be the projection with range M_r. If λ_r is nondegenerate, then M_r is one-dimensional. Generally, the degree of degeneracy of λ_r equals dim M_r. The previous statements concerning the orthogonality and completeness of the ψ_r can now be expressed by the equations

$$P_r P_s = \delta_{rs} P_r, \qquad \text{and} \quad \sum_r P_r = I. \tag{4–3}$$

A system of projections which satisfy such relations is sometimes called a decomposition of unity. In terms of the projections P_r, the operator A has the simple form $\Sigma \lambda_r P_r$ (Problem 7).

We have already stated what we mean by a simple spectrum. Now we shall take up this notion once more, and cast it into a different form, which at first sight may seem more complicated but which in the end will be the only useful form of expressing this notion for general operators.

Consider the set of all polynomials

$$u(A) = a_1 A^{n-1} + a_2 A^{n-2} + \cdots + a_n.$$

They form an algebra $\mathscr{A}$, that is a vector space with a multiplication law: If T_1 and $T_2 \in \mathscr{A}$, then $\lambda_1 T_1 + \lambda_2 T_2 \in \mathscr{A}$ for complex λ_1, λ_2 and $T_1 T_2 \in \mathscr{A}$.

The dimension of this vector space cannot exceed n since the operator A satisfies an algebraic equation of order n, that is, the Cayley equation:

$$\prod_{r=1}^{n} (\lambda_r - A) = 0.$$

If the dimension of $\mathscr{A}$ is exactly equal to n, then the spectrum of A is simple. If the dimension is less than n, it is degenerate.

Another equally useful way of characterizing the simple spectrum is the following: if g is a fixed vector in $\mathscr{H}$, we can consider the set of all the elements of the form $f = Tg$ with $T \in \mathscr{A}$. We denote this set by $\{\mathscr{A}g\}$. It is clearly a subspace of $\mathscr{H}$. The size of this subspace will depend on g as well as on $\mathscr{A}$. Concerning the dependence of g, it is convenient to select vectors for which dim $\{\mathscr{A}g\}$ is maximal. For such vectors the dimension of $\{\mathscr{A}g\}$ depends only on the structure of the algebra, and will therefore depend on its dimension. More precisely, we have the following theorem.

Theorem: *The spectrum of A is simple if and only if there exist vectors g such that $\{\mathscr{A}g\}$ is equal to the entire space.*

Instead of giving a proof of this theorem we merely make some heuristic remarks which can easily be expanded and sharpened to a complete proof (Problem 6).

The vectors g with the property that $\{\mathscr{A}g\} = \mathscr{H}$ are called *cyclic vectors* of the algebra $\mathscr{A}$. They are characterized by the property $P_r g \neq \mathbf{0}$ for all r. If the P_r are all one-dimensional, then $f = u(A)g = \sum_r u(\lambda_r)P_r g$.

By suitable choice of $u(\lambda_r)$ one can reach any arbitrary vector $f \in \mathscr{H}$. Thus we see that we may characterize the operators with simple spectrum by saying that they give the highest mobility of the vector Tg with $T \in \mathscr{A}$. The other extreme would be obtained if the spectrum of A is completely degenerate. Then the operator A is merely a multiple of the unit operator, and we have the least mobility: The degree of mobility of vectors Tg with $T \in \mathscr{A}$ thus measures the degree of degeneracy of the spectrum.

Both of the preceding definitions of the simple spectrum can, with suitable modifications, be transferred to the infinite-dimensional Hilbert space. Before we do this, we shall introduce the notion of the spectral measure (still for the finite-dimensional case).

Let Δ be a Borel set on the real line. To every set we can associate a projection $E(\Delta)$ defined by

$$E(\Delta) = \sum_{\lambda_r \in \Delta} P_r.$$

In this way we obtain a projection-valued set function, defined on all Borel sets and satisfying the relations

$$\begin{aligned} E(\Delta_1) \cup E(\Delta_2) &= E(\Delta_1 \cup \Delta_2), \\ E(\Delta_1) \cap E(\Delta_2) &= E(\Delta_1 \cap \Delta_2), \\ E(0) &= 0, \\ E(R^1) &= I. \end{aligned} \tag{4–4}$$

At the end of Chapter 3 we called a projection-valued set function with these properties a *spectral measure*. Thus we see that every self-adjoint operator A defines a unique spectral measure E. With every such measure we can also define, for any fixed vector f, a finite numerical-valued measure μ_f by the formula

$$\mu_f(\Delta) = (f, E(\Delta)f).$$

In our particular case (finite dimension of $\mathscr{H}$), every μ_f is a discrete Lebesgue-Stieltjes measure concentrated at the points λ_r. The weights ρ_r at the points λ_r depend on the choice of f, and they may be zero for certain vectors f. However, for cyclic vectors g we have

$$\mu_g(\lambda_r) - \mu_g(\lambda_r - 0) = (g, P_r g) \neq 0,$$

where we have used the notation $\mu_g(\lambda) \equiv \mu_g((-\infty, \lambda])$. From this remark we

see immediately that the measure μ_f for any f must be absolutely continuous with respect to any measure μ_g with g cyclic.

Thus, in the notation of Section 1-4,

$$\mu_f \prec \mu_g.$$

In particular if f is also a cyclic vector, we have

$$\mu_g \prec \mu_f;$$

the two measures are equivalent: $\mu_f \sim \mu_g$. One verifies easily with the Radon-Nikodym theorem that, conversely, if $\mu_f \sim \mu_g$, then f must be cyclic. We summarize this situation with the following theorem:

Theorem: *Two numerical spectral measures μ_{g_1} and μ_{g_2} are equivalent if both g_1 and g_2 are cyclic vectors. Every other numerical measure μ_f is inferior to them.*

All of the results in this section have analogues in the infinite-dimensional case, and the rest of this chapter is devoted to the explicit formulation of these analogues and their applications for establishing the spectral representation.

PROBLEMS

1. Let A be a self-adjoint operator in the finite-dimensional space $\mathscr{H}$. Then
$$A\psi_1 = \lambda_1\psi_1, \qquad A\psi_2 = \lambda_2\psi_2 \qquad \text{and} \qquad \lambda_1 \neq \lambda_2$$
imply that $(\psi_1, \psi_2) = 0$. Is this result also valid in infinite-dimensional spaces?
2. If λ is a root of multiplicity α of the secular equation $|A - \lambda \cdot I| = 0$, then there exist exactly α linearly independent solutions ψ of the equation $A\psi = \lambda\psi$.
3. If ψ_1 and ψ_2 are two linearly independent eigenvectors belonging to the same eigenvalue λ, then all vectors in the subspace spanned by ψ_1 and ψ_2 are eigenvectors with eigenvalue λ.
4. The correspondence $\Omega : f \to \{x_r\}$, where $x_r = (\psi_r, f)$ and ψ_r is a complete orthonormal system in $\mathscr{H}$, is one-to-one and isometric provided that the norm of the sequence $\{x_r\}$ is defined by
$$\|\{x_r\}\|^2 = \sum_{r=1}^{n} |x_r|^2.$$
5. A vector g is cyclic with respect to a self-adjoint operator A if and only if $P_r g \neq \mathbf{0}$ for all spectral projections P_r.
6. The spectrum of A is simple if and only if $\{\mathscr{A}g\} = \mathscr{H}$ for cyclic vectors g.
7. In a finite-dimensional space the self-adjoint operator A has the form $A = \sum \lambda_r P_r$, where P_r is the projection with range M_r and M_r is the linear subspace of vectors ψ_r which satisfy
$$(A \quad \lambda_r \cdot I)\psi_r \quad \mathbf{0}.$$

4-2. THE RESOLVENT AND THE SPECTRUM

In this section we consider a self-adjoint operator A in Hilbert space. A may be bounded or unbounded; in any case it is closed. For any complex $z = x + iy$, we consider the operator $A - z \cdot I$, and we denote by D its domain and by $\Delta(z)$ its range, so that $\Delta \equiv \Delta(0)$ is the range of A.

The equation $Af - zf = g$ establishes a correspondence between the elements of D and the elements of $\Delta(z)$. If this correspondence is one-to-one, then there exists the resolvent operator $R_z = (A - z \cdot I)^{-1}$ with domain $\Delta(z)$ and range D.

We adopt the following definition of the spectrum of the operator A: The values of z for which $\Delta(z) = \mathscr{H}$ are called *regular* values for A; all other values are called the *spectrum* of A. All the values $z = x + iy$, with $y \neq 0$, are regular values for A (Problems 1 and 2). Thus the spectrum of a self-adjoint operator A is always real; in particular the proper values are real.

For real values $z = \lambda$, $\Delta(\lambda)$ may or may not be equal to $\mathscr{H}$. There are four cases possible, depending on whether $\Delta(\lambda)$ is closed or not, and whether we have $\overline{\Delta(\lambda)} \subset \mathscr{H}$ or $\overline{\Delta(\lambda)} = \mathscr{H}$. We can thus divide the spectrum Λ into two parts, $\Lambda = \Lambda_c \dot{+} \Lambda_d$, called the *continuous* and the *discrete* part. If $\Delta(\lambda) \subset \overline{\Delta(\lambda)}$, then $\lambda \in \Lambda_c$ and if $\overline{\Delta(\lambda)} \subset \mathscr{H}$, then $\lambda \in \Lambda_d$. The four cases which arise is this way are given in Table 4-1.

Table 4-1

THE SPECTRUM OF A SELF-ADJOINT OPERATOR

Property of $\Delta(\lambda)$	Spectrum
$\Delta(\lambda) = \overline{\Delta(\lambda)} = \mathscr{H}$	$\lambda \notin \Lambda_c, \quad \lambda \notin \Lambda_d$
$\Delta(\lambda) \subset \overline{\Delta(\lambda)} = \mathscr{H}$	$\lambda \in \Lambda_c, \quad \lambda \notin \Lambda_d$
$\Delta(\lambda) = \overline{\Delta(\lambda)} \subset \mathscr{H}$	$\lambda \notin \Lambda_c, \quad \lambda \in \Lambda_d$
$\Delta(\lambda) \subset \overline{\Delta(\lambda)} \subset \mathscr{H}$	$\lambda \in \Lambda_c, \quad \lambda \in \Lambda_d$

We see from this table that the range $\Delta(\lambda)$ of the operator $A - \lambda \cdot I$ furnishes a convenient means to identify the structure of the spectrum of a self-adjoint operator.

This characterization does not say anything about the multiplicity of the spectrum. In the discrete spectrum, it is easy to verify that the dimension of $\Delta(\lambda)^{\perp}$ is exactly equal to the multiplicity of the eigenvalue λ (Problem 6). To characterize the multiplicity in the continuous part of Λ is more difficult. In order to do this, we need the functional calculus to which we devote much of the remaining part of this chapter.

We conclude this section with some remarks on the resolvent operator $R_z = (A - z \cdot I)^{-1}$. If z is a regular value for A (for instance, for all z with Im $z \neq 0$), then R_z is a bounded operator defined for all elements $g \in \mathscr{H} = \Delta(z)$.

From the two equivalent relations $(A - \lambda \cdot I)f = g$ and $R_\lambda g = f$, we easily obtain, for all $g \in \mathscr{H}$,

$$R_{z_1} g = R_{z_2}(A - z_2 \cdot I)R_{z_1} g,$$

$$R_{z_2} g = R_{z_2}(A - z_1 \cdot I)R_{z_1} g.$$

By taking the difference of the two equations we obtain

$$R_{z_1} - R_{z_2} = (z_1 - z_2)R_{z_2}R_{z_1}. \tag{4-5}$$

This is called the Hilbert relation. It follows immediately that two bounded resolvents commute:

$$R_{z_1}R_{z_2} = R_{z_2}R_{z_1}.$$

Finally one can prove the relation (Problem 7)

$$R_z^* = R_{z^*}.$$

PROBLEMS

1. The operator $(A - zI)^{-1}$, with A self-adjoint and $z = x + iy$ $(y \neq 0)$, exists and is bounded.
2. If $z = x + iy$ $(y \neq 0)$, then $\Delta(z) = \mathscr{H}$.
3. The solutions of the eigenvalue problem $A\psi = \lambda\psi$ are the orthogonal complement of $\Delta(\lambda)$.
4. The spectrum of the operator Q (Section 3-5) is the entire real line.
5. The point λ is in the continuous spectrum of the self-adjoint operator if and only if there exists a sequence of normalized vectors φ_n $(\|\varphi_n\| = 1)$ such that

$$\|(A - \lambda)\varphi_n\| \to 0 \qquad \text{for} \qquad n \to \infty.$$

6. The multiplicity of an eigenvalue $\lambda \in \Lambda_d$ of a self-adjoint operator is equal to the dimension of $\Delta(\lambda)^\perp$.
7. The resolvent R_z of a self-adjoint operator satisfies the relation $R_z^* = R_{z^*}$ for all $z \notin \Lambda$.

4-3. THE SPECTRAL THEOREM

At the end of Section 4-1 we introduced the notion of the spectral measure for the finite-dimensional case. We shall now generalize this notion to the operators in the infinite-dimensional Hilbert space. The fundamental spectral theorem may then be stated in the following way.

To every self-adjoint operator A there corresponds a unique spectral measure $\Delta \to E(\Delta)$ defined on the Borel sets of the real line R^1 such that

$$A = \int_{-\infty}^{+\infty} \lambda \, dE_\lambda, \tag{4–6}$$

where $E_\lambda \equiv E((-\infty, \lambda])$ and the integral is to be interpreted as the Lebesgue-Stieltjes integral valid for any $f \in D_A$

$$(f, Af) = \int_{-\infty}^{+\infty} \lambda \, d(f, E_\lambda f). \tag{4–7}$$

The proof of this important theorem is found in reference 1.

It suffices here to see that it is an obvious generalization of the corresponding theorem for the discrete case (Section 4-1).

The one-to-one correspondence of the spectral measures on the real line to the self-adjoint operators permits us to replace one by the other.

To every spectral measure on the real line belongs a *spectral family* of projections E_λ with $-\infty < \lambda < +\infty$.

The general projection of such a spectral family is defined $E_\lambda \equiv E((-\infty, \lambda])$. The spectral family satisfies the relations

$$\begin{aligned} E_\lambda &\leq E_\mu \qquad \text{for } \lambda < \mu, \\ E_{\lambda+0} &= E_\lambda, \\ E_{-\infty} &= 0, \\ E_{+\infty} &= I. \end{aligned} \tag{4–8}$$

If the spectral family is known, the spectral measure can be reconstructed by the formula

$$E(\Delta) = \int_\Delta dE_\lambda$$

for any Borel set Δ. This formula is an abbreviated notation for the numerical integral, valid for any $f \in \mathscr{H}$:

$$(f, E(\Delta)f) = \int_{-\infty}^{+\infty} \chi_\Delta(\lambda) \, d(f, E_\lambda f) \equiv \int_\Delta d(f, E_\lambda f)$$

PROBLEMS

1. If the spectrum Λ of a self-adjoint operator is continuous (that is Λ_d is the null set), then $(f, E_\lambda f)$ is a continuous function of λ for all vectors f.
2. The spectral measure $E(\Delta)$ of a self-adjoint operator A reduces the resolvent operator $R_z = (A - z \cdot I)^{-1}$: $R_z E(\Delta) \quad E(\Delta) R_z$.

4-4. THE FUNCTIONAL CALCULUS

The last formula of the preceding section is a special case of a much more general relation between certain functions $u(\lambda)$ of a real variable λ and linear operators in Hilbert space.

If T is a bounded operator defined in $D_T = \mathscr{H}$, then it is clear what we mean by the operator T^2. It is the operator which assigns to every vector f the vector $T^2 f = T(Tf)$. It is not difficult to extend this to any finite positive power of T, by a recursive definition: $T^n f = T(T^{n-1} f)$. If $u(\lambda) \equiv \lambda^n + a_1 \lambda^{n-1} + \cdots + a_n$ is a polynomial of λ, then we define the operator $u(T) = T^n + a_1 T^{n-1} + \cdots + a_n$ by setting

$$u(T)f = T^n f + a_1 T^{n-1} f + \cdots + a_n f.$$

This assignment of polynomials to operators satisfies the relations

$$\begin{aligned} (u_1 + u_2)(T) &= u_1(T) + u_2(T), \\ (u_1 u_2)(T) &= u_1(T) u_2(T), \\ (cu)(T) &= cu(T) \end{aligned} \tag{4–9}$$

for all complex c. Furthermore, all the operators $u(T)$ commute with each other.

The correspondence of functions $u(\lambda)$, with operators $u(T)$, which satisfies relations (4–9) is called a *functional calculus.* It is desirable to extend this calculus to the largest possible class of functions for self-adjoint operators. A convenient way to do this is the following.

We define $u(\lambda)$ as *measurable* with respect to the spectral family E_λ if for every $f \in \mathscr{H}$ the function $u(\lambda)$ is measurable with respect to the Lebesgue-Stieltjes measure defined by the spectral density functions $\rho_f = (f, E_\lambda f)$.

Similarly, we say $u(\lambda)$ is *integrable* with respect to the spectral family E_λ if for every $f \in \mathscr{H}$ the function $u(\lambda)$ is integrable with respect to the measure defined by $\rho_f(\lambda)$.

Let A be a self-adjoint linear operator and E_λ its spectral family. If $u(\lambda)$ is measurable and integrable with respect to E_λ, then we can define, for any pair of vectors $f, g \in \mathscr{H}$, the expression

$$L_g^*(f) \equiv \int_{-\infty}^{+\infty} u(\lambda)\, d(f, E_\lambda g),$$

and one verifies easily that $L_g(f)$ is a bounded linear functional of f. By Riesz' theorem there thus exists a unique vector g^* with the property $L_g(f) = (g^*, f)$.

The correspondence $g \to g^*$ defines a bounded linear operator $u(A)$ so that we have the formula

$$(f, u(A)g) = \int_{-\infty}^{+\infty} u(\lambda)\, d(f, E_\lambda g).$$

This will be written in an abbreviated notation as

$$u(A) = \int_{-\infty}^{+\infty} u(\lambda)\, dE_\lambda.$$

One can verify that the correspondence $u(\lambda) \to u(A)$ of functions with operators has the properties (4–9), (Problem 6).

The operator $u(A)$ is bounded if the function $u(\lambda)$ is essentially bounded with respect to E_λ; that is, if there exists a real number $M < \infty$ such that the set $\{\lambda : u(\lambda) < M\}$ has measure zero for all measures ρ_f. The greatest lower bound of the numbers M with this property is the bound of the operator $u(A)$ (Problem 1).

It is possible to extend the functional calculus to unbounded operators by restricting the vectors f and g to suitably defined dense linear manifolds. Some slight modifications of the relations (4–9) are then needed because of the restrictions of the domains of definition.

Some important applications of the functional calculus are the following examples:

1) The integral representation of the self-adjoint operator A with the spectral family λ is given by

$$A = \int_{-\infty}^{+\infty} \lambda\, dE_\lambda.$$

It is bounded if and only if

$$\int_{-\infty}^{+\infty} \lambda^2\, d(f, E_\lambda f)$$

exists for all $f \in \mathscr{H}$. If it is unbounded, then the domain of definition D_A is given by the set of vectors f for which

$$\int_{-\infty}^{+\infty} \lambda^2\, d(f, E_\lambda f) < \infty.$$

2) Let $\chi_\Delta(\lambda)$ be the characteristic function of the Borel set Δ. It is measurable and integrable with respect to E_λ. The operator

$$\chi_\Delta(A) \equiv \int_{-\infty}^{+\infty} \chi_\Delta(\lambda)\, dE_\lambda = \int_\Delta dE_\lambda \equiv E(\Delta)$$

defines the projection of the spectral measure associated with Δ.

3) For every real t and every self-adjoint operator A one can define

$$U_t = e^{iAt} = \int_{-\infty}^{+\infty} e^{i\lambda t}\, dE_\lambda. \tag{4–10}$$

One verifies that this is a family of unitary operators which satisfies

$$U_{t_1} U_{t_2} = U_{t_1 + t_2}.$$

This relation between self-adjoint operators and unitary one-parameter groups has a converse in the form of

Stone's theorem: *Every unitary one-parameter group U_t for which $(f, U_t g)$ is a continuous function in t for all $f, g \in \mathscr{H}$ defines a unique spectral measure such that*

$$U_t = \int_{-\infty}^{+\infty} e^{i\lambda t}\, dE_\lambda.$$

The self-adjoint operator A which corresponds to this spectral measure is called the *generating operator* of the group. We may then write the preceding relation equivalently $U_t = e^{iAt}$.

The set of all bounded operators of the form $u(A)$, with A some self-adjoint operator, forms an algebra $\mathscr{A}$. We shall denote it the algebra *generated* by A.

If $T_1, T_2 \in \mathscr{A}$, then $T_1 + T_2 \in \mathscr{A}$ and $T_1 T_2 \in \mathscr{A}$. Furthermore if $T \in \mathscr{A}$, then $\lambda T \in \mathscr{A}$ for all complex λ. The algebra is *abelian*; this means that for every pair of operators T_1 and T_2 one has $T_1 T_2 = T_2 T_1$. The algebra can also be characterized in the following equivalent way:

Let $\mathscr{S}$ be any set of self-adjoint operators; then we denote by $\mathscr{S}'$ the set of all bounded operators which commute with $\mathscr{S}$. The algebra generated by $\mathscr{S}$ is then the set $\mathscr{S}'' \equiv (\mathscr{S}')'$. The algebra $\mathscr{A}$ defined above is then also the algebra defined by $\mathscr{A} = \{A\}''$ (Problem 4). The fact that $\mathscr{A}$ is abelian is expressed by the relation $\mathscr{A} \subseteq \mathscr{A}'$. If $\mathscr{A} = \mathscr{A}'$, then the algebra is called *maximal abelian*. It then does not admit any abelian extension.

In Section 4-1 we stated that the self-adjoint operator A has simple spectrum if and only if the algebra generated by the operator A has maximal dimension. We can now transfer this property to the infinite dimensional case by defining: The operator A has simple spectrum if the algebra $\mathscr{A} = \{A\}''$ is a maximal abelian algebra: $\mathscr{A} = \mathscr{A}'$.

At this point we have succeeded in transferring the notion of simple spectrum to the infinite-dimensional case without making use of the notion of eigenvector.

PROBLEMS

1. The operator $u(A) = \int u(\lambda)\, dE_\lambda$ is bounded if and only if the function $u(\lambda)$ is essentially bounded.
2. The domain of definition of the unbounded operator $u(A)$ is the set of vectors f for which
$$\int_{-\infty}^{+\infty} |u(\lambda)|^2\, d(f, E_\lambda f) < \infty.$$
3. The operator $u(A)$ for A self-adjoint is unitary if and only if $|u(\lambda)| \quad 1$ a.e. with respect to the spectral family E_λ.

*4. The algebra $\mathscr{A} = \{A\}''$ consists of all the operators of the form $u(A)$ where $u(\lambda)$ is an essentially bounded measurable and integrable function with respect to the spectral family E_λ of A [2, Section 129].

5. If the spectrum of the self-adjoint operator A is discrete and $\{A\}'' = \mathscr{A} \subset \mathscr{A}'$, then there exists at least one degenerate eigenvalue λ of A.

6. The correspondence

$$u(\lambda) \to u(A) \equiv \int_{-\infty}^{+\infty} u(\lambda)\, dE_\lambda$$

is a functional calculus; that is, it satisfies relations (4–9).

4-5. SPECTRAL DENSITIES AND GENERATING VECTORS

In this section we shall study in more detail the spectral density function introduced in the preceding section. Let E_λ be a spectral family, and f a vector in $\mathscr{H}$; then we define the spectral density function $\sigma_f(\lambda) = (f, E_\lambda f)$. This function will depend on the spectral family E_λ on the one hand, and on the vector f on the other. We shall study the dependence on f for a fixed spectral family E_λ.

First we list a few simple properties of any function $\sigma(\lambda) = (f, E_\lambda f)$ which follow directly from the basic properties (4–8) of a spectral family.

$$\begin{aligned} &\sigma(\lambda_1) \leq \sigma(\lambda_2) \qquad \text{for } \lambda_1 < \lambda_2, \\ &\sigma(\lambda + 0) = \sigma(\lambda), \\ &\sigma(-\infty) = 0, \\ &\sigma(+\infty) = 1 \qquad \text{for } \|f\| = 1. \end{aligned} \tag{4–11}$$

Furthermore the function $\sigma(\lambda)$ is discontinuous for certain values $\lambda \in \Lambda_d$. For all other values of λ it is continuous. In particular for all values $\lambda \notin \Lambda$ the function $\sigma(\lambda)$ is constant.

Any function $\sigma(\lambda)$ with these properties defines a measure $\mu(\Delta)$ for all Borel subsets Δ of the real line through the formula:

$$\mu(\Delta) = \int \chi_\Delta(\lambda)\, d\sigma(\lambda).$$

Thus for each f we have defined a measure.

We shall now examine the dependence of this measure on the vector f. We recall from Section 1-2 that measures are a partially ordered set. A measure μ_1 is inferior with respect to μ_2 ($\mu_1 \prec \mu_2$) if μ_1 is absolutely continuous with respect to μ_2.

For the measures which we are studying there is another partial ordering possible by using the dependence of σ on the vector f. Let

$$\sigma_1(\lambda) = (f_1, E_\lambda f_1) \qquad \text{and} \qquad \sigma_2(\lambda) = (f_2, E_\lambda f_2).$$

To any vector f we can associate a subspace

$$M(f) = \overline{\{\mathscr{A}'f\}}$$

where the right-hand side denotes the subspace generated by all vectors of the form Sf with $S \in \mathscr{A}'$. If we denote by

$$M_1 \equiv M(f_1), \qquad M_2 \equiv M(f_2),$$

then we may define a partial ordering of the measure by denoting σ_1 inferior to σ_2 if $M_1 \subseteq M_2$. We have adopted a terminology which is justified in anticipation of the following.

Theorem: *Let E_λ be a spectral family and $f_1, f_2 \in \mathscr{H}$ two arbitrary vectors in $\mathscr{H}$; then the spectral density function σ_1 is absolutely continuous with respect to σ_2 if and only if $M_1 \subseteq M_2$* [3].

This theorem shows that the notions of partial ordering derived from absolute continuity and from the partial ordering of associated subspaces are equivalent. It follows from this that the measure associated with a cyclic vector of $\mathscr{A}'$ has a maximal property:

If g is a vector such that $\overline{\{\mathscr{A}'g\}} = \mathscr{H}$, then the measure defined by $\rho(\lambda) = (g, E_\lambda g)$ is maximal in the partially ordered set of measures. That is for any $f \in \mathscr{H}$, we have

$$\sigma_f \prec \rho.$$

It follows immediately from this remark that if g' is any other cyclic vector and ρ' the associated measure, then $\rho \sim \rho'$ (Problem 4). The spectral density functions for two different cyclic vectors define the same (maximal) measure class.

In conclusion of this subsection we can now give an alternate definition of the operator with simple spectrum which generalizes the one given in Section 4-1. We have defined an operator A to have simple spectrum if $\{A\}'' = \mathscr{A} = \mathscr{A}'$. An equivalent definition is possible with the cyclic vectors by using the following.

Theorem: *An operator A has simple spectrum if and only if there exists a cyclic vector for the algebra $\mathscr{A} = \{A\}''$* (Problem 5).

This theorem generalizes the corresponding elementary theorem for the finite-dimensional case.

PROBLEMS

1. If $\mathscr{A}$ is abelian and $M = \overline{\{\mathscr{A}'g\}}$, then the projection P with range M is contained in $\mathscr{A}$.
2. If $M \equiv \overline{\{\mathscr{A}'g\}} \subset \mathscr{H}$, then there exists a vector g_1, such that
$$M \subset \overline{\{\mathscr{A}'g_1\}}.$$
*3. There exists a cyclic vector g for $\mathscr{A}'$, such that
$$\overline{\{\mathscr{A}'g\}} = \mathscr{H}.$$
(Use Zorn's lemma.)
4. If g and g' are two cyclic vectors for $\mathscr{A}'$, then the associated measures ρ and ρ' are equivalent ($\rho \sim \rho'$).
5. $\mathscr{A} \equiv \{A\}'' = \mathscr{A}'$ if and only if there exists a vector g such that $\overline{\{\mathscr{A}g\}} = \mathscr{H}$. In that case the spectrum of A is simple.

4-6. THE SPECTRAL REPRESENTATION

This chapter started out with a discussion of the spectral representation in the finite-dimensional case. We have now all the tools on hand to demonstrate the existence of a spectral representation in the infinite-dimensional case. Let us recall the finite situation.

We have seen in Section 4-1 that any self-adjoint operator in an abstract space $\mathscr{H}$ defines an ℓ_n^2-space consisting of finite sequences $\{x_\nu\}$ ($\nu = 1, 2, \ldots, n$) together with an isometric mapping Ω of $\mathscr{H}$ onto ℓ_n^2 such that the transformed operator $\tilde{A} = \Omega A \Omega^{-1}$ is a multiplication operator.

When we try to transfer this theorem to the infinite-dimensional case, the first question that comes up is: what is the measure in the continuous part of the spectrum of A? From the remarks in Section 4-1 it seems fairly natural to suspect that only the class of equivalent measures will be uniquely determined, and that the measure which is thus defined is the measure associated with the cyclic vector.

We consider thus an operator A with simple spectrum, and define a measure over the spectrum with the spectral density function $\rho(\lambda) = (g, E_\lambda g)$. The space $L_\rho^2(\Lambda)$ consists of functions $u(\lambda)$ where $\lambda \in \Lambda$, over the spectrum Λ of the operator A. The norm is defined by $\|\{u(\lambda)\}\|^2 = \int |u(\lambda)|^2 \, d\rho(\lambda)$, with $\rho(\lambda) \equiv (g, E_\lambda g)$. In this expression E_λ is the uniquely determined spectral family of A, and g is a cyclic vector. To every $f \in \{\mathscr{A}g\}$, that is, to every f of the form $f = Tg$ with $T \in \mathscr{A}$, we can associate a function $u(\lambda)$ by the rule $T = u(A)$. Furthermore, because

$$\|f\|^2 = \|Tg\|^2 = \|u(A)g\|^2 = \int |u(\lambda)|^2 \, d\rho(\lambda),$$

we see that the correspondence $f \leftrightarrow \{u(\lambda)\} \in L^2_\rho(\Lambda)$ is an isometry from $\{\mathscr{A}g\}$ onto a dense linear subset of $L^2_\rho(\Lambda)$. Since $\{\mathscr{A}g\}$ is dense in $\mathscr{H}$, we can extend this correspondence by continuity to an isometric mapping of $\mathscr{H}$ onto $L^2_\rho(\Lambda)$. We denote this mapping by Ω.

What becomes of the operator A when it is transformed into an operator $\tilde{A}$ in $L^2_\rho(\Lambda)$? Since the functional calculus is multiplicative, the operator $Au(A)$ corresponds to the function $\lambda u(\lambda)$. This is true without qualification if $\lambda u(\lambda)$ is essentially bounded. If it is unbounded, certain precautions are required in order to take account of the restricted domain of definition. Let us therefore concentrate on the bounded case.

It follows then, from the definition of Ω, that

$$\Omega A \Omega^{-1}\{u(\lambda)\} = \Omega A f = \Omega A u(A) g = \{\lambda u(\lambda)\},$$

so that

$$\tilde{A}\{u(\lambda)\} = \{\lambda u(\lambda)\} \qquad \text{and} \qquad \tilde{A} = \Omega A \Omega^{-1}.$$

This is the spectral representation of the operator A.

The spectral representation is unique in the sense of equivalence. If $f \leftrightarrow \{u_1(\lambda)\}$ is another such representation, then there exists an equivalent density function $\rho_1 \sim \rho$, and the two representations are connected by a transformation

$$u_1(\lambda)\sqrt{\frac{d\rho_1}{d\rho}}\, e^{i\alpha(\lambda)} = u(\lambda),$$

where $d\rho_1/d\rho$ is the Radon-Nikodym derivative of the two equivalent measures.

The spectral representation has a generalization to a finite or countably infinite set of commuting self-adjoint operators. Let A_r $(r = 1, 2, \ldots)$ be such a set, and let Λ_r be the spectrum of A_r; then there exists a uniquely defined measure class $\{\rho\}$ on the Borel sets of the Cartesian product space $S = \Lambda_1 \times \Lambda_2 \times \cdots$ and an isometric mapping of $\mathscr{H}$ onto $L^2_\rho(S)$ such that if $f \leftrightarrow \{u(\lambda)\}$, where $\lambda = \{\lambda_1, \lambda_2, \ldots\} \in S$, then

$$\|f\|^2 = \int_S |u(\lambda)|^2 \, d\rho.$$

If we write as before $\{u(\lambda)\} = \Omega f$, then the transformed operators $\tilde{A}_r$ are defined by

$$\tilde{A}_r = \Omega A_r \Omega^{-1}.$$

One can prove that if $P_r(\Delta_r)$ is a spectral projection of the operator A_r, then $\tilde{P}_r(\Delta_r) \equiv \Omega P_r(\Delta_r)\Omega^{-1}$ is given explicitly by

$$\tilde{P}_r(\Delta_r)\{u(\lambda)\} = \chi_{\Delta_r}(\lambda_r)u(\lambda),$$

where $\chi_{\Delta_r}(\lambda_r)$ is the characteristic function of the set Δ_r. However, this does not mean that the operator $\tilde{A}_r$ is a multiplication operator in L^2. In order to

prove this property, a further assumption is needed which expresses something which we might describe as independence of the operators and which we shall not give in detail [3]. Under this additional assumption, one finds that

$$\tilde{A}_r\{u(\lambda_r)\} = \{\lambda_r u(\lambda)\}, \qquad (r = 1, 2, \ldots). \tag{4–12}$$

PROBLEMS

1. If $f = \{f(\lambda)\} \in L^2(-\infty, +\infty)$ and A is the operator $Af = \{-i(df/d\lambda)\}$ defined on a certain dense linear subset D_A of L^2 such that A is self-adjoint, then the transformation

$$\Omega f = \tilde{f}, \qquad \tilde{f}(\mu) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(\lambda) e^{i\lambda\mu}\, d\lambda$$

is isometric and transforms A into the spectral representation

$$\tilde{A} = \Omega A \Omega^{-1}, \qquad (\tilde{A}\tilde{f})(\mu) = \mu \tilde{f}(\mu).$$

*2. If two self-adjoint operators A and B commute, and if A has simple spectrum, then B is a function of A : $B = u(A)$. B has simple spectrum, too, if and only if the function $u(\lambda)$ has an inverse.

4-7. EIGENFUNCTION EXPANSIONS

Let us consider a self-adjoint operator A with spectrum Λ. From the preceding sections we know that such an operator defines a unique spectral measure $E(\Delta)$, $(\Delta \subseteq \Lambda)$ and that this spectral measure determines the operator. All the properties of the operator A are known if an explicit method is known for calculating the projections $E(\Delta)$ of the spectral measure. One such explicit method, which often works in practice, is obtained by utilizing the *eigenfunction expansion*. This method resembles in some respects the expansion in eigenvectors used for illustrative purposes in Section 4-1. The difference here is that we use solutions of the eigenvalue equation which fall outside the Hilbert space. We illustrate this in a special case.

Let $\mathscr{H} = L^2(-\infty, +\infty)$ be the space of square-integrable functions on the real line and A some self-adjoint operator in $\mathscr{H}$. The solutions $\varphi_n(x)$ of the equation $A\varphi_n = \lambda_n\varphi_n$ which are square-integrable are called eigenvectors of A, and they may be chosen so as to form an orthonormal system in $\mathscr{H}$. If this system is complete, then the spectrum of A is discrete, and we have essentially the case discussed in Section 4-1. If the system is not complete, then there may exist other solutions of the operator equation

$$A\varphi = \lambda\varphi \tag{4–13}$$

for which $\varphi \notin \mathscr{H}$. In order for this equation to make sense, it is evidently necessary to extend the domain of definition of the operator A to such func-

tions; this can often be done. For instance, if A is the differential operator P discussed in Section 3-6, then we may define it on functions $\varphi(x)$ which are not in L^2. The only property of $\varphi(x)$ which we need to define the operator $P = -i(d/dx)$ is that $\varphi(x)$ be differentiable. Such a function is, for instance, the exponential $\varphi(x) = e^{ikx}$ (k real), and one verifies that in this case one has an equation

$$P\varphi = k\varphi \qquad \text{for all } -\infty < k < +\infty.$$

It may be that there exists a complete set of eigenfunctions, that is, solutions of Eq. (4–12) which are not contained in $\mathscr{H}$. By "complete" we mean that the solutions depend on some (or several) parameters k : $\varphi(k, x)$, such that every vector $f(x)$ of $\mathscr{H}$ which is orthogonal to the eigenvectors $\varphi_n(x)$ is a linear superposition of the eigenfunctions $\varphi(k, x)$:

$$f(x) = \int_K \hat{f}(k)\varphi(k, x)\, d\mu(k),$$

where the integral extends to the entire range K of the parameter k. If such a complete set of eigenfunctions exists, then we can also normalize them suitably so that the norm of f satisfies Parseval's equation

$$\int_{-\infty}^{+\infty} |f(x)|^2\, dx = \int_K |\hat{f}(k)|^2\, d\mu(k).$$

For instance, in the above example with $A = P$, the system

$$\varphi(x) = \frac{1}{\sqrt{2\pi}} e^{ikx} \qquad (-\infty < k < +\infty)$$

is such a complete system, and the transformation

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_K \hat{f}(k) e^{ikx}\, dk$$

is simply the Fourier transformation of the function $f(x)$.

If such a complete system exists for all f orthogonal to the eigenvectors φ_n, then we say the operator A admits an *eigenfunction expansion*. It is then possible to prove that

$$(Af)(x) = \int_K \hat{f}(k)\lambda(k)\varphi(k, x)\, d\mu(k),$$

where $\lambda(k)$ is the eigenvalue belonging to $\varphi(k, x)$. When A is considered as an operator in the system of functions $\hat{f}(k)$, it is a multiplication operator. The eigenfunction expansion, if it exists, can thus serve the same purpose as the spectral representation.

Just as in the case of the Fourier transforms, there exists an inversion of the transformation (4–13) given by an equation such as

$$\hat{f}(k) = \int_{-\infty}^{+\infty} f(x)\varphi^*(k, x)\, dx.$$

The correspondence $f(x) \leftrightarrow \hat{f}(k)$ is thus an isometric mapping of the space $L^2(-\infty, +\infty)$ onto the space $L^2(K, \mu)$ such that A appears in the latter space as a multiplication operator.

The usefulness of this method of obtaining a spectral representation for self-adjoint operators is evident if the operator A is a differential operator. The solution of Eq. (4–13) is then obtained as the solution of an ordinary partial differential equation.

However, the expansion theorem is not generally true; and even if it is true, as, for instance, for certain partial differential operators, Eq. (4–13) does not suffice to determine the eigenfunctions uniquely. It is then necessary to add further conditions, which determine the eigenfunctions. For further detail on these questions the reader should refer to references 4 and 5.

The mathematical theory of eigenfunction expansions is not yet sufficiently developed to guarantee its availability in every case of practical interest. In general situations we must fall back on the spectral representation, which always exists. For certain special cases, however, especially for some elementary problems in one-particle quantum mechanics, the expansion theorem is available; and then it is a most convenient tool to calculate the spectrum and the spectral representation.

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PART 2

Physical Foundations

CHAPTER 5

THE PROPOSITIONAL CALCULUS

The first process, therefore, in the effectual study of the sciences, must be one of simplification and reduction of the results of previous investigations to a form in which the mind can grasp them.

J. C. MAXWELL,
On Faraday's lines of force

The topic of this chapter is the *propositional calculus of quantum mechanics*, sometimes also called (misleadingly) the logic of quantum mechanics. This calculus expresses the kinematic structure of physical systems and is quite independent of any dynamical process law. Already we notice on this general level the profound difference between classical and quantum mechanics, which will be placed into historical and philosophical context in Section 5-1. The appropriate tools for expressing this calculus are the *yes–no experiments*, also called *propositions*, which are introduced in Section 5-2. In the following section, 5-3, we list the principal structural properties of these propositions. The corresponding properties are then formulated for classical systems, and it is shown, in Section 5-4, that for such systems the lattice becomes a Boolean algebra. The notion of Boolean sublattice introduced in Section 5-5 is useful for the precise definition of the fundamental concept of *compatibility*.

A brief sketch of modular lattices is presented in Section 5-6, and it is pointed out that modularity, although more general than distributivity, is still too restrictive for certain physical systems. In Section 5-7 we connect the development with the parallel but more special topic of Section 2-5 on the lattice of subspaces. In particular it is shown that the formally different definition of compatibility of Section 2-5 is identical with that given in this chapter. The correct axiom (P) which replaces the distributive law of classical systems is finally enunciated in the last section, 5-8, together with the *atomicity axiom*, which is justified principally by its convenience.

5-1. HISTORIC–PHILOSOPHIC PRELUDE

Quantum mechanics has introduced into the description of nature such controversial novelties that a re-examination of the epistemological foundation of physical science has become a widely felt need. Indeed, some of the founders of this theory, notably Einstein, Schrödinger, and de Broglie, could not agree with the "orthodox" interpretation of quantum mechanics proposed by Born and elaborated by the so-called Copenhagen school.

Yet when the advent of quantum mechanics is viewed in a larger historical context, it is seen as one more step in a process of disintegration of the mechanistic view which began in the second half of the nineteenth century, and to which Einstein himself made decisive contributions. Classical mechanics originated in the seventeenth century, and its point of view dominated physical science for more than two hundred years. Newton replaced the anthropomorphic and qualitative physics of the middle ages by a general and quantitative process law which seemed to be the ideal of a physical law to which all other physical phenomena might eventually be reduced. This conviction was the driving motive behind most of the research of eighteenth- and nineteenth-century physics. Huygens wrote in 1690: "In true philosophy the causes of all natural phenomena are conceived in mechanical terms. We must do this, in my opinion, or give up all hope of ever understanding anything in physics." Nearly two hundred years later Helmholtz still believes that "To understand a phenomenon means nothing else than to reduce it to Newtonian laws. Then the necessity of explanation has been satisfied in a palpable way."

And indeed, who could doubt that the mechanical model would remain the ideal of physical science for all time to come, after two centuries of the most spectacular success? The difficulties of this program began with the advent of Maxwell's theory of the electromagnetic field. Although Maxwell was guided to some extent by mechanical analogies, the mechanistic point of view could not be carried through consistently. Not only would it entail a mechanical *ether* which had to have absurd physical properties, but the mechanical model was in the end found to be definitely in contradiction with the optical experiments by Michelson and Morley. H. Hertz was most explicit in announcing the departure from the mechanistic ideal by writing: "Maxwell's theory is nothing else than Maxwell's equations." Physicists began to realize that they could do physics just as well without ever mentioning the ether. With Einstein's special theory of relativity, this process was completed, and the ether with its mechanical properties quietly faded from sight.

But the special theory of relativity had introduced another radical novelty by showing that henceforth it was no longer admissible to consider space-time properties always as attributes of individual objects. The question: "What is the length of this rod?" has a unique answer only if it is specified with respect to what system of reference one determines the length. The same

is true for the duration of physical processes and the simultaneity of distant events. This meant one had to learn to think of space-time properties such as length and duration as *relations* rather than as *attributes*.

This process has gone much further with the advent of quantum mechanics. The discovery of the uncertainty relation by Heisenberg showed that the replacement of attributes by relations had to be extended even to the measurement of coordinates and momenta of a physical system if account were taken of the finite size of the quantum of action.

The question "What is the position?" or "What is the momentum?" of a particle becomes meaningful only in connection with a physical arrangement which, at least in principle, permits the determination of the quantity asked for. Bohr has shown, by a detailed analysis of many special cases, that physical arrangements which permit an objective determination of such quantities are in general incompatible, and he was led in this way to formulate the notion of *complementarity*. All this contributed to a complete disintegration of the mechanistic ideal.

The safe mechanical model of Huygens was replaced by the symbolism of mathematical formalism. This process was accompanied on the philosophical side by independent parallel developments.

In Austria Ernst Mach had published a series of historical–philosophical studies which tended to show that science is merely a description of relations between sensations. The radical antimetaphysical tendencies of Mach greatly stimulated a group of philosophers, known as the Vienna circle, who were prominent in the analysis of the new development in physics. A similar development in the form of a reaction to Kant's synthetic *a priori* was taking place elsewhere with such diverse representatives as Nietzsche, Poincaré and Duhem.

There was no lack of opposition to this tendency. Many viewed the disintegration process with alarm because the whole of science seemed to collapse like a house of cards. The French historian and philosopher A. Rey in 1907 gave expression to this feeling of failure of the scientific method with the words: "We can have a collection of empirical recipes; we can even systematize them for the convenience of memorizing them; but we have no cognition of the phenomena to which this system or these recipes are applied."

Max Planck, the founder of quantum theory, rejected the Machian conception of science as the most economical way of expressing relations between sensations. Planck on the contrary insisted on the "reality" corresponding to physical concepts.

The most violent opposition came from the ideologies. Both Nazism and Communism have declared open warfare on these "idealistic" tendencies in modern science, naturally for quite different reasons.

The new development seemed to becloud the concept of *reality*. What does it mean to affirm "reality" for a physical construct, if these constructs

dissolve into a collection of mathematical symbols, which to boot are not even unique?

We shall not attempt to review all the different answers which have been given to this disturbing question. We merely mention the question here to sketch the philosophical climate in which the evolution of quantum mechanics occurred.

We believe that, as far as physics is concerned, the answer to such questions will be largely irrelevant. Physics has been remarkably insensitive to metaphysical concerns. But there is one aspect which concerns us and to which we should pay attention. This is the new role assigned to mathematics in modern physical theories.

There is no doubt that the importance of mathematics in theoretical physics has increased with the collapse of the mechanistic model for physics. Not only has mathematics become more sophisticated and more intricate, but in addition it has acquired a kind of independence.

For instance, the basic physical notion of general covariance obtained its perfect expression only in the absolute differential calculus of Ricci and Levi-Civita. Quantum mechanics can only be formulated correctly by adopting formal techniques from functional analysis, notably the theory of Hilbert space.

In the absence of a clear-cut mechanical model, certain mathematical structures have risen to the status of a model in their own right. The most striking examples of this kind are found in recent trends toward classifying the different states of the elementary particle systems with the help of certain Lie algebras.

In view of these tendencies, it is necessary to have a sober look at the role of mathematics in physical theory, so that we can resist the temptation of a new form of rationalism which overestimates the significance of mathematics.

The prime source of scientific knowledge about the physical world is the experience gained by systematic observation of physical systems. Purely mathematical knowledge, although very useful for the organization of empirical raw material into a body of interrelated facts, is useless as a *source* of knowledge about the physical world. The reason for this is that mathematical truth is analytical truth; this means that it contains nothing more than what is already contained in the premises or the axioms. It is always certain, but, just because of this certainty, essentially tautological. Empirical truth, on the other hand, is *synthetic* truth. The general physical laws are arrived at by *induction* from observed facts, and therefore are never *certain* but only *verifiable for a finite number of instances.*

These general laws are formulated as axioms in a mathematical language. Conclusions are then drawn from these axioms by rigorous mathematical methods which lead to the prediction of other observable facts. These facts may be verified or not by observations. If they are not verified, the theory has

to be modified by modifying the axioms. For instance, the axiom of the invariance of the physical processes under space inversion predicted the spherical symmetry for the decay products of polarized radioactive atoms. The fact that this symmetry was not observed indicated a violation of parity conservation for weak interactions.

This somewhat schematic description of the role of mathematics and experience would have to be refined to be accurate. For instance, the facts which are observed are not just a haphazard collection of facts but are *selected* with a view to establishing general and simple regularities, that is, physical laws. Likewise, the mathematical axioms are to some extent arbitrary and must be selected by other criteria in addition to those mentioned above. A certain freedom is left to the creative theoretician which often can be a decisive element in the success of a theory.

The main problem in the selection of empirical material is the separation of relevant from irrelevant conditions. This is often made possible by isolating a sufficiently simple part from the rest of the physical world and studying the properties of the isolated part alone. We shall call such an isolated part a *physical system.* The simplest physical systems are those which consist of just one elementary particle, if we disregard its interactions with other particles.

The notion of the physical system as defined here becomes blurred in the general theory of relativity and in relativistic quantum mechanics. In the general theory of relativity one hopes to show that some mechanical properties such as inertia must depend on the state of the rest of the world (Mach's principle).. In relativistic quantum mechanics one must consider transitions between states with a variable number of particles. One is thus led to consider physical systems which normally would be called different as merely *different states* of one and the same system. These limitations of the concept of "system" need not concern us here since we are considering only nonrelativistic quantum mechanics.

A physical law which is obtained by the method sketched above may be expressed in the following form: If a system S is subject to conditions $A, B, \ldots$ then the effects $X, Y, \ldots$ can be observed. In this form it establishes a relation between the conditions and the effects.

The most general relation of this kind which can be formulated is a *probability relation.* There are two extreme cases possible: The effects are not correlated with the conditions, and they are distributed independently. (In common parlance this means there is *no* law which connects conditions and effects.) The other extreme case would be described thus: Every condition produces exactly one effect. (There is no scattering in the observed effects if the experiment is repeated.) This is still a probability connection but with dispersion zero. In all physical experiments one observes an intermediate situation. Measured quantities always fluctuate. It was an axiom of classical mechanics that, by increasing the accuracy of the measurements, one could,

for any system, reduce the dispersion of the measured effects below any arbitrary small amount. This axiom has been found false for certain elementary systems. This is an *empirical* fact, and is one of the pillars of quantum mechanics.

There is thus, as far as we know today, an irreducible statistical element in quantum mechanics quite in contrast with classical mechanics, where it is assumed that the statistical element, if it does appear, merely reflects our incomplete knowledge of the state of the system. This has often been considered an unsatisfactory feature of quantum mechanics. Seen historically, it is a further step in the "demechanization" of the physical laws.

There are those who long for a reestablishment of strict determinism in physics, be it for the reconciliation of some ideological faith, or for esthetic reasons. Quite soon after the discovery of quantum mechanics the question was raised as to whether there might exist "hidden parameters" not accessible to the usual observation and not affected by the gross manipulations in the conditioning experiments $A, B, \ldots$ We shall discuss this question of the hidden variables in great detail in Chapter 7. Here we shall just state that such attempts have failed and are bound to fail unless they spring from a much more profound knowledge of the physical microcosmos than anyone has at the present time.

In this chapter we shall introduce the statistical character of quantal systems as a basic axiom without further questions. Enough has been said in the above sketch of scientific methodology to obviate any further justification for this procedure. Its empirical justification will appear in the subsequent development of the theory.

5-2. YES–NO EXPERIMENTS

In this section we shall explain a mode of description of physical systems in terms of so-called "yes–no experiments."

Let us consider a physical system. This may be any specified system, but for illustrative purposes we shall occasionally speak about a proton. If we wish to determine the physical characteristics of a proton, we must perform a series of experiments which then in their ensemble will be a full operational equivalent for the construct *proton*. There are two complications which make it difficult to formalize this program into a convenient mathematical structure. First, physical experiments with a proton can be of a great many different kinds, giving results which are expressed in a variety of different ways. Secondly, the results of such experiments may turn out to be quite different for one and the same system depending on the "state" of the system. For instance, if we determine the momentum of a proton, we may obtain a variety of values, depending on the exact manner of the preparation of the system before the measurement was performed. On the other hand, if we measure its

rest mass by any method we always obtain the same value. There are thus properties which depend on the state and there are others which characterize the system and which therefore are independent of the state.

In order to overcome the first of these difficulties, we introduce a particular kind of experiment which we call yes–no experiments; these are observations which permit only *one* of two alternatives as an answer (hence the name "yes–no" experiment). Such experiments are part of the daily routine of every experimental physicist; for example, a counter which registers the presence of a particle within a certain region of space. What is perhaps less well known, however, is that every measurement on a physical system can be reduced, at least in principle, to the measurements with a certain number of yes–no experiments.

A typical example of this reduction of an experiment to yes–no experiments is the channel analyzer. The individual channels each define a yes–no experiment; and their *ensemble together* permits the measurement of an energy spectrum, for instance. Each measurable quantity has a certain range of values which may be indicated as a subset of the real line (or perhaps a Euclidean space). A determination of this quantity is obtained by dividing the real line into smaller intervals, and then deciding whether the measured value falls within any one of the intervals. By making the intervals sufficiently small, one can determine the value of the quantity to any desired accuracy.

If we wish to determine the position of the proton we would place a number of counters at various positions in space and register their response. This assembly of yes–no experiments will suffice to locate the proton to within the extension of one counter.

We shall introduce a terminology which will be useful in the discussion of general systems. A yes–no experiment which serves to select the values of a measurable physical quantity will be called a *filter* for this quantity. The name is clearly borrowed from the analogous situations encountered in frequency filters. We shall also refer to yes–no experiments simply as *propositions* of a physical system.

The second of the above-mentioned difficulties will be overcome if we investigate the properties of the propositions of a physical system which are *independent of the state* of the system. Evidently the individual propositions will not do that, since they can be either true or false. Such properties must therefore be found among the *relations* between different propositions. Let us illustrate this again with an example.

Suppose we have two propositions, a and b, which can be measured by two counters. Counter A locates a proton in the volume V_A and counter B locates the proton in the volume V_B. The responses of the counters A and B cannot be entirely independent of each other. This is obvious if for instance $V_a \subset V_b$. Then whenever the response to counter A is "yes," counter B must also respond with "yes" (assuming 100% efficiency of the counters).

Between certain pairs of propositions there exists thus a relation which we express as $a \subset b$; meaning: Whenever a is true, then b is true, too. What is important for us is that this relation is *independent* of the state of the system. It is thus the desired structural property which expresses a property of the system independent of its state.

5-3. THE PROPOSITIONAL CALCULUS

In this section we present in axiomatic form the structure properties of the propositions of a physical system which are independent of the state.

Let $\mathfrak{L}$ be the set of all propositions (yes–no experiments) $a, b, \ldots$ of a physical system. This set is partially ordered. We say a implies b and write $a \subseteq b$ if, whenever a is true it follows that b is true, too. The relation $\subseteq$ satisfies the following conditions:

$$\begin{aligned} &1) && a \subseteq a && \text{for all } a \in \mathfrak{L}; \\ &2) && a \subseteq b \text{ and } b \subseteq a && \text{implies } a = b; \\ &3) && a \subseteq b \text{ and } b \subseteq c && \text{implies } a \subseteq c. \end{aligned} \tag{I}$$

We note here that we have not yet defined what we mean by *equality* of two propositions. Rule (2) may therefore be regarded as a *definition* of equality. This definition is possible, since the simultaneous validity of the relations $a \subseteq b$ and $b \subseteq a$ is an equivalence relation which permits us to define the class of equivalent propositions. If we set $a = b$ we have essentially replaced the propositions by classes of equivalent propositions. In the physical interpretation this means that we have defined a proposition as a class of physical yes–no experiments, all of which measure the same proposition.

The next axiom asserts the existence of the *greatest lower bound* for any subset of propositions.

Let I be an index set and a_i $(i \in I)$ any subset of $\mathfrak{L}$, $a_i \in \mathfrak{L}$. Then there exists a proposition, denoted by $\bigcap_I a_i$ with the property

$$x \subseteq a_i \quad \text{for all } i \in I \Leftrightarrow x \subseteq \bigcap_I a_i. \tag{II}$$

The physical interpretation of this axiom requires considerably more explanation than does (I). Let us first consider the case that the set $\{a_i\}$ consists of just two elements which we call a and b. The proposition with the property (II) will then be denoted by $a \cap b$.†

† Note that the operation denoted by $a \cap b$ is identical with that used for set intersection in Chapter 1. Here it has a different meaning since the propositions $a, b, \ldots$ are not sets.

As a physical measurement $a \cap b$ denotes the measurement of "a and b." This is the proposition which is true if a is true *and* if b is true, and which is not true in all other cases. The existence of such a proposition is thus assured if it is possible to measure it, be it only in principle.

In a classical system there is no difficulty in measuring the proposition "a and b" if a and b can be separately measured. It suffices to measure both a *and* b and then we have also measured $a \cap b$. In fact $a \cap b$ is true if and only if both a and b are true.

This possibility in classical systems depends in an essential way on the property that measurements on such systems can be performed without modifying the state of the system. For quantal systems this is in general not possible, and then the measurement of the proposition $a \cap b$ may become obscure even if both a and b are separably measurable. The difficulty is this: If the measurement of $a \cap b$ is attempted by measuring first a, to be followed by a measurement of b, then we are not sure whether the first measurement of a may not have modified the state in such a way that the subsequent measurement of b may be affected. Such situations are easily exhibited in quantum mechanics.

It is possible to overcome this difficulty by the following procedure. Instead of making one pair of measurements a and b, we construct a filter for the proposition $a \cap b$ by using an infinite sequence of alternating pairs of filters for the propositions a and b respectively. This construction is symbolically represented in Fig. 5-1.

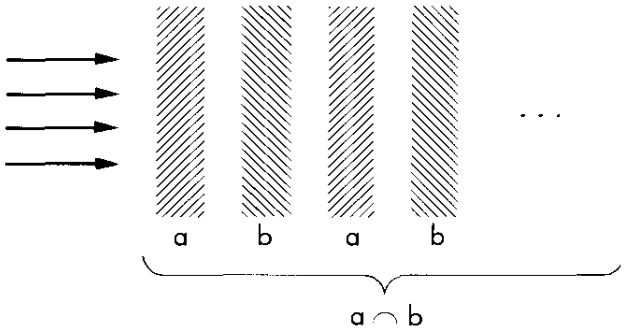


Fig. 5–1 Construction of the filter for the proposition $a \cap b$ in quantum mechanics.

The proposition $a \cap b$ is then true if the system passes this filter, and it is not true otherwise. Although infinite processes are, of course, not possible in actual physical measurements, the construction can be used as a base for an approximate determination of the proposition to any needed degree of accuracy.

It is just as easy to define the proposition $\bigcap_I a_i$ if I has a finite number of elements. With axiom II we require much more than that. We affirm the existence of the greatest lower bound even for an infinite family of propositions. There is no empirical correlate in the infinite conjunction implied in the definition of $\bigcap_I a_i$, since one can perform only a finite number of experiments. If we extend this definition to infinite sets, we transcend the proximately observable facts and we introduce *ideal elements* into the description of physical systems.

This is a procedure which is quite common in many other axiomatizations of pure or applied mathematics. For instance, in the calculus of probability it would correspond to the infinite additivity of the probability measure. It is justified by the resulting simplicity of the mathematical object thereby defined.

The axiom II implies the existence of a proposition $\emptyset$ with the property $\emptyset \subseteq a$ for all $a \in \mathscr{L}$. It is defined by

$$\emptyset = \bigcap_{a \in \mathscr{L}} a,$$

and it is called the *absurd proposition*, because it is always false. From this property its idealized nature is obvious.

The next axiom affirms the existence of the *orthocomplementation*.

To every $a \in \mathscr{L}$ there exists another proposition $a' \in \mathscr{L}$ such that

$$\begin{aligned} &1) && (a')' = a; \\ &2) && a' \cap a = \emptyset; \\ &3) && a \subseteq b \Leftrightarrow b' \subseteq a'. \end{aligned} \tag{III}$$

The physical interpretation of this axiom is quite easy, because the proposition a' is measured with exactly the same apparatus as a. The only difference is that the results are inverted: If a is true, then a' is false, and vice versa. We introduce here a strong negation denoted by "false" and distinguished from simply "not true." The property (1) is then obvious, while (2) expresses the law of the excluded middle. Property (3) is called Morgan's law in formal logic. Here we postulate it. The proposition a' is thus the (strong) negation of the proposition a. We could call it the proposition "not a."

From the three groups of axioms we immediately deduce the existence of the *least upper bound*. It is defined by

$$\bigcup_I a_i \equiv \left(\bigcap_I a_i'\right)', \tag{5-1}$$

and we verify easily that it satisfies

$$a_i \subseteq x \Leftrightarrow \bigcup_I a_i \subseteq x \qquad \text{for all } x \in \mathscr{L}. \tag{5-2}$$

(See Problem 1.)

The proposition $I \equiv \bigcup_{a \in \mathscr{L}} a$ is called the *trivial proposition* since it is always true (Problem 2). One can then prove that $x \cup x' = I$ for all $x \in \mathscr{L}$. (Problem 3.)

The proposition $a \cup b$ has the logical significance "a or b" and it is true if a or b, or both, are true.

Table 5-1

THE PROPOSITIONAL CALCULUS OF A PHYSICAL SYSTEM

Lattice operation	Interpretation
$a \subseteq b$	a implies b
a'	not a
$a \cap b$	a and b
$a \cup b$	a or b

A set $\mathscr{L}$ of elements which satisfy the axioms I, II, and III is called a complete, orthocomplemented lattice. We have thus postulated the following:

The propositions of a physical system are a complete, orthocomplemented lattice.

The structure of this lattice will be independent of the state of the physical system; the lattice describes the *intrinsic structure* of the system.

In Table 5-1 we summarize the fundamental relations in a lattice, together with their interpretation.

The propositional calculus of a physical system has a certain similarity to the corresponding calculus of ordinary logic. In the case of quantum mechanics, one often refers to this analogy and speaks of quantum logic in contradistinction to ordinary logic. This has unfortunately caused such confusion that we shall add a few words of explanation here to avoid any misunderstanding.

The calculus introduced here has an entirely different meaning from the analogous calculus used in formal logic. Our calculus is the formalization of a set of *empirical* relations which are obtained by making measurements on a physical system. It expresses an objectively given property of the physical world. It is thus the formalization of empirical facts, inductively arrived at and subject to the uncertainty of any such fact. The calculus of formal logic, on the other hand, is obtained by making an analysis of the meaning of propositions. It is true under all circumstances and even tautologically so. Thus, ordinary logic is used even in quantum mechanics of systems with a propositional calculus vastly different from that of formal logic. The two need have nothing in common. It turns out, however, that, if viewed as abstract structures, they have a great deal in common without being identical. Their most important difference is that the calculus of formal logic is Boolean, while that of physical propositions is Boolean only for classical systems (cf. Section 5-3 and references 14 through 20). The distinction between a formal logic and an empirical proposition system is exhibited most clearly in reference 16.

We shall occasionally use a graphical representation of lattices which is very convenient for analyzing simple finite examples of lattices. In this representation, propositions are denoted by points and the implication relation by a more or less vertical line. The simplest possible complete orthocomplemented lattice has the form given in Fig. 5-2.

Figure 5–2

PROBLEMS

1. If $\bigcup_I a_i \equiv (\bigcap_I a_i')'$, then

$$a_i \subseteq x \Leftrightarrow \bigcup_I a_i \subseteq x \qquad \text{for all } x \in \mathscr{L}.$$

2. The proposition

$$I = \bigcup_{a \in \mathscr{L}} a$$

has the property $I = \emptyset'$; consequently it is always true (trivial proposition).

3. $x \cup x' = I$ for all $x \in \mathscr{L}$.
4. If the two relations $x \subseteq a$ and $x \subseteq b$ imply one another, then $a = b$.
5. $(a \cap b)' = a' \cup b'$; $(a \cup b)' = a' \cap b'$.

5-4. CLASSICAL SYSTEMS AND BOOLEAN LATTICES

The propositional calculus so far developed is so general that it contains as yet no specific properties of physical systems. In fact, it does not even distinguish between classical and quantal systems. We shall now examine the additional properties of a lattice which will characterize the classical systems.

In classical mechanics, the state of a system is represented as a point in phase space, defined by the values $q_1, q_2, \ldots q_n, p_1, p_2, \ldots p_n$ of the coordinates and canonical momenta. We shall simply designate such a point by (q, p). Any measurable physical quantity will be represented by a real-valued Borel function $F(q, p)$. The elementary propositions associated with such a measurable quantity are then the propositions

$$F(q, p) \in \Delta,$$

where Δ is some Borel set of the real line. To every such proposition, one can associate in a unique manner a Borel set of the phase space

$$F^{-1}(\Delta) \equiv \{q, p : F(q, p) \in \Delta\}.$$

Conversely, to any Borel set S in the phase space, one can associate a proposition, for instance, $\chi_S(q, p) = 1$, where $\chi_S(q, p)$ is the characteristic function of the set S. Thus, every Borel set S in phase space represents a proposition of

the system. The proposition is true if $(q, p) \in S$. We see from this remark that in this case the greatest lower bound $a \cap b$ of two propositions corresponds to set intersection. Thus if S_x is the set which represents the proposition x, we have

$$S_{a \cap b} = S_a \cap S_b \qquad \text{and} \qquad S_{a'} = S_a' \quad \text{(complementary set)}.$$

The proposition $\emptyset$ is then represented by the null set and the proposition I by the entire phase space.

The postulated axioms are now elementary consequences from the theory of sets, except that II is valid only for countable families of propositions. In this case we replace II by II_σ.

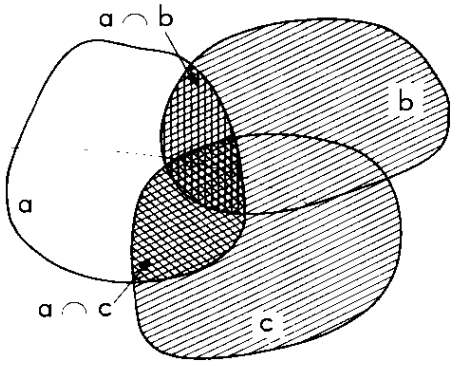


Fig. 5–3 Illustration of the distributive law: $a \cap (b \cup c) = (a \cap b) \cup (a \cap c)$.

The lattice $\mathscr{L}_c$ of a class of subsets satisfies, however, additional properties which are independent of the axioms I, II, and III, which we shall now enumerate: One verifies easily (cf. Fig. 5-3) that if $a, b, c \in \mathscr{L}_c$, then

$$\begin{aligned} a \cap (b \cup c) &= (a \cap b) \cup (a \cap c), \\ a \cup (b \cap c) &= (a \cup b) \cap (a \cup c). \end{aligned} \tag{D}$$

This is called the *distributive law*.

For our example we can verify, from our definition of propositions, the existence of *minimal propositions* (or "points") P, with the following property:

$$\emptyset \subset P \qquad \text{and} \qquad x \subset P \Rightarrow x = \emptyset \qquad (A_o).$$

We call such propositions *atomic*. They are represented by sets consisting of exactly one point, and every proposition a contains at least one such proposition.

The existence and meaning of atomic propositions in physical systems has been questioned by Birkhoff and von Neumann. In reference 3 they argue that it is operationally meaningless to say that the angular velocity of the moon around the earth (in radians per second) is a rational number. They assume that propositions are not Borel sets but classes of equivalent sets with respect to the Lebesgue measure in phase space, where two sets Δ_1 and Δ_2 are considered equivalent if their Lebesgue measure is equal. It is clear that the lattice of such classes of sets is nonatomic and it certainly contains fewer idealized elements than the class of all Borel sets.

However, in classical mechanics, this dictinction is not important, since even the classes of equivalent sets contain many elements which are probably just as difficult to associate with concrete propositions as some of the Borel sets. Furthermore, the lattice of Birkhoff and von Neumann can be embedded in an obvious way in the lattice of Borel sets, and so one always has the possibility of accordingly enlarging the lattice to an atomic lattice. Finally, only the atomic lattice represents really classical mechanics as it always has been understood, where the precise values (q, p) of the coordinates and momenta are used in the usual treatment of classical systems.

A lattice which satisfies I, II_σ, III, and A_0 is called an atomic, σ-complete Boolean lattice. We are thus led to postulate:

The propositions of a classical physical system are a σ-complete atomic Boolean lattice.

5-5. COMPATIBLE AND INCOMPATIBLE PROPOSITIONS

It is now time to identify the property which allows the distinction of classical from quantal systems. To this end we shall introduce a new concept, that of *compatibility* of propositions.

In classical systems all propositions are compatible. In the usual interpretation of this notion, it means that a simultaneous measurement of several propositions can be made without affecting the state of the system. This means specifically that the result of the measurement will be *independent of the order* in which the measurements are performed. This is naturally true only in an approximate sense; any measurement involves an interaction with the system. But in classical mechanics it is asserted that the effect of the disturbance of the state by the measurement can be reduced to a negligible amount, so that it may be omitted in a discussion of idealized experiments.

Since we have not yet defined and discussed the notion of "state" of a system, we shall, for the time being, define the notion of compatibility as equivalent to being "classical." In order to make this precise, we need a few definitions.

Let $\mathscr{L}$ be a lattice (orthocomplemented and complete; we shall not repeat these adjectives). A subset $\mathscr{L}_0 \subset \mathscr{L}$ is called a *sublattice* of $\mathscr{L}$ if it is again a lattice with respect to the operations which make $\mathscr{L}$ a lattice. Thus, in the lattice of Fig. 5-4, the subset $\emptyset, I$ is a sublattice but not the subset $(\emptyset, a)$, since a' and I are not in that subset.

One proves easily: If $\mathscr{L}_i$ $(i \in I)$ is a family of sublattices of a lattice $\mathscr{L}$, then the intersection $\bigcap_i \mathscr{L}_i$ is also a sublattice (Problem 1).

Now let $S \subset \mathscr{L}$ be any subset of $\mathscr{L}$ and denote by $\mathscr{L}_i$ the family of all the sublattices which contain S $(S \subseteq \mathscr{L}_i)$. Then the lattice $\mathscr{L}_0 = \bigcap_i \mathscr{L}_i$ is the smallest lattice which contains S. We shall call it the lattice *generated* by S. If $\mathscr{L}_0 = \mathscr{L}$, then the set S is called a *total* set.

A sublattice $\mathscr{L}_B \subset \mathscr{L}$ is called a Boolean sublattice if it satisfies the distributive law (D).

We now define a subset $S \subset \mathscr{L}$ as a *compatible set* of propositions if the lattice generated by S is a Boolean sublattice of $\mathscr{L}$.

Since a sublattice of any Boolean sublattice is again Boolean (Problem 2), we see that *every* subset of propositions in a classical system is compatible. This is just what we wanted to require of our definition of compatibility. Figure 5-5 illustrates this definition for a non-Boolean lattice.

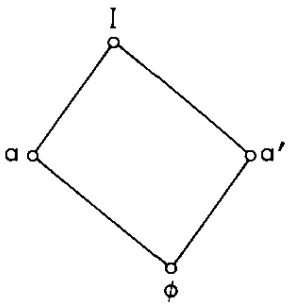


Fig. 5-4 Example of a lattice which contains a sublattice, for instance, $(\emptyset, I)$.

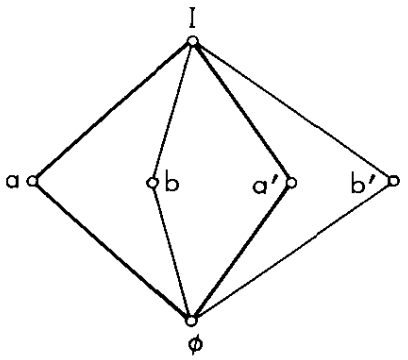


Fig. 5-5 A Boolean sublattice consisting of the elements $(\emptyset, I, a, a')$ in a non-Boolean lattice. It is generated by the subset $S = \{a\}$.

It is easy to prove that the two propositions a and a' are always compatible (Problem 3). This is physically very reasonable, since we have previously shown that these two propositions are measured with the same physical apparatus, and therefore they cannot disturb one another.

If two propositions a and b are compatible, that is, if the set $S = \{a, b\}$ generates a Boolean sublattice, we shall write $a \leftrightarrow b$. The notation indicates a symmetrical relationship. It is important to realize that the relationship of compatibility is not transitive. Thus if $a \leftrightarrow b$ and $b \leftrightarrow c$, we cannot in general assert $a \leftrightarrow c$.

The two ideal propositions $\emptyset$ and I have the property that they are compatible with any proposition (Problem 4). The set of propositions $\mathscr{C}$ which are compatible with all propositions of $\mathscr{L}$ is called the *center* of $\mathscr{L}$. It is a Boolean sublattice of $\mathscr{L}$ (Problem 5). In a Boolean lattice the center is identical with $\mathscr{L}$. If the center consists only of the elements $\emptyset$ and I, it is called *trivial*, and a lattice with trivial center is called *irreducible*. In all other cases the lattice is *reducible*.

The notion of irreducibility introduced here permits another interpretation which justifies the use of this term. In order to show this we introduce the notion of the *direct union* of two lattices. Let $\mathscr{L}_1$ and $\mathscr{L}_2$ be two lattices. We can define a new lattice $\mathscr{L}$ called the direct union of $\mathscr{L}_1$ and $\mathscr{L}_2$ by considering the elements of $\mathscr{L}$ as pairs of elements $\{x_1, x_2\}$ with $x_1 \in \mathscr{L}_1$ and $x_2 \in \mathscr{L}_2$.

The order relation in $\mathscr{L}$ is then defined by

$$\{x_1, x_2\} \subseteq \{y_1, y_2\} \qquad \text{if } x_1 \subseteq y_1 \quad \text{and} \quad x_2 \subseteq y_2.$$

With this order relation, it is possible to define unions and intersections in $\mathscr{L}$ by setting

$$\{x_1, x_2\} \cap \{y_1, y_2\} \equiv \{x_1 \cap y_1, x_2 \cap y_2\}$$

and

$$\{x_1, x_2\} \cup \{y_1, y_2\} \equiv \{x_1 \cup y_1, x_2 \cup y_2\}.$$

The lattice $\mathscr{L}$ obtained in this way is called the direct union. It contains the two lattices $\mathscr{L}_1$ and $\mathscr{L}_2$ as sublattices, since the set of elements $\{x_1, \emptyset_2\}$ is isomorphic with (has the same lattice structure as) $\mathscr{L}_1$ and the set of elements $\{\emptyset_1, x_2\}$ is isomorphic with $\mathscr{L}_2$.

This construction is easily generalized to any family of lattices: Let $\mathscr{L}_i$ $(i \in I)$ be a finite or infinite family of lattices. The direct union of the $\mathscr{L}_i$ is the lattice consisting of collections of elements $\{x_i\}$ with $x_i \subseteq \mathscr{L}_i$. A partial order in $\mathscr{L}$ is defined by

$$\{x_i\} \subseteq \{y_i\} \quad \text{if} \quad x_i \subseteq y_i \qquad \text{for all } i \in I.$$

If unions and intersections in $\mathscr{L}$ are defined by

$$\{x_i\} \cup \{y_i\} = \{x_i \cup y_i\}, \qquad \{x_i\} \cap \{y_i\} = \{x_i \cap y_i\},$$

then $\mathscr{L}$ becomes a lattice.

In the lattice of the first example, the elements $\{I_1, \emptyset_2\}$ and $\{\emptyset_1, I_2\}$ are in the center of $\mathscr{L}$ and they are different from the elements $\emptyset = \{\emptyset_1, \emptyset_2\}$ and $I = \{I_1, I_2\}$. Thus the center of $\mathscr{L}$ is nontrivial. For certain lattices (which we shall specify presently), one can prove a converse: If the center of a lattice $\mathscr{L}$ is nontrivial, then there exist at least two lattices such that $\mathscr{L}$ is the direct union of the two. It is possible to expand these remarks to a complete reduction theory analogous to the reduction theory of Hilbert spaces of group representations. We shall, however, not pursue these questions further until we have more fully specified the structure of the lattice of propositions.

PROBLEMS

1. If $\mathscr{L}_i$ $(i \in I)$ is a family of sublattices of a lattice, then $\bigcap_i \mathscr{L}_i$ is also a sublattice.
2. A sublattice of a Boolean lattice is again Boolean.
3. The two propositions a and a' are always compatible.
4. The two elements $\emptyset$ and I in a lattice $\mathscr{L}$ are compatible with any element $a \in \mathscr{L}$.
5. The center $\mathscr{C}$ of a lattice $\mathscr{L}$ is a Boolean sublattice of $\mathscr{L}$.

5-6. MODULARITY

The problem before us is the following: We know that the lattice of propositions cannot be Boolean if it should be more general than the lattice of a classical system; but we do not yet have any restriction which permits us to set a limit to the generalizations. What is this restriction?

Such a restriction should be motivated by physical considerations. Before we formulate it we shall briefly discuss in this section a proposal for such a restrictive axiom which is, however, physically untenable [3, 4]. This is the so-called *modular law.*

In any lattice one always has (Problem 1)

$$x \cup (y \cap z) \subseteq (x \cup y) \cap z \qquad \text{for } x \subseteq z.$$

If the lattice is such that for all $x \subseteq z$ we actually have equality in this relation, that is,

$$x \cup (y \cap z) = (x \cup y) \cap z \qquad \text{for all } x \subseteq z, \tag{M}$$

then we say that the lattice is a *modular* lattice. It is clear that a Boolean lattice is always modular. It is also easy to give examples of orthocomplemented lattices which are not modular. Two such examples are given in Fig. 5–6.

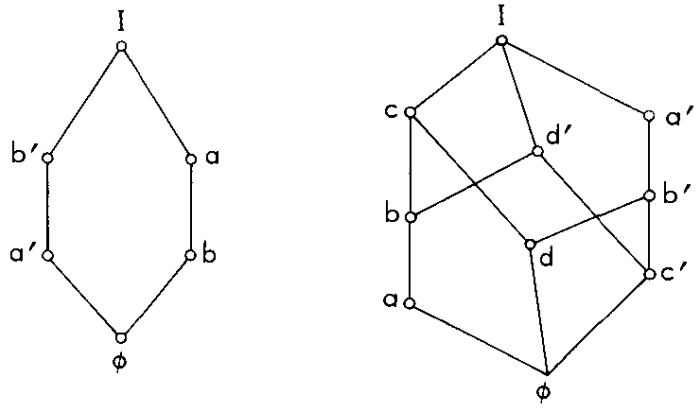


Fig. 5–6 Two examples of orthocomplemented nonmodular lattices.

The modularity postulate has much in its favor. For one thing, it is the best known of the possible generalizations of Boolean lattices. This, of course, would not suffice for a justification of its use as a physical axiom.

Birkhoff and von Neumann [3, 4] have tried to justify modularity by pointing out that on finite modular lattices one can define a dimension function $\nu(a)$ with the properties:

$$0 \leq \nu(a) \leq 1,$$

$$\nu(a) = 0 \qquad \text{if and only if } a = \emptyset,$$

$$\nu(a) = 1 \qquad \text{if and only if } a = I,$$

and

$$\nu(a) + \nu(b) = \nu(a \cup b) + \nu(a \cap b).$$

Such a function has the characteristic properties of a probability measure, and $v(a)$ would represent the *a priori* probability for finding the system with property a when nothing is specified as to its preparation. It is known that there are systems for which such a finite *a priori* probability does not exist. It would correspond classically to a system with a phase space of finite invariant measure. A particle moving in empty space does not admit a finite dimension function either in classical or in quantum mechanics. Thus this argument for the modularity of the proposition system is not convincing.

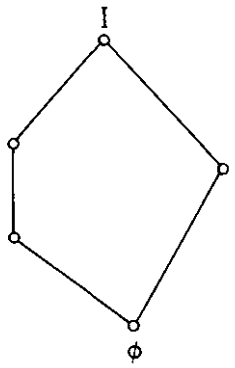
An argument against modularity is obtained from our analysis of the notion of localizability of a particle. This notion will be examined in Chapter 12, where it will be shown that, in the context of conventional quantum mechanics in Hilbert space, it is incompatible with modularity.

PROBLEMS

1. In any lattice one has

$$x \cup (y \cap z) \subseteq (x \cup y) \cap z \qquad \text{for } x \subseteq z.$$

2. The lattice given by the diagram below is not modular.



5-7. THE LATTICE OF SUBSPACES

It is high time we connected our lattice of propositions with the lattice of subspaces discussed in Section 2-5. We have already remarked that the lattice of subspaces of a Hilbert space is a complete orthocomplemented lattice. In that section we also introduced the notion of compatibility, but in a different way; and we must now show that it is identical with the definition used in this chapter. Finally, we shall answer the question whether the lattice of all subspaces is modular or not.

Let us begin with the notion of compatibility. Compatibility as defined in Section 2-5 is expressed very conveniently with the projections E and F, with ranges M and N, respectively. Indeed if $M \leftrightarrow N$, then $EF = FE$; that is, the projections commute (Problem 1).

Now it is not difficult to verify that the sublattice generated by two commuting projections is a Boolean lattice (Problem 2).

Conversely, if E and F are two projections generating a Boolean lattice, then one can show that they must be compatible in the sense of Section 2-5 (Problem 3). Thus the two definitions are equivalent.

Let us next examine the property of modularity. Here we must distinguish the finite- from the infinite-dimensional case. If the Hilbert space is finite-dimensional, then we can easily show that the lattice of subspaces is indeed modular.

To see this, let M, N, and K be three subspaces such that $M \subset K$. We have already established that, in any lattice,

$$M \cup (N \cap K) \subseteq (M \cup N) \cap K \qquad \text{if } M \subset K$$

(cf. Problem 1, Section 5-6). Thus, in order to demonstrate modularity, we need to show the inclusion in the reverse sense. If $\mathbf{a}$ is an arbitrary vector $\mathbf{a} \in (M \cup N) \cap K$, it follows from the definition of intersection that $\mathbf{a} \in M \cup N$ and $\mathbf{a} \in K$. But every vector in $M \cup N$ is a sum of a vector in M and a vector in N, because $M \cup N$ is finite-dimensional. Thus we may write $\mathbf{a} = \mathbf{b} + \mathbf{c}$ with $\mathbf{b} \in M$ and $\mathbf{c} \in N$. But according to the assumption $M \subset K$, we have also $\mathbf{b} \in K$. Thus $\mathbf{c} = \mathbf{a} - \mathbf{b} \in K$ and $\mathbf{c} \in N$. Therefore $\mathbf{c} \in K \cap N$, and we have shown that $\mathbf{a}$ is a sum of two vectors $\mathbf{b} \in M$ and $\mathbf{c} \in N \cap K$. This means that $\mathbf{a} \in M \cup (N \cap K)$, and thus

$$M \cup (N \cap K) = (M \cup N) \cap K.$$

Hence, the lattice is modular.

When we examine this demonstration, we observe that we have used the finite-dimensionality in an essential way, at the point where we wrote $\mathbf{a} = \mathbf{b} + \mathbf{c}$ with $\mathbf{b} \in M$ and $\mathbf{c} \in N$. This remark leads us easily to the construction of a counterexample if the two spaces M and N are infinite-dimensional.

Let us assume that $\mathbf{d} \in M \cup N$ and that $\mathbf{d}$ is a limit vector of vectors of the form $(\mathbf{a} + \mathbf{b})$ with $\mathbf{a} \in M$ and $\mathbf{b} \in N$, but that $\mathbf{d}$ is not itself of this form. Let us further assume, for simplicity, that $M \cap N = \emptyset$ and let K be the subspace generated by M and this vector $\mathbf{d}$. Every vector $\mathbf{x} \in N \cap K$ satisfies $\mathbf{x} = \lambda\mathbf{d} + \mathbf{b} \in N$ with $\mathbf{b} \in M$. But this is possible only under the stated conditions for $\mathbf{x} = 0$. Thus $N \cap K = \emptyset$. Therefore

$$M \cup (N \cap K) = M, \qquad \text{but} \qquad (M \cup N) \cap K = K \subset M.$$

Thus we conclude:

The subspaces of an infinite-dimensional Hilbert space are a nonmodular lattice.

PROBLEMS

1. Let M and N be the ranges of the projections E and F respectively; then (cf. Section 2-5)

$$M \leftrightarrow N \Leftrightarrow EF = FE.$$

2. The lattice generated by two commuting projections is Boolean.
3. If two projections E and F generate a Boolean sublattice of the lattice of all projections, then they satisfy

$$(E \cap F) \cup (E \cap F^{\perp}) = E \qquad \text{and} \qquad (F \cap E) \cup (F \cap E^{\perp}) = F.$$

5-8. PROPOSITION SYSTEMS

In this section we shall give the answer to the question formulated in Section 5-6 as to the nature of the axiom which is to be postulated in place of the distributive property. Several equivalent and apparently independent formulations of this axiom have been given [9, 10, 11, and 12].

Let us consider two propositions a and b such that a implies b: $a \subseteq b$. It is then reasonable to postulate that two such propositions are compatible with one another. That is, we postulate

$$a \subseteq b \Rightarrow a \leftrightarrow b \tag{P}$$

Let us first show that in a Hilbert space, this axiom is automatically satisfied. Thus, if E and F are two projections such that $E \subseteq F$, or $EF = E$, then $FE = (EF)^* = E^* = E = EF$. Thus, the two projections must commute; and, according to the preceding section, they are compatible.

Let us next verify that axiom (P) is independent of the others; that is, it actually excludes certain lattices which satisfy all the other axioms. Two examples of orthocompleted and complete lattice which do not satisfy (P) are given in Fig. 5–6 (a) and (b). Both of these lattices are nonmodular, and it is, in fact, easy to prove that modularity implies (P) (Problem 1). It seems, therefore, justified to call axiom (P) a *weak modularity*.

It follows immediately from axiom (P) that if $a \subseteq b'$, that is, if a and b are *disjoint*, then $a \leftrightarrow b$. Furthermore, one can prove that if $a \leftrightarrow b$, it follows also that $a \leftrightarrow b'$ (Problem 2). This means that disjoint propositions are always compatible.

A further consequence of axiom (P) is the following useful distributivity property:

If $\{a_i\}$ $(i \in I)$ *is any collection of propositions, and if* $a_i \leftrightarrow b$ *then*

$$b \cap \left(\bigcup_I a_i\right) = \bigcup_I (b \cap a_i) \qquad \textit{and} \qquad b \cup \left(\bigcap_I a_i\right) = \bigcap_I (b \cup a_i)$$

(Problem 3).

From this, one deduces easily that if $\{a_i\}$, $(i \in I)$, is any subset of elements, and if $a_i \leftrightarrow b$ for all $i \in I$, then

$$\bigcup_I a_i \leftrightarrow b \qquad \text{and} \qquad \bigcap_I a_i \leftrightarrow b$$

(Problem 4).

As a final theorem, we mention three other equivalent formulations of axiom (P):

1) *If we define by the segment* $[a, b]$ *the set of elements* x *such that* $a \subseteq x \subseteq b$, *then the mapping* $x \to x'_r \equiv (a \cup x') \cap b$ *is an orthocomplement for the segment* $[a, b]$ (see reference 9);
2) $a \perp b$, $a \perp c$; $a \cup b = a \cup c$; *and* $b \subseteq c \Rightarrow b = c$;
3) *the compatible complement* a' *is unique* (cf. reference 13).

Of these equivalent properties, the last (3) is especially interesting, since it is most easily interpretable in physical terms. These useful theorems simplify many steps in the study of such lattices.

The last axiom which we postulate for a proposition system is the atomicity axiom. It consists of two parts:

A_1: *For any proposition* $a \neq \emptyset$, *there exists a point* P (minimal proposition, cf. Section 5-4) *such that* $P \subseteq a$.

A_2: *If* Q *is a point, then*

$$a \subseteq x \subseteq a \cup Q \Rightarrow x = a \qquad \text{or} \qquad x = a \cup Q.$$

The physical justification for this axiom is not very strong; it is analogous to the justification which we have given for the atomicity in classical proposition systems. It is therefore desirable to draw as many conclusions as possible without the explicit use of A ($= A_1$ and A_2).

From now on we shall call a system of elements $\mathscr{L}$ which satisfies the axioms I, II, III, P, and A a *proposition system*. The kinematical structure which contains all the properties independent of the state of the system will be expressed entirely in the structure of the proposition system $\mathscr{L}$.

PROBLEMS

1. A modular orthocomplemented lattice satisfies axiom (P).

*2. The following statements are equivalent for a lattice which satisfies (P):
(1) $a \leftrightarrow b$.
(2) $a \leftrightarrow b'$.
(3) $(a \cap b') \cup b \quad (b \cap a') \cup a \quad a \cup b$.
(4) The four elements a, b, a', b' satisfy the distributive law for any combination.
(5) $(a \cap b) \cup (a \cap b') \cup (a' \cap b) \cup (a' \cap b') \quad I$.
(Cf. reference 9.)

*3. If a_i $(i \in I)$ is a subset of elements in a lattice satisfying (P), and if $a_i \leftrightarrow b$, then

$$b \cap \left(\bigcup_I a_i\right) = \bigcup_I (b \cap a_i) \qquad \text{and} \qquad b \cup \left(\bigcap_I a_i\right) = \bigcap_I (b \cup a_i)$$

for any $b \in \mathscr{L}$. (Cf reference 9.)

4. If a_i $(i \in I)$ is an arbitrary subset of a lattice satisfying the axiom (P), then $a_i \leftrightarrow b$ for all $i \in I$ implies

$$\bigcap_I a_i \leftrightarrow b \qquad \text{and} \qquad \bigcup_I a_i \leftrightarrow b.$$

REFERENCES

A readable account of some historical and epistemological questions concerning quantum mechanics is found in:

1. P. FRANK, *Modern Science and its Philosophy*. Collier Books (1961).

A valuable source book with many further references is

2. H. FEIGL AND M. BRODBECK, *Readings in the Philosophy of Science*. Appleton-Century-Crofts (1953).

The proposition calculus of quantum mechanics is given by:

3. G. BIRKHOFF AND J. VON NEUMANN, *Ann. Math.* **37**, 823 (1936).

Although lattice theory led to many interesting developments in mathematics, there was little impact of this branch of mathematics on physics. The little there is may be found in:

4. G. BIRKHOFF, "Lattices in Applied Mathematics." *Proc. Symp. Pure Math.* Vol. II, *Am. Math. Soc.* (1961); especially p. 155.

The notion of compatibility is found in:

5. P. JORDAN, *Arch. Math.* **2**, 166 (1950).

6. S. MAEDA, *J. Sci. Hirosh. Univ.* **A19**, 211 (1955).

For a convenient general introduction to lattice theory, without any physical applications, however, see the following two references:

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8. G. SZÁSZ, *Introduction to Lattice Theory*, 3rd ed. New York: Academic Press (1963).

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11. L. H. LOOMIS, *Mem. Amer. Math. Soc.* **18**, 36 (1955).

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14. P. MITTELSTAEDT, *Sitzungsber. der Bay. Akad. der Wissensch.*, München (1959).

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16. ———, *Philosophische Probleme der modernen Physik*, Mannheim, 1966; especially Chapter VI.

17. E. SCHEIBE, *Die kontingenten Aussagen der Physik*. Frankfurt, 1964.

A point of view differing from ours is expressed in:

18. P. DESTOUCHE-FÉVRIER, "La Structure des Theories Physiques." Paris: Presse Universitaire de France (1951).

19. F. V. WEIZSÄCKER, "Komplementarität und Logik," *Naturwiss.* **42**, 521, 545 (1955).

20. H. REICHENBACH, *Philosophical Foundations of Quantum Mechanics*, 3rd ed. Los Angeles: University of California Press, (1948).

CHAPTER 6

STATES AND OBSERVABLES

There are two kinds of truths. To the one kind belong statements so simple and clear that the opposite assertion obviously could not be defended. The other kind, the so-called "deep truths," are statements in which the opposite also contains deep truth.

NIELS BOHR

In this chapter we introduce three important notions, that of state, that of observable, and the superposition principle. In Section 6-1 we compare the classical with the quantum mechanical notion of state, and point out some of the limitations of this notion in the latter case. State is, however, a measurable physical quantity, and the general aspects of such measurements are described in Section 6-2. The insight gained from this description is transferred into the precise mathematical description of state in axiomatic form, and some conclusions are drawn in Section 6-3.

The important notion of observable is introduced in Section 6-4, and it is shown that the essential feature of this object is a σ-homomorphism from Borel sets on the real line into the lattice of propositions. The properties of observables are further discussed in Section 6-5, and such important properties as spectrum, range, separability, etc., are introduced. Section 6-6 introduces compatibility for observables as a straightforward generalization of that same notion for propositions. In Section 6-7 we introduce the functional calculus of observables, and prove a theorem of von Neumann in the generalized form of Varadarajan concerning systems of compatible observables.

Section 6-8 contains first a description and then a precise mathematical formulation of the superposition principle. The final Section 6-9 deals with superselection rules, where the superposition principle is not generally true.

6-1. THE NOTION OF STATE

The notion of the state of a physical system is so familiar from its use in classical mechanics and field theory that it has entered quantum mechanics almost without any further analysis. Yet this notion becomes substantially

modified in quantum mechanics, and it requires a much more careful analysis than that usually given for classical systems.

In order to exhibit this difference, let us for a minute examine the notion of state for a classical system. In a classical system we can distinguish certain properties which are independent of the state. Such properties appear in the description of the system as the number of degrees of freedom and the topological structure of the phase space. The dynamical property, which expresses itself in the structure of the Hamiltonian, is also independent of the state.

The state, on the other hand, appears as the *initial condition* which determines the solutions of the equations of motion of the system. In a classical mechanical system, the initial condition is determined by fixing the values of the positions and momenta, that is, by fixing a point in phase space. The evolution of the state is then described by the *orbit* which passes through this point in phase space (see Fig. 6–1).

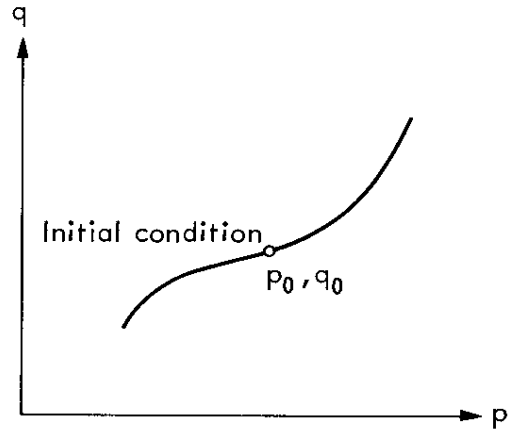

Fig. 6–1 Symbolic representation of a state in classical mechanics represented by the initial condition p_0, q_0 which determines an orbit.

The physical significance of this description for classical systems is this: If one prepares the system in such a way that at some time the initial conditions p_0, q_0 are realized, then the system evolves in time according to the unique orbit which passes through the point p_0, q_0 in phase space. At every moment it is then a state given by the values of p and q which are obtained for that value of time for this particular solution.

In quantum mechanics the specific description of the system in terms of the phase space is no longer possible. The structure that is independent of the state which replaces the classical phase space is the proposition system defined in Chapter 5.

The state of a quantum system is still a meaningful and useful notion if we attach this meaning closely to the empirical aspect of the state. This aspect is contained in the description: The state of a physical system is the result of a *preparation* of a system. The state thus embodies the specific history which preceded the instant to which the state refers. A preparation of a system is a series of manipulations which affect the system under consideration.

As simple as this description of the preparation of a state might appear at first sight, it is actually quite intricate because of the undefined notion of *affecting* a system. Without previous knowledge of the physical laws, it is not

immediately obvious whether certain physical conditions will affect a system or not.

Let us consider some examples to make this clear. If the system is a magnetic ion, then a static electric field will (in a very good approximation) have no observable effect on the state of the ion. However, if the electric field is *oscillating*, then the state may be markedly affected.

The photons emitted from a gas discharge tube might be affected by the intensity of the discharge, but again, in a good approximation, they are not.

We are thus led to the notion of *relevant* conditions for the preparation of a state. It is an empirical fact that some conditions are relevant and others are not; we stress here that we have no prior knowledge as to which of the conditions are relevant and which are not. The determination of the relevant conditions is a question of physics.

We summarize this discussion with a formal definition.

> ***Definition:*** *A state is the result of a series of physical manipulations on the system which constitute the preparation of the state. Two states are identical if the relevant conditions in the preparation of the state are identical.*

We shall add three remarks to this formal definition. The *distinction* between the system and its states cannot be maintained under all circumstances with the precision implied by this definition. The reason is that systems which we regard under normal circumstances as different may be considered as two *different states* of the *same* system. An example is a positronium and a system of two photons. We know that the former transforms spontaneously into the latter; and the adequate description for this process is that which assumes that a positronium and a pair of photons are two different states of one and the same system.

A similar situation is found in the description of a nucleon. A proton and a neutron may be considered two different physical systems, but a more unified and very useful description is obtained by considering them as two different states of a single system, called "nucleon." We speak then of isotopic spin, and we distinguish the two states by their isotopic spin value.

The second remark refers to the fact that there are certain conditions which are so obviously irrelevant that they are rarely considered seriously. For instance, only astrologists would include the phases of the moon as possible relevant conditions in the preparation of a micro system.

An important class of irrelevant physical conditions refers to the isotropy and homogeneity of space and time which are of basic importance for the objective verifiability of physical theories. For instance, it is a most fortunate fact that the *epoch* at which a state is prepared is usually irrelevant. This is very important for the possibility of measuring a state by a statistical series of experiments repeated at various times under otherwise identical conditions.

Likewise, the fact that an experiment on neutrinos, for instance, carried out in Geneva and in Brookhaven gives identical results means that the absolute *position in space* is not a relevant condition for the preparation of a state.

A final remark: The notion of state defined here has a limited, precise and technical meaning. It would lead to futile pseudo-problems if one tried to extend this meaning to situations where the notion is not applicable. Thus, it would be meaningless to speak about the state of the universe; and cosmological questions should therefore not be mixed into the kind of quantum mechanics that we discuss here.

6-2. THE MEASUREMENT OF THE STATE

A state is a measurable quantity. How can a state be determined by measurements? The measurements which are available are the set of yes–no experiments which form the propositions of the system. Let us suppose then that we try to determine these quantities.

Here we encounter a characteristic difficulty for quantum systems because not all elementary propositions are *simultaneously measurable*. The necessary and sufficient condition for this to be possible would be that every proposition is compatible with every other proposition. Since we shall see later that this is, in fact, not so, we cannot possibly determine the value of all the elementary propositions with a set of compatible measurements.

Thus, a state of a quantum system can only be measured if the system can be prepared an *unlimited number of times* in the same state. We have seen that the states of two systems are defined as identical if they are prepared under identical relevant conditions.

It is a fundamental fact that identical states do not yield identical results for the truth or falsehood of a proposition. Thus, a measurement of proposition a may sometimes give the value 1 (true) or 0 (false).

An example of such behavior is, for instance, found when one observes linearly polarized photons with an analyzer with its axis at 45° to the axis of the polarizer. It is possible to carry out such experiments with individual photons; and one observes that each individual photon either passes the analyzer or it does not. If a statistical study is made with a large number of photons, one observes that about half the photons pass through the analyzer and half are absorbed. It is, therefore, impossible to attribute to these photons the property of being polarized at 45°, nor is it possible to deny this property, since some of them do pass the analyzer.

From this example we see clearly that what we may expect in quantum mechanics is not a definite value for each of the elementary propositions a in a given state, but at the most a probability $p(a)$ for this value. This probability would be measured by making a large number n of experiments and recording

the number $n(a)$ of those experiments which give the value $+1$ for the proposition a. The probability in question would then be expected to be

$$p(a) = \lim_{n \to \infty} \frac{n(a)}{n}, \tag{6–1}$$

so that it could be determined in principle to an arbitrary degree of accuracy by making a sufficiently large number n of measurements.

It should be pointed out that this feature of elementary propositions is observed also for classical systems. Thus, for instance, if our initial prescription is to throw a die (without further detail), we observe one of the sides to turn up with a probability $\frac{1}{6}$. The difference between classical and quantal systems is that the classical state can be further determined by specifying further relevant conditions (such as throwing the die from a certain position in a certain direction and with a certain velocity) while for quantum systems such specification is usually not possible.

In any case we expect that the measured quantity is a probability function $p(a)$ defined on all the propositions. The physical interpretation which we attach to this function implies certain mathematical properties which we shall now enumerate.

6-3. DESCRIPTION OF STATES

According to the description of the preceding section, a state is mathematically determined by a real valued function $p(a)$ on all the propositions $a \in \mathscr{L}$. We shall require the following properties for the states $p(a)$:

1) $0 \leq p(a) \leq 1$.

2) $p(\emptyset) = 0, \qquad p(I) = 1$.

3) If $\{a_i\}$ is a sequence of propositions satisfying $a_i \subset a_k'$ for all pairs $(i \neq k)$, then $\sum_i p(a_i) = p(\bigcup a_i)$.

4) For any sequence $\{a_i\}$, $p(a_i) = 1$ implies $p(\bigcap a_i) = 1$.

5) (a) If $a \neq \emptyset$ then there exists a state p such that $p(a) \neq 0$.
(b) If $a \neq b$, then there exists a state p such that $p(a) \neq p(b)$.

Let us examine these axioms to determine to what extent they reflect the physical meaning of the state.

1) There is not much to say here, since this property is a direct consequence of the definition, Eq. (6–1).

2) $p(\emptyset) = 0$ means that the absurd proposition is always false and $p(I) = 1$ says that the trivial is always true. This is consistent with the idealized nature of these propositions.

3) This axiom is better discussed first in its finite form. Let, for instance, a and b be two propositions such that $a \subset b'$. We shall refer to such a pair as *disjoint*. Property (3) says then that

$$p(a) + p(b) = p(a \cup b). \tag{6–2}$$

Let us remember that the proposition $a \cup b$ has the physical interpretation of "a or b." In view of Eq. (6–1), the relation (6–2) is thus true if a and b are compatible and if

$$n(a) + n(b) = n(a \cup b).$$

The condition for this to hold is that $n(a \cap b) = 0$. But $a \cap b = \emptyset$, and thus condition (2) implies at least $n(a \cap b)/n \to 0$ (for $n \to \infty$). (The compatibility of a and b is a consequence of axiom (P), cf. Problem 1.)

Condition (3) is thus easily justified for two disjoint propositions, and hence for finite sequences of disjoint propositions. It is, however, postulated for infinite sequences, and this is a restriction which cannot be justified any longer by direct appeal to the experimental determination of $p(a)$. The extension to infinite sequences is a convenient mathematical axiom which corresponds exactly to the analogous axiom in Kolmogorov's theory of probability [1]. A simple consequence of (3) is:

If $a \leftrightarrow b$, then $p(a) + p(b) = p(a \cap b) + p(a \cup b)$. This relation is always true for any pair of elements if $p(a)$ is a probability function on a Boolean algebra of sets (Problem 3), but it need not be true for propositions which are not compatible.

The reader will have noticed that we are dealing with a kind of generalized probability. The classical probability is defined as a measure on a Boolean algebra of sets. The probability which we introduce here is a measure on a non-Boolean lattice. Some mathematical aspects of this notion have been studied by Varadarajan [2].

4) We discuss this property again first for two elements. Let $p(a) = p(b) = 1$. Then both propositions a and b are true. It is therefore reasonable to require that the proposition "a and b" also be true, that is, that

$$p(a) = p(b) = 1 \qquad \text{implies} \qquad p(a \cap b) = 1.$$

Property (4) is the generalization of this to an infinite sequence of propositions. Again, the same remarks apply that were made in connection with property (3), as to the idealized nature of this axiom.

For Boolean lattices property (4), when restricted to finite sequences, is a consequence of the others. This is no longer true for non-Boolean lattices (cf. Problem 4). We shall not always use property (4) in its infinite form in the following discussion. If we use only the finite form of (4), we shall replace it by

4)′ $$p(a) = p(b) = 1 \qquad \text{implies} \qquad p(a \cap b) = 1.$$

An immediate consequence of (4)′ and the other axioms is:

$$p(a) = p(b) = 0 \qquad \text{implies} \qquad p(a \cup b) = 0$$

(cf. Problem 5).

5) This is an axiom which guarantees that there are sufficiently many states. If it were not true, then a proposition a for which $p(a) = 0$ for all states would be, in a certain sense, unobservable. Likewise, if $p(a) = p(b)$ were true for all states, then the pair of propositions a, b would be physically indistinguishable; hence, it might as well be identified. It is possible that the lattice can be redefined in such a way that property (5) is always true. In this sense property (5) seems not a new physical property but merely a requirement which assumes the avoidance of redundancy.

The first question that ought to be settled is whether there exist states which possess the properties enumerated. This question is by no means easy to answer, because there exist examples of Boolean lattices which admit no states at all [3, p. 186]. It is thus not profitable to tackle this question in this general setting. In the more special context of complex quantum mechanics, we shall exhibit plenty of states, and in fact obtain all of them.

The states form a convex set. This means the following. If p_1 and p_2 are two different states, then

$$p = \lambda_1 p_1 + \lambda_2 p_2 \qquad \text{with } \lambda_1 + \lambda_2 = 1, \quad \lambda_1 > 0 \quad \text{and} \quad \lambda_2 > 0, \tag{6–3}$$

is again a state. This is easily verified (Problem 6). A state which is thus represented with the help of two others is said to be a *mixture*. A state which cannot be represented as a mixture of two others is said to be *pure*. The pure states are thus the extremal subset of a convex set.

We shall define the function $\sigma(a) \equiv p(a) - p^2(a)$ as the *dispersion* of the state. We shall sometimes also speak of the *overall dispersion* σ defined by

$$\sigma = \sup_{a \in \mathscr{L}} \sigma(a). \tag{6–4}$$

If $\sigma = 0$ we shall call the state *dispersion-free*. For such a state we have obviously the alternatives

$$p(a) = \begin{cases} 0, \\ 1. \end{cases} \tag{6–5}$$

The overall dispersion of a mixture of two different states is always > 0, so that dispersion-free states are always pure (cf. Problems 7 and 8). Pure states need not be dispersion-free, as we shall see later (Section 7-3).

PROBLEMS

1. Two disjoint propositions are compatible. That is $a \subset b' \Rightarrow a \leftrightarrow b$. [*Hint:* Use the result of Problem 2 in Section 5-8.]
2. If $a \leftrightarrow b$, then there exist three disjoint propositions a_1, b_1 and c such that

$$a = a_1 \cup c, \qquad b = b_1 \cup c.$$

They are given by

$$a_1 = a \cap b', \qquad b_1 = b \cap a', \qquad c = a \cap b.$$

3. For any pair $a, b \in \mathscr{L}$ and any state, $a \leftrightarrow b$ implies

$$p(a) + p(b) = p(a \cup b) + p(a \cap b).$$

(Use result of Problem 2, and axiom 3.)

4. If $\mathscr{L}$ is Boolean and $p(a)$ satisfies properties (1), (2), and (3), then

$$p(a) = p(b) = 1 \qquad \text{implies} \qquad p(a \cap b) = 1.$$

5. If $p(a) = p(b) = 0$, then $p(a \cup b) = 0$.
6. If p_1 and p_2 are two different states and λ_1, λ_2 two positive numbers such that $\lambda_1 + \lambda_2 = 1$, then $p = \lambda_1 p_1 + \lambda_2 p_2$ is also a state.
7. If p_1 and p_2 are two dispersion-free states, then their mixture $p = \lambda_1 p_1 + \lambda_2 p_2$ has dispersion $\sigma = \lambda_1 \lambda_2 (p_1 - p_2)^2$, where $\lambda_1 > 0$, $\lambda_2 > 0$, $\lambda_1 + \lambda_2 = 1$.
8. A dispersion-free state is always pure.

*9. Conditions (1), (2), (3), and (4) for states are equivalent to conditions (1), (2), and the following:

(3′) If $a \subset b'$, then $p(a) + p(b) = p(a \cup b)$;

(4′) If $p(a) = p(b) = 1$, then $p(a \cap b) = 1$.

(C) *Continuity.* For any increasing sequence $a_1 \subset a_2 \subset \cdots \subset a_t \subset \cdots$,

$$\lim_{n \to \infty} p(a_n) = p\left(\bigcup_n a_n\right)$$

(cf. reference 10).

6-4. THE NOTION OF OBSERVABLES

In physics an observation of a physical system consists in the manipulation of certain instruments (the measuring device) and the eventual reading (or recording) of a scale. The scale may consist of a continuum of values, or a discrete set, or both. The simplest "scale" would be the counter which registers the number of occurrences of certain elementary events. In any case, a measurement will give the answer to a number of elementary propositions corresponding to the different aggregates of values of the possible measuring result.

Since a measuring device is one experiment only, the question of compatibility cannot arise. Thus we expect all the elementary propositions associated with an observable to be mutually compatible. Moreover, we expect these propositions to be a Boolean algebra.

In order to formalize these properties, it is convenient to introduce the notion of a *σ-homomorphism.*

Definition: *A σ-homomorphism is a mapping from $B(R^1)$ (the Borel sets on the real line) into $\mathscr{L}$, such that, for all $\Delta \in B(R^1)$, one has $x: \Delta \to x(\Delta) \in \mathscr{L}$, satisfying the following conditions:*

1) $x(\emptyset) = \emptyset, \quad x(R^1) = I;$

2) $\Delta_1 \perp \Delta_2 \quad$ *implies* $\quad x(\Delta_1) \perp x(\Delta_2);$

3) *for any sequence Δ_i $(i = 1, 2, \ldots)$ such that $\Delta_i \perp \Delta_j$ for all pairs, we have*

$$x\left(\bigcup_i \Delta_i\right) = \bigcup_i x(\Delta_i).$$

Here we have used the notation $a \perp b$ for the disjoint relation $a \subset b'$ of a lattice.

All these properties, except the σ-additivity, flow directly from the heuristic meaning of an observable. The σ-additivity, property (3), can be justified only by the greater simplicity of the mathematical object thereby defined.

We shall call such a σ-homomorphism an *observable*; it is also sometimes called an *$\mathscr{L}$-valued measure* or a *random variable.* The last two terms suggest the relations to the spectral measure and the observable in quantum mechanics, on the one hand, and the relation to classical probability calculus on the other hand. The above definition is indeed a generalization of these concepts and it embraces them both.

In classical mechanics, for instance, the system defines a phase space Ω, and a random variable can be given by giving a Borel function $f(\omega)$ $(\omega \in \Omega)$ from Ω into the reals R^1. Since it is a Borel function, the set

$$f^{-1}(\Delta) \equiv \{\omega : f(\omega) \in \Delta\}$$

defines a Borel subset of Ω for any Borel subset of R^1. It is called the *inverse image* of Δ. The correspondence $\Delta \to f^{-1}(\Delta)$ defines a σ-homomorphism of the Borel sets on R^1 into those on Ω. Here the function f serves no other purpose than to establish this homomorphism via its inverse image. Thus, in order to rid the notion of observable of irrelevancies, it is advisable to leave out the function f altogether and concentrate on the homomorphism itself. Then one sees immediately that the fact that the image of the homomorphism is an algebra of subsets is irrelevant, too; it can just as well be any Boolean subalgebra of a (not necessarily Boolean) proposition system.

In this way we arrive at the abstract notion of an observable which can be used equally as well for classical as for quantal systems. In ordinary quantum mechanics, the propositions are the projection operators on some Hilbert space, and the observable becomes what we have called in Section 4-3 a spectral measure. Since every spectral measure determines a self-adjoint operator, it follows immediately that an observable is nothing else than a self-adjoint operator in that case, a well-known fact taught in all elementary texts of quantum mechanics.

It is easy to prove that the definition of an observable as given here implies that all the propositions $x(\Delta)$ are compatible with one another (Problem 1).

There is a converse of this. If a and b are two compatible propositions, then there exist an observable x and two Borel sets Δ_1 and Δ_2 such that $a = x(\Delta_1)$ and $b = x(\Delta_2)$.

For the proof, we select four arbitrary points on R^1 denoted by 1, 2, 3, and 4. For every set Δ which does *not* contain one or several of these points, we set $x(\Delta) = \emptyset$. For the others we define

$$x(\{1\}) = a \cap b', \qquad x(\{2\}) = b \cap a',$$
$$x(\{3\}) = a \cap b, \qquad x(\{4\}) = a' \cap b'.$$

Using compatibility of a and b, one verifies easily that

$$x(\{1, 3\}) = a, \qquad \text{and} \qquad x(\{2, 3\}) = b.$$

Thus $\Delta_1 = \{1, 3\}$, $\Delta_2 = \{2, 3\}$ will do what is claimed of them.

PROBLEMS

1. The range of an observable is a Boolean σ-subalgebra of propositions.
2. If a_t is an infinite sequence of mutually compatible propositions, then there exist an observable x and Borel sets Δ_t such that $a_t = x(\Delta_t)$.

6-5. PROPERTIES OF OBSERVABLES

For every state p, the observable x induces a numerical-valued measure $\alpha_x^p(\Delta)$ on the Borel sets defined by the formula

$$\alpha_x^p(\Delta) = p(x(\Delta)). \tag{6–6}$$

It represents the probability of finding the value of x in the set Δ when the system is in the state p. Physically it can be determined by performing a large number of measurements of the proposition $x(\Delta)$ on systems in the identical state p. We call it the *expectation value*. ■

A Borel set Δ will be called an x-null set if $\alpha_x^p(\Delta) = 0$ for all states p. Let $\{\Delta_i\}$ be the class of all open x-null sets. Then $\Delta_0 = \bigcup_i \Delta_i$ is also open and x-null. Its complement $\Lambda \equiv \Delta_0'$ is therefore closed, and it is called the *spectrum* of x. If Λ is compact, then x is called bounded and we define the bound of an observable as

$$\|x\| = \sup(|\lambda| : \lambda \in \Lambda).$$

The range of an observable x is the subset $\mathscr{B}_x \subset \mathscr{L}$ defined by

$$\mathscr{B}_x \equiv \{x : x = x(\Delta) \qquad \text{for some } \Delta \in B(R^1)\}.$$

It is easily verified that $\mathscr{B}_x$ is a Boolean sublattice of propositions in $\mathscr{L}$ (Problem 1).

At this point the natural question arises: What are the properties which characterize the Boolean sublattices $\mathscr{B}_x$? In other words, given a Boolean sublattice $\mathscr{B} \subset \mathscr{L}$, what additional property must it have in order that there exist an observable x such that $\mathscr{B} = \mathscr{B}_x$? For physical reasons we are interested in proposition systems $\mathscr{L}$ for which *every* Boolean sublattice $\mathscr{B}$ is a range of some observable.

This condition must evidently be a restriction on the size of the lattice $\mathscr{L}$, since we have seen already that finite and infinite Boolean lattices which are generated by a countable set are the range of some observable (cf. Problem 2 of Section 6-5). We shall now establish that this property is also necessary.

First we define the notion of *separability*. Let $\mathscr{S} \subset \mathscr{L}$ be a subset of mutually compatible propositions of $\mathscr{L}$. We denote by $\mathscr{B}(\mathscr{S})$ the Boolean sublattice generated by $\mathscr{S}$. We remind the reader that this is the smallest Boolean sublattice containing $\mathscr{S}$.

A Boolean sublattice $\mathscr{B} \subset \mathscr{L}$ is called *separable* if there exists a countable subset $a_i \in \mathscr{B}$ such that $\mathscr{B} = \mathscr{B}(\{a_i\})$. That is, there should exist in $\mathscr{B}$ a countable generating set.

We shall call a proposition system $\mathscr{L}$ *separable* if every Boolean sublattice of $\mathscr{L}$ is separable.

The usefulness of separability is revealed in the following:

Theorem: *A Boolean sublattice $\mathscr{B}$ of a proposition system $\mathscr{L}$ is separable if and only if there exists an observable x such that $\mathscr{B} = \mathscr{B}_x$.* (For the proof, cf. proposition 3.15 of reference 2.)

From here on we shall make the assumption that the proposition system $\mathscr{L}$ is separable. Every Boolean sublattice is then the range of some observable.

PROBLEMS

1. The range $\mathscr{B}_x$ of an observable is a Boolean sublattice of propositions.
2. Observables are partially ordered as follows: We say $x \propto y$ if $\mathscr{B}_x \subset \mathscr{B}_y$.

6-6. COMPATIBLE OBSERVABLES

The notion of compatibility for pairs of propositions is, as we have seen in Section 5-5, easily extended to sets of propositions. Thus we may also transfer it to pairs or sets of observables. We define:

Two observables x and y are *compatible* if every proposition of $\mathscr{B}_x$ is compatible with every proposition in $\mathscr{B}_y$.

We write in this case $x \leftrightarrow y$ and $\mathscr{B}_x \leftrightarrow \mathscr{B}_y$. The sublattice $\mathscr{B}(\mathscr{B}_x, \mathscr{B}_y)$, generated by the set $\mathscr{B}_x \cup \mathscr{B}_y$ of propositions, is then a Boolean sublattice. A family $\{x_i\}$ of observables is said to be compatible if $x_i \leftrightarrow x_k$ for every pair of $\{x_i\}$.

There is a special case which is of great interest in the following. If an observable x is such that $\mathscr{B}_x$ is a maximal Boolean lattice, then we say it is *complete*. Likewise, a system of observables x_i, all of which are compatible with one another, is called *complete* if the Boolean algebra $\mathscr{B}(\mathscr{B}_{x_i})$ generated by the ensemble of all $\mathscr{B}_{x_i}$ is maximal.

Every system of compatible observables can always be completed by adjoining to them a certain set of compatible observables.

PROBLEMS

1. Every Boolean sublattice can be extended to a maximal Boolean sublattice.
2. If $\{x_i\}$ is a compatible set of propositions, then either it is complete or it can be completed by adjoining a certain set of additional observables.
3. If $x \subseteq y$ (cf. Problem 2 of Section 6-6), then $x \leftrightarrow y$.

6-7. THE FUNCTIONAL CALCULUS FOR OBSERVABLES

There is an intuitive meaning to a function $u(x)$ of an observable x. If an observation of x yields the value ξ, then $u(x)$ should give the result $u(\xi)$. This of course does not suffice to define $u(x)$ as an observable. However, $u(\xi) \in \Delta$ if and only if $\xi \in u^{-1}(\Delta)$. From this we see that the natural definition of the observable $u(x)$ would be the homomorphism which sends the set $\Delta \in B(R^1)$ into $x(u^{-1}(\Delta))$. Thus we define:

Let $u(\xi)$ be a real-valued Borel function on R^1, and x an observable. We define the observable $u(x)$ as the mapping of $B(R^1)$ into $\mathscr{L}$ defined by $u(x) : \Delta \to u(x)(\Delta) \equiv x(u^{-1}(\Delta))$.

If Δ runs through all Borel sets $B(R^1)$, then $u^{-1}(\Delta)$ runs through a subclass of $B(R^1)$. It follows that $\mathscr{B}_{u(x)} \subseteq \mathscr{B}_x$.

More interesting is the converse of this expressed in the following:

Theorem: *If there are two observables x and y such that $\mathscr{B}_y \subseteq \mathscr{B}_x$, then there exists a Borel function u such that $y = u(x)$.*

For the proof of this theorem it is necessary to construct a Borel function $u(t)$ with the property

$$x(u^{-1}(\Delta)) = y(\Delta).$$

Let r_n $(n = 1, 2, \ldots)$ be an enumeration of the rational numbers. Set

$$b_n = y((-\infty, r_n)).$$

We shall show below that it is possible to construct Borel sets Δ_n with the properties

1) $b_n = x(\Delta_n)$;
2) $\Delta_i \subseteq \Delta_j$ whenever $i < j$;
3) $x\left(\bigcup_n \Delta_n\right) = I$.

For the moment we shall assume this construction possible. Denote by $X_0 \equiv \bigcup_n \Delta_n$ the union of all these sets Δ_n. For any $t \in X_0$ define

$$\bar{u}(t) = \inf \{r_n : t \in \Delta_n\}$$

We have then $\{t : \bar{u}(t) < s\} = \bigcup_{n : r_n < s} \Delta_n$, so that $\bar{u}(t)$ is a Borel function. If we define

$$u(t) = \begin{cases} \bar{u}(t) & \text{for } t \in X_0, \\ 0 & \text{for } t \in X_0', \end{cases}$$

then

$$\{t : u(t) < s\} = \begin{cases} \{t : \bar{u}(t) < s\} & \text{for } s \leq 0, \\ \{t : \bar{u}(t) < s\} \cup X_0' & \text{for } 0 < s, \end{cases}$$

so that $u(t)$ is also a Borel function. Furthermore

$$x(\{t : u(t) < s\}) = \bigcup_{n : r_n < s} x(\Delta_n) = \bigcup_{n : r_n < s} b_n = \bigcup_{n : r_n < s} y((-\infty, r_n))$$

$$= y((-\infty, s)) \qquad \text{for any real } s.$$

Since the sets $(-\infty, s)$ generate all the Borel sets, we conclude

$$x(u^{-1}(\Delta)) = y(\Delta) \qquad \text{for all } \Delta \in B(R^1).$$

Thus the function $u(t)$ does everything that is required of it, and the theorem is proved.

There remains the construction of the sets Δ_n with the three enumerated properties. We do this by induction. Let $\Delta_1, \Delta_2, \ldots, \Delta_n$ be so constructed that they satisfy conditions (1) and (2), and let $1', 2', \ldots, n'$ be a permutation of $1, 2, \ldots, n$ such that $r_{1'} < r_{2'} < \cdots < r_{n'}$.

We now use the hypothesis of the theorem. Since $b_{n+1} \in \mathscr{B}_y$ it follows from the hypothesis $\mathscr{B}_y \subseteq \mathscr{B}_x$ that $b_{n+1} \in \mathscr{B}_x$ also. Thus there exists a $\Delta \in B(R^1)$ such that $b_{n+1} = x(\Delta)$. We now distinguish three cases:

i) $r_{n+1} < r_{n'}$;

ii) there exists a μ such that $1 \leq \mu \leq n$ and $r_{\mu'} < r_{n+1} < r_{(\mu+1)'}$;

iii) $r_{n'} < r_{n+1}$.

We define,

in case (i), $\Delta_{n+1} = \Delta \cap \Delta_{n'}$,
in case (ii), $\Delta_{n+1} = \Delta_{\mu'} \cup (\Delta \cap \Delta_{(\mu+1)'})$,
in case (iii), $\Delta_{n+1} = \Delta_{n'} \cup \Delta$,

so that properties (1) and (2) are also satisfied for the sets $\Delta_1, \Delta_2, \ldots, \Delta_{n+1}$. We find

$$x\left(\bigcup_n \Delta_n\right) = \bigcup_n x(\Delta_n) = \bigcup_n b_n = \bigcup_n y((-\infty, r_n)) = I,$$

so that property (3) is also verified. This finishes the construction and thereby completes the proof of the theorem.

We finish this section with an important theorem from the calculus of observables. For self-adjoint operators, von Neumann has proved the theorem:

For every commuting family A_i $(i \in I)$ of self-adjoint operators there exist a self-adjoint operator x and Borel functions u_i such that $A_i = u_i(x)$.

This theorem can be (and has been) generalized for observables defined on lattices. Its generalization was conjectured by Mackey [4, p. 71] and its proof was given by Varadarajan [2].

With the result of the preceding theorems the proof becomes quite transparent, so we shall give it here.

Theorem (von Neumann–Varadarajan): *Let x_i $(i \in I)$ be a family of compatible observables in a separable lattice $\mathscr{L}$ so that $x_i \leftrightarrow x_j$ for all $i, j \in I$. Then there exist an observable x and Borel functions u_i such that $x_i = u_i(x)$.*

Proof: Let $\mathscr{B} \equiv \mathscr{B}(\mathscr{B}_{x_i})$ be the Boolean sublattice generated by the ranges $\mathscr{B}_{x_i}$ of the observables x_i. Since $\mathscr{L}$ is separable, $\mathscr{B}$ is separable too. By the theorem of Section 6-5 there exists an observable x such that $\mathscr{B} = \mathscr{B}_x$. Clearly $\mathscr{B}_{x_i} \subset \mathscr{B}_x$ and the theorem of Section 6-7 then tells us that there exist Borel functions u_i such that $x_i = u_i(x)$. This proves everything we needed.

It should be mentioned that this theorem is weaker than the one given by Varadarajan, since we have made stronger assumptions about the proposition system. The significance of this theorem is more mathematical than practical. The reason is that it is often easy to describe physical arrangements which

measure a set of commuting observables, while it may be practically impossible to describe such an arrangement for the observable x of which they are all functions. This difficulty is, however, only a practical one and must be sharply distinguished from the *impossibility* in principle of certain measurements to be discussed below.

The usefulness of the theorem for theoretical considerations is that it permits an extension of the functional calculus to systems of compatible observables (cf. Problems 4 and 5).

The extension of the functional calculus for noncompatible observables is an unsolved problem; thus it is not possible to give a meaning to the observable $(x + y)$ if x and y are noncompatible. An obvious way to attempt doing that would be through the method of expectation values. Thus if there exists an observable z with the property that

$$\alpha_z^p(\Delta) = \alpha_x^p(\Delta) + \alpha_y^p(\Delta) \qquad \text{for all states } p,$$

then one could define $z = x + y$. However, the existence of such a z cannot be proved with lattice-theoretical methods alone.

In Segal's method of axiomatic quantum mechanics [5], one starts with a noncommutative algebra of bounded observables rather than a lattice of propositions. Such an algebra is then equipped with a linear functional which is interpreted as expectation value; but the connection with the lattice of propositions is then lost.

The link between the lattice and the observables and their expectation values can be established explicitly only for conventional quantum mechanics in complex Hilbert spaces. The connecting link is the important theorem of Gleason [6] which so far has not been generalized sufficiently to be applicable for the more general situation envisaged here.

PROBLEMS

1. If x and y are two observables such that $\mathscr{B}_x = \mathscr{B}_y$, then there exist two Borel functions u and v such that $y = u(x)$ and $x = v(y)$.
2. If x is an observable and u_1 and u_2 are Borel functions on R^1, then we can define the Borel function $u = u_1 \circ u_2$ by setting $u(t) = u_1(u_2(t))$. The following relation is then true
$$u_1 \circ u_2(x) = u_1(u_2(x)).$$
3. If x defines the measure $\alpha_x^p(\Delta)$ in the state p, then $u(x)$ defines the measure
$$\alpha_{u(x)}^p(\Delta) = \alpha_x^p(u^{-1}(\Delta)).$$
4. Let x and y be two compatible observables; then there exist an observable z and Borel functions u and v such that
$$x = u(z), \qquad y = v(z).$$

We can define the observable $(x + y)$ by setting

$$w = u + v \qquad \text{and} \qquad (x + y) : \Delta \to z(w^{-1}(\Delta)).$$

Similarly we define the observable $x \cdot y$ by setting

$$w = u \cdot v \qquad \text{and} \qquad x \cdot y : \Delta \to z(w^{-1}(\Delta)).$$

5. Generalization of Problem 4: Let $x_1, \ldots, x_n$ be a finite set of compatible observables and let u_i be Borel functions and x an observable such that $x_i = u_i(x)$. Let $\phi(t_1, \ldots, t_n)$ be a Borel function on R^n. We define the Borel function $u(t) \equiv \phi(u_1(t), \ldots, u_n(t))$ and the σ-homomorphism

$$\phi(x_1, \ldots, x_n) : \Delta \to x(u^{-1}(\Delta)).$$

This defines an observable $\phi(x_1, \ldots, x_n)$.

This definition of the function of several compatible observables has the usual properties of a functional calculus (cf. Varadarajan [2], esp. Theorem 3.4).

6-8. THE SUPERPOSITION PRINCIPLE

In classical physics the principle of superposition is well known. It is a direct consequence of the linearity of certain equations of motion describing physical properties. Thus if $\varphi_1(x)$ and $\varphi_2(x)$ are two numerical functions describing two different physical processes of a linear system, then $\varphi(x) = \varphi_1(x) + \varphi_2(x)$ is again a solution describing another possible physical process.

The superposition principle of quantum mechanics has certain similarities with this classical form of the principle, at least when expressed in conventional quantum mechanics. Yet its physical content is radically different, and, in fact, contains the essential properties of quantum systems, to the extent that Dirac [7], in his well-known book on quantum mechanics, could introduce it as the fundamental principle of quantum mechanics from which much of the theory follows.

In order to illustrate the quantum mechanical superposition principle and its relation to the classical principle, let us examine a couple of examples.

One of the simplest examples is the polarization interference of light. For a classical light wave, the coherent superposition of two linearly polarized light waves will result in an elliptically polarized

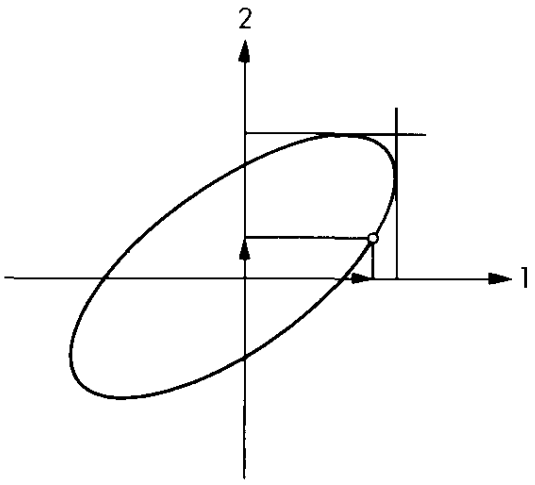

Fig. 6–2 Elliptically polarized light as a superposition of two linearly polarized components.

wave. The parameters of the elliptical polarization will depend not only on the relative intensity of the linearly polarized components, but also on the relative phase of these components (Fig. 6–2).

If the intensity of the interfering light is reduced, one may observe individual photons. Under constant intensity and phase conditions, each of the individual photons is in a definite state of (generally elliptical) polarization. Yet each of the photons partakes in some sense, to be made precise, of the properties of linear polarizations from which it was obtained. This can be seen by letting the elliptically polarized photon pass through an analyzer which determines linear polarization in one of two orthogonal directions. What one observes under these conditions is individual photons linearly polarized but distributed over the two alternatives with a certain probability. Thus each individual photon also potentially has the property of linear polarization in some direction. We shall therefore find it possible to consider elliptically polarized photons as a superposition of linearly polarized ones.

A similar situation is observed in an ordinary interference experiment such as the one sketched in Fig. 6–3.

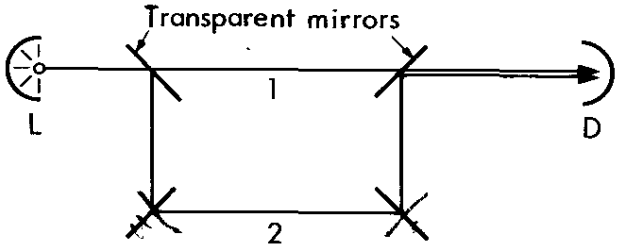

Fig. 6–3 Interference experiments.

Here a light source L sends light onto a partially transparent mirror which reflects half the intensity and transmits the rest. The original beam splits into two which are reunited at the detector D after having traversed different paths, 1 and 2.

Again this experiment can be carried out with individual photons, and then we find that the actual state of a photon in such an apparatus consists of a superposition of the states represented by the two paths, 1 and 2.

The quantum-mechanical description of the superposition principle must thus contain the following ingredients: For any pair of propositions a, b there must exist a number of propositions different from a as well as b, which imply the proposition "a and b." It is easiest to express this for the special case of atomic or minimal propositions.

We have defined minimal or atomic propositions in Section 5-4 as those propositions $e \neq \emptyset$ with the property:

$$x \subset e \qquad \text{implies} \qquad x = \emptyset.$$

Principle of Superposition. For any pair of atomic propositions e_1 and e_2 $(e_1 \neq e_2)$ there exists a third, e_3, such that $e_3 \neq e_1$, $e_3 \neq e_2$, and such that

$$e_1 \cup e_2 = e_1 \cup e_3 = e_2 \cup e_3. \tag{6-7}$$

The third atomic proposition e_3 which is here assumed to exist plays the role of one of the superpositions of e_1 and e_2. We shall, in fact, see later that there exists not only one but a one-parameter *family of propositions* such as e_3 which satisfy the relation (6–7). This fact gives rise to the phenomena of interference which are so characteristic in wave mechanics and which have led to the notion of the *wave nature* of matter.

Let us now examine some of the mathematical consequences of the principle of superposition. A first remark: A lattice which satisfies the principle of superposition cannot be Boolean. Indeed, let e_1, e_2 and e_3 be as in Eq. (6–7). If the lattice were Boolean, we would have, for instance,

$$e_3 \cap (e_1 \cup e_2) = (e_3 \cap e_1) \cup (e_3 \cap e_2).$$

But this relation cannot be right, as one sees from the following: Since e_1 and e_2 are two *different* minimal propositions, $e_1 \cap e_2 = \emptyset$. Hence the right-hand side is equal to $\emptyset \cup \emptyset = \emptyset$. But the left-hand side is equal to e_3 since $e_1 \cup e_2$ contains e_3. Thus the equation is incompatible with $e_3 \neq \emptyset$.

We can now understand why the validity of the superposition principle is so characteristic for quantum systems: It implies the non-Boolean character of the proposition system.

A further consequence is the following: The proposition e_3 which satisfies (6–7) can never be compatible with both e_1 and e_2. Indeed, it is quite easy to show that if $e_3 \leftrightarrow e_1$ and $e_3 \leftrightarrow e_2$, then e_3 satisfies a relation of distributivity (Problem 1):

$$e_3 \cap (e_1 \cup e_2) = (e_3 \cap e_1) \cup (e_3 \cap e_2),$$

which we have just shown to be incompatible with Eq. (6–7).

This property is quite significant in view of the question as to what extent a system which is known to have property e_3 may be considered to have simultaneously property e_1 or e_2 or both. We see that the answer to such questions would involve the simultaneous determination of incompatible propositions, a feat which we shall show generally to be impossible.

The foregoing does not exclude the possibility that the two propositions e_1 and e_2 may be compatible. This is, for instance, the case for the two examples which we have sketched in Figs. 6–2 and 6–3.

The questions which we touch here have been extensively discussed by Bohr in connection with a large variety of specific examples [8]. In all these examples, Bohr could show that the simultaneous determination of properties e_3 with either one of the two properties e_1 or e_2 would involve incompatible physical arrangements.

Here we have shown that this fundamental property expresses itself, in the mathematical structures of the proposition system, by the fact that the sublattice generated by e_1, e_2, and e_3 which satisfy (6–7) cannot be Boolean.

Finally, we want to discuss the relation of the superposition principle to the reducibility of proposition systems. In Section 5-5 we have introduced the notion of *center*, *reducibility* and *irreducibility*, and *direct union* of sublattices. Here we shall connect these concepts with the superposition principle.

Suppose that the lattice $\mathscr{L}$ is a direct union of two lattices $\mathscr{L}_1$ and $\mathscr{L}_2$, so that every element x of $\mathscr{L}$ can be written as a pair of elements $\{x_1, x_2\}$ with $x_1 \in \mathscr{L}_1$ and $x_2 \in \mathscr{L}_2$. Let us now consider a point (minimal proposition) $e_1 \in \mathscr{L}_1$, and denote by $\tilde{e}_1$ the element of the form $\{e_1, \emptyset_2\}$. Similarly, consider the element $\tilde{e}_2$ of the form $\{\emptyset_1, e_2\}$ where e_2 is a point in $\mathscr{L}_2$. If the superposition principle holds, then there must exist an element $\tilde{e}_3 \neq \emptyset$ such that

$$\tilde{e}_1 \cup \tilde{e}_2 = \tilde{e}_1 \cup \tilde{e}_3 = \tilde{e}_2 \cup \tilde{e}_3.$$

This is easily seen to be impossible. For such an element would be contained in $\tilde{e}_1 \cup \tilde{e}_2$. Therefore if we write $\tilde{e}_3 = \{x_1, x_2\}$, its two components x_1 and x_2 would have to satisfy $x_1 \subset e_1$ and $x_2 \subset e_2$. Since e_1 and e_2 are points, this implies $x_1 = \emptyset$, and $x_2 = \emptyset_2$. But this is incompatible with $\tilde{e}_3 \neq \emptyset$. We conclude with the following:

Theorem: *A proposition system which satisfies the principle of superposition for all pairs of points is irreducible.*

Since a proposition system with nontrivial center is reducible (Problem 2) we have immediately the following:

Corollary: *A proposition system which satisfies the principle of superposition for all pairs of points has trivial center.*

Since the center of a Boolean lattice is identical with the lattice itself (cf. Problem 5, Section 5-5), we see in this corollary again how the superposition principle implies the essential features of quantum mechanics.

The superposition principle is thus not a new axiom of quantum mechanics; it is merely a consequence of the non-Boolean structure of the proposition system. The detailed discussion of it in this section is given primarily in order to bring to light the connection with historical discussions of quantum mechanics.

PROBLEMS

1. If $x \leftrightarrow a$ and $x \leftrightarrow b$, then

$$x \cup (a \cap b) = (x \cup a) \cap (x \cup b)$$

and

$$x \cap (a \cup b) = (x \cap a) \cup (x \cap b).$$

2. A proposition system with nontrivial center is reducible.

6-9. SUPERSELECTION RULES

Whether the superposition principle is valid without restriction is a question of experience, and experience has shown that it is not universally valid [9]. When it is not valid we speak of *superselection rules.*

An example of a superselection rule is obtained from the neutron–proton system. These two elementary particles, which form the building blocks of all nuclei, are usually considered as two different states of one and the same nucleon system. This description, coupled with the isotopic spin formalism, results in certain simplifications in calculation. However, one must not overlook the fact that this description involves a superselection rule. It has never been possible to produce a state which could be considered a superposition of a neutron and a proton state. It is therefore a reasonable hypothesis that such a superposition does not exist and that the neutron–proton system gives rise to a reducible lattice of propositions.

Thus we must expect that the proposition system is reducible and that the superposition principle does not possess unrestricted validity. It is convenient to introduce the word *coherent* for all those propositions which form an irreducible sublattice of propositions.

A state p for a proposition system which is $\neq 0$ in at least two different coherent subsystems is always a mixture. This can be seen as follows: Let p be such a state, and let

$$\lambda_1 = p(\{I_1, \emptyset_2\}), \qquad \lambda_2 = p(\{\emptyset_1, I_2\}).$$

Since $p \neq 0$ in both coherent subsystems, we have $0 < \lambda_1$ and $0 < \lambda_2$. Furthermore, Property (3) for states (cf. Section 6-3) implies $\lambda_1 + \lambda_2 = 1$.

If $x = \{x_1, x_2\}$ is any proposition, then the functions $p_1(x)$ and $p_2(x)$, defined by

$$p_1(x) \equiv \frac{1}{\lambda_1} p(\{x_1, \emptyset_2\}) \qquad \text{and} \qquad p_2(x) \equiv \frac{1}{\lambda_2} p(\{\emptyset_1, x_2\}),$$

are easily seen to be different states. Furthermore, $p(x) = \lambda_1 p_1(x) + \lambda_2 p_2(x)$. This shows that $p(x)$ is indeed a mixture. It is possible to generalize this theorem to states which have components in a discrete or continuous family of superselection rules.

The occurrence of superselection rules in nature shows that the actual physical proposition systems take an intermediate position between the Boolean systems and the coherent systems. The Boolean systems characterize those systems with only classical mechanical properties. The coherent systems are those for which the quantum properties are universal and essential. This positioning of the actual physical proposition systems somewhere between the two extremes shows, in a most striking way, that the theory of quantum systems is a *generalization* of the classical theories, rather than (as it is often argued) in contradiction with them.

The fundamental cleavage between the two descriptions, which has caused so much concern, is thus resolved in the synthesis of an all-embracing theoretical frame which is flexible enough to accommodate all the known physical theories.

It will be our task in the following chapters to introduce further properties into this frame, which characterize specific physical systems.

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CHAPTER 7

HIDDEN VARIABLES

I reject the basic idea of contemporary statistical quantum theory, insofar as I do not believe that this fundamental concept will prove a useful basis for the whole of physics. . . . I am, in fact, firmly convinced that the essentially statistical character of contemporary quantum theory is solely to be ascribed to the fact that this theory operates with an incomplete description of physical systems.

A. EINSTEIN

The new epistemological situation underlying quantum mechanics is satisfactory, both from the standpoint of physics and from the broader standpoint of the conditions of human knowledge in general.

W. PAULI

In this short chapter we formulate the important question concerning the possible existence of hidden variables in quantum theory. A partial answer to this question can already be given at this state of the theory, and it is desirable to avoid confusing this problem with the specific form of conventional quantum mechanics. In Section 7-1 we show with a thought-experiment (due to Einstein) that it is in general not possible to assign definite values to all the observable quantities of a physical system. This leaves open the question whether there might not exist in principle unobservable quantities (hidden variables) which would account for the probabilistic feature of the observed states, due to our ignorance of these variables. After a short preparatory section (7-2) we give a precise definition of hidden variables in Section 7-3 and prove the theorem which shows that the existence of hidden variables of this kind is in contradiction with empirical facts. Two other proposals, which are not excluded by these considerations, are briefly discussed in the last section (7-4).

7-1. A THOUGHT EXPERIMENT

In Section 6-1 we analyzed the notion of the state of a physical system and characterized it as a *result of the preparation.* In Section 6-2 we pointed out that a state can be determined by measuring the values of a sufficient number of propositions. For each individual measurement the outcome is one of the two alternatives "yes" or "no"; but we have emphasized that a repetition of the experiment, prepared under identical relevant conditions, will not always produce identical results for the value of a given proposition.

Let us illustrate this situation by a thought experiment discussed by Einstein at the fifth Solvay Congress in 1927.

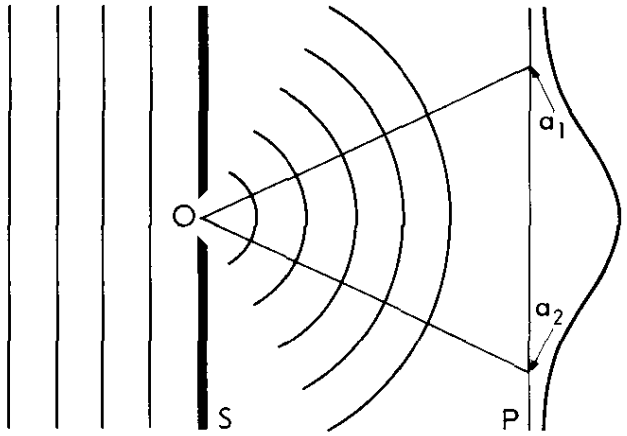

Fig. 7–1 Einstein's thought experiment.

A stream of particles, homogeneous in momentum, falls on a screen S with a small hole O, as shown in Fig. 7–1. Opposite the hole is a photographic plate P, which can detect the arrival of the particles. The intensity of the incident beam is assumed to be sufficiently low that individual events can be detected. If the hole is sufficiently small, particles will arrive at P separated by distances much larger than the diameter of the hole. The questions now arise: Does an individual particle actually have a *definite momentum* which, because it varies from case to case in a random manner, is not known; or does it have not a definite momentum but only a *probability distribution* which is revealed by the statistics of the measurements?

We can formulate this question in the language of propositional calculus. Let p_0 represent the state obtained by the preparation of the system after sending the particle through the hole in the screen. Let p_1 and p_2 be the states of the system after the particle has hit the screen at a_1, or a_2, respectively. These states are manifestly different from p_0 and from each other, since a measurement of the proposition "particle is at a_1" will be true with certainty in the state p_1 and false with certainty in the state p_2, while it has an intermediate value $p_0(a_1)$ in state p_0. Thus we have the following relations:

$$p_1(a_1) = p_2(a_2) = 1, \qquad p_1(a_2) = p_2(a_1) = 0;$$

$$0 < p_0(a_1) < 1, \qquad \text{and} \qquad 0 < p_0(a_2) < 1.$$

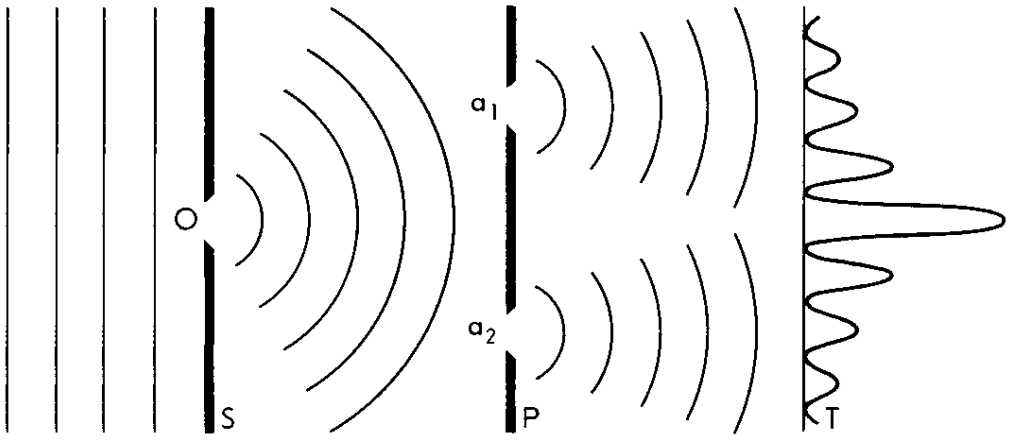

Fig. 7–2 Interference effects observed on screen T.

Since p_1 represents the state with the momentum of the particle in the direction Oa_1, the adequate description for the state for which the particle has definite but unknown momenta in the direction Oa_1, and Oa_2 would be the statistical mixture $\lambda_1 p_1 + \lambda_2 p_2$ with $\lambda_1 = p_o(a_1)$, $\lambda_2 = p_o(a_2)$. Generally, a screen P with a discrete (finite or infinite) set of points a_n would require a state

$$p = \sum \lambda_n p_n \qquad \text{with} \qquad \lambda_n = p_o(a_n). \tag{7–1}$$

However, whether the state is of this form or not can be decided by experiment. It suffices to replace two of the detectors a_1 and a_2 by holes, and observe the effect on a third screen T. The result, we know, is an interference pattern as indicated schematically in Fig. 7–2. However, the state expressed by Eq. (7–1) cannot be distinguished from a state where the two holes a_1 and a_2 are replaced by independent sources of particles. Such an arrangement would produce only two maxima in front of the two holes (as shown in Fig. 7–3), and this is quite different from the interference pattern of Fig. 7–2.

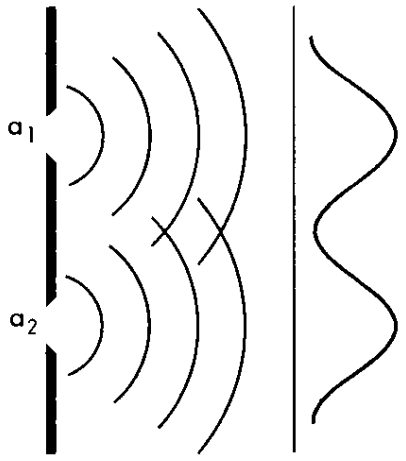

Fig. 7–3 Distribution of particles from two independent sources.

Thus, whether in this experiment the momenta have definite but unknown values can in principle be decided by an experiment and the answer is negative. We shall show later that this interdependence of mutually incompatible quantities is a quite general feature of quantum mechanics expressible quantitatively in the form of *uncertainty relations*.

The foregoing analysis merely shows that the actual state of the particle, after it has passed the hole O, is such that it does not allow the interpretation that the particle in this state has a definite (albeit unknown) momentum because such a state would behave differently in a subsequent experiment from the actual observed behavior. But this analysis does not exclude the possibility that the state in question might be the statistical mixture of *unknown* states, which cannot be produced with known physical equipment but which assign definite values to all measurable propositions. If this is the case for every state, we say that the system admits hidden variables. We shall give a formal definition of such systems in Section 7-3.

7-2. DISPERSION-FREE STATES

When actually observed, most real states show dispersion. This is true in quantum as well as in classical physics. This means that, when we observe a proposition a in a state p, we usually obtain a result $p(a)$ which lies between 0 and 1. We can give a sort of quantitative measure for the dispersion by defining the dispersion function $\sigma(a) = p(a) - p^2(a)$.

As shown in Fig. 7–4, the dispersion function has the value of zero for $p = 0$ or $p = 1$, and assumes its maximum value $\frac{1}{4}$ for $p = \frac{1}{2}$. It is thus an adequate measure of the degree of uncertainty associated with any particular value of p.

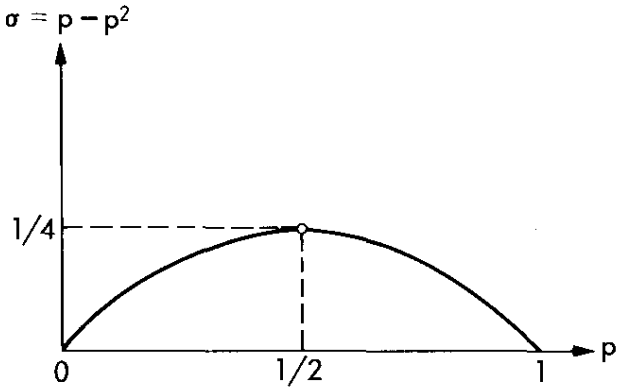

Fig. 7–4 The dispersion function.

We shall also define an *overall dispersion* σ for each state, defined by

$$\sigma = \sup_{a \in \mathscr{L}} \sigma(a). \qquad (7\text{–}2)$$

A state is called *dispersion-free* if $\sigma = 0$.

Physically, the existence of dispersion-free states is a question to be decided by experiment. In classical mechanics it is implicitly assumed that such states exist, at least in some idealized sense. Even if actual physical measurements on classical systems show dispersion for individual propositions, in classical physics nothing prevents us from assuming that such dispersion can be reduced further and further by a suitable refinement of the preparing experiment. In quantum physics this is not so, as we have seen in the discussion of Einstein's thought experiment of the preceding section. However, we can imagine that dispersion-free states, although not realizable physically, might still be useful as a mental construct for the formulation of a quantum mechanics based on a deeper level of causal processes. Such hypothetical states would then have the character of freely constructed mental images with no direct correlation with reality. Contact with reality

would appear only as derived consequences which might be obtained in a detailed dynamical theory involving such states. This would be a theory with *hidden variables*. In order to examine this question it is desirable to study some of the properties of dispersion-free states.

There is one property which can be immediately verified for dispersion-free states contained in the following

Proposition 1: *Every dispersion-free state is pure.*

Proof: Suppose the state p is a mixture. Then there exist two different states p_1 and p_2, as well as two positive numbers λ_1 and λ_2, such that $\lambda_1 + \lambda_2 = 1$ and $p = \lambda_1 p_1 + \lambda_2 p_2$. Since the two states p_1 and p_2 are different from one another, there exists a proposition a such that $p_1(a) \neq p_2(a)$ (cf. Property 5b of Section 6-3). Since the states are dispersion-free, there are two possibilities only: $p_1(a) = 1$, $p_2(a) = 0$ or $p_1(a) = 0$, $p_2(a) = 1$. In either case we have $\sigma(a) = \lambda_1\lambda_2 \neq 0$. Thus the state is not dispersion-free, contrary to the assumption. This proves the proposition.

The converse of this proposition is false. We shall later see many examples of pure states which are not dispersion-free. For coherent proposition systems (cf. Section 6-9 for this notion), we can even prove that:

Proposition 2: *On a nontrivial coherent proposition system there exists no dispersion-free state.*

Proof: Let us recall that a *coherent* proposition system $\mathscr{L}$ is defined as a system with trivial center. The center is the set of all propositions which are compatible with every other proposition in $\mathscr{L}$. If the center $\mathscr{C}$ is trivial, this means that it consists of only the two elements $\emptyset$ and I.

We base the proof on the following:

Lemma: *If there exists a dispersion-free state p in a proposition system, $\mathscr{L}$, then there exists a point e in the center of $\mathscr{L}$ such that $p(e) = 1$.*

Proof of Lemma: Let $\mathscr{L}_1$ be the subset of all propositions a_i ($i \in I$ = some index set) in $\mathscr{L}$ such that $p(a_i) = 1$, and let $a_0 = \bigcap_{i \in I} a_i$. By property (4) of Section 6-3, we also have that $p(a_0) = 1$, so that $a_0 \in \mathscr{L}_1$.

Now consider any $x \subseteq a_0$ but $x \neq a_0$. Since $p(x) = 1$ would imply $a_0 \subseteq x$ and hence $a_0 = x$, we must have $p(x) = 0$. Since x is compatible with x', it follows from the property of states that

$$p(x) + p(x') = p(x \cup x') = 1.$$

Since $p(x) = 0$, this means $p(x') = 1$, or $a_0 \subseteq x'$. It follows that

$$x = x \cap a_0 \subseteq x \cap x' = \emptyset.$$

Therefore $x = \emptyset$. This means that a_0 is a point, which we shall designate by e from now on.

Next we prove that e is compatible with every other proposition x in $\mathscr{L}$. If $x \in \mathscr{L}_1$, then $e \subseteq x$ and hence, by axiom (P) of Section 5-8, $e \leftrightarrow x$. If, on the other hand, $x \notin \mathscr{L}_1$, then, as we have just shown, $x' \in \mathscr{L}_1$ and so $e \leftrightarrow x'$. It follows then from a known theorem (cf. Problem 2 of Section 5-8) that $e \leftrightarrow x$ also. Thus we have, in all cases, $e \leftrightarrow x$. This proves the lemma.

The proof of Proposition 2 is then completed by observing that a trivial center cannot contain any point unless $\mathscr{L}$ is trivial itself. This proves Proposition 2.

7-3. HIDDEN VARIABLES

We must now express in mathematical language what we mean by a system that admits hidden variables. To this end we must generalize the description used in Section 7-1. The essential property of such a system is that every state which can be physically realized is a mixture of some dispersion-free states. In the general case the mixture may involve not just two states but a whole family of them. It is therefore necessary to introduce a measure space X, called the space of hidden variables, and a finite measure ρ defined on the Borel sets of X, and to consider mixtures of the form

$$p(a) = \int_X d\rho(\xi) p_\xi(a)$$

where $\xi \in X$ and $p_\xi(a)$ is a state which is at the same time a measurable function of ξ for all propositions a.

We shall now define a system with hidden variables in the following way:

Definition: *A physical system is said to admit hidden variables if there exists a measure space X together with a finite measure ρ (normalized so that $\rho(X) = 1$) on X such that every state p of the system can be represented as a mixture*

$$p(a) = \int_X d\rho(\xi) p_\xi(a) \tag{7–3}$$

of dispersion-free-states $p_\xi(a)$.

If the measure ρ is concentrated on a finite or countably infinite sequence of points ξ_i, then we obtain a representation in the form of a sum

$$p(a) = \sum_i \lambda_i p_i(a)$$

where

$$\lambda_i = \rho(\xi_i) \qquad \text{and} \qquad p_i(a) = p_{\xi_i}(a).$$

The variable $\xi \in X$ represents a variable which for a given state need never be known, and the states $p_{\xi_i}(a)$ are not necessarily producible by known physical equipment. For this reason we refer to these variables as *hidden*.

We shall now study the most important problem in connection with hidden variables: What are the physical properties of systems which admit hidden variables?

Two types of answers are possible. Either there are no observable physical properties which follow from the existence of hidden variables, or there are such observable physical properties. In the first case, the hidden variables have no physical significance, and their use for the description of physical systems is not a question of physics and would therefore not concern us here. In the second case, one may ask whether these physical consequences are in agreement with experience or not. If they are not in agreement, then the existence of hidden variables is empirically refuted.

There is one case where the answer can be given already without further work. It is the case of the coherent proposition system. In this case we have already shown that there do not even exist dispersion-free states (Proposition 2 of preceding section). For such simple systems, the question is thus already answered. However, the answer is more difficult to obtain if we have a system with superselection rules. It is contained in the following:

Theorem: *If a proposition system $\mathscr{L}$ admits hidden variables, then any pair of propositions a, b ($a \in \mathscr{L}$, $b \in \mathscr{L}$) is compatible: $a \leftrightarrow b$.*

Proof: The proof is based on the following:

Lemma: *If a proposition system admits hidden variables, then for any pair of propositions $a, b \in \mathscr{L}$ and any state p, one has*

$$p(a) + p(b) = p(a \cap b) + p(a \cup b). \tag{7–4}$$

Proof of Lemma: Since $\mathscr{L}$ admits hidden variables, every state is of the form

$$p(a) = \int_X d\rho(\xi) p_\xi(a), \tag{7–5}$$

where all states $p_\xi(a)$ are dispersion-free. It suffices thus to establish the relation in question for dispersion-free states. Thus let $p(a)$ be dispersion-free so that $p(a)$ is either 0 or 1. There are then four cases possible:

1. $p(a) = 0$, $p(b) = 0$,
2. $p(a) = 1$, $p(b) = 0$,
3. $p(a) = 0$, $p(b) = 1$,
4. $p(a) = 1$, $p(b) = 1$.

Let us examine each of these cases separately. Evidently (3) is reducible to (2) by interchanging the roles of a and b.

If $p(a) = p(b) = 0$, then $p(a \cap b) \leq p(a)$, and therefore $p(a \cap b) = 0$ also. On the other hand $p(a') = 1 = p(b')$. Thus by Property 4 of Section 6-3, $p(a' \cap b') = 1$. Since $(a \cup b)' = a' \cap b'$, we have

$$p(a \cup b) = 1 - p((a \cup b)') = 1 - p(a' \cap b') = 0.$$

Thus $p(a \cup b) = 0$ also, and the relation expressed in Eq. (7–4) is established.

Now let $p(a) = 1$ and $p(b) = 0$. It follows then that $p(a \cup b) \geq p(a) = 1$. Therefore $p(a \cup b) = 1$. Furthermore $p(a \cap b) \leq p(b) = 0$. Therefore $p(a \cap b) = 0$. Thus, again relation (7–4) is verified. Finally, assume $p(a) = p(b) = 1$. We then have

$$p(a') = 1 - p(a) = 0, \quad p(b') = 1 - p(b) = 0.$$

Furthermore,

$$p(a \cup b) = 1 - p(a' \cap b'), \quad p(a \cap b) = 1 - p(a' \cup b').$$

Therefore

$$p(a) + p(b) - p(a \cap b) - p(a \cup b)$$
$$= -[p(a' \cap b') + p(a' \cup b') - p(a') - p(b')].$$

The right-hand side is zero since it is an instance of Case 1. Thus the relation (7–4) is verified in this case also, and the lemma is proved.

We now proceed to the proof of the theorem. For every state we have, by repeated use of the lemma,

$$\begin{aligned} p((a \cap b') \cup b) &= p(a \cap b') + p(b) \\ &= p(a) + p(b') - p(a \cup b') + p(b) \\ &= p(a) + 1 - p(a \cup b') = p(a) + p(a' \cap b) \\ &= p(a \cup (a' \cap b)). \end{aligned}$$

Since this is true for every state we have, by Property 5b of Section 6-3,

$$(a \cap b') \cup b = (a' \cap b) \cup a.$$

This means (cf. Problem 2 of Section 5-8) $a \leftrightarrow b$, and this proves the theorem.

We may remark here that we have not used the axioms in full generality. For instance, we have used Property 4 only for a finite number of propositions, and we have not used the axiom of atomicity. This is very satisfactory since both of these axioms are only weakly justified empirically and were posited mainly for convenience.

The conclusion of the theorem is seen to be very strong, since it affirms compatibility for *all* pairs of propositions. Thus it suffices to exhibit a single pair of noncompatible propositions to establish that hidden variables are empirically refuted. Now we have seen that the occurrence of noncompatible propositions is the essence of quantum mechanics, since the lattice is Boolean and the system behaves classically if every pair of propositions is compatible. Because of this result we may simply affirm: A quantum system cannot admit hidden variables in the sense in which we have defined them. With this result the quest for hidden variables of this particular kind has found its definitive answer in the negative.

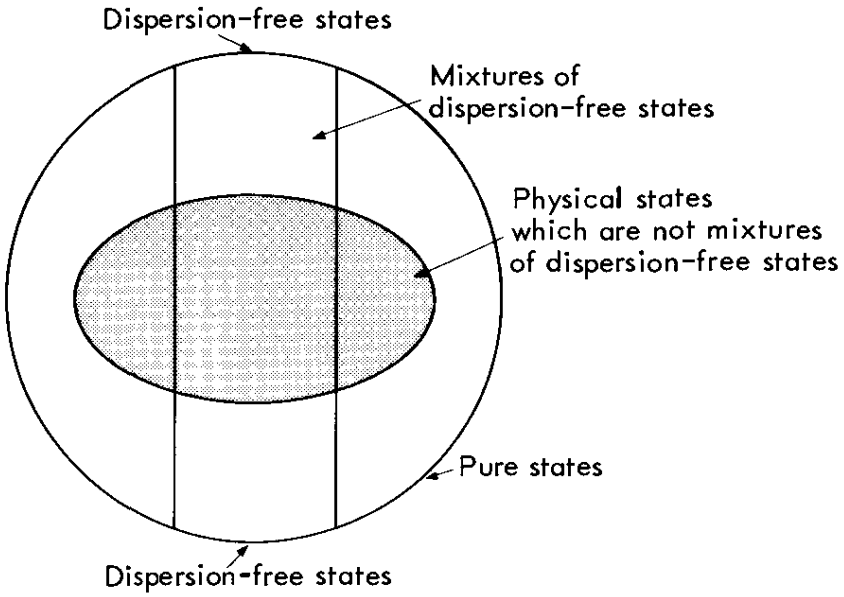

Fig. 7–5 The circular disk represents all the states. The physically realizable states are the circumference of the circle, and the dispersion-free states are the indicated subset of the circumference.

We can represent the result of this theorem with Fig. 7–5, which shows symbolically the different states and their relation to each other.

7-4. ALTERNATIVE WAYS OF INTRODUCING HIDDEN VARIABLES

It is clear from the foregoing considerations that any attempt at introducing hidden variables without leading to empirically refutable consequences would have to be done by giving up one or several of the axioms on which the theorems of Section 7-3 were based. Which of them should be given up is largely a matter of personal taste, and each of the chosen ways of doing so amounts to an alternative way of defining "hidden variables."

We shall briefly discuss two such possibilities which can serve for such a modified definition of hidden variables.

The first is due to G. Mackey, and it is based on the notion of "ε-dispersion-free states." A physical system is said to admit ε-dispersion-free states if for every $\varepsilon > 0$ there exists a state $p(a)$ such that the overall dispersion for this state defined by Eq. (7–2) is smaller than this ε.

A system can then be said to admit "quasi-hidden variables" if every state $p(a)$ admits a representation (7–5) where all the states $p_\xi(a)$ are ε-dispersion-free for any $\varepsilon > 0$.

So long as $\varepsilon \neq 0$, the proof which we have given in the previous section does not go through. On the other hand no example of a non-Boolean proposition system is known which admits such quasi-hidden variables.

Another way of avoiding the conclusions of the previous section is to modify the properties of the hypothetical dispersion-free states which are admitted in the representation (7–5).

An explicit example has been constructed by J. S. Bell [7]. The axiom which is violated in this example is (4) of Section 6-3. It is possible to construct other examples which violate other properties of states.

Of course none of these logical possibilities can be properly called theories with hidden variables unless they lead to empirically testable consequences which can be verified or refuted. As long as this is not done, the question concerning such generalized hidden variables remains rather academic. The merit of the considerations in Section 7-3 lies in the fact that they show that at least one class of hidden variables, the obvious and most natural one, can thus be empirically refuted.

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3. W. PAULI, *Louis de Broglie, Physicien et Penseur.* Paris: Albin Michel (1953).

The first "proof" of the impossibility of hidden variables in quantum mechanics is due to von Neumann:

4. J. VON NEUMANN, *Mathematische Grundlagen der Quantenmechanik.* Berlin: Springer (1932).

See also:

5. J. ALBERTSON, *Am. J. Phys.* **29,** 478 (1961).

The theorem of this chapter which is a strengthening of von Neumann's result was first stated and proved in:

6. J. M. JAUCH AND C. PIRON, *Helv. Phys. Acta* **36,** 827 (1963).
7. J. S. BELL, *Physics* **1,** 195 (1965).

The most recent discussion is found in:

8. B. Misra, *Nuovo Cim.* **47,** 841 (1967).

CHAPTER 8

PROPOSITION SYSTEMS AND PROJECTIVE GEOMETRIES

Ubi materia, ibi geometria.

J. KEPLER

In this chapter we begin the building of the bridge which connects the general quantum theory, as an abstract proposition system, with conventional quantum theory in a complex Hilbert space. This bridge is not yet complete. There are no convincing empirical grounds why our Hilbert space should be constructed over the field of the *complex numbers*. But it is possible to understand why we need linear vector spaces. The path leads *via* the mathematical theory of projective geometries which are defined in Section 8-1. We prepare the ground for a general representation theory of propositions in Section 8-2 by sketching a general reduction theory which leads to a simplification of the problem. The structure of the irreducible components is the subject of Section 8-3, where we demonstrate the general representation of these components as subspaces in a linear vector space over a field F.

The property of orthocomplementation leads to a restriction of the field. In Section 8-4 this restriction is stated and it is furthermore shown that orthocomplementation defines a definite Hermitian form in the vector space V. The vector space V thus becomes a metric space with positive definite metric. The metric, and especially its definite character, is thus directly traced to the axiom of orthocomplementation. The final section, 8-5, describes the representation of the proposition system in Hilbert space.

8-1. PROJECTIVE GEOMETRIES

In Sections 2-5 and 5-7 we showed that the subspaces of a Hilbert space are a lattice if the intersection of two subspaces is the set-intersection and the union of two subspaces is defined as the closed linear subspace spanned by them. It was pointed out that this lattice satisfies all the axioms of a proposition system; in particular it is orthocomplemented, atomic, and complete. This shows, first of all, that the axioms of a proposition system are self-consistent and, since conventional quantum mechanics can be formulated as a theory

using Hilbert space, that the axioms are realized in conventional quantum mechanics.

In this chapter we examine the converse question: Given the axioms of a proposition system, to what extent do they *determine* a realization in a vector space? Are there several independent and inequivalent realizations possible, and if so what are the physical reasons for choosing one over the other?

Let us admit to begin with that the full answer to this important question is not yet known. Certain inroads, however, have been made recently which permit a restriction of the problem. The essentials of the known results are as follows: It is possible to show that an irreducible proposition system can always be represented as the subspaces in a linear vector space of finite or countably infinitely many dimensions with coefficients from a field. However, not much is known about the physical implications of the *nature* of the field, or the uniqueness of this representation [14].

This result can be obtained by reducing the problem to another one which is part of a highly developed theory, namely, the theory of *projective geometries*.

It has been realized for a long time that the essential structural properties of a projective geometry are expressible in terms of the intersections and unions of the fundamental geometrical elements which can be built up from points, lines, planes, etc. Such a structure is an atomic lattice. Since a great deal is known about the structure of projective geometries and their realizations as subspaces, there is hope that this knowledge may be applicable for quantum-mechanical proposition systems, too. The difficulty which stands in the way of the execution of such a program is that a proposition system is not a projective geometry. What is missing is the modular law; a projective geometry is always defined as a modular lattice (cf. Section 5-6).

In the special case where the maximal element I is a finite union of points, this difficulty disappears, because one can demonstrate that such a finite proposition system is always modular. But for infinite proposition systems, that is, systems for which I is not a finite union of points, modularity is no longer compatible with the other axioms.

We could of course have retained modularity and given up some of the other axioms; but we have not done so for the reason that they are not suitable for the description of the physical reality. The possibilities which one could envisage would be the following:

The lattice of a proposition system is

1) A complete, modular, atomic but not orthocomplementable lattice. Such a lattice is, for instance, obtained by considering as elements all the linear manifolds (not necessarily closed) of an infinite-dimensional Hilbert space.

2) A complete, modular, orthocomplemented but nonatomic lattice. The existence of such lattices was discovered by von Neumann in the projections from a factor of type II, and they were called by him *continuous* geometries.

3) A complete, orthocomplemented, atomic but nonmodular lattice.

We can immediately exclude lattices of type (1) since the orthocomplementation is a property which can be very easily justified by the physical interpretation of the propositions.

The lattices of type (2) are not so easily rejected. We have already pointed out that atomicity is very difficult to justify on physical grounds, at least in the generality needed for the axiom system. For this reason von Neumann has on various occasions given serious consideration to lattices of type (2) as a possible generalization of conventional quantum mechanics. Indeed it seems impossible to exclude such lattices without further examination of the empirical material. The decisive property, which we have not yet considered, is what we shall call *localizability*. We shall show that a system which possesses this property, as we know to be the case for elementary particles, cannot have a modular lattice of propositions (cf. Section 12-7). This would then also exclude case (2), and there remains only possibility (3), which is precisely that which we have adopted for a general proposition system.

We are thus faced with the problem of how to relate a proposition system (which in general is nonmodular) to a projective geometry (which is modular). We shall find it convenient to adopt the following definition of a projective geometry which is valid in the finite as well as in the infinite case [2, 5].

Let E be a set of elements called points, and let there be a class G of subsets of E which have the following properties:

1) There exists a distinguished class of subsets called "lines" in G such that, to every pair of different points e_1 and e_2 in G, there exists exactly one line ℓ which contains e_1 and e_2.

2) Three points e_1, e_2, and e_3 form a triangle which has the following property: If e_4 is a point on the line through e_1 and e_2, and e_5 is a point on the line through e_2 and e_3, then e_4 and e_5 determine a line ℓ which contains one point, e_6, of the line through e_3 and e_1 (cf. Fig. 8–1).

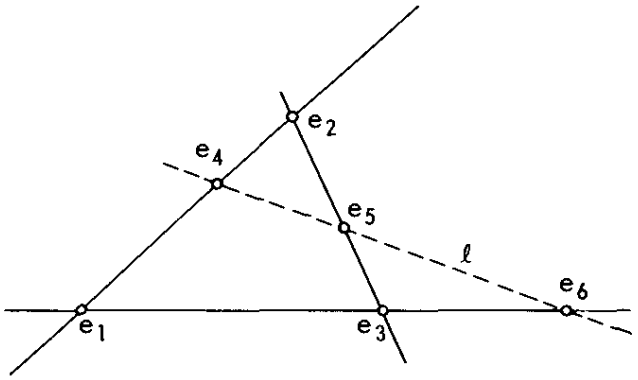

Fig. 8–1 The triangle axiom.

3) The necessary and sufficient condition that a subset of points a belongs to the class of subsets G is that it contain the line which passes through any pair of points from a.

If the partial ordering in G is defined by set inclusion, and if unions and intersections are defined as least upper bound and greatest lower bound, then one can prove that such a system G is an atomic modular lattice (not necessarily finite), and hence a projective geometry [2].

The principal problem to be discussed in the rest of this chapter, therefore, is how to relate a proposition system of a physical system to a projective geometry G, defined above. Before we attack this problem, it is convenient to develop the reduction theory of proposition systems, to be followed by the representation theory of irreducible proposition systems. The reduction theory is the object of the following section.

8-2. REDUCTION THEORY

A first important step towards the complete structure theory of proposition systems is the reduction theory, which we shall discuss in this section. The idea is the following: Every lattice $\mathscr{L}$ has a center $\mathscr{C}$ consisting of all those elements of $\mathscr{L}$ which are compatible with every other element in $\mathscr{L}$. In Boolean lattices the center is identical with $\mathscr{L}$. In more general lattices it is a proper subset of $\mathscr{L}$. The center always contains the elements $\emptyset$ and I of $\mathscr{L}$. If it contains only these two elements we call the center *trivial*. A lattice with trivial center is called *coherent* or *irreducible*.

If the center is not trivial, then there exists at least one element $z \in \mathscr{C}$ such that $z \neq \emptyset$ and $z \neq I$. It follows then from the axioms of a proposition system that $z' \in \mathscr{C}$ also (cf. Problem 2 of Section 5-8). Every element $a \in \mathscr{L}$ can then be decomposed according to the formulas $a_1 = a \cap z$ and $a_2 = a \cap z'$.

Since z and z' are in the center $\mathscr{C}$ of $\mathscr{L}$, the distributive law is valid for the expression

$$(a \cap z) \cup (a \cap z') = a \cap (z \cup z') = a.$$

Furthermore, $a_1 \cap a_2 = (a \cap z) \cap (a \cap z') = a \cap (z \cap z') = a \cap \emptyset = \emptyset$. Thus, every element a is decomposed by z into a pair $\{a_1, a_2\}$ of elements, and one finds that if $a = \{a_1, a_2\}$ and $b = \{b_1, b_2\}$ are two elements of $\mathscr{L}$, then (Problem 1)

$$a \cap b = \{a_1 \cap b_1, a_2 \cap b_2\} \qquad \text{and} \qquad a \cup b = \{a_1 \cup b_1, a_2 \cup b_2\}.$$

For the orthocomplement a' of a, one finds the decomposition $a' = \{a_1', a_2'\}$, where $a_1' = (a \cap z)' \cap z = a' \cap z$ and $a_2' = (a \cap z')' \cap z' = a' \cap z'$ (Problem 2).

We have thus constructed an explicit reduction of the lattice into two sublattices $\mathscr{L}_1$ and $\mathscr{L}_2$, such that $\mathscr{L}$ is the direct union of the lattices $\mathscr{L}_1$ and $\mathscr{L}_2$.

Both sublattices $\mathscr{L}_1$ and $\mathscr{L}_2$ by themselves satisfy all the axioms of a proposition system (Problem 4). Each of them contains a center, $\mathscr{C}_1$ and

$\mathscr{C}_2$ respectively, which may or may not be trivial. If both centers are trivial, the decomposition stops, and both $\mathscr{L}_1$ and $\mathscr{L}_2$ are irreducible. If $\mathscr{C}_1$, for instance, is not trivial, then the decomposition can be continued by choosing an element $z_1 \in \mathscr{C}_1$ such that $z_1 \neq \emptyset_1$ and $z_1 \neq I_1$, where $\emptyset_1$ is the null element and I_1 is the unit element of $\mathscr{L}_1$. Using this element one can then further reduce the sublattice $\mathscr{L}_1$, and so on.

The question presents itself whether the process will ever stop, and if it does, whether the resultant irreducible sublattices $\mathscr{L}_i$ are uniquely determined apart from a permutation.

These questions are easily answered in the affirmative if the lattice satisfies a finiteness condition: The unit element I is a finite union of compatible points,

$$\mathrm{I} = \bigcup_{i=1}^{n} e_i$$

(cf. Problem 5).

If the finite lattice is Boolean, then the irreducible lattices which are obtained in the reduction process each consist of exactly two elements. This is so because the only irreducible Boolean lattice is the trivial one consisting of two elements only.

A large class of infinite Boolean lattices can still be reduced to irreducible lattices in a similar way. When this is possible, we can label the irreducible components by an index i which runs through an index-space Ω, the *phase-space* of the system. Every proposition $x \in \mathscr{L}$ is then of the form $x = \{x_i\}$, with x_i either $\emptyset_i$ or I_i. If we let Δ be the subset of Ω defined by

$$\Delta \equiv \{i : x_i = I_i\},$$

we see that this defines a one-to-one correspondence between subsets of Δ and propositions $x \in \mathscr{L}$. The operation of union and intersection becomes set union and set intersection, and the entire lattice is isomorphically mapped into the lattice of the subsets of the phase space Ω. The null set of Ω corresponds to $\emptyset$ and the entire set corresponds to I.

The reduction theory of general Boolean lattices is not as complete as that, however. The strongest results are contained in the papers by Stone and by Loomis (cf. references 6 and 7), where it is shown that any Boolean lattice can be represented as the lattice of certain subsets of a set. In this general case one is very far from a complete reduction theory.

Let us now discuss the case of a non-Boolean lattice. We shall sketch only the main lines of the proof of the reduction theorem, referring for the details to reference 5.

One begins by establishing an equivalence relation between points in $\mathscr{L}$. Two points e_1 and e_2 are said to be *perspective* if there exists a third point $e_3 \subset e_1 \cup e_2$. One shows that perspectivity is an equivalence relation. (Only transitivity uses some deeper properties of the proposition system.) It is in

fact based on the following:

Lemma: *Given three points e_1, e_2, and e_3, which satisfy the property that $e_1 \cup e_2$ contains a point e_4 such that $e_4 \neq e_1$ and $e_4 \neq e_2$, and $e_2 \cup e_3$ contains a point e_5 such that $e_5 \neq e_2$ and $e_5 \neq e_3$, then e_4, e_5 define a line $\ell = e_4 \cup e_5$ which has exactly one point e_6 in common with $e_3 \cup e_1$* (cf. Fig. 8–1).

For the proof of this lemma, see reference 5. Now let e_a be any point and denote by $\{e_a\}$ the class of equivalent points containing e_a; then we can construct the element

$$z_a = \bigcup_{e \in \{e_a\}} e$$

which we shall denote in shorter fashion by $z_a = \bigcup e_a$. This element is contained in the center $\mathfrak{C}$ of $\mathfrak{L}$; in fact, it is the smallest element in $\mathfrak{C}$ which contains all the points e_a. We shall call it the *central cover* of e_a (Problem 6). Now it is not hard to demonstrate that the desired unique decomposition of an arbitrary $x \in \mathfrak{L}$ has the form

$$x = \bigcup x_a \qquad \text{with} \quad x_a = x \cap z_a.$$

It is easy to verify that the elements of the form $x_a = x \cap z_a$ are themselves an irreducible lattice, and that for any pair of elements $x = \bigcup x_a$ and $y = \bigcup y_a$, one has $x \cup y = \bigcup (x_a \cup y_a)$ and $x \cap y = \bigcup (x_a \cap y_a)$ (see reference 5). This reduction theorem simplifies the discussion of the representation theory of proposition systems. We can, in fact, now concentrate on the representation theory of irreducible lattices.

PROBLEMS

1. If z is a nontrivial element of the center $\mathfrak{C}$ of a lattice $\mathfrak{L}$, and we define for every element $x \in \mathfrak{L}$ the decomposition $x_1 = x \cap z$, $x_2 = x \cap z'$, then we have

$$(a \cap b)_1 = a_1 \cap b_1, \qquad (a \cup b)_1 = a_1 \cup b_1,$$

$$(a \cap b)_2 = a_2 \cap b_2, \qquad (a \cup b)_2 = a_2 \cup b_2.$$

2. For every $z \in \mathfrak{C}$ one has $a' \cap z = (a \cap z)' \cap z$.
3. A finite Boolean lattice has 2^n elements ($n = 1, 2, \ldots$). The elements of such a lattice are in one-to-one correspondence to the 2^n subsets of n elements.
4. If z is an element of the center $\mathfrak{C}$ of a proposition system $\mathfrak{L}$, then the set $\mathfrak{L}_1$ of elements of the form $a \cap z$, for all $a \in \mathfrak{L}$, is again a proposition system.
5. A lattice which satisfies a finite chain condition can be reduced in a unique way to the direct union of a finite set of irreducible lattices.

*6. The element $z_a = \bigcup e_a$ is contained in the center $\mathfrak{C}$ of $\mathfrak{L}$ and it is the smallest element in $\mathfrak{C}$ which contains any e_a (cf. reference 5).

8-3. THE STRUCTURE OF IRREDUCIBLE PROPOSITION SYSTEMS

We shall now study an irreducible lattice which is complete, atomic, orthocomplemented, and weakly modular (that is, it satisfies axiom (P) of Section 5-8). Irreducibility can be expressed in two equivalent forms (cf. Problem 1):

Either to every pair of points e_1, e_2 there exists a third e_3 such that

$$e_1 \cup e_2 = e_1 \cup e_3 = e_2 \cup e_3,$$

or the center $\mathfrak{C}$ is trivial.

In physical terms, irreducibility means the unrestricted validity of the superposition principle.

We shall introduce the notion of the dimension n of the system as the maximum number of compatible points whose union is equal to I. The dimension may be finite or infinite, and it is always > 0.

The structure of an irreducible proposition system is related to the structure of an (irreducible) projective geometry. The exact nature of this relation is contained in the following:

Theorem: *Every irreducible proposition system $\mathfrak{L}$ can be imbedded in a canonical way into a projective geometry G by a correspondence α which has the following properties:*

1) *α is a correspondence from $\mathfrak{L}$ into G.*
2) *The restriction of α to the points of $\mathfrak{L}$ is a mapping onto the points of G.*
3) *$a \subseteq b$ if and only if $\alpha(a) \subseteq \alpha(b)$.*
4) $\alpha\left(\bigcap_i a_i\right) = \bigcap_i \alpha(a_i)$.
5) $\alpha(a \cup e) = \alpha(a) \cup \alpha(e)$ *for any point $e \in \mathfrak{L}$.*

Proof: For the proof of this theorem, we utilize the definition of a projective geometry which we have given in Section 8-1. The set E in this definition will be taken as the set of all points in $\mathfrak{L}$. We *define* as $\alpha(a)$ the set of points contained in the proposition a. Let us verify that $\alpha(a)$ thus defined is indeed a set of the class of subsets which constitute the projective geometry G. According to the definition of G, such a subset must contain, with every pair of points, the line which passes through these points. This is evidently the case here, because every point of the line is $\subseteq a$ and hence contained in $\alpha(a)$.

Properties (2) and (3) are immediate consequences of the definition of α. Let us verify (4). The left-hand side consists of all the points contained in $\bigcap a_i$ and the right-hand side is equal to all the points contained in all the $\alpha(a_i)$ which is by definition equal to all the points in $\bigcap a_i$. Property (5) is a consequence of the fact that every point $e_1 \subseteq a \cup e$ but different from e is on

a line passing through e and a point in a. This is true if there exists a point $e_2 \subseteq a \cap (e \cup e_1)$ (cf. Problem 2). With this the theorem is proved.

We mention here for greater clarity that the union in an expression such as $\alpha(a) \cup \alpha(b)$ signifies the union with respect to the lattice structure of the projective geometry G. It does *not* follow from property (5) that for any pair of propositions a, b, one has $\alpha(a \cup b) = \alpha(a) \cup \alpha(b)$. In fact, in general one has $\alpha(a) \cup \alpha(b) \subset \alpha(a \cup b)$.

The theorem which we have now established enables us to reduce the study of the structure of a proposition system $\mathscr{L}$ to that of the projective geometry G into which any proposition system is thus canonically imbedded.

The structure of an irreducible projective geometry is completely determined by the following:

> ***Theorem:*** *If the projective geometry G has dimension $n \geq 3$, then there exists a linear vector space V with coefficients from a field (determined up to isomorphism) and a one-to-one correspondence between the elements of G and the linear manifolds of V. This correspondence preserves the partial order relation, and, in particular, maps points into one-dimensional subspaces of V.* (For the proof refer to reference 1, Chapter VII.)

With this theorem the first part of the analysis of the structure of proposition systems is accomplished. We may summarize it as follows:

Every proposition system is a unique direct union of irreducible proposition systems.

Every irreducible proposition system is imbedded in a canonical way into a projective geometry.

Every projective geometry is algebraically isomorphic with the linear manifolds of some linear vector space V with coefficients from a field. The nature of the field is, up to isomorphism, determined by the algebraic structure of the lattice. The field may be different for different components of a reducible lattice.

PROBLEMS

1. In a proposition system the two properties

   a) To every pair of points e_1, e_2 there exists a third such that

   $$e_1 \cup e_2 = e_1 \cup e_3 = e_2 \cup e_3; \quad \text{and}$$

   b) the center $\mathscr{C}$ is trivial

   are equivalent.

*2. Given a point e and an element $a \neq 0$ in a proposition system $\mathscr{L}$. Then every point $e_1 \subset a \cup e$ is situated on a line passing through e and a point $e_2 \subset a$ [5].

8-4. ORTHOCOMPLEMENTATION AND THE METRIC OF THE VECTOR SPACE

The theorem of the preceding section makes no statement about the nature of the field over which the vector space V is constructed. The field could be finite, discrete, or continuous. It could be commutative or not. Conventional quantum mechanics is constructed over a Hilbert space with coefficients from the complex numbers. It would be most desirable to understand and exhibit the physical basis for that particular choice in the conventional theory, but this has not yet been possible.

A certain restriction concerning the nature of the field comes from the postulate of orthocomplementation. The attentive reader will have noticed that the axiom of orthocomplementation has not yet been used for an irreducible proposition system in the analysis of the structure of such systems. This we shall do now. The aim of this section is thus to find out the restriction on the vector space V, which results from the existence of orthocomplementation.

A first example of such a restriction has been established by Birkhoff and von Neumann. In order to formulate their theorem we need a couple of definitions.

We shall define an involutive *antiautomorphism* of a field F as a mapping (denoted by *) of F onto F with the following properties:

$$(\alpha + \beta)^* = \alpha^* + \beta^*, \qquad (\alpha\beta)^* = \beta^*\alpha^*, \qquad \text{and} \qquad (\alpha^*)^* = \alpha,$$

for all $\alpha, \beta \in F$.

We shall call a *sesquilinear form* in V a mapping f of the cartesian product $V \times V$ into F such that for all $x_1, x_2, y_1, y_2 \in V$ and $\lambda \in F$,

$$f(x_1 + \lambda x_2, y) = f(x_1, y) + \lambda^* f(x_2, y),$$

$$f(x, y_1 + \lambda y_2) = f(x, y_1) + f(x, y_2)\lambda.$$

Such a form is called *Hermitian* if in addition

$$f(x, y) = f^*(y, x);$$

and it is called *definite* if

$$f(x, x) = 0 \qquad \text{implies} \qquad x = 0.$$

Birkhoff and von Neumann have demonstrated the following:

Theorem 1: *Let V be a vector space over a field F and let n be its dimension. If $3 \leq n < \infty$, then every orthocomplementation in V defines an antiautomorphism of F and a definite Hermitian form f such that every subspace can be represented by vectors x which satisfy $f(x, y_i) = 0$ for a certain family of vectors y_i* (cf. references 5 and 1).

The existence of a definite Hermitian form implies the existence of an involutive antiautomorphism. Not every field has this property. We see thus that in the finite case orthocomplementation implies a restriction on the field. The real, complex, and quaternionic fields all have this property and thus may be suitable candidates for the representation of proposition systems.

The following remarks outline the extension of the above theorem to the infinite case. A useful intermediate step is obtained from the following:

Theorem 2: *If the sesquilinear forms f and g over a vector space represent the same orthocomplementation, then there exists an element $\gamma \in F$ such that $g(x, y) = \gamma f(x, y)$ for all $x, y \in V$.* (Cf. reference 1, Proposition 2, p. 105.)

This theorem now permits the following construction: Let $\mathscr{L}$ be an infinite irreducible proposition system, and let G be the infinite projective geometry into which it is canonically imbedded. Denote by V the vector space over the field F which yields an isomorphic representation of G. Let V_0 be any three-dimensional subspace of V. The restriction of the orthocomplementation in V to V_0 defines an orthocomplementation in V_0, and since V_0 is finite-dimensional, it defines a Hermitian definite form $f_0(x, y)$.

Now let V_1 be any other finite-dimensional subspace of V which contains $V_0 : V_0 \subset V_1$. According to Theorem 1, there exists a Hermitian form $g_1(x, y)$ for which we denote the restriction to V_0 by $g_0(x, y)$. According to theorem 2, we can find a number $\gamma \in F$ such that

$$f_0(x, y) = \gamma g_0(x, y).$$

Thus if we define $f_1(x, y) \equiv \gamma g_1(x, y)$, we have found the uniquely determined Hermitian form which defines the orthocomplementation on V_1 and for which the restriction to V_0 is equal to $f_0(x, y)$.

We can now define a definite Hermitian form on the entire space V in the following way:

Let us define $V_1 \equiv V_0(x, y)$ as the linear subspace of V which is generated by V_0 and the two vectors x and $y \in V$, and denote by f_{V_1} the unique extension described in the preceding remarks of f_0 to the subspace V_1. Then we set

$$f(x, y) \equiv f_{V_1}(x, y).$$

This is, according to the definition, a definite Hermitian form on the entire space V. Moreover, if e is a one-dimensional subspace (or a point of the lattice), then the subspace e' consists of all those vectors x which satisfy

$$f(x, y) = 0 \qquad \text{for} \quad y \in e.$$

We see from these remarks that the orthocomplementation defines on V a definite Hermitian form, even if V is infinite-dimensional.

The usual assumption in conventional quantum mechanics of a definite metric is thus traced directly to the existence of the orthocomplementation. (For more details see reference 5.)

This result throws an interesting light on the various attempts at generalizing quantum field theory by postulating an indefinite metric in Hilbert space. While such formulations may indeed be possible, we see from the foregoing that nothing of an essential physical nature can be gained by it. Indeed, we may announce here quite generally that any physical theory (which admits orthocomplementation) represented in a Hilbert space with indefinite metric can be transcribed into another physically equivalent theory which operates in a Hilbert space with definite metric.

8-5. QUANTUM MECHANICS IN HILBERT SPACE

We have now completed the construction of the connection between the proposition system as an abstract lattice and its representation as a lattice of subspaces in some linear vector space with coefficients from some field. We obtain the proposition system of conventional quantum mechanics if for this field we choose the complex numbers, and for the antiautomorphism the ordinary complex conjugation.

Although it has not yet been possible to single out in full generality the empirical basis for the choice of complex numbers, the following remarks may be made concerning this choice. If the field contains the real numbers as a subfield, then the choice of field is severely limited by a celebrated mathematical theorem according to which there are only three fields which contain the reals as a subfield. These are the reals themselves, the complex numbers, and the quaternions. Quantum mechanics in real Hilbert space has been developed by Stueckelberg [10], and he has found that the empirical evidence points towards the existence of a superselection rule, which has the effect that at least for simple systems the proposition system is essentially equivalent to the system of subspaces in a complex Hilbert space.

It is more difficult to rule out quaternionic Hilbert spaces, and the possibility of a "quaternionic quantum mechanics" was seriously considered [11]. A rather decisive limitation comes from the relativistic form of quaternionic quantum mechanics, which can be shown, with a very plausible supplementary assumption, to be equivalent to complex quantum mechanics for a system consisting of just one particle [12].

From now on, therefore, we shall concentrate on quantum mechanics in complex Hilbert space. In this case elementary propositions are represented by projection operators or, equivalently, by closed linear subspaces. The intersection and unions are defined as set intersection and closed linear span of subspaces. The orthocomplement is defined with the fundamental Hermitian form f: If M is a subspace, then $M^{\perp}$ is the set of all vectors $x \in \mathcal{H}$ such that

$f(x, y) = 0$ for all $y \in M$. The Hermitian form $f(x, y)$ defines a scalar product of elements in $\mathscr{H}$ by setting

$$(x, y) \equiv f(x, y).$$

Two propositions are compatible if and only if their corresponding projection operators commute.

Observables are represented by σ-homomorphisms $\Delta \to E_\Delta$, which in this case are nothing else than spectral measures. Hence, in view of the one-to-one correspondence of spectral measures with self-adjoint linear operators, we may say: Observables *are* self-adjoint linear operators.

The states are σ-additive positive functionals on the projection operators. Gleason [13] has proved the important theorem that every such functional has the form

$$p(E) = \operatorname{Tr}(WE)$$

where Tr signifies the trace defined by the formula

$$\operatorname{Tr} X \equiv \sum_r (\varphi_r, X\varphi_r)$$

for any complete system of normalized orthogonal vectors φ_r. The operator W is a self-adjoint positive operator which satisfies the relations

$$W > 0, \qquad \operatorname{Tr} W = 1, \qquad \text{and} \qquad W^2 \leq W.$$

The state is pure if and only if the operator W satisfies the relation $W^2 = W$. In that case W is a projection operator of rank 1 (Problems 1 and 2).

We define the *expectation value* $p(A)$ of an observable A by setting

$$p(A) = \int_{-\infty}^{+\infty} \lambda \, d \operatorname{Tr}(E_\lambda W) \equiv \operatorname{Tr}(WA).$$

The expectation value is a linear functional on all the observables; that is, we always have

$$p(A + B) = p(A) + p(B),$$

whether A and B commute or not (Problem 5). The operator W is called the *density operator*. If W is a projection with one-dimensional range, and φ is a unit vector in that range, then φ is called the *state vector*. A state vector thus always represents a pure state. In such a state, the expectation value of the observable A is given by $p(A) = (\varphi, A\varphi)$. In the general case of a mixture there always exists an orthonormal family φ_r and positive numbers λ_r such that

$$p(A) = \sum_r \lambda_r(\varphi_r, A\varphi_r) \qquad \text{when} \quad \sum_r \lambda_r = 1$$

(Problem 6).

PROBLEMS

1. The state represented by the operator W is pure if and only if $W^2 = W$.
2. For a pure state W is a projection operator with one-dimensional range.
3. If W is pure, then there exists a normalized vector $\varphi \in \mathscr{H}$ such that the expectation value of any observable A is given by

$$\langle A \rangle = (\varphi, A\varphi).$$

4. If the state p is pure, then there exists a projection P of one-dimensional range such that $p(P) = 1$ and vice versa.
5. The expectation value $p(A)$ for any state is a linear functional on all observables:

$$p(A + B) = p(A) + p(B).$$

6. If p is any state, then there exists an orthonormal family of vectors (not necessarily complete) and real numbers $\lambda_r > 0$, such that

$$p(A) = \sum_r \lambda_r(\varphi_r, A\varphi_r) \qquad \text{with} \quad \sum_r \lambda_r = 1.$$

7. If A is an observable with spectrum Λ, then we always have $a \leq p(A) \leq b$, where a is the greatest lower bound and b the least upper bound of Λ.

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CHAPTER 9

SYMMETRIES AND GROUPS

Symmetry, as wide or as narrow as you may define its meaning, is one idea by which man through the ages has tried to comprehend and create order, beauty, and perfection.

H. WEYL

In this chapter we introduce the formal tools for the treatment of symmetries in physical systems. After a brief exposition of the meaning of symmetry in physics and its mathematical formulation (Section 9-1), we devote two sections, (9-2 and 9-3), to the theory of groups. What is offered here is a short recapitulation of the principal notions concerning abstract and Lie groups, and it does not replace a more thorough study of group theory. The basic group which concerns us here is the group of automorphisms of a proposition system, defined in Section 9-4. In Section 9-5 we show how states are transformed under this group and how this property can be used to make it into a topological group H. The symmetry groups G which we encounter in nature are, however, given by basic laws or by particular circumstances, and they are different from the group of automorphisms. There arises then the problem of the homomorphisms of G into H. We call these the projective representations of G (Section 9-6). Complete solutions of this problem are given for the case of Lie groups represented in the lattice of the subspaces of a Hilbert space. These are the most important cases for later applications.

9-1. THE MEANING OF SYMMETRY

The notion of symmetry has been of ever increasing importance in fundamental theoretical physics. The principles of symmetries are often the only guides into unknown territory, and in the realm of the known they furnish convenient shortcuts to important results.

Symmetries pervade the whole of physics. They are important in the classical as well as the quantum domain. They are expressions of the immutable laws which make physics as a science possible, and they are the most

profound structural properties of space and time, the arena of the physical phenomena.

A symmetry has an immediate intuitive appeal and can often be recognized at a very early stage of a physical theory. But the notion of symmetry can also be given a precise mathematical sense which is crystallized, so to speak, in the notion of the group. Mathematics has developed the theory of abstract groups to a high degree of perfection, and in the formulation of physical symmetries the theory of groups is an indispensable tool.

If we analyze the notion of symmetry, we find that it is based on two other more primitive notions, that of *transformation* and that of *invariance*. We say that we have a symmetry if there exist certain transformations of the elements of a set which leave one or several relations among these elements unchanged.

The lattice of a proposition system $\mathscr{L}$ furnishes excellent examples of symmetries. In order to show this, we introduce the notion of a *morphism* of a lattice $\mathscr{L}_1$ onto another one $\mathscr{L}_2$.

A *morphism* m for the lattices $\mathscr{L}_1$ and $\mathscr{L}_2$ is a bijective (that is one-to-one) mapping of $\mathscr{L}_1$ onto $\mathscr{L}_2$ with the following two properties:

1) $a \subseteq b$ implies $m(a) \subseteq m(b)$, and vice versa.

2) $m(a') = m(a)'$ for every $a \in \mathscr{L}_1$.

If two lattices are connected by a morphism then they are said to be isomorphic.†

Since the mapping m is bijective, there exists an inverse mapping m^{-1} with domain $\mathscr{L}_2$ and range $\mathscr{L}_1$, and this inverse is also a morphism.

In the special case that $\mathscr{L}_1 = \mathscr{L}_2 = \mathscr{L}$, the mapping is a permutation of the elements of $\mathscr{L}$ and m becomes an *automorphism*.

If there exist automorphisms of a lattice, we say the lattice has symmetries.

If m_1 and m_2 are two different automorphisms of a lattice, then the mapping which is obtained by carrying out first m_1 followed by m_2 is again an automorphism denoted by $m_2 m_1$, and called the product of m_1 with m_2. The set M of all automorphisms of $\mathscr{L}$ is thus a family of morphisms which is closed under the operations of the product and the inverse. Such a family of transformations is called a group.

The algebraic structure of the group of automorphisms of $\mathscr{L}$ embodies a great deal of the structure of $\mathscr{L}$. It is therefore of some interest to study the structure of groups quite independently of the structure of the objects which the elements of the group transform. Some of the elements of the structure of groups are discussed in the following two sections.

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† It should be remarked that morphisms in the mathematical literature are usually given a more general meaning than the one adopted here. A morphism in the general sense need be neither one-to-one nor onto. Here we do not need it in this generality.

9-2. ABSTRACT GROUPS

An abstract group is a finite or infinite set of objects called the elements of the group endowed with an algebraic structure as follows: To every pair of elements $r, s \in G$ there corresponds a unique element $rs \in G$ such that:

1) $(rs)t = r(st)$ (associative law).

2) There exists a neutral element $e \in G$ such that, for all $r \in G$, $er = re = r$.

3) To every r there exists a unique inverse r^{-1} such that $rr^{-1} = r^{-1}r = e$.

The order of the elements in an expression such as rs is important because in general $rs \neq sr$. If $rs = sr$, we say the elements commute. A group for which all pairs of elements commute is called commutative or *abelian*.

The set of elements in G which commute with every element in G is called the *center* Z of G. Abelian groups are thus characterized by the property $Z = G$. The neutral element e certainly belongs to the center. Furthermore, if z_1, z_2 are two elements $\in Z$, then $z_1z_2r = z_1rz_2 = rz_1z_2$, so that $z_1z_2 \in Z$. Likewise if $z \in Z$, then $zr = rz$, from which it follows that $rz^{-1} = z^{-1}r$. Thus $z^{-1} \in Z$. We see from these remarks that the center Z is itself an abelian group, and since $Z \subseteq G$ we call it a *subgroup* of G.

In general, a subset $H \subset G$ is called a subgroup of G, if it is itself a group under the group operations of G.

There always exist two trivial subgroups, namely, $H = \{e\}$ and $H = G$. In the first case H consists of the single element e (evidently a group), and in the second case it consists of all the elements of G. An easy way to construct nontrivial subgroups of a group is the following: Take any element $a \in G$ $(a \neq e)$ and form the successive powers of a, $a^2 = aa$, $a^3 = aa^2$, etc. If there exists an n such that $a^n = e$, we obtain a finite subgroup of a special kind called a *cyclic* group. If there exists no such n, then we obtain an infinite cyclic subgroup.

If H is a subgroup of G, and r an element of G which is not contained in H, then we denote by $rH = R_\ell$ the set of elements of the form rx for all $x \in H$ and fixed r. It is called a *left coset* of H. It has no elements in common with H. If there exists a further element $s \in G$ such that $s \notin H$ and $s \notin rH$, then we can construct a further left coset $S_\ell = sH$. By continuing this process we can exhaust the entire group G and arrive at a decomposition of G as a union of disjoint subsets,

$$G = H \cup R_\ell \cup S_\ell \cup \cdots$$

One can do the same thing by using *right cosets* instead, for instance, $R_r = Hr$, etc.; one then obtains a decomposition of G into right cosets

$$G = H \cup R_r \cup S_r \cup \cdots$$

These two decompositions become identical if every left coset is equal to some right coset, and vice versa. The necessary and sufficient condition for

this to be the case is that $rH = Hr$ for all $r \in G$. This means that for any $x \in H$ there exists another $y \in H$ such that $rx = yr$. A subgroup with this property is called an *invariant subgroup* of G.

If H is an invariant subgroup, then the cosets are themselves a group. A group operation can be defined between two cosets R and S by selecting any two elements $r \in R$ and $s \in S$. Then the product rs lies in a coset RS. This notation is justified if the coset RS does not depend on the choice of $r \in R$ nor on the choice of $s \in S$. For this to be the case, it is necessary and sufficient that H be an invariant subgroup of G. The product can then be transferred to the cosets themselves. The group properties are easily verified (Problem 1). The group of cosets with respect to an invariant subgroup H is called the *factor group*, and is denoted by G/H.

If we have two groups G_1 and G_2, and if there exists a correspondence $r_1 \to r_2$ between elements $r_1 \in G_1$ and $r_2 \in G_2$ such that $r_1 \to r_2$ and $s_1 \to s_2$ implies $r_1 s_1 \to r_2 s_2$, we have a *homomorphism* of G_1 into G_2. The homomorphism is *onto* if every element of G_2 is the image of some element in G_1. The group G_2 is then the homomorphic image of the group G_1.

The group G_2 may be considered to reflect some but not all of the properties of G_1. It is indistinguishable from G_1 as an abstract object if the homomorphism is one-to-one. In that case the two groups are said to be isomorphic.

If the two groups are identical, that is if $G_1 = G_2$, then an isomorphism is called an automorphism (cf. Problems 4 and 5).

PROBLEMS

1. The cosets with respect to an invariant subgroup $H \subset G$ are a group.
2. If $G_1 \to G_2$ is a homomorphism, then the set of elements H which are mapped into the neutral element $e_2 \in G_2$ is an invariant subgroup and there exists a natural isomorphism between G/H and G_2.
3. The center Z is an invariant subgroup of G.
4. The transformation $r \to srs^{-1}$ for fixed $s \in G$ is an automorphism of G which leaves the center pointwise invariant. This is called an inner automorphism.
5. There are automorphisms which are not inner: The simplest example is the cyclic group of three elements, $e : a, a^2, a^3 = e$. The automorphism $a \to a^2$ is not inner.
6. Every abstract group is isomorphic to some transformation group. Such an isomorphism can be implemented by considering the left translation L_r of the group space associated with the element r and defined by

$$L_r : s \to rs.$$

We have then for any pair r_1, r_2,

$$L_{r_1} L_{r_2} \quad L_{r_1 r_2}.$$

9-3. TOPOLOGICAL GROUPS

The abstract groups defined in the preceding section can be endowed with a topology. The group is then simultaneously an abstract group and a topological space. It is then meaningful to consider groups such that the product rs^{-1} of two elements is a continuous function of both of the elements. If this is the case we speak of a *topological group* [3]. If the topology is the trivial discrete topology, then we speak of a discrete topological group. More interesting for the applications are certain continuous groups called Lie groups which have a wide range of applications.

a) Lie groups. For Lie groups the topology is locally that of a finite-dimensional linear manifold. This means that for every element $r_0 \in G$ there exists a neighborhood N_0 which is the continuous and one-to-one image of some neighborhood of a finite-dimensional Euclidean space. If n is the dimension of this space, then every element $r \in N_0$ can be represented as a set of n real numbers $\rho_1, \rho_2, \ldots, \rho_n$. It suffices to introduce cartesian coordinates in the Euclidean space and use the coordinates of the representative point for r in that space. These coordinates can, of course, be chosen in many different ways. In any case we can write the group relations as a set of functional equations between the parameters. For instance, let s be a second element of the group with the parameters $\sigma_1, \sigma_2, \ldots, \sigma_n$, and assume furthermore that $t = rs \in N_0$; then we can express the law of the group multiplication in the form

$$\tau_i = f_i(\rho_1, \ldots, \rho_n; \sigma_1, \ldots, \sigma_n) \qquad (i = 1, 2, \ldots, n), \tag{9–1}$$

where $\tau_1, \tau_2, \ldots, \tau_n$ are the parameters for the element $t = rs$.

The f_i are n continuous functions of the $2n$ variables $\rho_1, \ldots, \sigma_n$. For Lie groups the parameters can be chosen in such a way that the functions f_i are not only continuous but also analytic in a suitable neighborhood. They then admit derivatives to any order. It is natural in this case to study the relation of the local properties of Lie groups to the global properties, that is, the structure of the group in the large. It turns out that the local properties determine to a large extent the properties of the group in the large, and the remaining ambiguity can be completely characterized.

b) Local properties of Lie groups. We adopt the following notation. The labels $r, s, \ldots$ for the group elements are used simultaneously for the set of parameters in some parametrization of the group. Thus $r = \{\rho_1, \rho_2, \ldots, \rho_n\}$ We choose the parameters so that the neutral element has the parameters $e = \{0, 0, \ldots, 0\}$. Equation (9–1) will then appear in the abbreviated form $t = f(r, s)$. The local properties in the neighborhood N_0 of an arbitrary element r_0 can always be related to the neighborhood of the neutral element by the transformation $r_0^{-1}N_0$. Thus it suffices to study the neighborhood of the identity.

A curve which passes through the neutral element is a continuous function $r(\alpha)$ of the real variable α in some neighborhood of $\alpha = 0$, and such that $r(0) = e$. A curve is a one-parameter subgroup if the parameter can be chosen such that $r(\alpha)r(\beta) = r(\alpha + \beta)$ in some neighborhood of 0. In that case the functions $r(\alpha)$ are analytic and we can define the tangent vector as a vector in Euclidean space with the components $a_i = (d\rho_i/d\alpha)_{\alpha=0}$.

If we differentiate the equation (9–1) with respect to the parameter α, we obtain the differential equation

$$\frac{d\rho_i}{d\alpha} = \sum_{k=1}^{n} \theta_{ik}(r)a_k \tag{9–2}$$

where

$$\theta_{ik}(r) = \left(\frac{\partial f_i(r, s)}{\partial \sigma_k}\right)_{s=e}.$$

Thus every one-parameter subgroup of a Lie group satisfies a differential equation (9–2); and conversely, every solution of this differential equation is a one-parameter subgroup.

Consider two arbitrary local one-parameter subgroups $r(\alpha)$ and $s(\beta)$ with the tangent vectors **a** and **b** respectively. We use vector notation. In a particular coordinate system the vector **a** has components $a_i = (d\rho_i/d\alpha)_{\alpha=0}$ where $\rho_1, \rho_2, \ldots, \rho_n$ are the coordinates of the point r. We define the commutant

$$q(\alpha; a, b) \equiv r(\alpha)s(\alpha)r^{-1}(\alpha)s^{-1}(\alpha)$$

and the infinitesimal commutant

$$[a, b] = \lim_{\alpha \to 0} \frac{1}{\alpha^2} q(\alpha; a, b). \tag{9–3}$$

This expression is antisymmetrical in its arguments

$$[a, b] = -[b, a], \tag{9–4}$$

and it satisfies the Jacobi identity

$$[[a, b], c] + [[b, c], a] + [[c, a], b] = 0. \tag{9–5}$$

If the group is abelian, then the bracket $[a, b] = 0$. If it is not abelian, then its value is some sort of measure of the deviation from commutativity in the group. In any case the bracket expression $[a, b]$ is again a tangent vector, and it defines an algebraic structure property of the tangent vectors of a Lie group. Such an algebra which satisfies the relations (9–4) and (9–5) is called a *Lie algebra* or an infinitesimal Lie group.

The structure of a Lie algebra can be expressed explicitly by referring it to a particular coordinate system. Let $\mathbf{a}_i$ $(i = 1, \ldots, n)$ be a base of tangent vectors, where $\mathbf{a}_i$ is the tangent vector in the direction i of the local coordinate

axis (*not* the component of a vector **a**!). Then the explicit evaluation of the commutant gives the following result [3]:

$$[\mathbf{a}_i, \mathbf{a}_j] = \sum_{k=1}^{n} c_{ij}^k \mathbf{a}_k, \tag{9–6}$$

where

$$c_{ij}^k = \left(\frac{\partial f_k}{\partial \rho_i \partial \sigma_j} - \frac{\partial f_k}{\partial \rho_j \partial \sigma_i} \right)_{r=s=e} \tag{9–7}$$

are the *structure constants* of the Lie algebra. From the expression (9–7) one sees immediately that the structure constants are antisymmetrical in the lower indices

$$c_{ij}^k = -c_{ji}^k. \tag{9–4}$$

Furthermore, they satisfy

$$\sum_{m=1}^{n} (c_{mk}^l c_{ij}^m + c_{mi}^l c_{jk}^m + c_{mj}^l c_{ki}^m) = 0, \tag{9–5}$$

as a consequence of the Jacobi identity.

In the theory of Lie groups, one proves that the structure constants determine the structure of the group completely in a suitable neighborhood of the neutral element. This is the essential result of the *local* theory of Lie groups.

We turn now to global properties.

c) The global properties of Lie groups. Let G be a Lie group and r and s two arbitrary elements of G. These two elements are said to be connected if there exists a continuous curve $x(\alpha) \in G$ $(0 \leq \alpha \leq 1)$ such that $x(0) = r$ and $x(1) = s$. The set of all the elements which are connected with the neutral element e is an invariant subgroup G_0 of G, called the connected component of G (cf. Problem 2).

A connected group is said to be *simply connected* if every closed curve in the group can be contracted to a point. This means that if $r(\alpha)$ $(0 \leq \alpha \leq 1)$ is closed $(r(0) = r(1))$ then there exists a continuous function $r(\alpha, \beta)$ of the two variables α, β $(0 \leq \beta \leq 1)$ such that

$$r(\alpha, 1) \equiv r(\alpha) \qquad \text{and} \qquad r(\alpha, 0) = r(0, 0).$$

If this is not the case, then G_0 is said to be multiply connected.

According to a fundamental theorem on Lie groups there exists for every connected, multiply-connected Lie group G_0 a unique simply-connected *universal covering group* G^* with the following properties:

1) G_0 is the homomorphic image of G^*;

2) the kernel of the homomorphism $G^* \to G_0$ is an invariant discrete subgroup N of the center of G^*.

This theorem then spells out in detail to what extent the Lie algebra determines the global structure of the Lie group. Every connected Lie group is a subgroup of its universal covering group. The structure constants determine the nature of the covering group, but they allow no general conclusion as to the connectedness of the group.

There is one more topological property which is of great importance in the applications of groups to quantum mechanics. A topological group, seen as a topological space, may be either compact or noncompact. A topological space is *compact* if every infinite sequence has a convergent subsequence. Since the structure constants determine the covering group completely, it must be possible to determine whether this group is compact or not from an examination of these constants alone; this is indeed the case. We shall be content with this general remark here. For greater details we refer the reader to reference 3.

PROBLEMS

1. The group of the real numbers (called the real line) consists of all real numbers under the group operation of addition. It is a one-parameter abelian group. Its structure constants are identically zero. The group is connected, simply connected, and noncompact.
2. The connected component G_0 of Lie group G is an invariant subgroup of G.
3. The circle group consists of the real numbers φ $(0 \leq \varphi \leq 2\pi)$ under the operation of addition modulo 2π. Its Lie algebra is identical with that of the real line. The group is connected, multiply connected, and compact.
4. The real line is the universal covering group G^* of the circle group G. The kernel of the homomorphism $G^* \to G$ is the cyclic group of infinite order.
5. The Euclidean motions in a two-dimensional plane are a three-parameter nonabelian group. It is connected, multiply connected, and noncompact.
6. The rotations of three-dimensional Euclidean space are a three-parameter Lie group. It is nonabelian, connected, doubly connected, and compact. The kernel of the homomorphism $G^* \to G_0$ is the cyclic group Z_2 of order 2 (cf. Section 13-3, especially Problem 3).
7. The rotation-reflection group of the three-dimensional Euclidean space consists of two disconnected components.

9-4. THE AUTOMORPHISMS OF A PROPOSITION SYSTEM

As we have seen, by way of illustration of the notion of symmetry in Section 9-1, there exists a group of automorphisms of a lattice $\mathscr{L}$. Automorphisms m are one-to-one mappings of $\mathscr{L}$ onto itself with the properties

1) $a \subseteq b$ if and only if $m(a) \subseteq m(b)$;

2) $m(a') = m(a)'$.

It follows immediately that an automorphism admits an inverse m^{-1} which is also an automorphism. If $a_1 = m(a)$, then the inverse m^{-1} is defined by $m^{-1}(a_1) = a$. Thus if $a_1 \subseteq b_1$, then by property (1), $m^{-1}(a_1) \subseteq m^{-1}(b_1)$. Property (2) read from right to left then gives $m^{-1}(a_1') = m^{-1}(a_1)'$.

We shall now show that an automorphism leaves not only the partial ordering intact, but it leaves the entire lattice structure invariant. We prove first:

Lemma 1: $m(\bigcup a_i) = \bigcup m(a_i)$ *and* $m(\bigcap a_i) = \bigcap m(a_i)$.

Proof: We have, from the definition of union, $a_i \subseteq \bigcup a_i$ for all i. Thus by property (1) it follows that $m(a_i) \subseteq m(\bigcup a_i)$, and by the definition of the union we obtain $m(a_i) \subseteq \bigcup m(a_i) \subseteq m(\bigcup a_i)$. From the first of these two inclusion relations we obtain $a_i \subseteq m^{-1} \bigcup m(a_i)$, by observing that m^{-1} is also an automorphism. Consequently, by taking unions and applying m again,

$$m(\bigcup a_i) \subseteq \bigcup m(a_i).$$

Comparing this with the previous inclusion in the reverse sense, we conclude

$$m(\bigcup a_i) = \bigcup m(a_i). \qquad \text{Q.E.D.}$$

The proof of the second assertion of the lemma is similar.

From Lemma 1 it follows immediately that $m(\emptyset) = \emptyset$ and $m(I) = I$. Furthermore if a is compatible with b : $a \leftrightarrow b$, then $m(a) \leftrightarrow m(b)$ and conversely. To see this, it suffices to remark that compatibility is expressible entirely with the relations $\bigcup$ and $\bigcap$. These relations are invariant under an automorphism m, and so is compatibility. The converse follows again from the fact that m^{-1} is also an automorphism.

Another corollary is that a point e is transformed by an automorphism into a point $m(e)$. Suppose indeed that $x \subset m(e)$. It follows then that $m^{-1}(x) \subset e$, and since e is a point, $m^{-1}(x) = \emptyset$. This implies that $x = m(\emptyset) = \emptyset$. Thus $m(e)$ is a point.

Lemma 2: *An automorphism is completely determined by its restriction to the points.*

Proof: The assertion is a direct consequence of the fact that every proposition is the union of its points. Thus if $a = \bigcup e_i$, then $m(a) = m(\bigcup e_i) = \bigcup m(e_i)$, by Lemma 1. This proves Lemma 2.

In Section 8-2 we defined the central cover of a point e as the union of all the points e_i which are coherent with e: $z = \bigcup e_i$. Let us denote by a *coherent component* the segment $[\emptyset, z]$, consisting of all elements x of the lattice which satisfy $\emptyset \subseteq x \subseteq z$. What happens to the coherent components under an automorphism? The answer is contained in Lemma 3.

Lemma 3: *The image of a coherent component under an automorphism is again a coherent component.*

Proof: If z is the union of coherent points. Then $m(z)$ is also a union of coherent points, since coherence is invariant under an automorphism. This proves Lemma 3.

We have now obtained the following characterization of an automorphism of a lattice: Let $\mathscr{L}$ be a lattice and $\mathscr{L}_\alpha$ its (uniquely determined) coherent components. An automorphism induces a permutation of the coherent components. If $m(\alpha)$ is the index of the component with index α, then the automorphism induces a morphism between the lattice $\mathscr{L}_\alpha$ and the lattice $\mathscr{L}_{m(\alpha)}$.

At this point we obtain a further characterization of automorphisms if we make use of the fundamental theorem of projective geometry. We have seen that every projective geometry admits a representation as subspaces of a linear vector space V with coefficients over a field F. Let $u_1 \in V_1$; we say the correspondence $Su_1 = u_2 \in V_2$ of the vector space V_1 onto V_2 is a *semilinear* transformation if $S(u_1 + v_1) = Su_1 + Sv_1$ and $S(fu) = f^s u$ for every element $f \in F$, where f^s is the image of f under an automorphism of the field F. It is clear that every semilinear transformation of V_1 onto V_2 induces a morphism which maps the lattice of subspaces from V_1 onto the lattice of subspaces from V_2. The fundamental theorem of projective geometry affirms the converse: Every morphism of $\mathscr{L}_1$ onto $\mathscr{L}_2$ is induced by a semilinear transformation of V_1 onto V_2, provided the dimension of V_1 and V_2 is at least three [4]. With this we have arrived at the following fundamental theorem.

Theorem (Wigner)*: Every automorphism m of a lattice of propositions represented by a family of vector spaces V_α of dimension at least three, maps every coherent space V_α onto another one $V_{m(\alpha)}$ by a semilinear transformation* [7], [8], [9].

In the special case of quantum mechanics, the vector spaces V_α are all Hilbert spaces over the complex numbers. The only automorphisms of the complex numbers are the identity and the complex conjugation. We speak then of *linear* or *antilinear* transformations of the vector space V.

PROBLEMS

1. An automorphism of a lattice has always at least two fixed elements.
2. If a and b are fixed elements of an automorphism m of $\mathscr{L}$, then the segment $[a, b]$ is invariant under m. (The segment is defined as the set of elements x such that $a \subseteq x \subseteq b$.)
3. If an automorphism m of subspaces in a complex Hilbert space is a square of another automorphism, then m is induced by a *linear* transformation of the Hilbert space.

9-5. TRANSFORMATION OF STATES

Every automorphism in a lattice $\mathscr{L}$ induces a transformation of the states on $\mathscr{L}$. It is defined as follows: Let $a \to m(a)$ be an automorphism of $\mathscr{L}$ and *define* $p^m(a) \equiv p(m^{-1}(a))$. Then we can easily verify that $p^m(a)$ is also a state (Problem 1).

The important application of this realization of the automorphisms of $\mathscr{L}$ is the definition of a topology on the group M of automorphisms.

For every $\varepsilon > 0$ we can define an ε-neighborhood N_ε of the identity $e \in M$ by setting

$$N_\varepsilon = \{m : |p^m(a) - p(a)| < \varepsilon \quad \text{for all } a \text{ and all } p\}.$$

This system of neighborhoods satisfies the conditions of Theorem 10 in reference 3, so that this theorem is applicable and we have thereby defined a topological group M of automorphisms.

It now becomes meaningful to speak of *connected automorphisms*. Two automorphisms m_1 and m_2 are said to be connected if there exists a continuous mapping $m(\alpha)$ from the interval [0, 1] into M such that $m(0) = m_1$ and $m(1) = m_2$.

The elements $m \in M$ which are connected with the identity $e \in M$ are an invariant subgroup $M_0 \subset M$, called the *connected component* of M (Problem 2).

We can now use continuity arguments to prove the following:

> ***Theorem:*** *If $\mathscr{L}$ is the discrete direct union of several coherent sublattices $\mathscr{L}_i$, then every automorphism m which is connected to the identity transforms each $\mathscr{L}_i$ onto itself* (Problem 3).

The topology of the group M of automorphisms is involved too when we speak about the (projective) representation of a group G. We define: A continuous homomorphism of a topological group G into M is called a *projective representation* of G.

Let $r \to U_r$ be a representation of a group G with elements r in the automorphisms M of a lattice $\mathscr{L}$. We shall say that the pair $(\mathscr{L}, U)$ is an *elementary system* if

$$U_r a = a \text{ for all } r \qquad \text{implies } a = \emptyset \quad \text{or} \quad a = I.$$

It is then easy to prove (Problem 5): Every elementary system with respect to a connected group G is necessarily coherent.

PROBLEMS

1. If $p(a)$ is a state on the lattice $\mathscr{L}$ and $a \to m(a)$ is an automorphism of $\mathscr{L}$, then $p^m(a) \equiv p(m^{-1}(a))$ is also a state.
2. The connected component M_0 of the automorphisms M of a lattice is an invariant subgroup of M.

*3. If $\mathscr{L}$ is a finite direct union of irreducible lattices $\mathscr{L}_i$, then an automorphism m which is connected with the identity maps each $\mathscr{L}_i$ onto itself ([6], Theorem 1.2).

4. If the state p is pure, then p^m is pure, too.

*5. If G is a connected group and $\mathscr{L}$ an elementary system with respect to G, then $\mathscr{L}$ is necessarily coherent [6].

9-6. PROJECTIVE REPRESENTATION OF GROUPS

From now on we shall concentrate on the projective representations of symmetry groups in Hilbert space and we shall study the representation in a connected component of the lattice of subspaces.

We have thus a group G and a homomorphism U_r into the automorphisms M of the lattice of subspaces in some Hilbert space. Every such automorphism is induced by a semilinear transformation which we denote also by U_r. U_r is determined only up to a numerical factor. By choosing this factor conveniently, we can always make U_r unitary or antiunitary. If we concentrate first on the connected component of a Lie group we can even assume that U_r is unitary. Under these conditions the operator U_r is only determined up to an arbitrary phase factor. The composition law for the representation of the group G may therefore be written in the form

$$U_r U_s = \omega(r, s) U_{rs}, \tag{9–8}$$

where $\omega(r, s)$ is a complex number of magnitude 1.

The problem of the projective representation of a symmetry group is thus to find a continuous mapping of G into the group of unitary operators U_r which satisfies a relation such as Eq. (9–8).

It is useful to point out here that the exact values of the numbers $\omega(r, s)$ have no significance because the operators U_r are, as we have said, only determined up to phase factors of magnitude 1. It is therefore appropriate to introduce the notion of *equivalent phase factors*.

If we carry out the transformation $U_r \to U'_r = \phi(r) U_r$ ($|\phi(r)| = 1$), then the new operators U'_r satisfy $U'_r U'_s = \omega'(r, s) U'_{rs}$ with

$$\omega'(r, s) = \omega(r, s) \frac{\phi(rs)}{\phi(r)\phi(s)}. \tag{9–9}$$

Two factors which are related to one another by the relation (9–9) are said to be *equivalent*. We easily verify that this is indeed an equivalence relation, and we shall write $\omega \sim \omega'$ (Problem 1). If every factor is ~ 1, the factor ω is irrelevant and can be removed. In this case and in this case only, it is possible to reduce the problem of the projective representations to that of a vector representation. One of the major problems in the theory of

projective representations of a group is to determine all the classes of *inequivalent* phase factors.

The functions $\omega(r, s)$ are not entirely arbitrary, since G is a group and satisfies the associative law. If we consider three elements r, s, and $t \in G$, and we write the equation $(rs)t = r(st)$ in the projective representation, then we find

$$\omega(r, s)\omega(rs, t) = \omega(s, t)\omega(r, st). \tag{9–10}$$

We can furthermore introduce a normalization of an arbitrary overall phase factor by assuming $U_e = I$. From this it follows that

$$1 = \omega(r, e) = \omega(e, r) \qquad \text{for all} \quad r \in G. \tag{9–11}$$

Every solution of these two equations furnishes us a possible phase factor. The problem is thus reduced to finding all the equivalent classes of complex-valued functions $\omega(r, s)$ of magnitude 1, which satisfy conditions (9–10) and (9–11).

The problem can be broken up into two others, a local one and a global one. The local problem deals with the classes of inequivalent phase factors in a neighborhood of the identity. The global problem deals with the extension of these factors to the entire group.

In the theory of the Lie groups, the determination of all local factors reduces to a relatively simple problem in vector algebra. Here we shall give merely a sketch of the solution of this problem. For greater details we refer the reader to references 2 and 8.

One first shows that within the class of equivalent factors it is always possible to choose a canonical factor such that all one-parameter subgroups are represented as vector representations. Thus for such a factor a one-parameter subgroup $r(\alpha)$, where $r(\alpha_1)r(\alpha_2) = r(\alpha_1 + \alpha_2)$, would be represented by unitary operators $r(\alpha) \to U_\alpha$ such that $U_{\alpha_1}U_{\alpha_2} = U_{\alpha_1 + \alpha_2}$. Moreover, the representation is continuous, and we can therefore, via Stone's theorem, associate with every one-parameter subgroup a unique self-adjoint operator A through the relation $U_\alpha = e^{i\alpha A}$. We may regard the self-adjoint operator A as the representation of the tangent vector $\mathbf{a}$ corresponding to the one-parameter subgroup $r(\alpha)$. If $r \to U_r$ were a true vector representation for the group, then one could show that the Lie algebra for the tangent vectors is faithfully represented by the self-adjoint operators A in the following sense: To a complete family of tangent vectors $\mathbf{a}_i$ there corresponds a complete set of self-adjoint operators A_i such that to the Lie bracket $[\mathbf{a}_i, \mathbf{a}_j]$ of two tangent vectors there corresponds the commutator of A_i and A_j multiplied with i. Thus, if the Lie algebra has the basic structure equation

$$[\mathbf{a}_i, \mathbf{a}_j] = \sum_{m}^{n} c_{ij}^{m}\mathbf{a}_m, \tag{9–12}$$

then the self-adjoint operators A_i corresponding to a_i satisfy commutator relations

$$i[A_i, A_j] = \sum_{m=1}^{n} c_{ij}^m A_m. \qquad (9\text{–}12)'$$

However, if we are dealing with a projective representation, then we obtain, by differentiating Eq. (9–8), a commutator relation such as

$$i[A_i, A_j] = \sum_{m=1}^{n} c_{ij}^m A_m + \beta_{ij} \cdot I. \qquad (9\text{–}13)$$

It differs from the relation (9–12)′ by the additional terms on the right-hand side. These terms come from the phase-factors in Eq. (9–8). In fact, one finds

$$\beta_{ij} = \left(\frac{\partial \xi(r, s)}{\partial \rho_j \partial \sigma_i} - \frac{\partial \xi(r, s)}{\partial \rho_i \partial \sigma_j}\right)_{r=s=e},$$

where $\omega(r, s) = e^{i\xi(r, s)}$. We see from this expression, as well as from Eq. (9–13), that the β_{ij} are antisymmetrical:

$$\beta_{ij} = -\beta_{ji}. \qquad (9\text{–}14)$$

From the associative law, for instance by differentiating Eq. (9–12), we further obtain the relation

$$\sum_{k=1}^{n} (c_{ij}^k \beta_{lk} + c_{jl}^k \beta_{ik} + c_{li}^k \beta_{jk}) = 0. \qquad (9\text{–}15)$$

Every solution of the identities (9–14) and (9–15) will be called a *local factor*. Every local factor can be extended by integration to a factor in a suitable neighborhood of the identity.

It follows readily from the Jacobi identity (9–5) that, if β_{ij} is a solution of the relations (9–14) and (9–15), then

$$\beta'_{ij} = \beta_{ij} + \sum_{k=1}^{n} \lambda_k c_{ij}^k \qquad \text{with } \lambda_k \text{ real}, \qquad (9\text{–}16)$$

is again such a solution. The corresponding factors are in the same equivalence class, and any two factors in the same equivalence class lead to local factors related by a set of equations (9–16) with some real constants λ_k.

From these results it is easily seen that the equivalence classes of local factors form a linear vector space. If the structure constants are identically zero (abelian groups), then this vector space has the dimension n^* of the antisymmetrical matrices of n dimensions, that is $n^* = \frac{1}{2}n(n-1)$. If the structure constants are different from zero, then this dimension is reduced by the dimension of the antisymmetrical matrices spanned by the structure constants. Thus we have generally $n^* \leq \frac{1}{2}n(n-1)$.

The determination of all local factors is thus obtained as the solution of a set of linear equations.

By a suitable choice of the parameters on the group, the factors in the neighborhood of the neutral element may be written in the form

$$\omega(r, s) = e^{i\xi(r, s)}$$

with

$$\xi(r, s) = \tfrac{1}{2} \sum_{i, j} \beta_{ij} \rho_i \sigma_j. \tag{9–17}$$

The determination of the factors on the entire group is easy when the group is simply connected, because of the following result due to Bargmann: On a simply connected group every local factor determines a factor on the entire group. Moreover, in every class of equivalent factors there exist continuous and differentiable factors [9]. With this result the determination of the projective representations of simply connected Lie groups is completed.

PROBLEMS

1. The formula

$$\omega'(r, s) = \omega(r, s) \frac{\phi(rs)}{\phi(r)\phi(s)}$$

establishes an equivalence relation between two factors of projective representations of a group.

2. For a one-parameter abelian group, every projective representation is equivalent to a vector representation.

3. Consider the translation group of the Euclidean plane, described by pairs of real numbers (α, β) with the composition law (vector addition)

$$(\alpha_1, \beta_1)(\alpha_2, \beta_2) = (\alpha_1 + \alpha_2, \beta_1 + \beta_2).$$

This group is abelian, connected, simply connected, and noncompact, and of dimension $n = 2$.

There exists a one-parameter family of nonequivalent classes of factors. Let $(\alpha, \beta) \to W(\alpha, \beta)$ be any of the projective representations, so that

$$W(\alpha_1, \beta_1)W(\alpha_2, \beta_2) = \omega(\alpha_1, \alpha_2; \beta_1, \beta_2)W(\alpha_1 + \alpha_2, \beta_1 + \beta_2).$$

In each of the equivalence classes we can then choose a factor of the form

$$\omega(\alpha_1, \alpha_2; \beta_1, \beta_2) \quad e^{i\xi(\alpha_1, \alpha_2; \beta_1, \beta_2)},$$

$$\xi(\alpha_1, \alpha_2; \beta_1, \beta_2) \quad \frac{\kappa}{2}(\alpha_1\beta_2 \quad \alpha_2\beta_1)$$

with κ some arbitrary real number.

4. Consider the rotation group in three dimensions. It is nonabelian, connected, doubly connected, and compact. Its dimension is $n = 3$. The three infinitesimal rotations along the three orthogonal axes are a complete system of tangent vectors. They satisfy the commutation rules

$$[A_1, A_2] = i(A_3 + \beta_3 \cdot I),$$
$$[A_2, A_3] = i(A_1 + \beta_1 \cdot I),$$
$$[A_3, A_1] = i(A_2 + \beta_2 \cdot I).$$

Show, by a suitable choice of local factors, that every local factor is equivalent to the factor 0, so that every projective representation of the rotation group is locally equivalent to a vector representation.

REFERENCES

All the essentials of group theory needed for this chapter can be found in a context of physical applications in:

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For the theory of topological groups, the standard reference is

3. L. PONTRYAGIN, *Topological Groups*. Princeton: Princeton University Press (1958).

The fundamental theorem of projective geometry which is used here is found for instance in:

4. E. ARTIN, *Geometric Algebra*. New York: Academic Press (1957); Theorem 2.26, p. 88.

Wigner's theorem has been proved many times by different methods; see the following:

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A complete list and critical evaluation of all the references (up to 1963) concerning Wigner's theorem are found in:

8. U. UHLHORN, *Arkiv Fysik* **23**, 307 (1963).
9. V. BARGMANN, *Ann. of Math.* **59**, 1 (1952).

CHAPTER 10

THE DYNAMICAL STRUCTURE

The objective world simply is, it does not happen. Only to the gaze of my consciousness, crawling up along the life-line of my body, does a section of this world come to life as a fleeting image in space which continually changes in time.

H. WEYL

The dynamical structure of a physical system contains the law which governs the time evolution of the states (Section 10-1). For the conservative system this law is a homomorphism of the additive group of real numbers into the automorphisms of a proposition system. The application of results from previous chapters readily permits us to derive, without any further assumptions, the Schrödinger equation (Section 10-2) which we cast into the different but equivalent forms corresponding to the Schrödinger, Heisenberg, and Dirac pictures (Section 10-3). The last section (10-4) contains some remarks concerning the dynamical law for nonconservative systems.

10-1. THE TIME EVOLUTION OF A SYSTEM

Until now we have considered merely the kinematic aspect of quantum physical systems. This aspect refers to properties which can be measured at one particular instant of time. We have so far completely ignored the time evolution of the state of a system. This time evolution contains the *dynamical aspects* of the system.

It is perhaps not superfluous to point out that the reference to the properties at "one instant of time" is an abstraction which can never be completely satisfied for real observations or real physical systems. All measurements *take time*; some measurements may even take a very long time. For such measurements the notion of the "state at a given instant" or similar notions (which refer to a certain definite value of time) may become very difficult to define. In such cases the practical distinction between the kinematic and dynamical aspects of the system may be obscured. Nevertheless this distinction can be maintained as an idealization.

A second difficulty in the application of this notion is encountered in relativistic quantum mechanics where it is not possible to give an absolute meaning to the notion of simultaneity of distant events. This is one of the difficulties of a relativistic quantum mechanics for nontrivial systems, and it can only be dealt with within the framework of a field theory where time is a local parameter and not an overall variable as in the nonrelativistic case. This is one of the reasons why we are forced to restrict our discussion to nonrelativistic physical systems.

The dynamical property of a physical system expresses itself as a transformation of the state at some time $t = 0$ to the state at some other time $t \neq 0$. What can we say about the nature of this transformation?

In the classical mechanics of conservative systems, the state evolves in accordance with the solution of some first-order differential equation in the canonical variables. For such systems, the state at one instant of time determines the state at any other instant. It is not unreasonable to assume a similar behavior for quantum mechanical systems, modified only with respect to the quantum mechanical meaning of "state" as given in Section 6-1.

We expect, then, that any given state $p = p_0$ at time $t = 0$ will uniquely determine another state p_t at time $t \neq 0$, and that the transformation $p \to p_t$ is continuous in the topology induced by the states.

We shall speak of conservative systems if the transformation $p \to p_t$ does not depend on the value of the initial time (which we have here chosen to be $t = 0$). For such systems we may say more explicitly: The correspondence $p_t \to p_{t+\tau}$ depends only on τ and not on t.

This general property does not yet sufficiently determine the character of the time evolution of quantum systems. Just as a continuous curve in phase space is a much more general object than the solution of a differential equation, so it is with the time evolution of states in quantum systems: Continuity alone gives very little information as to the character of the transformation $p \to p_t$.

We therefore supplement continuity with a very important and far-reaching further assumption: The time evolution of a physical system is induced by a symmetry transformation of the proposition system.

Let us discuss what this assumption means from the physical point of view. If time evolution is a symmetry transformation, then the physical structure of the proposition system is indistinguishable at two different values of the time. This expresses the homogeneity of time. For isolated systems this property is equivalent to the existence of immutable dynamical laws. With such systems it is not possible to determine, by physical measurements, an absolute value of the time; only time differences are accessible to measurements. Whether there are systems which are, in this sense, homogeneous in time is of course a matter of experience, and it is indeed one of the fundamental experiences about the physical world that this is the case.

These considerations lead us therefore to the following formulation of the basic dynamical law for a conservative quantum system:

The evolution $p \to p_t$ of the state is induced by a continuous symmetry transformation of the lattice of propositions. This means that there exists an automorphism $a \to a^t$ of the lattice $\mathscr{L}$ of propositions, such that

$$p_t(a^t) = p(a).$$

Moreover, this automorphism is a continuous function of the parameter t.

We should emphasize here that this specification of the time evolution is certainly correct for a certain class of systems, those which correspond classically to the conservative systems; but it need not be true for *all* systems. Indeed, systems which during their evolution are subject to external influences may deviate from the behavior of conservative systems in two important respects: They may evolve in a manner which depends on the *absolute value* of the time, and their evolution may not necessarily be induced by a *symmetry transformation* of the proposition system. The second of these modifications has hardly been considered; yet it is possible to give quite elementary examples where this behavior must certainly occur (cf. Section 11-9). It is expected to occur always when the quantal nature of the external interacting system is not negligible.

We shall here be primarily concerned with the behavior of conservative systems which comprise a very large and important class. For such systems the description can be made much more specific.

10-2. THE DYNAMICAL GROUP

We shall now assume that we are dealing with a conservative system described by a proposition system which can be represented as the subspaces in a Hilbert space. The time evolution of such a system is described by a continuous homomorphism of the one-parameter group of the real numbers into the automorphisms of the proposition system. According to the discussion in the preceding chapter, such a homomorphism can be induced by a unitary vector transformation of Hilbert space which maps the real line continuously into a one-parameter group of unitary operators U_t $(-\infty < t < +\infty)$:

$$U_{t_1} U_{t_2} = U_{t_1 + t_2} \qquad \text{and} \qquad U_t^* = U_{-t}, \tag{10–1}$$

and $(\varphi, U_t\psi)$ is a continuous function of the real variable t. Under this group, observables, and in particular projections, transform according to

$$A \to U_t A U_t^{-1}. \tag{10–2}$$

The transformed state p_t is then defined by

$$p_t(U_t A U_t^{-1}) = p(A). \tag{10–3}$$

In Hilbert space this becomes

$$\mathrm{Tr}\,(W_t U_t A U_t^{-1}) = \mathrm{Tr}\,(WA). \tag{10–4}$$

Since this relation must be true for all A, in particular for all projections, we obtain, by using the cyclic invariance of the trace,

$$W_t = U_t W U_t^{-1}. \tag{10–5}$$

In particular if the state is pure and if it is represented by a state vector ψ in the range of W, then the time evolution $\psi \to \psi_t$ of the state is given by the unitary transformation

$$\psi_t = U_t \psi. \tag{10–6}$$

We call the particular homomorphism $t \to U_t$ the *dynamical group* of the system. The dynamical group is thus more than a mere abstract group. As an abstract group, it would merely be the additive group of real numbers. As a homomorphism it is a particular one-parameter family of unitary transformations of Hilbert space. We can further characterize the dynamical group by expressing it in infinitesimal form: The linear manifold of vectors $\psi \in \mathscr{H}$ for which

$$i \lim_{t \to 0} \frac{1}{t} (U_t - I)\psi = H\psi \tag{10–7}$$

exists is the domain of a self-adjoint linear operator H defined by the operation on the left-hand side of Eq. (10–7) (cf. Problem 1). The operator H is called the evolution operator or *Hamiltonian* of the system. With this operator we may write, according to Stone's theorem, $U_t = e^{-iHt}$.

Equation (10–5) can now be written in infinitesimal form by formal expansion of $U_t = e^{-iHt}$. In this way we obtain

$$i \frac{dW_t}{dt} = [H, W_t] \equiv HW_t - W_t H. \tag{10–5$'$}$$

Similarly, we obtain for Eq. (10–6),

$$i \frac{d\psi_t}{dt} = H\psi_t. \tag{10–6$'$}$$

This is called the *Schrödinger equation* of the system.

The two descriptions are completely equivalent. The connecting link is furnished by the spectral measure associated with the self-adjoint operator H. Indeed, if we know this spectral measure, then we can attain the finite form through the formula

$$U_t = \int_{-\infty}^{+\infty} e^{-i\lambda t}\, dE_\lambda,$$

where E_λ is the uniquely determined spectral family of the operator H (cf. Section 4-4). It is evident from this that the spectral measure of the Hamiltonian contains the dynamical structure of the system.

PROBLEMS

1. The operator
$$i \lim_{t \to 0} \frac{1}{t} (U_t - I)\psi$$
is defined on a dense linear manifold and there defines a self-adjoint linear operator.
2. If H commutes with a state W, then W is constant in time.
3. A pure state which is stationary is necessarily an eigenstate of the operator H.
4. If H has only continuous spectrum, then there does not exist a stationary state.

10-3. DIFFERENT DESCRIPTIONS OF THE TIME EVOLUTION

In the practical calculations of the evolution of the states of a system, it is often convenient to have different but equivalent descriptions of this process. If we choose the description corresponding to Eqs. (10–5) and (10–6), we say that we are using the *Schrödinger picture.*

Another description, called the *Heisenberg picture*, is obtained if we retain the states *fixed* but instead change the *observables* in such a way that all expectation values are identical with the expectation values calculated in the Schrödinger picture. Thus we introduce new time-dependent operators A_t representing observables, and determined in such a way that

$$\mathrm{Tr}\,(W_t A) = \mathrm{Tr}\,(W A_t). \qquad (10\text{–}4)'$$

If we substitute the expression (10–5) for W_t and use the fact that the relation (10–4)′ must be an identity, valid for any observable, we obtain

$$A_t = U_t^{-1} A U_t. \qquad (10\text{–}8)$$

This is the time dependence of an observable in the Heisenberg picture. The states W, and consequently also the state vectors ψ, are then independent of time.

In many practical calculations a third description is even more important than either of the two preceding ones. This description is in a sense intermediate between the two, where part of the time evolution appears as a change of the state, and another part as a change of the observables. Let us assume that the Hamiltonian for the system is a sum of two terms $H = H_0 + V$, and let us define the evolution operators corresponding to H_0 and to H by setting

$$U_t = e^{iH_0 t}, \qquad V_t = e^{iHt}. \qquad (10\text{–}9)$$

Table 10-1

THE THREE PICTURES FOR THE TIME EVOLUTION OF A CONSERVATIVE PHYSICAL SYSTEM. NOTATIONS:

$$U_t = e^{-iH_0t},\ V_t = e^{-iHt},\ V = H - H_0,\ V(t) = U_t^{-1}VU_t$$

	Differential forms			Integrated forms		
	State-vectors	Density operators	Observables	State-vectors	Density operators	Observables
Schrödinger picture	$i\dot{\psi} = H\psi$	$i\dot{W} = [H, W]$	$\dot{A} = 0$	$\psi_t = V_t\psi$	$W_t = V_tWV_t^{-1}$	A
Heisenberg picture	$\dot{\psi} = 0$	$\dot{W} = 0$	$i\dot{A} = [A, H]$	ψ	W	$A_t = V_t^{-1}AV_t$
Dirac picture	$i\dot{\psi} = V(t)\psi$	$i\dot{W} = [V(t), W]$	$i\dot{A} = [A, H_0]$	$\psi(t) = U_t^{-1}V_t\psi$	$W(t) = U_t^{-1}V_tWV_t^{-1}U_t$	$A(t) = U_t^{-1}AU_t$

Let us then introduce a time-dependence of an observable

$$A(t) = U_t^{-1} A U_t. \tag{10–10}$$

This formula is identical with (10–8), but it has a different meaning because the operator U_t is the evolution operator corresponding to the Hamiltonian H_0. We can now determine the time dependence of the state $W(t)$ such that

$$\mathrm{Tr}\,(W(t)A(t)) = \mathrm{Tr}\,(W_t A). \tag{10–11}$$

A short calculation then gives the result

$$W(t) = U_t^{-1} V_t W V_t^{-1} U_t. \tag{10–12}$$

We shall refer to this description as the *Dirac picture.* In much of the current literature it is also called the *interaction picture.*

We can also express the different pictures in the infinitesimal forms. For instance, the time dependence of an observable in the Heisenberg picture satisfies a differential equation given by

$$i \frac{dA_t}{dt} = [A_t, H], \tag{10–13}$$

while the density operator is of course constant and thus satisfies $(dW_t/dt) = 0$. Similarly, we find for the Dirac picture

$$i \frac{dA(t)}{dt} = [A(t), H_0] \tag{10–14}$$

and

$$i \frac{dW(t)}{dt} = [V(t), W], \tag{10–15}$$

where $V(t) = U_t^{-1} V U_t$ is the interaction operator in the Dirac picture.

A pure state represented in the Dirac picture is then a solution of the differential equation

$$i\dot{\psi}(t) = V(t)\psi(t), \tag{10–16}$$

and such a solution can be given in the form

$$\psi(t) = U_t^{-1} V_t \psi. \tag{10–17}$$

The different forms are collected for convenience in Table 10-1.

10-4. NONCONSERVATIVE SYSTEMS

The conservative systems which we have described so far are systems which interact with the external world through constant forces and which do not react back on this world at all. Examples of such systems which we shall

study in greater detail later on are, for instance, a particle in a constant external field of force or a spin carrying a magnetic moment in an external magnetic field. The effect of the external forces is then entirely incorporated in the nature of the Hamiltonian which expresses the dynamical law of the system.

We must bear in mind that such systems are always some sort of approximation, whether because the external forces are not constant, or because there *is* some reaction of the system back to the external world. In many situations the approximation is a very good one indeed, and we need not concern ourselves with these limitations at all. The theory for conservative systems is then fully applicable and gives excellent results. But there are also situations of great physical interest where the approximation for conservative systems is no longer applicable. We can imagine two causes for a breakdown of this approximation. One may be due to a time variation of the external forces which act on the system; the other may be due to the reaction of the system back to the external world.

These situations are of course well known from classical mechanics. There it is often possible to reduce a nonconservative system to a conservative one by enlarging the system so that it contains not only the original system but also the *source* of the external force. But in many situations this procedure is not practicable, and it is then desirable to have a generalization of the dynamical law for nonconservative systems. This same need exists in dealing with quantum-mechanical systems. But in such systems the situation is even more complicated because of the following circumstance: If two classical systems interact and both of them are, at the beginning of the interaction, in a pure state, then after the end of the interaction each separate component is still in a pure state. If the same problem is considered for quantum systems, one finds that after the interaction the component systems are, in general, in a mixture, even if before the interaction they were in a pure state. This is a property of quantum systems which is of fundamental importance in the theory of measurement. We shall discuss this in great detail in the next chapter.

In this section we shall concentrate instead on the modifications needed when we are dealing with time-dependent external forces, and we can still neglect the reaction of the system back to the source of the forces.

We could describe such a system by saying that its dynamical law changes from one moment to the next so that it is still expressible in a differential form, but with a Hamiltonian $H(t)$ which depends explicitly on time. Thus, instead of Eq. (10–5)′ describing the evolution of a state, we would expect an equation

$$i\frac{dW_t}{dt} = [H(t), W_t]; \tag{10–18}$$

and similarly, instead of (10–6)′, we should have

$$i\frac{d\psi_t}{dt} = H(t)\psi_t. \tag{10–19}$$

For such systems it is no longer possible to give a simple expression for the integrated form of the dynamical law, although states at different times are still connected by unitary transformations which depend on time but which no longer have the group property. Thus while we can still write $\psi_t = U_t\psi$, we must admit that $U_{t_1}U_{t_2} \neq U_{t_1+t_2}$.

There does not yet exist a general integration theory for the solutions of Eq. (10–18) or Eq. (10–19), and it is only possible to discuss individual cases or approximation methods.

CHAPTER 11

THE MEASURING PROCESS

That things have a quality in themselves quite apart from interpretation and subjectivity, is an idle hypothesis: It would presuppose that to interpret and to be a subject are not essential, that a thing detached from all relations is still a thing.

F. NIETZSCHE,
in *The Will to Power*

In this chapter we give an analysis of the process of measurement. The characteristic limitations of the accuracy of measurements in the form of the uncertainty relations (Section 11–1) is traced to the interaction of the measuring device and the system (Sections 11-2 and 11-3). In order to analyze this effect we describe the characteristic properties of a measuring device in Section 11-4. The following sections, 11-5 and 11-6, introduce the notation of equivalent states, events, and data. In a mathematical interlude we sketch the theory of the tensor product (Section 11-7), followed by Section 11-8 on the union and separation of system. All the tools are then on hand to analyze in detail the measuring process on a particular and simple model (Section 11-9). In the last section, 11-10, we describe three paradoxes of the measuring process.

11-1. UNCERTAINTY RELATIONS

The deeper understanding of quantum phenomena began with the discovery of the uncertainty relations [1]. From the earliest beginnings in the discussion of the uncertainty relations, it was recognized that the analysis of these relations, which restrict the precision of measurement, must be somehow related to the inevitable interaction between measuring device and the system during the process of measurement.

In our formulation of quantum mechanics, the actual behavior of a physical system under the process of measurement is already incorporated in the empirically given structure of the proposition system. It is therefore not surprising that the uncertainty relations appear, at this stage of our presen-

tation, as a purely mathematical consequence of the properties of observables. In this section we shall demonstrate this.

Let A and B stand for two observables, which need not be compatible. They are represented by self-adjoint operators which need not commute. In order to avoid inessential complications, we shall assume that the two operators are bounded so that their domain of definition is the entire Hilbert space. Let us consider a general state given by the density operator W, and define the expectation values

$$a \equiv \text{Tr } WA, \qquad b \equiv \text{Tr } WB. \tag{11–1}$$

The mean square deviation of the observable A in the state W is then defined by

$$(\Delta a)^2 \equiv \text{Tr } W(A - a)^2. \tag{11–2}$$

Similarly, we define

$$(\Delta b)^2 \equiv \text{Tr } W(B - b)^2. \tag{11–3}$$

The uncertainty relation is an inequality for the product of Δa with Δb. We write $A_0 = A - a$ and $B_0 = B - b$. Then we have, by definition,

$$\text{Tr } WA_0 = \text{Tr } WB_0 = 0.$$

In order to obtain such an inequality we consider the operator $T \equiv A_0 + i\rho B_0$, with ρ real. Since A and B are self-adjoint and bounded, $T^* = A_0 - i\rho B_0$. It follows from this that $\text{Tr } WTT^* = \text{Tr } T^*WT > 0$ for all values of ρ. In order to see this, it suffices to recall that the trace of any operator X, if it exists, can be calculated with the formula

$$\text{Tr } X = \sum_r (\varphi_r, X\varphi_r)$$

for some arbitrary, complete, orthonormal system of vectors φ_r. Thus

$$\text{Tr } T^*WT = \sum_r (\varphi_r, T^*WT\varphi_r) = \sum_r (T\varphi_r, WT\varphi_r).$$

Let $\psi_r = T\varphi_r$; then we have finally

$$\text{Tr } T^*WT = \sum_r (\psi_r, W\psi_r). \tag{11–4}$$

The system ψ_r is in general neither complete nor orthogonal, but this does not matter. What does matter is that every term $(\psi_r, W\psi_r)$ is positive. Therefore the trace in question is expressed as a sum of positive terms. Thus we have found

$$\text{Tr } WTT^* \equiv \text{Tr } WA_0^2 - i\rho \text{ Tr } W[A_0, B_0] + \rho^2 \text{ Tr } WB_0^2 \geq 0. \tag{11–5}$$

The right-hand side is a quadratic form in ρ which is thus positive definite. This implies that its determinant must be positive, too. Since A_0 and B_0 are both self-adjoint, the operator $[A_0, B_0] = [A, B]$ which occurs in Eq. (11–5) is

antiself-adjoint. We can then define a new self-adjoint operator C by setting $[A, B] = iC$. We obtain the real quadratic form

$$(\Delta a)^2 + \rho \operatorname{Tr} WC + \rho^2(\Delta b)^2 \geq 0.$$

The positive definiteness of this quadratic expression in ρ implies that

$$(\Delta a)^2(\Delta b)^2 \geq \tfrac{1}{4}(\operatorname{Tr} WC)^2, \tag{11–6}$$

or, after taking square roots,

$$(\Delta a)(\Delta b) \geq \tfrac{1}{2}|\operatorname{Tr} WC|. \tag{11–7}$$

This is the general uncertainty relation. It gives a limitation on the value of the product of the root-mean-square deviation for any two observables. In the event that A and B do not commute, then $C \neq 0$, and there exist, in general, states such that the right-hand side is positive (and not zero). In case C is a positive operator (which will be seen to occur in the most important application), then this will occur for any state. In this case we have what we might call an *absolute* uncertainty relation: The two observables in question can *never* be measured with an arbitrary simultaneous accuracy.

The difficulty in the interpretation of the uncertainty relation stems from the fact that A and B might be observables which admit an arbitrarily small mean square deviation for certain states. The uncertainty relation implies, then, that this can never occur for the same state. For such cases the observable A separately, as well as the observable B separately, can be measured with unrestricted accuracy. However, if we desire to measure A and B simultaneously, we find that the two measurements must be disturbing each other in precisely such a way that the uncertainty relation is satisfied. This behavior, which for classical systems is completely unknown, gives rise to the often discussed conjecture whether the actual values of the observables are perhaps determined, but unknown and unknowable because the measuring process interferes with the state of the system.

This point of view is closely related to the possible existence of hidden variables which we have already discussed in Chapter 7. But in this case the hidden aspect of the state would even have a subjective character, depending on the state of information which we have about the system. That this would lead to quite inadmissible consequences can be seen, for instance, by the fact that the state would be different for two different observers who have different information about one and the same system. This would amount to a denial of objectively valid physical laws throughout the world of microsystems, something for which we have at present no evidence, and no need [9].

We shall therefore take the position that the correct interpretation of the uncertainty relation is that an observable in a given state need not have a definite value even though the observable is capable of assuming definite values for other states. The value of an observable may be not only ambi-

guous, it may even be *undetermined*, and this is as much an irreducible attribute of a state as specific values were in classical physics.

We observe here a significant difference between quantum and classical physics. The situation has often been described by saying that in quantum mechanics it is not possible to ignore the reaction of the measuring device on the system. This interaction, so we are told, produces an *uncontrollable effect* on the system, so that the actual values of the observables remain partially hidden from us. Although this discussion of the interaction of the measuring device and system has been most useful in attracting our attention to the fact that we are dealing with physical objects and not with a mathematical model, the introduction of an *uncontrollable* reaction of one on the other has given a misleading impression. It is not an uncontrollable effect which causes the uncertainty relation; on the contrary, the time evolution of the joint system, consisting of measuring device and original system, may be completely controlled and determined by a fixed physical arrangement. It is the laws of quantum mechanics as they are embodied in the structure properties of the proposition system which cause this result.

A complete understanding of these laws can only be obtained by following them through their effects on the measuring process, and this is precisely what we shall do in the following sections.

11-2. GENERAL DESCRIPTION OF THE MEASURING PROCESS

All the information which we have about physical systems is obtained from observations and measurements on such systems. Observations consist in bringing the system under examination in contact with some other system, the observer, or some measuring device M, and observing the reaction of the system on the observer. The general setup of a measurement on a physical system S has thus schematically the form indicated in Fig. 11–1.

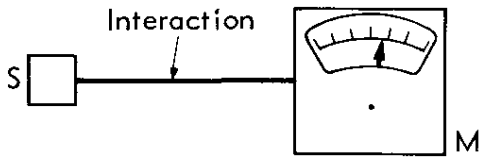

Fig. 11–1 Schematic representation of the interaction between measuring device M and system S.

Let us point out at the outset two important features which we shall encounter throughout the discussion on the quantum-mechanical measuring process. The first of these concerns the fact that the measuring device M, if it is to be of any use at all, must interact somehow with the system S. But an interaction always acts both ways. Not only does S influence M, thereby producing the desired measurable effect, but also M acts on S, producing an effect on S with no particularly desirable consequences. In fact, this back-effect on S seems to be the cause of much of the difficulty in the interpretation of quantum mechanics.

The second point to be mentioned here is that, in a complete measurement, the schematic arrangement of Fig. 11–1 is an oversimplification. If the measurement is to be useful there must be a further observation on M, which we shall call "reading the scale." Such further observations may be made at a later time by examining a permanent record of some sort, but in any case, if they are to be of some use for the construction of a scientific theory they must, at some point, enter the consciousness of a scientific observer.

This appearance of the "conscious observer" in a full description of the measuring process is a disturbing element, since it seems to introduce into the process of reconstructing the objective physical laws a foreign subjective element. It is essential in the construction of an objective science that it be freed from anthropomorphic elements. This requirement of objectivity of the physical science of microobjects can actually be satisfied because of the fact that the last stages of observation which we have designated symbolically as "reading the scale" take place on the classical level. On this level the measuring process also follows the general scheme of Fig. 11–1, with one important difference. The interconnection between S and M acts only in one direction, namely from S to M. The reverse action from M to S, although always present, is not important because its effect can always be reduced to a negligible amount. This is an essential feature of the classical measuring process which distinguishes it fundamentally from the quantum mechanical measuring process, where this reaction is not negligible.

The insensitivity of the system with respect to its observation when "reading the scale" has the consequence that all the data furnished by a macroscopic measuring device have an objective meaning. By this we mean that the "scale can be read" by a number of different observers who can communicate and establish that they read concurrent results. The physical fact is "objectivized," as we might say. The individual observer, although necessary for completing an actual observation, can now fade into the background; and we retain only the objectively verifiable content of the observation. These are the building bricks of man's theory of the physical world.

The situation which we encounter here is very similar to the description of a physical event in space and time with respect to some coordinate system. Although a coordinate description of such events is usually necessary, their objective character and their spatio-temporal interrelations are objective properties quite independent of the particular choice of such a description.

11-3. DESCRIPTION OF THE MEASURING PROCESS FOR QUANTUM-MECHANICAL SYSTEMS

As we have pointed out in the preceding section, the quantum-mechanical measuring process will affect the system. We shall now examine the effect of this reaction more carefully. Let us begin with two examples.

First we consider the measurement of the position of some elementary particle by a counter with a finite sensitive volume. After the measurement has been performed and the counter has recorded the presence of a particle inside its sensitive volume, we know for certain that the particle, at the instant of the triggering, is actually inside the sensitive volume. By this we mean the following: Suppose we repeated the measurement immediately after it has occurred (this is of course an idealization, since counters are notorious for having a dead time after they are triggered), then we would with *certainty* observe the particle inside the volume of the counter.

In the second example, we consider a momentum measurement with a counter which analyzes the pulse height of a recoil particle. Here the situation is quite different. The experiment will permit us to determine the value of the momentum only *before* the collision occurred. If we repeat the measurement immediately after it has occurred, then we find that the momentum of the particle will have a quite different value from its measured value. The very act of measurement has changed the momentum, and it is this change which produced the observable effect.

We shall call a measurement which will give the same value when immediately repeated a measurement of the *first kind.* The second example is then a measurement of the *second kind* [3].

From now on we shall be primarily concerned with measurements of the first kind. They are easier to discuss, yet they exhibit the characteristic quantum features which we want to explore here.

Measurements of the first kind can be used for *preparing* a state with definite values for certain observables. If they are used in this way we speak of *filters.* For the preparation of such a state, the condition imposed by the measuring device becomes a *relevant* condition in the preparation of the state (cf. Section 6-1). The states before and after the measurement are not the same, even if the duration of the measurement can be considered negligible. The change in the state must be attributed to the interaction of the system with the measuring device.

We shall now obtain a formula for the change of the state by a measurement of the first kind. Let us begin with a simple special case where the observable to be measured is represented by a self-adjoint operator A with nondegenerate eigenvalues. Let ψ_r be the eigenvectors of A, and denote by P_r the projection which contains ψ_r in its range. The operator A may then be represented in the form

$$A = \sum a_r P_r, \tag{11–8}$$

where a_r denotes the eigenvalues of A.

A measurement of the quantity A in a system in the state W will give the result a_r with a probability which is given by

$$p(P_r) = \operatorname{Tr} W P_r. \tag{11–9}$$

If the measurement is of the first kind, then the repetition of a measurement which yielded the value a_r will reproduce this value with certainty. If the measurement is not used as a filter—that is, if it is not used to select a certain subensemble of systems which have definite values for A—then the state of the system after the measurement will be a mixture of the pure states ψ_r with probabilities as expressed by Eq. (11–9).

The density operator for this mixture is given by

$$W' = \sum_r P_r W P_r. \tag{11–10}$$

To see this we verify that for projections P with one-dimensional range we have

$$PWP = (\mathrm{Tr}\, WP)P.$$

Let ψ by a unit vector in the range of P, and let f be an arbitrary vector. We have then, by definition of the projection operator P,

$$PWPf = (\psi, W\psi)(\psi, f)\psi = (\psi, W\psi)Pf.$$

Thus it suffices to show that

$$(\psi, W\psi) = \mathrm{Tr}\, WP.$$

This can be verified by evaluating the trace in a special orthonormal system ψ_r, which is so chosen that its first vector $\psi_1 = \psi$. We have then, because P has one-dimensional range, $P\psi_r = 0$ for all $r \neq 1$. Thus the infinite sum in the evaluation of the trace reduces to one single term, the term on the left-hand side of the last equation. With this we have established formula (11–10) for the case that the ranges of all P_r are one-dimensional.

If the eigenvalues a_r of the observable A are degenerate, then the state of the system referring to a subspace associated with an a_r depends on the detailed nature of the measuring equipment. The degeneracy leaves us with a certain freedom of choice for the state after the measurement, which cannot be removed without a detailed knowledge of the actual measuring equipment used. In such cases the measurement of one and the same observable with *different equipment* may result in different states after the interaction.

It is therefore convenient to introduce the notion of the *ideal measurement* which affects the state in a minimal way, and for which the state after the measurement is still given by formula (11–10) but without the requirement that the projection operators P_r be one-dimensional.

For the special case of the ideal measurement of a projection operator E, we shall then obtain for the state after measurement the density operator

$$W' = EWE + E'WE', \tag{11–11}$$

where $E' = I - E$ and W is the density operator before the measurement. If the projection operator E is used to describe a filter, then we shall call it a

passive filter if after the filter process the state is given by

$$W' = \frac{1}{\operatorname{Tr} WE} EWE. \tag{11–12}$$

This state is obtained if we prepare the state W, and add to the conditions which prepare this state the further relevant condition that the measurement of the property represented by E must be true.

When we examine the change of the state as expressed, for instance, in Eq. (11–11), we observe an important point. This change is quite different from the change of the state due to the time-evolution of a system, which is expressed by a formula such as

$$W_t = e^{-iHt} W e^{iHt}, \tag{11–13}$$

with some Hamiltonian operator H. The fundamental character of the difference between (11–11) and (11–13) can be seen by the fact that the transformation $W \to W_t$ is unitary, while $W \to W'$ usually is not. For instance, if the state W is pure and E does not commute with W, then W' is always a mixture (cf. Problem 1).

There is one special case when the observation of a property E does not affect the state, namely, when E commutes with W. If E commutes with W, we may in fact write $EWE = WE$ and $E'WE' = WE'$; therefore $W' = EWE + E'WE' = WE + WE' = W(E + E') = W$. This condition is also necessary. Indeed, if $W' = W$, then $WE = W'E \overset{\vee}{=} EWE \overset{\vee}{=} EW' = EW$. Thus we have established:

> *The necessary and sufficient condition such that an ideal measurement of a proposition represented by the projection operator E does not* disturb *a state W is that E commute with W.*

The measurements which do not disturb the state are thus very special cases; in general we must expect a change which leads to a density operator W' which is not unitarily equivalent to the operator W.

This behavior of the state under measurement is at first sight very strange, because in Chapter 10 we derived the unitary transformation of states under very general conditions. Even if the system is subject to variable external forces, we must expect such a unitary transformation of the change. It seems as if the unity of the description of the physical laws is broken at this point: If we have the system under its own influence the state changes in one way, given by (11–13); if we observe or measure something on the state, the state changes in another entirely different way, given by (11–11).

We might suppose this difference to be due to the interaction of the system S with the measuring device M. The difficulty with this explanation is that one is always at liberty to consider the time evolution of the combined system, consisting of S and M. This combined system, if left undisturbed by outside

influences, then evolves in time according to Eq. (11–13) where the operator H is now the total Hamiltonian of the combined system. That such an operator must exist follows from the fact that the combined system $S + M$ is also subject to the laws of quantum mechanics, even if it is, as in most practical cases, a very complicated system. The complication should not detract us from the essence of the question, namely, how to reconcile the two different behaviors of the state vectors without violating the unity of the laws of nature.

We shall analyze and answer this question in the subsequent sections of this chapter.

PROBLEMS

1. If W is pure and E is a projection which does not commute with W, then $W' = EWE + E'WE'$ is a mixture.
2. A repetition of a measurement E on a state W will not disturb the state W' obtained after the first measurement of E.

11-4. PROPERTIES OF THE MEASURING DEVICE

The general description of the measuring process that we have given in the preceding section did not specify the nature of the measuring device M. This we shall do now.

It is clear that not every system M will be suitable as a measuring apparatus. In order to fulfill its function of determining the measurable physical properties of the system S, it must satisfy certain conditions which we shall formulate now.

If we examine any measuring apparatus M commonly used for the measurements of quantum systems S, then we observe at once a common feature: Every measuring device is usually a large system, producing macroscopic effects which can be observed or recorded with equipment for which the quantum effects are completely irrelevant. For instance, if our apparatus M is a counter of some sort, it will contain a large number of molecules in an unstable state which can be triggered by the micro-event to be measured. The triggering then produces a chain reaction which may lead, for instance, to a potential drop on a capacitor, and eventually recorded in some mechanical counter. The resulting large-scale effect in the last stage of the measurement can then be read off by any observer without interfering in the least with the state of the apparatus. The final stage of the observation can therefore be described completely in classical terms alone.

This last remark is very important, and it has played an essential part in the analysis of the measuring process given, for instance, by Bohr [8]. It is

this classical aspect of the measuring device which enables us to establish the objective aspects of the state of a system, and it is from such objectively given ingredients that the physical laws governing the microsystems must be reconstructed.

Thus we must assume that measuring devices are usually constructed out of macroscopic parts which can be adequately described by classical laws; yet this device must be sensitive to the quantum features of the system S. This is often accomplished by the use of metastable systems which can be triggered by micro-events, which subsequently are amplified to macro-events. A typical example is the bubble chamber using a superheated liquid as the metastable macrosystem. A single micro-event in the form of the ionization of an atom may be sufficient to trigger the sequence of events which lead to the formation of a bubble.

The classical aspect of the measuring device which we have stressed here is usually associated with its macroscopic features. We must, however, be on guard not to confuse the two. To be sure, most macroscopic objects—that is, objects which consist of a very large number of microsystems—do, in most situations, behave according to the classical laws of physics. But this is not necessarily so. There are macro-objects which exhibit quantal features, and there are micro-objects which, for certain types of observations, behave classically. The part of the measuring system which amplifies the triggered event to a macroscopic phenomenon is therefore a convenient device which enables us to observe and register this event, but it is not absolutely indispensable for the completion of a measurement. This means that the characteristic difficulties in understanding the measuring process are not to be attributed to the inevitable complication of an amplifying device; they are already present in the microscopic part of the measuring equipment.

In order to make this explicit, it is convenient to divide the measuring device M into two parts, $M = m + A$. Here m denotes the "little" measuring device, that is, that part which is truly responsible for the measurement of the system M; and A represents the *amplifying* part of M. Part A may be disconnected in thought or sometimes in reality from the little measuring device, without impairing the essential part of the measuring process.

For instance, if our measuring equipment is the photographic plate, the little measuring device m may be a single silver-halide complex, while the amplifying device A may be an individual grain, containing a large number of atoms. The record of an event may be triggered by a single ionization process and stored as a latent image long before the amplification A in the form of the development of the plate is put into effect.

The system $S + m$ which really performs the measurement must satisfy further restrictions. The function of the measurement consists in transferring certain properties of the system S to the system m, in such a way that a mere observation on the system m (by means of the amplifier A) will permit us to

draw certain conclusions as to the state of the system S. There must therefore exist a correlation between the events on M and the states of S. The measuring device can then distinguish states of S which are correlated with observable events in M.

In a measurement of the first kind, we have the additional requirement that a repetition of the measurement immediately after it has occurred will reproduce the same result. This means that the system S is left after the measurement in the state registered by M.

We have now listed the essential properties which we must require of the measuring device for a measurement of the first kind.

11-5. EQUIVALENT STATES

In this section we shall now examine in detail the modification in the description of states which results from a restricted system of observables. In the preceding section we have pointed out that the observables which are measured by a measuring device must be of a classical nature in order that the measurement have an objective character. This means that one and the same device M can, in general, measure only a restricted class of observables, all of which must commute with one another. This has the consequence that certain states which may be represented by different density operators may actually be indistinguishable with respect to this system of observables.

The natural way of describing this situation is by introducing a theory of equivalence classes of states. We shall first do this quite generally, without the requirement that we are dealing with classical observables, and shall specialize later for classical observables.

Let $\mathscr{S}$ be a system of observables. We say that two states W_1 and W_2 are *equivalent* with respect to $\mathscr{S}$ if

$$\operatorname{Tr} AW_1 = \operatorname{Tr} AW_2 \tag{11–14}$$

for all $A \in \mathscr{S}$. We shall write for two states equivalent with respect to $\mathscr{S}$: $W_1 \sim W_2(\mathscr{S})$. If two states are equivalent in this sense, then no measurement with observables from $\mathscr{S}$ can distinguish the two states. It is not difficult to show (Problem 1) that $W_1 \sim W_2$ is an equivalence relation. We can therefore divide the set of all states into classes of equivalent states.

From the physical point of view, the selection of an individual representative inside a class of equivalent states is irrelevant; any choice will be equally good. It is therefore quite natural to consider the states with respect to a system $\mathscr{S}$ not as one of the members of the class but as the classes themselves. By this procedure we remove the redundancy in the description of the state, and we restore the one-to-one correspondence between the physical notion of state and its mathematical description.

Let us denote by $[W]$ the class of the states which are all equivalent to W. We shall call the redundant states W the *microstates* and the classes of equivalent states $[W]$ the *macrostates.*

The operation of the mixture of states can be transferred from the microstates to the macrostates. This means we claim the property expressed in the formula

$$[\lambda_1 W_1 + \lambda_2 W_2] = \lambda_1 [W_1] + \lambda_2 [W_2]. \tag{11-15}$$

This formula implies the following:

$$W_1 \sim W_1' \qquad \text{and} \qquad W_2 \sim W_2'$$

and if

$$W = \lambda_1 W_1 + \lambda_2 W_2, \qquad W' = \lambda_1 W_1' + \lambda_2 W_2',$$

then $W \sim W'$. Due to this property it is possible to transfer the process of mixing from the microstates to the macrostates, as we have indicated with the notation of the right-hand side of (11–15).

In order to prove this property, we mention that it is sufficient to verify it for the projections contained in $\mathscr{S}$. Let $\mathscr{S}_P$ denote the projections in $\mathscr{S}$. We want to show that

$$\operatorname{Tr} EW = \operatorname{Tr} EW' \qquad \text{for all } E \in \mathscr{S}_P.$$

This we see by using the linearity property of the trace through the following sequence of steps:

$$\begin{aligned} \operatorname{Tr} EW &= \operatorname{Tr} E(\lambda_1 W_1 + \lambda_2 W_2) \\ &= \lambda_1 \operatorname{Tr} EW_1 + \lambda_2 \operatorname{Tr} EW_2 \\ &= \lambda_1 \operatorname{Tr} EW_1' + \lambda_2 \operatorname{Tr} EW_2' \\ &= \operatorname{Tr} E(\lambda_1 W_1' + \lambda_2 W_2') = \operatorname{Tr} EW'. \end{aligned}$$

In the third step we have made use of the fact that $W_1 \sim W_1'$ and $W_2 \sim W_2'(\mathscr{S})$. Thus the property is verified.

We shall have occasion to use a corollary which states that if $W_1 \sim W_2$, then any mixture $W = \lambda_1 W_1 + \lambda_2 W_2$ is in the same equivalence class $[W_1] = [W_2]$. The equivalence classes are thus closed against the operation of mixing. This implies that every class which contains more than one microstate contains mixtures.

An important question which will concern us now is this: What happens to the macrostates during a measurement? We know what happens to microstates. If, for instance, the state is W before the measurement, then after the measurement of E it is

$$W^E \equiv EWE + E'WE', \tag{11-16}$$

where we have written $E' = I - E$.

Let $[W]$ be the class which contains W and $[W^E]$ the class which contains W^E. We shall now determine under what condition the class $[W^E]$ is independent of the representative W in the class $[W]$. Thus we choose two members $W_1, W_2 \in [W]$ from the same class, so that $W_1 \sim W_2$. The condition that $W_1^E \sim W_2^E$ is that for any $F \in \mathscr{S}_P$ we have

$$\operatorname{Tr} F(EW_1E + E'W_1E') = \operatorname{Tr} F(EW_2E + E'W_2E').$$

By using the invariance property of the trace under cyclic permutations of the operators, we can change this into

$$\operatorname{Tr} (EFE + E'FE')W_1 = \operatorname{Tr} (EFE + E'FE')W_2.$$

This must be true for all projection operators $F \in \mathscr{S}_P$. This is true for all equivalent pairs W_1, W_2 if and only if

$$F^E \equiv EFE + E'FE' \in \mathscr{S}. \tag{11–17}$$

This, then, is the condition which guarantees that the macrostates are not broken up under the process of measurement.

We shall be particularly interested in the case of an abelian set of observables. In that case $F^E \equiv F$, and so condition (11–17) is always true. When this condition is satisfied we may transfer the process of change under measurements from the micro- to the macrostates and we can write a formula

$$[W^E] = [W]^E$$

where the right-hand side denotes the class which contains the element W^E.

We are now also in a position to answer the question under what condition a state is left invariant under all the measurements. The condition for this is that

$$[W]^E = [W] \qquad \text{or} \qquad W^E \sim W \qquad \text{for all } W \in [W].$$

This means that for all $E \in \mathscr{S}_P$ and all $F \in \mathscr{S}_P$ we must have

$$\operatorname{Tr} FW^E = \operatorname{Tr} FW = \operatorname{Tr} F^E W.$$

A sufficient condition for this to hold is

$$F^E \equiv EFE + E'FE' = F \tag{11–18}$$

for all $E, F \in \mathscr{S}_P$. If we require invariance for every state, then this condition is also necessary (Problem 2).

Since invariance of the states under measurements is a property of idealized classical systems, we shall call a state which is invariant under all measurements a *classical state*.

For a classical system the relation (11–18) is always satisfied since E and F commute. It follows that in a classical system every state is a classical state.

PROBLEMS

1. The relation $W_1 \sim W_2(\mathscr{S})$ is an equivalence relation.
2. If $\mathrm{Tr}\, AW = \mathrm{Tr}\, BW$ for all states W, then $A = B$.

11-6. EVENTS AND DATA

One of the chief difficulties in the epistemology of quantum mechanics is its apparent inadequacy for describing events. The fact that there are systems which do not admit dispersion-free states leads to the inevitable and irreducible probability statements regarding the occurrence of certain events. Such events may be the measurements associated with yes–no experiments, and as such they may be macroscopic phenomena. The individual occurence of such phenomena is then completely outside the scope of the theory; only the probabilities for such events can be accounted for in our description of the state.

In order to understand this problem better we may compare it with the classical situation. The occurrence of probability statements in the description of states is not unknown in classical mechanics. Most systems, with a large number of degrees of freedom, are much better described with states which are not dispersion-free.

To illustrate this, suppose we want to describe the state of a thrown die before it is examined to learn what number it shows. Such a system is in a state determined by the conditions of the throw, but this state can only be described by a probability function as to the occurrence on top of one of the six sides. The initial condition or preparation which determined this state could be described by a rule such as: Throw die in the air not higher than so and so, and let it come to rest on the table.

From our experience with classical objects such as dice, we know that this description results in a probability statement for the outcome of the throw merely because it is not precise enough. We know from experience with similar systems that the specification of the preparation (throwing a die) can be made more precise, enough so as to determine the outcome of the throw with certainty. It is possible to add other relevant conditions to the prescription for preparing the state. For instance, we might specify the exact position, direction of throw, air currents in the vicinity, angular momentum, and many other variables, to such a degree of precision that the result of the throw will always be the same under the same conditions and we can predict it with certainty. In this case the state has no dispersion any more.

If we examine this question for quantum systems, then we find that it is not always possible to add conditions which permit the preparation of states without dispersion. Adding further conditions may indeed change the state but it will not make it dispersion-free.

The classical states show dispersion not because of any intrinsic occurrence of probabilities, but because the prescriptions for preparing the states already involve probabilities. This gives us justification for considering the probabilities as expressions of our ignorance of the finer features of the state. We do not have any doubt that a die, when it has come to rest, does indeed show one of the numbers before we look at it; the final act of observation does not produce this number—it merely uncovers a fact which has already occurred.

It is convenient to have a special technical terminology for the description of such facts to which we want to ascribe reality before they are observed. We shall call them *events*. The important property of events is that they represent objectively given phenomena capable of being determined by observations which in no way interfere with the state of the system. When an event has been observed we call it a *datum*.

While in classical mechanics every physical property which, after an observation, is found to be true, may be called an event (because we can always arrange it so that such an observation does not affect the state), the situation is more complex in quantum mechanics. It was pointed out by Einstein that we may have events in quantum mechanics, too [8]. Einstein used the term "element of reality" for the description of properties which we have called events. There are, however, also properties which do not have this element of reality and which cannot be called events. It is of the utmost importance in the analysis of the measuring process to be able to distinguish between the two kinds of properties.

Let W be a state and E a projection representing a yes–no experiment. The property E is an event if and only if the measurement of E does not affect the state W. We have previously shown that this is the case if and only if W commutes with E. We may then affirm that each individual system of an ensemble of identically prepared systems in the state W realizes one or several of the events; which of these events are in fact realized for an individual system is determined in principle by making measurements of all the events E on that individual system. Since none of the measurements change the state, all the results which are obtained pertain to that one system in the unchangeable state W.

A little more delicate is the question concerning events if the system of observables is a restricted class of operators $\mathscr{S}$. As we have seen in the preceding section, the proper description of states in this case consists of the classes of equivalent states, that is, the macrostates. We are then entitled to affirm that a projection E is an event in the state W if $[W^E] \equiv [W]^E = [W]$. Thus the observation E may very well change the states in one and the same class but it does not change the class. This condition is weaker than the one we had for microstates. W need not commute with E; it is only necessary that it leave the macrostate unchanged, to be an event.

This remark will be very important in the analysis of the measuring process, since the necessary classical feature of the measuring equipment implies the restriction of the observables of the measuring device to an abelian subset of all the observables.

11-7. MATHEMATICAL INTERLUDE: THE TENSOR PRODUCT

In the following parts of the analysis of the measuring process, we need to apply the theory of the tensor product of Hilbert spaces, which we shall develop in this section. The tensor product is involved whenever we consider the union or separation of two subsystems; a process which occurs precisely during a measurement; the two systems in this case are the system to be measured on the one hand and the measuring equipment on the other.

The reason for the occurrence of the tensor product may be seen from the following remarks. Let S_1 and S_2 be two systems, and let $\mathscr{S}_1$ be a complete set of commuting observables of S_1, and $\mathscr{S}_2$ such a set for S_2. Every observable $A_1 \in \mathscr{S}_1$ is naturally also an observable on the joint system $S_1 + S_2$. The same is true for every observable $A_2 \in \mathscr{S}_2$. Furthermore every observable A_1 commutes with every observable A_2 and $\{\mathscr{S}_1, \mathscr{S}_2\}$ is a complete set of commuting observables for $S_1 + S_2$.

We must thus find a description which will incorporate these characteristic properties of the union of two systems. This can be done in the spectral representation for the two systems $\mathscr{S}_1$ and $\mathscr{S}_2$, for instance, as follows: Let Λ_1 be the Cartesian product of the spectra of a complete commuting set of some of the observables $\mathscr{S}_1$; and similarly, let Λ_2 be the corresponding product of the spectra of some of the observables $\mathscr{S}_2$.

The Hilbert space $\mathscr{H}_1$ of the spectral representation for $\mathscr{S}_1$ consists of square-integrable functions $\varphi_1(\lambda_1)$ with $\lambda_1 \in \Lambda_1$. Similarly the Hilbert space $\mathscr{H}_2$ of the spectral representation for $\mathscr{S}_2$ consists of square-integrable functions $\varphi_2(\lambda_2)$ with $\lambda_2 \in \Lambda_2$. The Hilbert space $\mathscr{G}$ of the spectral representation for the set $\{\mathscr{S}_1, \mathscr{S}_2\}$ is then a set of functions $\varphi(\lambda_1, \lambda_2)$, square-integrable over the Cartesian product space $\Lambda_1 \times \Lambda_2$.

The measure ρ for the space $\Lambda_1 \times \Lambda_2$ may be taken as the product measure $\rho_1\rho_2$ of the measures for the spaces Λ_1 and Λ_2 separately.

In this way we arrive quite naturally at the notion of the *tensor product*. Associated with the pair of spaces $\mathscr{H}_1$ and $\mathscr{H}_2$, we have constructed another space $\mathscr{G}$, the tensor product of $\mathscr{H}_1$ and $\mathscr{H}_2$, which in some respect generalizes the notion of product.

The same $\mathscr{G}$ contains a certain subset of vectors, those of the form $\psi(\lambda_1, \lambda_2) = \psi_1(\lambda_1)\psi_2(\lambda_2)$. This subset is the image of a bilinear mapping of pairs of vectors $\psi_1 \in \mathscr{H}_1$ and $\psi_2 \in \mathscr{H}_2$ into $\mathscr{G}$. Furthermore, this image set is a complete set of vectors in $\mathscr{G}$ in the sense that every vector in $\mathscr{G}$ can be written as a linear combination of vectors of the form $\psi_1(\lambda_1)\psi_2(\lambda_2)$.

These last two remarks will permit us to free ourselves from the particular construction of the tensor product which we have adopted here for illustrative purposes. We shall now proceed to a formal and abstract definition of the tensor products.

Let $\mathscr{H}_1$ and $\mathscr{H}_2$ be two Hilbert spaces. The tensor product $\mathscr{G} = \mathscr{H}_1 \otimes \mathscr{H}_2$ *is a Hilbert space together with a bilinear mapping φ from the topological product $\mathscr{H}_1 \times \mathscr{H}_2$ into $\mathscr{G}$, such that*

1) *the set of all vectors $\varphi(f_1, f_2)$* (where $f_1 \in \mathscr{H}_1, f_2 \in \mathscr{H}_2$) spans $\mathscr{G}$;
2) $(\varphi(f_1, f_2), \varphi(g_1, g_2)) = (f_1, g_1)(f_2, g_2)$ *for all $f_1, g_1 \in \mathscr{H}_1$, and for all $f_2, g_2 \in \mathscr{H}_2$.*

A few remarks on this definition and the notation may enhance the reader's understanding of them:

We are using two different kinds of products, the *topological* product $\mathscr{H}_1 \times \mathscr{H}_2$, and the *tensor* product $\mathscr{H}_1 \otimes \mathscr{H}_2$, which should not be confused. The first consists simply of the pairs of vectors $\{f_1, f_2\}$ with $f_1 \in \mathscr{H}_1$ and $f_2 \in \mathscr{H}_2$. The second is a Hilbert space $\mathscr{G}$ together with a bilinear mapping φ which satisfies the two conditions indicated above.

We have designated the scalar product in $\mathscr{G}$ with the same bracket notation as the scalar product in $\mathscr{H}_1$ and $\mathscr{H}_2$. The reader should not confuse the two.

It is important to note that the image of the bilinear mapping φ is not the entire Hilbert space $\mathscr{G}$; it is only a proper subset of $\mathscr{G}$. However, this subset is total in the sense that it spans the entire space $\mathscr{G}$.

The definition need not be restricted to the product of two spaces. Indeed, we may define the tensor product of a finite number n of spaces $\mathscr{G} = \mathscr{H}_1 \otimes \mathscr{H}_2 \otimes \cdots \otimes \mathscr{H}_n$ as a Hilbert space $\mathscr{G}$ together with a multilinear mapping from $\mathscr{H}_1 \times \mathscr{H}_2 \times \cdots \times \mathscr{H}_n$ into $\mathscr{G}$ which satisfies

1′) the set of all vectors $\varphi(f_1, f_2, \ldots, f_n)(f_r \in \mathscr{H}_r)$ spans $\mathscr{G}$;

2′) $(\varphi(f_1, f_2, \ldots, f_n), \varphi(g_1, g_2, \ldots, g_n)) = (f_1, g_1)(f_2, g_2) \cdots (f_n, g_n)$ for all $f_r, g_r \in \mathscr{H}_r$ $(r = 1, 2, \ldots, n)$.

We have already proved the existence of the tensor product for $n = 2$ by the construction employed in our example at the beginning of this section. We now need only verify that this construction does indeed satisfy the conditions (1) and (2) of the definition (Problem 1).

The tensor product is unique in the following precise sense: Let $\mathscr{H}_1$ and $\mathscr{H}_2$ be two Hilbert spaces and denote by $\mathscr{G}$ and $\mathscr{G}'$ two different tensor products with the associated bilinear mappings φ and φ' respectively; then there exists a unique isometric operator U with domain $\mathscr{G}$ and range $\mathscr{G}'$, such that

$$U\varphi(f_1, f_2) = \varphi'(f_1, f_2) \qquad \text{for all } f_1 \in \mathscr{H}_1, f_2 \in \mathscr{H}_2. \tag{11-19}$$

This uniqueness property of the tensor product is very important for its physical interpretation. The projection operators in $\mathscr{G}$ are the yes–no experiments for the joint system. The representation of the Hilbert space is determined only up to unitary equivalence by the lattice structure of the propositions. Then the uniqueness of the tensor product means that the physical property of the joint system, insofar as it is contained in the algebraic structure of the lattice of propositions, is entirely determined by the structure of the component systems.

An explicit construction of the tensor product, independent of any particular reference system, can be given as follows:

We define first the notion of the *conjugate linear* transformation T from $\mathscr{H}_2$ into $\mathscr{H}_1$. Such a T is required to satisfy

$$\begin{aligned} T(f_2 + g_2) &= Tf_2 + Tg_2, \\ T(\lambda f_2) &= \lambda^* Tf_2, \end{aligned} \tag{11–20}$$

for all $f_2, g_2 \in \mathscr{H}_2$.

Let $\{\psi_r\}$ be a complete orthonormal system in $\mathscr{H}_2$, and define the norm

$$\|T\|^2 \equiv \sum_{r=1}^{\infty} \|T\psi_r\|^2. \tag{11–21}$$

The sum on the right-hand side need not be finite, but it is independent of the choice of the orthonormal system $\{\psi_r\}$ (Problem 2). This norm satisfies the parallelogram identity (cf. Section 2-2, Problem 3), so that it can be derived from a scalar product as follows:

$$(T, S) \equiv \sum_{r=1}^{\infty} (T\psi_r, S\psi_r). \tag{11–22}$$

The set of all conjugate linear mappings T, with $\|T\| < \infty$, are therefore a Hilbert space $\mathscr{G}$. Moreover there exists a bilinear mapping φ from $\mathscr{H}_1 \times \mathscr{H}_2$ into $\mathscr{G}$ by setting, for each pair of vectors f_1, f_2,

$$Tg_2 = (g_2, f_2)f_1. \tag{11–23}$$

We denote this particular T by $f_1 \otimes f_2$. Its norm is $\|f_1 \otimes f_2\| = \|f_1\|\|f_2\|$ (Problem 3).

Now let $T = f_1 \otimes f_2$ and $S = g_1 \otimes g_2$; then one verifies easily that (Problem 3)

$$(T, S) = (f_1, g_1)(f_2, g_2). \tag{11–24}$$

Thus we have completed the construction of the tensor product: The elements of the space $\mathscr{G}$ are the conjugate linear mappings of $\mathscr{H}_2$ into $\mathscr{H}_1$ with finite norm, and the bilinear mapping φ is given by Eq. (11–23).

To every $T \in \mathcal{G}$ we can uniquely associate another conjugate linear mapping $T^{\#}$ from $\mathcal{H}_1$ into $\mathcal{H}_2$ by the formula

$$(f_1, Tf_2) = (f_2, T^{\#}f_1).$$

This mapping is unique because of Riesz' theorem (Section 3-1).

One verifies (Problem 5) the following rules of this correspondence:

$$T^{\#\#} = T, \qquad \|T^{\#}\| = \|T\|,$$

$$(T + S)^{\#} = T^{\#} + S^{\#}, \qquad (\lambda T)^{\#} = \lambda T^{\#}.$$

If $T = f_1 \otimes f_2$, so that, according to Eq. (11–23), $Tg_2 = (g_2, f_2)f_1$, then we find that

$$(g_1, Tg_2) = (g_1, f_1)(g_2, f_2) = (g_2, T^{\#}g_1);$$

therefore we must have $T^{\#}g_1 = (g_1, f_1)f_2$. It is suggestive to denote this particular $T^{\#}$ by $T^{\#} = f_2 \otimes f_1$.

The notion of the product can be extended from the vectors to the linear operators. Thus, if we have two bounded operators A_1 and A_2, where A_1 operates in $\mathcal{H}_1$ and A_2 operates in $\mathcal{H}_2$, then we may define for every $T = f_1 \otimes f_2$ the operation

$$(A_1 \otimes A_2)(f_1 \otimes f_2) = Af_1 \otimes Af_2.$$

This definition of $A_1 \otimes A_2$ can be extended by linearity to the entire space $\mathcal{G}$. Then we have, for every $T \in \mathcal{G}$, the formula (Problem 6)

$$(A_1 \otimes A_2)T = A_1 T A_2^{*}, \tag{11–25}$$

where A_2^{*} is the Hermitian conjugate of A_2.

This completes the construction of the tensor product.

PROBLEMS

1. The construction of the tensor product by means of the spectral representation of two complete sets of commuting operators used in the first part of this section does satisfy the formal definition of the tensor product.
2. If T is a conjugate linear mapping of a Hilbert space $\mathcal{H}_2$ into another $\mathcal{H}_1$, then

$$\sum_{r=1}^{\infty} \|T\psi_r\|^2 = \sum_{r=1}^{\infty} \|T\psi_r'\|^2,$$

where $\{\psi_r\}$ and $\{\psi_r'\}$ are two arbitrary complete orthonormal systems in $\mathcal{H}_2$.

3. If $f_1 \otimes f_2$ is defined as the conjugate linear mapping T given by

$$Tg_2 = (g_2, f_2)f_1,$$

and the scalar product of two such mappings is defined by

$$(T, S) = \sum_{r=1}^{\infty} (T\psi_r, S\psi_r),$$

then

$$(f_1 \otimes f_2, g_1 \otimes g_2) = (f_1, g_1)(f_2, g_2)$$

and

$$\|f_1 \otimes f_2\| = \|f_1\|\|f_2\|.$$

4. If T is a conjugate linear mapping from $\mathscr{H}_2$ into $\mathscr{H}_1$, then $T^\#$ defined by $(f_1, Tf_2) = (f_2, T^\# f_1)$ for all $f_1 \in \mathscr{H}_1$, $f_2 \in \mathscr{H}_2$ is a uniquely determined conjugate linear mapping of $\mathscr{H}_1$ into $\mathscr{H}_2$.
5. The correspondence $T \to T^\#$ satisfies the rules

$$T^{\#\#} = T, \qquad \|T^\#\| = \|T\|,$$
$$(T + S)^\# = T^\# + S^\#, \qquad (\lambda T)^\# = \lambda T^\#.$$

6. If A_1 is a bounded operator in $\mathscr{H}_1$ and A_2 a similar operator in $\mathscr{H}_2$, then $A_1 \otimes A_2 T = A_1 T A_2^*$ for every $T \in \mathscr{H}_1 \otimes \mathscr{H}_2$.

11-8. THE UNION AND SEPARATION OF SYSTEMS

We shall now consider two coherent systems S_1 and S_2. The joint system we denote by $S_1 + S_2$. The principal question that we want to answer here is how the states of the component systems are related to the states of the joint system, and vice versa.

Let us begin with the first part of the question. The states of the component system shall be given by their respective density operators W_1 and W_2. We wish to know what the state is if we consider the two components together as a joint system. The criterion for answering this question is a physical one: If we measure observables which refer to only one of the components we must obtain the same result whether we consider them measured on the joint system or on the component system.

We shall denote by A_1 an observable which refers to the component S_1. As an observable on S_1 it is a self-adjoint operator in the Hilbert space $\mathscr{H}_1$ pertaining to the system S_1. But as an observable on the joint system $S_1 + S_2$, it is a self-adjoint operator in the Hilbert space $\mathscr{G} = \mathscr{H}_1 \otimes \mathscr{H}_2$ pertaining to the joint system. Since it is an observable on S_1 alone, it must be the identity operator I_2 in $\mathscr{H}_2$. That is, it must have the form $\mathbf{A}_1 = A_1 \otimes I_2$. Similarly an observable on the joint system which refers only to system S_2 must have the form $\mathbf{A}_2 = I_1 \otimes A_2$.

Let W_1 be the state of system S_1 and W_2 the state of system S_2. The joint system $S_1 + S_2$ is then in a state W for which we now want to determine the manner of its dependence on W_1 and W_2. The conditions which W must

satisfy are thus

$$\mathrm{Tr}\,\mathbf{A}_1 W = \mathrm{Tr}_1 A_1 W_1 \qquad \mathrm{Tr}\,\mathbf{A}_2 W = \mathrm{Tr}_2 A_2 W_2. \tag{11-26}$$

Here we have, for greater clarity, introduced the notation Tr_1 and Tr_2 for traces which refer only to $\mathscr{H}_1$ and $\mathscr{H}_2$, respectively.

One possible solution of Eq. (11–26) is given by $W = W_1 \otimes W_2$, as one may verify immediately. In general this is not the only solution. Physically this means that the state of the compound system $S_1 + S_2$ cannot be completely determined by measurements on the component systems alone. There are thus physically distinguishable properties which express themselves as correlations between observation on S_1 and S_2. Such correlations are nonexistent for the state $W_1 \otimes W_2$.

There is one exception: If one of the states W_1 or W_2 is pure (Problem 1), then the states W_1 and W_2 determine the state of the compound system uniquely.

Let us now examine the reverse problem: Given W, determine W_1 and W_2 such that Eqs: (11–26) hold. This problem always has a unique solution. Let us first demonstrate the uniqueness of the solution. Let W, W_1, and W_2 be three density operators satisfying Eq. (11–26) for all A_1 and A_2. Let us assume that W, W_1', and W_2' is another set of such operators satisfying also the conditions (11–26). We find then that

$$\mathrm{Tr}_1\, A_1 W_1 = \mathrm{Tr}_1\, A_1 W_1' \tag{11-27}$$

for all observables $A_1 \in \mathscr{S}_1$. Since S_1 was assumed to be a coherent system, this means that (11–27) must be true for all projections P, in particular one-dimensional ones. Let P be such a projection and φ a unit vector in its range. Then we obtain from Eq. (11–27)

$$(\varphi, W_1 \varphi) = (\varphi, W_1' \varphi)$$

for all φ. This is possible only if $W_1 = W_1'$. Q.E.D.

Similarly one proves $W_2 = W_2'$. This proves uniqueness.

Let us next assume that W is a mixture, for instance, $W = \lambda U + \mu V$. Let U_1 and U_2 be the component states determined by U, and similarly let V_1 and V_2 be the component states determined by V. The linearity of the connection (11–26) between W and W_1, W_2 then results immediately in the statement: The component states W_1 and W_2 corresponding to the state W are given by

$$W_1 = \lambda U_1 + \mu V_1, \qquad W_2 = \lambda U_2 + \mu V_2. \tag{11-28}$$

This shows in particular that the component states can be pure only if W is pure.

In any case we need only determine the component states for pure states W; for the mixtures they can, by means of Eq. (11–28), be calculated immediately in terms of the pure states contained in the mixture.

Let us then assume that W is pure and denote by Φ the vector in $\mathscr{G}$ contained in the range of W. Φ is thus an antilinear mapping of $\mathscr{H}_2$ into $\mathscr{H}_1$. We assume Φ normalized, so that $\|\Phi\| = 1$. Let us choose a complete orthonormal system $\Phi_n \in \mathscr{G}$ such that $\Phi_1 \equiv \Phi$. We then obtain

$$\operatorname{Tr} \mathbf{A}_2 W = \sum_n (\Phi_n, \mathbf{A}_2 W \Phi_n) = (\Phi, \mathbf{A}_2 \Phi).$$

Since $\mathbf{A}_2 = I_1 \otimes A_2$ we use Eq. (11–25) and obtain

$$\mathbf{A}_2 \Phi = \Phi A_2^* = \Phi A_2.$$

Therefore

$$(\Phi, \mathbf{A}_2 \Phi) = \operatorname{Tr}_1 \Phi^* \Phi A_2$$

which shows that $W_2 = \Phi^{\#}\Phi$. In a similar way we evaluate W_1. The result is

$$W_1 = \Phi\Phi^{\#}, \qquad W_2 = \Phi^{\#}\Phi. \tag{11–29}$$

In the general case in which W is a mixture of orthogonal states Φ_n with weights λ_n, the component states are

$$W_1 = \sum \lambda_n \Phi_n \Phi_n^{\#} \qquad \text{and} \qquad W_2 = \sum \lambda_n \Phi_n^{\#} \Phi_n. \tag{11–30}$$

We shall refer to Eqs. (11–29) and (11–30) as the *reduction formulas*, and the states W_1, W_2 are called the *reduced* (or component) *states*.

Let us now discuss the reduction formula (11–29) in a little more detail. Consider first the case that $\Phi = \varphi \otimes \psi$ where φ and ψ are both normalized and $\varphi \in \mathscr{H}_1$, $\psi \in \mathscr{H}_2$. From the definition of Φ and $\Phi^{\#}$ it follows that

$$\Phi^{\#}\varphi = (\varphi, \varphi)\psi = \psi,$$

$$\Phi\psi = (\psi, \psi)\varphi = \varphi.$$

Thus $\Phi\Phi^{\#}\varphi = \varphi$ and $\Phi^{\#}\Phi\psi = \psi$. Furthermore, if φ_1 is orthogonal to φ, so that $(\varphi_1, \varphi) = 0$, then

$$\Phi^{\#}\varphi_1 = (\varphi_1, \varphi)\psi = 0$$

so that $\Phi\Phi^{\#}\varphi_1 = 0$. Similarly if ψ_1 is orthogonal to ψ,Φ then $\Phi^{\#}\Phi\psi_1 = 0$. In this case we find that $\Phi\Phi^{\#} = P$ is a projection in $\mathscr{H}_1$ with one-dimensional range containing φ. Similarly $\Phi^{\#}\Phi = Q$ is a projection in $\mathscr{H}_2$ with one-dimensional range, containing ψ. This means if the compound state has the form $\Phi = \varphi \otimes \psi$, then the reduced states are pure. The converse we have already seen, and so we have established:

The reduced states are pure if and only if the pure state Φ is of the form $\varphi \otimes \psi$.

Let us now consider the case in which the compound state is still pure, but not of this form. Then we know from the previous discussion that neither W_1 nor W_2 can be pure. Let $\Phi\Phi^{\#} \equiv W_1 = \sum_r \alpha_r P_r$ with P_r projections with

one-dimensional range and $\alpha_r > 0, \sum_r \alpha_r = 1$. Define $\psi_r = (1/\sqrt{\alpha_r})\Phi^{\#}\varphi_r$, where φ_r is a normalized vector in the range of P_r. We have then

$$\|\psi_r\|^2 = \frac{1}{\alpha_r}\|\Phi^{\#}\varphi_r\|^2 = \frac{1}{\alpha_r}(\varphi_r, \Phi\Phi^{\#}\varphi_r) = 1,$$

and

$$W_2\psi_r = \frac{1}{\sqrt{\alpha_r}}\Phi^{\#}\Phi\Phi^{\#}\varphi_r = \frac{1}{\sqrt{\alpha_r}}\Phi^{\#}W_1\varphi_r = \sqrt{\alpha_r}\,\Phi^{\#}\varphi_r = \alpha_r\psi_r.$$

Thus ψ_r is a normalized eigenvector of W_2 with eigenvalue α_r. Furthermore every eigenvector of W_2 is of this form. It follows from this that $W_2 \equiv \Phi^{\#}\Phi$ has the form $W_2 = \sum_r \alpha_r Q_r$ with $Q_r\psi_r = \psi_r$.

If we complete the vectors φ_r and ψ_s to complete orthonormal systems in $\mathscr{H}_1$ and $\mathscr{H}_2$ respectively, we obtain such a system in $\mathscr{G}$ in the form $\varphi_r \otimes \psi_s$. By substituting the definition of $\varphi_r \otimes \psi_s$ as an antilinear mapping of $\mathscr{H}_2$ into $\mathscr{H}_1$ we find

$$(\Phi, \varphi_r \otimes \psi_s) = \sum_t (\Phi\psi_t, (\varphi_r \otimes \psi_s)\psi_t) = (\Phi\psi_s, \varphi_r) = \sqrt{\alpha_r}\,\delta_{rs}.$$

This means Φ has the development

$$\Phi = \sum_r \sqrt{\alpha_r}\,\varphi_r \otimes \psi_r. \tag{11–31}$$

We have thus established the following result:

If Φ is a general vector in $\mathscr{G}$, then there exists an orthonormal system $\{\varphi_r\}$ in $\mathscr{H}_1$, a similar system $\{\psi_s\}$ in $\mathscr{H}_2$ and positive numbers α_r such that

$$\Phi = \sum_r \sqrt{\alpha_r}\,\varphi_r \otimes \psi_r, \qquad \Phi^{\#}\Phi = \sum_r \alpha_r P_r,$$

$$\Phi\Phi^{\#} = \sum_s \alpha_s Q_s, \qquad P_r\varphi_r = \varphi_r, \qquad Q_s\psi_s = \psi_s.$$

With this result we have established the *normal form* of the reduction of the pure state Φ of the compound state to its component states.

PROBLEMS

1. If W_1 is pure and if

$$\operatorname{Tr} \mathbf{A}_1 W = \operatorname{Tr}_1 A_1 W_1, \qquad \operatorname{Tr} \mathbf{A}_2 W = \operatorname{Tr}_2 A_2 W_2$$

for all observables A_1 and A_2, then $W = W_1 \otimes W_2$.

2. Let W_1, W_2 be the reduced states of the state W. If W_1 is pure, then W_2 is pure too.

3. If $P = \Phi\Phi^{\#}$ is a projection of one-dimensional range, then $Q \quad \Phi^{\#}\Phi$ is also a projection of one-dimensional range.

11-9. A MODEL OF THE MEASURING PROCESS

In this section we shall return to physics and complete the analysis of the process of measurement on a model which is so designed that it permits an explicit description of the state of the system *and* the measuring device during the entire measuring process. The measuring device is here assumed in the simplest form, so that its quantum character is not obscured by the complexity of a large system. The purpose of the model is to show the consistency of measurement in the quantum description of the entire system.

In order for the model to represent the essential features of the measurement, it must satisfy the conditions laid down in Section 11-4. The system thus consists of two parts, the system $S_1 = S$ on which a state is to be measured, and a microscopic but classical measuring device $S_2 = m$.

For the system S_1 we take a system represented by a two-dimensional state vector. Let φ_+ and φ_- be two orthogonal vectors in this space which are the eigenstates of the quantity to be measured.

The system S_2 is assumed to be described by a three-dimensional Hilbert space. It contains the vector ψ_0 which we shall call the *neutral state* of m and two more orthogonal vectors ψ_+ and ψ_-. The vector ψ_+ represents the "pointer reading" indicating system S_1 to be in state φ_+. Similarly ψ_- is the indicator for state φ_-.

If before interaction the system $S + m$ is in the pure state

$$\Phi_{+0} \equiv \varphi_+ \otimes \psi_0,$$

then after the measurement is completed the system $S + m$ is in the pure state

$$\Phi_+ = \mathcal{U}\Phi_{+0} = \varphi_+ \otimes \psi_+, \tag{11–32}$$

where $\mathcal{U}$ is some unitary operator. Similarly the initial state $\Phi_{-0} \equiv \varphi_- \otimes \psi_0$ is, after the interaction, given by

$$\Phi_- = \mathcal{U}\Phi_{-0} = \varphi_- \otimes \psi_-. \tag{11–33}$$

These formulas describe the characteristic behavior of a measurement of the first kind in the context of this model.

We now take the general initial state of the form

$$\Phi_0 = \alpha_+\Phi_{+0} + \alpha_-\Phi_{-0}.$$

Since the transformation $\mathcal{U}$ is linear, we can obtain the final state after the measurement in this case by linear superposition of the final states (11–32) and (11–33):

$$\Phi = \mathcal{U}\Phi_0 = \alpha_+\varphi_+ \otimes \psi_+ + \alpha_-\varphi_- \otimes \psi_-. \tag{11–34}$$

After the measurement is completed we can imagine the interaction between S and m removed. The reading of the scale consists in amplifying the record contained in m and deducing from it the state of S.

The state of m, to be read with the amplifier, is obtained from the pure state (11–34) by reducing that state to the system m. We use the reduction formulas of the previous section. In this case their application is especially easy since (11–34) is already in the normal form (11–31). The only slight generalization here is that the coefficients $\alpha_\pm$ are complex numbers (in Eq. 11–31 they were real); however, an adjustment of the phases of $\varphi_\pm, \psi_\pm$ will reduce them to reals.

Thus we may write for the reduced states

$$\begin{aligned} W_1 &= |\alpha_+|^2 P_+ + |\alpha_-|^2 P_-, \\ W_2 &= |\alpha_+|^2 Q_+ + |\alpha_-|^2 Q_-, \end{aligned} \tag{11–35}$$

where $P_\pm$ and $Q_\pm$ are the projections containing $\varphi_\pm, \psi_\pm$ respectively. We see that both states have become mixtures. Since m (as well as $m + A$) is a classical system, the state is a classical state. No further observation on m will modify the state, and the measurement has become an objective record. According to Section 11-6, each individual system m which may be used in a statistic of the measurement realizes one of the two alternatives. These alternatives are thus events in the sense of Section 11-6, and their amplification will make them data. There is no question of any superposition here. The reduction of the state to the system m has wiped out any phase relations.

Moreover, we have a measurement since the events in m and those in S are correlated. If m is in the state ψ_+, then S is necessarily in the state φ_+. In order to see this, we calculate the expectation value for the cross correlation expressed by the proposition P_+ *and* Q_- and represented by the projection $P_+ \otimes Q_-$. It is given by

$$(\Phi, P_+ \otimes Q_- \Phi) = 0. \tag{11–36}$$

Therefore the event ψ_+ is strictly correlated with φ_+, and ψ_- is similarly correlated with φ_-. Thus in the reduction formulas we see the true origin of the probability statements in the quantum-mechanical measuring process.

A difficulty seems to appear for this interpretation if we include the system S in the measuring device. In this case there is no occasion to reduce the pure state Φ to that of a mixture. If we do this, then the observable projections of the joint system are Π_+ with range $\varphi_+ \otimes \psi_+$ and Π_- with range $\varphi_- \otimes \psi_-$ and, in our model, there are no others. The abelian system $\mathscr{S}$ of observables on this system consists of all linear combinations of these two projections. In this case we are in the situation where the pure state Φ is contained in a class of equivalent microstates. These states contain the state

$$W = |\alpha_+|^2 \Pi_+ + |\alpha_-|^2 \Pi_-, \tag{11–37}$$

since

$$\operatorname{Tr} W\Pi_+ = (\Phi, \Pi_+ \Phi) = |\alpha_+|^2$$

and

$$\operatorname{Tr} W\Pi_- = (\Phi, \Pi_- \Phi) = |\alpha_-|^2.$$

Thus the final state is again a probability distribution of events, this time described by the projections $\Pi_{\pm}$. In this case the probability statement comes in through the theory of equivalent states.

11-10. THREE PARADOXES

a) Schrödinger's cat. In a paper entitled "The Present State of Quantum Mechanics," Schrödinger wrote a criticism of the orthodox view of quantum mechanics [2]. He pointed out that this view would imply rather grotesque situations for macroscopic events, and he illustrated it with an example involving a cat. This example has been reformulated by many other authors in more or less equivalent forms, and it has to this day been considered by many an unsolved paradox. Here we shall give a literal translation of Schrödinger's cat paradox. Schrödinger writes:

"A cat is placed in a steel chamber, together with the following hellish contraption (which must be protected against direct interference by the cat): In a Geiger counter there is a tiny amount of radioactive substance, so tiny that maybe within an hour one of the atoms decays, but equally probably none of them decays. If one decays then the counter triggers and via a relay activates a little hammer which breaks a container of cyanide. If one has left this entire system for an hour, then one would say that the cat is still living if no atom has decayed. The first decay would have poisoned it. The ψ-function of the entire system would express this by containing equal parts of the living and dead cat.

"The typical feature in these cases is that an indeterminacy is transferred from the atomic to the crude macroscopic level, which then can be *decided* by direct observation. This prevents us from accepting a "blurred model" so naively as a picture of reality. By itself it is not at all unclear or contradictory. There is a difference between a blurred or poorly focussed photograph and a picture of clouds or fog patches."

The paradoxical aspect of this example is to be found in the supposed reduction of the state from a superposition of macroscopically distinct alternatives to one of the events during the act of observation.

b) Einstein's element of physical reality. Einstein has been not only one of the founders of quantum mechanics, but also one of its strongest critics. His critique does not concern the existing theory as such, which he recognizes as satisfactory as far as it goes in the description of physical phenomena. He questions its completeness. The paradox of Einstein, Podolsky, and Rosen [12] is one of the most striking forms in which this question is expressed.

The authors take the position that physics is concerned with the description of "physical reality" and they affirm that an objective reality exists which does not depend on our observation. *A priori* we do not know what it is, so

they say, but this precisely is the task of physics: to establish the properties of the existing physical reality.

They are aware that this position requires a meaningful definition of "physical reality." This is, of course, not easy and it is probably impossible in physical terms alone.

However, certain elements of physical reality can, so they affirm, be given a precise meaning. Indeed, if the value of a physical quantity for a physical system can be determined with certainty without in any manner whatsoever perturbing the state of the system, then this quantity has for them an element of "physical reality" in that system.

The authors then proceed to contruct an example which seems to lead to the conclusion that quantum mechanics is in contradiction with a complete description of all elements of physical reality. We reproduce this example here in a simplified form.

Let us assume that we have two systems I and II, which at a given time can interact with each other. We assume that the states of each system are completely described by a two-dimensional vector space. Let $\varphi_\pm$ represent a complete orthonormal set of vectors in the first space and $\psi_\pm$ a similar set in the second space. Let us further assume that the interaction between the two systems is such that at some time the (pure) state of the joint system is given by

$$\Phi = \frac{1}{\sqrt{2}} [(\varphi_+ \otimes \psi_+) + (\varphi_- \otimes \psi_-)]. \tag{11–38}$$

We now assume that the two systems can be isolated from each other, for instance by separating them spatially, so that any observation carried out on one of the component systems cannot have any physical effect on the other system.

After this separation the state is still given by Eq. (11–38). If we now measure on system I whether it is in the state φ_+ or φ_-, we find that it is in $\varphi_\pm$ with probability $\frac{1}{2}$. The interesting point is that a measurement of $\varphi_\pm$ constitutes at the same time a measurement of $\psi_\pm$ on system II. Indeed, according to the general theory of the measuring process, we know that whenever a measurement on system I has given the result φ_+, any future measurement on system II will give the result ψ_+. Since the two systems are physically separated we have a means of determining the state of system II "without in any manner whatsoever perturbing the state" of that system. According to the criterion of Einstein, Podolsky, and Rosen, the quantity with the eigenstates $\psi_\pm$ of system II must therefore have an element of physical reality.

The value of this quantity is of course not known before the measurement on system I is completed, but that does not invalidate the conclusion that it has a definite value, since one can determine it by a measurement carried out

entirely on system I. Moreover this definite value must have had the same element of reality even *before* the measurement on system I was carried out, since a measurement on system I cannot produce any physical effect whatsoever on system II and thus cannot change the reality of a physical quantity in that system.

We are thus driven to the conclusion that the system (I + II) is in a mixture of two different states, namely, the states $\varphi_+ \otimes \psi_+$ and $\varphi_- \otimes \psi_-$ mixed, with probabilities $\frac{1}{2}$. But such a state is different from the state expressed by Eq. (11–38). Thus the acceptance of the notion of "physical reality" has led us to a contradiction.

This paradox can be given still another form. It is possible to carry out a simultaneous change of coordinate systems in the vector spaces referring to systems I and II respectively in such a way that the vector Φ remains invariant. This means we can find other orthonormal pairs $\varphi'_\pm$ and $\psi'_\pm$ such that

$$\Phi = \frac{1}{\sqrt{2}} (\varphi'_+ \otimes \psi'_+ + \varphi'_- \otimes \psi'_-). \qquad (11\text{–}38)'$$

The same reasoning that was applied for the form (11–38) can now be repeated identically for the representation (11–38)′, with the conclusion that system II is in one of the arbitrary states $\psi'_\pm$. But a system cannot be simultaneously in two different states; hence we have encountered another contradiction.

Einstein, Podolsky, and Rosen have drawn the conclusion from this paradox that quantum mechanics does not furnish a complete description of the physical reality of individual systems but merely describes the statistical properties of ensembles of systems.

This paradox was discussed by Bohr [13], who showed that it could not be considered a refutation of the basic principles of quantum mechanics but that it merely revealed the limits of the traditional concepts of natural philosophy. In a rejoinder [14] Einstein admits the logical possibility of Bohr's viewpoint, but reaffirms his belief in and preference for another point of view.

c) Wigner's friend. In 1962 Wigner added a new element to the paradoxes already known by including consciousness for the physical systems involved [15]. The situation discussed by Wigner is identical with that of formula (11–34), in Section (11–9), except that Wigner endows system II (the measuring apparatus) with the facility of consciousness. He then proceeds to introduce the ultimate observer Ω who observes and communicates with the (conscious) apparatus II. When Ω asks II what he has observed, he will receive the answer that he has observed the state φ_+ (as the case may be) and this with probability $|\alpha_+|^2$. All this is quite satisfactory and in agreement with the theory of measurement.

However, Wigner now inquires what would happen if Ω asked his friend (system II): "What did you feel just *before* I asked you?" Then the friend will answer, "I told you already I observed φ_+ (or φ_-)," as the case may be. In other words, the question whether his friend did observe φ_+ or φ_- was already present in his consciousness before Ω asked him. But at that moment there was no question of any interference of the observer Ω into the natural process of evolution of the two interacting systems; thus its state at that time must have been the superposition (11–34).

But this does not seem to be compatible with the information directly accessible to the conscious friend who is aware of his state before he was asked by the observer what his state is.

For if his awareness is correct, then the state of I + II *before* Ω asked his friend, was already a mixture of the two states $(\varphi_+ \otimes \psi_+)$ and $(\varphi_- \otimes \psi_-)$ and not the superposition (11–34).

Wigner considers this paradox an indication of the influence of consciousness on the physicochemical conditions of living systems. He finds such an influence entirely in accord with the general principle of action and reaction, since it is known that these physicochemical conditions have in turn a profound influence on conscious sensations.

d) Discussion of the paradoxes. The similarity between the three paradoxes is obvious. In all three cases one considers two interacting systems, and the paradox is produced by obtaining some information on the state of one of the systems which seems to be in contradiction with the state obtained from the principle of superposition. The difference in the three cases refers only to the *method* of obtaining this information.

In case (a) one appeals to the common-sense notion that a cat is either dead or alive, and that no other state which would leave us undecided about these two alternatives can occur.

In case (b) the information about system II is obtained by looking at the other system I and using the known correlation of observations in I with those in II.

Finally in case (c) we have the "consciousness" of system II which, seemingly without outside interference, is capable of determining the state of II by introspection.

Having thus stressed the similarity, we now pay attention to the differences. Here one sees at once that (b) stands in a class apart, since in this case only does one obtain information about the system through an outside observer which interacts with the system (I + II). To be sure, the interaction is assumed to affect only system I and not system II, about which we thus obtain information without outside interference.

Case (b) differs from the other two in another respect. In cases (a) and (c) one appeals to notions which are outside the confines of physics. To "be

alive" or to "be conscious" are presumably certain states of very complicated physical systems, but it is impossible to express in physical terms what these states are.

In paradox (b), on the other hand, an effort is made to reduce the problem entirely to physical terms. For this reason it is easier to discuss this case and we shall do it first.

If science is possible then there is nothing paradoxical about the physical world, and insofar as quantum mechanics is a correct physical theory it cannot contain paradoxes. Thus if paradoxes seem to appear, they must originate either from an inconsistent (and hence incorrect) physical theory, or they must indicate the limitation of concepts in physics which have acquired their meaning outside the domain of physics. In case (b) we can exclude the second possibility, and so we can discuss this case entirely within existing physical theory, without first having to interpret the physical content of nonphysical concepts.

What does quantum mechanics tell us about the state of the physical systems I, II, and (I + II) after a third observer has carried out a measurement of the quantities $P_\pm$ on system I?

We use the notation and the theory of Sections 11–8 and 11–9. This theory tells us that after measurement of the quantity $P_\pm$, the system is in the state $W_\mathrm{I} \otimes W_\mathrm{II}$, where W_I and W_II are the reductions of the state $W = P_\phi$ to the subsystems I and II respectively. This result is a direct consequence of the analysis of Section 11–9, the only difference being that the system is now (I + II) while the apparatus is the observer Ω.

The effect of the observer Ω on the system (I + II) was thus to change the state W of that system to the state $W_\mathrm{I} \otimes W_\mathrm{II}$. This change of the state of the entire system is exactly the same as the change which would have been obtained by measuring the quantity $Q_\pm$ of system II. We see now quite clearly that the attempt at restricting the observation to I is illusory. The effect on the entire system is exactly the same, whether we observe $P_\pm$ in system I or $Q_\pm$ in system II. To be sure, in neither case is the state of subsystem I or subsystem II modified in any manner whatsoever. This state is *before* and *after* the measurement given by W_I for I and W_II for II.

The paradox originates in our habit of thinking that the states of two subsystems determine uniquely the state of the composite system. As we have shown in Section 11-8, this is usually not the case. In the present example the two *different* states $W = P_\phi$ and $W_\mathrm{I} \otimes W_\mathrm{II}$ have the same reductions to the systems I and II and the measurement of either $P_\pm$ *or* $Q_\pm$ changes the state W of the combined system to the state $(W_\mathrm{I} \otimes W_\mathrm{II})$.

This shows that the application of Einstein's criterion of physical reality becomes ambiguous. It all depends how we want to interpret the condition "in any manner whatsoever." If we refer it only to the states of the subsystems I or II, it is obviously fulfilled; if we refer it to the entire system (I + II), it is

not. In no case is there a contradiction of the uncertainty relation, because, as we have seen, a measurement of $P_{\pm}$ has exactly the same effect on the states as a measurement of $Q_{\pm}$.

Thus the "paradox" of Einstein, Podolsky, and Rosen does not reveal any contradiction of quantum mechanics; it merely emphasizes in a most striking way the essential nonclassical consequences of the quantum-mechanical superposition of states. It is this very superposition principle which leads to the ambiguity in the application of Einstein's criterion of "physical reality."

Let us now turn to the more difficult discussion of paradoxes (a) and (c). The difficulty in these cases stems from the fact that the outside observer is pushed into the background. In case (a) he may merely be needed to verify whether the cat is dead or alive, an observation which may reasonably be assumed to have no effect whatsoever on the biological state of the cat. In case (c) he is even entirely superfluous since consciousness becomes aware of itself by introspection. Of course this faculty of observing the state of II without any observer is obtained here with properties which are difficult to express in physical terms, namely, "being alive" in case (a) and "being conscious" in case (c). In either case the alternatives of the microscopic system are transferred to the crude macroscopic level and thus are no longer subject to the quantum-mechanical ambiguities associated with coherent interferences of two different states.

One might reformulate the Schrödinger cat paradox by using only the macroscopic features of system II. Such a reformulation has been given, for instance, by Einstein (cf. reference 8, reply to criticisms), who replaced the "hellish contraption" of Schrödinger by a moving film strip which records the event of the radioactive decay in a permanent, macroscopic, and unobserved record. In this form the paradox is formulated entirely within the confines of physics, and yet at first sight it seems to retain its paradoxical character.

The essential point here is that system II, which contains this recording device, can be made as large as one wishes. In a subsequent observation on this system, the inevitable interaction of the outside observer with system II can therefore be made as small as one wishes, and thus (one is tempted to conclude) it can be neglected altogether.

It would, however, be incorrect to neglect it altogether. For we must not forget that the distinction between state W and state $W_{\mathrm{I}} \otimes W_{\mathrm{II}}$ becomes increasingly difficult to detect with the increase in size of the whole apparatus, and it is precisely this distinction which is under discussion here. The theory of the preceding two sections has shown with sufficient generality that the remaining interaction between II and an outside observer Ω is in fact the essential effect which will indeed obliterate the distinction between the two states.

If the information of the recording device does have objective validity, that is, if it can be communicated, then this very property makes it impossible to distinguish between the two states W and $W_{\mathrm{I}} \otimes W_{\mathrm{II}}$.

Thus the paradox of Schrödinger's cat can be resolved when it is reformulated entirely in physical terms.

Wigner's friend could be treated in the same manner with the same conclusion, but this would not meet the heart of Wigner's problem. As long as one insists on including consciousness as a property of quantum-mechanical systems, the outsider observer Ω can be dispensed with altogether and then we have no answer to the paradox. Must we conclude from this, as Wigner does, that quantum mechanics, as we know it now, would be inapplicable for systems with consciousness? The answer to such a question obviously presupposes a characterization and analysis of "consciousness" in physical terms, a task which seems to transcend the present limitations of physics.

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PART 3
Elementary Particles

CHAPTER 12

THE ELEMENTARY PARTICLE IN ONE DIMENSION

I shall never forget the thrill which I experienced when I succeeded in condensing Heisenberg's ideas on quantum conditions in the mysterious equation

$$pq - qp = h/2\pi i,$$

which is the center of wave mechanics and was later found to imply the uncertainty relation.

MAX BORN, *Physics and Metaphysics*,
Joule Memorial Lecture, 1950

In this chapter we begin the quantum theory of elementary particles. The central notion is localizability, which we introduce in Section 12-1 for the particle in one dimension. Closely related to it is the notion of homogeneity of space (Section 12-2) which leads in a natural manner to the canonical commutation rules (Section 12-3) and the systems of imprimitivities. The definition of elementary particle is given in Section 12-4. In Section 12-5 we treat the relation between Galilei invariance and the equation of motion for an elementary particle. The theory of the harmonic oscillator follows as an illustrative example, in Section 12-6. In the following section (12-7) we give a modern version of the harmonic oscillator in a Hilbert space of analytic functions, which has lately become important in the treatment of coherence phenomena. In the final section (12-8) we take up once more the question of modularity of the proposition system left open in Chapter 5.

12-1. LOCALIZABILITY

The atomic hypothesis is based on the idea that the constituents of matter are elementary indivisible entities, the atoms, whose properties determine the behavior of the bulk of matter. Although this hypothesis was strikingly successful, especially in the development of the kinetic theory of heat, crystal structure, atomic and molecular structure, it had to undergo a number of modifications and refinements in the course of the development of physics in the last fifty years. One of the most significant aspects of the present state of

knowledge about elementary particles is the fact that the known constituents of matter, which would merit this label, can be transformed into each other, and most can decay into other particles. Only very few of them are known to be stable. These phenomena force us to question the very notion of an elementary particle as a suitable notion for a basic theory.

In a nonrelativistic theory, as we develop it here, with a definite, although limited, domain of validity it is quite possible to retain the notion of elementary particle as a useful basic concept. It is meaningful to study the behavior of the center of mass of a complex nucleus even if we know such a nucleus to be a *composite system* of many nucleons. It is equally meaningful to study the properties of a muonic atom even if we know that it will decay in 10^{-6} sec. It is in this sense that we shall here develop the nonrelativistic quantum theory of elementary particles.

The key concept in the theory of elementary particles is *localizability* to which we have to turn our attention first. We begin with a description of the term.

One of the basic features of the physical world is its occurrence in a physical space of three dimensions. This physical space is the "arena" of the events in physical systems. A careful examination of the preceding chapters shows that so far we have nowhere introduced this fact as an essential element in the theory. This we must do now.

Localizability of an elementary particle means first of all a special property of the proposition system. This system must contain a class of propositions which answer the question whether the particle is in this or in that volume element of physical space. We are familiar with this from classical mechanics, where the corresponding propositions are represented by the Boolean algebra of the Borel subsets in the three-dimensional Euclidean space. How must we represent these propositions in quantum mechanics?

We must first examine the question whether propositions concerning the location of a particle in different volume elements are compatible or not. The answer must be sought through experience with counters which locate particles in various regions in space, and we can only record the fact that so far all our experience is consistent with the assumption that all these propositions are indeed compatible.

We shall point out here, however, that this experience is of course limited to relatively large volume elements, and no systematic study has ever been made of this question. The possibility of a quantum mechanics of localizable systems, for which not all propositions expressing localization are mutually compatible, is a distinct possibility. It would imply a far more profound modification of quantum mechanics than has ever been contemplated.

Let us proceed then on the traditional assumption that the propositions locating a particle in various domains Δ of physical space are all compatible. We represent them therefore by a projection-valued measure $\Delta \to E_\Delta$ which satisfies the properties to be explained and enumerated now. We shall do

this in this chapter for the case in which the physical space is one-dimensional. The Δ are then Borel sets on the real line. If Δ_1 and Δ_2 are two Borel sets on the real line, then the proposition that the system is located in the intersection $\Delta_1 \cap \Delta_2$ is represented by $E_{\Delta_1} \cap E_{\Delta_2}$. Since E_{Δ_1} and E_{Δ_2} are compatible, this same proposition is also given by $E_{\Delta_1}E_{\Delta_2} \equiv E_{\Delta_1} \cap E_{\Delta_2}$.

Similarly the proposition $E_{\Delta_1} \cup E_{\Delta_2}$ may also be represented by $E_{\Delta_1} \cup E_{\Delta_2} \equiv E_{\Delta_1} + E_{\Delta_2} - E_{\Delta_1}E_{\Delta_2}$. Finally if we denote the complementary Borel set as usual by Δ' and the complementary proposition $I - E$ by E', we must have $E_{\Delta'} = E'_{\Delta}$. By generalizing the additivity property to a countable sequence of Borel sets, we obtain the fundamental relations for the propositions which localize a physical system:

$$\begin{aligned} E_{\Delta_1 \cap \Delta_2} &= E_{\Delta_1} \cap E_{\Delta_2}, \\ E_{\Delta_1 \cup \Delta_2} &= E_{\Delta_1} \cup E_{\Delta_2}, \\ \sum_i E_{\Delta_i} &= E_{\cup \Delta_i} \qquad \text{for any sequence of disjoint } \Delta_i, \\ E_{\Delta'} &= E'_{\Delta}. \end{aligned} \tag{12–1}$$

A special case of the last relation is obtained by choosing for Δ the null set $\emptyset$, so that $\emptyset' = \Lambda$, the entire real line:

$$E_{\Lambda} = E'_{\emptyset} = I. \tag{12–2}$$

We see thus that the physical concept of localizability leads in a natural way to a *spectral measure* over the real line Λ.

According to the fundamental theorem quoted in Section 4-3, every spectral measure defines a self-adjoint operator Q. The operator defined by the spectral measure (Eq. 12–1) is called the *position* operator. It is a self-adjoint operator with a continuous spectrum extending over the entire real line.

12-2. HOMOGENEITY

Two of the basic properties of physical space are its homogeneity and isotropy. Both of these properties express the fact that physical space has no observable physical properties. This means that different points in physical space are physically indistinguishable. For a particle moving in a one-dimensional space, we can express homogeneity by requiring that a translation of the space Λ by an arbitrary amount α will induce a symmetry transformation in the proposition system.

In order to express this in a formula, we introduce the notation $[\Delta]\alpha$ for the set $\{\lambda : \lambda - \alpha \in \Delta\}$; that is, the set translated as a whole by the amount α. If the space Λ is physically homogeneous, we must require that there exist unitary operators U_α such that

$$E_{[\Delta]\alpha} = U_\alpha^{-1} E_\Delta U_\alpha. \tag{12–3}$$

The unitary operators U_α depend continuously on the parameter α and we can choose the as yet undetermined phase of U_α in such a way that they form a continuous vector representation of the additive group of real numbers:

$$U_\alpha U_\beta = U_{\alpha+\beta}. \tag{12–4}$$

According to Stone's theorem, such a group uniquely determines a self-adjoint operator P such that

$$U_\alpha = e^{i\alpha P}. \tag{12–5}$$

We shall call P the *displacement operator.*

The relation (12–3) is fundamental. It is the precise mathematical expression of the notion of localizability in a *homogeneous* space. In the following we shall develop a number of consequences and other equivalent forms of this fundamental property.

First of all we can transform Eq. (12–3) into another equivalent but more symmetrical form as follows: The self-adjoint operator Q may also be considered as a generator of a one-parameter group representation by setting

$$V_\beta = e^{i\beta Q} \equiv \int_{-\infty}^{+\infty} e^{i\beta\mu}\, dE_\mu.$$

We then obtain from Eqs. (12–3) and (12–4),

$$\begin{aligned} U_\alpha V_\beta U_\alpha^{-1} &= \int_{-\infty}^{+\infty} e^{i\beta\mu}\, d(U_\alpha E_\mu U_\alpha^{-1}) \\ &= \int_{-\infty}^{+\infty} e^{i\beta\mu}\, dE_{\mu-\alpha} \\ &= \int_{-\infty}^{+\infty} e^{i\beta(\mu+\alpha)}\, dE_\mu = e^{i\alpha\beta} V_\beta \end{aligned}$$

or

$$U_\alpha V_\beta = e^{i\alpha\beta} V_\beta U_\alpha. \tag{12–6}$$

Relation (12–6) is the canonical commutation rule in Weyl's form. In this form the symmetry between the two groups is more apparent than in the form of Eq. (12–3). We see at once, for instance, that the group V_β induces in the spectral measure of P also a displacement in the opposite direction. Thus if F_Δ are the spectral projections of the operator P, we have

$$V_\beta F_\Delta V_\beta^{-1} = F_{[\Delta]\beta}. \tag{12–7}$$

We can throw the canonical commutation rule (12–6) into still another form by expressing it in terms of the generators of the unitary groups. The

generator P is defined on all vectors f for which the limit

$$\lim_{\alpha \to 0} \frac{1}{i\alpha} (U_\alpha - I)f = Pf$$

exists, while Q is defined for the vectors f which admit the limit

$$\lim_{\beta \to 0} \frac{1}{i\beta} (V_\beta - I)f = Qf.$$

From these definitions and Eq. (12–3), we easily obtain the commutation rule (cf. Problem 2)

$$[Q, P]f = if. \tag{12–8}$$

In order to give this equation a meaning, we must have $Qf \in D_P$ and $Pf \in D_Q$. The domain D of such vectors **f** is everywhere dense (Problem 1), and the restriction of Q or P to D is essentially self-adjoint (Problem 3).

PROBLEMS

1. There exists a dense domain D of vectors **f** which satisfy $Pf \in D_Q$ and $Qf \in D_P$, where D_Q is the domain of Q and D_P is the domain of P.
2. If U_α and V_β are two one-parameter unitary group representations satisfying Eq. (12–3), then their infinitesimal generators P and Q respectively satisfy the canonical commutation rule

   $$[Q, P]f = if,$$

   for all $f \in D$ where D is the domain of Problem 1.

*3. The restriction of Q to the domain D is essentially self-adjoint, so is the restriction of P to D.

*4. ***Theorem*** (Plessner): *The spectrum of P and the spectrum of Q are absolutely continuous* (cf. reference 2).

12-3. THE CANONICAL COMMUTATION RULES

We have seen that the notion of localizability in a one-dimensional homogeneous space lead in a natural way to a pair of self-adjoint operators P and Q, which on a dense subset D of the entire Hilbert space satisfy the relation

$$[Q, P]f = if \qquad \text{for all } f \in D. \tag{12–9}$$

We shall now examine the mathematical aspects of this canonical commutation rule. In many discussions it is written simply as an operator relation

$$[Q, P] = i \cdot I. \tag{12–10}$$

We shall do this too, occasionally, but in doing so we must always bear in mind that this relation is only valid on the dense set D, and that the restriction of P or Q to D is only essentially self-adjoint. Failure to take account of these important restrictions can cause pseudo problems in the form of paradoxes.

The principal mathematical problem of the canonical commutation rules is connected with the question of the possible irreducible representations of the canonical commutation rules as in Eq. (12–9).

We first construct an explicit representation. Let us assume that there exists a generating vector g for the operator Q, so that its spectrum is simple (cf. Section 4-5). There then exists a spectral representation of Q, and in this representation the vectors $f \in \mathscr{H}$ are given by functions $\psi(x)$ on the real line $(-\infty < x < +\infty)$ such that $\psi(x) \in L^2(-\infty, +\infty)$ and

$$(Q\psi)(x) = x\psi(x). \tag{12–11}$$

A possible expression for P in this representation is given by

$$(P\psi)(x) = -i\frac{d\psi(x)}{dx}. \tag{12–12}$$

The domain D on which the commutation rules are satisfied is determined by the following conditions:

$$\begin{aligned} &1)\quad \psi(x) \in D_Q, \\ &2)\quad \psi(x) \text{ is differentiable a.e.,} \\ &3)\quad \psi'(x) \in D_Q. \end{aligned} \tag{12–13}$$

With these restrictions on the domain, the following operations can be carried out:

$$(PQ\psi)(x) = -i\frac{d}{dx}(x\psi(x)) = -i\psi(x) - ix\frac{d\psi(x)}{dx},$$

$$(QP\psi)(x) = -ix\frac{d\psi(x)}{dx},$$

so that, for all such $\psi(x)$,

$$[Q, P]\psi(x) = i\psi(x).$$

We have thus constructed the *Schrödinger representation* of the canonical commutation rules.

The exponential form of this representation, that is, the representation of relation (12–6), is given by the formulas

$$\begin{aligned} (U_\alpha\psi)(x) &= \psi(x + \alpha) \\ (V_\beta\psi)(x) &= e^{i\beta x}\psi(x). \end{aligned} \tag{12–14}$$

It follows from these formulas that

$$(U_\alpha V_\beta \psi)(x) = e^{i\beta(x+\alpha)}\psi(x + \alpha),$$
$$(V_\beta U_\alpha \psi)(x) = e^{i\beta x}\psi(x + \alpha),$$

and we have verified Eq. (12-6).

We turn now to the question of the uniqueness of the irreducible representation of the commutation rules. This question is much easier to answer for the representation of Weyl's commutation rules than for the unbounded ones. For Weyl's form, von Neumann has proved the uniqueness of the irreducible representation up to unitary equivalence [1]. Many other proofs have been given since. We may thus state the

> ***Theorem*** (von Neumann): *Every irreducible representation of the commutation relations* $U_\alpha V_\beta = e^{i\alpha\beta} V_\beta U_\alpha$ *is unitarily equivalent to the Schrödinger representation* (Eq. 12–14).

We shall not prove this theorem here, but we shall show that it is a corollary of another theorem, of much greater generality, due to Frobenius and Mackey, which plays a very important role in quantum mechanics. This is the theorem on *systems of imprimitivities.* This notion appears in the following way:

Given a topological space M (the "configuration space" of the particle) together with a locally compact transformation group G which acts transitively on M. This means there exists a function $(q, x) \equiv [q]x$ on $M \times G$ ($q \in M, x \in G$) with values in M with the following properties:

a) For each fixed $x \in G$ the function $q \to [q]x$ is a one-to-one and continuous mapping of M onto itself.

b) $[[q]x_1]x_2 = [q]x_1x_2$ for all $x_1, x_2 \in G$ and all q.

c) $[q]e = q$.

d) if $q_1, q_2 \in M$, there exists an $x \in G$ such that $[q_1]x = q_2$ (transitivity).

Let us further assume that we are given a projection-valued measure on the Borel sets of M and a representation of the group G, $x \to U_x$ such that

$$U_x^{-1} E_\Delta U_x = E_{[\Delta]x}, \tag{12–15}$$

where $[\Delta]x$ denotes the set $\{q : [q]x^{-1} \in \Delta\}$ obtained from Δ by the action of the group element x on the configuration space.

A projection-valued measure $\Delta \to E_\Delta$ which satisfies the fundamental relation (12-15) is called a *transitive system of imprimitivities* for the representation $x \to U_x$ based on the space M.

A comparison of (12-15) with (12-3) shows immediately that the propositions E_Δ representing the localization of a particle in the Borel sets Δ are a transitive system of imprimitivities based on the real line Λ. Here the group G is the translation group of Λ. It is obviously transitive.

The greater generality of the imprimitivity system, which is so useful for later application, is that we admit for M any topological space and for G any group which acts continuously and transitively on M.

For every M and every group G, we can always construct a special system of imprimitivities called the *canonical* system, defined in the following way:

Let $\mu(\Delta)$ be a measure on M with the property $\mu_x(\Delta) \equiv \mu([\Delta]x) \sim \mu(\Delta)$. This means that all the measures which are obtained by the action of the group on the space M are equivalent to one another. One can prove that such a measure always exists and that it is unique up to equivalence. For instance, in the example of system (12–3), the measure in question is simply Lebesgue measure on the real line. In this particular case the measure is even *invariant* under the translations. What we need is, however, only the weaker condition $\mu_x(\Delta) \sim \mu(\Delta)$. We call such a measure *quasi-invariant* under the group G.

Such a measure defines the unique Radon-Nikodym derivative (cf. Section 1-4) $d\mu_x/d\mu$, which is an a.e. positive bounded function for all $x \in G$.

We can then define a Hilbert space $L_\mu(M)$ consisting of all complex valued measurable functions $f(q)$ over M which are square-integrable:

$$\int_M |f(q)|^2 \, d\mu < \infty.$$

The transformation U_x defined by

$$(U_x f)(q) = \sqrt{(d\mu_x/d\mu)} f([q]x) \tag{12–16}$$

is then easily verified to be unitary.

We define the projection-valued measure $\Delta \to E_\Delta$ by setting

$$(E_\Delta f)(q) = 1_\Delta(q) f(q), \tag{12–17}$$

where $1_\Delta(q)$ is the characteristic function of the set Δ

$$1_\Delta(q) = \begin{cases} 1 & \text{for } q \in \Delta, \\ 0 & \text{for } q \notin \Delta. \end{cases}$$

This measure defines a system of imprimitivities with respect to the representation $x \to U_x$. To see this, it suffices to verify the equation (Problem 5)

$$(U_x^{-1} E_\Delta U_x f)(q) = (E_{[\Delta]x} f)(q). \tag{12–18}$$

We shall call it a *canonical system of imprimitivities.*

This procedure of constructing systems of imprimitivities can be generalized as follows: we consider an arbitrary point $q_0 \in M$ together with the subgroup G_0 of G which consists of all those transformations which leave the point q_0 invariant. We shall denote the elements of this subgroup G_0 by

means of Greek letters so that

$$[q_0]\xi = q_0 \qquad \forall\ \xi \in G_0,$$

and we call G_0 the "little group."

The choice of the point q_0 is arbitrary. The group will of course depend on that choice. However, the group associated with another choice q_0' will be a conjugate subgroup (Problem 6).

Next we consider an irreducible representation $\xi \to L_\xi$ of G_0 by unitary operators L_ξ in a Hilbert space $\mathscr{H}_0$. We can now construct a new Hilbert space $\mathscr{H}^{\mathrm{L}}$ in the following way. The elements of $\mathscr{H}^{\mathrm{L}}$ are functions $f(x)$ on the group G with values in $\mathscr{H}$ which satisfy the following conditions:

a) $(f(x), g)$ is a measurable function for all $g \in \mathscr{H}_0$.

b) for all $x \in G$ and all $\xi \in G_0$, one has

$$f(\xi x) = L_\xi f(x).$$

c) $\int_M \|f(x)\|^2\, d\mu(q) < \infty.$

Property (c) needs an explanation. The functions $f(x)$ are defined on the group G but the integration is extended over the space M. This is possible because of condition (b), the quantity $\|f(x)\|^2$ is constant on all right cosets and the latter are in one-to-one correspondence with the points $q \in M$ (Problem 7). Since every element $x \in G$ is in exactly one right coset, there exists a natural homomorphism from G to M which is given explicitly by $x \to [q_0]x$.

For the same reason, we can also define the scalar product between two functions $F = \{f(x)\}$ and $G = \{g(x)\}$ by writing

$$(F, G) = \int_M (f(x), g(x))\, d\mu(q).$$

If addition and multiplication is defined by

$$F + G = \{f(x) + g(x)\}$$

$$\lambda F = \{\lambda f(x)\},$$

we obtain a Hilbert space $\mathscr{H}^{\mathrm{L}}$. For each $x \in G$ we define a unitary operator U_x^{L} by setting

$$(U_x^{\mathrm{L}} f)(y) = f(yx)\sqrt{\rho_x(y)}. \qquad (12\text{–}16)'$$

Here we have denoted by $\rho_x(y)$ the Radon-Nikodym derivative of the measure $\mu_x(\Delta) \equiv \mu([\Delta]x)$ with respect to the measure $\mu(\Delta)$.

It is now easily verified that the operators U^{L} are a unitary representation of the group G in the space $\mathscr{H}^{\mathrm{L}}$. It is called an *induced* representation.

Equipped with this representation, we can define a generalized irreducible canonical system of imprimitivities by setting

$$(E_\Delta f)(x) = 1_\Delta([q_0]x)f(x). \qquad (12\text{–}17)'$$

The verification of the relation

$$((U_x^{\mathrm{L}})^{-1}E_\Delta U_x^{\mathrm{L}}f)(y) = (E_{[\Delta]x}f)(y) \qquad (12\text{–}18)'$$

is then just as easy as that of the corresponding relation (12–18).

There exists a very powerful theorem which states that every irreducible system of imprimitivities is unitarily equivalent to one of the canonical ones that we have constructed.

More explicitly, if $\Delta \to E_\Delta$ is such a system, where E_Δ are projections in the representation space $\mathscr{H}$ of the representation $x \to U_x$, then there exists an irreducible unitary representation L of the little group and a unitary mapping W which maps $\mathscr{H}$ onto $\mathscr{H}^{\mathrm{L}}$ such that the image system of imprimitivities under this mapping is a canonical one [5, 6].

For the proof of the uniqueness of the commutation rules in Weyl's form, we need only a special case of this theorem. For in this particular case, the space M is the real line and the group G its one-parameter translation group, the little group G_0 is the trivial group $\{e\}$ and its representation is unity. Thus the particular irreducible imprimitivity system (12–3) is unique (up to unitary equivalence) and this establishes the uniqueness of the commutation rules (12–6) in the same sense.

This theorem has many useful applications. For instance the uniqueness theorem of the canonical commutation rules in Weyl's form (12–6) is a corollary of the imprimitivity theorem. Indeed any irreducible representation of (12–6) will determine a system of imprimitivities which is obtained from (12–6) by choosing for the E_Δ the spectral projections of U_α. Since such a system is unique up to unitary equivalence, the same is true for the representation of (12–6).

The more general imprimitivity theorem permits the definition of localizability in other than Euclidean spaces, for instance on the surface of a sphere. This notion is also needed for the quantum mechanics of systems subject to constraints where position operators may not exist.

We have now established the uniqueness of the representations of Weyl's commutation rules (12–6) on the basis of the imprimitivity theorem. Every such representation furnishes also a representation of the canonical commutation rules (12–10). But the converse is not true; the uniqueness of (12–6) does not imply the uniqueness of (12–10). The reason for this asymmetry is the fact that operators which satisfy relations such as (12–10) cannot both be bounded (cf. Problem 4). Hence they are never definable on the entire Hilbert space. When this is the case, then the relations (12–10) do not imply the relations (12–6) even if Q and P are essentially self-adjoint on their respective domains.

It is possible to impose additional conditions on the operators P and Q, so that their representations also become unique. Such additional conditions have been formulated by Rellich [7], Dixmier [8], Sz.-Nagy *et al.* [9], and Kilpi [10]. Unfortunately none of these conditions have any obvious physical interpretation.

PROBLEMS

*1. The Schrödinger representation of the canonical commutation rules defines two essentially self-adjoint operators on the domain D given by the three conditions (12–13) (cf. reference 4).

2. An irreducible representation of a system of imprimitivities determines a maximal abelian von Neumann algebra $\mathcal{A} = \{E_\Delta\}''$ generated by the projections E_Δ.

3. In any irreducible representation of the canonical commutation rules $[Q, P] = i$, the spectrum of Q and P is simple.

4. The symmetrical operators Q and P which satisfy $[Q, P] = i$ on some dense domain cannot both be bounded.

5. Define E_Δ and U_x as in Eq. (12–17) and (12–16); then

$$U_x^{-1} E_\Delta U_x = E_{[\Delta]x}.$$

6. If G_1 is the subgroup of G which leaves $q_1 \in M$ invariant and G_2 is similarly defined for another point $q_2 \in M$, then the two groups G_1 and G_2 are similar: There exists an element $x \in G$ such that $G_2 = x^{-1} G_1 x$.

7. If G_0 is a subgroup of G acting an a homogeneous space M, then the right cosets of G_0 are in one-to-one correspondence with the points $q \in M$. This correspondence is a homeomorphism.

12-4. THE ELEMENTARY PARTICLE

With the representation theory of the canonical commutation rules out of the way, we can now give a precise definition of the notion of an "elementary particle." Let M be the three-dimensional Euclidean space and G the translation group in M. We define:

> *A localizable system with the system of imprimitivities* $\{E_\Delta, U_x\}$ *describes an* elementary particle *if the system of imprimitivities is irreducible.*

Irreducibility means that the only operators which commute with the entire system $\{E_\Delta, U_x\}$ are the multiples of the unit operator. Thus $\{E_\Delta, U_x\}' = \{\lambda I\}$ for elementary particles.

It is convenient to generalize this notion slightly in order to accommodate systems with spins, where the "nonelementary" aspect can be absorbed into

a finite-dimensional matrix algebra. Thus we define:

A localizable system is quasi-elementary *if the ring of bounded operators* $\{E_\Delta, U_x\}'$ *is isomorphic to a finite-dimensional matrix algebra.*

Whether such systems exist in nature is a question of experience. As far as we know there are many systems which have this property to a very good degree of approximation. However, one justifiably doubts whether the notion can have an absolute and fundamental significance. A great many particles such as nucleons, mesons, electrons in very energetic collisions behave more like systems with an internal structure which would require, for its complete description, the introduction of many more degrees of freedom than there would be available from the operators $\{E_\Delta, U_x\}$. Notwithstanding this reservation, the notion of elementary particles is certainly useful for a large number of physical systems even if it is only approximate.

12-5. VELOCITY AND GALILEI INVARIANCE

The postulates of localizability and homogeneity have led us to a fairly complete description of the kinematical aspect of an elementary particle. As to the dynamical characteristics we know that the state of an isolated elementary particle will evolve according to the solution of a Schrödinger equation, expressed by a unitary group $U_t = e^{-iHt}$. But the principles which we have enunciated so far will give us no information about the nature of the evolution operator H. We shall now introduce new principles which will give us such information.

We begin with the definition of the *velocity*. As an observable, the velocity must be represented by a self-adjoint operator. It can be obtained from the position operator $Q(t) = U_t^{-1} Q U_t$ in the Heisenberg picture by a formal differentiation with respect to the time t. In this way we find that $\dot{Q}(0) \equiv \dot{Q}$ is given by

$$\dot{Q} = i[H, Q]. \tag{12–19}$$

In this equation we have ignored questions pertaining to the domains associated with the unbounded operators. Such questions would have to be discussed if the arguments in this section were to be made mathematically rigorous.

It is seen from this definition that the velocity will in general depend on H. Conversely if we impose certain properties on $\dot{Q}$, then we must expect that they will restrict the evolution operator H.

In order to motivate the conditions which we shall impose on $\dot{Q}$, we consider for a moment the classical situation. The velocity $\dot{Q}$ depends on the system of reference with respect to which the velocity is measured. Thus if we change the system of reference to a new system which moves with the

constant velocity v with respect to the old system then the velocity of a particle will change according to

$$\dot{Q} \to \dot{Q} + v. \tag{12–20}$$

It is well known that the classical equations of motion are invariant under this transformation. We are thus led to consider the same transformation (12–20) in quantum mechanics, supplemented by the condition $Q \to Q$. We shall refer to such a transformation as the *Galilei transformation.*

In analogy to the classical principle of Galilei invariance, we would expect that in nonrelativistic quantum mechanics the transformation (12–20) should have a special significance. Inspired by this analogy we may formulate a *principle of Galilei invariance*:

> *The Galilei transformations* (12–20) *induce symmetry transformations in the lattice of propositions.*

Let us now examine the consequences of this principle for an elementary particle in a one-dimensional space.

If Eq. (12–20) is a symmetry transformation, then this means that there exists a one-parameter unitary group G_v with the properties

$$\dot{Q} + v = G_v \dot{Q} G_v^{-1} \tag{12–21}$$

and

$$G_{v_1} G_{v_2} = G_{v_1 + v_2}. \tag{12–22}$$

Furthermore, since Q remains unchanged under Galilei transformation, G_v commutes with Q. Since the system is elementary, this implies that G_v is a function of Q. By Stone's theorem we may write $G_v = e^{iKv}$ with $K = u(Q)$, where u is some Borel function on the real line.

We can go a step further if we combine the Galilei transformation with the displacements discussed in the preceding sections. We define the two-parameter family of unitary operators $W(\alpha, v)$ with the properties

$$\begin{aligned} Q + \alpha &= W(\alpha, v) Q W^{-1}(\alpha, v), \\ \dot{Q} + v &= W(\alpha, v) \dot{Q} W^{-1}(\alpha, v). \end{aligned} \tag{12–23}$$

This shows that $W(\alpha, v)$ is a projective representation of the translation of the plane:

$$W(\alpha_1, v_1) W(\alpha_2, v_2) = \omega(\alpha_1, \alpha_2; v_1, v_2) W(\alpha_1 + \alpha_2, v_1 + v_2). \tag{12–24}$$

According to the general theory of such representations (cf. Section 9-6), it is possible to choose the arbitrary phase factors in the definition of W in such a way that the factor ω in Eq. (12-24) assumes the form

$$\omega(\alpha_1, \alpha_2; v_1, v_2) = e^{i(\mu/2)(\alpha_1 v_2 - \alpha_2 v_1)}, \tag{12–25}$$

where μ is an arbitrary real constant which distinguishes the different inequivalent projective representations of the two-dimensional translation groups.

The two one-parameter subgroups U_α and G_v are recovered by specializing the parameter values according to

$$U_\alpha = W(\alpha, 0), \qquad G_v^{-1} = W(0, v). \tag{12–26}$$

Specialized to these two subgroups, the relations (12–24) and (12–25) become

$$U_\alpha G_v^{-1} = e^{i\mu\alpha v} G_v^{-1} U_\alpha. \tag{12–27}$$

Comparison of this equation with Eq. (12–6) shows that a possible solution is obtained by setting

$$G_v^{-1} = V_{\mu v} = e^{i\mu v Q}; \tag{12–28}$$

and we conclude from the representation theorem of the preceding section that every other solution must be unitarily equivalent to it.

Before we proceed further, we shall examine the case $\mu = 0$. In this case we see from (12–27) that G_v commutes with U_α. According to the remark following Eq. (12–22), it also commutes with Q and hence with V_β. Since the system is supposed to be an elementary particle we conclude that G_v must be a multiple of the identity. But this is impossible, since it contradicts Eq. (12–21). Hence, we conclude $\mu \neq 0$ [11].

Proceeding now with the expression (12–28), we find that

$$\frac{1}{\mu} P + v = \frac{1}{\mu} G_v P G_v^{-1}. \tag{12–29}$$

By taking the difference of (12–29) and (12–21), we obtain the result that $(1/\mu)P - \dot{Q}$ commutes with G_v and therefore with Q, and so it can only be a function $u(Q)$ of Q. We have thus derived the fundamental relation

$$\dot{Q} = \frac{1}{\mu} P + u(Q). \tag{12–30}$$

The function $u(Q)$ depends on the representation of P. For a given Q we can always find a representation of P such that $u(Q) = 0$. In order to see this, it suffices to show that there exists a canonical transformation S which commutes with Q and which transforms P according to $SPS^{-1} = P - \mu u(Q)$ (Problem 1). Thus, replacing P by SPS^{-1} we find the relationship

$$\dot{Q} = \frac{1}{\mu} P. \tag{12–31}$$

If we combine this result with Eq. (12–19), we find

$$\frac{1}{\mu} P = i[H, Q]. \tag{12–32}$$

From the commutation rules for P and Q, it follows that the operator $H_0 = (1/2\mu)P^2$ satisfies

$$\frac{1}{\mu} P = i[H_0, Q]. \tag{12–33}$$

Thus by taking the difference between Eqs. (12–33) and (12–32), we find that $H - H_0$ commutes with Q. Since we assumed that our system is an elementary particle, it follows that $H - H_0$ is a function of Q. Let us denote it by $v(Q)$.

We have thus found the most general evolution operator which is compatible with the principle of Galilei invariance. It has the form

$$H = \frac{1}{2\mu} P^2 + v(Q). \tag{12–34}$$

Moreover, we have shown that the displacement operator P is proportional to the velocity operator $\dot{Q}$. (More precisely, we can always adopt a representation so that it is.) The function $v(Q)$ can be interpreted as the effect of an external force acting on the particle. Classically it would represent the potential of that force. The function $v(Q)$ might even depend explicitly on time. In that case the evolution of the state is no longer described by a group, and some modification in the preceding derivation is necessary.

For the special case in which H is invariant under displacements, the function $v(Q)$ must reduce to a constant. We shall refer to this case as a *free* particle.

We see from the foregoing that localizability and Galilei invariance, in the form which we have given it, lead to a one-parameter family of elementary particles distinguished by the real parameter μ.

Let us now study the physical significance of the parameter μ. In order to do this we refer to the classical aspects of an elementary particle. Classically such a system would be described by the movement of a point in configuration space, which in our example is the real line. It is therefore natural to identify the classical motion of the particle with the motion of the expectation value of the position operator. We shall denote this value by x, so that

$$x = \operatorname{Tr} WQ, \tag{12–35}$$

where W is the density operator for the quantum-mechanical state. The velocity is then given by

$$\frac{dx}{dt} = \operatorname{Tr} \dot{W}Q = \operatorname{Tr} W\dot{Q} = i \operatorname{Tr} W[H, Q] = \frac{1}{\mu} \operatorname{Tr} WP,$$

and for the momentum we find

$$m \frac{dx}{dt} = \frac{m}{\mu} \operatorname{Tr} WP, \tag{12–36}$$

where m is the mass of the particle. We thus see that the operator $p = (m/\mu)P$ may be interpreted as the momentum operator. The quantity m/μ which connects the displacement operator with the momentum operator is a fundamental universal constant of the theory, which can be determined by any experiment which relates the measurement of a wavelength (for instance, a diffraction) to that of a momentum or energy. This constant is Planck's constant

$$\frac{m}{\mu} = \hbar = \frac{h}{2\pi}.$$

It has the approximate value

$$\hbar \simeq 1.05 \times 10^{-27} \text{ erg sec.}$$

We can pursue the classical limit even further. If we calculate the second derivative of x with the same method, we obtain

$$m \frac{d^2x}{dt^2} = -\hbar \operatorname{Tr}\left(W \frac{dv}{dQ}\right). \tag{12–37}$$

The operator $\hbar v(Q) \equiv v(Q)$ may thus be interpreted as the potential energy of the particle. Consistently with this we would interpret

$$\frac{\hbar}{2\mu} P^2 = \frac{1}{2m} p^2 \tag{12–38}$$

as the kinetic energy, and $\hbar H$ as the total energy of the particle.

The relations which we have now established lead to a simple rule which permits the transition from a classical to a quantum system. If, in the classical analogue of a spinless one-particle problem, we have a total energy of the form

$$E(p, q) = (1/2m)p^2 + V(q),$$

then we obtain the quantum mechanical evolution operator for such a system by reinterpreting the quantities p and q according to the formulas

$$p = \hbar P, \qquad q = Q, \qquad E = \hbar H.$$

PROBLEM

1. If Q and P are canonical operators, there exists a unitary operator S which commutes with Q and which transforms P according to

$$SPS^{-1} = P + v(Q),$$

where v is an arbitrary Borel function of a real variable.

12-6. THE HARMONIC OSCILLATOR

The simple harmonic oscillator in classical mechanics is a mechanical system of one degree of freedom with a total energy expression of the form

$$E = \frac{1}{2m} p^2 + \frac{f}{2} x^2. \tag{12–39}$$

According to the rule of the preceding section, the quantum-mechanical harmonic oscillator is characterized by the position operator Q, the displacement operator $P = (1/\hbar)p$ and the evolution operator

$$H = \frac{1}{2\mu} P^2 + \frac{f}{2\hbar} Q^2. \tag{12–40}$$

We define the characteristic frequency ω of the oscillator

$$\omega = \sqrt{\frac{f}{m}} = \sqrt{\frac{f}{\mu\hbar}}, \tag{12–41}$$

and carry out the canonical transformation

$$Q \to \sqrt[4]{\frac{f\mu}{\hbar}}\, Q, \qquad P \to \sqrt[4]{\frac{\hbar}{\mu f}}\, P;$$

then we obtain for H in the new variables the expression

$$H = \frac{\omega}{2} (P^2 + Q^2). \tag{12–42}$$

The properties of this operator can be established in considerable detail. For the following calculations we shall omit the constant ω and reintroduce it in the final result.

It is easily seen that the operator H is a positive definite operator, since, for any $\psi \in D_P$ and $\psi \in D_Q$,

$$(\psi, H\psi) = \tfrac{1}{2} \|P\psi\|^2 + \tfrac{1}{2} \|Q\psi\|^2 > 0.$$

The operator H is also strictly positive since from $(\psi, H\psi) = 0$, it would follow that $P\psi = Q\psi = 0$, which is impossible because of the commutation rules given by Eq. (12–10).

Next we show that the operator H has at least one eigenvalue. To this end we introduce the "annihilation" and "creation" operators defined by

$$a = \frac{1}{\sqrt{2}} (Q + iP), \qquad a^* = \frac{1}{\sqrt{2}} (Q - iP). \tag{12–43}$$

On a dense domain of $\mathcal{H}$, these operators satisfy the commutation rules

$$[a, a^*] = 1. \tag{12–44}$$

Furthermore, we have the relations

$$a^*a = \tfrac{1}{2}(P^2 + Q^2 - 1); \qquad aa^* = \tfrac{1}{2}(P^2 + Q^2 + 1),$$

so that

$$H = \tfrac{1}{2}(a^*a + aa^*) = a^*a + \tfrac{1}{2} \equiv N + \tfrac{1}{2}. \tag{12–45}$$

Let ψ_0 be a normalized vector which satisfies

$$a\psi_0 = 0 \tag{12–46}$$

When this equation is expressed in the Schrödinger representation, we find that $\psi_0(x)$ is the solution of the differential equation

$$x\psi_0(x) + \frac{d\psi_0(x)}{dx} = 0. \tag{12–47}$$

The solution of this equation is given by

$$\psi_0(x) = Ae^{-(x^2/2)}. \tag{12–48}$$

The real integration constant A is determined by normalization:

$$1 = \int_{-\infty}^{+\infty} |\psi_0(x)|^2 \, dx = A^2 \int_{-\infty}^{+\infty} e^{-x^2} \, dx = A^2\sqrt{\pi}$$

or

$$A = \frac{1}{\sqrt[4]{\pi}},$$

so that

$$\psi_0(x) = \frac{1}{\sqrt[4]{\pi}} e^{-(x^2/2)}. \tag{12–49}$$

This normalized vector of the space $\mathscr{H} = L^2(-\infty, +\infty)$ is thus an eigenvector of N with the eigenvalue 0.

We can obtain a whole series of further eigenvectors if we use the commutation rules (12–44) which yield the two formulas

$$Na = a(N - 1), \qquad Na^* = a^*(N + 1). \tag{12–50}$$

Consider now the vector $\psi_1 = a^*\psi_0$. It satisfies

$$Na^*\psi_0 = a^*(N + 1)\psi_0 = a^*\psi_0.$$

It is thus an eigenvector of N to the eigenvalue 1. Furthermore

$$\begin{aligned} \|a^*\psi_0\|^2 &= (\psi_0, aa^*\psi_0) \\ &= (\psi_0, (1 + a^*a)\psi_0) \\ &= \|\psi_0\|^2 = 1, \end{aligned}$$

so that it is also normalized.

We can continue this process and define the vector

$$\psi_n = \frac{1}{\sqrt{n!}} (a^*)^n \psi_0.$$

It is eigenvector of N to the eigenvalue n and it is normalized (Problem 1)

$$N\psi_n = n\psi_n \qquad \|\psi_n\| = 1.$$

In this manner we have obtained an infinite sequence of normalized eigenvectors of N, one for each of the nonnegative integers n.

The eigenfunctions can be expressed explicitly in the Schrödinger representation.

$$\psi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} \left(x - \frac{d}{dx}\right)^n e^{-x^2/2}. \tag{12–51}$$

The execution of the differential operator leads to an expression of the form

$$\left(x - \frac{d}{dx}\right)^n e^{-x^2/2} = H_n(x) e^{-x^2/2},$$

where $H_n(x)$ is a polynomial of the nth degree in the variable x, the so-called Hermite polynomial.

Explicit evaluation of the first few polynomials give:

$$H_0(x) = 1; \qquad H_1(x) = 2x;$$

$$H_2(x) = 4x^2 - 2;$$

$$H_3(x) = 8x^3 - 12x.$$

The general formula is (Problem 2)

$$H_n(x) = \sum_{k=0}^{[n/2]} \frac{(-1)^k n!}{k!(n-2k)!} (2x)^{n-2k},$$

where $[n/2]$ denotes the greatest integer $\leq n/2$. These polynomials satisfy the differential equation

$$H_n'' - 2xH_n' + 2nH_n = 0,$$

and the recursion relation

$$H_{n+1} - 2xH_n + 2nH_{n-1} = 0.$$

We shall now show that the system of eigenvectors $\psi_n(x)$, $(n = 0, 1, 2, \ldots)$, is complete in $\mathscr{H}$ if P and Q are irreducible in $\mathscr{H}$. To this end let $\mathscr{H}_0 \subseteq \mathscr{H}$ be the space spanned by the vectors ψ_n and denote by E the projection with range $\mathscr{H}_0 = E\mathscr{H}$. If $f \in \mathscr{H}_0^{\perp}$, then $(f, \psi_n) = 0$ for all n. Since

$$(af, \psi_n) = (f, a^*\psi_n) = \sqrt{\frac{(n+1)!}{n!}} (f, \psi_{n+1}) = 0,$$

and

$$(a^*f, \psi_n) = (f, a\psi_n) = \sqrt{\frac{(n-1)!}{n!}}\,(f, \psi_n) = 0,$$

it follows that $\mathscr{H}_0$ and $\mathscr{H}_0^{\perp}$ are invariant under a and a^*. Thus the projection E reduces a and a^*; consequently it also reduces

$$Q = \frac{1}{\sqrt{2}}\,(a + a^*)$$

and

$$P = \frac{1}{i\sqrt{2}}\,(a - a^*).$$

Since Q and P are irreducible, it follows that $E = 0$ or $E = I$. The first alternative is impossible; hence $E = I$. This means that

$$(f, \psi_n) = 0 \qquad \text{for all } n \qquad \text{implies } f = \theta,$$

and we have proved that the system ψ_n is a complete system.

With this the operator $H = (\omega/2)(Q^2 + P^2)$ is completely analyzed with the result: There exists a complete system of eigenvectors ψ_n with the eigenvalues $\lambda_n = \omega(n + \frac{1}{2})$ with $n = 0, 1, 2, \ldots$ Each eigenvalue is nondegenerate.

PROBLEMS

1. The vector $\psi_n = (1/\sqrt{n!})\,(a^*)^n\psi_0$ is a normalized eigenvector of $N = a^*a$ with eigenvalues n.
2. $(x - (d/dx))^n e^{-(x^2/2)} = H_n(x)e^{-(x^2/2)}$, where

$$H_n(x) = \sum_{k=0}^{[n/2]} \frac{(-1)^k n!}{k!(n-2k)!}\,(2x)^{n-2k},$$

   and $[n/2]$ denotes the largest integer $\leq n/2$.
3. The calculation of the eigenfunctions and eigenvalues of the evolution operator

$$H = \frac{1}{2}P^2 + \frac{\lambda}{2}Q^2, \qquad \text{with } \lambda > 0,$$

   can be reduced to that of the harmonic oscillator by the substitutions

$$P \to \sqrt[4]{\lambda}\,P, \qquad Q \to \frac{1}{\sqrt[4]{\lambda}}\,Q.$$

4. The eigenfunctions of the operator $H = \frac{1}{2}P^2 + \frac{1}{2}Q^2 + Qa$, with a real, can be determined by carrying out the substitution $Q \to Q + a$.

12-7. A HILBERT SPACE OF ANALYTICAL FUNCTIONS [13]

The great similarity of the commutation relations for the operators a and a^* with those for Q and P raises the question whether the operators a, a^* may be represented as differential and multiplication operators in a suitably defined Hilbert space analogously to the Schrödinger representation of the operators Q and P. In such a space the vector ψ_0 would be represented by the function $f(z) = 1$ (since $a\psi_0 = 0$) and ψ_n would have to be represented by

$$\frac{1}{\sqrt{n!}} z^n \equiv u_n(z);$$

naturally the linear combination $\psi = \sum_n c_n \psi_n$, with $\sum_n |c_n|^2 < \infty$, would be represented by the entire analytical function

$$f(z) = \sum_n \frac{c_n}{\sqrt{n!}} z^n.$$

Such functions are clearly a linear vector space. In order to have a Hilbert space, it is necessary to complete this structure of linear vector space by a scalar product between any two such functions f, g. This product must be consistent with the fact that a^* is the Hermitian conjugate of a. Thus we must have, for any pair of vectors f, g from the domain of a and a^*,

$$\left(f, \frac{dg}{dz}\right) = (zf, g). \tag{12–52}$$

In particular, for the functions $u_n = \{u_n(z)\}$, we must have $(u_n, u_m) = \delta_{nm}$. If we write the scalar product in the form

$$(f, g) = \int f^*(z) g(z)\, d\mu(z), \tag{12–53}$$

then $d\mu(z)$ is a positive measure in the complex z-plane C which is completely determined by the preceding conditions. Indeed from these conditions it follows that

$$(z^n, z^m) = \sqrt{n!m!}\, \delta_{nm}. \tag{12–54}$$

In particular, for $n = m$,

$$\int_C |z|^{2n}\, d\mu(z) = n!. \tag{12–54}'$$

The set of equations (12–54)′ are the conditions for a moment problem. As is well known from the theory of this problem, these conditions determine the positive measure $d\mu(z)$ uniquely. The measure which has this property for all values of n is

$$d\mu(z) = \frac{1}{\pi} e^{-|z|^2} dx\, dy.$$

where $z = x + iy$ and $dx\,dy$ denotes the Lebesgue measure in the complex z-plane.

We denote the Hilbert space thus constructed by $\mathscr{F}$. It is isomorphic to the space $\mathscr{H}$ spanned by the eigenvectors ψ_n of the harmonic oscillator. The explicit form of the isomorphism is given by the formula:

$$f(z) = \sum_{n=0}^{\infty} \frac{(\psi_n, f)}{\sqrt{n!}} z^n. \tag{12–55}$$

This realization has some remarkable properties which we shall briefly sketch here.

The space $\mathscr{F}$ is a function space, but because its elements are *analytical* functions, the space differs in some respects from an L^2-space of complex-valued functions. We recall that, in the latter space, it is not the functions themselves which are the elements of the space but rather classes of equivalent functions, where two functions are called equivalent if they differ at most on a set of measure zero.

In the space $\mathscr{F}$, on the other hand, every element is represented by exactly one function and not by a class of equivalent functions. This is so because two analytical functions which differ at most on a set of measure zero are identical. Another consequence of the same order is the fact that if a sequence of functions $f_n(z)$ converges in the mean to a limit function $f(z)$, then the functions converge pointwise to $f(z)$.

To the particular vector $f = \psi_0$ corresponds the function $f(z) = 1$. The operators a and a^* are represented by d/dz and by z, respectively.

The harmonic-oscillator problem in this representation is defined by the evolution operator $H = a^*a = z(d/dz)$. The eigenvectors $\varphi_n(z)$ are thus the properly normalized solutions of the differential equation

$$z \frac{d}{dz} \varphi_n(z) = n\varphi_n(z), \tag{12–56}$$

given by $\varphi_n(z) = (z^n/\sqrt{n!})$.

A characteristic property of this space is the existence of a family of principal vectors e_α for each value of the complex number $\alpha = \alpha_1 + i\alpha_2$. They are defined in the following manner. For each value of α we consider the bounded linear functional (cf. Problem 6)

$$L_\alpha(f) = f(\alpha). \tag{12–57}$$

According to the theorem of Riesz (cf. Section 3-1), every such functional determines a unique vector $e_\alpha \in \mathscr{F}$ such that

$$(e_\alpha, f) = f(\alpha). \tag{12–58}$$

From $(a^*f)(z) = zf(z)$ we find

$$(e_\alpha, a^*f) = \alpha f(\alpha) = (ae_\alpha, f) = (\alpha^* e_\alpha, f)$$

for all $f \in \mathscr{F}$. Thus $ae_\alpha = \alpha^* e_\alpha$. When this relation is expressed in $\mathscr{F}$ it reads

$$\frac{de_\alpha(z)}{dz} = a^* e_\alpha(z),$$

from which we obtain

$$e_\alpha(z) = e^{\alpha^* z}. \tag{12–59}$$

Here we have already chosen the correct normalization factor which is determined by the condition $(e_\alpha, e_\alpha) = e_\alpha(\alpha)$. This may be rewritten and verified as the identity

$$\frac{1}{\pi}\int e^{\alpha z^* + \alpha^* z - |z|^2}\, dx\, dy = e^{|\alpha|^2}. \tag{12–60}$$

The expression (12–59) leads to the remarkable reproducing property for any analytical function $f(z) \in \mathscr{F}$:

$$f(\alpha) = \frac{1}{\pi}\int e^{\alpha z^* - |z|^2} f(z)\, dx\, dy. \tag{12–61}$$

If we choose for f in (12–58) the function e_β, we obtain the relation

$$(e_\alpha, e_\beta) = e^{\beta^* \alpha}. \tag{12–62}$$

The normalized vectors $\psi_\alpha \equiv (1/\|e_\alpha\|)e_\alpha$ are thus given by

$$\psi_\alpha = e^{-(1/2)|\alpha|^2 + \alpha^* z}. \tag{12–63}$$

It is easy to see that the set of vectors e_α is total in f. Indeed if f were orthogonal to all of them, it would have to satisfy $(e_\alpha, f) = f(\alpha) = 0$ for all α; that is, $f = 0$.

On the other hand, the vectors e_α are linearly dependent. This can be seen most easily from the relation $(e_z, e_\beta) = e_\beta(z)$. When the integration on the left is written out explicitly, one obtains

$$\int e_z^*(\alpha) e_\beta(\alpha)\, d\mu(\alpha) = e_\beta(z).$$

Using $e_z^*(\alpha) = e_\alpha(z)$ (cf. Eq. 12–59), this relation becomes

$$\int e_\alpha(z) e_\beta(\alpha)\, d\mu(\alpha) = e_\beta(z), \tag{12–64}$$

which expresses $e_\beta(z)$ linearly in terms of the $e_\alpha(z)$. In spite of this linear dependence of the vectors, it is possible to give a unique expansion of every vector f in terms of the e_α:

$$f = \int c(\alpha) e_\alpha\, d\mu(\alpha), \tag{12–65}$$

provided we subject the $c(\alpha)$ to the additional condition that $c(\alpha)$ be an analytical function of α contained in $\mathscr{F}$. Indeed from the relation (12–65) we can calculate $c(\alpha) = f(\alpha)$. Uniqueness then follows from the completeness relation of the e_α.

It follows from these remarks that any finite set of the vectors e_α is necessarily linearly independent. This gives us the possibility of an intrinsic construction of the Hilbert space $\mathscr{F}$.

Let $e_{\alpha_i} \equiv e_i$ and define the scalar product of two finite linear combinations $f = \sum_{i=1}^{n} \lambda_i e_i$, $g = \sum_{k=1}^{m} \mu_k e_k$ by setting

$$(f, g) = \sum_{i,k} \lambda_i^* \mu_k e^{\alpha_k^* \alpha_i}.$$

This set of vectors provided with this scalar product are a linear manifold $\mathscr{M}$ with a scalar product. This is called a pre-Hilbert space. It can be completed to a Hilbert space by adjoining the limit points. This is the space $\mathscr{F}$.

The remarkable property of the e_α of behaving like a coordinate system, although they are linearly dependent, is brought to light even more explicitly by the fact that in the space $\mathscr{F}$ every linear operator T such that $e_\alpha \in D_T$ is an integral operator and its matrix elements are given by

$$T(\alpha, \beta) \equiv (e_\alpha, Te_\beta). \tag{12–66}$$

We have already seen this for the identity operator for which $T(\alpha, \beta) = e^{\beta^* \alpha}$ (cf. Eq. 12–61). For the general case we prove it by evaluating

$$\begin{aligned}(Tf)(\alpha) &= (e_\alpha, Tf) = (T^* e_\alpha, f) \\ &= \int (T^* e_\alpha)^*(\beta) f(\beta)\, d\mu(\beta) \\ &= \int (Te_\beta)(\alpha) f(\beta)\, d\mu(\beta) \\ &= \int (e_\alpha, Te_\beta) f(\beta)\, d\mu(\beta).\end{aligned}$$

Here we have used the identity $(Te_\beta)^*(\alpha) = (T^* e_\alpha)(\beta)$, which is left as a problem (7).

The states ψ_α are especially useful in connection with the study of coherence properties of radiation (cf. reference 14).

PROBLEMS

1. The vectors e_α have a representation

$$e_\alpha = \frac{(\alpha^*)^n}{\sqrt{n!}} \psi_n$$

[*Hint:* Use the relation $(e_\alpha, f) = f(\alpha)$ together with Eq. (12–55).]

2. Define $U_{\alpha_1} = e^{i\alpha_1 P}$, $V_{\alpha_2} = e^{i\alpha_2 Q}$ and

$$W(\alpha) \equiv e^{-(i/2)\alpha_1\alpha_2} U_{\alpha_1} V_{\alpha_2} \qquad (\alpha = \alpha_1 + i\alpha_2);$$

then

$$W(\alpha)W(\beta) = e^{(i/2)(\alpha_1\beta_2 - \alpha_2\beta_1)} W(\alpha + \beta).$$

3. For each $\alpha = \alpha_1 + i\alpha_2$, one finds

$$W(\alpha)QW^{-1}(\alpha) = Q + \alpha_1, \qquad W(\alpha)PW^{-1}(\alpha) = P - \alpha_2.$$

4. The vector ψ_α can be obtained from ψ_0 by the "translation" $\psi_\alpha = W^{-1}(\alpha)\psi_0$.
5. For any $f \in \mathscr{H}$ one has, for the corresponding $f(z) \in \mathscr{F}$,

$$f(\alpha) = e^{(1/2)|\alpha|^2}(\psi_0, W(\alpha)f).$$

The correspondence L_α, which associates for each $\alpha \in C$ and for each $f(z) \in \mathscr{F}$ the number $f(\alpha)$ is a bounded linear functional.

6. The bound of the linear functional L_α is $e^{(1/2)|\alpha|^2}$. From this one obtains the inequality

$$f(z) \leq e^{(1/2)|z|^2} \|f\|,$$

valid for all $f \in \mathscr{F}$.

7. For any linear operator T in $\mathscr{F}$ such that $e_\alpha \in D_T$ we have

$$(Te_\beta)^*(\alpha) = (T^* e_\alpha)(\beta).$$

12-8. LOCALIZABILITY AND MODULARITY

In Section 5-6 we discussed the notion of modularity, and we stated there without proof that modularity is incompatible with localizability. In this section we shall give the proof of this assertion. It involves studying the structure of the lattice generated by the projection operators of Q and P.

Let us denote by E_Δ the spectral projection of the spectral measure of Q associated with the Borel set Δ on the real line. Similarly we denote by F_Δ the corresponding spectral projection of P. We define the lattice L generated by E_Δ and F_Δ as the smallest lattice of projections which is complete and closed under countably infinite operations of unions and intersections of projections in L. The intersection of any pair of projections $X, Y \in L$ is defined by

$$X \cap Y = \lim_{n \to \infty} (XY)^n,$$

and the union is defined by

$$X \cup Y = I - (I - X) \cap (I - Y).$$

If X_n is any sequence of projections in L then by definition the projections $\bigcap X_n$ and $\bigcup X_n$ are also in L. Furthermore L contains all the projections E_Δ and F_Δ, and it is the smallest lattice with these properties.

The question which we wish to answer here is whether the lattice L thus defined is modular or not. If L were identical with the lattice of all projections, our task would be finished, because we have shown in Section 5-7 that this lattice is nonmodular. But it is not certain whether this is the case, and so we must employ more powerful results to prove the nonmodularity of L.

The crucial property which we need for this proof is the $\bigcap$-continuity and its dual, the $\bigcup$-continuity, which we shall formulate now.

A lattice is called $\bigcap$-continuous if, for every nondecreasing sequence $\cdots \leq a_{n-1} \leq a_n \leq a_{n+1} \leq \cdots$ and every $b \in \mathscr{L}$, we have

$$b \cap \left(\bigcup_n a_n\right) = \bigcup_n (b \cap a_n).$$

A lattice is called $\bigcup$-continuous if, for every nonincreasing sequence $\cdots \geq a_{n-1} \geq a_n \geq a_{n+1} \geq \cdots$ and every $b \in \mathscr{L}$, we have

$$b \cup \left(\bigcap_n a_n\right) = \bigcap_n (b \cup a_n).$$

We are now equipped to understand the meaning of the following theorem of Kaplansky [12]:

Theorem (Kaplansky): *A complete, orthocomplemented, modular lattice is $\bigcap$-continuous and $\bigcup$-continuous.*

The relevance of this theorem for our problem is evident since the lattice defined above is complete and orthocomplemented. Hence if it is also modular, it satisfies the hypotheses of the theorem and therefore also its conclusion. Thus let us examine whether the lattice $\mathscr{L}$ is $\bigcap$-continuous and $\bigcup$-continuous.

To this end we consider the increasing series of Borel sets

$$\Delta_n = \{\lambda : -n \leq \lambda \leq +n\}.$$

We have

$$\cdots < \Delta_{n-1} < \Delta_n < \Delta_{n+1} < \cdots,$$

and consequently also, for $E_n \equiv E_{\Delta_n}$,

$$\cdots \leq E_{n-1} \leq E_n \leq E_{n+1} \leq \cdots.$$

Furthermore we find that $\bigcup_n E_n = I$. Now let b be represented by a projection $F \equiv F_\Delta$ where Δ is a fixed finite interval on the real line. We then find from $\bigcap$-continuity the relation

$$F \cap \left(\bigcup_n E_n\right) \equiv F = \bigcup_n (F \cap E_n).$$

But this relation is easily seen to be impossible, for the simple reason that every one of the terms $F \cap E_n$ on the right-hand side is the zero projection.

This last property can be seen as follows. If ψ is a vector contained in the range of $F \cap E_n$, then this ψ would appear in the x-representation as a function which vanishes outside the finite interval $\Delta = (-n, +n)$. Its Fourier transform also would vanish outside the finite interval Δ. One can show that such a function must be identically zero. Hence $F \cap E_n = 0$.

With this we have shown that the hypothesis that L is modular is incorrect; hence L is not modular. We have thereby justified the choice of a weaker axiom for the structure of the lattice of propositions.

It should be mentioned that we have proved the nonmodularity of the proposition system only in the context of the usual Hilbert-space formulation of quantum mechanics, under the assumption that the system is localizable. The question of whether localizability can be formulated within a modular lattice of propositions in a more general setting remains open.

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CHAPTER 13

THE ELEMENTARY PARTICLE WITHOUT SPIN

After having reached an opinion for a special case, one gradually modifies the circumstances of this case in one's imagination as far as possible, and in so doing tries to stick to the original opinion as closely as one can.

E. MACH

This chapter is devoted to the quantum mechanics of the spinless elementary particle in three-dimensional space. The first two sections introduce the notions of *localizability, homogeneity* and *isotropy*. The first two are notions which are easily recognized as straightforward generalizations of the analogous notions in one dimension treated in the preceding chapter. The greater richness of the three-dimensional space is mirrored in the new notion of isotropy. It originates from the complexity of the rotation group which is discussed in some detail in Section 13-3. The dynamical structure is introduced as in the preceding chapter via the notion of Galilei invariance (Section 13-4), which largely determines the structure of the evolution operator H. In the following section (13-5) we discuss gauge transformations and we show that gauge invariance is a consequence of Galilei invariance as formulated here. The question of the localization of various observable quantities leads us to the general definition of the densities of observables of which the probability density and the probability current are special cases. The last two sections are devoted to space inversion (13-7) and time reversal (13-8).

13-1. LOCALIZABILITY

In this section we shall formulate the notion of localizability in a Euclidean space of three dimensions. This notion is a generalization of the content of Section 12-1 of the preceding chapter. We aim at a complete quantum-mechanical description of an elementary particle which moves in the three-dimensional physical space E_3. Let us briefly recapitulate the basic concepts which are needed for such a description.

As we explained in Section 12-1, the notion of *localizability* is described by a function $\Delta \to E_\Delta$ which associates with every Borel subset Δ from E_3

a projection operator. The Borel sets Δ are subsets of E_3 and the projections E_Δ are projections representing the yes–no experiments to find the particle in the subsets Δ. We assume again, as before, that these elementary propositions are all compatible and that, therefore, the projection operators all commute with one another. From this property follow the fundamental relations (12–1), which say that the correspondence $\Delta \to E_\Delta$ is a projection-valued measure.

There is an important difference between this measure and the one defined in the preceding chapter. The latter was defined on the Borel sets of the real line, the former on the Borel sets of E_3. A projection-valued measure on the real line defines via the spectral theorem a self-adjoint operator, the position operator.

In E_3 it is also possible to define an operator if the measure $\Delta \to E_\Delta$ represents an elementary system. We define the system as "elementary" if the projections E_Δ generate a maximal abelian von Neumann algebra $\mathscr{A}$, so that

$$\{E_\Delta\}'' = \mathscr{A} = \mathscr{A}'. \tag{13–1}$$

According to a theorem of von Neumann [1], a maximal abelian algebra can always be generated by a single self-adjoint operator X such that $\{X\}'' = \mathscr{A}$. However, such an operator has no physical interpretation. There is no experiment known which would effectuate a measurement of the quantity represented by such an X. From the physical point of view this X is therefore not very useful.

Much more useful are the position operators associated with the three Cartesian coordinates of a point in E_3. We can define them as follows:

Let $E_\lambda^{(r)}$ $(r = 1, 2, 3)$ be the projections associated with the sets

$$\Delta = \{x_1, x_2, x_3 \mid x_r < \lambda\} \qquad (r = 1, 2, 3), \tag{13–2}$$

where x_r are the Cartesian coordinates of a point in E_3. It follows from this definition that

$$E_{\lambda_1}^{(r)} \leq E_{\lambda_2}^{(r)} \qquad \text{for } \lambda_1 < \lambda_2 \qquad \text{and} \qquad E_{-\infty}^{(r)} = 0, \qquad E_{+\infty}^{(r)} = I. \tag{13–3}$$

Thus the $E_\lambda^{(r)}$ are, for each $r = 1, 2, 3$, a spectral family and therefore they define three operators Q_r $(r = 1, 2, 3)$. These operators represent the Cartesian coordinates of the particle. More generally, if $u(x)$ is a measurable function with respect to the measure $\Delta \to E_\Delta$, that is, such that for any $f \in L^2(E_3)$ the function is measurable in the ordinary sense with respect to the numerical measure $\Delta \to \mu_f(\Delta) \equiv (f, E_\Delta f)$, then we may define an operator $u(Q)$ by setting for any f

$$(f, u(Q)f) = \int_{E_3} u(x)\, d\mu_f, \qquad \text{for all } f \in L^2(E_3).$$

We might symbolically write for this operator

$$u(Q) = \int_{E_3} u(x)\, dE.$$

This notation should be interpreted as an abbreviation of the preceding equation.

Just as we have done in Section 12-3, we can construct a special representation, the Schrödinger representation of the projection-valued measure $\Delta \to E_\Delta$ and the operators Q_r. It is defined in the Hilbert space $L^2(E_3)$ of Lebesgue square-integrable complex-valued functions $\psi(x)$. The projection operators E_Δ then operate on the functions $\psi(x)$ according to the formula

$$(E_\Delta \psi)(x) = 1_\Delta(x)\psi(x), \tag{13–4}$$

where $1_\Delta(x)$ is the characteristic function of the set Δ, defined by

$$1_\Delta(x) = \begin{cases} 1 & \text{for } x \in \Delta, \\ 0 & \text{for } x \notin \Delta. \end{cases}$$

In this representation the operators Q_r appear as multiplication operators:

$$(Q_r\psi)(x) = x_r\psi(x) \qquad (r = 1, 2, 3),$$

while for any function $u(Q)$ we have

$$(u(Q)\psi)(x) = u(x)\psi(x).$$

The operator $u(Q)$ is self-adjoint if the $u(x)$ is a real-valued Borel function and the spectral projections P_Δ of $u(Q)$ are then given by the formula

$$P_\Delta = E_{u^{-1}(\Delta)}. \tag{13–5}$$

13-2. HOMOGENEITY AND ISOTROPY

We must now express the physically fundamental properties of *homogeneity* and *isotropy* of the physical space. We begin with homogeneity and we formulate it by generalizing the notions introduced in Section 12-2.

The translation by a vector $\boldsymbol{\alpha}$ transports every Borel set Δ into the set $[\Delta]\boldsymbol{\alpha} \equiv \Delta + \boldsymbol{\alpha}$. It consists of all the points of the form $\mathbf{x} + \boldsymbol{\alpha}$ with $\mathbf{x} \in \Delta$. This transformation is physically indifferent if there exist unitary operators U_α, such that

$$E_{\Delta+\alpha} = U_\alpha^{-1} E_\Delta U_\alpha. \tag{13–6}$$

The operators U_α are only determined up to an arbitrary phase factor. A choice of this factor is possible, so that the U_α are a (projective) representa-

tion of the three-dimensional translation group

$$U_{\alpha_1}U_{\alpha_2} = \omega(\alpha_1, \alpha_2)U_{\alpha_1+\alpha_2}. \tag{13–7}$$

According to the theorem of Bargmann, there are three different classes of such projective representations possible. In our case only the class which contains the vector representation ($\omega \equiv 1$) can occur. This is so because the physical space is not only homogeneous; it is also isotropic. Thus we shall proceed to the notion of *isotropy*.

A rotation R of E_3 is a transformation of the point with coordinates x_r into the point with the coordinates

$$x_r' = \sum_{s=1}^{3} R_{rs}x_s, \tag{13–8}$$

where R_{rs} is a real orthogonal matrix. Every Borel set Δ transforms under the operation R into another one $\Delta' = [\Delta]R$ consisting of all the points $\mathbf{x}' = R\mathbf{x}$ with $\mathbf{x} \in \Delta$. Isotropy of the physical space is then taken to mean that there exists a set of unitary operators U_R such that for every Δ

$$E_{[\Delta]R} = U_R^{-1}E_\Delta U_R. \tag{13–9}$$

The U_R too are a (projective) representation of the rotation group

$$U_{R_1}U_{R_2} = \omega(R_1, R_2)U_{R_1R_2}. \tag{13–10}$$

We have shown in Section 9-6, Problem 4, that every such representation is equivalent to a vector representation of the universal covering group. This means that a suitable choice of the phase factors in U_R will reduce the factor ω in Eq. (13–10) to ± 1.

The two groups of translations and rotations can be welded together into a single six-parameter group of Euclidean motions of E_3. Let (α, R) represent the general element of this group consisting of the rotation R, followed by the translation α. The composition law of this group is then given by

$$(\alpha_1, R_1)(\alpha_2, R_2) = (\alpha_1 + R_1\alpha_2, R_1R_2) = (\alpha', R'). \tag{13–11}$$

Let Δ' be the set obtained from Δ by the operation (α, R). Then the two kinds of symmetries lead to the condition

$$E_{\Delta'} = W^{-1}(\alpha, R)E_\Delta W(\alpha, R), \tag{13–12}$$

where $W(\alpha, R)$ is a (projective) representation of the group of Euclidean motions in E_3. It was shown by Bargmann (cf. reference in Section 9-6) that there exists locally only one class of projective representations of this group, and it contains the vector representation. Thus we may assume that, at least locally, we have the relations

$$W(\alpha_1, R)W(\alpha_2, R) = W(\alpha_1 + R_1\alpha_2, R_1R_2). \tag{13–13}$$

An explicit representation of this relation is obtained from the Schrödinger representation by setting

$$(W(\alpha, R)\psi)(R\mathbf{x} + \alpha) = \psi(\mathbf{x}). \tag{13–14}$$

With this definition of $W(\alpha, R)$, Eq. (13–13) is identically satisfied. Furthermore, the $W(\alpha, R)$ thereby defined is unitary (Problems 1 and 2).

The relation (13–13), which holds in a suitable neighborhood of the identity, can actually be extended to the entire group of Euclidean motions (Problem 3). This shows incidentally that only the single-valued representations can be obtained in the form (13–14).

The operators $W(\alpha, R)$, together with the projection-valued measure $\Delta \to E_\Delta$ defined by Eq. (13–4) are the canonical system of imprimitivities for the representation $(\alpha, R) \to W(\alpha, R)$ based on the Euclidean space E_3 (cf. Section 12-3, Problem 4).

It is useful to remember at this point that the condition (13–12) determines the canonical representation $W(\alpha, R)$ only up to unitary equivalence. In fact, let Ω be any unitary operator which commutes with all the E_Δ. Then $\Omega^{-1}W(\alpha, R)\Omega$ is another representation of the Euclidean group which has the same property (13–12) (see Problem 5).

Let us now consider the subgroup of the translations only; that is, the elements of the form (α, I). They are represented through Eq. (13–14) by a subgroup $U_\alpha \equiv W(\alpha, I)$ which acts on $\psi(\mathbf{x})$ according to

$$(U_\alpha\psi)(\mathbf{x} + \alpha) = \psi(\mathbf{x}). \tag{13–15}$$

The U_α, together with the $V_\beta = e^{i\beta \cdot \mathbf{Q}}$, furnish us a representation of the three-dimensional canonical commutation rules in Weyl's form:

$$U_\alpha V_\beta = e^{i\alpha \cdot \beta} V_\beta U_\alpha. \tag{13–16}$$

The infinitesimal generators $\mathbf{P}$ of the group U_α defined by

$$U_\alpha = e^{i\alpha \cdot \mathbf{P}} \tag{13–17}$$

satisfy the canonical commutation rules

$$[Q_r, P_s] = i\delta_{rs}. \tag{13–18}$$

The same precaution as in the one-dimensional case is necessary here. The left-hand side of Eq. (13–18) is only defined on a dense set D on which both operators Q_r and P_s are essentially self-adjoint. On this domain the commutator $[Q_r, P_s]$ is equal to $i\delta_{rs}$. The latter is a bounded essentially antiself-adjoint operator which admits a unique extension to the entire Hilbert space.

A reasoning similar to that employed in Section 12-3 then shows that in the Schrödinger representation, these operators appear in the form

$$(Q_r\psi)(\mathbf{x}) = x_r\psi(\mathbf{x}_r), \qquad (P_s\psi)(\mathbf{x}) = -i\frac{\partial}{\partial x_s}\psi(\mathbf{x}). \tag{13–19}$$

We have now recovered the usual wave-mechanical description of an elementary particle in three-dimensional Euclidean space by starting from the notion of localizability.

Compared to the one-dimensional case we have an additional feature: The natural symmetry group of the system contains a compact subgroup, the three-parameter rotation group. This fact permits an important simplification of many problems in elementary particle physics. We shall devote the following section to the study of this feature.

PROBLEMS

1. The operators $W(\alpha, R)$ defined by Eq. (13–14) satisfy the relation (13–13).
2. The operator $W(\alpha, R)$ of Eq. (13–14) is unitary in the space $L^2(E_3)$.
3. The relation (13–13) can be extended to the entire group for the representation (13–14).
4. The projections defined by $(E_\Delta\psi)(\mathbf{x}) = 1_\Delta(\mathbf{x})\psi(x)$ satisfy the relation

$$E_{\Delta'} = W^{-1}(\alpha, R)E_\Delta W(\alpha, R),$$

with $W(\alpha, R)$ defined by (13–14) and $\Delta' = [\Delta](\alpha, R)$ the translated domain.

5. If $W(\alpha, R)$ is the representation (13–14) of the Euclidean group, then

$$(W'(\alpha, R)\psi)(R\mathbf{x} + \alpha) = e^{i[\omega(\mathbf{x}) - \omega(R\mathbf{x} + \alpha)]}\psi(\mathbf{x})$$

defines a new representation, where $\omega(\mathbf{x})$ is an arbitrary real-valued measurable function of $\mathbf{x}$. The new representation is connected with the old one by a unitary transformation Ω:

$$W'(\alpha, R) = \Omega^{-1}W(\alpha, R)\Omega,$$

with Ω defined by

$$(\Omega\psi)(\mathbf{x}) = e^{i\omega(\mathbf{x})}\psi(\mathbf{x}).$$

$W'(\alpha, R)$ also satisfies Eq. (13–12).

13-3. ROTATIONS AS KINEMATICAL SYMMETRIES

The natural invariance group of the particle in E_3 is the Euclidean group of motions of this space. This is a six-parameter Lie group which contains the translations as an invariant abelian subgroup. We have seen in the preceding section that the translations are generated by three self-adjoint displacement operators P_r $(r = 1, 2, 3)$.

In this section we shall study the three-parameter subgroup of the rotations. This subgroup is neither invariant nor abelian. On the other hand it is compact, and this feature makes it possible to study its representations with relatively elementary means. With the three parameters are associated three

generators, which are a representation of the nonabelian Lie algebra of this group. In Cartesian coordinates the three generators are proportional to the three observables which are the components of *angular momentum.*

However, the infinitesimal or local properties of this group are not the only ones of physical interest. The investigation of the global properties shows that the rotation group is doubly-connected. This property has important physical consequences which we shall study in the following chapter.

Let us begin with some basic facts on rotations. A rotation is a transformation of the Euclidean space E_3 which associates with every point $\mathbf{x}$ with Cartesian coordinates x_r another point $\mathbf{x}'$ with Cartesian coordinates x'_r:

$$x'_r = \sum_{s=1}^{3} R_{rs} x_s. \tag{13–20}$$

Here the R_{rs} are a set of nine real numbers which satisfy the six relations

$$\sum_{t=1}^{3} R_{tr} R_{ts} = \delta_{rs}, \tag{13–21}$$

from which follow also the relations

$$\sum_{t=1}^{3} R_{rt} R_{st} = \delta_{rs}. \tag{13–22}$$

It is often convenient to introduce a matrix notation in which the last three equations appear in the shorter form

$$\mathbf{x}' = R\mathbf{x} \qquad \text{and} \qquad R^{\sim} R = R R^{\sim} = I. \tag{13–23}$$

The letter R stands for the matrix with components R_{rs} and $R^{\sim}$ is the transposed matrix with components $(R^{\sim})_{rs} = R_{sr}$. Eqs. (13–21) and (13–22) show that the matrix R has an inverse. In fact they also show that $(\det R)^2 = 1$ and $R^{-1} = R^{\sim}$. From this it follows that $\det R = \pm 1$. We shall in this section be primarily concerned with the *proper rotations* for which $\det R = +1$, and we shall refer to them as rotations without qualification.

If R_1 and R_2 are two rotations, then the rotation $R_1 R_2$ is the matrix product of R_1 and R_2. It is clearly again a rotation. Thus the rotations form a group, the rotation group.

The rotation matrices R depend on nine real parameters which, in addition, satisfy the six relations (13–21) or (13–22). They therefore contain three independent parameters. It is often convenient to have an explicit parametrization of the rotations which associates with every rotation a point in a three-dimensional parameter space. This can be and has been done in many different ways. We shall adopt one such representation which has the additional advantage of a simple geometrical interpretation.

Every rotation R admits a vector $\boldsymbol{\alpha}$ which satisfies $R\boldsymbol{\alpha} = \boldsymbol{\alpha}$ (Problem 1). This invariant $\boldsymbol{\alpha}$ determines the *rotation axis.* If this axis is chosen as the

3-axis of a Cartesian coordinate system, the rotation matrix has the form

$$R = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{13–24}$$

The parameter φ is the rotation angle. We can represent the rotation R by a point with coordinates $\boldsymbol{\varphi} = \varphi\boldsymbol{\alpha}$ ($|\boldsymbol{\alpha}| = 1$) such that $|\boldsymbol{\varphi}| = \varphi$. These points are in the interior of a sphere of radius π. The points on the surface of the sphere represent rotations with angle $\varphi = \pm\pi$. Two such rotations at opposite ends of a diameter are identical since the corresponding matrices R are identical.

We can introduce a topology in this group space by defining as open sets the interiors of Euclidean spheres. The group operations are then continuous, and the rotation group becomes a topological group. It is easily seen that it is connected. The rotations R_φ around a fixed rotation axis $\boldsymbol{\alpha}$ and variable angle φ are one-parameter subgroups. We have

$$R_{\varphi_1} R_{\varphi_2} = R_{[\varphi_1 + \varphi_2]} \tag{13–25}$$

where $[\varphi_1 + \varphi_2] = \varphi_1 + \varphi_2 \pmod{2\pi}$. Thus these one-parameter subgroups are all isomorphic to the circle group (cf. Section 9-3, Problem 3), and to every one we can associate an antisymmetric real transformation of E_3 by the definition

$$A = \lim_{\varphi \to 0} \frac{1}{\varphi} (R_\varphi - I). \tag{13–26}$$

We shall call the operator A an infinitesimal rotation around the axis $\boldsymbol{\alpha}$. In the special coordinate system used for the representation (13–24), A is easily calculated and it has the form

$$A = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{13–27}$$

The special rotations around the axes 1, 2, and 3 respectively are represented by the special antisymmetrical matrices

$$A_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad A_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{13–28}$$

These matrices satisfy the commutation rules

$$[A_1, A_2] = A_3, \qquad [A_2, A_3] = A_1, \qquad [A_3, A_1] = A_2. \tag{13–29}$$

This set of commutation rules constitutes the Lie algebra of the rotation group.

With the three fundamental infinitesimal rotations we can construct the infinitesimal rotation A around any axis $\boldsymbol{\alpha}$ ($|\boldsymbol{\alpha}| = 1$) by the rule

$$A = \boldsymbol{\alpha} \cdot \mathbf{A} \equiv \alpha_1 A_1 + \alpha_2 A_2 + \alpha_3 A_3.$$

It is then easily verified, by integrating the differential equation (13–26), that the rotation $R_{\boldsymbol{\varphi}}$ has the form

$$R_{\boldsymbol{\varphi}} = e^{A\varphi} = e^{\boldsymbol{\alpha} \cdot \mathbf{A}\varphi} = e^{\boldsymbol{\varphi} \cdot \mathbf{A}}. \tag{13–30}$$

With this form we have "parametrized" the rotation group. An arbitrary rotation is written explicitly as a function of the three parameters φ_1, φ_2, φ_3 which represent the rotation (cf. Problem 5).

Let us now proceed to the interpretation of the rotation as a kinematical symmetry for an elementary particle. According to the preceding section, such a symmetry is expressed by a system of relations for the projection-valued measure $\Delta \to E_\Delta$:

$$E_{[\Delta]R} = U_R^{-1} E_\Delta U_R. \tag{13–31}$$

Here Δ is an arbitrary Borel set of E_3, $[\Delta]R$ the set $\{\mathbf{x} \mid R^{-1}\mathbf{x} \in \Delta\}$, and $U_R = W(0, R)$ the representation of the rotation group obtained by restricting the representation $W(\boldsymbol{\alpha}, R)$ of the Euclidean group to the rotations alone.

If the particle is elementary, the representation $W(\boldsymbol{\alpha}, R)$ is, according to the imprimitivity theorem, unique (up to unitary equivalence) and consequently so is U_R. We shall now study this representation.

First, we note that the representation is, according to the theorem of Bargmann (cf. Section 9-6), locally equivalent to a vector representation, so that we may assume

$$U_{R_1} U_{R_2} = U_{R_1 R_2} \tag{13–32}$$

in a suitable neighborhood of the identity. The operator U_R is explicitly given in the space $L^2(E_3)$ by the formula

$$(U_R \psi)(R\mathbf{x}) = \psi(\mathbf{x}), \tag{13–33}$$

from which it can be seen that the relation (13–32) is valid for the entire group.

This representation is reducible. Let us determine its irreducible parts. To this end it is convenient to introduce polar coordinates r, ω. Here

$$r = \sqrt{x_1^2 + x_2^2 + x_3^2}$$

is the distance of the point $\mathbf{x}$ from the origin, and ω represents a point on the unit sphere. If $\omega' = R\omega$ is the corresponding point after the rotation, we have

$$(U_R \psi)(r, \omega') = \psi(r, \omega). \tag{13–34}$$

Thus the rotation affects only the angular part of the function ψ. It is thus possible to discuss the representations U_R by studying their effects on L^2

functions on the unit sphere Ω. These functions form a Hilbert space $L^2(\Omega)$. Any function $f(\omega) \in L^2(\Omega)$ can be developed in a complete orthonormal system of such functions. A system which is especially convenient for the problem on hand consists of the *spherical harmonics* $\mathscr{Y}_l^m(\omega)$, where e and m are integers and $l = 0, 1, 2, \ldots ; -l \leq m \leq l$. An explicit definition of the spherical harmonics is given by

$$\mathscr{Y}_l^m(\omega) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\frac{\sin^m\theta e^{im\varphi}}{2^l l!}\left(\frac{d}{d\xi}\right)^{l+m}(\xi^2-1)^l. \qquad (13\text{–}35)$$

Here $\xi = \cos\theta$; θ is the polar angle, and φ the azimuth of the point ω on the unit sphere.

One shows in standard texts [2, 3] that the spherical harmonics are a complete orthonormal system of normalized functions on the sphere. That is, we have

$$\int_\Omega \mathscr{Y}_l^{m*}(\omega)\mathscr{Y}_{l'}^{m'}(\omega)\,d\omega = \delta_{ll'}\delta_{mm'}, \qquad (13\text{–}36)$$

and any function $f(\omega)$ in $L^2(\Omega)$ admits a convergent development

$$f(\omega) = \sum_{l=0}^{\infty}\sum_{m=-l}^{+l} C_l^m \mathscr{Y}_l^m(\omega), \qquad (13\text{–}37)$$

with

$$C_l^m = \int_\Omega \mathscr{Y}_l^{m*}(\omega) f(\omega)\,d\omega. \qquad (13\text{–}38)$$

Under rotations the $2l+1$ functions $\mathscr{Y}_l^m$ for fixed l transform irreducibly among themselves, such that

$$(U_R\mathscr{Y}_l^m) = \sum_{m'=-l}^{+l} D_{m'm}^l(R)\mathscr{Y}_l^{m'}(\omega) \qquad (13\text{–}39)$$

where

$$D_{m'm}^l(\omega) = \int_\Omega \mathscr{Y}_l^{m'*}(\omega) U_R \mathscr{Y}_l^m(\omega)\,d\omega. \qquad (13\text{–}40)$$

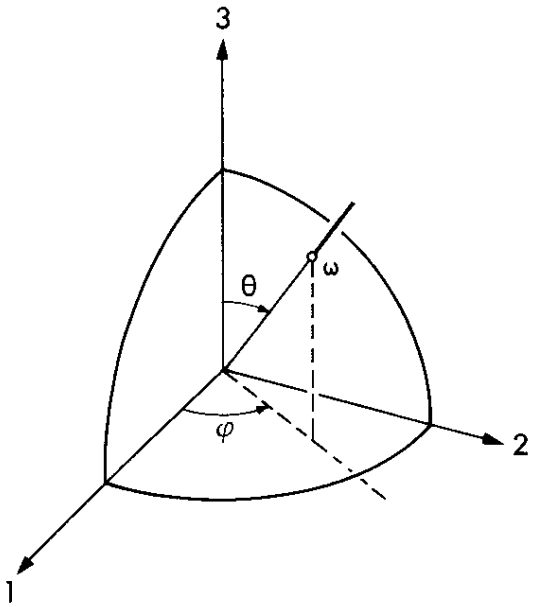

Fig. 13–1 The polar angle θ and the azimuth φ of the point ω on the unit sphere.

These formulas give the explicit reduction of the canonical representation U_R on the unit sphere into its irreducible parts. This result illustrates the usefulness of the spherical harmonics.

It is easy to see that, with the exception of the trivial case $l = 0$, all these representations are faithful (Problem 2). It is more difficult to show that these are the only faithful representations of the rotation group. The usual procedure for this demonstration is to reduce the problem to an algebraic

one, and to discuss the representations of the associated Lie algebra. To this end one writes $U_R = e^{-i\boldsymbol{\alpha}\cdot\mathbf{L}\varphi}$ where $\boldsymbol{\alpha}$ is the unit vector in the direction of the rotation axis and L_r are three self-adjoint operators defined by

$$\boldsymbol{\alpha}\cdot\mathbf{L} = \lim_{\varphi\to 0}\frac{i}{\varphi}(U_R - I).$$

Since U_R is a representation of the rotation group, the operators satisfy the same commutation rules as the operators iA_r, that is,

$$[L_1, L_2] = iL_3, \ldots .$$

Using the definition of U_R, one finds that

$$L_1 = Q_2P_3 - Q_3P_2, \qquad L_2 = Q_3P_1 - Q_1P_3, \qquad L_3 = Q_1P_2 - Q_2P_1.$$

One can determine with elementary algebraic methods all the irreducible matrices L_3 which satisfy these commutation rules.

With this method one obtains not only the representations given above in the finite form, but another infinite set associated with half-integer values for l. This set furnishes, however, not a representation of the rotation group, but only of its simply-connected covering group. It is sometimes referred to as the double-valued representation of the rotation group.

In order to see explicitly that the rotation group is not simply- but doubly-connected, we consider the parametrization introduced before in the φ-sphere. The order of connectedness is the number of inequivalent classes of closed paths in the group. A closed path is equivalent to another if it can be transformed into the other by continuous deformation.

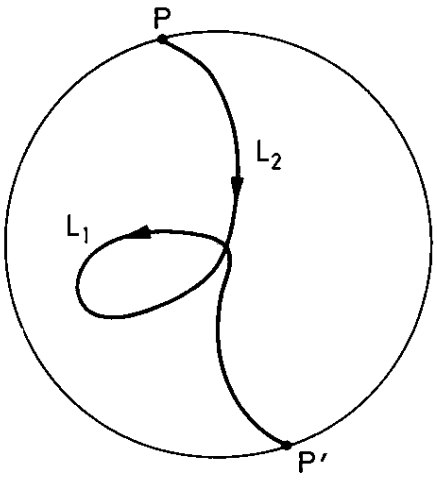

Fig. 13–2 Inequivalent paths in the rotation group.

Figure 13–2 shows two closed paths L_1 and L_2 which are inequivalent. Indeed, L_1 is easily seen to contract continuously into the unit element while L_2 cannot be so contracted. The path L_2 is closed because the point P and its opposite P' are to be identified.

Every closed path intersects the surface of the sphere in an even number of points. If $2n$ is this number, then the path can be continuously contracted

into a point if n is even and it cannot be so contracted if n is odd (Problem 3). Hence there are exactly two classes of inequivalent paths: The rotation group is doubly-connected.

The simply-connected universal covering group is a larger group than the rotation group. It also has more representations. Yet its Lie algebra is identical with that of the rotation group. This is the reason for the doubling of the number of representations when one uses the algebraic method for their construction.

Having thus established that all the irreducible representations of the rotation group appear in the representation U_R, we now proceed to the transformation of operators under rotations. First we recall the basic relation for the projection-valued measure:

$$E_{[\Delta]R} = U_R^{-1} E_\Delta U_R.$$

It follows from this relation that for any complex-valued function $u(\mathbf{x})$, measurable with respect to the measure E_Δ, we have, for any $f \in \mathscr{H}$, $(f, u(\mathbf{Q})f) = \int u(\mathbf{x})\, d\mu_f$, where μ_f is the numerical-valued measure $\Delta \to \mu_f(\Delta) = (f, E_\Delta f)$. It follows from this that

$$\begin{aligned}(f, U_R u(\mathbf{Q}) U_R^{-1} f) &= \int u(\mathbf{x})\, d\mu_{U_R^{-1}f} \\ &= \int u(Rx)\, d\mu_f \\ &= (f, u(R\mathbf{Q})f).\end{aligned}$$

Since this relation is true for any f, we have established the operator relation

$$U_R u(\mathbf{Q}) U_R^{-1} = u(R\mathbf{Q}). \tag{13–41}$$

In particular, for $u = Q_r$, we find

$$U_R Q_r U_R^{-1} \equiv Q_r' = \sum_{s=1}^{3} R_{rs} Q_s. \tag{13–42}$$

It follows from this and the canonical commutation rules that

$$U_R P_r U_R^{-1} \equiv P_r' = \sum_{s=1}^{3} R_{rs} P_s. \tag{13–43}$$

This result may be generalized. Any operator triplet X_r which transforms under rotations according to

$$X_r' = U_R X_r U_R^{-1} = \sum_{s=1}^{3} R_{rs} X_s, \tag{13–44}$$

is called a *vector* operator. The L_r $(r = 1, 2, 3)$ are such a triplet (Problem 4).

In a similar way one can introduce tensor operators of any rank. Once the transformation law of the fundamental set Q_r and P_s is determined, the transformation law of any operator which is a function of them is also determined. If the system is irreducible (elementary particle), then this includes every operator.

With this we conclude this discussion of the rotations as kinematical symmetries and proceed to the dynamical characteristics of the one-particle system.

PROBLEMS

1. Every rotation matrix R admits a real eigenvector α with eigenvalue 1, so that for this α we have $R\alpha = \alpha$. The secular determinant $\det(R - \lambda I)$ always has one root $\lambda = 1$.
2. The representations $R \to D^j_{m'm}(R)$ of the rotation group are faithful. That is, if $D^j_{m'm}(R) = \delta_{m'm}$, then $R = I$.
3. Every closed path in the rotation group can be continuously contracted into a point if the number n of rotations by the angle π contained in the path is even. If this number is odd, the path cannot be so contracted.
4. The operators $L_1 = Q_2P_3 - Q_3P_2$ and their cyclic permutations are a set of vector operators. They satisfy relations

$$U_R L_r U_R^{-1} = \sum_{s=1}^{3} R_{rs} L_s.$$

5. The matrix R_φ for the rotation with angle φ around the rotation axis $\alpha = (\alpha_1, \alpha_2, \alpha_3)$, $(|\alpha| = 1)$, is given explicitly by the formula

$$R_\varphi = I + A \sin\varphi + A^2(1 - \cos\varphi)$$

with

$$A = \alpha \cdot \mathbf{A} = \begin{pmatrix} 0 & -\alpha_3 & \alpha_2 \\ \alpha_3 & 0 & -\alpha_1 \\ -\alpha_2 & \alpha_1 & 0 \end{pmatrix}.$$

13-4. VELOCITY AND GALILEI INVARIANCE

Let A be any observable not depending explicitly on time. We can define a velocity of A, denoted by $\dot{A}$, by requiring that for any state ψ_t,

$$\frac{d}{dt}(\psi_t, A\psi_t) = (\psi_0, \dot{A}\psi_0). \tag{13-45}$$

In this expression ψ_t is the time-dependent state vector in the Schrödinger picture (cf. Section 10-3) which satisfies a Schrödinger equation

$$i\dot{\psi}_t = H\psi_t. \tag{13-46}$$

It follows from this definition of $\dot{A}$ that for every $\psi = \psi_0$,

$$i(\psi, [H, A]\psi) = (\psi, \dot{A}\psi)$$

or

$$\dot{A} = i[H, A]. \tag{13-47}$$

In particular, if A is one of the position operators Q_r, we may define the *velocity* operator

$$\dot{Q}_r = i[H, Q_r]. \tag{13-48}$$

It is only defined if the operator H is known. In general both H and Q_r are unbounded operators. Thus $\dot{Q}_r$ is defined only on a dense set which we assume to be so large that $\dot{Q}_r$ is essentially self-adjoint. Of all known examples which have been studied, this is the case. We shall denote both $\dot{Q}_r$ of (13–48) and its self-adjoint extension by the same symbol.

The $\dot{Q}_r$ thus defined are observables and their expectation values can be measured.

If an observer O has measured the observable $\dot{Q}_r$ and has found a value α_r, then an observer O' in relative motion with velocity v_r with respect to O, who measures $\dot{Q}_r$ on the same system, will observe the value $\alpha_r + v_r$. This would be the expectation value of $\dot{Q}_r + v_r$ if the same state had been prepared by the observer O'. Thus the connection between the two systems are obtained via the Galilei transformation which transforms position and velocity according to

$$Q_r \to Q_r, \qquad \dot{Q}_r \to \dot{Q}_r + v_r. \tag{13-49}$$

We shall define the system as *Galilei invariant* if this transformation is a kinematical symmetry; that is, if there exists a unitary operator $G_{\mathbf{v}}$ which commutes with Q_r and for which

$$G_{\mathbf{v}}\dot{Q}_r G_{\mathbf{v}}^{-1} = \dot{Q}_r + v_r. \tag{13-50}$$

This definition implies certain restrictions on the nature of the operators $\dot{Q}_r$ and hence also on the operator H which is involved in the definition of $\dot{Q}_r$. For instance Eq. (13–50) implies that the spectrum of $\dot{Q}_r$ is continuous and extends from $-\infty$ to $+\infty$.

Let us now determine the operators H which are admitted by particles satisfying Galilei invariance. We do this under the assumption that we are dealing with an *elementary* system, so that the position operators Q_r generate a maximal abelian algebra.

If we combine the Galilei transformations (13–49) with the displacements, we obtain a six-parameter group of translations. We define the family of unitary operators $W(\boldsymbol{\alpha}, \mathbf{v})$ with the properties

$$\begin{aligned} Q_r + \alpha_r &= W(\boldsymbol{\alpha}, \mathbf{v})\, Q_r W^{-1}(\boldsymbol{\alpha}, \mathbf{v}), \\ \dot{Q}_r + v_r &= W(\boldsymbol{\alpha}, \mathbf{v})\, \dot{Q}_r W^{-1}(\boldsymbol{\alpha}, \mathbf{v}). \end{aligned} \tag{13-51}$$

It follows from this that the $W(\boldsymbol{\alpha}, \mathbf{v})$ are a projective representation of the six-dimensional vector space

$$W(\boldsymbol{\alpha}_1, \mathbf{v}_1)W(\boldsymbol{\alpha}_2, \mathbf{v}_2) = \omega(\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2; \mathbf{v}_1, \mathbf{v}_2)W(\boldsymbol{\alpha}_1 + \boldsymbol{\alpha}_2, \mathbf{v}_1 + \mathbf{v}_2). \quad (13\text{–}52)$$

According to the general theory of such representations developed in Section 9-6, it is possible to determine the as yet arbitrary phase factors of W in such a way that the factor ω in (13–52) assumes the form

$$\omega(\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2; \mathbf{v}_1, \mathbf{v}_2) = e^{i(\mu/2)(\boldsymbol{\alpha}_1 \cdot \mathbf{v}_2 - \boldsymbol{\alpha}_2 \cdot \mathbf{v}_1)}, \quad (13\text{–}53)$$

where μ is an arbitrary real constant $\neq 0$. There exists also a representation for $\mu = 0$, but it is reducible and does not describe elementary particles.

The two-parameter subgroups U_α and $G_\mathbf{v}$ are obtained by specializing the parameter values

$$U_\alpha = W(\boldsymbol{\alpha}, 0) \qquad \text{and} \qquad G_\mathbf{v}^{-1} = W(0, \mathbf{v}). \quad (13\text{–}54)$$

For these two subgroups, the relation (13–53) becomes

$$U_\alpha G_\mathbf{v}^{-1} = e^{i\mu\boldsymbol{\alpha} \cdot \mathbf{v}} G_\mathbf{v}^{-1} U_\alpha. \quad (13\text{–}55)$$

If we set $\mu\mathbf{v} = \boldsymbol{\beta}$ and $V_\beta = G_{\beta/\mu}^{-1}$, we obtain from (13–55) the canonical commutation rules in Weyl's form. It follows in particular that

$$\frac{1}{\mu} P_r + v_r = \frac{1}{\mu} G_\mathbf{v} P_r G_\mathbf{v}^{-1}. \quad (13\text{–}56)$$

By comparing this with Eq. (13–50) we see that $(1/\mu)P_r$ and $\dot{Q}_r$ have the same commutation rules with $G_\mathbf{v}$. Their difference commutes with $G_\mathbf{v}$; thus it must be a function of the Q_r alone. Hence we find the important relation

$$\mu\dot{Q}_r = P_r - a_r \qquad (r = 1, 2, 3) \quad (13\text{–}57)$$

where $a_r(\mathbf{Q})$ are three functions of Q_1, Q_2, Q_3, which may depend explicitly on time.

From the relation (13–57) we obtain the commutation rules

$$\mu[Q_r, \dot{Q}_s] = i\delta_{rs}, \quad (13\text{–}58)$$

and it follows from them, that the operator $H_0 = (\mu/2)\dot{Q}^2$ satisfies

$$i[H_0, Q_s] = \dot{Q}_s. \quad (13\text{–}59)$$

Consequently, in view of (13–48), $H - H_0$ commutes with Q_s, hence it must be a function $v(\mathbf{Q})$ of the Q_r, which may even depend on time.

We have now shown that the evolution operator H must have the form

$$H = \frac{1}{2\mu} (\mathbf{P} - \mathbf{a})^2 + v. \quad (13\text{–}60)$$

We have thus arrived at the main result of this section. Every localizable elementary physical system which satisfies Galilei invariance in the sense of (13–50) evolves in time according to Eq. (13–46), with H as given by Eq. (13–60).

The operators $\mathbf{a}(\mathbf{Q})$ and $v(\mathbf{Q})$ are not entirely determined by Eqs. (13–57) and (13–60) since the quantities P_r and H are not determined by their commutation properties. The remaining ambiguity is closely connected with the gauge invariance of the theory which we shall discuss in the next section.

The physical interpretation of this result is analogous to the case of the particle in one dimension. The parameter μ is proportional to the mass m of the particle $m = \hbar\mu$. The proportionality factor $\hbar$ is Planck's constant divided by 2π. The operator $\mathbf{p} = \hbar\mathbf{P}$ represents the momentum of the particle. The operators $\mathbf{a}$ and v represent the effects of external forces on the motion of the particles. These forces are the quantum mechanical analogues of the forces due to an arbitrary external electromagnetic field. The identification is completed by identifying $(c\hbar/e)\mathbf{a} = \mathbf{A}$ with the vector potential and $(\hbar/e)v = V$ with the scalar potential of this field. Here e is the electric charge of the particle which, for an electron, has the value -4.8×10^{-10} esu.

It is interesting to note that the principle of Galilei invariance as stated at the beginning of this section limits the possible nature of external forces to those of electromagnetic origin.

13-5. GAUGE TRANSFORMATIONS AND GAUGE INVARIANCE

In classical electrodynamics it is shown that the electromagnetic field determines the potentials only up to a gauge transformation

$$\begin{aligned} \frac{1}{c}\mathbf{A} &\to \frac{1}{c}\mathbf{A} + \nabla\phi, \\ V &\to V - \frac{\partial\phi}{\partial t}. \end{aligned} \tag{13–61}$$

It is therefore natural to expect that this classical property correspond to a certain invariance property of the system characterized by the evolution operator H of Eq. (13–60). This indeed is the case. The invariance property is called gauge invariance.

Let Ω be the unitary operator defined in the Schrödinger representation by

$$(\Omega\psi)(\mathbf{x}) = e^{i\phi(\mathbf{x})}\psi(\mathbf{x}). \tag{13–62}$$

Here $\phi(\mathbf{x})$ is an arbitrary differential function of $\mathbf{x}$ which may depend explicitly on time. Under this transformation the operator P transforms according to (cf. Problem 1)

$$\Omega\mathbf{P}\Omega^{-1} = \mathbf{P} - \nabla\phi. \tag{13–63}$$

Let us now determine the effect of such a transformation on the Schrödinger equation. To this end we define $\varphi_t = \Omega\psi_t$ and we find by an elementary calculation (Problem 2) that

$$i\dot{\varphi}_t = G\varphi_t, \tag{13–64}$$

with

$$G = \Omega H\Omega^{-1} + i\left(\frac{d}{dt}\,\Omega\right)\Omega^{-1}. \tag{13–65}$$

The explicit evaluation of this expression gives

$$G = \frac{1}{2\mu}\,(\mathbf{P} - (\mathbf{a} + \nabla\phi))^2 + v - \frac{\partial\phi}{\partial t}, \tag{13–66}$$

where ϕ is now considered as a (possibly time-dependent) function of the operators Q_r.

Thus we find that the effect of the transformation Ω is exactly the same as that of a gauge transformation. Motivated by this example we can now express explicitly what we mean by *gauge invariance*:

A quantum mechanical theory is gauge invariant if every gauge transformation of the electromagnetic potentials can be induced by a unitary transformation of the Hilbert space of state vectors.

We have thus shown in this section that a one-particle theory which satisfies the principle of Galilei invariance is automatically gauge invariant.

When we consider the effect of gauge transformation on operator functions of $\mathbf{Q}$ and $\mathbf{P}$, we may distinguish three types of quantities.

1) Operators which are invariant under the general transformations Ω and gauge transformations. For example the operators Q_r themselves.
2) Operators, such as $\dot{Q}_r$ and H, which transform identically under Ω and gauge transformations.
3) Operators which transform differently under Ω and gauge transformations.

We shall call quantities which belong to one of the groups 1 and 2 *gauge-invariant* quantities. Thus, according to this definition, the evolution operator G (see Eq. 13–66) is gauge invariant, but the vector potentials A_r or the displacement operators P_r are not (cf. Problem 4).

In classical physics it is known that only gauge invariant quantities are observable. Thus it is reasonable to assume that only gauge invariant operators can represent observables in quantum mechanics. According to this assumption, the P_r are not observables but the $\dot{Q}_r$ are, and they represent the cartesian components of the velocity. The operators which represent the *momentum* of a particle are $m\dot{Q} = \hbar(P_r - a_r)$, and they, too, are gauge invariant and thus observable.

PROBLEMS

1. Let Ω be the unitary operator defined by

$$(\Omega)\psi(\mathbf{x}) = e^{i\phi(\mathbf{x})}\psi(\mathbf{x}),$$

where ϕ is a differentiable and real-valued function. Then

$$\Omega\mathbf{P}\Omega^{-1} = \mathbf{P} - \nabla\phi.$$

2. If $\varphi_t = \Omega\psi_t$, and ψ_t satisfies the Schrödinger equation $i\dot{\psi}_t = H\psi_t$, then φ_t satisfies an equation

$$i\dot{\varphi}_t = G\varphi_t, \qquad \text{with } G = \Omega H\Omega^{-1} + i\left(\frac{d}{dt}\,\Omega\right)\Omega^{-1}.$$

3. If for every observable A we define

$$\dot{A} = i[H, A] + \frac{\partial A}{\partial t},$$

we have for the acceleration $\ddot{\mathbf{Q}}$ the relation

$$\mu\ddot{\mathbf{Q}} = \ddot{Q} \times (\nabla \times \mathbf{a}) - \left(\nabla V + \frac{\partial \mathbf{a}}{\partial t}\right).$$

4. Both velocity and acceleration are gauge invariant quantities but the displacement operator $\mathbf{P}$ is not. Under gauge transformations the latter transforms according to $\mathbf{P} \to \mathbf{P} + \nabla\phi$.

13-6. DENSITY AND CURRENT OF AN OBSERVABLE

Localizability, as we have previously formulated it, implies the existence of a family of propositions represented by projection operators E_Δ. Each of these projections represents the proposition that the localizable system is contained in the Borel subset Δ of the three-dimensional Euclidean space E_3.

This concept permits the definition of a density of probability in the space E_3. We may define this quantity, for instance, in the following manner. Let $\mathbf{x}$ be a point in E_3 and let $\Delta = V$ be a volume element containing $\mathbf{x}$. We may for instance choose for V a cube centered at the point $\mathbf{x}$. Let $\psi(\mathbf{x})$ be the Schrödinger function for a pure state. The probability of finding the system in the volume element V is then given by $(\psi, E_V\psi)$. We define the *probability density* by

$$\rho(\mathbf{x}) = \lim_{V \to 0} \frac{1}{V}(\psi, E_V\psi). \tag{13–67}$$

It is normalized: $\int \rho(\mathbf{x})\, d^3x = 1$, and positive definite: $\rho(\mathbf{x}) \geq 0$. In general the probability density is a function of time. But it satisfies a differential

conservation law, the continuity equation, which connects the time variation of $\rho(\mathbf{x})$ with a suitably defined probability current $\mathbf{j}(\mathbf{x})$:

$$\dot{\rho}(\mathbf{x}) + \nabla \mathbf{j}(\mathbf{x}) = 0. \tag{13-68}$$

The expression for the current is determined by this continuity equation up to a numerical vector field with vanishing divergence, and is given by

$$\mathbf{j}(\mathbf{x}) = \frac{1}{2\mu i}\{\psi^*(\mathbf{x})(\nabla - i\mathbf{a})\psi(\mathbf{x}) - \psi(\mathbf{x})(\nabla + i\mathbf{a})\psi^*(\mathbf{x})\}. \tag{13-69}$$

Equation (13–68) is then an elementary consequence of the Schrödinger equation

$$i\dot{\psi}(\mathbf{x}) = -\frac{1}{2\mu}(\nabla - ia)^2\psi + v\psi. \tag{13-70}$$

Expression (13–69) can be related to the velocity operator $\dot{\mathbf{Q}}$ defined previously. Indeed, if we define

$$\dot{\mathbf{Q}}(V) = \tfrac{1}{2}(E_V\dot{\mathbf{Q}} + \dot{\mathbf{Q}}E_V), \tag{13-71}$$

then we verify without difficulty that

$$\mathbf{j}(\mathbf{x}) = \lim_{V \to 0} \frac{1}{V}(\psi, \dot{\mathbf{Q}}(V)\psi) \tag{13-72}$$

where $\dot{\mathbf{Q}}$ stands for the operator $(1/\mu)(\mathbf{P} - \mathbf{a}) = (1/\mu i)(\nabla - i\mathbf{a})$.

More generally, let $\mathcal{O}$ be any observable and define

$$\mathcal{O}(V) \equiv \tfrac{1}{2}(E_V\mathcal{O} + \mathcal{O}E_V); \tag{13-73}$$

then the quantity

$$\mathcal{O}(\mathbf{x}) \equiv \lim_{V \to 0} \frac{1}{V}(\psi, \mathcal{O}(V)\psi) \tag{13-74}$$

defines the density of the quantity $\mathcal{O}$ at the position $\mathbf{x}$. It can be given explicitly if we define $\varphi(\mathbf{x}) = (\mathcal{O}\psi)(\mathbf{x})$. It then has the form

$$\mathcal{O}(\mathbf{x}) = \tfrac{1}{2}(\varphi^*(\mathbf{x})\psi(\mathbf{x}) + \psi^*(\mathbf{x})\varphi(\mathbf{x})) = \operatorname{Re}\varphi^*(\mathbf{x})\psi(\mathbf{x}). \tag{13-75}$$

That this expression is a generalization of the probability density $\rho(\mathbf{x})$ can be seen by taking for $\mathcal{O}$ the unit operator I.

The corresponding current can also be defined by

$$\mathcal{J}_0(\mathbf{x}) \equiv \frac{1}{4\mu i}\left(\varphi^*(\mathbf{x})(\nabla - i\mathbf{a})\psi(\mathbf{x}) - \psi(\mathbf{x})(\nabla + i\mathbf{a})\varphi^*(\mathbf{x})\right)$$

$$+ \frac{1}{4\mu i}\left(\psi^*(\mathbf{x})(\nabla - i\mathbf{a})\varphi(\mathbf{x}) - \varphi(\mathbf{x})(\nabla + i\mathbf{a})\psi^*(\mathbf{x})\right). \tag{13-76}$$

However, only if $\mathcal{O}$ commutes with H does it satisfy a continuity equation

$$\dot{\mathcal{O}}(\mathbf{x}) + \nabla \cdot \mathcal{J}_0(\mathbf{x}) = 0. \tag{13–77}$$

As an example we may calculate the density of angular momentum (in units of $\hbar$) by choosing for $\mathcal{O}$ the vector operator

$$\mathcal{O} = \mathbf{Q} \times \mathbf{P} \equiv \mathbf{L}, \tag{13–78}$$

with the components $\mathcal{O}_1 = Q_2P_3 - Q_3P_2$, etc. We find after a short calculation (Problem 1) for the angular momentum density, the expression

$$\mathbf{L}(\mathbf{x}) = \mu\mathbf{x} \times \mathbf{j}(\mathbf{x}), \tag{13–79}$$

which is just what one would have expected from the physical interpretation of the current operator $\mathbf{j}(\mathbf{x})$.

For an observable $\mathcal{O}$ which does not commute with the evolution operator H the definition of the probability current is less useful, since the continuity equation (13–77) is no longer correct. The expression (13–77), instead of being equal to zero, is then equal to a nonvanishing term representing the sources or sinks of the quantity $\mathcal{O}$ resulting from the action of the external fields.

PROBLEMS

1. The angular momentum density $\mathbf{L}(\mathbf{x})$ for a spinless elementary particle is given by
$$\mathbf{L}(\mathbf{x}) = \mu\mathbf{x} \times \mathbf{j}(\mathbf{x})$$
2. If $\psi(\mathbf{x})$ is a function of $r = \sqrt{x_1^2 + x_2^2 + x_3^2}$ alone, then the angular momentum density is identically zero.
3. $(\psi, \dot{\mathbf{Q}}\psi) = \int \mathbf{j}(\mathbf{x})\, d^3x$ for all pure states $\psi(\mathbf{x})$.
4. For any observable $\mathcal{O}$ the density $\mathcal{O}(\mathbf{x})$ and the current $\mathcal{J}_0(\mathbf{x})$ are real quantities.

13-7. SPACE INVERSION

In order to simplify the notation we shall consider the one-dimensional case. The generalization to three dimensions is then obvious. The transformation

$$Q \to -Q = Q', \qquad P \to -P = P' \tag{13–80}$$

is called a space inversion. It leaves the commutation rules invariant. The following discussion is formal and, mathematically, not completely rigorous. If the operators Q and P are unitarily equivalent to the Schrödinger

representation, then the following formal discussion could be carried through in full mathematical rigor, if we expressed it in terms of the bounded operators $U_\alpha = e^{i\alpha P}$ and $V_\beta = e^{i\beta Q}$.

We shall continue the discussion in the unbounded form, however, benefitting thereby from some formal simplification.

Since Q' and P' satisfy the same commutation rules, there exists a unitary operator Π with the property

$$\Pi Q \Pi^{-1} = -Q, \qquad \Pi P \Pi^{-1} = -P. \tag{13–81}$$

We shall now determine this operator Π. In order to do this it is useful to consider the transformation (13–80) as a special case of a rotation

$$\begin{aligned} Q \to Q' &= \cos \alpha Q + \sin \alpha P, \\ P \to P' &= -\sin \alpha Q + \cos \alpha P. \end{aligned} \tag{13–82}$$

This transformation is easily seen also to be canonical, so that there exists a unitary one-parameter group U_α such that

$$Q' = U_\alpha Q U_\alpha^{-1}, \qquad P' = U_\alpha P U_\alpha^{-1}. \tag{13–83}$$

The $U_\alpha = e^{i\alpha A}$ can be determined easily if we consider the infinitesimal part:

$$\begin{aligned} Q' &= Q + \alpha P + \cdots = Q + i\alpha[A, Q] + \cdots, \\ P' &= P - \alpha Q + \cdots = P + i\alpha[A, P] + \cdots. \end{aligned}$$

It follows from this that A must satisfy the commutation relations

$$\begin{aligned} P &= i[A, Q], \\ -Q &= i[A, P]. \end{aligned} \tag{13–84}$$

The formal solution of these relations is obtained by setting, for A,

$$A = \tfrac{1}{2}(P^2 + Q^2). \tag{13–85}$$

Thus

$$U_\alpha = e^{i(\alpha/2)(P^2+Q^2)}. \tag{13–86}$$

For the special value $\alpha = \pi$ we find the space inversion operator

$$\Pi = e^{i(\pi/2)(P^2 + Q^2)}. \tag{13–87}$$

It is interesting to note that for $\alpha = \pi/2$, we obtain a transformation

$$\Phi = e^{i(\pi/4)(P^2+Q^2)}$$

with the following properties

$$\Phi Q \Phi^{-1} = P, \qquad \Phi P \Phi^{-1} = -Q, \qquad \text{and} \qquad \Phi^2 = \Pi.$$

The transformation Φ is called the *Fourier transformation* (cf. Problems 1 through 5). If the evolution operator H has the property that it commutes with the space inversion operator Π, then the space inversion constitutes a dynamical symmetry of the system.

A dynamical symmetry in an extended sense is present even if the evolution operator H does not commute with Π but changes under $H \to \Pi H \Pi^{-1}$ into another operator which can be obtained from the original one by the transformation $\mathbf{a} \to -\mathbf{a}$ and $v \to v$.

Physically this latter transformation represents the space inversion operation of the external electromagnetic field, and the invariance in this extended sense expresses the fact that the original system in the original field has the same dynamical structure as the space-inverted system in the space-inverted field.

It is immediately seen that an evolution operator H of the form (13–60) does have this invariance property, and we have thus established that Galilei invariance implies not only gauge invariance, but also the extended dynamical invariance under space inversion.

PROBLEMS

1. The Fourier transformation Φ has, in the spectral representation of Q, the explicit form

$$(\Phi\psi)(x) = \int \langle x|\ \Phi\ |x'\rangle \psi(x')\, dx'$$

with $\langle x|\ \Phi\ |x'\rangle = (1/(2\pi)^{1/2})\, e^{ixx'}$.

2. If

$$\varphi_n = \frac{1}{\sqrt{n!}} (A^*)^n \varphi_0 \qquad \text{where } A = \frac{1}{\sqrt{2}} (Q + iP) \text{ and } A\varphi_0 = 0,$$

then $\Phi\varphi_n = i^n \varphi_n$.

3. Every vector $f \in \mathscr{H}$ permits a unique decomposition into four vectors

$$f = f_1 + f_2 + f_3 + f_4$$

such that $\Phi f_n = i^n f_n$.

4. The Fourier transformation Φ satisfies the properties

$$\Phi^2 = \Pi, \qquad \Phi^4 = I.$$

5. If $\varphi_n(x)$ is the vector

$$\varphi_n \qquad \frac{1}{\sqrt{n!}} (A^*)^n \varphi_0$$

in the spectral representation of Q, then the operator U_α (13–86) may be represented as an integral operator with the kernel

$$\langle x|\, U_\alpha \,|x'\rangle = \sum_{n=0}^{\infty} \varphi_n^*(x) e^{i(\alpha/2)(n+1/2)} \varphi_n(x').$$

6. The space inversion operator Π commutes with the angular momentum operators L_r $(r = 1, 2, 3)$:

$$L_1 = Q_2 P_3 - Q_3 P_2, \ldots .$$

7. If $\psi(r, \vartheta, \varphi)$ is the polar-coordinate representation of a wave function, then $(\Pi\psi)(r, \vartheta, \varphi) = \psi(r, \pi - \vartheta, \varphi + \pi)$. In particular,

$$\Pi \mathcal{Y}_l^m = (-1)^l \mathcal{Y}_l^m.$$

13-8. TIME REVERSAL

The time-reversal transformation is defined by $Q \to Q$, $\dot{Q} \to -\dot{Q}$. It is immediately seen that the evolution operator as given by Eq. (13–60) is invariant under this transformation. It follows from this that it cannot be a unitary transformation. If it were, we could conclude, from the definition of $\dot{Q} = i[H, Q]$, that $\dot{Q}$ must be invariant too, contrary to the defining property of the time-reversal transformation.

Let us examine whether there exists an anti-unitary transformation which generates the time-reversal transformation. Such a transformation does indeed exist. If we define by T the complex conjugation of the state in the spectral representation of Q, that is, the transformation which assigns to any vector $\psi(x)$ the vector

$$(T\psi)(x) = \psi^*(x), \tag{13–88}$$

then we find that

$$PT = -TP, \qquad QT = TQ, \qquad \text{and} \qquad T^2 = I.$$

Furthermore, $THT^{-1} = (1/2\mu)(P + a(Q))^2 + v(Q)$. The evolution operator is thus invariant under time reversal if the external fields $a(Q)$ and $v(Q)$ are transformed simultaneously into $-a(Q)$ and $v(Q)$.

Since $\mu\dot{Q} - P = -a(Q)$, this implies that $\dot{Q}$ transforms into $-\dot{Q}$ under the transformation T, as it must.

A special case, which is of great importance in some applications, is the case of scalar interactions in three dimensions. The evolution operator is then always equivalent to the operator

$$H = \frac{1}{2\mu} \mathbf{P}^2 + v(\mathbf{Q})$$

for a suitable choice of the gauge. The form invariance of this operator under gauge transformations has the consequence that to every solution ψ_t of the Schrödinger equation there corresponds another one which is related to the first by a time-reversal transformation. The time-reversed solution φ_t is defined by

$$\varphi_t = T\psi_{-t}. \tag{13-89}$$

We verify that with ψ_t this is also a solution of the Schrödinger equation. Thus let $i\dot{\psi}_t = H\psi_t$. Applying T on both sides of the equation, we find

$$T(i\dot{\psi}_t) = -iT\dot{\psi}_t = TH\psi_t = HT\psi_t.$$

Here we have used the fact that T is anti-unitary and that it commutes with H. Since $d\psi_t/dt = -d\psi_t/d(-t)$, we may write the above result also in the form

$$i\dot{\varphi}_t = H\varphi_t \qquad \text{with } \varphi_t = T\psi_{-t}.$$

This shows that φ_t represents the time-reversed solution of the Schrödinger equation.

It is interesting to examine the effect of time reversal on the angular-momentum operator. It is not difficult to verify (Problem 1) that

$$T\mathbf{L} = -\mathbf{L}T. \tag{13-90}$$

It follows from this that (up to a phase factor)

$$T\mathcal{Y}_l^m = \mathcal{Y}_l^{-m}. \tag{13-91}$$

For the particular choice of phases adopted in Eq. (13–35), the phase factor is $+1$ as written in the last equation.

PROBLEMS

1. The angular-momentum operator anticommutes with the time-reversal operator:

$$T\mathbf{L} = -\mathbf{L}T.$$

2. If $H\psi = E\psi$, and E is nondegenerate, then the solution ψ is proportional to a real function in the spectral representation of Q.
3. The time-reversal transformation T commutes with the rotations and the space inversion:

$$TU_R = U_R T, \qquad \text{and} \qquad T\Pi = +\Pi T.$$

[*Note:* In the derivation of these relations it is essential to use the antilinear property of T.]

4. In the spectral representation of P, the time-reversal transformation has the form

$$(T\varphi)(k) = \varphi^*(-k).$$

5. If T commutes with H, and if there exists an eigenstate ψ of the evolution operator $H\psi = E\psi$ with a current density $\mathbf{j}(\mathbf{x})$ not identically zero, then the eigenvalue E is necessarily degenerate. [*Hint:* A solution of $H\psi = E\psi$ with $\mathbf{j}(\mathbf{x}) \neq 0$ is necessarily complex. The operator T then generates another solution.]

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CHAPTER 14

PARTICLES WITH SPIN

Das ist ja ein ganz witziger Einfall.

W. PAULI to R. de L. Kronig,
January 8, 1925

In this chapter the nonrelativistic theory of a particle is refined to the theory of a particle with spin. The case of spin $\frac{1}{2}$ is considered in detail, being at once the simplest and the most fundamental one. In Section 14-1 we prepare the physical and mathematical background for the description of "quasi-elementary" particles, that is, particles which have some sort of internal degree of freedom. These general considerations are then specialized in Section 14-2 to the elementary theory of a particle with spin $\frac{1}{2}$. The aspect of the spin as an intrinsic angular momentum is then related to the representation theory of the rotation group in Section 14-3. How the spin and the orbital angular momentum combine to the resultant total angular momentum is explained in Section 14-4. We sketch in Section 14-6 the effect of external electric and magnetic fields on the dynamical structure of a particle with spin $\frac{1}{2}$ which leads to the observable phenomena of hyperfine splitting and anomalous Zeeman effects. The case of a general spin is considered in the last section (14-7), where it is shown that the entire kinematics of a particle with *any* spin can be obtained from the imprimitivity theorem.

14-1. SPIN, A NONCLASSICAL DEGREE OF FREEDOM

In Section 13-1 we gave a definition of an elementary particle as a localizable system for which the position observables constitute a complete system of compatible observables. In mathematical terms this can be expressed in two different, but equivalent, ways. In order to do this, it is convenient to introduce the abelian von Neumann algebra generated by the projection-valued measure $\Delta \to E_\Delta$, where Δ is a Borel set in the Euclidean space E_3 of three dimensions and E_Δ is the projection representing the elementary proposition: "The particle is in the set Δ." The algebra $\mathcal{A}$ generated by this set is defined by the formula $\mathcal{A} = \{E_\Delta\}''$, which says that $\mathcal{A}$ is the double

commutant of the family of projections E_Δ. $\mathscr{A}$ consists of all functions $u(\mathbf{Q})$ defined by

$$(f, u(\mathbf{Q})f) = \int u(\mathbf{x})\, d\mu_f, \qquad \text{where} \quad \mu_f(\Delta) = (f, E_\Delta f),$$

is the measure induced by the projections E_Δ for any fixed vector $\mathbf{f}$.

The statement that E_Δ is a complete system of compatible observables is expressed in full rigor and extreme simplicity by the relation (cf. Eq. (13–1))

$$\mathscr{A} = \mathscr{A}', \tag{14–1}$$

which says that $\mathscr{A}$ is a maximal abelian algebra.

We have previously shown that this property can also be expressed in terms of the cyclic vector g. In fact, Eq. (14–1) is equivalent to the statement that the family of projections E_Δ admits a cyclic vector: There exists a vector g with the property that the linear manifold

$$D_g \equiv \{\mathscr{A}g\} \tag{14–2}$$

is dense in $\mathscr{H}$: $\bar{D}_g = \mathscr{H}$.

Whether there exist elementary particles is ultimately a matter of experience. There is nothing in the axioms of quantum mechanics which would throw any light on this question. We shall see that electrons, for instance, are not elementary in this sense. They have an internal degree of freedom, called spin, which one must include in a complete set of compatible observables.

But even for systems which in a first approximation may be considered "elementary," the notion may have only a limited validity.

We can illustrate this point by discussing a few examples: A He nucleus in its ground state can, to a good approximation, be considered an elementary particle in the sense just described. But we know that this notion represents only an approximation, which is fully adequate for the description of all low-energy phenomena, but which is no longer valid for very high-energy processes. This reason is that a He nucleus is a complex structure with internal degrees of freedom, which we may conveniently ignore as long as we focus our attention only on the ground state. These internal degrees of freedom make themselves felt in processes of excitation and dissociation which may occur at high energies.

As a second example, we consider the π-meson. Again, if we consider a π-meson of a definite charge, we may, to a good approximation, consider it an elementary particle in the above sense, but only as long as we ignore its instability against decay into other particles. Furthermore we observe that π-mesons occur in nature in three varieties of charge, $+e$, $-e$, and 0, and of masses very nearly equal. For this reason physicists have for a long time adopted the point of view that the π-meson might really be not an elementary system but rather a threefold degenerate version of a larger system. The

additional degrees of freedom which need to be added in order to obtain a full description of the system are, in this case, known as the *isotopic spin*. This point of view has proved very fruitful for the discussion of the so-called *strong interactions*, because it is found that these interactions are invariant under rotations in the isotopic spin-space.

Finally we mention one of the most interesting cases of additional degeneracy from the domain of weak interactions. This is the system of the neutral K-mesons. There are two neutral particles K_0 and $\overline{K}_0$ which have identical mass and no electric charge; they appear in different reactions and they decay differently. What is more striking is that they may occur in coherent superpositions.

Historically the earliest example known of a system which is not elementary in the above sense is furnished by the electron. Soon after the discovery of quantum mechanics, it was realized that the number of terms found, for instance in the analysis of the Zeeman effect for alkali atoms, was actually twice as large as the number one would have expected on the assumption of elementarity for the electron. This doubling was first attributed to a residual angular momentum of the core electron [1]. This interpretation was, however, soon found to be wrong, and the doubling of the states was recognized to be a double degeneracy of the states of the electron itself. Furthermore it was found that the doubly degenerate states transform under space rotations like the two-component representation of the group $SU(2)$, the unitary group in two variables with determinant 1. This is the simply-connected universal covering group of the rotation group of E_3.

In physical language this means that the electron carries with it an intrinsic angular momentum, different from the orbital angular momentum. For this additional intrinsic angular momentum, the word "spin" is quite generally used today.

14-2. THE DESCRIPTION OF A PARTICLE WITH SPIN $\frac{1}{2}$

In this section we shall now consider the kinematics of a particle with spin $\frac{1}{2}$, a system for which the electron is a typical example.

Let $\Delta \to E_\Delta$ be the projection-valued measure describing localizability of the system and let $\mathscr{A} = \{E_\Delta\}''$ be the von Neumann algebra generated by the E_Δ. Since the spectrum of this algebra is degenerate there does no longer exist a cyclic vector. Indeed a vector g_1 with the property that the measure $\mu_1(\Delta) \equiv \mu_{g_1}(\Delta) = (g_1, E_\Delta g_1)$ is maximal defines a linear manifold $D_{g_1} = \{\mathscr{A} g_1\}$, the closure of which, $M_1 \equiv M(g_1) = \bar{D}_{g_1}$, is a proper subspace of the Hilbert space.

Let E_1 be the projection with range M_1, and $E_2 = I - E_1$ the projection with range $M_1^\perp = M_2$. In M_2 we can choose a second maximal vector g_2 such that the measure $\mu_2(\Delta) = (g_2, E_\Delta g_2)$ is also maximal. It is therefore

equivalent to μ_1. The invariance of the measures μ_1 and μ_2 under translations implies that both these measures are equivalent to Lebesgue measure in E_3. If the algebra $\mathscr{A}$ is doubly degenerate, then the vector g_2 generates the entire space $M(g_2)$ so that

$$M_2 \equiv M(g_2) = \overline{\{\mathscr{A} g_2\}}.$$

This is the situation which is found for electrons.

Let $\psi \in \mathscr{H}$ be an arbitrary unit vector in $\mathscr{H}$, representing, for instance, a pure state of the electron system, and $\psi = \psi_1 + \psi_2$ the unique decomposition with $\psi_1 = E_1\psi$, $\psi_2 = E_2\psi$. Furthermore, let $\mathscr{A}_1 = \mathscr{A}E_1 = E_1\mathscr{A}E_1$ and $\mathscr{A}_2 = \mathscr{A}E_2 = E_2\mathscr{A}E_2$ be the reduction of $\mathscr{A}$ to the subspaces M_1 and M_2 respectively. Then $\mathscr{A}_1$ is maximal abelian in M_1 and $\mathscr{A}_2$ is maximal abelian in M_2. Hence the vector ψ_1 admits a spectral representation $\psi_1 = \{\psi_1(\mathbf{x})\}$ and so does $\psi_2 = \{\psi_2(\mathbf{x})\}$.

We have thus verified that the pure states of the doubly degenerate electron system permit a unique description in terms of pairs of functions $\psi = \{\psi_1(\mathbf{x}), \psi_2(\mathbf{x})\}$. The square of the norm of the vector ψ is then equal to the sum of the square of the norms of ψ_1 and ψ_2:

$$\|\psi\|^2 = \|\psi_1\|^2 + \|\psi_2\|^2 = \int (|\psi_1(\mathbf{x})|^2 + |\psi_2(\mathbf{x})|^2)\, d^3x. \qquad (14\text{–}3)$$

A slightly more abstract description is obtained by noting that for each value of $\mathbf{x}$ the two complex numbers $\psi_1(\mathbf{x})$ and $\psi_2(\mathbf{x})$ may be regarded as the two components in a two-dimensional Hilbert space $\mathscr{H}_2$. We may therefore describe the spectral representation of a doubly degenerate localizable system by giving for each $\mathbf{x}$ a vector $\psi(\mathbf{x})$ in some Hilbert space $\mathscr{H}_2(\mathbf{x})$. Such a family of vectors $\psi = \{\psi(\mathbf{x})\}$ with the norm defined by

$$\|\psi\|^2 = \int \|\psi(\mathbf{x})\|^2\, d^3x$$

form a Hilbert space $\mathscr{H}$ which is called the *direct integral* of the spaces $\mathscr{H}_2(\mathbf{x})$.

Instead of a family of two-dimensional spaces, we may also choose a standard space $\mathscr{H}_2$ (independent of $\mathbf{x}$). If $f \in L^2(E_3)$ and $u \in \mathscr{H}_2$, we can define a vector $\varphi(f, u) \in \mathscr{H}$ by setting $\varphi(\mathbf{x}) = \{\varphi_1(\mathbf{x}), \varphi_2(\mathbf{x})\}$, where φ_1 and φ_2 are proportional to the components of u in a fixed coordinate system (u_1, u_2) in $\mathscr{H}_2$. That is

$$\varphi_1(\mathbf{x}) = \lambda_1 f(\mathbf{x}), \qquad \varphi_2(\mathbf{x}) = \lambda_2 f(\mathbf{x})$$

with

$$\lambda_1 = (u_1, u), \quad \lambda_2 = (u_2, u) \qquad \text{and} \qquad (u_1, u_2) = 0.$$

The following facts are easily verified:

1) The mapping $\varphi(f, u)$ from $L^2(E_3) \times \mathscr{H}_2$ into $\mathscr{H}$ is bilinear in f and u.

2) Every vector of $\mathscr{H}$ is a linear combination of vectors of the form $\varphi(f, u) \equiv f \otimes u$.

We have previously shown (Section 11-7) that these properties characterize the tensor product of the two spaces $L^2(E_3)$ and $\mathscr{H}_2$. Thus we see: The pure states are unit vectors in the tensor product $L^2(E_3) \otimes \mathscr{H}_2$.

Furthermore, because the space $\mathscr{H}_2$ is two-dimensional, every pure state in $\mathscr{H}$ is the linear combination of exactly two states of the form $\varphi(f, u)$. Indeed, let u_1 and u_2 be an orthonormal coordinate system in $\mathscr{H}_2$. We then verify easily that the pure state

$$\psi(\mathbf{x}) \equiv \{\psi_1(\mathbf{x}), \psi_2(\mathbf{x})\}$$

is represented by

$$\psi(\mathbf{x}) = \psi_1(\mathbf{x})u_1 + \psi_2(\mathbf{x})u_2 \tag{14–4}$$

provided we choose for u_1 and u_2 the special representations

$$u_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{and} \qquad u_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

In the following, both representations of the vectors in $\mathscr{H}$ will be used interchangeably. The transition from one to the other is given by formula (14–4).

The fact that pure states for a particle with spin are unit vectors in a direct product space of $L^2(E_3)$ and the two-dimensional spin space $\mathscr{H}_2$ has interesting consequences when we consider the reduction of the states to these two factor spaces.

For instance, we may ask the question: What is the spin state of a particle which is in the pure state (14–4)? Similarly we may ask: What is the state in the space $L^2(E_3)$? We encounter here again the problem of the reduction of the state of a system in a product space to one of its factor spaces. This problem is identical with the problem of the reduction of states in the measuring process. We have solved it in detail in Section 11-8 and we can take over the solution here in full. From the general theory of Section 11-8 we know that a pure state in a product space is in general a mixture in one of the factor spaces and is therefore best represented by the density matrix.

We express the result in the notation of Section 11-8 by introducing $\mathscr{H}^{\mathrm{I}} = L^2(E_3)$, $\mathscr{H}^{\mathrm{II}} = \mathscr{H}_2$, and $W = P_\psi$ for the pure state (14–4). A simple calculation then gives for the reduced states W^{I}, W^{II} the expressions (cf. Problems 1, 2)

$$W^{\mathrm{I}} = \|\psi_1\|^2 P_{\psi_1} + \|\psi_2\|^2 P_{\psi_2}, \tag{14–5}$$

$$W^{\mathrm{II}} = \begin{pmatrix} (\psi_1, \psi_1) & (\psi_1, \psi_2) \\ (\psi_2, \psi_1) & (\psi_2, \psi_2) \end{pmatrix}. \tag{14–6}$$

From these expressions we can verify immediately what we know already from the general reduction theory: The reduced states W^{I} and W^{II} are pure if and only if the pure state ψ is of the form $f \otimes u$ where $f \in L^2(E_3)$ and $u \in \mathscr{H}_2$ (Problems 3, 4).

The matrix W^{II} represents the spin state for the entire system. We may physically also speak of the spin states of the particles inside a volume element Δ. It is then convenient to define the spin-state density $W^{II}(\mathbf{x})$ defined by the matrix

$$W^{II}(\mathbf{x}) = \begin{pmatrix} |\psi_1(\mathbf{x})|^2 & \psi_1^*(\mathbf{x})\psi_2(\mathbf{x}) \\ \psi_2^*(\mathbf{x})\psi_1(\mathbf{x}) & |\psi_2(\mathbf{x})|^2 \end{pmatrix}. \tag{14–7}$$

This expression is normalized so that

$$\mathrm{Tr} \int W^{II}(\mathbf{x})\, d^3x = 1.$$

The spin-state density is always a pure state since $\det W^{II}(\mathbf{x}) = 0$; therefore $W^{II}(x)$ is of rank 1. However, the spin state of a finite volume element, given by

$$W_\Delta^{II} = \int_\Delta W^{II}(\mathbf{x})\, d^3x \tag{14–8}$$

is in general a mixture.

An interesting illustration of these properties of the spin which was of great importance in the development of the spin theory is the Stern-Gerlach and related types of experiments. These experiments are based on the fact that the magnetic properties associated with the different spin states permit modifications of the components $\psi_1(\mathbf{x})$ and $\psi_2(\mathbf{x})$ by external magnetic fields.

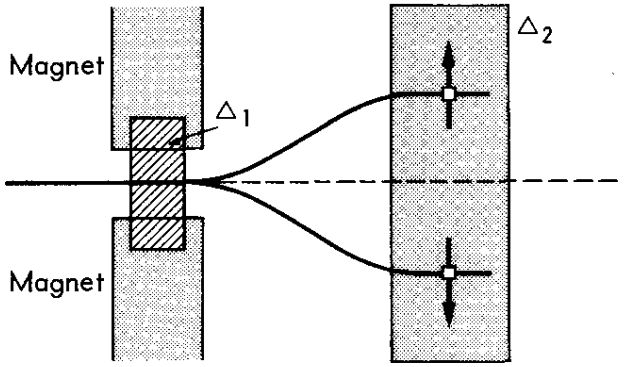

Fig. 14–1 Schematic representation of the Stern-Gerlach experiment.

For instance, in the Stern-Gerlach experiment an atom carrying the spin of a single electron is subject to an inhomogeneous magnetic field which separates the wave function $\psi_1(\mathbf{x})$ from $\psi_2(\mathbf{x})$ (cf. Fig. 14–1). In the region Δ_1 the pure state of the system is represented by a pair of functions of the form

$$\psi(\mathbf{x}) = f(\mathbf{x}) \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix}.$$

The spin state for Δ_1 is pure too, and it is given by

$$u = \lambda_1 u_1 + \lambda_2 u_2.$$

In the region Δ_2 the state $\psi(\mathbf{x})$ is still pure but it is given by a pair of functions

$$\psi(\mathbf{x}) = \begin{pmatrix} \psi_1(\mathbf{x}) \\ \psi_2(\mathbf{x}) \end{pmatrix} \qquad \text{with} \quad (\psi_1, \psi_2) = 0.$$

The spin state for Δ_2 is now a mixture of the states u_1 and u_2 with the respective probabilities

$$\int_{\Delta_2} |\psi_1(\mathbf{x})|^2 \, d^3x \qquad \text{and} \qquad \int_{\Delta_2} |\psi_2(\mathbf{x})|^2 \, d^3x.$$

PROBLEMS

1. Let $\mathscr{H} = \mathscr{H}^{\mathrm{I}} \otimes \mathscr{H}^{\mathrm{II}}$ where $\mathscr{H}^{\mathrm{I}} = L^2(E_3)$ and $\mathscr{H}^{\mathrm{II}} = \mathscr{H}_n$ is a finite (n)-dimensional Hilbert space. The reduction of a pure state $\psi \in \mathscr{H}$ to $\mathscr{H}^{\mathrm{I}}$ has the form

$$W^{\mathrm{I}} = \sum \|\psi_r\|^2 P_{\psi_r}$$

where ψ_r is the rth component of ψ in the direct product space $\mathscr{H}$.

2. Under the assumptions of Problem 1, the reduction of the pure state W to the space $\mathscr{H}^{\mathrm{II}}$ is given by the matrix of Gram

$$W^{\mathrm{II}}_{rs} = (\psi_r, \psi_s) \qquad (r, s = 1, \ldots, n).$$

3. If W^{I} and W^{II} of the preceding problems are pure, then the matrix W^{II}_{rs} is of rank one and all the functions $\psi_r(\mathbf{x})$ are proportional: $\psi_r(\mathbf{x}) = \lambda_r f(\mathbf{x})$.

4. If W^{I} and W^{II} are pure, then ψ is of the form $\psi = f \otimes u$ with $\lambda_r f(\mathbf{x}) = \psi_r(\mathbf{x})$ and

$$u = \sum_{r=1}^{n} \lambda_r u_r.$$

14-3. SPIN AND ROTATIONS

So far we have formulated only the mathematical aspect of the degeneracy caused by an internal degree of freedom. Now we must proceed to express in mathematical terms that this internal degree of freedom is an intrinsic angular momentum, in short, a spin.

This property implies a definite transformation law of the spin components under space rotations: The spin-space $\mathscr{H}_2$ will undergo, under space rotations, a linear transformation which furnishes a projective representation of the rotation group. The problem of finding the transformation of the spin is thus reduced to a mathematical one: Find all the projective representations of the rotation group in a two-dimensional complex space. The solution of this problem is unique up to a similarity transformation: There exists exactly one class of equivalent representations of the rotation group. We shall now determine this representation.

There are essentially two methods which one may employ in determining the unique two-dimensional projective representation of the rotation group. One of them emphasizes the *global* point of view, the other the *local* one.

The global method is based on the fact that the rotation group G is doubly connected and that its simply connected universal covering group is $SU(2)$, the group of unimodular unitary transformations in a two-dimensional complex space. Every such transformation U induces, in fact, a rotation in E_3 in the following manner: We represent a vector in $\mathscr{H}_2$ by two complex numbers (z_1, z_2) and write for U,

$$\begin{aligned} z_1' &= \alpha z_1 + \beta z_2 \\ z_2' &= -\beta^* z_1 + \alpha^* z_2, \end{aligned} \tag{14–9}$$

where α, β are two complex numbers subject to the condition

$$\alpha^*\alpha + \beta^*\beta = 1. \tag{14–10}$$

It follows from Eq. (14–9) that the quantities

$$\begin{aligned} s_1 &= z_1^* z_2 + z_2^* z_1 \\ s_2 &= -i(z_1^* z_2 - z_2^* z_1) \\ s_3 &= z_1^* z_1 - z_2^* z_2 \end{aligned} \tag{14–11}$$

undergo a linear transformation with real coefficients if the z_1, z_2 are transformed according to Eq. (14–9). Furthermore the Euclidean length $\sqrt{s_1^2 + s_2^2 + s_3^2}$ is left invariant under this transformation. One finds, in fact, that (Problem 1)

$$\sqrt{s_1'^2 + s_2'^2 + s_3'^2} = (\alpha^*\alpha + \beta^*\beta)\sqrt{s_1^2 + s_2^2 + s_3^2}. \tag{14–12}$$

Thus to every transformation U there corresponds exactly one rotation. Evidently the same rotation corresponds to the transformations U and $-U$. Furthermore to every rotation R there corresponds exactly one such pair of transformations $U(R)$ in $\mathscr{H}_2$ (Problem 2).

It follows from this that the transformations $U(R)$ constitute a ray representation of the rotations:

$$U(R_1)U(R_2) = \pm U(R_1R_2). \tag{14–13}$$

Let us now examine this representation from the local point of view. Locally, the rotation group G and the group $SU(2)$ are isomorphic. This means there exist neighborhoods of the identity in the two groups and a one-to-one correspondence of these neighborhoods which is left invariant under the group operations. This local structure is completely characterized by the Lie algebra, which for the rotation group is given by

$$[L_1, L_2] = iL_3, \ldots \text{cycl.} \tag{14–14}$$

Here and subsequently, we indicate by "... cycl." the other two equations which are obtained by cyclic rotations of the indices.

A solution of these commutation rules by two-dimensional matrices may be obtained in the form

$$L_r = 2\sigma_r \qquad (r = 1, 2, 3),$$

where

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{14–15}$$

are the Pauli spin-matrices. They satisfy, in addition to the relation (14–14), the stronger relations

$$\begin{aligned} \sigma_1\sigma_2 &= i\sigma_3 = -\sigma_2\sigma_1, \ldots \text{ cycl.}, \\ \sigma_r^2 &= I \qquad (r = 1, 2, 3). \end{aligned} \tag{14–16}$$

One can prove that the irreducible representations (14–15) of the commutation relations are unique up to equivalence. This is expressed in the form of the following:

> ***Theorem.*** *If σ_r' $(r = 1, 2, 3)$ is an irreducible representation of the algebraic relations* (14–16), *then there exists a nonsingular transformation S such that*
>
> $$\sigma_r' = S\sigma_r S^{-1} \qquad (r = 1, 2, 3)$$
>
> *where σ_r are the Pauli spin matrices* (14–15).

If σ_r' are Hermitian matrices, then S is unitary. For the proof of the theorem see Problems 3, 4, 5, and 6.

The uniqueness of the representations of (14–14) can be also demonstrated by construction of all the representations of (14–14) with algebraic methods. We shall here sketch this method. More details can be found in many textbooks, since this is one of the oldest methods which has been used for this purpose.

We observe first that the operator $\mathbf{L}^2 \equiv L_1^2 + L_2^2 + L_3^2$ commutes with all three components L_σ and it is therefore a multiple of the unity. We denote it by $\kappa^2 \cdot I$. Since $\mathbf{L}^2$ is a sum of squares, it is a positive operator. Therefore $\kappa^2 \geq 0$, so that κ is real. We introduce the raising and lowering operators

$$L_\pm = L_1 \pm iL_2. \tag{14–17}$$

They satisfy the commutation rules

$$[L_3, L_\pm] = \pm L_\pm, \qquad [L_+, L_-] = 2L_3. \tag{14–18}$$

Let $|m\rangle$ represent an eigenvector of L_3 with eigenvalue m, so that

$$L_3|m\rangle = m|m\rangle. \tag{14–19}$$

It follows from the relations (14–18) that

$$L_3 L_+ |m\rangle = (L_+ L_3 + L_+)|m\rangle = (m + 1)L_+ |m\rangle. \qquad (14\text{–}20)$$

This shows that $L_+ |m\rangle$ is also eigenvector of L_3 with eigenvalue $m + 1$. Thus we may write $L_+ |m\rangle = \lambda_m |m + 1\rangle$ where λ_m is some numerical constant to be determined. One proves in a similar way that $L_- |m\rangle = \mu_m |m - 1\rangle$, where μ_m is some other numerical constant. Since L_+ and L_- are adjoints of one another it follows immediately that $\lambda_m = \mu^*_{m+1}$. Furthermore, from

$$L_- L_+ = L_1^2 + L_2^2 + i[L_1, L_2] = \mathbf{L}^2 - L_3^2 - L_3,$$

it follows that

$$|\mu_{m+1}|^2 = |\lambda_m|^2 = \kappa^2 - m(m + 1).$$

From this equation one sees immediately that the sequence (m) is bounded above and below. Since $\operatorname{Tr} L_3 = 0$ (cf. Problem 3), the values of m must be symmetrically distributed between positive and negative values. This is only possible if $\kappa^2 = l(l + 1)$ and $-l \leq m \leq +l$ with l one of the values $l = 0, \frac{1}{2}, 1, 3/2, \ldots$ It follows that $|\lambda_m|^2 = l(l + 1) - m(m + 1)$ and the arbitrary phase can be fixed such that

$$\mu_{m+1} = \lambda_m = \sqrt{l(l + 1) - m(m + 1)}.$$

We have thus constructed the matrix representation of the operators L_r in a $(2l + 1)$-dimensional space for $l = 0, \frac{1}{2}, 1, 3/2, \ldots$, etc. We summarize the result:

$$\begin{aligned} L_3 |m\rangle &= m |m\rangle \\ L_+ |m\rangle &= \lambda_m |m + 1\rangle \\ L_- |m\rangle &= \lambda_{m-1} |m - 1\rangle \end{aligned} \qquad (14\text{–}21)$$

with $\lambda_m = \sqrt{l(l + 1) - m(m + 1)}$.

One verifies that one finds the representation (14–15) by specializing: $l = \frac{1}{2}$.

Returning to this special case $l = \frac{1}{2}$ once more, we can now easily establish the connection between the local and the global approach. Since the rotation R_φ with the parameter vector $\boldsymbol{\varphi}$ is generated by the infinitesimal rotation in the direction of $\boldsymbol{\varphi}$, we find immediately that this rotation is represented by $R_\varphi \to \pm U_\varphi$ with

$$U_\varphi = e^{(i/2)\boldsymbol{\varphi} \cdot \boldsymbol{\sigma}}. \qquad (14\text{–}22)$$

The last relation is very useful for obtaining an explicit formula for the matrix U_φ. If we write

$$\sigma_\alpha = (\boldsymbol{\alpha} \cdot \boldsymbol{\sigma}) \qquad \left(\boldsymbol{\alpha} = \frac{1}{\varphi} \boldsymbol{\varphi} \quad \text{and} \quad \varphi = |\boldsymbol{\varphi}|\right),$$

we have

$$U_\varphi = \cos\frac{\varphi}{2} + i\sigma_\alpha \sin\frac{\varphi}{2}, \tag{14–23}$$

or explicitly

$$U_\varphi = \begin{pmatrix} \cos\dfrac{\varphi}{2} + i\alpha_3 \sin\dfrac{\varphi}{2}, & i(\alpha_1 - i\alpha_2)\sin\dfrac{\varphi}{2} \\ i(\alpha_1 + i\alpha_2)\sin\dfrac{\varphi}{2}, & \cos\dfrac{\varphi}{2} - i\alpha_3 \sin\dfrac{\varphi}{2} \end{pmatrix} \tag{14–24}$$

so that, in the notation of (14–9),

$$\alpha = \cos\frac{\varphi}{2} + i\alpha_3 \sin\frac{\varphi}{2}, \qquad \beta = (\alpha_2 + i\alpha_1)\sin\frac{\varphi}{2}. \tag{14–25}$$

This transformation law of the spin components is now to be combined with the other effect of space rotations on the state vector to obtain the general transformation law for the state vectors. We define the transformed vector $\psi' \equiv R\psi$ by the equation

$$(R\psi)(R\mathbf{x}) = U(R)\psi(\mathbf{x}). \tag{14–26}$$

This definition of the transformed state vector $R\psi$ is made in such a way that for two rotations R_1 and R_2, we find the composition law

$$(R_1R_2\psi)(R_1R_2\mathbf{x}) = U(R_1)U(R_2)\psi(\mathbf{x}). \tag{14–27}$$

PROBLEMS

1. If s_r $(r = 1, 2, 3)$ are defined according to (14–11), then the linear transformation $s_r \to s'_r$ of the variables s_r induced by (14–9) is such that

$$s_1'^2 + s_2'^2 + s_3'^2 = (\alpha^*\alpha + \beta^*\beta)^2(s_1^2 + s_2^2 + s_3^2).$$

2. The correspondence between rotations R in E_3 and unimodular unitary transformations U in $\mathscr{H}_2$ is such that to every pair of transformations $\pm U$, one rotation corresponds exactly.
3. If L_r $(r = 1, 2, 3)$ is any set of matrices satisfying (14–14), then

$$\operatorname{Tr} L_\sigma = 0.$$

4. Any set σ_r satisfying Eq. (14–16) is linearly independent:

$$\sum_{r=1}^{3} \lambda_r\sigma_r = 0 \qquad \text{implies} \qquad \lambda_r = 0.$$

5. Every representation of the relation (14–16) is equivalent to a Hermitian one.
6. Every irreducible Hermitian representation of (14–16) is of dimension two, and every two such representations are unitarily equivalent.

7. Two rotations R_{φ} and $R_{\varphi'}$ have the composition law $R_{\varphi} \cdot R_{\varphi'} = R_{\psi}$, where the rotation angle of R_{ψ} is $\psi = |\boldsymbol{\psi}|$ and is given by

$$\cos\frac{\psi}{2} = \cos\frac{\varphi}{2}\cos\frac{\varphi'}{2} - (\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}')\sin\frac{\varphi}{2}\sin\frac{\varphi'}{2}$$

with

$$\boldsymbol{\alpha} = \frac{1}{\varphi}\boldsymbol{\varphi}, \qquad \boldsymbol{\alpha} = \frac{1}{\varphi'}\boldsymbol{\varphi}'.$$

14-4. SPIN AND ORBITAL ANGULAR MOMENTUM

The combination of spin and orbital angular momentum gives rise to a number of interesting phenomena which are caused by the fact that in general neither the spin nor the orbital angular momentum are separately conserved in the time evolution of the system.

For a particle without spin we have found that in a spherically symmetrical external field the evolution operator H commutes with the angular momentum operators L_r $(r = 1, 2, 3)$. For a particle with spin this need no longer be the case. Instead, another quantity, the *total* angular momentum, has this property.

In order to formulate this conservation law it is convenient to change the notation. We retain the notation L_r $(r = 1, 2, 3)$ for the three components of the *orbital* angular momentum. They are defined as before as the three operators with the components L_r. The spin angular momentum components we designate by $S_r = \frac{1}{2}\sigma_r$ $(r = 1, 2, 3)$. We then define the *total angular* momentum $\mathbf{J}$ in vector notation by

$$\mathbf{J} = \mathbf{L} + \mathbf{S}. \tag{14–28}$$

For an infinitesimal rotation with parameters α we then have

$$R\psi = \psi - \boldsymbol{\alpha}\cdot\mathbf{J}\psi + \cdots \tag{14–29}$$

In an external field which is spherically symmetric the rotations leave the evolution operator H invariant. It follows that the infinitesimal parts of the rotations commute also with H:

$$[\mathbf{J}, H] = 0. \tag{14–30}$$

This equation expresses the conservation of angular momentum in quantum mechanics.

For spinless systems we have shown that the possible values for the total angular momentum in units of $\hbar$ are given by $L^2 = l(l+1)$ where l assumes one of the values $l = 0, 1, 2, \ldots$. We shall now examine the corresponding question in a system with spin $s = \frac{1}{2}$. From (14–28) we find

$$\mathbf{J}^2 = \mathbf{L}^2 + \mathbf{S}^2 + 2\mathbf{L}\cdot\mathbf{S}. \tag{14–31}$$

Let us examine the properties of this operator in a subspace spanned by the $2l + 1$ eigenvectors of L_3 and the $2s + 1 = 2$ eigenvectors of S_3. We designate these vectors in the $2(2l + 1)$-dimensional product space characterized by fixed values for $\mathbf{L}^2 = l(l + 1)$ and $\mathbf{S}^2 = \frac{3}{4}$.

Let us examine the operator (14–31). Since the values of $\mathbf{L}^2$ and $\mathbf{S}^2$ are fixed we must concentrate our attention on the operator $X = \mathbf{L} \cdot \mathbf{S}$. An elementary calculation, using the commutation rules of $\mathbf{L}$ and $\mathbf{S}$, yields the relation

$$X^2 + \tfrac{1}{2}X = \tfrac{1}{4}\mathbf{L}^2 = \tfrac{1}{4}l(l + 1). \tag{14–32}$$

This shows immediately that the $2(21 + 1)$-dimensional matrix X has only two different eigenvalues which we may denote by x_1 and x_2. They are the two roots of the quadratic equation

$$x^2 + \tfrac{1}{2}x - \tfrac{1}{4}l(l + 1) = 0$$

$$x_1 = \tfrac{1}{2}l, \qquad x_2 = -\tfrac{1}{2}(l + 1).$$

It follows from this result that if we write $\mathbf{J}^2 = j(j + 1)$ then j may assume exactly two values which are determimed by the two equations:

$$j(j + 1) = l(l + 1) + \tfrac{3}{4} - l = (l + \tfrac{1}{2})(l + \tfrac{3}{2})$$

$$j(j + 1) = l(l + 1) + \tfrac{3}{4} - (l + 1) = (l - \tfrac{1}{2})(l + \tfrac{1}{2}).$$

Thus the two possible values of j are $l \pm \frac{1}{2}$.

This is the composition law of a spin $s = \frac{1}{2}$ with an orbital angular momentum l: The resultant angular momentum j assumes only the two values $j = l \pm \frac{1}{2}$. This composition law is a special case of a more general law which governs the composition of any two angular momenta $\mathbf{j}_1$ and $\mathbf{j}_2$ to a result $\mathbf{J} = \mathbf{j}_1 + \mathbf{j}_2$. If $\mathbf{j}_1^2 = j_1(j_1 + 1)$ and $\mathbf{j}_2^2 = j_2(j_2 + 1)$, then $\mathbf{J}^2 = j(j + 1)$ assumes the values $j = j_1 + j_2, j_1 + j_2 - 1, \ldots, |j_1 - j_2|$. The proof of this is given in many references (e.g. [3]).

PROBLEMS

1. If $\mathbf{L}^2 = l(l + 1)$ and $\mathbf{S}^2 = s(s + 1)$ then $\mathbf{L} \cdot \mathbf{S}$ may assume the values

$$\mathbf{L} \cdot \mathbf{S} = \frac{j(j + 1) - l(l + 1) - s(s + 1)}{2}, \qquad j = l + s, l + s - 1, \ldots, |l - s|.$$

2. Two spins $\boldsymbol{S}^{(1)}$ and $\boldsymbol{S}^{(2)}$, each of value $s = \frac{1}{2}$ may combine into a triplet and a singlet system of total angular momentum $j = 1$ or $j = 0$ respectively.
3. The values j resulting from the combination of two angular momenta are either all half integers or all integers.

14-5. SPIN UNDER SPACE REFLECTION AND TIME INVERSION

We shall now examine the effect on a spin of the transformations of space reflection and time inversion.

The space reflection σ is defined by the transformation:

$$\mathbf{Q} \to -\mathbf{Q}, \qquad \mathbf{P} \to -\mathbf{P}, \qquad \text{and} \qquad \mathbf{S} \to \mathbf{S}. \tag{14–33}$$

It is evident that this is a canonical transformation: The commutation rules are invariant and there exists a unitary transformation U such that

$$\begin{aligned} U\mathbf{Q}U^{-1} &= -\mathbf{Q} \\ U\mathbf{P}U^{-1} &= -\mathbf{P} \\ [U, S] &= 0. \end{aligned} \tag{14–34}$$

The transformation U with these properties is given by the same expression (13–87) as for the particle without spin.

The time inversion τ is defined by the transformation

$$\mathbf{Q} \to \mathbf{Q}, \qquad \mathbf{P} \to -\mathbf{P}, \qquad \text{and} \qquad \mathbf{S} \to -\mathbf{S}. \tag{14–35}$$

Just as in the spinless case it follows that the operator which produces this transformation must be antiunitary. But it is not simply given by complex conjugation as in the spinless case.

This is so because the spin-matrices do not all reverse the sign under complex conjugation; only S_2 does. Thus the transformation of complex conjugation must be combined with a unitary transformation which commutes with $\mathbf{Q}$ and $\mathbf{P}$ and S_2 and anticommutes with S_1 and S_3. This transformation has the form σ_2. The time reversal transformation is thus finally given in the form $T = \sigma_2 K$, where K stands for the operation of complex conjugation in the x-representation. With this expression for T we find indeed

$$\begin{aligned} T\mathbf{Q}T^{-1} &= \mathbf{Q} \\ T\mathbf{P}T^{-1} &= -\mathbf{P} \\ T\mathbf{S}T^{-1} &= -\mathbf{S}. \end{aligned} \tag{14–36}$$

We mention incidentally that $T^2 = -I$, a relation which follows from the fact that

$$K^2 = I \qquad \text{and} \qquad K\sigma_2 K = -\sigma_2,$$

since σ_2 is purely imaginary. Thus a repetition of the transformation of time reversal does not restore the wave function of a pure state but it replaces it by its negative. The state is thereby not affected since it is represented by a

ray in Hilbert space and both ψ and $-\psi$ are evidently in the same ray. This is in contrast to the case without spin where $T^2 = +I$. The generalization of this result for general spin is left as a problem (5).

PROBLEMS

1. In the standard representation of any angular momentum the complex conjugation operation K has the effect

$$L_1^c \equiv KL_1K = L_1$$

$$L_2^c \equiv KL_2K = -L_2$$

$$L_3^c \equiv KL_3K = L_3.$$

2. The unitary operator X with the property

$$XL_rX^{-1} = -L_r^c$$

is given by

$$X = e^{i\pi L_2}.$$

3. For the operator X of problem (2) one has $KXK = X$.
4. For a fixed value l for the angular momentum operator ($L^2 = l(l+1)$; $l = 0, \frac{1}{2}, 1, \ldots$) we have

$$X^2 = (-1)^{2l}I.$$

5. For a particle with a spin of value s the time inversion operator T has the property

$$T^2 = (-1)^{2s}I.$$

6. If T is a time inversion operator then $T' = e^{i\alpha}T$ for any real α is, too. Furthermore

$$T'^2 = T^2.$$

7. Let $H = (1/2\mu)\mathbf{P}^2 + v(Q)$ be the evolution operator for a spinning particle of spin $\frac{1}{2}$ in an external *electric* field. (No magnetic field, $\mathbf{a} = 0$). For such a system every eigenstate of H is at least doubly degenerate (Kramer's degeneracy). (Hint: Consider the transformation T, show that it commutes with H and that for any eigenvector ψ of H, ψ and $T\psi$ are in different rays.)

14-6. SPIN IN AN EXTERNAL FORCE FIELD

In this section we shall examine the dynamical structure of a spin in an external field of force. In other words we shall determine the most general form of the evolution operator H in the presence of a spin. We have shown in Section 13-4 that under the hypothesis of Galilei invariance the evolution

operator for a spinless particle must necessarily be of the form (13–60). In the case of a spin the arguments which led to this expression are no longer valid, since we used explicitly that the position operator generates a maximal abelian algebra. In the presence of a spin degree of freedom this is not the case and the evolution operator may assume other forms involving the spin operator. We shall now examine the other possibilities.

The possibilities for the other forms of H are restricted if we impose the conditions that the evolution operator be invariant not only under rotations but also under space reflections and time inversions.

We shall first of all assume that in the absence of an external field the evolution is governed by the operator H_0 as it follows from Galilei invariance for each spin-component separately. The spin-degree of freedom is thus affected only in the presence of an external field.

We consider the case of a static field only. There are two vectors which must be considered: $\mathbf{e} = -\nabla v$ and $\mathbf{h} = \nabla \times \mathbf{a}$. Under space-inversion $\mathbf{e}$ behaves like a polar vector and $\mathbf{h}$ like an axial vector. Under time reversal $\mathbf{e}$ is invariant while $\mathbf{h}$ changes sign.

There are exactly two invariants which can be formed with $\mathbf{e}$, $\mathbf{h}$ and the other dynamical variables. They are of the form (Problem 1)

$$H_1 = -\alpha(\mathbf{e} \cdot \dot{\mathbf{Q}} \times \mathbf{S}), \qquad H_2 = -\beta(\mathbf{h} \cdot \mathbf{S}). \tag{14–37}$$

Here α and β are two constants to be determined by experiments. Invariance arguments alone do not suffice for their determination. The values obtained for them from the spectra for the atoms are

$$\alpha = \frac{1}{2}\frac{\hbar}{mc^2}, \qquad \beta = \frac{\hbar}{m} = \frac{1}{\mu}. \tag{14–38}$$

In conventional units where the external field $\mathbf{e}$ is measured in e.s.u. units, $\mathbf{h}$ in gauss, and the energy operator is given in ergs, they take on the values

$$\alpha = \frac{e}{2}\left(\frac{\hbar}{mc}\right)^2, \qquad \beta = \frac{e\hbar}{mc}. \tag{14–38$'$}$$

The fact that in these expressions the constant c, the velocity of light, appears explicitly indicates that they cannot be calculated in a purely non-relativistic theory. On the other hand, in the relativistic theory of the electron they can be calculated, and they are found to be in agreement with the experimental values.

The actual value of these constants played an important role in the early days of quantum mechanics. Indeed the value β is twice as large as one would expect on the basis of a simple model of the electron, giving rise to the remarkable phenomenon of the anomalous Zeeman effect.

On the other hand the constant α, also called the spin-orbit constant, is half as large as one would expect on the basis of the magnetic field in the rest system of the electron due to the electric field **e**. This factor $\frac{1}{2}$ was explained by Thomas on the basis of a more exact quasi-relativistic spin theory. It is often referred to as the *Thomas factor* [4].

In a spherical external field $v(r)$ the term H_1 can be transformed since

$$\nabla v = \mathbf{Q} \frac{1}{r} \frac{dv}{dr};$$

therefore

$$H_1 = \alpha(\mathbf{S} \cdot \mathbf{L}) \frac{1}{r} \frac{dv}{dr}.$$

In this form it is seen that the term H_1 produces a rotation-invariant coupling between spin and orbital angular momenta. This term is responsible for the fine-structure splitting of the energy levels in the atoms.

PROBLEMS

1. For a particle with spin $\frac{1}{2}$ the only invariants which, under space rotations, space reflections, and time inversion, depend on the external forces through **e** and **h**, are of the form

$$\mathbf{e} \cdot (\dot{\mathbf{Q}} \times \mathbf{S}) \qquad \text{and} \qquad (\mathbf{h} \cdot \mathbf{S}).$$

2. The hyperfine interaction is zero for an electron with orbital angular momentum $l = 0$.
3. A charged particle with charge e is placed in a uniform magnetic field **H**. The additional term in the energy operator (= $\hbar$ times the evolution operator) which is linear in **H** is of the form

$$-\frac{e\hbar}{2mc}(\mathbf{H} \cdot \mathbf{L})$$

where **L** is the orbital angular momentum.

4. A spin $\frac{1}{2}$ in a uniform magnetic field **H** is governed by the evolution operator

$$\mathbf{H}_1 = -\frac{e}{2mc}(\mathbf{H} \cdot \mathbf{S})$$

so that for any state W in the two-dimensional spin space

$$i\dot{W} \quad [H_1, W] \qquad \omega[(\alpha \cdot \mathbf{S}), W]$$

where ω $eH/2mc$ is the *Larmor frequency* and α $(1/H)\mathbf{H}$ is the unit vector in the direction of the magnetic field.

5. Define the spin vector **S** with components

$$S_r = \text{Tr } W\sigma_r \qquad (r = 1, 2, 3).$$

It has the length

$$\mathbf{S}^2 \equiv \sum_{r=1}^{3} S_r^2 = 2 \text{ Tr } W^2 - 1.$$

6. For a spin in a uniform magnetic field **H** (cf. Problem 4), the spin vector of an electron satisfies the equation of motion $\dot{\mathbf{s}} = \omega(\mathbf{s} \times \boldsymbol{\alpha})$, where $\omega = eH/2mc$ (Larmor precession).

14-7. ELEMENTARY PARTICLE WITH ARBITRARY SPIN

In this last section we shall return to the case of the free particle but with an arbitrary value of the spin. We could, in principle, pursue the same road that we have used for the case of spin $\frac{1}{2}$. However, we shall not do this here, but shall instead use this occasion to show how the imprimitivity theorem, which we quoted in Section 12-3, is sufficient to furnish us a classification of all the possible types of elementary particles which can occur in nature. Let us review the content of this theorem and apply it to the case we wish to study.

We are given a group G and a homogeneous space M. In our case G is the group of Euclidean motions (or, rather, is a simply-connected covering group), and M is the three-dimensional Euclidean space. Both are separable and locally compact, and M has an invariant measure. The action of the group on M is expressed as a continuous function from $M \times G$ to M which, in the example, is transitive. If $q \in M$ and $x \in G$, this function is denoted by $[q]x$.

A system of imprimitivities is a σ-additive projection-valued measure on the Borel sets of M and a representation $x \to U_x$ of G by unitary operators all in a Hilbert space and such that

$$U_x^{-1} E_\Delta U_x = E_{[\Delta]x}. \tag{14–39}$$

The physical interpretation of such a system is as follows: The E_Δ represent the propositions of finding the particle in the set Δ and property (14–39) expresses the homogeneity and isotropy of the physical space in which the particle is located. An *irreducible* representation of such a system then represents an *elementary* particle. We therefore wish to know all the irreducible representations of the system (14–39). The answer is contained in the imprimitivity theorem (cf. Section 12-3).

Let q_0 be an arbitrary point of G and let G_0 be the set of all elements $\xi \in G$ which leave the point q_0 fixed: In our example the set G will consist of the subgroup of all rotations with a rotation axis passing through q_0.

Thus G_0 is simply the rotation group (which we shall always replace by its covering group). The elements $\xi \in G_0$ can thus be identified with the rotations R, while a general element $x \in G$ is represented by (R, α), which means the rotation R followed by the translation given by the vector α. With this convention the composition law of the Euclidean group is given by

$$(R_1, \alpha_1)(R_2, \alpha_2) = (R_1R_2, \alpha_1 + R_1\alpha_2). \tag{14–40}$$

We shall continue with the general notation, however, until it is necessary to use specific properties of G and M.

Let $\xi \to L_\xi$ be a particular irreducible representation of the little group G_0 in a Hilbert space $\mathscr{H}_0$. The induced representation consists of operators which act on functions $f(x)$ on the group with values in $\mathscr{H}_0$ and satisfying

$$f(\xi x) = L_\xi f(x). \tag{14–41}$$

Let μ be the quasi-invariant measure on M, and define the equivalent measure μ_x by setting $\mu_x(\Delta) \equiv \mu([\Delta]x)$. Let $\rho_x(y)$ be the Radon-Nikodym derivative of μ_x with respect to μ. We then define

$$(U^L_x f)(y) = \sqrt{\rho_x(y)}\, f(yx). \tag{14–42}$$

(In our case we may take Lebesgue measure and assume $\rho_x(y) = 1$, but for the time being we retain the more general formulas.) One can then prove that (14–42) is a unitary representation of G. Furthermore we have also obtained a canonical system of imprimitivities by setting

$$(E_\Delta f)(x) = \mathbf{1}_\Delta([q_0]x) f(x). \tag{14–43}$$

The last two formulas contain the entire kinematics of nonrelativistic elementary particles. However, in this form they have little resemblance to what one might have expected as a generalization of the spin $\frac{1}{2}$ case.

This generalization would have looked as follows: The representation space $\mathscr{H} = \mathscr{L}^2_\mu(M, \mathscr{H}_0)$ is the Hilbert space of functions $F(q)$ over M with values in a "spin space" $\mathscr{H}_0$ of finite dimensions. If $D(R)$ is the irreducible representation of G_0 with that dimension, then $U_{(R,\alpha)}$ acts on such functions according to

$$(U_{(R,\alpha)}F)(q) = D(R)F([q](R, \alpha)), \tag{14–44}$$

and the projections E_Δ are given by

$$(E_\Delta F)(q) = \mathbf{1}_\Delta(q)F(q). \tag{14–45}$$

The chief difference between the last two pairs of equations is that in one case we are dealing with functions over the group G and in the other case with functions over the space M.

We shall now show that these two representations of the system of imprimitivities are nevertheless equivalent in the sense that there exists an isometric linear mapping from $\mathscr{H}^L$ onto $\mathscr{H}$ which transforms the two systems into each other.

Let $F(q)$ be a vector valued function over q. We can change it into a function over the group by writing $q = [q_0]x$. But as a function of x it would in general not satisfy Eq. (14–41). In order to obtain this relation we proceed as follows: Let $x \to B(x)$ be a function from G to the unitary operators in $\mathscr{H}_0$ which satisfies the identity

$$B(\xi x) = L_\xi B(x) \qquad \forall\, \xi \in G_0,\ x \in G. \tag{14–46}$$

We then define

$$f(x) = B(x)F([q_0]x), \tag{14–47}$$

and verify without effort that *this* function does satisfy Eq. (14–41). Conversely, if $f(x)$ is given, we can define a function $F(q)$ by the formula

$$F([q_0]x) = B^{-1}(x)f(x), \tag{14–48}$$

and again it is routine to verify that the F thus defined is indeed a function on the right coset $q = [q_0]x$ only.

We have thus established a one-to-one correspondence between $\mathscr{H}^L$ and $\mathscr{L}^2_\mu(M, \mathscr{H}_0)$ which is linear and isometric. If we define this mapping by Ω which takes $\mathscr{H}^L$ to $\mathscr{L}^2_\mu(M, \mathscr{H}_0)$, then we can calculate in a straightforward manner the form of the representation U_x in $\mathscr{L}^2_\mu(M, \mathscr{H}_0)$ defined by

$$U_x = \Omega U^L_x \Omega^{-1}. \tag{14–49}$$

The result is

$$(U_x F)(q) = B^{-1}(y)B(yx)\sqrt{\rho_x(y)}\, F([q]x) \tag{14–50}$$

with $q = [q_0]y$. We find that for each fixed x there appears a unitary operator

$$Q_x(y) \equiv B^{-1}(y)B(yx).$$

Both $Q_x(y)$ and the numerical factor $\rho_x(y)$ satisfy a functional equation which can be obtained from (14–50) by the simple device of expressing the fact that U_x is a representation of G. Thus if we operate on the left twice, once with U_{x_1} and then with U_{x_2} and then compare the result with the operation $U_{x_1x_2}$, we find the identities:

$$\rho_{x_1}(y)\rho_{x_2}(yx_1) = \rho_{x_1x_2}(y), \tag{14–51}$$

$$Q_{x_1}(y)Q_{x_2}(yx_1) = Q_{x_1x_2}(y). \tag{14–52}$$

We have now brought U_x into the form

$$(U_x F)(q) = Q_x(y)\sqrt{\rho_x(y)}\, F([q]x). \tag{14–53}$$

This begins to resemble Eq. (14–44), but is not yet identical with it. In order to bring it into the final form we need to use special properties of the Euclidean group.

First we make somewhat less arbitrary the definition of $B(x)$ and thus of $Q_x(y)$. To this end we choose in each right coset (remember M is in one-to-one correspondence with the right cosets) an arbitrary element x_0 so that $q = [q_0]x_0$. Then we fix $B(x)$ on each coset by setting $B(x_0) = I$. We then obtain

$$B(x) = B(xx_0^{-1}x_0) = L_{xx_0^{-1}}B(x_0),$$

since $xx_0^{-1} \in G_0$. Thus, using $B(x_0) = I$, we have an explicit formula for $B(x)$:

$$B(x) = L_{xx_0^{-1}}. \tag{14–54}$$

From this we find the standard form of

$$Q_x(q) \equiv Q_x(y) = L^{-1}_{yy_0^{-1}}L_{(yx)(yx)_0^{-1}} \qquad (q = [q_0]y). \tag{14–55}$$

The last step consists now in showing that for the Euclidean group the representative element x_0 in the coset q can be so chosen that $Q_x(q)$ becomes simply $L_{(R,\,0)}$ (independent of q).

If $x = (R_1, \boldsymbol{\alpha})$ we choose $x_0 = (I, R^{-1}\boldsymbol{\alpha})$ and find, from the composition law (14–40), that

$$x = \xi x_0 \qquad \text{with} \quad \xi = (R, 0) \in G_0.$$

Let the element $y = (S, \boldsymbol{\beta})$ be similarly written. Then we find

$$yy_0^{-1} = (S, 0),\ yx = (SR, \boldsymbol{\beta} + S\boldsymbol{\alpha})$$

$$(yx)_0 = (I, R^{-1}S^{-1}\boldsymbol{\beta} + R^{-1}\boldsymbol{\alpha})$$

$$(yx)(yx)_0^{-1} = (SR, 0).$$

Substituting all these results into (14–55) we find

$$Q_x(q) = L_{(R,\,0)}. \tag{14–56}$$

This is the desired result. It suffices to identify $L_{(R,\,0)}$ with $D(R)$ of Eq. (14–44). The equivalence is therefore established and our expectations are fully justified. We have now also the assurance that the properties of localizability and homogeneity are sufficient to determine in a general way the kinematics of the system. The only arbitrariness which is left is the positive integer $n = \dim \mathscr{H}'_0$ which determines the spin of the particle by the formula $S = (n - 1)/2$.

REFERENCES

The early history of the discovery of the spin is recounted in the following papers:

1. R. KRONIG, "The Turning Point," *Pauli Memorial Volume*. New York: Interscience (1960); p. 5.
2. B. L. VAN DER WAERDEN, "The Exclusion Principle and Spin." Ibid. (1960), p. 199.

Angular momenta in quantum mechanics are discussed in many good textbooks. We refer, for instance, to:

3. A. MESSIAH, *Mécanique Quantique*. Paris: Dunod (1960); especially Volume 2, Chapter XIII.
4. L. H. THOMAS, *Nature* **117**, 514 (1926); *Phil. Mag.* **17**, 3 (1927).

CHAPTER 15

IDENTICAL PARTICLES

"This must be the wood, where things have no names. I wonder what'll become of my *name when I go in?"*

LEWIS CARROLL,
Alice in Wonderland

The formal theory of welding several similar particles into a single system is developed in Section 15-1. The central notion is the *tensor product* of the Hilbert spaces, referring to the individual particles, a notion which was already introduced in connection with the measuring process in Section 11-7. Here we extend it to several factors, and study some superficial aspects of the structure of the von Neumann algebras generated by the observables for such a system.

In Section 15-2 we develop the theory of the tensor product with several factors in somewhat greater detail and generality, in order to have the tools ready for expressing the notion of identity in quantum mechanics, introduced in the following section (15-3). Great care is taken to emphasize the difference in meaning for this notion in quantum mechanics and in classical mechanics. It is then formalized in the proper mathematical language for a system of two particles.

In Section 15-4 we begin the treatment of *any number* of identical particles. We introduce the two classes of statistics corresponding to the symmetrical and the antisymmetrical subspaces of the tensor product space. The possibility of intermediate cases (parastatistics) is mentioned, and it is shown that the existence of a complete set of commuting observables is not compatible with parastatistics. The formal treatment of the Bose gas is the subject of Section 15-5, and the Fermi gas, that of Section 15-6.

15-1. ASSEMBLY OF SEVERAL PARTICLES

The preceding sections were concerned with the quantum theory of a single particle. We now turn to the theory of an assembly of several particles. We begin with the theory of two particles; the generalization to an arbitrary finite number of particles is then easy.

When we consider a physical system consisting of two particles, we are dealing with a special case of the union of two systems into a joint larger system. The theory of this process was discussed in detail in Section 11-7, in connection with the measuring process. Although the purpose here is different, we can take over the formalism of that section in full.

Let $\mathscr{S}_1$ be the set of all observables of particle 1. They are represented by a family of self-adjoint operators in a Hilbert space $\mathscr{H}_1$. We shall assume that there are no superselection rules, so that $\mathscr{S}_1'' \equiv \mathscr{N}_1 = \mathscr{B}(\mathscr{H}_1)$. This means that the von Neumann algebra generated by $\mathscr{S}_1$ is the set of all bounded operators over $\mathscr{H}_1$.

Let $\mathscr{S}_2$ be the corresponding set of operators for particle 2, and assume also $\mathscr{S}_2'' \equiv \mathscr{N}_2 = \mathscr{B}(\mathscr{H}_2)$.

The kinematical independence of the two sets of observables expresses itself with the equation

$$\mathscr{S}_1 \subseteq \mathscr{S}_2', \tag{15–1}$$

which is equivalent to the statement that any observable from the set $\mathscr{S}_1$ is compatible with any observable from the set $\mathscr{S}_2$.

Let us now consider the joint system (1 + 2). Denote by $\mathscr{S}$ the set of all observables for this system. Every such observable is a self-adjoint operator in the tensor product space. This set contains, first of all, observables of the form $A_1 \otimes I_2$ with $A_1 \in \mathscr{S}_1$ and I_2 the identity in $\mathscr{H}_2$ which represents the measurement of the quantity A_1 on the joint system (1 + 2). Likewise, it will contain the observable $I_1 \otimes A_2$ with I_1 the identity in $\mathscr{H}_1$ and $A_2 \in \mathscr{S}_2$. This observable represents the observation of A_2 on the joint system. Since these last two operators commute, they can be measured independently, and such a measurement constitutes also a measurement of their product $A_1 \otimes A_2$, which is thus also an observable.

However, not every observable is of the form $A_1 \otimes A_2$. For instance, for two particles the total energy is not of this form, even in the absence of a dynamical interaction. In fact, any quantity which is additive in the constituent parts cannot be of this form. We have thus

$$\mathscr{S}_1 \times \mathscr{S}_2 \subset \mathscr{S} \tag{15–2}$$

where $\mathscr{S}_1 \times \mathscr{S}_2$ denotes the set of observables of the form $A_1 \otimes A_2$; $A_1 \in \mathscr{S}_1$, $A_2 \in \mathscr{S}_2$.

Let us define the *tensor product* of two von Neumann algebras $\mathscr{N}_1 \otimes \mathscr{N}_2$ as the algebra generated by elements of the form $T_1 \otimes T_2$ with $T_1 \in \mathscr{N}_1$ and $T_2 \in \mathscr{N}_2$. In the notation adopted with Eq. (15–2) we may thus write

$$\mathscr{N}_1 \otimes \mathscr{N}_2 = (\mathscr{N}_1 \times \mathscr{N}_2)''. \tag{15–3}$$

From Eq. (15–2) it follows first that

$$\mathscr{S}' \subseteq (\mathscr{S}_1 \times \mathscr{S}_2)'. \tag{15–4}$$

One can prove furthermore [1] that

$$(\mathscr{S}_1 \times \mathscr{S}_2)' = (\mathscr{N}_1 \times \mathscr{N}_2)'. \tag{15–5}$$

Hence, combining Eqs. (15–4) and (15–5), we find

$$\mathscr{S}' \subseteq (\mathscr{N}_1 \times \mathscr{N}_2)'. \tag{15–6}$$

From this equation we obtain, after once more taking the commutant,

$$(\mathscr{N}_1 \times \mathscr{N}_2)'' \equiv \mathscr{N}_1 \otimes \mathscr{N}_2 \subseteq \mathscr{S}'' = \mathscr{N}, \tag{15–7}$$

where $\mathscr{N}$ is the von Neumann algebra generated by all the observables $\mathscr{S}$ on the system.

Let us examine the commutant of $\mathscr{N}$. According to Eq. (15–7), we obtain

$$\mathscr{N}' \subseteq (\mathscr{N}_1 \otimes \mathscr{N}_2)' = \mathscr{N}_1' \otimes \mathscr{N}_2'.$$

The affirmation contained in the last equality sign is by no means obvious. It can be proved only for the so-called *semi-finite* algebras [2]. Fortunately this hypothesis is satisfied for our case where $\mathscr{N}_1 = \mathscr{B}(\mathscr{H}_1)$ and $\mathscr{N}_2 = \mathscr{B}(\mathscr{H}_2)$. These algebras are known to be semifinite [3].

Since $\mathscr{N}_1$ and $\mathscr{N}_2$ are both irreducible, it follows from Eq. (15–7) that

$$\mathscr{N}' = \{\lambda I\}.$$

Thus $\mathscr{N}$ is irreducible too and $\mathscr{N}$ consists of all bounded operators over $\mathscr{G} = \mathscr{H}_1 \otimes \mathscr{H}_2$. We summarize this result with the following:

> ***Theorem:*** *If $\mathscr{S}_1$ is a set of self-adjoint operators in $\mathscr{H}_1$ generating the algebra of all bounded operators in $\mathscr{H}_1$: $\mathscr{S}_1'' \equiv \mathscr{N}_1 = \mathscr{B}(\mathscr{H}_1)$, and if $\mathscr{S}_2$ is a similar set of operators in $\mathscr{H}_2$, then the set of operators $A_1 \otimes A_2$ in the product space $\mathscr{G} = \mathscr{H}_1 \otimes \mathscr{H}_2$, with $A_1 \in \mathscr{S}_1$ and $A_2 \in \mathscr{S}_2$, generates the algebra of all bounded operators in $\mathscr{G}$.*

With this theorem established, we can now proceed with the description of the system of two particles. Let $\mathscr{C}_1 \subset \mathscr{S}_1$ be a complete system of compatible observables in $\mathscr{S}_1$, that is, a system of commuting self-adjoint operators from $\mathscr{S}_1$ such that $\mathscr{C}_1'' \equiv \mathscr{A}_1 = \mathscr{A}_1'$. For an elementary particle such a system always exists (cf. the definition of elementary particle in Section 12-4). We denote by Λ_1 the Cartesian product of the spectra of the system of operators in $\mathscr{C}_1$.

Let $\mathscr{C}_2 \subset \mathscr{S}_2$ be a similar set in $\mathscr{S}_2$, and Λ_2 the Cartesian product of the spectra of the operators in $\mathscr{C}_2$.

The spectral representation of the set $\mathscr{C}_1$ is given by functions $\psi_1(\lambda_1)$ $(\lambda_1 \in \Lambda_1)$ in the Hilbert space $L^2_{\rho_1}(\Lambda_1)$, where ρ_1 is a measure in the uniquely defined measure class determined by $\mathscr{C}_1$ in the space Λ_1.

Similarly the spectral representation of $\mathscr{C}_2$ is given by functions $\psi_2(\lambda_2)$, $(\lambda_2 \in \Lambda_2)$ in the Hilbert space $L^2_{\rho_2}(\Lambda_2)$.

Every operator $A_1 \in \mathscr{C}_1$ may be amplified to an operator $A_1 \otimes I_2$ in $\mathscr{G} = \mathscr{H}_1 \otimes \mathscr{H}_2$. Similarly every operator $A_2 \in \mathscr{C}_2$ in $\mathscr{H}_2$ may be amplified to an operator $I_1 \otimes A_2$ in $\mathscr{G}$. We shall denote these sets of amplified operators again by $\mathscr{C}_1$ and $\mathscr{C}_2$. Their union will be denoted by $\mathscr{C} = \mathscr{C}_1 \cup \mathscr{C}_2$. It is now possible to prove that if $\mathscr{C}_1$ and $\mathscr{C}_2$ are both complete sets of commuting operators in $\mathscr{H}_1$, $\mathscr{H}_2$ respectively, then $\mathscr{C}$ is a complete commuting set of operators in $\mathscr{G} = \mathscr{H}_1 \otimes \mathscr{H}_2$ (Problem 1).

The spectral representation of this set is then given by functions $\psi(\lambda_1 \lambda_2) \in L^2_\rho(\Lambda_1 \times \Lambda_2)$ over the Cartesian product space $\Lambda_1 \times \Lambda_2$, where ρ is the product measure $\rho_1 \times \rho_2$.

In most calculations in applications one chooses the position and the spin for the sets $\mathscr{C}$ so that for particles with spin $\frac{1}{2}$, for instance, $\lambda = \{\mathbf{x}, s\}$ ($\mathbf{x} \in E_3$, $s = \pm 1$). For elementary particles with spin $\frac{1}{2}$ this set is always a complete set of commuting observables by the definition of elementarity.

The foregoing considerations can easily be extended to the case of any finite number of particles. Successive applications of the preceding theorem established for two Hilbert spaces gives the following result:

> ***Theorem:*** *If $\mathscr{S}_i$ is a set of self-adjoint operators in $\mathscr{H}_i$ generating the algebra of all bounded operators in $\mathscr{H}_i$ ($i = 1, \ldots, n$) so that $\mathscr{S}_i'' = \mathscr{N}_i = \mathscr{B}(\mathscr{H}_i)$, then the set of operators $A_1 \otimes A_2 \otimes \cdots \otimes A_n$ in the product space $\mathscr{G} = \mathscr{H}_1 \otimes \mathscr{H}_2 \otimes \cdots \otimes \mathscr{H}_n$ with $A_i \in \mathscr{S}_i$ generates the algebra of all bounded operators in $\mathscr{G}$.*

With the same reasoning one can establish that if $\mathscr{C}_i \subset \mathscr{S}_i$ are a complete set of commuting operators in $\mathscr{H}_i$, then, after amplification of the operators from $\mathscr{H}_i$ to $\mathscr{G}$, we can affirm that $\mathscr{C}_1 \cup \mathscr{C}_2 \cup \cdots \cup \mathscr{C}_n$ is a complete set of commuting operators in $\mathscr{G}$. The spectral representation for this set is given by functions $\psi(\lambda_1, \lambda_2, \ldots, \lambda_n)$ in a space $L^2_\rho(\Lambda_1 \times \Lambda_2 \times \cdots \times \Lambda_n)$, where ρ is the product measure $\rho = \rho_1 \times \rho_2 \times \cdots \times \rho_n$ of the measures ρ_i induced in Λ_i by $\mathscr{C}_i$.

PROBLEMS

*1. If $\mathscr{C}_1$ is a complete abelian set of self-adjoint operators in a Hilbert space $\mathscr{H}_1$, and $\mathscr{C}_2$ is a similar set in $\mathscr{H}_2$, then the set of operators $A_1 \otimes I_2$, $I_1 \otimes A_2$, with $A_1 \in \mathscr{C}_1$ and $A_2 \in \mathscr{C}_2$ is a complete abelian set in $\mathscr{H}_1 \otimes \mathscr{H}_2$. [*Hint*: Show that $g = g_1 \otimes g_2$ is a cyclic vector in $\mathscr{G}$ if $g_1 \in \mathscr{H}_1$, $g_2 \in \mathscr{H}_2$ are cyclic vectors for $\mathscr{A}_1$ and $\mathscr{A}_2$.]

*2. If $\psi_1(\lambda_1) \in L^2_{\rho_1}(\Lambda_1)$ is the spectral representation for a set of operators $\mathscr{C}_1$ in a Hilbert space $\mathscr{H}_1$ and $\psi_2(\lambda_2) \in L^2_{\rho_2}(\Lambda_2)$ a similar representation for another set $\mathscr{C}_2$ in another Hilbert space $\mathscr{H}_2$, then $\psi(\lambda_1, \lambda_2) \in L^2_\rho(\Lambda_1 \times \Lambda_2)$ is a spectral representation for the set $\mathscr{C}_1 \cup \mathscr{C}_2$ in the Hilbert space $\mathscr{H}_1 \otimes \mathscr{H}_2$. Furthermore the measure $\rho \quad \rho_1 \times \rho_2$ [consult: J. M. Jauch and B. Misra, *Helv. Phys. Acta* **38,** 30 (1965)].

15-2. MATHEMATICAL DIGRESSION: THE MULTIPLE TENSOR PRODUCT

The theorems stated at the end of the last section make use of the multiple tensor product which we have not yet discussed explicitly. We can, of course, always proceed by iteration, using the abstract definition of the product of two spaces given in Section 11-7. However, it is desirable, especially for the treatment of identical particles, to treat all the individual subsystems and their Hilbert space on a symmetrical basis. For this reason we shall briefly sketch here how the multiple tensor product may be defined for any number of factors in a symmetrical manner.

We recall the definition of the tensor product given in Section 11-7. That such an object exists can always be shown by explicitly constructing it. There are some advantages in constructing the tensor product as a function space independently of any representation of the Hilbert spaces, since its uniqueness is then much easier to prove and certain general aspects of the tensor product become very transparent.

We define a bounded conjugate multilinear functional on the Cartesian product $\mathscr{H}_1 \times \mathscr{H}_2 \times \cdots \times \mathscr{H}_f$ as a complex-valued function

$$T(x_1, x_2, \ldots, x_f) \qquad (x_1 \in \mathscr{H}_1, x_2 \in \mathscr{H}_2, \ldots x_f \in \mathscr{H}_f)$$

with the following properties:

$$T(x_1, \ldots, x_i + y_i, \ldots, x_f) = T(x_1, \ldots x_i, \ldots x_f) + T(x_1 \ldots y_i, \ldots x_f)$$

$$T(x_1, x_2, \ldots \lambda x_i, \ldots x_f) = \lambda^* T(x_1, x_2, \ldots x_i, \ldots x_f),$$

$$|T(x_1, x_2, \ldots, x_f)| \leq C\|x_1\|\|x_2\| \cdots \|x_f\| \qquad (C < \infty).$$

Such functionals always exist, for instance,

$$T(x_1, x_2, \ldots, x_f) = (x_1, a_1)(x_2, a_2) \cdots (x_f, a_f) \tag{15–8}$$

for an arbitrary set of vectors $a_i \in \mathscr{H}_i$. We denote this particular functional by

$$T = a_1 \otimes a_2 \otimes \cdots \otimes a_f.$$

The notation anticipates the role which it is going to play in the construction of the tensor product.

We first note that the set of all bounded functionals is a linear vector space: If T and S are two such functionals, then so is $(T + S)$, as well as λT for all complex λ. The axioms of the vector space for these operations are verified.

Next let us define the scalar product of two functionals T and S. We define

$$(T, S) \qquad \sum_{r_1 \cdots r_f} T(\varphi_{r_1}, \varphi_{r_2} \cdots \varphi_{r_f})^* S(\varphi_{r_1}, \varphi_{r_2} \cdots \varphi_{r_f})$$

where $\varphi_{r_i} \in \mathscr{H}_i$ is a complete orthonormal system in $\mathscr{H}_i$. The indicated sum need not be convergent. We can prove (by Schwartz's inequality) its convergence if we admit only such functionals T for which $(T, T) < \infty$. This is the case, for instance, for the special functional $T = a_1 \otimes a_2 \otimes \cdots \otimes a_f$ for which we find easily

$$(T, T) = \|a_1\|^2 \|a_2\|^2 \cdots \|a_f\|^2.$$

It is then possible to prove that the indicated sum in the definition of (T, S) is actually independent of any particular choice of the orthonormal systems φ_{r_i}.

Let us now consider the set of all functionals T of the form $T = a_1 \otimes a_2 \otimes \cdots \otimes a_f$. The set of all finite linear combinations of such functionals is then a linear manifold. The closure in the norm topology of this manifold is a Hilbert space $\mathscr{G}_f$ and this space is the tensor product of the spaces $\mathscr{H}_1, \mathscr{H}_2, \ldots, \mathscr{H}_f$.

The separability of this space is not hard to prove. We note that this construction can be carried through with some caution for an infinite sequence of spaces. The caution refers to the convergence of infinite products as shown by Eq. (15–8). Separability is, however, in general not true. We shall not use the infinite product.

In the next section we shall need certain subspaces of the space $\mathscr{G}_f$ which we define as follows: To each $T \in \mathscr{G}_f$ of the form $T = a_1 \otimes a_2 \otimes \cdots \otimes a_f$ we can associate PT defined by

$$PT = a_{i_1} \otimes a_{i_2} \otimes \cdots \otimes a_{i_f},$$

where P stands for the permutation

$$P = \begin{pmatrix} 1 & 2 & \cdots & f \\ i_1 & i_2 & \cdots & i_f \end{pmatrix}.$$

We then define

$$T_+ = \frac{1}{f!} \sum_P PT \equiv \Pi_+ T,$$

where the summation is extended to all permutations P. The operator Π_+ thus defined on all T of the special form $a_1 \otimes a_2 \otimes \cdots \otimes a_f$ can be extended by linearity to the entire space $\mathscr{G}_f$, and it is a projection operator on this space. Its range defines a linear subspace $\mathscr{G}_f^+ \equiv \Pi_+ \mathscr{G}_f$.

In a similar way we define the space

$$\mathscr{G}_f^- \equiv \Pi_- \mathscr{G}_f = \frac{1}{f!} \sum_P \delta_P P \mathscr{G}_f.$$

Here the δ_P are the signature of the permutations P, and the sum extends over all permutations.

15-3. THE NOTION OF IDENTITY IN QUANTUM MECHANICS

The elementary particles known to occur in nature fall into a finite number of distinct classes. The members of one and the same class all have the same properties. It would be possible logically that every individual particle have certain identifying characteristics which would enable us to distinguish it, at least in principle, from all the other particles in the same class. This does not seem to be the case.

The problem of identity which we are facing here has for thousands of years been one of the most baffling in metaphysical speculations. It separated the schoolmen who were involved in the great controversy of the reality of universals. Thomas Aquinas held that the only difference between identical material objects was accidental, their essences being considered by him exactly alike. Duns Scotus, on the other hand, held that there were always differences in essence between two different individual things. This same view was held by Leibnitz who defended it in the celebrated correspondence with Clark against the views of Newton and his followers. In modern philosophy the problem still exists in a modified form in the question concerning the meaning of proper names for individual objects [9].

In physics the problem reappears as an empirical question: "Can two individual physical systems always be distinguished, or are there systems which are exactly alike?"

This is a question which can be brought down from the purely speculative level to the empirical level. It suffices to remind us how we would establish a difference between two physical systems. The only way we can establish a difference is by measuring the properties of the two systems and to see whether they show any difference.

Here a first difficulty appears which we must overcome before we can use this criterion. It is obvious that two systems cannot give the same results for all the measurable properties if they are not in the same state. We can only expect identical results for identical systems if they were prepared exactly the same way, that is, if their states are identical. This remark leads us to emphasize again the distinction between *extrinsic properties* which depend on the state of the system and *intrinsic properties* which are independent of the state. This distinction corresponds exactly to the *accidental* and *essential* qualities of the scholastic philosophers.

It is also the same distinction that we made in Chapter 5 where we showed that intrinsic properties are expressed in the lattice structure of the proposition system. For elementary particles the proposition system can be completely characterized by the property of localizability and the value of a few constants such as mass, charge, and spin (and possibly some others).

We are thus led to define identity for elementary particles in the following sense: Two elementary particles are identical if they agree in all their intrinsic properties.

In this sense two electrons, for instance, are identical and so are two protons or two neutrons. But a negaton (negative electron) differs from its positive counterpart, the positon, in the sign of the charge. Likewise an electron differs from a muon by the value of its mass and its lifetime, although the two particles seem to be identical in all the other intrinsic properties.

There is an important difference between the notion of identity in classical and in quantum mechanics to which we want to draw particular attention. Although classical particles may be identical in the above sense, they can still be distinguished from each other by their extrinsic properties, for instance their initial conditions at a given instant of time. A pair of such particles can, for instance, be distinguished, and thus identified, at all times by the fact that the initial state evolves continuously in time. The evolution of the states in classical mechanics is such that at any later time we can keep track of a particle with given initial conditions by following it along a continuous path in phase space. Thus, although two particles may be mechanically identical, they can in a classical system be identified at all times. We might say the particles can be "named" and, although the names are purely conventional, they serve at least to distinguish them from each other.

This possibility disappears for quantum systems. In such systems there is no orbit which could be retraced by continuity to some initial value. In fact, if the wave functions of the two particles overlap to any extent, they intertwine so thoroughly that their identity is lost. Thus in quantum mechanics the identification by initial conditions is not possible. This is the reason why the notion of identity in quantum physics is more fundamental than in classical physics.

Let us now express this notion in mathematical terms. We begin with the case of two particles. Let $\mathscr{S}_1$ be the set of observables for one of the particles. They are a family of self-adjoint operators in a Hilbert space $\mathscr{H}_1$. Let $\mathscr{S}_2$ be a similar set of operators in a second Hilbert space $\mathscr{H}_2$. The two sets are in every respect identical; they are merely two copies of the same set of observables.

The observables of the joint system will be a set of self-adjoint operators $\mathscr{S}$ in the Hilbert space $\mathscr{G} \equiv \mathscr{H}_1 \otimes \mathscr{H}_2$. If the two particles are merely similar but not identical, then $\mathscr{S}$ consists of operators of the form $A_1 \otimes A_2$, $A_1 \in \mathscr{S}_1$, $A_2 \in \mathscr{S}_2$, and functions of them. If the particles are identical, on the other hand, not all these operators can be observables because some of them distinguish between particle 1 and 2. Only those operators which do not distinguish between the two particles can be observables.

We can express this in a mathematical language by introducing the permutation operator P which interchanges the two particles. To this operator there corresponds a unitary transformation U_P of the Hilbert space defined as follows: Let f be a vector in $\mathscr{G}$ of the form $f = f_1 \otimes f_2$ with $f_1 \in \mathscr{H}_1$,

$f_2 \in \mathscr{H}_2$. To every such vector we associate another one $U_P f = f_2 \otimes f_1$. This defines the operator U_P on all vectors of the form $f_1 \otimes f_2$. We now extend the operator U_P by linearity to all linear combinations of vectors of this form and obtain in this manner the operator U_P in the entire Hilbert space $\mathscr{G}$. It is easily shown that U_P is unitary (Problem 1).

Let W be a state and $A \in \mathscr{S}$ an observable for the joint system. The expectation value of A is then $\langle A \rangle = \operatorname{Tr} WA$. If we carry out the transformation U_P the state changes to $W' = U_P W U_P^{-1}$. For this state the expectation value of the observable A is

$$\langle A \rangle' = \operatorname{Tr} U_P W U_P^{-1} A = \operatorname{Tr} W U_P^{-1} A U_P. \tag{15–9}$$

We shall now make the assumption that the observables are *separated* by the states. By this we mean: If A_1 and A_2 are two different observables, then there exists a state W such that

$$\operatorname{Tr} WA_1 \neq \operatorname{Tr} WA_2. \tag{15–10}$$

Since Eq. (15–9) should be true for any state, it follows from Eq. (15–10) that

$$A = U_P^{-1} A U_P, \tag{15–11}$$

or U_P commutes with A.

Thus we see that only operators A which commute with U_P can represent observables of a system with two identical particles. The operators must be symmetrical in the individual particle variables. An operator which does have this property is, for instance, $A \otimes I_2 + I_1 \otimes A$. Another one is $A_1 \otimes A_2 + A_2 \otimes A_1$.

Since the observables commute with U_P, they also commute with every function of U_P. We define the two projection operators (Problem 4):

$$\Pi_+ = \tfrac{1}{2}(I + U_P), \qquad \Pi_- = \tfrac{1}{2}(I - U_P). \tag{15–12}$$

Every observable $A \in \mathscr{S}$ commutes with them and it follows that the projections $\Pi_\pm$ reduce all the $A \in \mathscr{S}$. If there are no superselection rules, then the only projections which reduce all the observables are 0 or I. In this case only two possibilities exist:

$$\begin{aligned} &1) \quad \Pi_+ = I, \ \Pi_- = 0, \quad U_P = I, \\ &2) \quad \Pi_- = I, \ \Pi_+ = 0, \quad U_P = -I. \end{aligned} \tag{15–13}$$

In the first case the states and the operators are all reduced to the subspace

$$\mathscr{G}_+ = \Pi_+ \mathscr{G}. \tag{15–14}_+$$

In the second case they are reduced to the subspace

$$\mathscr{G}_- = \Pi_- \mathscr{G}. \tag{15–14}_-$$

If we choose a spectral representation $\varphi(\lambda_1, \lambda_2)$ with respect to some spectral set $\Lambda_1 \times \Lambda_2$ for the system (1 + 2) the functions $\varphi(\lambda_1, \lambda_2)$ satisfy

$$\varphi(\lambda_1, \lambda_2) = \varphi(\lambda_2, \lambda_1) \qquad \text{in case 1} \qquad (15\text{–}15)_+$$

and

$$\varphi(\lambda_1, \lambda_2) = -\varphi(\lambda_2, \lambda_1) \qquad \text{in case 2.} \qquad (15\text{–}15)_-$$

The two cases can be physically distinguished, for instance, by the analysis of the spectrum of a two-particle system. In case (1) one speaks of Einstein-Bose statistics, in case (2) of Fermi-Dirac statistics.

It is known empirically that all the particles which have an integral multiple of the value of the spin fall under case (1), while all particles with half-integer value for the spin fall under case (2). Thus electrons satisfy Fermi-Dirac statistics [4, 5]. This relation between spin and statistics can be deduced from the relativistic theory of many-particle systems. So far it has not been possible to do the same within the limitations of the non-relativistic theory. Thus in a nonrelativistic theory we must adopt it as an empirical fact.

PROBLEMS

1. The linear operator U_P defined on the set of vectors $f \in \mathcal{G} \equiv \mathcal{H}_1 \otimes \mathcal{H}_2$ of the form $f = f_1 \otimes f_2$ is unitary.
2. The eigenvalues of U_P of Problem 1 are ± 1.
3. If $A = A_1 \otimes A_2$, then $U_P^{-1} A U_P = A_2 \otimes A_1$.
4. The two operators $\Pi_\tau = \frac{1}{2}(I + U_P)$ are projections which commute with all observables of a system of two identical particles.

*5. Every system of two identical particles admits a complete set of commuting observables. [*Hint*: Establish $\mathcal{S}' \to \mathcal{S}''$, and use Lemma 1, p. 704, Reference 8.]

6. If $\mathcal{S}_n$ is the set of observables for n identical particles satisfying Einstein-Bose or Fermi-Dirac statistics, then the set of operators $\mathcal{S}_n \times \mathcal{S}_1$ in $\mathcal{H}_n^{\pm} \otimes \mathcal{H}_1$ have nonabelian superselection rules.

15-4. SYSTEMS OF SEVERAL IDENTICAL PARTICLES

In the last section we deduced from the notion of identity that a system of two identical particles can fall into one of two physically distinguishable classes, the symmetrical or the antisymmetrical class. We now examine the system of several identical particles. We introduce a slight change of notation. The observables for any one of the single particles will be denoted by $\mathcal{S}_1$. They are operators in the Hilbert space $\mathcal{H}_1$. The Hilbert space for the combined system of n identical particles is the n-fold tensor product $\mathcal{H}_n \equiv \mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_1$. The set of observables $\mathcal{S}$ is a set of self-

adjoint linear operators in the space $\mathscr{H}_n$. The identity of the particles restricts this set to those operators which are symmetrical under the permutation of the n-particle variables. A general permutation is

$$P = \begin{pmatrix} 1 & 2 & \dots & n \\ i_1 & i_2 & \dots & i_n \end{pmatrix}.$$

It changes 1 into i_1, 2 into i_2, etc. To every such permutation we associate a unitary operator U_P operating in $\mathscr{H}_n$. When operating on a vector $\mathbf{f}$ of the form $f = f_1 \otimes f_2 \otimes \cdots \otimes f_n$, it changes it into $U_P f = f_{i_1} \otimes f_{i_2} \otimes \cdots \otimes f_{i_n}$. U_P is then extended to the entire space $\mathscr{H}_n$ by linearity. The U_P thus defined are a unitary representation of the permutation group (Problem 7).

The representation $P \to U_P$ is reducible. Not all the irreducible representations contained in U_P are needed. Physically important are the two subspaces of $\mathscr{H}_n$ which contain the symmetrical and the antisymmetrical vectors.

A vector $\mathbf{f}$ is symmetrical if $U_P f = f$ for all permutations P. It is antisymmetrical if $U_P f = \delta_P f$. The projection Π_+ on the symmetrical subspace is defined by

$$\Pi_+ = \frac{1}{n!} \sum_P U_P. \qquad (15\text{–}16)_+$$

The projection on the antisymmetrical space is

$$\Pi_- = \frac{1}{n!} \sum_P \delta_P U_P, \qquad (15\text{–}16)_-$$

where the summations are extended over all $n!$ permutations P and δ_P is $+1$ or -1 according to whether P is even or odd (Problem 1).

For identical particles we must have

$$[A, U_P] = 0 \qquad (15\text{–}17)$$

for all $A \in \mathscr{S}$ and all U_P (Problem 3). It follows immediately that the projections $\Pi_\pm$ reduce the observables:

$$[A, \Pi_\pm] = 0. \qquad (15\text{–}18)$$

There exist other projections which reduce U_P and A. This shows that there occur other irreducible representations in U_P besides the symmetrical and antisymmetrical ones. Physically they are of no importance since every kind of particle falls into one of the two classes $\Pi_+ = I$, $\Pi_- = 0$, or $\Pi_+ = 0$, $\Pi_- = I$. Thus the subspace in which the observables A operate is either $\mathscr{H}_n^\pm = \Pi_\pm \mathscr{H}_n$. The first case corresponds to Einstein-Bose statistics, the second to Fermi-Dirac statistics.

The question has often been discussed whether some particles might obey a *parastatistics* where the observables are reduced to some of the other

reducing subspaces. So far there has been no experimental indication that such parastatistics occur in nature. Parastatistics can be excluded if one makes the assumption that there exists at least one complete system of commuting observables in $\mathscr{S}$. (Cf. Problems 4, 5, and 6.)

PROBLEMS

1. The operators $\Pi_+ \equiv \frac{1}{n!}\sum_P U_P, \qquad \Pi_- \equiv \frac{1}{n!}\sum_P \delta_P U_P$

   are projections which commute with all the observables of the system of n identical particles.
2. If $\mathscr{S}$ are the observables of a system of n identical particles and if the states separate the observables, then for all permutations P

$$[A, U_P] = 0 \qquad \text{for all} \quad A \in \mathscr{S}.$$

3. The projections $\Pi_\pm$ reduce the operators U_P:

$$[\Pi_\pm, U_P] = 0 \qquad \text{for all } P.$$

*4. There exists a complete system of commuting observables in the set $\mathscr{S}$ of all observables if and only if $\mathscr{S}' \subset \mathscr{S}''$ [cf. J. M. Jauch and B. Misra, reference 5].
5. If $\mathscr{S}' \subset \mathscr{S}''$, then the set of operators which commute with all the observables commute with each other (abelian superselection rules).
6. A system of identical particles with abelian superselection rules obeys either Einstein-Bose or Fermi-Dirac statistics.
7. The operators U_P defined in $\mathscr{H}_n$ are a faithful representation of the permutation group.
8. The reduction of U_P to the subspaces $\mathscr{H}_n^\pm \equiv \Pi_\pm \mathscr{H}_n$ is an abelian representation of the permutation group.

15-5. THE BOSE GAS

We now consider an assembly of n identical noninteracting particles satisfying the Einstein-Bose statistics. Such a system will be called a *free Bose gas*. The Hilbert space for this system is $\mathscr{H}_n^+ = \Pi_+ \mathscr{H}_n$. Let φ_r $(r = 1, 2, \ldots)$ be a complete orthonormal system of vectors in $\mathscr{H}_1$. With such a system we can construct a complete orthonormal system in $\mathscr{H}_n$ in the form

$$\varphi_{r_1} \otimes \varphi_{r_2} \otimes \cdots \otimes \varphi_{r_n}$$

(Problem 1). Every such vector when projected with Π_+ into the subspace $\mathscr{H}_n^+$ yields a vector

$$\varphi[r_1 r_2 \cdots r_n] \equiv \Pi_+ \varphi_{r_1} \otimes \varphi_{r_2} \otimes \cdots \otimes \varphi_{r_n}. \tag{15-19}$$

These vectors are still orthogonal and complete, but in general they are not normalized. In order to normalize them, we introduce a new notation.

Let n_1 be the number of indices among the $r_1 r_2 \cdots r_n$ which are equal to 1; similarly let n_2 be the number of such indices equal to 2, and so on. The following facts follow then from the definition of Eq. (15–19).

a) $n_1 + n_2 + \cdots + n_r + \cdots = n$.

b) Two $\varphi[r_1 r_2 \cdots r_n]$ are equal if and only if the corresponding $n_1, n_2, \ldots, n_r, \ldots$ are equal.

c)

$$\|\varphi[r_1 r_2 \cdots r_n]\|^2 = \frac{1}{n!} \sum_P \delta_{r_1 r_{i_1}} \delta_{r_2 r_{i_2}} \cdots \delta_{r_n r_{i_n}} = \frac{n_1! n_2! \cdots n_r! \cdots}{n!} \tag{15–20}$$

(Problem 2). Because of (b) we may replace the index $[r_1 r_2 \cdots r_n]$ by $\{n\} \equiv \{n_1 n_2 \cdots n_r \cdots\}$ and we obtain with

$$\varphi(\{n\}) \equiv \varphi(n_1 n_2 \cdots n_r \cdots) \equiv \sqrt{\frac{n_1! n_2! \cdots n_r! \cdots}{n!}}\, \Pi_+ \varphi_{r_1} \otimes \varphi_{r_2} \otimes \cdots \otimes \varphi_{r_n} \tag{15–21}$$

a complete orthonormal system of vectors in $\mathscr{H}_n^+$. Since every observable is a self-adjoint operator which is reduced by Π_+ it is possible to express it entirely in the system (15–21). A representation in this system is called an *occupation number representation.*

So far we have considered the number n, the total number of particles, as fixed. There are several advantages in dropping this restriction and considering a much larger system with an undetermined number of particles. Such a system is described in the *direct sum* of the Hilbert spaces $\mathscr{H}_n^+$ ($n = 0, 1, 2, \ldots, \infty$) called the *Fock space.* We define it as follows: A vector $F \in \mathscr{H}_0^+ \oplus \mathscr{H}_1^+ \oplus \cdots \oplus \mathscr{H}_n^+ \oplus \cdots$ is a finite or infinite sequence of vectors $f_n \in \mathscr{H}_n^+$, subject to the condition

$$\|F\|^2 \equiv \sum_{n=0}^{\infty} \|f_n\|^2 < \infty. \tag{15–22}$$

The scalar product of two vectors $F = \{f_n\}$ and $G = \{g_n\}$ is then defined by

$$(F, G) = \sum_{n=0}^{\infty} (f_n, g_n). \tag{15–23}$$

Addition and multiplication with scalars is defined by

$$F + G = \{f_n + g_n\}, \qquad \lambda F = \{\lambda f_n\}. \tag{15–24}$$

The set of all sequences $F = \{f_n\}$ with these properties thus have the structure of a Hilbert space. The vectors in the space $\mathscr{H}_0$ represent the system in the state with no particle. We shall assume that this state is nondegenerate so that $\mathscr{H}_0$ is a one-dimensional subspace. We call it the *vacuum state*. The vectors $\varphi_n \equiv \varphi(n_1 n_2 \cdots n_r \cdots)$ defined in Eq. (15–21) are vectors in the space $\mathscr{H}_n (n = n_1 + n_2 + \cdots + n_r + \cdots)$; as such they may also be considered as vectors F in the Fock space

$$F = \{f_k\}, \qquad f_k = \begin{cases} 0, & k \neq n, \\ \varphi_n, & k = n. \end{cases}$$

It is now possible to introduce a set of operators in the Fock space which permit a description of a Bose gas in terms of harmonic oscillators. We define for each $r = 1, 2, \ldots,$

$$\begin{aligned} a_r \varphi(n_1 n_2 \cdots n_r \cdots) &= \sqrt{n_r}\, \varphi(n_1 n_2 \cdots n_r - 1 \cdots), \\ a_r^* \varphi(n_1 n_2 \cdots n_r \cdots) &= \sqrt{n_r + 1}\, \varphi(n_1 n_2 \cdots n_r + 1 \cdots), \end{aligned} \tag{15–25}$$

and we call a_r a *destruction operator* and a_r^* a *creation operator*. From these definitions follows

$$a_r \varphi(0, 0, \ldots 0, \ldots) = 0, \tag{15–26}$$

and for any pair we find

$$\begin{aligned} &\big(\varphi(n_1 n_2 \cdots n_r \cdots), a_r \varphi(n_1' n_2' \cdots n_r')\big) \\ &\qquad = \big(a_r^* \varphi(n_1 n_2 \cdots n_r \cdots), \varphi(n_1' n_2' \cdots n_r' \cdots)\big) \\ &\qquad = \sqrt{n_r + 1}\, \delta_{n_1 n_1'} \delta_{n_2 n_2'} \cdots \delta_{n_r + 1, n_r'} \cdots \end{aligned} \tag{15–27}$$

Thus the operator a_r^* is the Hermitian conjugate of a_r. The operators a_r, a_r^* satisfy the commutation rules (Problem 3):

$$\begin{aligned} [a_r, a_s] &= [a_r^*, a_s^*] = 0, \\ [a_r, a_s^*] &= \delta_{rs}. \end{aligned} \tag{15–28}$$

Furthermore, the operator $N_r \equiv a_r^* a_r$ satisfies

$$N_r \varphi(n_1 n_2 \cdots n_r \cdots) = n_r \varphi(n_1 n_2 \cdots n_r \cdots). \tag{15–29}$$

This justifies calling it the *number operator* for the state r. The *total number operator* is then defined by

$$N = \sum_{r=1}^{\infty} N_r. \tag{15–30}$$

We recognize in this formulation that the free Bose gas is kinematically indistinguishable from an independent collection of distinct harmonic oscillators. The numbers n_r correspond to the excitation of the r^{th} oscillator

to the state n_r. Just as we have done for the simple harmonic oscillator, so we can show here that the vacuum state vector is a cyclic vector: By using Eq. (15–25) we obtain

$$\varphi(n_1 n_2 \cdots n_r \cdots) = \frac{1}{\sqrt{n_1!\, n_2! \cdots n_r! \cdots}} (a_1^*)^{n_1}(a_2^*)^{n_2} \cdots (a_r^*)^{n_r} \cdots, \tag{15–31}$$

where $\varphi(0) = \varphi(0, 0, \ldots, 0, \ldots)$.

Let us now consider the energy of the free Bose gas. By assumption the evolution operator and therefore the energy for a state in $\mathscr{H}_n$ is given by an operator of the form $H = H_1 + H_2 + \cdots + H_n + \cdots$, where $H_r = I \otimes I \otimes \cdots \otimes H_0 \otimes \cdots$, and where H_0 is the energy of one single boson. In order to treat this problem with relatively elementary mathematical means, it is convenient to assume that H_0 has only a discrete spectrum. We choose then for our orthonormal system φ_r the eigenvectors of the operator H_0:

$$H_0 \varphi_r = \varepsilon_r \varphi_r. \tag{15–32}$$

We find then

$$H\varphi(n_1 n_2 \cdots n_r \cdots) = (n_1 \varepsilon_1 + n_2 \varepsilon_2 + \cdots)\varphi(n_1 n_2 \cdots n_r \cdots).$$

By using the number operator (15–29) we can write, therefore, for H the expression

$$H = \varepsilon_1 a_1^* a_1 + \varepsilon_2 a_2^* a_2 + \cdots + \varepsilon_r a_r^* a_r + \cdots. \tag{15–33}$$

From this we see that also the dynamical structure of a free Bose gas is identical with that of a collection of harmonic oscillators.

Equation (15–33) is a special case of an energy operator of the form

$$H = \sum_{r,\, s} A_{rs} a_r^* a_s. \tag{15–34}$$

It corresponds to a system of bosons in an external force-field. If V is the additional term in the one-particle energy we find, by taking matrix elements of (15–34) between any two one-particle states,

$$(\varphi_r, V\varphi_s) = \left(a_r^* \varphi(0), \sum_{r_1,\, s_1} A_{r_1 s_1} a_{r_1}^* a_{s_1} a_s^* \varphi(0)\right).$$

The right-hand side can be evaluated using the commutation rules and the definition (15–26) of the vacuum state, and it is thus found to be equal to A_{rs}. Thus we have generally a relation between the one-particle energy operator and Eq. (15–34) in the form

$$(\varphi_r, V\varphi_s) = A_{rs}. \tag{15–35}$$

The energy (Eq. 15–33) is clearly a special case of this for the diagonal one-particle energy operator $V = H_0$ satisfying Eq. (15–32).

In a similar way we can express more general types of operators in the occupation number representation. For instance, an energy operator, which is the sum of operators between pairs of particles (two-body interaction), would have the form

$$H = \sum_{\substack{r_1 r_2 \\ s_1 s_2}} A_{r_1 r_2 | s_1 s_2} a_{r_1}^* a_{r_2}^* a_{s_1} a_{s_2}. \tag{15–36}$$

By a calculation which generalizes the arguments given above, one finds for the coefficients the expression

$$A_{r_1 r_2 | s_1 s_2} = (\varphi_{r_1} \otimes \varphi_{r_2}, V \varphi_{s_1} \otimes \varphi_{s_2}) \tag{15–37}$$

which relates them to the two-particle interaction operator V considered as an operator in the space $\mathscr{H}_2 = \mathscr{H}_1 \otimes \mathscr{H}_1$. It is not hard to see how this result can be generalized to many-body interactions of any kind.

We have thus succeeded in transcribing the entire theory of a system of interacting identical bosons into the theory of a system of interacting and distinct harmonic oscillators.

We may remark here, by way of a historical digression, that this result establishes the connection with the original formulation of quantum theory which treated the statistics of a gas of photons as a system of harmonic oscillators with discrete energy levels (black-body radiation). In this treatment the oscillators were represented as the normal modes of the electromagnetic field in a finite enclosure. These normal modes correspond to our choice of base vectors φ_r in $\mathscr{H}_1$ which diagonalize the free energy operator H_0.

PROBLEMS

1. If $\varphi_r \in \mathscr{H}_1$ is a complete orthonormal system in $\mathscr{H}_1$, then $\varphi_{r_1} \otimes \varphi_{r_2} \otimes \cdots \otimes \varphi_{r_n}$ is such a system in $\mathscr{H}_n = \mathscr{H}_1 \otimes \mathscr{H}_2 \otimes \cdots \otimes \mathscr{H}_n$.
2. For any two vectors of the form of Eq. (15–19) we have

$$(\varphi[r_1 r_2 \cdots r_n], \varphi[s_1 s_2 \cdots s_n]) = \frac{n_1! n_2! \cdots n_r! \cdots}{n!} \delta_{n_1 m_1} \delta_{n_2 m_2} \cdots \delta_{n_r m_r} \cdots$$

   where

   n_r is the number of r_i equal to $r = 1, 2, \ldots,$

   m_s is the number of s_k equal to $s = 1, 2, \ldots,$

   and

$$n = n_1 + n_2 + \cdots + n_r + \cdots = m_1 + m_2 + \cdots + m_r + \cdots.$$

3. The operators a_r, a_r^* defined by Eq. (15–25) are Hermitian conjugates of one another and they satisfy the commutation rules (15–28).

15-6. THE FERMI GAS

An assembly of n identical noninteracting particles satisfying the Fermi-Dirac statistics will be called a free Fermi gas. The Hilbert space for this system is $\mathscr{H}_n^- = \Pi_-\mathscr{H}_n$. For any complete orthonormal system $\{\varphi_n\} \in \mathscr{H}_1$ we define another such system in $\mathscr{H}_n^-$ from the vectors

$$\varphi[r_1 r_2 \cdots r_n] = \frac{1}{n!}\sum_P \delta_P U_P \varphi_{r_1} \otimes \varphi_{r_2} \otimes \cdots \otimes \varphi_{r_n}$$

$$\equiv \Pi_- \varphi_{r_1} \otimes \varphi_{r_2} \otimes \cdots \otimes \varphi_{r_n}. \tag{15–38}$$

If any two indices $r_i = r_k$ for $i \neq k$, then the corresponding $\varphi[r_1 r_2 \cdots r_n]$ is identically zero. We may therefore assume that the indices are all different from one another.

If we denote by n_1 ($= 0$ or 1) the number of indices among the $r_1, r_2, \ldots, r_n$ which are equal to 1, we obtain in complete analogy to the properties for the Bose gas,

a) $n_1 + n_2 + \cdots + n_r + \cdots = n$.

b) Two $\varphi[r_1 r_2 \cdots r_n]$, with corresponding numbers n_r equal, differ at most by a sign.

c) $\|\varphi[r_1 r_2 \cdots r_n]\|^2 = 1/n!$.

We call the numbers n_r the occupation numbers of the Fermi gas and we define the complete orthonormal system

$$\varphi(n_1 n_2 \cdots n_r \cdots) \equiv \frac{1}{\sqrt{n!}} \Pi_- \varphi_{r_1} \otimes \varphi_{r_2} \otimes \cdots \otimes \varphi_{r_n} \tag{15–39}$$

as the natural basis for the occupation-number representation.

Just as we have done for the Bose gas, so we can also introduce here the Fock space consisting of sequences of vectors $F = \{f_n\}$ ($f_n \in \mathscr{H}_n^-$), satisfying Eq. (15–22). Addition and scalar multiplications are defined by Eqs. (15–23) and (15–24), and the vacuum state $\varphi(0)$ is the unique unit vector in the one-dimensional space $\mathscr{H}_0$.

We can now introduce, in analogy to Eq. (15–25), the annihilation and creation operators a_r and a_r^* by defining

$$\begin{aligned} a_r\varphi(n_1 n_2 \cdots n_r \cdots) &= (-1)^{s_r} n_r \varphi(n_1 n_2 \cdots n_r - 1 \cdots) \\ a_r^*\varphi(n_1 n_2 \cdots n_r \cdots) &= (-1)^{s_r}(1 - n_r)\varphi(n_1 n_2 \cdots n_r + 1 \cdots) \end{aligned} \tag{15–40}$$

where

$$s_r = \sum_{k=1}^{r-1} n_k.$$

From these definitions it follows that

$$a_r\varphi(0) = 0 \tag{15–41}$$

and for any pair of vectors φ we find

$$(\varphi(n_1 n_2 \cdots n_r \cdots), a_r \varphi(n_1' n_2' \cdots n_r')) = (a_r^* \varphi(n_1 n_2 \cdots n_r \cdots), \varphi(n_1' n_2' \cdots n_r' \cdots)). \quad (15\text{–}42)$$

Thus the operator a_r^* is the Hermitian conjugate of a_r. Furthermore, the operators a_r satisfy the commutation rules

$$\begin{aligned} \{a_r, a_s\} &= \{a_r^*, a_s^*\} = 0 \\ \{a_r, a_s^*\} &= \delta_{rs}. \end{aligned} \quad (15\text{–}43)$$

Here we have introduced the anticommutator brackets defined by $\{A, B\} \equiv AB + BA$.

The operator $N_r \equiv a_r^* a_r$ is the number operator for the state r. It is diagonal in the representation which we have adopted, and it has the two eigenvalues 0 and 1. The *total number operator* is then defined by

$$N = \sum_{r=1}^{\infty} N_r. \quad (15\text{–}44)$$

In complete analogy to Eq. (15–31), we can obtain any vector φ by operating with creation operators on the vacuum state $\varphi(0)$:

$$\varphi(n_1 n_2 \cdots n_r \cdots) = (a_1^*)^{n_1} (a_2^*)^{n_2} \cdots (a_r^*)^{n_r} \cdots \varphi(0). \quad (15\text{–}45)$$

The normalization factor is here superfluous since all the $n_r!$ are equal to 1. [*Note:* $0! = 1$.]

The energy of the free Fermi gas will be given by an operator $H = H_1 + H_2 + \cdots + H_r + \cdots$, where $H_r = I \otimes I \otimes \cdots \otimes H_0 \otimes \cdots$, and where H_0 is the energy for a single fermion. We assume that H_0 has a discrete spectrum only, and we write φ_r for the complete system of eigenvectors for H_0:

$$H_0 \varphi_r = \varepsilon_r \varphi_r. \quad (15\text{–}46)$$

We find then, for H in the occupation-number representation, the expression

$$H = \varepsilon_1 a_1^* a_1 + \varepsilon_2 a_2^* a_2 + \cdots + \varepsilon_r a_r^* a_r + \cdots \quad (15\text{–}47)$$

which is formally identical with Eq. (15–33). The content is, however, quite different, in spite of the apparent similarity, since the operators a_r for the Fermi system satisfy different commutation rules. Thus the possible values for the energy eigenvalues are

$$E = \varepsilon_1 n_1 + \varepsilon_2 n_2 + \cdots + \varepsilon_r n_r + \cdots, \quad (15\text{–}48)$$

where the n_r can assume only the values $n_r = 0, 1$, $\sum n_r = n$.

For the interacting Fermi system we may have additional terms in the energy operators of the form of either Eq. (15–34) or Eq. (15–36). The

formulas (15–35) and (15–37) which we have derived for the constants occurring in the interaction energy remain exactly the same.

A new feature appears in the free Fermi gas in that the lowest value of the energy is not simply given by $E_0 = n\varepsilon_1$ (we assume $\varepsilon_1 \leq \varepsilon_2 \leq \cdots$) as in the Bose gas but instead by the expression

$$E_0 = \varepsilon_1 + \varepsilon_2 + \cdots + \varepsilon_n.$$

This different behavior for the ground-state energy has important observable physical consequences. For the atomic electrons, for instance, it is the reason for the shell structure of the periodic system which led Pauli to the discovery of the exclusion principle [5].

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